Large-scale Mathematical Optimization

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INF580

About the course

- **Aims of lectures:** theory, algorithms, some code
  won't repeat much of MAP557
- **Aims of TD:** modelling abilities in practice
  with AMPL and Python
- **Warning:**
  some disconnection between lectures and TD is normal
  some theoretical topics do not lend themselves to implementation
- Lectures/TD: (generally) on fri afternoon
- **Exam:** mini-project (individual/pairs) or oral exam

http://www.lix.polytechnique.fr/~liberti/teaching/dix/inf580

Outline

Outline

What is *Mathematical Optimization*?

- Mathematics of solving optimization problems
- Formal language: Mathematical Programming (MP)
- Sentences: descriptions of optimization problems
- Interpreted by solution algorithms ("solvers")
- As expressive as any imperative language
- Shifts focus from *algorithmics* to *modelling*

Why *Large-scale*?

- Any process can be optimized
- Social, technical and business processes are complex
- Computer power limits model precision
- Nowadays, need to solve very precise models
  $\Rightarrow$ *increase in model size*
- $\Rightarrow$ algorithmic complexity must grow slowly with size
- Focus on LP algs and heuristics
- Investigate LP relaxations & dimensionality reduction methods

The syllabus

- Which optimization problems can be solved?
  a tour of 20th century logic
- Complexity of optimization problems
  basics of theoretical computer science
- Distance geometry
  modern large-scale optimization and data science techniques
- Random projections
  new approaches to approximately solving large-scale problems
- Sparsity and ℓ_1 minimization
  integrality out of continuity
- Further topics
  as time allows

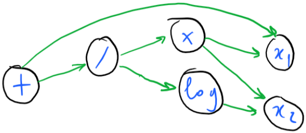
MP Formulations

Given functions $f, g_1, \ldots, g_m : \mathbb{Q}^n \to \mathbb{Q}$ and $Z \subseteq \{1, \ldots, n\}$

$$\left.\begin{array}{rrcl} \min_x & f(x) & & \\ \forall i \leq m & g_i(x) & \leq & 0 \\ \forall j \in Z & x_j & \in & \mathbb{Z} \end{array}\right\} \quad [P]$$

- More general than it looks:
  - $\max f(x) = -\min -f(x)$
  - $g_i(x) = 0 \quad \Leftrightarrow \quad (g_i(x) \leq 0 \wedge -g_i(x) \leq 0)$
  - $L \leq x \leq U \quad \Leftrightarrow \quad (L - x \leq 0 \wedge x - U \leq 0)$
- f, g_i represented by *expression DAGs*

$$x_1 + \frac{x_1 x_2}{\log(x_2)}$$



Class of all formulations P: $\mathbb{MP}$

Semantics of MP formulations

- $[\![P]\!]$ = optimum (or optima) of P
- Given $P \in \mathbb{MP}$, there are *three possibilities*:
  $[\![P]\!]$ exists, P is unbounded, P is infeasible
- *P is feasible* iff $[\![P]\!]$ exists or P is unbounded
  otherwise it is infeasible
- *P has an optimum* iff $[\![P]\!]$ exists
  otherwise it is infeasible or unbounded
- Example:

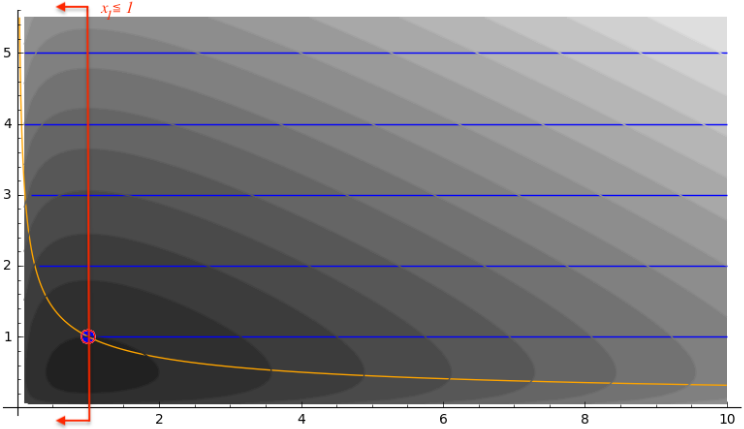
$$\left.\begin{array}{rrcl} \min & x_1 + 2x_2 - \log(x_1 x_2) & & \\ & x_1 x_2^2 & \ge & 1 \\ & x_1 & \in & [0,1] \\ & x_2 & \in & \mathbb{N} \end{array}\right\}$$

Exercise

Code this toy MP in AMPL and solve it with BARON

Example: solution “by inspection”

$$P \equiv \min\{x_1 + 2x_2 - \log(x_1 x_2) \mid x_1 x_2^2 \geq 1 \wedge 0 \leq x_1 \leq 1 \wedge x_2 \in \mathbb{N}\}$$



$$[\![P]\!] = (\mathsf{opt}(P), \mathsf{val}(P)) \qquad \mathsf{opt}(P) = (1,1) \qquad \mathsf{val}(P) = 3$$

Feasibility and optimality

- Feasibility problem: $[g(x) \leq 0]$
  can be written as the MP $[\min\{0 \mid g(x) \leq 0]\}$
- Bounded MP $[\min\{f(x) \mid g(x) \leq 0\}]$:
  bisection on f_0 in feas. prob. $[f(x) \leq f_0 \wedge g(x) \leq 0]$
- Unbounded MP: not equivalent to feasibility
  in general, cannot prove unboundedness

Bisection algorithm

- $P \equiv \min\{f(x) \mid \forall i \in I \; g_i(x) \le 0 \wedge x \in X\}$
- Assume global opt x^* of P has value $f(x^*)$ between given lower/upper bounds
- Reformulate P to a parametrized feasibility problem $Q(f_0) \equiv \{x \in X \mid f(x) \le f_0 \wedge \forall i \in I \; g_i(x) \le 0\}$

Bisection algorithm for *optimal value*

Input: lower & upper bound for f_0
while lower and upper bounds differ by $> \epsilon$ **do**
    let f_0 be midway between bounds
    if $Q(f_0)$ is feasible **then**
        update *upper* bound to f_0
    else
        update *lower* bound to f_0
    end if
end while

- solve an optimization problem with calls to feasibility oracle
- need only $\lceil \log_2 \left(\frac{\mathrm{UB}-\mathrm{LB}}{\epsilon}\right) \rceil$ calls to oracle

Exercise

Solve the toy MP using this bisection algorithm in AMPL

Bisection algorithm for *optimum*

Input: lower & upper bounds for f_0,
candidate global optimum $\hat{x}$
while lower and upper bounds differ by $> \epsilon$ **do**
  let f_0 be midway between bounds
  if $Q(f_0)$ is feasible **then**
    find a feasible point x'
    if $f(x')$ better than $f(\hat{x})$ **then**
      update $\hat{x}$ to x'
      update *upper* bound to $f(\hat{x})$
    end if
  else
    update *lower* bound to f_0
  end if
end while

Exercise

Solve the toy MP using this bisection algorithm in AMPL

Bisection algorithm for MP (formal)

Given:

- an optimization problem in *minimization* form

  for maximization have to switch a few things: which ones?
- global optimal value approximation tolerance $\epsilon > 0$
- lower bound $\underline{f}$, upper bound $\bar{f}$
- a feasibility algorithm $\mathcal{F}$ which

  finds an element in a set or certifies emptyness up to ϵ

Bisection algorithm for MP (formal)

let $(\hat{x}, \hat{f}) = (\textsf{uninitialized}, \bar{f})$
while $\bar{f} - \underline{f} > \epsilon$ **do**
  let $f_0 = (\underline{f} + \bar{f})/2$
  $(x', f') = \mathcal{F}(Q(f_0))$
  if $(x', f') \neq (\varnothing, \varnothing)$ **then**
    if $f' < \hat{f}$ **then**
      update $(\hat{x}, \hat{f}) \leftarrow (x', f')$
      update $\bar{f} \leftarrow \hat{f}$
    end if
  else
    update $\underline{f} \leftarrow f_0$
  end if
end while

Subsection 1

MP language

Entities of a MP formulation

- Sets of indices
- Parameters
  problem input, or *instance*
- Decision variables
  will encode the solution after solver execution
- Objective function
- Constraints

MP Example

Linear Program (LP) in standard form

- m, n: number of rows and columns
  corresponding index sets $I = \{1, \ldots, m\}, J = \{1, \ldots, n\}$
- $c \in \mathbb{R}^n$, $b \in \mathbb{R}^m$, A an $m \times n$ matrix
- $x \in \mathbb{R}^n$
- $\min_x c^\top x$
- $Ax = b \quad \wedge \quad x \geq 0$

Exercise

Code this example in AMPL and solve it with CPLEX

MP language implementations

- Humans model with quantifiers ($\forall$, $\sum$,...)
  e.g. $\forall i \in I \ \sum_{j \in J} a_{ij} x_j \le b_i$
  structured formulation
- Solution algorithms accept lists of explicit constraints
  e.g. $4x_1 + 1.5x_2 + x_6 \le 2$
  flat formulation
- **Translation from structured to flat formulation**
- MP language implementations
  AMPL, GAMS, Matlab+YALMIP,
  Python+amplpy/cvxpy, Julia+JuMP, ...

Exercise

Use AMPL to derive the flat formulation from the standard form LP

AMPL

- AMPL = A Mathematical Programming Language
- Syntax similar to human notation
- Bare-bone programming language

  e.g. no function calls
- Commercial & closed-source
  - extremely rapid prototyping
  - we get free licenses for this course
  - free open-source AMPL sub-dialect in GLPK `glpsol`
- Can also use Python+amplpy/cvxpy, or Julia+JuMP

Exercise

Formulate and solve the standard form LP using Python+amplpy

Subsection 2

Solvers

Solvers

- Solver:
  a solution algorithm for a whole subclass of MP
  examples: BARON, CPLEX
- Take formulation P as input
- Output $\llbracket P \rrbracket$ *and possibly other information*
- Trade-off between generality and efficiency
  fast solvers for large MP subclasses: unlikely

Some subclasses of MP

(i) Linear Programming (LP)
   f, g_i linear, $Z = \varnothing$

(ii) Mixed-Integer LP (MILP)
   f, g_i linear, $Z \neq \varnothing$

(iii) Nonlinear Programming (NLP)
   some nonlinearity in f, g_i, $Z = \varnothing$
   f, g_i convex: convex NLP (cNLP)

(iv) Mixed-Integer NLP (MINLP)
   some nonlinearity in f, g_i, $Z \neq \varnothing$
   f, g_i convex: convex MINLP (cMINLP)

$$\left.\begin{array}{rrcl} \min & f(x) & & \\ \forall i \le m & g_i(x) & \le & 0 \\ \forall j \in Z & x_j & \in & \mathbb{Z} \end{array}\right\} \quad [P]$$

And their solvers

(i) Linear Programming (LP)
simplex algorithm, interior point method (IPM)
Implementations: CPLEX, GLPK, CLP

(ii) Mixed-Integer LP (MILP)
cutting plane alg., Branch-and-Bound (BB)
Implementations: CPLEX, GuRoBi

(iii) Nonlinear Programming (NLP)
IPM, gradient descent (cNLP), spatial BB (sBB)
Implementations: IPOPT (cNLP), Baron, Couenne

(iv) Mixed-Integer NLP (MINLP)
outer approximation (cMINLP), sBB
Implementations: Bonmin (cMINLP), Baron, Couenne

Subsection 3

MP systematics

Types of MP

Continuous variables:

- LP (linear functions)
- QP (quadratic objective over affine sets)
- QCP (linear objective over quadratic sets)
- QCQP (quadratic objective over quadratic sets)
- cNLP (convex sets, convex objective)
- SOCP (LP over 2nd order cone)
- SDP (LP over PSD cone)
- CPP (LP over copositive cone)
- NLP (nonlinear functions)

Types of MP

Mixed-integer variables:

- IP (integer programming), MIP (mixed-integer programming)
- *extensions:* MILP, MIQP, MIQCP, MIQCQP, cMINLP, MINLP
- BLP (LP over $\{0,1\}^n$)
- BQP (QP over $\{0,1\}^n$)

Some more "exotic" classes:

- MOP (multiple objective functions)
- BLevP (optimization constraints)
- SIP (semi-infinite programming)
  Example: nonlinear constraint $y \geq x^2$ equivalent to infinite linear constraint set $\forall p \in \mathbb{R}\ (y \geq 2px - p^2)$

Subsection 4

Some applications

Some application fields

- Production industry
  planning, scheduling, allocation, ...
- Transportation & logistics
  facility location, routing, rostering, ...
- Service industry
  pricing, strategy, product placement, ...
- Energy industry
  power flow optimization, monitoring smart grids, ...
- Machine Learning & Artificial Intelligence
  clustering, support vector machines, ANN training, ...
- Biochemistry & medicine
  protein structure, blending, tomography, ...
- Mathematics
  Kissing number, packing of geometrical objects, ...

Easy example

A bank needs to invest C gazillion dollars, and focuses on two types of investments: one, imaginatively called (a), guarantees a 15% return, while the other, riskier and called, surprise surprise, (b), is set to a 25%. At least one fourth of the budget C must be invested in (a), and the quantity invested in (b) cannot be more than double the quantity invested in (a). How do we choose how much to invest in (a) and (b) so that revenue is maximized?

Modelling school

First question to ask oneself is: **What are the decision variables?**

Easy example

- Parameters:
  - budget C
  - return on investment on (a): 15%, on (b): 25%
- Decision variables:
  - x_a = budget invested in (a)
  - x_b = budget invested in (b)
- Objective function: $1.15\,x_a + 1.25\,x_b$
- Constraints:
  - $x_a + x_b = C$
  - $x_a \geq C/4$
  - $x_b \leq 2x_a$

Easy example: remarks

- *Missing trivial constraints*:
  verify that $x_a = C + 1$, $x_b = -1$ satisfies constraints
  forgot $x \geq 0$
- *No numbers in formulations*:
  replace numbers by parameter symbols

$$\left.\begin{array}{rrcl} \max\limits_{x_a, x_b \geq 0} & c_a x_a + c_b x_b & & \\ & x_a + x_b & = & C \\ & x_a & \geq & pC \\ & d x_a - x_b & \geq & 0 \end{array}\right\}$$

- *Formulation generality*:
  extend to n investments:

$$\left.\begin{array}{rrcl} \max\limits_{x \geq 0} & \sum\limits_{j \leq n} c_j x_j & & \\ & \sum\limits_{j \leq n} x_j & = & C \\ & x_1 & \geq & pC \\ & d x_1 - x_2 & \geq & 0 \end{array}\right\}$$

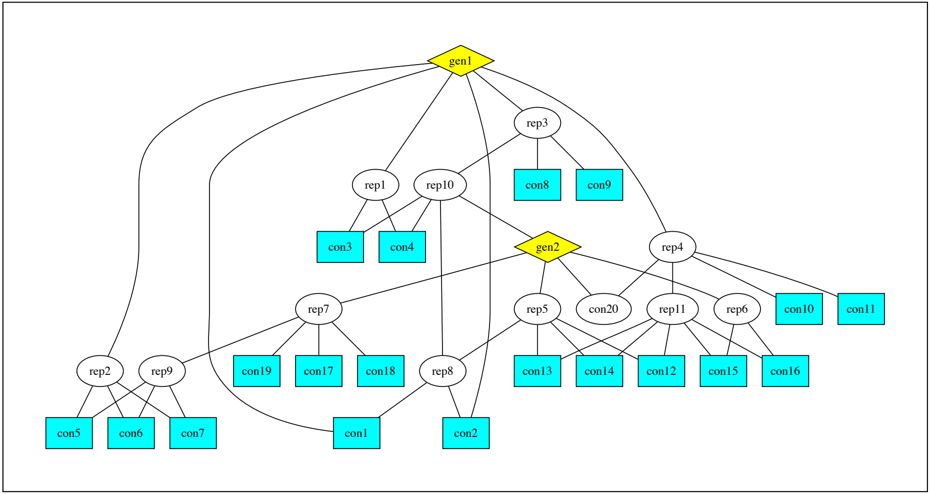
Example: monitoring an electrical grid

An electricity distribution company wants to monitor certain quantities at the lines of its grid by placing measuring devices at the buses. There are three types of buses: consumer, generator, and repeater. There are five types of devices:

- A: installed at any bus, and monitors all incident lines (cost: 0.9MEUR)
- B: installed at consumer and repeater buses, and monitors two incident lines (cost: 0.5MEUR)
- C: installed at generator buses only, and monitors one incident line (cost: 0.3MEUR)
- D: installed at repeater buses only, and monitors one incident line (cost: 0.2MEUR)
- E: installed at consumer buses only, and monitors one incident line (cost: 0.3MEUR).

Provide a least-cost installation plan for the devices at the buses, so that all lines are monitored by at least one device.

Example: the electrical grid



Example: formulation

- Index sets:
  - V: set of buses v
  - E: set of lines $\{u, v\}$
  - A: set of *directed* lines (u, v)
  - $\forall u \in V$ let N_u = buses adjacent to u
  - D: set of device types
  - D_M: device types covering > 1 line
  - $D_1 = D \smallsetminus D_M$
- Parameters:
  - $\forall v \in V \quad b_v =$ bus type
  - $\forall d \in D \quad c_d =$ device cost

Example: formulation

- Decision variables
  - $\forall d \in D, v \in V \quad x_{dv} = 1$
    iff device type d installed at bus v
  - $\forall d \in D, (u,v) \in A \quad y_{duv} = 1$
    iff device type d installed at bus u measures line $\{u, v\}$
  - all variables are binary
- Objective function

$$\min_{x,y} \sum_{d \in D} \sum_{v \in V} c_d x_{dv}$$

Example: formulation

- Constraints
  - device types:

$$\begin{aligned}
\forall v \in V \quad b_v = \mathsf{gen} \quad &\rightarrow \quad x_{\mathsf{B}v} = 0 \\
\forall v \in V \quad b_v \in \{\mathsf{con}, \mathsf{rep}\} \quad &\rightarrow \quad x_{\mathsf{C}v} = 0 \\
\forall v \in V \quad b_v \in \{\mathsf{gen}, \mathsf{con}\} \quad &\rightarrow \quad x_{\mathsf{D}v} = 0 \\
\forall v \in V \quad b_v \in \{\mathsf{gen}, \mathsf{rep}\} \quad &\rightarrow \quad x_{\mathsf{E}v} = 0
\end{aligned}$$

  - at most one device of any type at each bus

$$\forall v \in V \quad \sum_{d \in D} x_{dv} \leq 1$$

Example: formulation

- Constraints
  - A: every line incident to installed device is monitored

$$\forall u \in V, v \in N_u \quad y_{\mathsf{A}uv} = x_{\mathsf{A}u}$$

  - B: two monitored lines incident to installed device

$$\forall u \in V \quad \sum_{v \in N_u} y_{\mathsf{B}uv} = \min(2, |N_u|) x_{\mathsf{B}u}$$

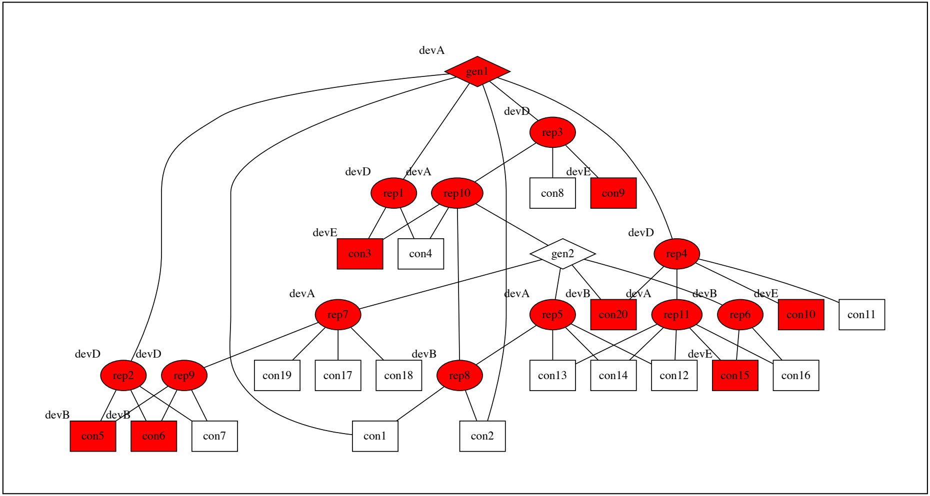
  - C,D,E: one monitored line incident to installed device

$$\forall d \in D_1, u \in V \quad \sum_{v \in N_u} y_{duv} = x_{du}$$

  - line is monitored

$$\forall \{u,v\} \in E \quad \sum_{d \in D} y_{duv} + \sum_{e \in D} y_{evu} \geq 1$$

Example: solution



all lines monitored, no redundancy, cost 9.2MEUR

Outline

Can we solve MPs?

- "Solve MPs": is there an algorithm $\mathcal{D}$ s.t.:

$$\forall P \in \mathbb{MP} \quad \mathcal{D}(P) = \begin{cases} \mathsf{infeasible} & P \text{ is infeasible} \\ \mathsf{unbounded} & P \text{ is unbounded} \\ [\![P]\!] & \text{otherwise} \end{cases}$$

- I.e. does there exist a single, all-powerful solver?

Subsection 1

Formal systems

Formal systems (FS)

- A *formal system* consists of:
  - an *alphabet*
  - a *formal grammar*
    allowing the determination of *formulæ* and *sentences*
  - a set A of *axioms* (given sentences)
  - a set R of *inference rules*
    allowing the derivation of new sentences from old ones
- A *theory* T is the smallest set of sentences that is obtained by recursively applying R to A

[Smullyan, Th. of Formal Systems, 1961]

Examples

- *Alphabets*:
  $\mathscr{B} = \{\text{␣}, 0, 1\}$, $\mathscr{N} = \mathscr{B} \cup \{2, 3, \ldots, \}$, $\mathscr{V} = \{x_0, x_1, x_2, \ldots\}$
  $\mathscr{E} = \{(,), +, -, \times, \div, \square^{\square}, \exp, \log, \sin\} \cup \mathscr{N} \cup \mathscr{V}$
  $\mathscr{P}\mathscr{A}_1 = \{\forall, \exists, \vee, \wedge, \neg, =\} \cup \mathscr{E}$,
  $\mathscr{M}\mathscr{P} = \{\min, \max, \sum, \prod, \leq, \geq\} \cup \mathscr{P}\mathscr{A}_1$
- *An expression grammar*:

$$\begin{array}{rcl}
\texttt{expr} & : & \texttt{term} + \texttt{expr} \;\mid\; \texttt{term} - \texttt{expr} \;\mid\; \texttt{term} \\
\texttt{term} & : & \texttt{factor} \times \texttt{term} \;\mid\; \texttt{factor} \div \texttt{term} \;\mid\; \texttt{factor} \\
\texttt{factor} & : & \texttt{power}^{\texttt{power}} \;\mid\; \texttt{power} \\
\texttt{power} & : & \log(\texttt{unr}) \mid \exp(\texttt{unr}) \mid \sin(\texttt{unr}) \mid (-\texttt{unr}) \mid \texttt{unr} \\
\texttt{unr} & : & (\texttt{expr}) \;\mid\; \mathscr{N} \;\mid\; \mathscr{V}
\end{array}$$

  e.g. $(1 - \sin(x)^2)^{(1/2)}$:
  $\texttt{expr} = \texttt{term} = \texttt{factor} = \texttt{power}^{\texttt{power}} = \texttt{unr}^{\texttt{unr}} = (\texttt{expr})^{(\texttt{expr})} =$
  $(\texttt{term} - \texttt{expr})^{(\texttt{term})} = (\texttt{factor} - \texttt{term})^{(\texttt{factor}\div\texttt{factor})} = \ldots$
- *Axioms*: see later
- *Inference rules*:
  modus ponens, symbol replacement, $A \vdash A \wedge A$, $A \vdash A \vee A$, $\ldots$

Example: PA1

- Theory: 1st order provable sentences about $\mathbb{N}$
- Alphabet: $+, \times, \wedge, \vee, \rightarrow, \forall, \exists, \neg, =, 0, S(\cdot)$ and variable names
- Peano's Axioms:
  1. $\forall x\ (0 \neq S(x))$
  2. $\forall x, y\ (S(x) = S(y) \rightarrow x = y)$
  3. $\forall x\ (x + 0 = x)$
  4. $\forall x\ (x \times 0 = 0)$
  5. $\forall x, y\ (x + S(y) = S(x + y))$
  6. $\forall x, y\ (x \times S(y) = x \times y + x)$
  7. axiom schema over all $(k+1)$-ary ϕ: $\forall y = (y_1, \ldots, y_k)$ $(\phi(0, y) \wedge \forall x(\phi(x, y) \rightarrow \phi(S(x), y))) \rightarrow \forall x \phi(x, y)$
- Inference: see `https://en.wikipedia.org/wiki/List_of_rules_of_inference`
  e.g. *modus ponens* $(P \wedge (P \rightarrow Q)) \rightarrow Q$
- Generates ring $(\mathbb{N}, +, \times)$ and arithmetical proofs
  e.g. $\exists x \in \mathbb{N}^n\ \forall i\ (p_i(x) \leq 0)$ (polynomial MINLP feasibility)

Example of PA1 derivation

Thm.

$\forall x\ (x = x)$

Proof

A3	$\forall x$	$x + 0 = x$	[1]
logic	$\forall t, r, s$	$t = r \to (t = s \to r = s)$	[2]
1, 2	$\forall x$	$x + 0 = x \to (x + 0 = x \to x = x)$	[3]
1, 3, mp	$\forall x$	$x + 0 = x \to x = x$	[4]
1, 4, mp	$\forall x$	$x = x$	QED

Notes:

- truth tables of $A \to B$ and $(\neg A) \vee B$ are the same
- logic indicates a "logical theorem"

  [equality] $(t = r \wedge t = s) \to r = s$; [truth tables] $t = r \to (t = s \to r = s)$
- mp indicates application of *modus ponens*
- all derivations are completely syntactical

Example: Reals

- Theory: 1st order provable sentences about $\mathbb{R}$
- Alphabet: $+, \times, \wedge, \vee, \forall, \exists, =, <, \leq, 0, 1$,variable names
- Axioms: field and order
- Inference: see
  https://en.wikipedia.org/wiki/List_of_rules_of_inference
  e.g. *modus ponens* $(P \wedge (P \to Q)) \to Q$
- Generates polynomial rings $\mathbb{R}[X_1, \ldots, X_k]$ (for all k)
  e.g. $\exists x \in \mathbb{R}^n \; \forall i \; (p_i(x) \leq 0)$ (polynomial NLP feasibility)

Relevance of FSs to MP

Given a FS $\mathcal{F}$:

- A *decision problem* is a set P of sentences
  Decide if a given sentence f belongs to P
- Decidability in formal systems:
  $$P \equiv \text{provable sentences}$$
- *Proof of f*: finite sequence of sentences ending with f
  sentences: axioms, or derived from predecessors by inference rules
- PA1: decide if sentence f about $\mathbb{N}$ has a proof
  e.g. $\exists x \in \mathbb{Z}^n \; \forall i \; p_i(x) \leq 0 \quad$ (polynomial p)
- Reals: decide if sentence f about $\mathbb{R}$ has a proof
  e.g. $\exists x \in \mathbb{R}^n \; \forall i \; p_i(x) \leq 0 \quad$ (polynomial p)
- Formal study of MINLP/NLP feasibility

Decidability, computability, solvability

- *Decidability*: applies to decision problems
- *Computability*: applies to function evaluation
  - Is the function mapping i to the i-th prime integer computable?
  - Is the function mapping Cantor's CH to 1 if provable in ZFC axiom system and to 0 otherwise computable?
- *Solvability*: applies to other problems

  E.g. to optimization problems

Completeness and decidability

- *Complete* FS $\mathcal{F}$:
  for any $f \in \mathcal{F}$, either f or $\neg f$ is provable
  otherwise $\mathcal{F}$ is *incomplete*
- *Decidable* FS $\mathcal{F}$:
  $\exists$ algorithm $\mathcal{D}$ s.t.

$$\forall f \in \mathcal{F} \begin{cases} \mathcal{D}(f) = 1 & \text{iff } f \text{ is provable} \\ \mathcal{D}(f) = 0 & \text{iff } f \text{ is not provable} \end{cases}$$

  otherwise $\mathcal{F}$ is *undecidable*

Example: PA1

- Gödel's 1st incompleteness theorem:
  PA1 is incomplete
- Turing's theorem:
  PA1 is undecidable
- $\Rightarrow$ PA1 is incomplete and undecidable

Subsection 2

Gödel

Gödel's 1st incompleteness theorem

- $\mathcal{F}$: any FS extending PA1
- **Thm.** $\boxed{\mathcal{F} \text{ complete iff inconsistent}}$
- ϕ: sentence "ϕ not provable in $\mathcal{F}$"
  denoted $\mathcal{F} \nvdash \phi$; it can be constructed *in $\mathcal{F}$* *(hard part of thm.)*
  - $\vdash$: "is provable" in PA1; $\vdash$: in meta-language
  - *Assume $\mathcal{F}$ is complete:* either $\mathcal{F} \vdash \phi$ or $\mathcal{F} \vdash \neg\phi$
  - If $\mathcal{F} \vdash \phi$ then $\mathcal{F} \vdash (\mathcal{F} \nvdash \phi)$ i.e. $\mathcal{F} \nvdash \phi$, contradiction
  - If $\mathcal{F} \vdash \neg\phi$ then $\mathcal{F} \vdash \neg(\mathcal{F} \nvdash \phi)$ i.e. $\mathcal{F} \vdash (\mathcal{F} \vdash \phi)$
    this implies $\mathcal{F} \vdash \phi$, i.e. $\mathcal{F} \vdash (\phi \wedge \neg\phi)$, $\mathcal{F}$ inconsistent
  - *Assume $\mathcal{F}$ is inconsistent:* any sentence is provable,
    i.e. $\mathcal{F}$ complete
    proof: $P \wedge \neg P$, hence P and $\neg P$, in particular for any Q we have
    $P \vee Q$,
    whence Q (since $\neg P$ and $P \vee Q$), implying $P \wedge \neg P \to Q$
- If we want PA1 to be consistent, it must be incomplete
- **Warning:** $\mathcal{F} \nvdash \phi \;\equiv\; \neg(\mathcal{F} \vdash \phi) \;\not\equiv\; \mathcal{F} \vdash \neg\phi$

Gödel's encoding

- For $\psi \in \mathsf{PA1}$, $\ulcorner \psi \urcorner \in \mathbb{N}$

  an integer which encodes the sentence

  called "Gödel number" of the sentence

- $\ulcorner \cdot \urcorner$ is an injective map

  many ways to define $\ulcorner \cdot \urcorner$

- Inverse: $\langle \ulcorner \phi \urcorner \rangle = \phi$

  ϕ is the sentence corresponding to Gödel number $\ulcorner \phi \urcorner$

- Encode/decode in $\mathbb{N}$ any sentence of a formal system

Gödel's self-referential sentence ϕ

- For integers x, y $\boxed{\exists g \in \mathbb{N}\ \langle g \rangle \equiv}$ $\mathsf{proof}(x, y)$:
  $\langle x \rangle$ is a proof in PA1 for the sentence $\langle y \rangle$
- For integers m, n, p $\boxed{\exists g \in \mathbb{N}\ g =}$ $\mathsf{sost}(m, n, p) =$
  Gödel number of the sentence obtained by replacing in $\langle m \rangle$ the free variable symbol with Gödel number n with the Gödel number p *(note that this operation replaces a symbol with a number)*
- let y be the Gödel number of the variable symbol "y"
  i.e. $\mathrm{y} = \ulcorner y \urcorner \in \mathbb{N}$
- $\gamma(y) \equiv \neg \exists x \in \mathbb{N}\ \mathsf{proof}(x, \mathsf{sost}(y, \mathrm{y}, y))$:
  $\gamma(y)$: there is no proof in PA1 for the sentence obtained by replacing, in the sentence $\langle y \rangle$, every free variable symbol "y" with the integer assigned to the free variable y
- let $q = \ulcorner \gamma(y) \urcorner$, consider $\phi \equiv \gamma(q)$
  note $\phi \equiv \neg \exists x \in \mathbb{N}\ \mathsf{proof}(x, \mathsf{sost}(q, \mathrm{y}, q))$

Gödel's self-referential sentence ϕ

$$\phi \equiv \neg \exists x \in \mathbb{N}\ \mathsf{proof}(x, \mathsf{sost}(q, \mathrm{y}, q))$$

- Let $\ulcorner \psi \urcorner \equiv \mathsf{sost}(q, \mathrm{y}, q)$

  ψ derived by replacing the free variable symbol "y" in $\langle q \rangle$ with q
- $\phi \equiv$ "there is no proof in PA1 for the sentence ψ"
- How did we obtain ϕ? Since $\phi \equiv \gamma(q)$,

  ϕ derived by replacing the free variable symbol "y" in $\gamma(y)$ with q
- ***Only difference between ϕ and ψ:*** $\boxed{\gamma(y) \textit{ instead of } \langle q \rangle}$
- **But recall that** $q = \ulcorner \gamma(y) \urcorner$, i.e. $\boxed{\langle q \rangle \equiv \gamma(y)}$
- So, in fact, $\psi \equiv \phi$
- Hence ϕ states "ϕ is not provable in PA1"

Note: *the replacement of y with q in meta-language is encoded by* $\mathsf{sost}()$ *in* PA1

Subsection 3

Turing

Turing machines

- Turing Machine (TM): *computation model*
  - infinite tape with cells storing finite alphabet letters
  - head reads/writes/skips i-th cell, moves left/right
  - states=program (e.g. if s write 0, move left, change to state t)
  - initial tape content: input, final tape content: output
  - final state $\perp$: termination (*nontermination denoted* $\varnothing$)
  - can model PA1
- $\exists$ universal TM (UTM) U s.t.
  - given the "program" of a TM T and an input x
  - U "simulates" T running on x
- $\Rightarrow$ The basis of the modern computer
- HALTING PROBLEM (HP): given TM M & input x, is $M(x) = \perp$?

  $\boxed{\textit{Does a given TM terminate on its input?}}$
- Turing's theorem: HP is undecidable

Computable functions

- TM T on input x yielding output y: write $T(x) = y$
- If a TM T terminates on all input, $T(\cdot)$ is *computable*
  a.k.a. "total computable"
- If a function is not computable, then it's *uncomputable*
- If T only terminates on some input, $T(\cdot)$ is *partial computable*
  denote $T(x) = \varnothing$ (undefined) if T does not terminate on input x

Turing's proof

- Enumerate all TMs: $(M_i \mid i \in \mathbb{N})$
- Halting function $\mathsf{halt}(i, \ell) = \begin{cases} 1 & \text{if } M_i(\ell) = \bot \\ 0 & \text{if } M_i(\ell) = \varnothing \end{cases}$
- Show $\mathsf{halt} \neq F$ for any total computable $F(i, \ell)$:
  - define $G(i) = 0$ if $F(i, i) = 0$ or undefined ($\varnothing$) othw

    G is partial computable because F is computable
  - let M_j be the TM computing G

    for any i, $M_j(i) = \bot$ iff $G(i) = 0$ (since $G(i)$ undefined othw)
  - consider $\mathsf{halt}(j, j)$:
    - $\mathsf{halt}(j, j) = 1 \to M_j(j) = \bot \to G(j) = 0 \to F(j, j) = 0$
    - $\mathsf{halt}(j, j) = 0 \to M_j(j) = \varnothing \to G(j) = \varnothing \to F(j, j) \neq 0$
  - so $\mathsf{halt}(j, j) \neq F(j, j)$ for all j
- halt is uncomputable

Turing and Gödel

- Consider TM called "provable" with input $\alpha \in \mathsf{PA1}$:
  `while(1) {i=0; if` $\mathsf{proof}(\mathtt{i}, \ulcorner\alpha\urcorner)$ `return` YES`; else i=i+1}`
- $\mathsf{provable}(\alpha) = \mathsf{YES}$ iff $\mathsf{PA1} \vdash \alpha$
- termination of provable $\Rightarrow$ decidability in PA1
- Gödel's ϕ is not provable
  $\Rightarrow \mathsf{provable}(\phi) = \varnothing$
  $\Rightarrow$ PA1 is undecidable

PA1 incomplete and undecidable

Subsection 4

Tarski

Example: Reals

- Tarski's theorem: Reals is complete
- Algorithm:
  constructs solution sets (YES) or derives contradictions(NO)
  ⇒ provides proofs or contradictions for all sentences
- ⇒ Reals is complete and also decidable
  since every complete theory is decidable

Completeness $\Rightarrow$ decidability

- Given $\phi \in \mathcal{F}$

```
i = 0
while 1 do
    if proof(i, ⌜φ⌝) then
        return YES
    else if proof(i, ⌜¬φ⌝) then
        return NO
    end if
    i = i + 1
end while
```

- Since $\mathcal{F}$ complete, alg. terminates on all ϕ

Tarski's theorem

- Algorithm based on quantifier elimination
- *Feasible sets of polynomial systems* $p(x) \leq 0$ *have finitely many connected components*
- Each connected component recursively built of cylinders over points or intervals
  extremities: pts., $\pm\infty$*, algebraic curves at previous recursion levels*
- In some sense, generalization of Reals in $\mathbb{R}^1$

Dense linear orders

Given a sentence ϕ in DLO *(similar to Reals in one dimension)*

- Reduce to DNF w/clauses $\exists x_i\, q_i(x)$ where $q_i = \bigwedge q_{ij}$
- Each q_{ij} has form $s = t$ or $s < t$ (s, t vars or consts)
  - s, t both constants:
    $s < t$, $s = t$ verified and replaced by 1 or 0
  - s, t the same variable x_i:
    $s < t$ replaced by 0, $s = t$ replaced by 1
  - if s is x_i and t is not:
    $s = t$ means "replace x_i by t" (eliminate x_i)
  - remaining case:
    q_i conjunction of $s < x_i$ and $x_i < t$:
    replace by $s < t$ (eliminate x_i)
- q_i no longer depends on x_i, rewrite $\exists x_i\, q_i$ as q_i
- Repeat over vars. x_i, obtain real intervals or contradictions

Quantifier elimination!

Subsection 5

Completeness and incompleteness

Decidability and completeness

- PA1 is incomplete and undecidable
- Reals is complete and decidable
- Are there FS $\mathcal{F}$ that are:
  - incomplete and decidable?
  - complete and undecidable?

    this case already discussed, answer is NO

Incomplete and decidable (trivial)

- NoInference:
  Any FS with $<\infty$ axiom schemata and no inference rules
- Only possible proofs: sequences of axioms
- Only provable sentences: axioms
- For any other sentence f: no proof of f or $\neg f$
- Trivial decision algorithm:
  given f, output YES if f is a finite axiom sequence,
  NO otherwise
- NoInference is incomplete and decidable

Incomplete and decidable (nontrivial)

- ACF: Algebraically Closed Fields (e.g. $\mathbb{C}$)
  field axioms + "every polynomial splits" schema
- Theorem: ACF is incomplete
  - ACF_p: $\mathsf{ACF} \wedge \mathsf{C}_p \equiv [\sum_{j \leq p} 1 = 0]$ (with p prime)
  - Claim: $\forall p$ (prime) C_p independent of ACF
    - suppose proof of C_p or $\neg\mathsf{C}_p$ possible for p
    - then either $\mathsf{ACF} \wedge \neg\mathsf{C}_p$ or $\mathsf{ACF} \wedge \mathsf{C}_p$ inconsistent
    - but $\exists$ field of *any* prime characteristic p
    - $\mathsf{ACF} \wedge \mathsf{C}_p$ and $\mathsf{ACF} \wedge \neg\mathsf{C}_p$ consistent for all p
- Theorem: ACF is decidable
  Decision algorithm $\mathcal{D}(\psi)$ for ACF:
  - if $\psi \equiv C_p$ or $\neg C_p$ for some prime p, return NO
  - else run quantifier elimination on ψ'
    ψ' obtained by replacing $\sum_{j \leq p} 1$ by 0 whenever possible in ψ
- $\Rightarrow$ ACF is incomplete and decidable

The two meanings of *completeness*

- WARNING!!!
  "complete" is used in two different ways in logic
  1. Gödel's 1st incompleteness theorem
     FS $\mathcal{F}$ complete$_1$ if ϕ or $\neg\phi$ provable $\forall\phi$
  2. Gödel's completeness$_2$ theorem
     - A: set of sentences in $\mathcal{F}$
     - M a *model* of $\mathcal{F}$ (domain of values for var symbols)
     - A^M: each var in A replaced by corresp. value
     - $\exists M$ s.t. A^M is true $\Rightarrow$ A consistent

       partial converse: corollary of Gödel's completeness thm
     - Complete$_2$ FS: $\forall M\,(A^M) \Rightarrow \mathcal{F} \vdash A$
     - *Gödel's completeness theorem:*
       1$^{\text{st}}$ order logic is complete$_2$
     - Note the strong assumption "$\forall M$"

       incompleteness theorem only considers $M = \mathbb{N}$
- *Pay attention when reading literature/websites*

Subsection 6

MP solvability

The issue

- Proved PA1 incomplete and undecidable
- Proved Reals complete and decidable
- But MP feasibility problems are *existential statements*

$$\exists x \text{ s.t. } g(x) \leq 0 \ ?$$

- PA1 and Reals also involve universal quantifiers
  $\Rightarrow$ *MP feasibility provides smaller theories*
- For Reals, if larger theory complete and decidable, smaller theory also complete and decidable
- For PA1, larger theory incomplete and undecidable, but smaller theory might be complete or decidable!

Polynomial equations in integers

- Consider the feasibility-only MP

$$\min\{0 \mid \forall i \le m \; g_i(x) = 0 \land x \in \mathbb{Z}^n\}$$

  with $g_i(x)$ multivariate polynomials in x

- Rewrite as a *Diophantine equation* (DE):

$$\exists x \in \mathbb{Z}^n \quad \sum_{i \le m} (g_i(x))^2 = 0 \qquad (1)$$

- Can restrict to $\mathbb{N}$ wlog, i.e. Eq. (1) $\in$ PA1
  write $x_i = x_i^+ - x_i^-$ where $x_i^+, x_i^- \in \mathbb{N}^n$
- Formulæ of PA1 are generally undecidable
  but is the subclass (1) *of PA1 decidable or not?*

Hilbert's 10th problem

- Hilbert:

  > *Given a Diophantine equation with any number of unknowns and with integer coefficients: devise a process which could determine by a finite number of operations whether the equation is solvable in integers*

- Davis & Putnam: *conjecture DEs are undecidable*
  - consider set $\mathbb{RE}$ of *recursively enumerable* (r.e.) sets
  - $R \subseteq \mathbb{N}$ is in $\mathbb{RE}$ if $\exists$ TM listing all and only elements in R
    let $\mathbb{TM} = \{T : \mathbb{N} \to \mathbb{N} \mid T \text{ is a TM}\}$; then
    $\forall R \in \mathbb{RE}\ \exists T \in \mathbb{TM}\ (\operatorname{ran} T = R)$
  - some $\mathbb{RE}$ sets are undecidable, e.g. $R = \{\ulcorner\phi\urcorner \mid \mathsf{PA1} \vdash \phi\}$
    r.e.: list all proofs; undecidable: by Gödel's thm
    "listing elements of set" and "proving if element in set" are very different problems!
  - for each $R \in \mathbb{RE}$ show $\exists$ polynomial $p(r,x)$ s.t.
    $$r \in R \leftrightarrow \exists x \in \mathbb{N}^n\ p(r,x) = 0$$
  - if we can prove this, $\exists$ undecidable DEs
    othw for any $r \in \mathbb{N}$ can decide if $r \in R$ by finding $x \in \mathbb{N}^n$ s.t. $p(r,x) = 0$

Proof strategy

- Strategy: "model" r.e. sets with polynomial equations in integers
- D&P+Robinson: universal quantifiers removed, but eqn system involves exponentials
- Matiyasevich: exploits exponential growth of Pell's equation solutions to remove exponentials
- $\Rightarrow$ DPRM theorem, implying DE undecidable

  Negative answer to Hilbert's 10th problem

Structure of the DPRM theorem

- Gödel's proof of his 1st incompleteness thm.

  r.e. sets $\equiv$ DEs with $< \infty$ $\exists$ and bounded $\forall$ quantifiers

- Davis' normal form

  one bounded quantifier suffices: $\exists x_0 \forall a \leq x_0 \exists x\ p(a,x) = 0$

  - (2 bnd qnt $\equiv$ 1 bnd qnt on pairs) and induction

- Robinson's idea

  get rid of bounded universal quant. by using exponent vars

  - *idea:* $[\exists x_0 \forall a \leq x_0 \exists x\ p(a,x) = 0]$ " $\rightarrow$ " $\left[\exists x \prod_{a \leq x_0} p(a,x) = 0\right]$
  - precise encoding needs variables in exponents

- Matyiasevic's contribution

  express $c = b^a$ using polynomials

  - use Pell's equation $x^2 - dy^2 = 1$
  - solutions (x_n, y_n) satisfy $x_n + y_n\sqrt{d} = (x_1 + y_1\sqrt{d})^n$
  - x_n, y_n grow exponentially with n

MP is unsolvable

- We know that if $R \in \mathbb{RE}$ then $\exists T \in \mathbb{TM}$ s.t. $\operatorname{ran} T = R$, we need the converse!
- Lemma: $\forall T \in \mathbb{TM}\ \operatorname{ran} T \in \mathbb{RE}$
- *Consider list of all TMs* $(M_i \mid i \in \mathbb{N})$

  if $M_i(x) = \perp$ at t-th execution step, write $M_i^t(x) = \perp$
- Yields all sets in $\mathbb{RE} = (R_i \mid i \in \mathbb{N})$ by dovetailing

  at k-th round, perform k-th step of $M_i(1)$, $(k-1)$-st of $M_i(2)$, ..., 1-st of $M_i(k)$

  $\Rightarrow \forall k \in \mathbb{N}, \ell \leq k$ if $M_i^\ell(k - \ell + 1) = \perp$ then let $R_i \leftarrow R_i \cup \{k - \ell + 1\}$

  $\Rightarrow R_i = \{k - \ell + 1 \mid \exists k \in \mathbb{N}, \ell \leq k\ (M_i^\ell(k - \ell + 1) = \perp)\}$ $\square$
- DPRM theorem: $\forall R \in \mathbb{RE}$, R represented by poly eqn
- By lemma, can choose UTM M_i with $\operatorname{ran} M_i = R_i \in \mathbb{RE}$

  $\Rightarrow \exists$ Universal DE (UDE), say $U(r, x) = 0$
- $\min\{0 \mid U(r, x) = 0 \wedge x \in \mathbb{N}^n\}$:

  undecidable (feasibility) MP
- $\min\limits_{x \in \mathbb{N}^n} (U(r, x))^2$: unsolvable (optimization) MP

Common misconception

"Since $\mathbb{N}$ is contained in $\mathbb{R}$, how is it possible that Reals is decidable but DE (= Reals $\cap\, \mathbb{N}$, right?) is not?"

After all, if a problem contains a hard subproblem, it's hard by inclusion, right?

- Can you express DE $p(x) = 0 \wedge x \in \mathbb{N}$ in Reals?
  - $p(x) = 0$ belongs to both DE and Reals, OK
  - "$x \in \mathbb{N}$" in Reals?

    $\Leftarrow$ find poly $q(x)$ s.t. $\exists x\ q(x) = 0$ iff $x \in \mathbb{N}^n$
  - $q(x) = x(x-1)\cdots(x-a)$ only good for $\{0, 1, \ldots, a\}$

    $q(x) = \prod_{i \in \omega}(x - i)$ is ∞ly long, invalid
  - IMPOSSIBLE!

    if it were possible, DE would be decidable, contradiction
  - $\Rightarrow$ Reals $\not\supseteq$ DE

MIQCP is undecidable

- [Jeroslow 1973]: MIQCP:

$$\left.\begin{array}{rrcl} \min & c^\top x & & \\ \forall i \le m & x^\top Q^i x + {a_i}^\top x + b_i & \ge & 0 \\ & x & \in & \mathbb{Z}^n \end{array}\right\} \qquad (\dagger)$$

  is undecidable

  Proof:

  - Let $U(r,x)=0$ be an UDE
  - $P(r) \equiv \min\{u \mid (1-u)U(r,x)=0 \wedge u \in \{0,1\} \wedge x \in \mathbb{Z}^n\}$

    $P(r)$ describes an unsolvable problem
  - Linearize every product $x_i x_j$ by y_{ij} and add $y_{ij}=x_i x_j$

    until only degree 1 and 2 left
  - Obtain instances of MIQCP ($\dagger$) for every r

Some MIQCQPs are decidable

- If each Q_i is diagonal PSD, decidable [Witzgall 1963]

- If x are bounded in $[x^L, x^U] \cap \mathbb{Z}^n$, decidable

  can express $x \in \{\lceil x^L \rceil, \lceil x^L \rceil + 1, \ldots, \lfloor x^U \rfloor\}$ by polynomial

$$\forall i \le m \qquad \prod_{x_i^L \le i \le x_i^U} (x - i) = 0$$

  turn into poly system in $\mathbb{R}$ (in Reals, decidable)

- $\Rightarrow$ *Bounded (vars)* easier than *unbounded* (for $\mathbb{Z}$)

- [MIQP decision vers.] is decidable

$$\left.\begin{array}{rrcl} & x^\top Q x + c^\top x & \le & \gamma \\ & Ax & \ge & b \\ \forall j \in Z & x_j & \in & \mathbb{Z} \end{array}\right\} \qquad \text{(in \textbf{NP} [Del Pia et al. 2014])}$$

NLP is undecidable

We can't represent unbounded subsets of $\mathbb{N}$ by polynomials
But we can if we allow some transcendental functions

$$x \in \mathbb{Z} \quad \longleftrightarrow \quad \sin(\pi x) = 0$$

- Constrained NLP is undecidable:

$$\min\{0 \mid U(a,x) = 0 \wedge \forall j \le n \ \sin(\pi x_j) = 0\}$$

- Even with just one nonlinear constraint:

$$\min\{0 \mid (U(a,x))^2 + \sum_{j \le n} (\sin(\pi x_j))^2 = 0\}$$

- Unconstrained NLP is undecidable:

$$\min (U(a,x))^2 + \sum_{j \le n} (\sin(\pi x_j))^2$$

- Box-constrained NLP is undecidable (*boundedness doesn't help*):

$$\min\{(U(a, \tan x_1, \ldots, \tan x_n))^2 + \sum_{j \le n} (\sin(\pi \tan x_j))^2 \mid -\frac{\pi}{2} \le x \le \frac{\pi}{2}\}$$

Some NLPs are decidable

- All polynomial NLPs are decidable

  by decidability of Reals

- Quadratic Programming (QP) is decidable over $\mathbb{Q}$

$$\left.\begin{array}{rrcl} \min & x^\top Q x & + & c^\top x \\ & Ax & \geq & b \end{array}\right\} \qquad (P)$$

- *Bricks of the proof*
  - if Q is PSD, $[\![P]\!] \in \mathbb{Q}$
    1. *remove inactive constr., active are eqn, use to replace vars*
    2. *work out KKT conditions, they are linear in rational coefficients*
    3. $\Rightarrow$ *solution is rational*
  - $\exists$ polytime IPM for solving P [Renegar&Shub 1992]
  - *unbounded case treated in* [Vavasis 1990]
- $\Rightarrow$ [QP decision version] is in **NP**

  $\Rightarrow$ QP is decidable over $\mathbb{Q}$

Rationals

- [Robinson 1949]:
  RT (1st ord. theory over $\mathbb{Q}$) is undecidable
- [Pheidas 2000]: *existential* theory of $\mathbb{Q}$ (ERT) is open
  can we decide whether $p(x) = 0$ has solutions in $\mathbb{Q}$? Boh!
- [Matyiasevich 1993]:
  - equivalence between DEH and ERT
  - DEH = [DE restricted to homogeneous polynomials]
  - *but we don't know whether DEH is decidable*

Note that Diophantus solved DE in positive rationals

Outline

Worst-case algorithmic complexity

- Computational complexity theory:
  worst-case time/space taken by an algorithm to complete
- Given an algorithm $\mathcal{A}$
  - e.g. to determine whether a graph $G = (V, E)$ is connected or not
  - input: G; size of input: $\nu = |V| + |E|$
- How does $\mathsf{cpu}(\mathcal{A})$ vary with ν?
  - $\mathsf{cpu}(\mathcal{A}) = O(\log \nu)$: logarithmic (sublinear)
  - $\mathsf{cpu}(\mathcal{A}) = O(\log^k \nu)$ for fixed k: polylogarithmic
  - $\mathsf{cpu}(\mathcal{A}) = O(\nu)$: linear
  - $\mathsf{cpu}(\mathcal{A}) = O(\nu^2)$: quadratic
  - $\mathsf{cpu}(\mathcal{A}) = O(\nu^k)$ for fixed k: polytime
  - $\mathsf{cpu}(\mathcal{A}) = O(2^\nu)$: exponential
- polytime $\leftrightarrow$ efficient
- exponential $\leftrightarrow$ inefficient

The "$O(\cdot)$" calculus

$$\forall f, g : \mathbb{N} \to \mathbb{N} \quad f <_O g \quad \leftrightarrow \quad \exists n \in \mathbb{N}\, \forall \nu > n\, (f(\nu) < g(\nu))$$

$$\forall g : \mathbb{N} \to \mathbb{N} \quad O(g) \quad = \quad \{f : \mathbb{N} \to \mathbb{N} \mid \exists C \in \mathbb{N}\, (f <_O Cg)\}$$

$$\forall f, g : \mathbb{N} \to \mathbb{N} \quad O(f) < O(g) \quad \leftrightarrow \quad f \in O(g) \;\wedge\; g \notin O(f)$$

Are polytime algorithms “efficient”?

- Why are polynomials special?
- Many different variants of Turing Machines (TM)
  more tapes, more heads, . . .
- Polytime is *invariant* to all definitions of TM
  e.g. TM with ∞ly many tapes: simulate with a single tape running along diagonals, similarly to dovetailing
- In practice, $O(\nu)$-$O(\nu^3)$ is an acceptable range covering most practically useful efficient algorithms
- Many exponential algorithms are also usable in practice for limited sizes
- Sublinear algorithms aren't allowed to read their whole input!

Instances and problems

- An input to an algorithm $\mathcal{A}$: *instance*
- Collection of all inputs for $\mathcal{A}$: *problem*

  in general, a problem P *is an infinite set of instances*
- $\mathcal{A}$ *solves* P if $\mathcal{A}$ solves every instance of P
  - There are problems which no algorithm can solve
  - A problem can be solved by different algorithms
- Given P find complexity of *best alg.* $\mathcal{A}$ solving P

$$\min_{<_O}\{\mathsf{cpu}(\mathcal{A}) \mid \mathcal{A} \text{ solves } P\}$$

- We (generally) don't know how to search over all algs for P

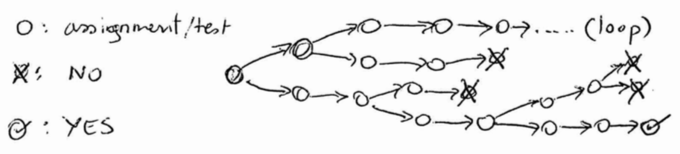
  sometimes we can find complexity bounds

Complexity classes: **P**, **NP**

- Focus on *decision problems*
- If ∃ polytime algorithm for P, then $P \in \boxed{\mathbf{P}}$
- If there is a polytime checkable *certificate* for all YES instances of P, then $P \in \boxed{\mathbf{NP}}$
  e.g. problem: shortest s—t path with fewer than K edges in a graph; path itself is a certificate: it can be checked whether it has fewer than K edges in time proportional to K, which is smaller than the size of the graph
- No-one knows whether $\mathbf{P} = \mathbf{NP}$: we think not
  NO *instances of some probs in* **NP** *don't seem to have polytime certificates*
- **NP** includes problems for which we don't think a polytime algorithm exists
  e.g. k-CLIQUE, SUBSET-SUM, KNAPSACK, HAMILTONIAN CYCLE, SAT, ...

Equivalent definition of **NP**

- $\boxed{\textbf{NP}\text{: problems solved by } \textit{nondeterministic} \text{ polytime TM}}$



nondeterministic: follow all paths concurrently, stop at first YES

- Equivalence with previous definition
  - ($\Rightarrow$) Assume $\exists$ polysized certificate for every YES instance. Nondeterministic polytime algorithm: concurrently explore all possible polysized certificates, call verification oracle for each, determine YES/NO.
  - ($\Leftarrow$) Run nondeterministic polytime algorithm: trace will look like a tree (branchings at tests, loops unrolled) with polytime depth. If YES there will be a terminating polysized sequence of steps from start to termination, serving as a polysized certificate

Subsection 1

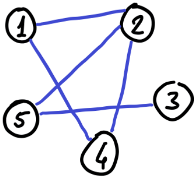
Some combinatorial problems in **NP**

k-STABLE

- Instance: $(G = (V, E), k)$
- Problem: determine if G has a *stable set* of size k
  - A subset $U \subseteq V$ is *stable* if $G[U]$ is *empty*
  - For $G = (V, E)$ and $U \subseteq V$, the *subgraph of G induced by U* is

$$G[U] = (U, \{\{u, v\} \in E \mid u, v \in U\})$$

  - $G = (V, E)$ is *empty* if $E = \varnothing$



- 1-STABLE? YES (every graph with ≥ 1 vertices is YES)
- 2-STABLE? YES (every non-complete graph is YES)
- 3-STABLE? NO

  polytime certificate for the absence of a k-stable?

MP formulations for STABLE

Variables? Objective? Constraints?

MP formulations for STABLE

Variables? Objective? Constraints?

- Decision variables: $\forall j \in V \quad x_j = \begin{cases} 1 & j \in k\text{-stable} \\ 0 & \text{otherwise} \end{cases}$

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$$\forall \{i,j\} \in E \quad x_i + x_j \le 1$$

MP formulations for STABLE

Variables? Objective? Constraints?

- Decision variables: $\forall j \in V \quad x_j = \begin{cases} 1 & j \in k\text{-stable} \\ 0 & \text{otherwise} \end{cases}$
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- "$\exists$ a k-stable"

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$$\forall \{i,j\} \in E \quad x_i + x_j \le 1$$

- "$\exists$ a k-stable"

$$\sum_{i \in V} x_i = k$$

MP formulations for STABLE

- *Pure feasibility problem:*

$$\left.\begin{array}{rrcl} & \sum\limits_{i\in V} x_i & = & k \\ \forall\{i,j\}\in E & x_i + x_j & \le & 1 \\ & x & \in & \{0,1\}^n \end{array}\right\}$$

MP formulations for STABLE

- *Pure feasibility problem:*

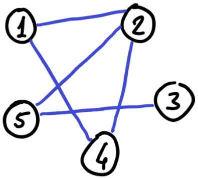
$$\left.\begin{array}{rrcl} & \sum\limits_{i\in V} x_i & = & k \\ \forall\{i,j\}\in E & x_i + x_j & \le & 1 \\ & x & \in & \{0,1\}^n \end{array}\right\}$$

- Max Stable:

$$\left.\begin{array}{rrcl} \max & \sum\limits_{i\in V} x_i & & \\ \forall\{i,j\}\in E & x_i + x_j & \le & 1 \\ & x & \in & \{0,1\}^n \end{array}\right\}$$

k-CLIQUE

- Instance: $(G = (V, E), k)$
- Problem: determine whether G has a *clique* of size k



- 1-CLIQUE? YES (every graph with ≥ 1 vertices is YES)
- 2-CLIQUE? YES (every non-empty graph is YES)
- 3-CLIQUE? YES (triangle $\{1, 2, 4\}$ is a certificate)
  certificate can be checked in $O(k^2) < O(n^2)$ (k fixed)
- $>$ 4-CLIQUE? NO
  polytime certificate for the absence of a k-clique?

MP formulations for CLIQUE

Variables? Objective? Constraints?

MP formulations for CLIQUE

Variables? Objective? Constraints?

- Decision variables: $\forall j \in V \quad x_j = \begin{cases} 1 & j \in k\text{-clique} \\ 0 & \text{otherwise} \end{cases}$

MP formulations for CLIQUE

Variables? Objective? Constraints?

- Decision variables: $\forall j \in V \quad x_j = \begin{cases} 1 & j \in k\text{-clique} \\ 0 & \text{otherwise} \end{cases}$
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MP formulations for CLIQUE

Variables? Objective? Constraints?

- Decision variables: $\forall j \in V \quad x_j = \begin{cases} 1 & j \in k\text{-clique} \\ 0 & \text{otherwise} \end{cases}$
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- Constraints:
  - "$\exists$ a k-clique"

$$\sum_{i \in V} x_i = k$$

MP formulations for CLIQUE

Variables? Objective? Constraints?

- Decision variables: $\forall j \in V \quad x_j = \begin{cases} 1 & j \in k\text{-clique} \\ 0 & \text{otherwise} \end{cases}$
- no objective (pure feasibility MP)
- Constraints:
  - "$\exists$ a k-clique"

$$\sum_{i \in V} x_i = k$$

  - for $G = (V, E)$, the *complement graph* $\bar{G} = (V, \bar{E})$ has

$$\bar{E} = \{\{u, v\} \mid \{u, v\} \notin E\}$$

  - $\boxed{\textbf{Prop.: } C \text{ clique in } G \Leftrightarrow C \text{ stable in } \bar{G}}$

MP formulations for CLIQUE

Variables? Objective? Constraints?

- Decision variables: $\forall j \in V \quad x_j = \begin{cases} 1 & j \in k\text{-clique} \\ 0 & \text{otherwise} \end{cases}$
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- Constraints:
  - "$\exists$ a k-clique"

$$\sum_{i \in V} x_i = k$$

  - for $G = (V, E)$, the *complement graph* $\bar{G} = (V, \bar{E})$ has

$$\bar{E} = \{\{u, v\} \mid \{u, v\} \notin E\}$$

  - $\boxed{\textbf{Prop.: } C \text{ clique in } G \Leftrightarrow C \text{ stable in } \bar{G}}$
  - $\Rightarrow$ use constraints for k-stable in $\bar{G}$:
    "if $\{i, j\} \in \bar{E}$ then $\neg(x_i = x_j = 1)$"

$$\forall \{i, j\} \notin E \quad x_i + x_j \leq 1$$

MP formulations for CLIQUE

- *Pure feasibility problem:*

$$\left.\begin{array}{rrcl} & \sum\limits_{i\in V} x_i & = & k \\ \forall \{i,j\} \not\in E & x_i + x_j & \le & 1 \\ & x & \in & \{0,1\}^n \end{array}\right\}$$

MP formulations for CLIQUE

- *Pure feasibility problem:*

$$\left.\begin{array}{rrcl} & \sum\limits_{i\in V} x_i & = & k \\ \forall \{i,j\} \not\in E & x_i + x_j & \le & 1 \\ & x & \in & \{0,1\}^n \end{array}\right\}$$

- MAX CLIQUE:

$$\left.\begin{array}{rrcl} \max & \sum\limits_{i\in V} x_i & & \\ \forall \{i,j\} \not\in E & x_i + x_j & \le & 1 \\ & x & \in & \{0,1\}^n \end{array}\right\}$$

Notice the tiny difference with STABLE

AMPL code for Max Clique

File `clique.mod`

```
# clique.mod
param n integer, > 0;
set V := 1..n;
set E within {V,V};
var x{V} binary;
maximize clique_card: sum{j in V} x[j];
subject to notstable{i in V, j in V : i<j and (i,j) not in E}:
  x[i] + x[j] <= 1;
```

File `clique.dat`

```
# clique.dat
param n := 5;
set E := (1,2) (1,4) (2,4) (2,5) (3,5);
```

AMPL code for MAX CLIQUE

File `clique.run`:

```
# clique.run
model clique.mod;
data clique.dat;
option solver cplex;
solve;
printf "C =";
for {j in V : x[j] > 0} {
  printf " %d", j;
}
printf "\n";
```

Run with "`ampl clique.run`" on command line

```
CPLEX 12.8.0.0: optimal integer solution; objective 3
0 MIP simplex iterations
0 branch-and-bound nodes
C = 1 2 4
```

Code and test the formulation for MAX STABLE

SUBSET-SUM

- Instance: list $a = (a_1, \dots, a_n) \in \mathbb{N}^n$ and $b \in \mathbb{N}$
- Problem: is there $J \subseteq \{1, \dots, n\}$ such that $\sum_{j \in J} a_j = b$?

- $a = (1, 1, 1, 4, 5)$, $b = 3$: YES with $J = \{1, 2, 3\}$

  all $b \in \{0, \dots, 12\}$ yield YES *instances*
- $a = (3, 6, 9, 12)$, $b = 20$: NO

MP formulations for SUBSET-SUM

Variables? Objective? Constraints?

MP formulations for SUBSET-SUM

Variables? Objective? Constraints?

- *Pure feasibility problem*:

$$\left.\begin{array}{rcl} \sum\limits_{j\le n} a_j x_j & = & b \\ x & \in & \{0,1\}^n \end{array}\right\}$$

AMPL code for SUBSET-SUM

File subsetsum.mod

```
# subsetsum.mod
param n integer, > 0;
set N := 1..n;
param a{N} integer, >= 0;
param b integer, >= 0;
var x{N} binary;
subject to subsetsum: sum{j in N} a[j]*x[j] = b;
```

File subsetsum.dat

```
# subsetsum.dat
param n := 5;
param a :=
1  1
2  1
3  1
4  4
5  5
;
param b := 3;
```

Code your own subsetsum.run!

KNAPSACK

- Instance: $c, w \in \mathbb{N}^n$, $K \in \mathbb{N}$
- Problem:
  find $J \subseteq \{1, \ldots, n\}$ s.t. $c(J) \leq K$ and $w(J)$ is maximum
  - *notation:* $c(J) = \sum_{j \in J} c_j$ *(similarly for* $w(J)$*)*
  - natively expressed as an optimization problem

- $n = 3$, $c = (5, 6, 7)$, $w = (3, 4, 5)$, $K = 11$
  - $c(J) \leq 11$ feasible for J in $\varnothing, \{j\}, \{1, 2\}$
  - $w(\varnothing) = 0, w(\{1, 2\}) = 3 + 4 = 7, w(\{j\}) \leq 5$ for $j \leq 3$

    $\Rightarrow J_{\mathsf{max}} = \{1, 2\}$
- $K = 4$: trivial solution ($J = \varnothing$)

MP formulation for KNAPSACK

Variables? Objective? Constraints?

MP formulation for KNAPSACK

Variables? Objective? Constraints?

$$\left.\begin{array}{rcl} \max \displaystyle\sum_{j\le n} w_j x_j & & \\ \displaystyle\sum_{j\le n} c_j x_j & \le & K \\ x & \in & \{0,1\}^n \end{array}\right\}$$

AMPL code for KNAPSACK

File `knapsack.mod`

```
# knapsack.mod
param n integer, > 0;
set N := 1..n;
param c{N} integer;
param w{N} integer;
param K integer, >= 0;
var x{N} binary;
maximize value: sum{j in N} w[j]*x[j];
subject to knapsack: sum{j in N} c[j]*x[j] <= K;
```

File `knapsack.dat`

```
# knapsack.dat
param n := 3;
param : c w :=
1  5 3
2  6 4
3  7 5 ;
param K := 11;
```

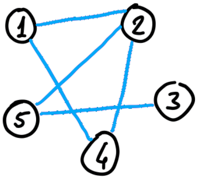
Code your own `knapsack.run`!

Hamiltonian Cycle

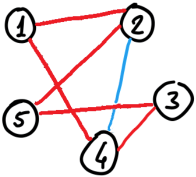
- Instance: $G = (V, E)$
- Problem: does G have a *Hamiltonian cycle*?

  cycle covering every $v \in V$ exactly once

NO



YES (cert. $1 \to 2 \to 5 \to 3 \to 4 \to 1$)



MP formulation for Hamiltonian Cycle

Variables? Objective? Constraints?

MP formulation for HAMILTONIAN CYCLE

Variables? Objective? Constraints?

$$\forall i \in V \quad \sum_{\substack{j \in V \\ \{i,j\} \in E}} x_{ij} = 1 \tag{2}$$

$$\forall j \in V \quad \sum_{\substack{i \in V \\ \{i,j\} \in E}} x_{ij} = 1 \tag{3}$$

$$\forall \varnothing \subsetneq S \subsetneq V \quad \sum_{\substack{i \in S, j \notin S \\ \{i,j\} \in E}} x_{ij} \geq 1 \tag{4}$$

WARNING: Eq. (4) is a second order statement!

quantified over sets

yields exponentially large set of constraints

AMPL code for Hamiltonian Cycle

File `hamiltonian.mod`

```
# hamiltonian.mod
param n integer, > 0;
set V default 1..n, ordered;
set E within {V,V};
set A := E union {i in V, j in V : (j,i) in E};
# index set for nontrivial subsets of V
set PV := 1..2**n-2;
# nontrivial subsets of V
set S{k in PV} := {i in V: (k div 2**(ord(i)-1)) mod 2 = 1};

var x{A} binary;
subject to successor{i in V} :
  sum{j in V : (i,j) in A} x[i,j] = 1;
subject to predecessor{j in V} :
  sum{i in V : (i,j) in A} x[i,j] = 1;

# breaking non-hamiltonian cycles
subject to breakcycles{k in PV}:
  sum{i in S[k], j in V diff S[k]: (i,j) in A} x[i,j] >= 1;
```

Code your own `.dat` and `.run` files!

Satisfiability (SAT)

- Instance: boolean logic sentence f in CNF

$$\bigwedge_{i \leq m} \bigvee_{j \in C_i} \ell_j$$

  where $\ell_j \in \{x_j, \bar{x}_j\}$ for $j \leq n$
- Problem: is there $\phi : x \to \{0,1\}^n$ s.t. $\phi(f) = 1$?

- $f \equiv (x_1 \vee \bar{x}_2 \vee x_3) \wedge (\bar{x}_1 \vee x_2)$

  $x_1 = x_2 = 1$, $x_3 = 0$ is a YES certificate
- $f \equiv (x_1 \vee x_2) \wedge (\bar{x}_1 \vee \bar{x}_2) \wedge (\bar{x}_1 \vee x_2) \wedge (x_1 \vee \bar{x}_2)$

ϕ	$x = (1,1)$	$x = (0,0)$	$x = (1,0)$	$x = (0,1)$
false	C_2	C_1	C_3	C_4

MP formulation for SAT

Variables? Objective? Constraints?

MP formulation for SAT

Variables? Objective? Constraints?

Algorithm $\hat{\rho}$ to generate MP from given SAT sentence $\bigwedge\limits_{i \le m} \bigvee\limits_{j \in C_i} \ell_j$:

MP formulation for SAT

Variables? Objective? Constraints?

Algorithm $\hat{\rho}$ to generate MP from given SAT sentence $\bigwedge_{i \le m} \bigvee_{j \in C_i} \ell_j$:

- Literals $\ell_j \in \{x_j, \bar{x}_j\}$: *decision variables in* $\{0,1\}$

$$\hat{\rho}(\ell_j) \quad \longmapsto \quad \begin{cases} x_j & \text{if } \ell_j \equiv x_j \\ 1 - x_j & \text{if } \ell_j \equiv \bar{x}_j \end{cases}$$

- Clauses $\Gamma_i \equiv \bigvee_{j \in C_i} \ell_j$: *constraints*

$$\hat{\rho}(\Gamma_i) \quad \longmapsto \quad \sum_{j \in C_i} \hat{\rho}(\ell_j) \ge 1$$

- Conjunction: *feasibility-only ILP*

$$\hat{\rho}\big(\bigwedge_i \Gamma_i\big) \quad \longmapsto \quad \forall i \le m \quad \hat{\rho}(\Gamma_i)$$

MP formulation for SAT

- **Prop.**: SAT instance q is YES iff ILP instance $\hat{\rho}(q)$ is YES
- *Proof:* Let $L = (\ell'_1, \ldots, \ell'_n)$ be a solution of SAT. Then $x^* = (x^*_1, \ldots, x^*_n)$ where $x^*_j = 1$ iff $\ell'_j = x_j = \mathsf{true}$ and $x^*_j = 0$ iff $\ell'_j = \bar{x}_j = \mathsf{true}$ is a feasible solution of ILP (satisfies each clause constraint by definition of $\hat{\rho}$).

  Conversely: if x solves ILP, then form solution L of SAT by mapping $x^*_j = 1$ to true and $x^*_j = 0$ to false, result follows again by defn of $\hat{\rho}$.

AMPL code for SAT?

Using $\hat{\rho}$ we can only obtain flat formulations

Example: file `sat.run` (flat formulation) for instance
$(x_1 \vee \bar{x}_2 \vee x_3) \wedge (\bar{x}_1 \vee x_2)$

```
# sat.run
var x{1..3} binary;
subject to con1: x[1] + (1-x[2]) + x[3] >= 1;
subject to con2: (1-x[1])+ x[2] >= 1;
option solver cplex;
solve;
display x, solve_result;
```

Subsection 2

NP-hardness

NP-Hardness

- Do *hard* problems exist? Depends on $\mathbf{P} \neq \mathbf{NP}$
- Next best thing: define *hardest problem in* **NP**
- Defn.: Problem P is **NP**-*hard* if $\forall Q \in \mathbf{NP}\ \exists$ polytime alg. ρ_Q:

  $$\boxed{q \in Q \mapsto \rho_Q(q) \in P \text{ with } q \text{ YES iff } \rho_Q(q) \text{ YES}}$$

  $\rho_Q : Q \to P$ is called a *polynomial reduction* from Q to P
- Prop.: P is hardest for **NP**
  1. run best alg. for P on $\rho_Q(q)$, get answer $\alpha \in \{\mathsf{YES}, \mathsf{NO}\}$
  2. return α as answer for q
  3. so Q cannot be harder than P
  4. $\forall Q \in \mathbf{NP} \Rightarrow$ no problem in **NP** is harder than P
- If P is in **NP** and is **NP**-hard, it is called **NP**-*complete*
- *Reduction: "model" Q using "language" of P*
- Every problem in **NP** reduces to SAT [Cook 1971]

Cook's theorem

Theorem 1: If a set S of strings is accepted by some nondeterministic Turing machine within polynomial time, then S is P-reducible to {DNF tautologies}.

Boolean decision variables store TM dynamics

Proposition symbols:

$P^i_{s,t}$ for $1 \le i \le \ell$, $1 \le s,t \le T$. $P^i_{s,t}$ is true iff tape square number s at step t contains the symbol σ_i.

Q^i_t for $1 \le i \le r$, $1 \le t \le T$. Q^i_t is true iff at step t the machine is in state q_i.

$S_{s,t}$ for $1 \le s,t \le T$ is true iff at time t square number s is scanned by the tape head.

Definition of TM dynamics in CNF

B_t asserts that at time t one and only one square is scanned:

$$B_t = (S_{1,t} \vee S_{2,t} \vee \dots \vee S_{T,t}) \,\&\, [\mathop{\&}_{1 \le i < j \le T} (\neg S_{i,t} \vee \neg S_{j,t})]$$

$G^t_{i,j}$ asserts that if at time t the machine is in state q_i scanning symbol σ_j, then at time $t+1$ the machine is in state q_k, where q_k is the state given by the transition function for M.

$$G^t_{i,j} = \mathop{\&}_{s=1}^{T} (\neg Q^i_t \vee \neg S_{s,t} \vee \neg P^j_{s,t} \vee Q^k_{t+1})$$

Description of a dynamical system using a declarative programming language (SAT) — what MP is all about!

The MP version of Cook's theorem

Thm.

Any problem P in **NP** can be polynomially reduced to a MILP

Proof

Since $P \in \mathbf{NP}$, every YES instance $\pi \in P$ must have a polynomial-time (say $p^P(|\pi|)$) verifiable certificate c_π (wlog assume it is a $\{0,1\}$ string), with length bounded by a polynomial (say $q^P(|\pi|)$). This means that a deterministic TM M_P verifying c_π will reach termination in polytime $p^P(\pi)$. Let κ be such that $p^P, q^P \in O(n^\kappa)$. We define a MILP on binary variables holding the content of the tape of M_P as it changes according to the transition function of M_P, such that the tape contains: (i) "NO" in the first cell, and π in the subsequent $|\pi|$ cells, at the initial step $k = 0$; (ii) "YES" in the first cell at the final step $k = n^\kappa$. Then the MILP is feasible iff π is a YES instance of P. This provides a polytime reduction from P to MILP.

Cook's theorem: sets and params

- Model a deterministic TM dynamics using MILP
- M_P is a 5-tuple $(Q, \Sigma, s, F, \delta)$:
  states, alphabet, initial, final, transition
- Transition function $\delta : Q \smallsetminus F \times \Sigma \to Q \times \Sigma \times \{-1, 1\}$
  δ: state ℓ, symbol $j \mapsto$ state ℓ', symbol j', direction d
- M_P polytime: terminates in n^κ , where $n = |\pi|$
- *Index sets:*
  states Q, characters Σ, tape cells I, steps K
- *Parameters:*
  initial tape string (NO, π)
  YES written in cell 1 when M_P in final state

Cook's theorem: decision vars

- $\forall i \in I, j \in \Sigma, k \in K$
  $t_{ijk} = 1$ *iff* *<u>tape</u>* *cell* i *contains symbol* j *at step* k
- $\forall i \in I, k \in K$
  $h_{ik} = 1$ *iff* *<u>head</u>* *is at tape cell* i *at step* k
- $\forall \ell \in Q, k \in K$
  $q_{\ell k} = 1$ *iff* M_P *is in* *<u>state</u>* ℓ *at step* k

Cook's theorem: constraints (informal)

1. *Initialization:*
   1.1 initial string (NO, π) on tape at step $k = 0$
   1.2 M_P in initial state s at step $k = 0$
   1.3 initial head position on cell $i = 0$ at $k = 0$
2. *Execution:*
   2.1 $\forall i, k$: cell i has exactly one symbol j at step k
   2.2 $\forall k$: M_P is in exactly one state ℓ
   2.3 $\forall k$: tape head M_P is at exactly one cell i
   2.4 $\forall i, k$: if cell i changes symbol between steps k and $k + 1$, head must be on cell i at step k
   2.5 $\forall k, i, j$: cell i and symbol j in state k lead to cells, symbol and states given by transition function δ
3. *Termination:*
   3.1 M_P terminates at step $k \leq n^k$ w/YES written in cell 1

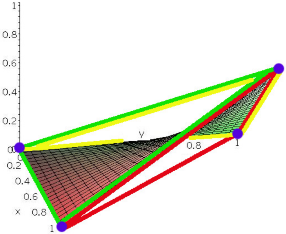
Cook's theorem: constraints

1. *Initialization:*
   1.1 $(t_{1,\mathrm{NO},0} = 1) \wedge (\forall i > 1 \quad t_{i,\pi_i,0} = 1)$
   1.2 $q_{s,0} = 1$
   1.3 $h_{0,0} = 1$
2. *Execution:*
   2.1 $\forall i, k \quad \sum_j t_{ijk} = 1$
   2.2 $\forall k \quad \sum_\ell q_{\ell k} = 1$
   2.3 $\forall k \quad \sum_i h_{ik} = 1$
   2.4 $\forall i, j \neq j', k < n^\kappa \quad t_{ijk}\, t_{i,j',k+1} \leq h_{ik}$

   2.5 $\forall i, \ell, \ell', j, j', k, d$ s.t. $(\ell', j', d) = \delta(\ell, j)$
   $$h_{ik}\, q_{\ell k}\, t_{ijk} = h_{i+d,k+1}\, q_{\ell',k+1}\, t_{i,j',k+1}$$
3. *Termination:*
   3.1 $(t_{1,\mathrm{YES},n^\kappa} = 1) \wedge \left(\sum_{f \in F, k} \quad q_{fk} = 1 \right)$

Cook's theorem: linearization

- MP in previous slide: MINLP not MILP
- Fortet's inequalities for products of binary vars:
  For $x, y \in \{0,1\}$ and $z \in [0,1]$
  $z = xy \Leftrightarrow z \le x \wedge z \le y \wedge z \ge x + y - 1$



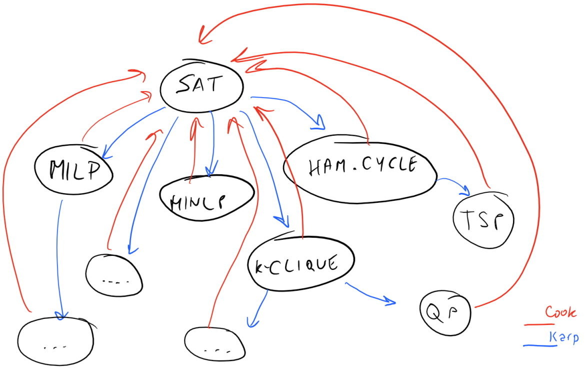
- MILP is feasibility only
- MILP has polynomial size
- $\Rightarrow$ *MILP is* **NP***-hard*

Reduction graph

After Cook's theorem

To prove **NP**-hardness of a new problem P, pick a known **NP**-hard problem Q that "looks similar enough" to P and find a polynomial reduction ρ_Q from Q to P [Karp 1972]

Why it works: suppose P easier than Q, solve Q by calling $\mathrm{Alg}_P \circ \rho_Q$, conclude Q as easy as P, contradiction since Q hardest in **NP**



Example of polynomial reduction

- STABLE: given $G = (V, E)$ and $k \in \mathbb{N}$, does it contain a stable set of size k?
- Assuming k-CLIQUE is **NP**-complete, reduce from it
  - Given instance (G, k) of CLIQUE consider the *complement graph* (computable in polytime)

$$\bar{G} = (V, \bar{E} = \{\{i, j\} \mid i, j \in V \wedge \{i, j\} \notin E\})$$

  - **Prop.**: G has a clique of size k iff $\bar{G}$ has a stable set of size k
  - $\rho(G) = \bar{G}$ a polynomial reduction CLIQUE $\to$ STABLE
- $\Rightarrow$ STABLE is **NP**-hard
- STABLE is also in **NP**
  $U \subseteq V$ is a stable set iff $E(G[U]) = \varnothing$ (polytime verification)
- $\Rightarrow$ STABLE is **NP**-complete

Subsection 3

Complexity of solving MP formulations

LP is in **P**

- Khachian's algorithm (Ellipsoid method)
- Karmarkar's algorithm
- IPM with crossover
  IPM: penalize $x \geq 0$ by $-\beta \log(x)$, polysized sequence of subproblems
  crossover: polytime number of simplex pivots get to opt
- No known pivot rule makes simplex alg. polytime!

  greedy pivot has exponential complexity on Klee-Minty cube

(Recall) MILP is **NP**-hard

- SAT **NP**-hard by Cook's theorem, reduce from SAT

$$\bigwedge_{i \le m} \bigvee_{j \in C_i} \ell_j$$

  where ℓ_j is either x_j or $\bar{x}_j \equiv \neg x_j$

- Polynomial reduction $\hat{\rho}$

SAT	x_j	$\bar{x}_j$	$\vee$	$\wedge$
MILP	x_j	$1 - x_j$	$+$	≥ 1

- E.g. $\hat{\rho}$ maps $(x_1 \vee x_2) \wedge (\bar{x}_2 \vee x_3)$ to

$$\min\{0 \mid x_1 + x_2 \ge 1 \wedge x_3 - x_2 \ge 0 \wedge x \in \{0,1\}^3\}$$

- SAT is YES iff MILP is feasible

Complexity of Quadratic Programming (QP)

$$\left.\begin{array}{rcl} \min\ \ x^\top Q x & + & c^\top x \\ Ax & \ge & b \end{array}\right\}$$

- Quadratic obj, linear constrs, continuous vars
- Many applications (e.g. portfolio selection)
- If Q has at least one negative eigenvalue, **NP**-hard
- Decision problem: "is the min. obj. fun. value ≤ 0?"
- If Q PSD then objective is convex, problem is in **P**
  KKT conditions become linear system, data in $\mathbb{Q} \Rightarrow$ soln in $\mathbb{Q}$

QP is **NP**-hard

- By reduction from SAT, let σ be an instance of SAT
- $\hat\rho(\sigma, x) \ge 1$: linear constraints of (SAT $\to$ MILP) reduction
- Consider QP subclass

$$\left.\begin{array}{ll} \min & f(x) = \sum\limits_{j \le n} x_j(1 - x_j) \\ & \hat\rho(\sigma, x) \ge 1 \\ & 0 \le x \le 1 \end{array}\right\} \quad (\dagger)$$

- **Claim**: σ is YES iff val($\dagger$)$\equiv$ opt. obj. fun. val. of $(\dagger) = 0$
- *Proof:*
  - assume σ YES with soln. x^*, then $x^* \in \{0,1\}^n$, hence $f(x^*) = 0$, since $f(x) \ge 0$ for all x, val($\dagger$) $= 0$
  - assume σ NO, suppose val($\dagger$) $= 0$, then $(\dagger)$ feasible with soln. x', since $f(x') = 0$ then $x' \in \{0,1\}$, feasible in SAT hence σ is YES, contradiction

Box-constrained QP is **NP**-hard

$$\left.\min_{x\in[x^L,x^U]} \quad x^\top Q x \quad + \quad c^\top x \right\}$$

- Add surplus vars v to SAT→MILP constraints:
  $\hat\rho(\sigma, x) - 1 - v = 0$
  (denote by $\forall i \le m \ (a_i^\top x - b_i - v_i = 0)$)
- Consider special QP subclass

$$\left.\begin{array}{rl} \min & \sum\limits_{j\le n} x_j(1-x_j) + \sum\limits_{i\le m} (a_i^\top x - b_i - v_i)^2 \\ & 0 \le x \le 1, v \ge 0 \end{array}\right\}$$

- Issue: v not bounded above
- Reduce from 3SAT, get ≤ 3 literals per clause
  $\Rightarrow$ *can consider* $0 \le v \le 2$

cQKP is **NP**-hard

- continuous Quadratic Knapsack Problem (cQKP)

$$\left.\begin{array}{rcl} \min \quad f(x) = x^\top Q x & + & c^\top x \\ \sum\limits_{j \le n} a_j x_j & = & \gamma \\ x & \in & [0,1]^n, \end{array}\right\}$$

- Reduction from SUBSET-SUM

  given list $a \in \mathbb{Q}^n$ and γ, is there $J \subseteq \{1,\ldots,n\}$ s.t. $\sum\limits_{j \in J} a_j = \gamma$?

  reduce to cQKP subclass with $f(x) = \sum_j x_j(1 - x_j)$

- σ is a YES instance of SUBSET-SUM
  - let $x^*_j = 1$ iff $j \in J$, $x^*_j = 0$ otherwise
  - feasible by construction
  - f is non-negative on $[0,1]^n$ and $f(x^*) = 0$: optimum
- σ is a NO instance of SUBSET-SUM
  - suppose $\mathsf{opt}(\text{cQKP}) = x^*$ with $f(x^*) = 0$
  - then $x^* \in \{0,1\}^n$ because $f(x^*) = 0$
  - feasibility of $x^* \Rightarrow J = \mathsf{supp}(x^*)$ solves σ, contradiction $\Rightarrow f(x^*) > 0$

QP on a simplex is **NP**-hard

$$\left.\begin{array}{rrcl} \min & f(x) = x^\top Q x & + & c^\top x \\ & \sum\limits_{j \le n} x_j & = & 1 \\ \forall j \le n & x_j & \ge & 0 \end{array}\right\}$$

- Reduce MAX CLIQUE to subclass with $f(x) = -\sum\limits_{\{i,j\} \in E} x_i x_j$

  Motzkin-Straus formulation (MSF):

$$\max\{ \sum_{\{i,j\} \in E} x_i x_j \mid \sum_{j \in V} x_j = 1 \wedge x \ge 0 \}$$

- Theorem [Motzkin& Straus 1964]

  > Let C be the maximum clique of the instance $G = (V, E)$ of MAX CLIQUE
  >
  > $\exists x^* \in \mathsf{opt}\,(\text{MSF})$ with $f^* = f(x^*) = \frac{1}{2} - \frac{1}{2\omega(G)}$
  >
  > $\forall j \in V \qquad x_j^* = \begin{cases} \frac{1}{\omega(G)} & \text{if } j \in C \\ 0 & \text{otherwise} \end{cases}$

- $\omega(G)$: size of max clique in G

Proof of the Motzkin-Straus theorem

$$x^* \in \mathsf{arg}(\max_{\substack{\sum_j x_j = 1 \\ x \geq 0}} \sum_{ij \in E} x_i x_j) \text{ s.t. } |C = \{j \in V \mid x_j^* > 0\}| \text{ smallest } (\ddagger)$$

1. $\boxed{\textit{C is a clique}}$
   - Suppose $1, 2 \in C$ but $\{1, 2\} \not\in E$, then $x_1^*, x_2^* > 0$, can perturb x^* by $\epsilon \in [-x_1^*, x_2^*]$, get $x^\epsilon = (x_1^* + \epsilon, x_2^* - \epsilon, x_3^*, x_4^*, \ldots)$, feasible w.r.t. simplex and bound constraints
   - $\{1, 2\} \not\in E \Rightarrow x_1 x_2$ does not appear in $f(x) \Rightarrow f(x^\epsilon)$ depends at worst linearly on ϵ; by local optimality of x^*, f achieves max for $\epsilon = 0$, in interior of its range $\Rightarrow f(x^\epsilon)$ constant w.r.t. ϵ. Hence $f(x^\epsilon)$ is globally optimal for all ϵ
   - setting $\epsilon = -x_1^*$ or $= x_2^*$ yields global optima with more zero components than x^*, against assumption $(\ddagger)$, hence $\{1, 2\} \in E[C]$; by relabeling C is a clique

Proof of the Motzkin-Straus theorem

$$x^* \in \mathsf{arg}(\max_{\substack{\sum_j x_j = 1 \\ x \geq 0}} \sum_{ij \in E} x_i x_j) \text{ s.t. } |C = \{j \in V \mid x_j^* > 0\}| \text{ smallest } (\ddagger)$$

2. $\boxed{|C| = \omega(G)}$

- square the simplex constraint $\sum_j x_j = 1$, get

$$\psi(x) \equiv \sum_{j \in V} x_j^2 + 2 \sum_{i<j \in V} x_i x_j = 1$$

- by construction $x_j^* = 0$ for $j \notin C \Rightarrow$

$$\psi(x^*) = \sum_{j \in C} (x_j^*)^2 + 2 \sum_{i<j \in C} x_i^* x_j^* = \sum_{j \in C} (x_j^*)^2 + 2f(x^*) = 1$$

- $\psi(x) = 1$ for all feasible x, so $f(x)$ achieves maximum when $\sum_{j \in C} (x_j^*)^2$ is minimum, i.e. $x_j^* = \frac{1}{|C|}$ for all $j \in C$
- again by simplex constraint

$$2f(x^*) = 1 - \sum_{j \in C} (x_j^*)^2 = 1 - |C| \frac{1}{|C|^2} = 1 - \frac{1}{|C|} \leq 1 - \frac{1}{\omega(G)}$$

so $f(x^*)$ attains max $\left(\frac{1}{2} - \frac{1}{2|C|}\right)$ when $|C| = \omega(G) \Rightarrow \forall j \in C \; x_j = \frac{1}{\omega(G)}$

Copositive programming

- StQP: $\min x^\top Q x : \sum_j x_j = 1 \wedge x \geq 0$
  $\boldsymbol{NP}$-hard by Motzkin-Straus
- Linearize: $X = xx^\top$
  replace $x_i x_j$ by X_{ij} and add constraints $X_{ij} = x_i x_j$
- Define $A \bullet B = \mathsf{tr}(A^\top B) = \sum_{i,j} A_{ij} B_{ij}$
  write StQP (linearized) objective as $\min Q \bullet X$
- Let $C = \{X \mid X = xx^\top \wedge x \geq 0\}$, $\bar{C} = \mathsf{conv}(C)$
- $\sum_j x_j = 1 \Leftrightarrow (\sum_j x_j)^2 = 1^2 \Leftrightarrow \mathbf{1} \bullet X = 1$
- StQP $\equiv \min Q \bullet X : \mathbf{1} \bullet X = 1 \wedge X \in C$
  linear obj. $\Rightarrow$ optima attained at extrema of feas. set
  $\Rightarrow$ can replace C by its convex hull $\bar{C}$

  $\bar{C}$ is a completely positive cone
- Dual $\equiv \max y : Q - y\mathbf{1} \in \bar{C}^* = \{A \mid \forall x \geq 0 \ (x^\top A x \geq 0)\}$
  $\bar{C}^*$ is a copositive cone
- $\Rightarrow$ Pair of **NP**-hard cNLPs!

An exercise and a project idea

> *You, a private investment banker, are seeing a customer. She tells you "I have 3,450,000$ I don't need in the next three years. Invest them in low-risk assets so I get at least 2.5% return per year."*
>
> *Model the problem of determining the required portfolio. Missing data are part of the fun (and of real life).*

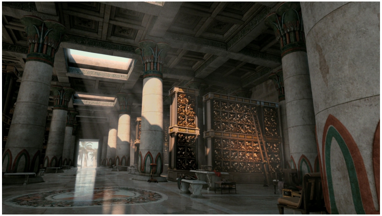
[What are the decision varis, objective, constraints? What data are missing?]

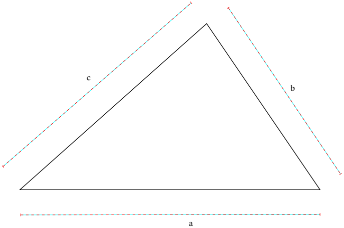
Project idea 1: Consider the MILP formulation for Max Clique and the Motzkin-Straus formulation. Can the latter have multiple global optima? If so, do they all characterize a maximum clique? What do local optima characterize? Pursue a computational study to answer these questions, then check [Gibbons et al., *Mathematics of Operations Research*, **22**:754-768, 1997] and [Pelillo & Jagota, *J. Artif. Neural Networks*, **2**:411-420, 1995]

Outline

A gem in Distance Geometry

- *Heron's theorem*
- Heron lived around year 0
- Hung out at Alexandria's library



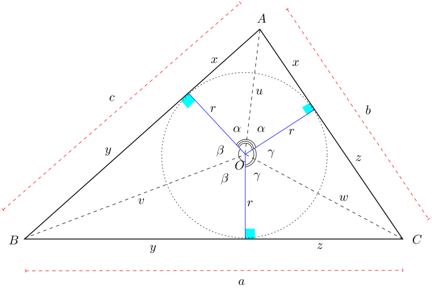


$$A = \sqrt{s(s-a)(s-b)(s-c)}$$

- $A =$ area of triangle
- $s = \frac{1}{2}(a+b+c)$

Useful to measure areas of agricultural land

Heron's theorem: *Proof* [M. Edwards, high school student, 2007]



A. $2\alpha + 2\beta + 2\gamma = 2\pi \Rightarrow \alpha + \beta + \gamma = \pi$

$$\begin{aligned} r + ix &= ue^{i\alpha} \\ r + iy &= ve^{i\beta} \\ r + iz &= we^{i\gamma} \end{aligned}$$

$\Rightarrow (r+ix)(r+iy)(r+iz) = (uvw)e^{i(\alpha+\beta+\gamma)} = uvw\, e^{i\pi} = -uvw \in \mathbb{R}$

$\Rightarrow \mathrm{Im}((r+ix)(r+iy)(r+iz)) = 0$

$\Rightarrow r^2(x+y+z) = xyz \Rightarrow r = \sqrt{\frac{xyz}{x+y+z}}$

B. $s = \frac{1}{2}(a+b+c) = \frac{1}{2}(2x+2y+2z) = x+y+z$

$$\begin{aligned} s - a &= x + y + z - y - z = x \\ s - b &= x + y + z - x - z = y \\ s - c &= x + y + z - x - y = z \end{aligned}$$

$$\Rightarrow \quad \mathcal{A} = \frac{1}{2}(ra + rb + rc) = r\frac{a+b+c}{2} = rs = \sqrt{s(s-a)(s-b)(s-c)}$$

Subsection 1

The universal isometric embedding

Representing metric spaces in $\mathbb{R}^n$

- Given metric space (X, d) with dist. matrix (DM) $D = (d_{ij})$, embed X in some $\mathbb{R}^K$ so it has the same DM
- Consider i-th row $x_i = (d_{i1}, \ldots, d_{in})$ of D
- Embed $i \in X$ by vector $U^D(i) = x_i \in \mathbb{R}^n$
  define $U^D : \{1, \ldots, n\} \to \mathbb{R}^n$ s.t. $U^D(i) = x_i$
- Thm.: (U^D, ℓ_∞) is a metric space with DM D
  i.e. $\forall i, j \le n \; \|x_i - x_j\|_\infty = d_{ij}$
- U^D is called Universal Isometric Embedding (UIE)
- Practical issue: *embedding is high-dimensional ($\mathbb{R}^n$)*

[Kuratowski 1935]

Proof

- Consider $i, j \in X$ with distance $d(i,j) = d_{ij}$
- Then

$$\|x_i - x_j\|_\infty = \max_{k \le n} |d_{ik} - d_{jk}| \le \max_{k \le n} |d_{ij}| = d_{ij}$$

ineq. $\le$ above from triangular inequalities in metric space:

$$\begin{array}{lll} \forall k & d_{ik} \le d_{ij} + d_{jk} & \wedge \quad d_{jk} \le d_{ij} + d_{ik} \\ \Rightarrow & d_{ik} - d_{jk} \le d_{ij} & \wedge \quad d_{jk} - d_{ik} \le d_{ij} \\ \Rightarrow & |d_{ik} - d_{jk}| \le d_{ij} & \end{array}$$

If valid $\forall k$ then valid for $\max_k$

- $\max |d_{ik} - d_{jk}|$ over $k \le n$ achieved when $k \in \{i, j\}$

$$\Rightarrow \|x_i - x_j\|_\infty = d_{ij}$$

Subsection 2

Dimension reduction

Schoenberg's theorem

- [I. Schoenberg, *Remarks to Maurice Fréchet's article "Sur la définition axiomatique d'une classe d'espaces distanciés vectoriellement applicable sur l'espace de Hilbert"*, Ann. Math., 1935]
- **Question**: Given $n \times n$ symmetric matrix D, what are necessary and sufficient conditions s.t. D is a Euclidean DM (EDM) corresponding to n points $x_1, \ldots, x_n \in \mathbb{R}^K$ with K minimum?
- Necessary and sufficient conditions for an EDM
  Thm.
  $D = (d_{ij})$ is an EDM iff $\frac{1}{2}(d_{1i}^2 + d_{1j}^2 - d_{ij}^2 \mid 2 \le i, j \le n)$ is PSD (of rank K)
- Yields important result in data science:
  Classic Multidimensional Scaling

Gram matrices and EDMs

- Realization: $n \times K$ matrix $x = (x_1, \ldots, x_n) \subseteq \mathbb{R}^K$
- Gram matrix of x: $G = xx^\top = (x_i \cdot x_j)$

  Lemma: *(i) $G \succeq 0$; (i) each $M \succeq 0$ is a Gram matrix of some x*
- Theorem: *given rlz x, Gram matrix G and EDM D satisfy*

$$G = -\frac{1}{2} J D^2 J \qquad (\S)$$

- In the theorem, $D^2 = (d_{ij}^2)$ and

$$J = I_n - \tfrac{1}{n}\mathbf{1}\mathbf{1}^\top = \begin{pmatrix} 1-\frac{1}{n} & -\frac{1}{n} & \cdots & -\frac{1}{n} \\ -\frac{1}{n} & 1-\frac{1}{n} & \cdots & -\frac{1}{n} \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{n} & -\frac{1}{n} & \cdots & 1-\frac{1}{n} \end{pmatrix}$$

- This is a variant of Schoenberg's theorem

Multidimensional scaling (MDS)

- Often get approximate EDMs $\tilde{D}$ from raw data
  (i.e. matrices that are not EDMs, but they are "not too far")
  (they measure dissimilarities, discrepancies, differences)
- $\tilde{G} = -\frac{1}{2}J\tilde{D}^2J$ is an approximate Gram matrix
- Approximate Gram $\Rightarrow$ spectral decomposition $P\tilde{\Lambda}P^\top$ has $\tilde{\Lambda} \not\geq 0$
- Let Λ be a PSD diagonal matrix closest to $\tilde{\Lambda}$:
  Λ *obtained from* $\tilde{\Lambda}$ *by zeroing negative components*
- $x = P\sqrt{\Lambda}$ is an "approximate realization" of $\tilde{D}$
- Denote $x = \mathrm{MDS}(D)$

Classic MDS: Main result

1. Prove lemma: matrix is Gram iff it is PSD
2. Prove theorem: $G = -\frac{1}{2} J D^2 J$

Proof of lemma

- *Gram* $\subseteq$ *PSD*
  - x is an $n \times K$ real matrix
  - $G = xx^\top$ its Gram matrix
  - For each $y \in \mathbb{R}^n$ we have
    $$yGy^\top = y(xx^\top)y^\top = (yx)(x^\top y^\top) = (yx)(yx)^\top = \|yx\|_2^2 \geq 0$$
  - $\Rightarrow G \succeq 0$
- *PSD* $\subseteq$ *Gram*
  - Let $G \succeq 0$ be $n \times n$
  - *Spectral decomposition*: $G = P\Lambda P^\top$
    (P orthogonal, $\Lambda \geq 0$ diagonal)
  - $\Lambda \geq 0 \Rightarrow \sqrt{\Lambda} \in \mathbb{R}^{n\times n}$
  - $G = P\Lambda P^\top = (P\sqrt{\Lambda})(\sqrt{\Lambda}^\top P^\top) = (P\sqrt{\Lambda})(P\sqrt{\Lambda})^\top$
  - Let $x = P\sqrt{\Lambda}$, then G is the Gram matrix of x

Proof of theorem (1/2)

- Let $G = xx^\top$, translate x so that centroid $\frac{1}{n}\sum_j x_j = 0$
- Expand: $d_{ij}^2 = \|x_i - x_j\|_2^2 = (x_i - x_j)(x_i - x_j) = x_i x_i + x_j x_j - 2x_i x_j \qquad (*)$
- Aim at "inverting" $(*)$ to express $x_i x_j$ in function of d_{ij}^2
- Sum $(*)$ over i: $\sum_i d_{ij}^2 = \sum_i x_i x_i + n x_j x_j - 2x_j \cancel{\sum_i x_i}$ 0 by zero centroid
- Similarly for j and divide by n, get:

$$\begin{aligned} \frac{1}{n}\sum_{i \le n} d_{ij}^2 &= \frac{1}{n}\sum_{i \le n} x_i x_i + x_j x_j \qquad (\dagger) \\ \frac{1}{n}\sum_{j \le n} d_{ij}^2 &= x_i x_i + \frac{1}{n}\sum_{j \le n} x_j x_j \qquad (\ddagger) \end{aligned}$$

- Sum $(\dagger)$ over j, get:

$$\frac{1}{n}\sum_{i,j} d_{ij}^2 = n\frac{1}{n}\sum_i x_i x_i + \sum_j x_j x_j = 2\sum_i x_i x_i$$

- Divide by n, get:

$$\frac{1}{n^2}\sum_{i,j} d_{ij}^2 = \frac{2}{n}\sum_i x_i x_i \qquad (**)$$

Proof of theorem (2/2)

- Rearrange $(*)$, $(\dagger)$, $(\ddagger)$ as follows:

$$
\begin{aligned}
2x_ix_j &= x_ix_i + x_jx_j - d_{ij}^2 && (5)\\
x_ix_i &= \frac{1}{n}\sum_j d_{ij}^2 - \frac{1}{n}\sum_j x_jx_j && (6)\\
x_jx_j &= \frac{1}{n}\sum_i d_{ij}^2 - \frac{1}{n}\sum_i x_ix_i && (7)
\end{aligned}
$$

- Replace LHS of Eq. (6)-(7) in RHS of Eq. (5), get

$$2x_ix_j = \frac{1}{n}\sum_k d_{ik}^2 + \frac{1}{n}\sum_k d_{kj}^2 - d_{ij}^2 - \frac{2}{n}\sum_k x_kx_k$$

- By $(**)$ replace $\frac{2}{n}\sum_i x_ix_i$ with $\frac{1}{n^2}\sum_{i,j} d_{ij}^2$, get

$$2x_ix_j = \frac{1}{n}\sum_k (d_{ik}^2 + d_{kj}^2) - d_{ij}^2 - \frac{1}{n^2}\sum_{h,k} d_{hk}^2 \qquad (\S)$$

  which expresses x_ix_j in function of D
- Finally, show RHS of $(\S)$ is (i,j)-th entry of $-JD^2J$

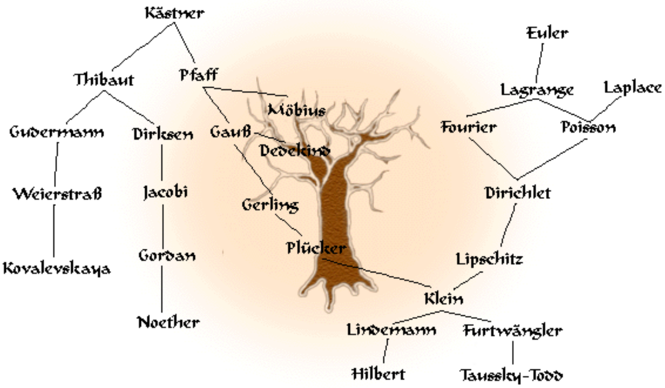
  See lecture notes, Thm. 10.3.5

Principal Component Analysis (PCA)

- Given an approximate EDM D
- find $x = \text{MDS}(D)$
- However, you want $x = P\sqrt{\Lambda}$ in K dimensions
  but $\mathsf{rank}(\Lambda) > K$
- Only keep K largest components of Λ
  zero the rest
- Get realization in desired space
- Denote $x = \text{PCA}(D, K)$

Example 1/3

Mathematical genealogy skeleton



Example 2/3

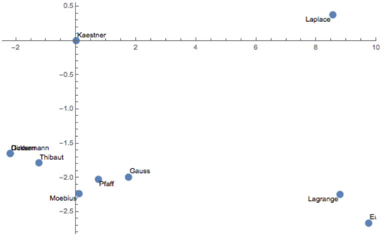
A partial view

	Euler	Thibaut	Pfaff	Lagrange	Laplace	Möbius	Gudermann	Dirksen
Kästner	10	1	1	9	8	2	2	2
Euler		11	9	1	3	10	12	12
Thibaut			2	10	10	3	1	1
Pfaff				8	8	1	3	3
Lagrange					2	9	11	11
Laplace						9	11	11
Möbius							4	4
Gudermann								2
Dirksen								

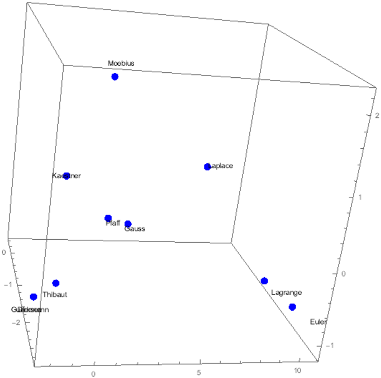
$$D = \begin{pmatrix} 0 & 10 & 1 & 1 & 9 & 8 & 2 & 2 & 2 & 2 \\ 10 & 0 & 11 & 9 & 1 & 3 & 10 & 12 & 12 & 8 \\ 1 & 11 & 0 & 2 & 10 & 10 & 3 & 1 & 1 & 3 \\ 1 & 9 & 2 & 0 & 8 & 8 & 1 & 3 & 3 & 1 \\ 9 & 1 & 10 & 8 & 0 & 2 & 9 & 11 & 11 & 7 \\ 8 & 3 & 10 & 8 & 2 & 0 & 9 & 11 & 11 & 7 \\ 2 & 10 & 3 & 1 & 9 & 9 & 0 & 4 & 4 & 2 \\ 2 & 12 & 1 & 3 & 11 & 11 & 4 & 0 & 2 & 4 \\ 2 & 12 & 1 & 3 & 11 & 11 & 4 & 2 & 0 & 4 \\ 2 & 8 & 3 & 1 & 7 & 7 & 2 & 4 & 4 & 0 \end{pmatrix}$$

Example 3/3

In 2D



In 3D

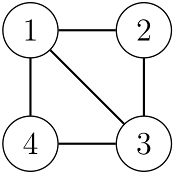


Subsection 3

Dealing with incomplete metrics

Partial metrics

- If your metric space is missing some distances
- Get incomplete EDM D
- Cannot define vectors $U^D(i)$ in UIE
- *Note*: D defines a graph

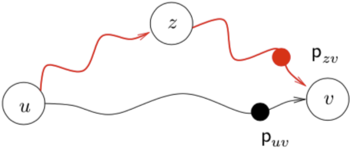


$$D = \begin{pmatrix} 0 & 1 & \sqrt{2} & 1 \\ 1 & 0 & 1 & \boxed{?} \\ \sqrt{2} & 1 & 0 & 1 \\ 1 & \boxed{?} & 1 & 0 \end{pmatrix}$$

- Complete graph with shortest path (SP) distances: $d_{24} = 2$

Floyd-Warshall algorithm 1/2

- Given $n \times n$ partial matrix D computes *all shortest path lengths*
- For each triplet z, u, v of vertices in the graph, test: *when going $u \to v$, is it convenient to pass through z?*



- If so, then change the path length
- Complete missing entries d_{uv} in D shortest path lengths $u \to v$
- Denote $\bar{D} = \text{FloydWarshall}(D)$

Floyd-Warshall algorithm 2/2

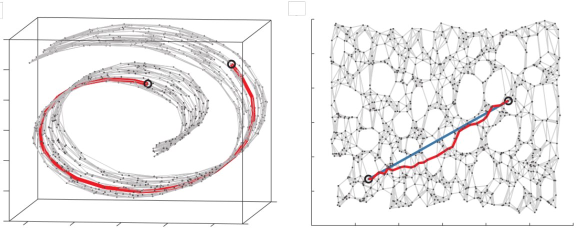
```
# initialization
for u ≤ n, v ≤ n do
  if d_uv =? then
    d_uv ← ∞
  end if
end for
# main loop (outer loop must be on triangulation vertex)
for z ≤ n do
  for u ≤ n do
    for v ≤ n do
      if d_uv > d_uz + d_zv then
        d_uv ← d_uz + d_zv
      end if
    end for
  end for
end for
```

Subsection 4

The Isomap heuristic

Isomap embedding in $\mathbb{R}^K$

- Given a partial EDM D
  1. $\bar{D} = \text{FloydWarshall}(D)$
  2. $x = \text{PCA}(\bar{D}, K)$
- Intuition of why it works well:



- Denote $x = \text{Isomap}(D, K)$

[Tenenbaum et al., *Science*, 2000]

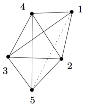
Subsection 5

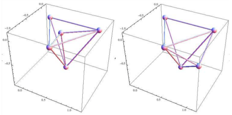
Distance geometry problem

The Distance Geometry Problem (DGP)

Given $K \in \mathbb{N}$ *and* $G = (V, E, d)$ *with* $d : E \to \mathbb{R}_+$,
find $x : V \to \mathbb{R}^K$ *s.t.*

$$\forall \{i, j\} \in E \quad \|x_i - x_j\|_2^2 = d_{ij}^2$$

Given a weighted graph 

, draw it so edges are drawn as segments with lengths = weights 

Some applications

- clock synchronization ($K = 1$)
- sensor network localization ($K = 2$)
- molecular structure from distance data ($K = 3$)
- autonomous underwater vehicles ($K = 3$)
- EDM completion (whatever K)
- finding graph embeddings (whatever K)

Clock synchronization

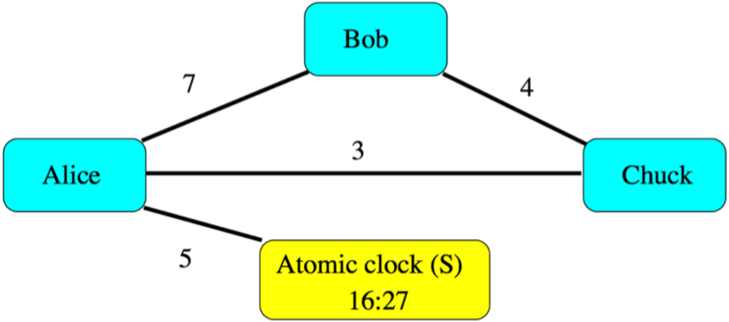
From [Singer, *Appl. Comput. Harmon. Anal.* 2011]

Determine a set of unknown timestamps from partial measurements of their time differences

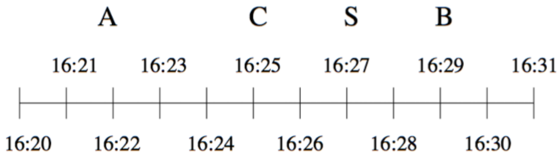
- $K = 1$
- V: timestamps
- $\{u, v\} \in E$ if known time difference between u, v
- d: values of the time differences

Used in time synchronization of distributed networks

Clock synchronization



$\downarrow$



Sensor network localization

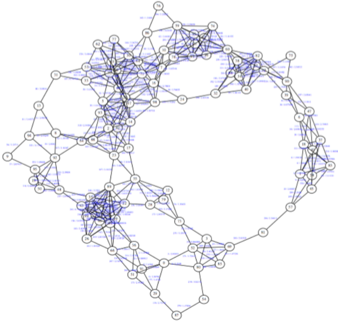
From [Yemini, *Proc. CDSN*, 1978]

The positioning problem arises when it is necessary to locate a set of geographically distributed objects using measurements of the distances between some object pairs

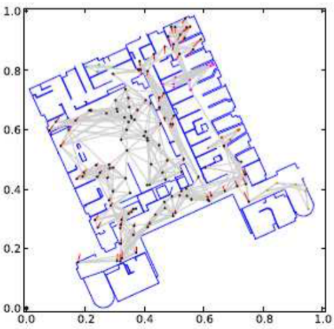
- $K = 2$
- V: (mobile) sensors
- $\{u, v\} \in E$ iff distance between u, v is measured
- d: distance values

Used whenever GPS not viable (e.g. underwater)
$d_{uv} \mathrel{\propto\!\!\!\sim}$ battery consumption in P2P communication betw. u, v

Sensor network localization

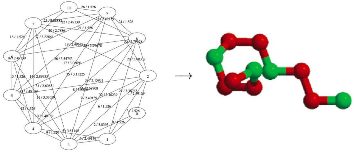


$\longrightarrow$



Molecular structure from distance data

From [Liberti et al., *SIAM Rev.*, 2014]



- $K = 3$
- V: atoms
- $\{u, v\} \in E$ iff distance between u, v is known
- d: distance values

Used whenever X-ray crystallography does not apply (e.g. liquid)
Covalent bond lengths and angles known precisely
Distances $\lessapprox 5.5$ measured approximately by NMR

Graph embeddings

- Relational knowledge best represented by graphs
- *We have fast algorithms for clustering vectors*
- **Task**: represent a graph in $\mathbb{R}^n$
- "Graph embeddings" and "distance geometry": almost synonyms
- Used in Natural Language Processing (NLP)
  obtain "word vectors" & "sentence vectors"

Project idea 2: create a graph-of-words from a sentence, enrich it with semantic distances, then use the DG methods in these lectures to embed the graph in a low-dimensional space; then evaluate sentence similarity using vector angles

Complexity

- DGP_1 with $d : E \to \mathbb{Q}_+$ is in **NP**
  - if instance YES $\exists$ realization $x \in \mathbb{R}^{n\times 1}$
  - if some component $x_i \notin \mathbb{Q}$ translate x so $x_i \in \mathbb{Q}$
  - consider some other x_j
  - let $\ell = |\text{sh. path } p : i \to j| = \sum\limits_{\{u,v\}\in p} (-1)^{s_{uv}} d_{uv} \in \mathbb{Q}$
    for some $s_{uv} \in \{0, 1\}$
  - then $x_j = x_i \pm \ell \to x_j \in \mathbb{Q}$ $(\forall j)$
  - $\Rightarrow$ polytime verification of

$$\forall \{i,j\} \in E \quad |x_i - x_j| = d_{ij}$$

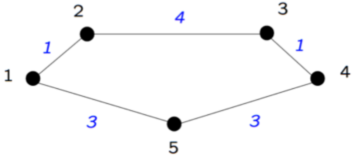
- DGP_K may not be in **NP** for $K > 1$
  don't know how to polytime check $\|x_i - x_j\|_2 = d_{ij}$ for $x \notin \mathbb{Q}^{nK}$

Hardness

PARTITION *is* **NP**-*hard*

Given $a = (a_1, \ldots, a_n) \in \mathbb{N}^n$, $\exists\, I \subseteq \{1, \ldots, n\}$ s.t. $\sum\limits_{i \in I} a_i = \sum\limits_{i \notin I} a_i$?

- Reduce PARTITION to DGP_1 on single-cycle graphs
- $a \longrightarrow$ cycle C
  $V(C) = \{1, \ldots, n\}$, $E(C) = \{\{1,2\}, \ldots, \{n,1\}\}$
- For $i < n$ let $d_{i,i+1} = a_i$
  For $i = n$, let $d_{n,n+1} = d_{n1} = a_n$
- *E.g. for* $a = (1,4,1,3,3)$, *get cycle graph:*



[Saxe, 1979]

PARTITION is YES $\Rightarrow$ DGP$_1$ is YES

- **Given**: $I \subset \{1, \ldots, n\}$ s.t. $\sum_{i \in I} a_i = \sum_{i \notin I} a_i$
- **Construct**: realization x of C in $\mathbb{R}$
  1. $x_1 = 0$ `// start`
  2. **induction step**: suppose x_i known
     if $i \in I$

     let $x_{i+1} = x_i + d_{i,i+1}$ `// go right`

     else

     let $x_{i+1} = x_i - d_{i,i+1}$ `// go left`
- **Correctness proof**: by the same induction
  but careful when $i = n$: have to show $x_{n+1} = x_1$

PARTITION is YES $\Rightarrow$ DGP$_1$ is YES

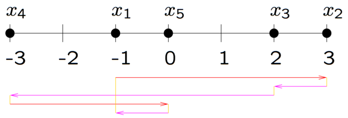
Proof that $x_{n+1} = x_1$:

$$
\begin{aligned}
(1) = \sum_{i \in I} (x_{i+1} - x_i) &= \sum_{i \in I} d_{i,i+1} = \\
= \sum_{i \in I} a_i &= \sum_{i \notin I} a_i = \\
= \sum_{i \notin I} d_{i,i+1} &= \sum_{i \notin I} (x_i - x_{i+1}) = (2)
\end{aligned}
$$

$$
\begin{aligned}
(1) = (2) \Rightarrow \sum_{i \in I} (x_{i+1} - x_i) = \sum_{i \notin I} (x_i - x_{i+1}) \Rightarrow \sum_{i \leq n} (x_{i+1} - x_i) &= 0 \\
\Rightarrow (x_{n+1} - x_n) + (x_n - x_{n-1}) + \cdots + (x_3 - x_2) + (x_2 - x_1) &= 0 \\
\Rightarrow x_{n+1} &= x_1
\end{aligned}
$$

PARTITION is NO $\Rightarrow$ DGP$_1$ is NO

- By contradiction: suppose DGP$_1$ is YES, x realization of C
- $F = \{\{u,v\} \in E(C) \mid x_u \le x_v\}$,
  $E(C) \smallsetminus F = \{\{u,v\} \in E(C) \mid x_u > x_v\}$
- Trace $x_1, \ldots, x_n$: follow edges in F ($\rightarrow$) and in $E(C) \smallsetminus F$ ($\leftarrow$)



DGP$_1$ instance is YES $\Rightarrow$

$$\begin{aligned}
\sum_{\{u,v\}\in F} (x_v - x_u) &= \sum_{\{u,v\}\notin F} (x_u - x_v) \\
\sum_{\{u,v\}\in F} |x_u - x_v| &= \sum_{\{u,v\}\notin F} |x_u - x_v| \\
\sum_{\{u,v\}\in F} d_{uv} &= \sum_{\{u,v\}\notin F} d_{uv}
\end{aligned}$$

- Let $J = \{i < n \mid \{i, i+1\} \in F\} \cup \{n \mid \{n,1\} \in F\}$

$$\Rightarrow \quad \sum_{i \in J} a_i = \sum_{i \notin J} a_i$$

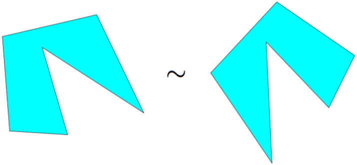
- So J solves Partition instance, contradiction
- $\Rightarrow$ DGP is **NP**-hard, DGP$_1$ is **NP**-complete

Number of solutions

- (G, K): DGP instance
- $\tilde{X} \subseteq \mathbb{R}^{Kn}$: set of solutions
- *Congruence*: composition of translations, rotations, reflections
- $C =$ set of congruences in $\mathbb{R}^K$
- $x \sim y$ means $\exists \rho \in C \ (y = \rho x)$:
  distances in x are preserved in y through ρ
- $\Rightarrow$ if $|\tilde{X}| > 0$, $|\tilde{X}| = 2^{\aleph_0}$

Number of solutions modulo congruences

- Congruence is an *equivalence relation* $\sim$ on $\tilde{X}$ (reflexive, symmetric, transitive)



- Partitions $\tilde{X}$ into *equivalence classes*
- $X = \tilde{X}/\sim$
  sets of representatives of equivalence classes
- **Focus on** $|X|$ **rather than** $|\tilde{X}|$

Rigidity, flexibility and $|X|$

- infeasible $\Leftrightarrow |X| = 0$
- rigid graph $\Leftrightarrow |X| < \aleph_0$
- globally rigid graph $\Leftrightarrow |X| = 1$
- flexible graph $\Leftrightarrow |X| = 2^{\aleph_0}$
- $|X| = \aleph_0$: impossible by Milnor's theorem

Milnor's theorem implies $|X| \neq \aleph_0$

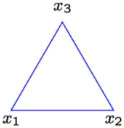
- System S of polynomial equations of degree 2

$$\forall i \leq m \quad p_i(x_1, \ldots, x_{nK}) = 0$$

- Let X be the set of $x \in \mathbb{R}^{nK}$ satisfying S
- **Number of connected components of X is $O(3^{nK})$** [Milnor 1964]
- Assume $|X|$ is countable; then G cannot be flexible
  $\Rightarrow$ *each incongruent rlz is in a separate component*
  $\Rightarrow$ by Milnor's theorem, there's finitely many of them

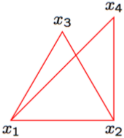
Examples

$V^1 = \{1, 2, 3\}$
$E^1 = \{\{u, v\} \mid u < v\}$
$d^1 = 1$



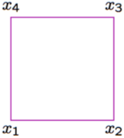
ρ congruence in $\mathbb{R}^2$
$\Rightarrow \rho x$ valid realization
$|X| = 1$

$V^2 = V^1 \cup \{4\}$
$E^2 = E^1 \cup \{\{1, 4\}, \{2, 4\}\}$
$d^2 = 1 \wedge d_{14} = \sqrt{2}$



ρ reflects x_4 wrt $\overline{x_1, x_2}$
$\Rightarrow \rho x$ valid realization
$|X| = 2$ (,)

$V^3 = V^2$
$E^3 = \{\{u, u+1\} | u \leq 3\} \cup \{1, 4\}$
$d^1 = 1$



ρ rotates $\overline{x_2 x_3}$, $\overline{x_1 x_4}$ by θ
$\Rightarrow \rho x$ valid realization
$|X|$ is uncountable
(, , , , ...)

Subsection 6

Distance geometry in MP

DGP formulations and methods

- System of equations
- Unconstrained global optimization (GO)
- Constrained global optimization
- SDP relaxations and their properties
- Diagonal dominance
- Concentration of measure in SDP
- Isomap for DGP

System of quadratic equations

$$\forall \{u,v\} \in E \quad \|x_u - x_v\|^2 = d_{uv}^2 \tag{8}$$

Computationally: useless
reformulate using slacks:

$$\min_{x,s} \Big\{ \sum_{\{u,v\} \in E} s_{uv}^2 \;\Big|\; \forall \{u,v\} \in E \quad \|x_u - x_v\|^2 = d_{uv}^2 + s_{uv} \Big\} \tag{9}$$

Unconstrained Global Optimization

$$\min_x \sum_{\{u,v\}\in E} (\|x_u - x_v\|^2 - d_{uv}^2)^2 \tag{10}$$

$\boxed{\text{Globally optimal obj. fun. value of (10) is 0 iff } x \text{ solves (8)}}$

Computational experiments in [Liberti et al., 2006]:

- GO solvers from >15 years ago
- randomly generated protein data: ≤ 50 atoms
- cubic crystallographic grids: ≤ 64 atoms

Constrained global optimization

- $\min_x \sum\limits_{\{u,v\}\in E} |\|x_u - x_v\|^2 - d_{uv}^2|$ exactly reformulates (8)
- Relax objective f to concave part, remove constant term, rewrite $\min -f$ as $-\max f$

$\min_x \sum_{uv}(d_{uv}^2 - \|x_u - x_v\|_2^2) = \sum_{uv} d_{uv}^2 - \max_x \sum_{uv} \|x_u - x_v\|_2^2$

- Reformulate convex part of obj. fun. to convex constraints

$$\forall\{u,v\} \in E \ \|x_u - x_v\|_2^2 \le d_{uv}^2$$

- Exact reformulation *("push-and-pull")*

$$\left.\begin{array}{rl} \max_x & \sum\limits_{\{u,v\}\in E} \|x_u - x_v\|^2 \\ \forall\{u,v\} \in E & \|x_u - x_v\|^2 \le d_{uv}^2 \end{array}\right\} \quad (11)$$

Theorem (Activity)

At a glob. opt. x^* of a YES *instance, all constraints of (11) are active*

Push-and-pull linearization

Linearization of nonlinear terms $\|x_i - x_j\|_2^2$
for all $\{i,j\} \in E$:

$$\Rightarrow \quad \forall \{i,j\} \in E \quad \|x_i\|_2^2 + \|x_j\|_2^2 - 2x_i \cdot x_j = d_{ij}^2$$

$$\Rightarrow \left\{ \begin{array}{rcl} \forall \{i,j\} \in E \quad X_{ii} + X_{jj} - 2X_{ij} & = & d_{ij}^2 \\ X & = & x\,x^\top \end{array} \right.$$

Relaxation

$$
\begin{array}{rrcl}
 & X & = & x\,x^\top \\
\Rightarrow & X - x\,x^\top & = & 0 \\
\text{(relax)} \quad \Rightarrow & X - x\,x^\top & \succeq & 0
\end{array}
$$

$$\mathsf{Schur}(X, x) = \begin{pmatrix} I_K & x^\top \\ x & X \end{pmatrix} \succeq 0$$

If x does not appear elsewhere $\Rightarrow$ get rid of it (e.g. choose $x = 0$):

replace $\mathsf{Schur}(X, x) \succeq 0$ *by* $X \succeq 0$

SDP relaxation

- Relaxation:

$$\begin{array}{rrcl} & \min F \bullet X & & \\ \forall \{i,j\} \in E & X_{ii} + X_{jj} - 2X_{ij} & = & d_{ij}^2 \\ & X & \succeq & 0 \end{array}$$

- Note SDP $\equiv$ linear obj. s.t. linear constrs $\wedge$ PSD cone
- DGP linearization/relaxation only defines feasible set
- Note $F \bullet X = \mathsf{tr}(F^\top X) = \sum_{ij} F_{ij} X_{ij}$
- Can we choose a "good" objective function F?

Some possible objective functions

- For protein conformation:

$$\min \sum_{\{i,j\} \in E} (X_{ii} + X_{jj} - 2X_{ij})$$

  with $=$ changed to $\geq$ in constraints *(or* max *and* $\leq$*)*
  "push-and-pull" relaxation

- [Ye, 2003], application to wireless sensors localization

$$\min \mathsf{tr}(X)$$

  $\mathsf{tr}(X) = \mathsf{tr}(P^{-1}\Lambda P) = \mathsf{tr}(P^{-1}P\Lambda) = \mathsf{tr}(\Lambda) = \sum_i \lambda_i$
  $\Rightarrow$ *hope to minimize rank*

- How about "just random"?

How do you choose?

for want of some better criterion...

TEST!

- Download protein files from Protein Data Bank (PDB)

  they contain atom realizations

- Mimick a Nuclear Magnetic Resonance experiment

  Keep only pairwise distances < 5.5

- Try and reconstruct the protein shape from those weighted graphs

- Quality evaluation of results:
  - $\mathrm{LDE}(x) = \max_{\{i,j\}\in E} |\, \|x_i - x_j\| - d_{ij} \,|$
  - $\mathrm{MDE}(x) = \frac{1}{|E|} \sum_{\{i,j\}\in E} |\, \|x_i - x_j\| - d_{ij} \,|$

Empirical choice

- *Ye* faster but often imprecise
- *Random* good but nondeterministic
- *Push-and-Pull*: can relax $X_{ii} + X_{jj} - 2X_{ij} = d_{ij}^2$ to $X_{ii} + X_{jj} - 2X_{ij} \geq d_{ij}^2$
  easier to satisfy feasibility, useful later on
- Heuristic: add $+\eta \mathsf{tr}(X)$ to objective, with $\eta \ll 1$
  might help minimize solution rank
- $\min \sum\limits_{\{i,j\} \in E} (X_{ii} + X_{jj} - 2X_{ij}) + \eta \mathsf{tr}(X)$
  appears to be a good objective function

When solving real problems maths may not be enough
use common sense too

Retrieving realizations in $\mathbb{R}^K$

- SDP relaxation yields $n \times n$ PSD matrix X^*
- We need $n \times K$ realization matrix x^*
- Recall $PSD \Leftrightarrow Gram$
- Apply PCA to X^*, keep K largest comps, get x'
- This yields solutions with errors
- Use x' as starting pt for local NLP solver

Later on: Barvinok's Naive Algorithm, *an SDP-specific alternative to PCA*

When SDP solvers hit their size limit

- **SDP solver: technological bottleneck**
- Can we use an LP solver instead?
- Diagonally Dominant (DD) matrices are PSD
- Not *vice versa*: inner approximate PSD cone $Y \succeq 0$
- *Idea by A.A. Ahmadi [Ahmadi & Hall 2015]*

Diagonally dominant matrices

$n \times n$ symmetric matrix X is DD if

$$\forall i \le n \quad X_{ii} \ge \sum_{j \ne i} |X_{ij}|.$$

E.g. $\begin{pmatrix} 1 & 0.1 & -0.2 & 0 & 0.04 & 0 \\ 0.1 & 1 & -0.05 & 0.1 & 0 & 0 \\ -0.2 & -0.05 & 1 & 0.1 & 0.01 & 0 \\ 0 & 0.1 & 0.1 & 1 & 0.2 & 0.3 \\ 0.04 & 0 & 0.01 & 0.2 & 1 & -0.3 \\ 0 & 0 & 0 & 0.3 & -0.3 & 1 \end{pmatrix}$

Gershgorin's circle theorem

- Let A be symmetric $n \times n$
- $\forall i \leq n$ let $R_i = \sum_{j \neq i} |A_{ij}|$ and $I_i = [A_{ii} - R_i, A_{ii} + R_i]$
- Then $\forall \lambda$ eigenvalue of $A \quad \exists i \leq n$ s.t. $\lambda \in I_i$

<u>*Proof*</u>

- Let λ be an eigenvalue of A with eigenvector y
- Normalize y s.t. $\exists i \leq n\ y_i = 1$ and $\forall j \neq i\ |y_j| \leq 1$
  let $i = \arg\max_j |y_j|$, *divide* y *by* $\mathrm{sgn}(y_i)|y_i|$
- $Ay = \lambda y \Rightarrow \sum_{j \leq n : j \neq i} A_{ij} y_j + A_{ii} y_i = \sum_{j \leq n : j \neq i} A_{ij} y_j + A_{ii} = \lambda y_i = \lambda$
- Hence $\sum_{j \leq n : j \neq i} A_{ij} y_j = \lambda - A_{ii}$
- Triangle+Cauchy-Schwarz inequalities & $\forall j \neq i\ |y_j| \leq 1 \Rightarrow$
  $|\lambda - A_{ii}| = |\sum_{j \leq n : j \neq i} A_{ij} y_j| \leq \sum_{j \leq n : j \neq i} |A_{ij}|\,|y_j| \leq \sum_{j \leq n : j \neq i} |A_{ij}| = R_i$
  hence $\lambda \in I_i$

DD $\Rightarrow$ PSD

- Assume A is DD, λ an eigenvalue of A
- $\Rightarrow \forall i \leq n \quad A_{ii} \geq \sum_{j \neq i} |A_{ij}| = R_i$
- $\Rightarrow \forall i \leq n \quad A_{ii} - R_i \geq 0$
- By Gershgorin's circle theorem $\lambda \geq 0$
- $\Rightarrow A$ is PSD

DD Linearization

$$\forall i \le n \quad X_{ii} \ge \sum_{j \ne i} |X_{ij}| \qquad (*)$$

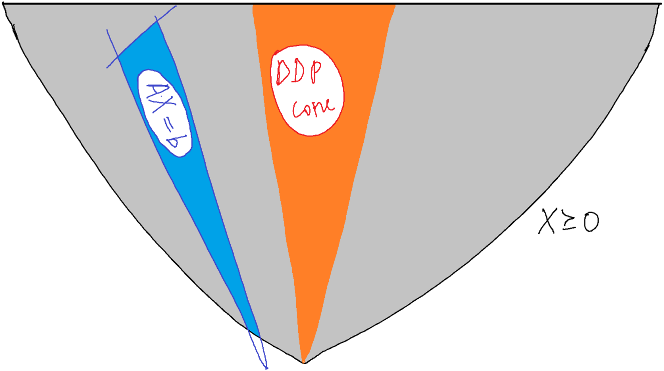
- linearize $|\cdot|$ by additional matrix var T
  $\Rightarrow$ *write $|X|$ as T*
- $\Rightarrow (*)$ becomes
$$X_{ii} \ge \sum_{j \ne i} T_{ij}$$
- add "sandwich" constraints $-T \le X \le T$
- Can easily prove $(*)$ in case $X \ge 0$ or $X \le 0$:
$$\begin{aligned} X_{ii} &\ge \sum_{j \ne i} T_{ij} \ge \sum_{j \ne i} X_{ij} \\ X_{ii} &\ge \sum_{j \ne i} T_{ij} \ge \sum_{j \ne i} -X_{ij} \end{aligned}$$
- General case requires polyhedral analysis

DD Programming (DDP)

$$\left.\begin{array}{rcl} \forall \{i,j\} \in E \quad X_{ii} + X_{jj} - 2X_{ij} & = & d_{ij}^2 \\ X & \text{is} & \text{DD} \end{array}\right\}$$

$$\Rightarrow \left\{\begin{array}{rcl} \forall \{i,j\} \in E \quad X_{ii} + X_{jj} - 2X_{ij} & = & d_{ij}^2 \\ \forall i \le n \qquad\qquad \sum\limits_{\substack{j \le n \\ j \ne i}} T_{ij} & \le & X_{ii} \\ -T \le X & \le & T \end{array}\right.$$

The issue with inner approximations



DDP could be infeasible!

Exploit push-and-pull

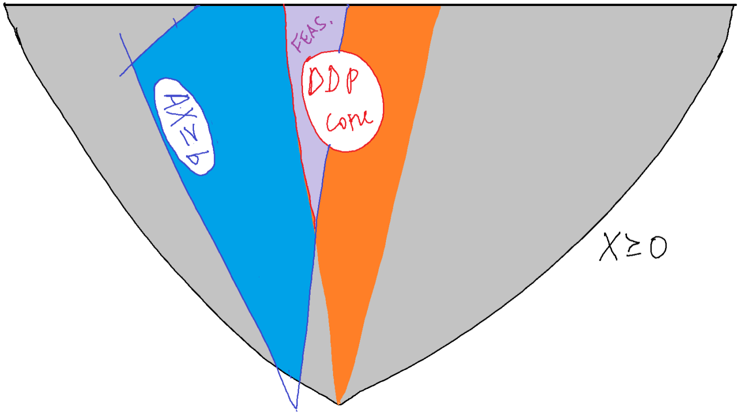
- Enlarge the feasible region
- From

$$\forall \{i,j\} \in E \quad X_{ii} + X_{jj} - 2X_{ij} = d_{ij}^2$$

- Use "push" objective $\min \sum\limits_{ij \in E} X_{ii} + X_{jj} - 2X_{ij}$
- Relax to

$$\forall \{i,j\} \in E \quad X_{ii} + X_{jj} - 2X_{ij} \geq d_{ij}^2$$

Hope to achieve LP feasibility



DDP formulation for the DGP

$$\left.\begin{array}{rrcl}
\min & \sum\limits_{\{i,j\}\in E}(X_{ii}+X_{jj}-2X_{ij}) & & \\
\forall\{i,j\}\in E & X_{ii}+X_{jj}-2X_{ij} & \ge & d_{ij}^2 \\
\forall i\le n & \sum\limits_{\substack{j\le n\\ j\ne i}} T_{ij} & \le & X_{ii} \\
 & -T\le X & \le & T \\
 & T & \ge & 0
\end{array}\right\}$$

Solve, then retrieve solution in $\mathbb{R}^K$ with PCA

Subsection 7

DGP cones

Cones

- Set C is a *cone* if:

$$\forall A, B \in C,\ \alpha, \beta \geq 0 \quad \alpha A + \beta B \in C$$

- If C is a cone, the *dual cone* is

$$C^* = \{y \mid \forall x \in C\ \langle x, y \rangle \geq 0\}$$

vectors making acute angles with all elements of C

- If $C \subset \mathbb{S}_n$ (set $n \times n$ symmetric matrices)

$$C^* = \{Y \mid \forall X \in C\ (Y \bullet X \geq 0)\}$$

- A $n \times n$ matrix cone C is *finitely generated* by $\mathcal{X} \subset \mathbb{R}^n$ if

$$\mathcal{X} = \{x_1, \ldots, x_p\} \wedge \quad \forall X \in C\ \exists \delta \in \mathbb{R}^p_+\ X = \sum_{\ell \leq p} \delta_\ell\, x_\ell {x_\ell}^\top$$

Representations of $\mathbb{DD}$

- Consider $E_{ii}, E_{ij}^+, E_{ij}^-$ in $\mathbb{S}_n$
  Define $\mathcal{E}_0 = \{E_{ii} \mid i \leq n\}$, $\mathcal{E}_1 = \{E_{ij}^{\pm} \mid i < j\}$, $\mathcal{E} = \mathcal{E}_0 \cup \mathcal{E}_1$
- $E_{ii} = \mathsf{diag}(0, \ldots, 0, 1_i, 0, \ldots, 0)$
- E_{ij}^+ has minor $\begin{pmatrix} 1_{ii} & 1_{ij} \\ 1_{ji} & 1_{jj} \end{pmatrix}$, 0 elsewhere
- E_{ij}^- has minor $\begin{pmatrix} 1_{ii} & -1_{ij} \\ -1_{ji} & 1_{jj} \end{pmatrix}$, 0 elsewhere
- **Thm.** $\mathbb{DD}$ = cone generated by $\mathcal{E}$ [Barker & Carlson 1975]
  Pf. *Rays in $\mathcal{E}$ are extreme, all DD matrices generated by $\mathcal{E}$*
- **Cor.** $\mathbb{DD}$ finitely gen. by
  $\mathcal{X}_{\mathbb{DD}} = \{e_i \mid i \leq n\} \cup \{(e_i \pm e_j) \mid i < j \leq n\}$
  Pf. *Verify $E_{ii} = e_i e_i^\top$, $E_{ij}^{\pm} = (e_i \pm e_j)(e_i \pm e_j)^\top$, where e_i is the i-th std basis element of $\mathbb{R}^n$*

Finitely generated dual cone representation

Thm. If C finitely gen. by $\mathcal{X}$, then

$$C^* = \{Y \in \mathbb{S}^n \mid \forall x \in \mathcal{X}\ (Y \bullet xx^\top \geq 0)\}$$

recall $C^* \triangleq \{Y \in \mathbb{S}^n \mid \forall X \in C \quad Y \bullet X \geq 0\}$

- ($\supseteq$) Let Y s.t. $\forall x \in \mathcal{X}\ (Y \bullet xx^\top \geq 0)$
  - $\forall X \in C$, $X = \sum_{x \in \mathcal{X}} \delta_x xx^\top$ (by fin. gen.)
  - hence $Y \bullet X = \sum_x \delta_x Y \bullet xx^\top \geq 0$ (by defn. of Y)
  - whence $Y \in C^*$ (by defn. of C^*)
- ($\subseteq$) Suppose $Z \in C^* \smallsetminus \{Y \mid \forall x \in \mathcal{X}\ (Y \bullet xx^\top \geq 0)\}$
  - then $\exists \mathcal{X}' \subset \mathcal{X}$ s.t. $\forall x \in \mathcal{X}'\ (Z \bullet xx^\top < 0)$
  - consider any $Y = \sum_{x \in \mathcal{X}'} \delta_x xx^\top \in C$ with $\delta \geq 0$
  - then $Z \bullet Y = \sum_{x \in \mathcal{X}'} \delta_x Z \bullet xx^\top < 0$ so $Z \notin C^*$
  - contradiction $\Rightarrow C^* = \{Y \mid \forall x \in \mathcal{X}\ (Y \bullet xx^\top \geq 0)\}$

Dual cone constraints

- **Remark**: for $v \in \mathbb{R}^n$, $X \bullet vv^\top = v^\top X v$
- Use finitely generated dual cone theorem
- Decision variable matrix X
- Constraints:

$$\forall v \in \mathcal{X} \quad v^\top X v \geq 0$$

- **Cor.** $\mathbb{DD}^* \supset \mathbb{PSD}$

  Pf. $X \in \mathbb{PSD}$ iff $\forall v \in \mathbb{R}^n \; vXv \geq 0$, so certainly valid $\forall v \in \mathcal{X}$
- If $|\mathcal{X}|$ polysized, get compact formulation

  otherwise use column generation
- $|\mathcal{X}_{\mathbb{DD}}| = |\mathcal{E}| = O(n^2)$

Dual cone DDP formulation for DGP

$$\left.\begin{array}{rrcl} \min & \sum\limits_{\{i,j\}\in E} (X_{ii} + X_{jj} - 2X_{ij}) & & \\ \forall \{i,j\} \in E & X_{ii} + X_{jj} - 2X_{ij} & = & d_{ij}^2 \\ \forall v \in \mathcal{X}_{\mathbb{DD}} & v^\top X v & \geq & 0 \end{array}\right\}$$

- $v^\top X v \geq 0$ for $v \in \mathcal{X}_{\mathbb{DD}}$ equivalent to:

$$\begin{array}{rrcl} \forall i \leq n & X_{ii} & \geq & 0 \\ \forall \{i,j\} \notin E & X_{ii} + X_{jj} - 2X_{ij} & \geq & 0 \\ \forall i < j & X_{ii} + X_{jj} + 2X_{ij} & \geq & 0 \end{array}$$

Note we went back to equality "pull" constraints (why?)

Quantifier $\forall \{i,j\} \notin E$ should be $\forall i < j$ but we already have those constraints $\forall \{i,j\} \in E$

Properties

- SDP relaxes original problem
- DualDDP relaxes SDP
  hence also relaxes original problem
- Yields tight obj fun bounds w.r.t. SDP
- Solutions may have large negative rank
  in some applications, retrieving feasible solutions may be difficult

Project idea 3: Apply the DG methods seen in these lectures in order to control a fleet of submarine robots (for each time instant $t \in T$ they define a different distance graph)

Subsection 8

Barvinok's Naive Algorithm

Concentration of measure

From [Barvinok, 1997]

> *The value of a "well behaved" function at a random point of a "big" probability space X is "very close" to the mean value of the function.*

and

> *In a sense, measure concentration can be considered as an extension of the law of large numbers.*

Concentration of measure

Given Lipschitz function $f : X \to \mathbb{R}$ s.t.

$$\forall x, y \in X \quad |f(x) - f(y)| \leq L\|x - y\|_2$$

for some $L \geq 0$, there is *concentration of measure* if $\exists$ constants c, C s.t.

$$\forall \varepsilon > 0 \quad \mathsf{P}_x(|f(x) - \mathsf{E}(f)| > \varepsilon) \leq c\, e^{-C\varepsilon^2/L^2}$$

where $\mathsf{E}(\cdot)$ is w.r.t. given Borel measure μ over X

$\equiv$ *"discrepancy from mean is unlikely"*

Barvinok's theorem

Consider:

- for each $k \leq m$, manifolds $\mathcal{X}_k = \{x \in \mathbb{R}^n \mid x^\top Q^k x = a_k\}$
  where $m \leq \mathsf{poly}(n)$
- feasibility problem $F \equiv \left[\bigcap_{k \leq m} \mathcal{X}_k \overset{?}{\neq} \varnothing\right]$
- SDP relaxation $\forall k \leq m \; (Q^k \bullet X = a_k) \wedge X \succeq 0$ with soln. $\bar{X}$
- Algorithm: $T \leftarrow \mathsf{factor}(\bar{X})$; $\quad y \sim \mathsf{N}^n(0,1)$; $\quad x' \leftarrow Ty$

Then:

- $\exists c > 0,\ n_0 \in \mathbb{N}$ such that $\forall n \geq n_0$

$$\mathsf{Prob}\left(\forall k \leq m \quad \mathsf{dist}(x', \mathcal{X}_k) \leq c\sqrt{\|\bar{X}\|_2 \ln n}\right) \geq 0.9.$$

Algorithmic application

- x' is "close" to each $\mathcal{X}_k$: *try local descent from x'*
- $\Rightarrow$ Feasible QP solution from an SDP relaxation

Elements of Barvinok's formula

$$\mathsf{Prob}\left(\forall k \le m \quad \mathsf{dist}(x', \mathcal{X}_k) \le c\sqrt{\|\bar{X}\|_2 \ln n}\right) \ge 0.9.$$

- $\sqrt{\|\bar{X}\|_2}$ arises from T (a factor of $\bar{X}$)
- $\sqrt{\ln n}$ arises from concentration of measure
- 0.9 follows by adjusting parameter values in "union bound"

Application to the DGP

- $\forall \{i,j\} \in E \quad \mathcal{X}_{ij} = \{x \mid \|x_i - x_j\|_2^2 = d_{ij}^2\}$
- DGP can be written as $\bigcap_{\{i,j\}\in E} \mathcal{X}_{ij} \stackrel{?}{\neq} \varnothing$
- SDP relaxation $X_{ii} + X_{jj} - 2X_{ij} = d_{ij}^2 \wedge X \succeq 0$ with soln. $\bar{X}$

- Difference with Barvinok: $x \in \mathbb{R}^{Kn}$, $\mathrm{rk}(\bar{X}) \leq K$
- IDEA: sample $y \sim \mathsf{N}^{nK}(0, \frac{1}{\sqrt{K}})$
- **Thm.** *Barvinok's theorem works in rank K*

Proof structure

- Show that, on average, $\forall k \le m\ \mathsf{tr}((Ty)^\top Q^k (Ty)) = Q^k \bullet \bar{X} = a_k$
  - compute multivariate integrals
  - bilinear terms disappear because y normally distributed
  - decompose multivariate int. to a sum of univariate int.
- Exploit concentration of measure to show errors happen rarely
  - a couple of technical lemmata yielding bounds
  - $\Rightarrow$ bound Gaussian measure μ of ε-neighbourhoods of

$$
\begin{aligned}
A_i^- &= \{y \in \mathbb{R}^{n\times K} \mid \mathcal{Q}^i(Ty) \le Q^i \bullet \bar{X}\} \\
A_i^+ &= \{y \in \mathbb{R}^{n\times K} \mid \mathcal{Q}^i(Ty) \ge Q^i \bullet \bar{X}\} \\
A_i &= \{y \in \mathbb{R}^{n\times K} \mid \mathcal{Q}^i(Ty) = Q^i \bullet \bar{X}\}.
\end{aligned}
$$

  - use "union bound" for measure of $A_i^-(\varepsilon) \cap A_i^+(\varepsilon)$
  - show $A_i^-(\varepsilon) \cap A_i^+(\varepsilon) = A_i(\varepsilon)$
  - use "union bound" to measure intersections of $A_i(\varepsilon)$
  - appropriate values for some parameters $\Rightarrow$ result

The heuristic

1. Solve SDP relaxation of DGP, get soln. $\bar{X}$
   use DDP+LP if SDP+IPM too slow

2. a. $T = \mathsf{factor}(\bar{X})$
   b. $y \sim \mathsf{N}^{nK}(0, \frac{1}{\sqrt{K}})$
   c. $x' = Ty$

3. Use x' as starting point for a local NLP solver on formulation

$$\min_x \sum_{\{i,j\} \in E} \left(\|x_i - x_j\|^2 - d_{ij}^2 \right)^2$$

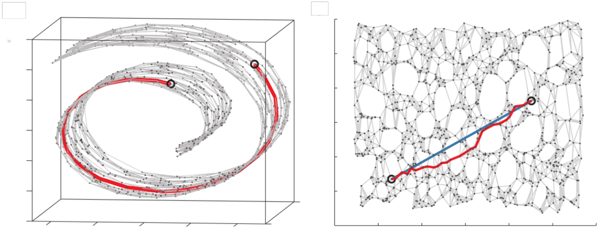
   and return improved solution x

Subsection 9

Isomap revisited

Isomap for the DGP

- Given DGP instance $(K, G = (V, E, d))$:
  1. $D =$ square weighted adjacency matrix of G
  2. $\bar{D} =$ completion of D
  3. $x' = \mathrm{PCA}(\bar{D}, K)$
  4. $x =$ locally optimal solution closest to x



- Step 4 is the "refinement step"

  calls a local solver for the DGP with starting point x'
- Vary Step 2 to generate Isomap-based heuristics

Variants for Step 2

A. Floyd-Warshall all-shortest-paths algorithm on G
(classic Isomap)

B. Find a spanning tree (SPT) of G and compute a random realization in $\bar{x} \in \mathbb{R}^K$, use its sqEDM

C. Solve a push-and-pull SDP/DDP/DualDDP to find a realization $x' \in \mathbb{R}^n$, use its sqEDM

Project idea 4: implement and test at least 6 different variants of Isomap for DGP: the three above, and at least three new ones of your own conception

Subsection 10

Summary

Matrix reformulations

- Quadratic nonconvex too difficult?
- *Solve SDP relaxation*
- SDP relaxation too large?
- *Solve DDP approximation*
- Get $n \times n$ matrix solution, need $K \times n$!

Solution rank reduction methods

- Multidimensional Scaling (MDS)
- Principal Component Analysis (PCA)
- Barvinok's naive algorithm (BNA)
- Isomap

All provide good starting points for local solvers

Can also use them for general dimensionality reduction:
they map n vectors in $\mathbb{R}^n \longrightarrow n$ vectors in $\mathbb{R}^K$

Outline

The gist of random projections (RP)

- Let A be a $m \times n$ data matrix (columns in $\mathbb{R}^m$, $m \gg 1$)
- T short & fat, normally sampled componentwise

$$\underbrace{\begin{pmatrix} \vdots\,\vdots\,\vdots & \quad & \vdots\,\vdots\,\vdots \end{pmatrix}}_{T} \underbrace{\begin{pmatrix} \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \end{pmatrix}}_{A} = \underbrace{\begin{pmatrix} \vdots & \vdots & \vdots \end{pmatrix}}_{TA}$$

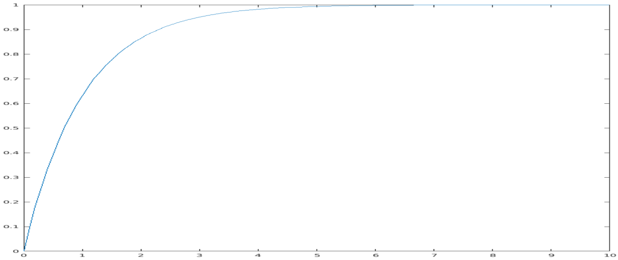
- Then $\forall i < j \;\; \|A_i - A_j\|_2 \approx \|TA_i - TA_j\|_2$ "wahp"

wahp

"wahp" = "with arbitrarily high probability"

the probability of E_k (depending on some parameter k)
approaches 1 *"exponentially fast"* as k increases

$$\mathbf{P}(E_k) \geq 1 - O(e^{-k})$$



Johnson-Lindenstrauss Lemma (JLL)

Thm.

Given $A \subseteq \mathbb{R}^m$ with $|A| = n$ and $\varepsilon > 0$ there is $k = O(\frac{1}{\varepsilon^2} \ln n)$ and a $k \times m$ matrix T s.t.

$$\forall x, y \in A \quad (1-\varepsilon)\|x-y\| \ \leq \ \|Tx - Ty\| \ \leq \ (1+\varepsilon)\|x-y\|$$

If $k \times m$ matrix T is sampled componentwise from $\mathsf{N}(0, \frac{1}{\sqrt{k}})$, then

$$\mathbf{P}(A \text{ and } TA \text{ approximately congruent}) \geq \frac{1}{n}$$

(nontrivial) — result follows by probabilistic method

Note that $1/\sqrt{k}$ is the standard deviation, not the variance

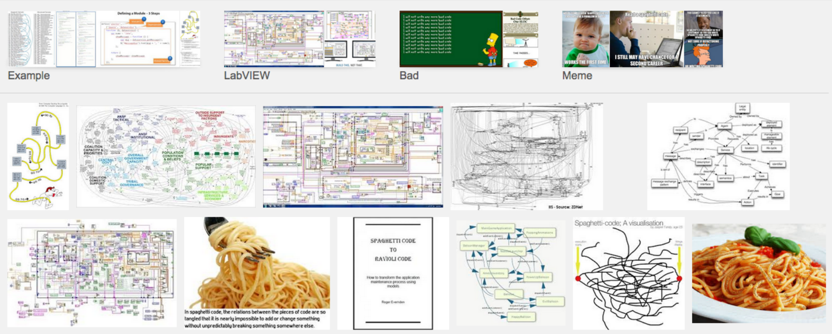
In practice

- $\mathbf{P}(A \text{ and } TA \text{ approximately congruent}) \geq \frac{1}{n}$
- re-sampling sufficiently many times gives wahp
- Empirically, sample T few times (once will do)
  $\mathbb{E}_T(\|Tx - Ty\|) = \|x - y\|$
  probability of error decreases wahp

Surprising fact:

$\boxed{k \text{ is independent of the original number of dimensions } m}$

Clustering Google images

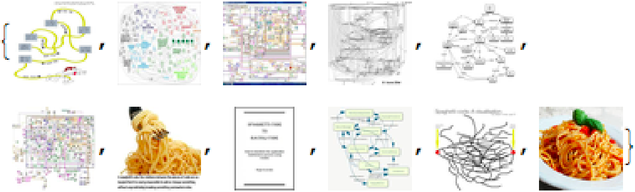


[L. & Lavor, 2017]

Clustering without RPs

```
VHimg = Map[Flatten[ImageData[#]] &, Himg];
```

Out[28]=



```
VHcl = Timing[ClusteringComponents[VHimg, 3, 1]]
Out[29]= {0.405908, {1, 2, 2, 2, 2, 2, 3, 2, 2, 2, 3}}
```

Too slow!

Clustering with RPs

```
Get["Projection.m"];
VKimg = JohnsonLindenstrauss[VHimg, 0.1];
VKcl = Timing[ClusteringComponents[VKimg, 3, 1]]
Out[34]= {0.002232, {1, 2, 2, 2, 2, 2, 3, 2, 2, 2, 3}}
```

From 0.405s CPU time to 0.00232s

Same clustering

Projecting formulations

- Given:
  - $F(p, x)$: MP formulation with params p & vars x
  - $\mathsf{sol}(F)$: solution of F
  - $\mathscr{C}$: formulation class (e.g. LP, NLP, MILP, MINLP)
  - Given RP T, define $T\,F(p, x)$ as
    $$F(Tp, x) \text{ or } F(Tp, Tx)$$
- Want to show: $\forall F \in \mathscr{C}$ $\mathsf{sol}(F) \approx \mathsf{sol}(TF)$ wahp
- Issues:
  - RPs project points not vars/constrs
  - approximate congruence $\neq$ feasibility/optimality
  - JLL applies to finite pt sets, vars encode ∞ pts

- Today we see this for $\mathscr{C} = \text{LP}$
- Can also be applied to QP, SDP, QCQP, and more

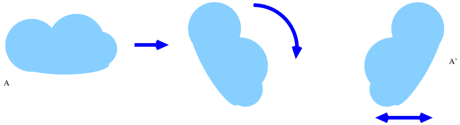
Subsection 1

Random projection theory

The shape of a set of points

- **Lose dimensions but not too much accuracy**
  Given $A_1, \ldots, A_n \in \mathbb{R}^m$ find $k \ll m$ and $A'_1, \ldots, A'_n \in \mathbb{R}^k$ s.t.
  A and A' "have almost the same shape"

- What is the shape of a set of points?



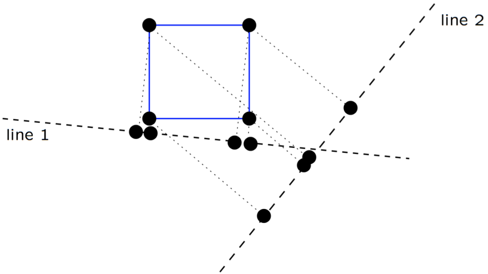
congruence $\Leftrightarrow$ *same shape:* $\|A_i - A_j\| = \|A'_i - A'_j\|$

- *Approximate congruence* $\equiv$ *small distortion:*
  A, A' have *almost the same shape* if
  $\forall i < j \leq n \quad (1-\varepsilon)\|A_i - A_j\| \leq \|A'_i - A'_j\| \leq (1+\varepsilon)\|A_i - A_j\|$
  for some small $\varepsilon > 0$

Assume norms are all Euclidean

Losing dimensions = "projection"

In the plane, hopeless



In 3D: no better

Recall the JLL

Thm.

Given $A \subseteq \mathbb{R}^m$ with $|A| = n$ and $\varepsilon > 0$ there is $k = O(\frac{1}{\varepsilon^2} \ln n)$ and a $k \times m$ matrix T s.t.

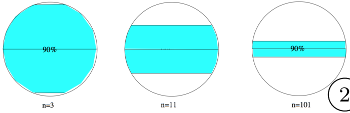
$$\forall x, y \in A \quad (1-\varepsilon)\|x-y\| \ \leq \ \|Tx - Ty\| \ \leq \ (1+\varepsilon)\|x-y\|$$

Approximate congruence: proof sketch

1

Thm.

Let T be a $k \times m$ RP sampled from $\mathsf{N}(0, \frac{1}{\sqrt{k}})$, and $u \in \mathbb{R}^m$ s.t. $\|u\| = 1$. Then $\mathbb{E}(\|Tu\|^2) = \|u\|^2$



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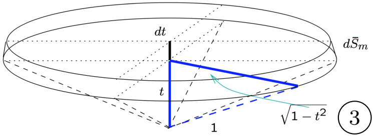

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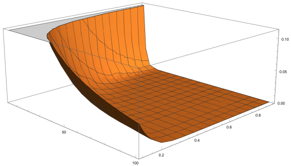

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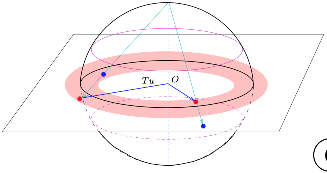


6

RPs preserve norms on average

Thm.

Let T be a $k \times m$ rectangular matrix with each component sampled from $\mathsf{N}(0, \frac{1}{\sqrt{k}})$, and $u \in \mathbb{R}^m$ s.t. $\|u\| = 1$. Then $\mathbb{E}(\|Tu\|^2) = 1$

Proof

- Let $v = Tu$, i.e. $\forall i \leq k$ let $v_i = \sum_{j \leq n} T_{ij} u_j$
- $\mathbb{E}(v_i) = \mathbb{E}\left(\sum_{j \leq m} T_{ij} u_j\right) = \sum_{j \leq m} \mathbb{E}(T_{ij}) u_j = 0$
- $\mathsf{Var}(v_i) = \sum_{j \leq m} \mathsf{Var}(T_{ij} u_j) = \sum_{j \leq m} \mathsf{Var}(T_{ij}) u_j^2 = \sum_{j \leq m} \frac{u_j^2}{k} = \frac{1}{k}\|u\|^2 = \frac{1}{k}$
- $\frac{1}{k} = \mathsf{Var}(v_i) = \mathbb{E}(v_i^2 - (\mathbb{E}(v_i))^2) = \mathbb{E}(v_i^2 - 0) = \mathbb{E}(v_i^2)$
- $\mathbb{E}(\|Tu\|^2) = \mathbb{E}(\|v\|^2) = \mathbb{E}\left(\sum_{i \leq k} v_i^2\right) = \sum_{i \leq k} \mathbb{E}(v_i^2) = \sum_{i \leq k} \frac{1}{k} = 1$

Can we argue that the variance decreases wahp?

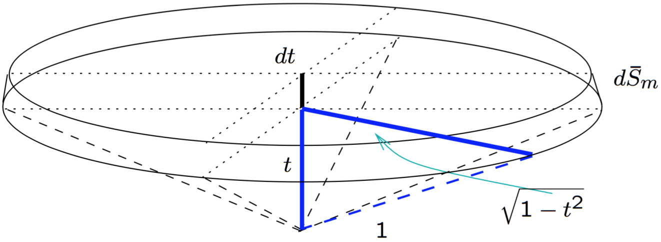
Surface area of a slice of hypersphere

$\bar{S}_m(r)$: surface of m-dimensional sphere of radius r

$$\bar{S}_m(r) = \frac{2\pi^{m/2} r^{m-1}}{\Gamma(m/2)} \qquad S_m \triangleq \bar{S}_m(1)$$

Lateral surface of infinitesimally high hypercylinder

$$d\bar{S}_m(t) = S_{m-1}(1-t^2)^{\frac{m-2}{2}} dt$$

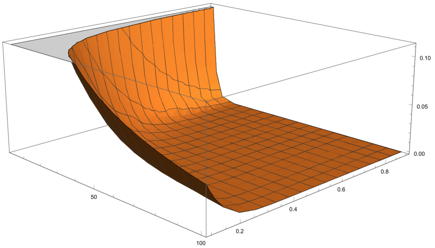


Area of polar caps

$$\mathcal{A}^{\mathrm{pc}} = 2\int_t^1 d\bar{S}_m(s) = 2S_{m-1}\int_t^1 (1-s^2)^{\frac{m-2}{2}}\,ds$$

$$1 + x \le e^x \text{ for all } x \qquad \text{and} \qquad \int\limits_t^1 f(s)ds \le \int\limits_t^\infty f(s)ds \text{ for } f \ge 0$$

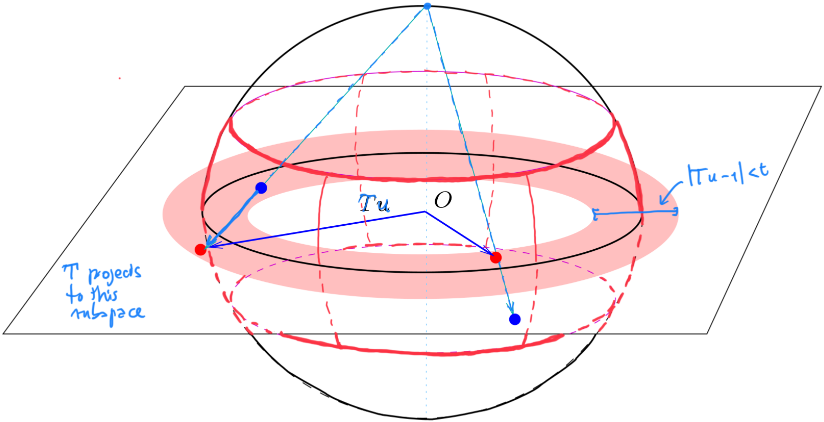
$$\Rightarrow \mathcal{A}^{\mathrm{pc}} \le 2S_{m-1}\int_t^\infty e^{-\frac{m-2}{2}s^2}ds = \frac{2S_{m-1}}{\sqrt{m-2}}\sqrt{\frac{\pi}{2}}\,\mathsf{erfc}\left(\frac{\sqrt{m-2}t}{\sqrt{2}}\right) \text{“}\approx\text{”} O(e^{-t^2})$$



- **Polar caps area decreases as $m \to \infty$ with t fixed**
- **Concentration of measure of the equatorial band**

An intuitive explanation

- Polar caps area $\mu(\mathcal{A}_t^m) = \mu(\{u \in \mathbb{S}^{m-1} \mid |u_m| > t\})$ decreases with t fixed as $m \to \infty \Rightarrow$ area of equatorial band $\bar{\mathcal{A}}_t^m$ increases with same conditions
- $T\bar{\mathcal{A}}_t^m = \{u \in \mathbb{S}^{m-1} \mid \left|\|Tu\|^2 - 1\right| \leq t\}$ has concentration of measure (if T is stereographic)



Intermezzo: The union bound

- Events $E_1, \ldots, E_k$ such that $\mathbf{P}(E_i) \geq 1 - p$ for each $i \leq k$
- What is $\mathbf{P}(\text{all } E_i)$?
- $\mathbf{P}(\text{all } E_i) = 1 - \mathbf{P}(\text{at least one } \neg E_i) \Rightarrow$

$$\mathbf{P}\Big(\bigwedge_{i \leq k} E_i\Big) = 1 - \mathbf{P}\Big(\bigvee_{i \leq k} (\neg E_i)\Big) \geq$$

$$\geq 1 - \sum_{i=1}^{k} \mathbf{P}(\neg E_i) \geq 1 - \sum_{i=1}^{k} (1 - (1 - p)) = 1 - kp$$

- So $\mathbf{P}(\text{all } E_i) \geq 1 - kp$

A syntactical explanation for $k = O(\varepsilon^{-2} \ln n)$

- B = set of unit vectors; by "intuitive explanation"
  $\Rightarrow \forall u \in B \; \exists C > 0$ s.t. $\mathbf{P}(1 - t \le \|Tu\| \le 1 + t) \ge 1 - e^{-Ct^2}$
- By union bound:
  $\Rightarrow \mathbf{P}(\forall u \in B \; 1 - t \le \|Tu\| \le 1 + t) \ge 1 - |B| e^{-Ct^2}$
- Prob. $\in [0, 1] \Rightarrow$ require $1 - |B| e^{-Ct^2} > 0$:
  $\Rightarrow |B| e^{-Ct^2} < 1$
- (arbitrarily) Let $t = \varepsilon \sqrt{k}$:
  $\Rightarrow |B| e^{-C\varepsilon^2 k} < 1$
- $\Rightarrow \boxed{k > C\varepsilon^{-2} \ln(|B|)}$

Apply to vector differences

- Let $A \subset \mathbb{R}^m$, $|A| = n$
- $\forall x, y \in A$ we have

  $$\|Tx - Ty\|^2 = \|T(x-y)\|^2 = \|x-y\|^2 \Big\|T\frac{x-y}{\|x-y\|}\Big\|^2 = \|x-y\|^2\|Tu\|^2$$

  where $\|u\|_2 = 1$
- $\mathbb{E}(\|Tu\|^2) = \|u\| = 1 \Rightarrow \boxed{\mathbb{E}(\|Tx - Ty\|^2) = \|x-y\|^2}$
- Let $B = \{\frac{x-y}{\|x-y\|} \mid x, y \in A\}$
  $|B| = O(n^2) \Rightarrow k = C\varepsilon^{-2}\ln(n)$ for some constant C
- By concentration of measure on $T\bar{\mathcal{A}}^m$, $\exists \varepsilon \in (0,1)$ s.t.

  $$(1-\varepsilon)\|x-y\|^2 \leq \|Tx - Ty\|^2 \leq (1+\varepsilon)\|x-y\|^2 \quad (*)$$

  holds with positive probability
- **Probabilistic method**: $\exists T$ such that $(*)$ holds
  $\Rightarrow$ *JLL follows*

Randomized algorithm

- Distortion has low probability [Gupta 02]:

$$\begin{array}{lcl} \forall x, y \in A \quad \mathbf{P}(\|Tx - Ty\| \le (1-\varepsilon)\|x-y\|) & \le & 1/n^2 \\ \forall x, y \in A \quad \mathbf{P}(\|Tx - Ty\| \ge (1+\varepsilon)\|x-y\|) & \le & 1/n^2 \end{array}$$

- Probability $\exists$ pair $x, y \in A$ distorting Euclidean distance: *union bound over* $\binom{n}{2}$ *pairs*

$$\begin{array}{rcl} \mathbf{P}(\neg(A \text{ and } TA \text{ have almost the same shape})) & \le & \binom{n}{2}\frac{2}{n^2} = 1 - \frac{1}{n} \\ \mathbf{P}(A \text{ and } TA \text{ have almost the same shape}) & \ge & 1/n \end{array}$$

- Algorithm:
  - $\mathbf{P}(\exists x, y \in A$ with large JLL discrepancy$) \le 1 - 1/n$
  - Consider $t > 1$ independent samplings of random RP T
  - Probability that all have large discrepancy: $\le (1 - 1/n)^t$
  - Choose t so at least one T will be good with prob. ≥ 0.99:
    $(1 - 1/n)^t \le 1 - 0.99 = 0.01$ yields $t \ge \ln(0.01)/\ln(1 - 1/n)$
    if $n = 100$, get $t \ge 459$

Subsection 2

Projecting LP feasibility

Pure feasibility LP: easy cases

Thm.

$T : \mathbb{R}^m \to \mathbb{R}^k$ a RP, and $b, A_1, \ldots, A_n \in \mathbb{R}^m$. For any given vector $x \in X$, we have:

(i) If $b = \sum_{i=1}^{n} x_i A_i$ then $Tb = \sum_{i=1}^{n} x_i T A_i$

by linearity of T

(ii) If $b \neq \sum_{i=1}^{n} x_i A_i$ then $\mathbf{P}\left(Tb \neq \sum_{i=1}^{n} x_i T A_i \right) \geq 1 - 2e^{-\mathcal{C}k}$

by JLL applied to $\|b - \sum_i x_i A_i\|$

(iii) If $b \neq \sum_{i=1}^{n} y_i A_i$ for all $y \in X \subseteq \mathbb{R}^n$, where $|X|$ is finite, then

$$\mathbf{P}\left(\forall y \in X \; Tb \neq \textstyle\sum_{i=1}^{n} y_i T A_i \right) \geq 1 - 2|X|e^{-\mathcal{C}k}$$

for some constant $\mathcal{C} > 0$ (independent of n, k)

by union bound

[Vu et al., Math of OR, 2018]

Separating hyperplanes

When $|X|$ is large, project separating hyperplanes instead

- **Convex $C \subseteq \mathbb{R}^m$, $x \notin C$:**
  then $\exists$ hyperplane c separating x from C
- In particular, true if $C = \mathsf{cone}(A_1, \ldots, A_n)$ for $A \subseteq \mathbb{R}^m$
- **Can show $x \in C \Leftrightarrow Tx \in TC$ with high probability**
- As above, if $x \in C$ then $Tx \in TC$ by linearity of T
  Difficult part is proving the converse
- Can also project point-to-cone distances

Projection of separating hyperplanes

Thm.

Given $c, b, A_1, \ldots, A_n \in \mathbb{R}^m$ of unit norm s.t. $b \notin \mathsf{cone}\{A_1, \ldots, A_n\}$ pointed, $\varepsilon > 0$, $c \in \mathbb{R}^m$ s.t. $c^\top b < -\varepsilon$, $c^\top A_i \geq \varepsilon$ $(i \leq n)$, and T a RP:

$$\mathbf{P}\left[Tb \notin \mathsf{cone}\{TA_1, \ldots, TA_n\}\right] \geq 1 - 4(n+1)e^{-\mathcal{C}(\varepsilon^2 - \varepsilon^3)k}$$

for some constant $\mathcal{C}$.

Proof

Let $\mathscr{A}$ be the event that T approximately preserves $\|c - \chi\|^2$ and $\|c + \chi\|^2$ for all $\chi \in \{b, A_1, \ldots, A_n\}$. Since $\mathscr{A}$ consists of $2(n+1)$ events, by the JLL ("squared variant") and the union bound, we get

$$\mathbf{P}(\mathscr{A}) \geq 1 - 4(n+1)e^{-\mathcal{C}(\varepsilon^2 - \varepsilon^3)k}$$

Now consider $\chi = b$

$$\begin{aligned}
\langle Tc, Tb \rangle &= \frac{1}{4}(\|T(c+b)\|^2 - \|T(c-b)\|^2) \\
\text{by JLL} \quad &\leq \frac{1}{4}(\|c+b\|^2 - \|c-b\|^2) + \frac{\varepsilon}{4}(\|c+b\|^2 + \|c-b\|^2) \\
&= c^\top b + \varepsilon < 0
\end{aligned}$$

and similarly $\langle Tc, TA_i \rangle \geq 0$

[Vu et al., Math. OR, 2018]

The feasibility projection theorem

Thm.

Given $\delta > 0$, $\exists$ sufficiently large $m \leq n$ such that:

for any LFP input A, b where A is $m \times n$

we can sample a random $k \times m$ matrix T with $k \ll m$

and

$$\mathbf{P}(\text{orig. LFP feasible} \iff \text{proj. LFP feasible}) \geq 1 - \delta$$

Subsection 3

Projecting LP optimality

Notation

- $P \equiv \min\{cx \mid Ax = b \wedge x \geq 0\}$ *(original problem)*
- $TP \equiv \min\{cx \mid TAx = Tb \wedge x \geq 0\}$ *(projected problem)*
- $v(P)$ = optimal objective function value of P
- $v(TP)$ = optimal objective function value of TP

The optimality projection theorem

- Assume $\mathsf{feas}(P)$ is bounded
- Assume all optima of P satisfy $\sum_j x_j \leq \theta$ for some given $\theta > 0$
  (prevents unboundedness)

Thm.

Given $\gamma > 0$,

$$v(P) - \gamma \leq v(TP) \leq v(P) \qquad (*)$$

holds with arbitrarily high probability (w.a.h.p.)

more precisely, $(*)$ holds with prob. $1 - 4ne^{-\mathcal{C}(\varepsilon^2-\varepsilon^3)k}$ where $\varepsilon = \gamma/(2(\theta+1)\eta)$ and $\eta = O(\|y\|_2)$ where y is a dual optimal solution of P having minimum norm

The easy part

Show $v(TP) \leq v(P)$:

- Constraints of P: $Ax = b \ \wedge \ x \geq 0$
- Constraints of TP: $TAx = Tb \ \wedge \ x \geq 0$
- $\Rightarrow$ constraints of TP are lin. comb. of constraints of P
- $\Rightarrow$ any solution of P is feasible in TP
  (btw, the converse holds almost never)
- P and TP have the same objective function
- $\Rightarrow$ TP is a **relaxation** of $P \Rightarrow v(TP) \leq v(P)$

The hard part (sketch)

- Eq. (12) equivalent to P for $\gamma = 0$

$$\left.\begin{array}{rcl} cx & \leq & v(P) - \gamma \\ Ax & = & b \\ x & \geq & 0 \end{array}\right\} \tag{12}$$

Note: for $\gamma > 0$, Eq. (12) is infeasible

- By feasibility projection theorem,

$$\left.\begin{array}{rcl} cx & \leq & v(P) - \gamma \\ TAx & = & Tb \\ x & \geq & 0 \end{array}\right\}$$

is infeasible w.a.h.p. for $\gamma > 0$

- Re-state: $cx < v(P) - \gamma \wedge TAx = Tb \wedge x \geq 0$ infeasible w.a.h.p.
- $\Rightarrow cx \geq v(P) - \gamma$ holds w.a.h.p. for $x \in \mathsf{feas}(TP)$
- $\Rightarrow v(P) - \gamma \leq v(TP)$

Subsection 4

Solution retrieval

Projected solutions are infeasible in P

- $Ax = b \;\Rightarrow\; TAx = Tb$ by linearity
- However,
  Thm.
  $\boxed{\text{For } x \geq 0 \text{ s.t. } TAx = Tb,\ Ax = b \text{ with probability zero}}$

  if not, an x belonging to $(n-k)$-dim. subspace would belong to an $(n-m)$-dim. subspace (with $k \ll m$) with positive probability
- Can't get solution for original LFP using projected LFP!

Solution retrieval by duality

- Primal $\min\{c^\top x \mid Ax = b \wedge x \geq 0\} \Rightarrow$ dual $\max\{b^\top y \mid A^\top y \leq c\}$
- Let $x' = \mathsf{sol}(TP)$ and $y' = \mathsf{sol}(\mathsf{dual}(TP))$
- $\Rightarrow (TA)^\top y' = (A^\top T^\top) y' = A^\top (T^\top y') \leq c$
- $\Rightarrow T^\top y'$ is a solution of $\mathsf{dual}(P)$
- $\Rightarrow$ we can compute an optimal basis J for P
- Solve $A_J x_J = b$, get x_J, obtain a solution x^* of P
- *Won't work in practice: errors in computing J*

Solution retrieval by projected basis

- H: optimal basis of TP
  we can trust that — given by solver
- $|H| = k \Rightarrow A_H$ is $m \times k$ (tall and slim)
- Pseudoinverse: solve $k \times k$ system $A_H^\top A_H x_H = A_H^\top b$
  $\Rightarrow x_H = (A_H^\top A_H)^{-1} A_H^\top b$
- let $x = (x_H, 0)$
- *Can prove small feasibility error wahp*
- **ISSUE**: may be slightly infeasible
  empirically: $x \not\geq 0$ *but* $x^- = \min(0, x) \to 0$ *as* $k \to \infty$

Project idea 5: Test the output of duality and projected basis retrieval methods on a set of 50 random large feasible standard-form LPs: you should find that the duality method is worse than the projected basis method. Formulate a reasoned hypothesis about the reason why this happens

Projected LP duals

- The dual of $\mathsf{P} \equiv \min\{cx \mid Ax = b \wedge x \geq 0\}$ is
  $\mathsf{D} \equiv \max\{yb \mid yA \leq c\}$
- A projected dual on $y \in \mathbb{R}^m$ can be derived as follows:
  $\max\{(yT^\top)Tb \mid (yT^\top)TA \leq c\}$
- Replacing $u = yT^\top \in \mathbb{R}^k$, we obtain
  $T\mathsf{D} \equiv \max\{u\bar{b} \mid u\bar{A} \leq c\}$ where $\bar{b} = Tb$, $\bar{A} = TA$
- Theory [D'Ambrosio et al. *MPB* 2020]:
  - if original dual is feasible, projected dual is feasible
  - approximation guarantees on projected dual objective function
  - retrieval: if $\bar{u} \in \arg\mathrm{opt}(T\mathsf{D})$, let $\tilde{y} = \bar{u}T$, $\tilde{y}$ is feasible in D

Project idea 6: Develop an algorithm for finding a candidate solution x' of P from $\tilde{y}$. Sample 50 random large standard form LP instances, solve P, $T\mathsf{P}$, $T\mathsf{D}$ for each instance. Collect soln. x^* from P, $\tilde{x}$ from $T\mathsf{P}$, x' from $T\mathsf{D}$, then compute objective function value and feasibility error w.r.t. P of $x^*, \tilde{x}, x'$. Plot all this data in function of the number of rows of A and ε

Subsection 5

Application to quantile regression

Conditional random variables

- random variable B conditional on $A_1, \ldots, A_p$
- assume B depends linearly on $\{A_j \mid j \leq p\}$
- want to find $x_1, \ldots, x_n \in \mathbb{R}$ s.t.

$$B = \sum_{j \leq p} x_j A_j$$

- use samples $b, a_1, \ldots, a_p \in \mathbb{R}^m$ to find estimates
- a^i = row, a_j = column

Sample statistics

- expectation:

$$\hat{\mu} = \operatorname*{arg\,min}_{\mu \in \mathbb{R}} \sum_{i \le m} (b_i - \boxed{\mu})^2$$

- conditional expectation (*linear regression*):

$$\hat{\nu} = \operatorname*{arg\,min}_{\nu \in \mathbb{R}^p} \sum_{i \le m} (b_i - \boxed{\nu a^i})^2$$

- sample median:

$$\begin{aligned} \hat{\xi} &= \operatorname*{arg\,min}_{\xi \in \mathbb{R}} \sum_{i \le m} |b_i - \xi| \\ &= \operatorname*{arg\,min}_{\xi \in \mathbb{R}} \sum_{i \le m} \left(\frac{1}{2} \max(b_i - \xi, 0) - \frac{1}{2} \min(b_i - \xi, 0) \right) \end{aligned}$$

- conditional sample median: *similarly*

Quantile regression

- sample τ-quantile:

$$\hat{\xi} = \operatorname*{arg\,min}_{\xi \in \mathbb{R}} \sum_{i \leq m} (\tau \max(b_i - \xi, 0) - (1 - \tau) \min(b_i - \xi, 0))$$

- conditional sample τ-quantile (*quantile regression*):

$$\hat{\beta} = \operatorname*{arg\,min}_{\beta \in \mathbb{R}^p} \sum_{i \leq m} \left(\tau \max(b_i - \beta a^i, 0) - (1 - \tau) \min(b_i - \beta a^i, 0)\right)$$

Linear Programming formulation

Let $A = (a_j \mid j \le n)$; then

$$\left.\begin{array}{rrcl} \hat{\beta} = \mathsf{arg\,min} & \tau u^+ + (1-\tau)u^- & & \\ & A(\beta^+ - \beta^-) + u^+ - u^- & = & b \\ & \beta, u & \ge & 0 \end{array}\right\}$$

- **parameters**: A is $m \times p$, $b \in \mathbb{R}^m$, $\tau \in \mathbb{R}$
- **decision variables**: $\beta^+, \beta^- \in \mathbb{R}^p$, $u^+, u^- \in \mathbb{R}^m$
- LP constraint matrix is $m \times (2p + 2m)$
  density: $p/(p+m)$ — can be high

Project idea 7: Test the application of RPs on at 50 large random MultiCommodity Flow (MCF) problems. Plot the ratio of projected to original objective, retrieved to original objective, and infeasibility errors in function of the number of rows of the equality system $Ax = b$ and ε. Is MCF a good application testbed for RP?

Large datasets

- Russia Longitudinal Monitoring Survey `hh1995f`
  - $m = 3783$, $p = 855$
  - $A = \texttt{hf1995f}$, $b = \log \text{avg}(A)$
  - 18.5% dense
  - poorly scaled data, CPLEX yields infeasible (!!!) after around 70s CPU
  - `quantreg` in R fails
- 14596 RGB photos on my HD, scaled to 90×90 pixels
  - $m = 14596$, $p = 24300$
  - each row of A is an image vector, $b = \sum A$
  - 62.4% dense
  - CPLEX killed by OS after ≈30min (presumably for lack of RAM) on 16GB
  - could not load dataset in R

Electricity prices

- Every hour over 365 days in 2015 (8760 rows)
- From 22 countries (columns) from the European zone

	orig	proj
1	5.82e-01	5.69e-01
2	9.46e-02	0
3	0	0
4	1.06-01	1.18e-01
5	2.73e-04	6.92e-05
6	-4.81e-06	-2.07e-05
7	1.32e-01	1.36e-01
8	0	0
9	0	0
10	0	0
11	-3.46e-08	-2.45e-05
12	0	0
13	5.66e-02	5.49e-02
14	-2.50e-04	2.91e-03
15	2.86e-02	2.81e-02
16	0	0
17	0	0
18	0	9.35e-02
19	0	0
20	2.23e-09	0
21	0	-7.99e-06

- Permutation (18,2) (21,20) applied to proj gives same nonzero pattern and reduces ℓ_2 error from 0.13 to 0.01
- For every proj solution I found I could always find a permutation with this property!!
- . . . On closer inspection, many columns reported equal data
- *Small numerical error*
- *Approximate solutions respect Nonzero pattern*
- LP too small for approximation to have an impact on CPU time

Outline

Subsection 1

Motivation

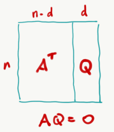
Coding problem for costly channels

- Task:
  send long sparse vector $y \in \mathbb{R}^n$ on costly channel
  1. construct $m \times n$ encoding matrix A with $m \leq n$
     both parties know A
  2. encode $b = Ay \in \mathbb{R}^m$
  3. send b
- Decode by finding sparsest x s.t. $Ax = b$
  can we expect $x \approx y$, i.e. small $\|x - y\|$?
- Summary:
  1. given long sparse vector y
  2. shorten it to b, send b
  3. upon receiveing b, recover long sparse vector y

Coding problem for noisy channels

- Task: send vector $w \in \mathbb{R}^d$ on a noisy channel
- *Encoding:* $n \times d$ matrix Q with $n > d$, send $z = Qw \in \mathbb{R}^n$

  both parties know Q
- Error prob. e: $e\,n$ components of z sent wrong
- *Receive (wrong) vector $\bar{z} = z + x$ where x is sparse*
- Can we recover z?



  - Choose $m \times n$ matrix A s.t. $m = n - d$ and $AQ = 0$
  - Let $b = A\bar{z} = A(z + x) = A(Qw + x) = AQw + Ax = Ax$
  - *Suppose we can find sparsest x' s.t. $Ax' = b$*
  - $\Rightarrow$ we can recover $z' = \bar{z} - x'$
- Recover $w' = (Q^\top Q)^{-1} Q^\top z'$ (pseudoinverse)

  What is the likelihood of getting small $\|w - w'\|$?

Summary: 1. given short dense vector w, 2. lengthen it to z for redundancy; 3. send z and receive $\bar{z} = z + x$; 4. find long sparse error vector x using short vector $b = A\bar{z}$; 5. recover z' then w'

What these tasks have in common

- Given matrix A with fewer rows than columns
- Given vector b
- Find sparsest solution x^* of $Ax = b$

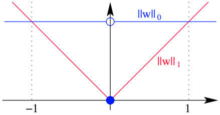
- Note: $Ax = b$ feasible iff $\mathsf{rank}(A) = \mathsf{rank}(A|b)$

Subsection 2

Basis pursuit

Sparsest solution of a linear system

- Problem $P^0(A,b) \equiv \min\{\|x\|_0 \mid Ax = b\}$ is **NP**-hard
  Reduction from EXACT COVER BY 3-SETS [Garey&Johnson 1979, A6[MP5]]
  MILP: $\min\{\sum_j y_j \mid \forall j \ -My_j \le x_j \le My_j \ \wedge \ Ax = b \ \wedge \ y \in \{0,1\}^n\}$
- $P^1(A,b) \equiv \min\{\|x\|_1 \mid Ax = b\}$ is a relaxation

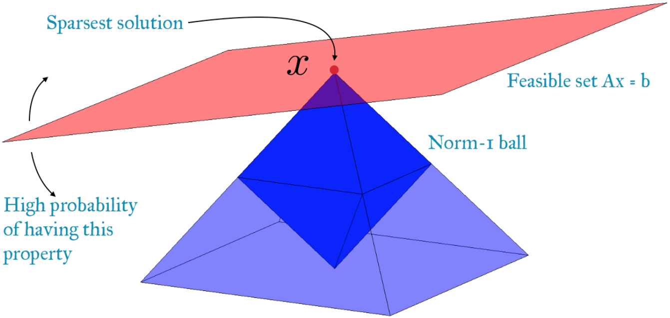


- Reformulate to LP:

$$\boxed{\left.\begin{array}{rrcl} \min & \sum\limits_{j \le n} & s_j & \\ \forall j \le n & -s_j \le & x_j & \le s_j \\ & Ax & = & b \end{array}\right\} \quad (\dagger)}$$

- Empirical observation: P^1 often finds optimum of P^0
  Too often for this to be a coincidence
- Theoretical justification by Candès, Tao, Donoho
  Mathematics of sparsity, Compressed sensing, Compressive sampling
- Note: we always assume $b \neq 0$ in $P^0(A,b)$ and $P^1(A,b)$

Graphical intuition 1

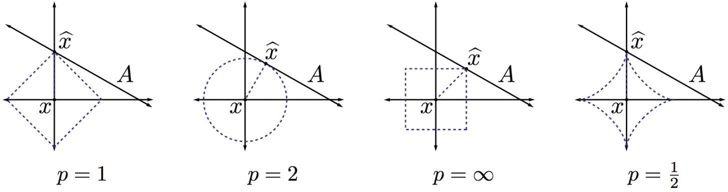


- Wouldn't work with ℓ_2, ℓ_∞ norms

  $Ax = b$ flat at poles — "zero probability of sparse solution"

Warning: *this is not a proof, and ∃ cases not explained by this drawing* [Candès 2014]

Graphical intuition 2

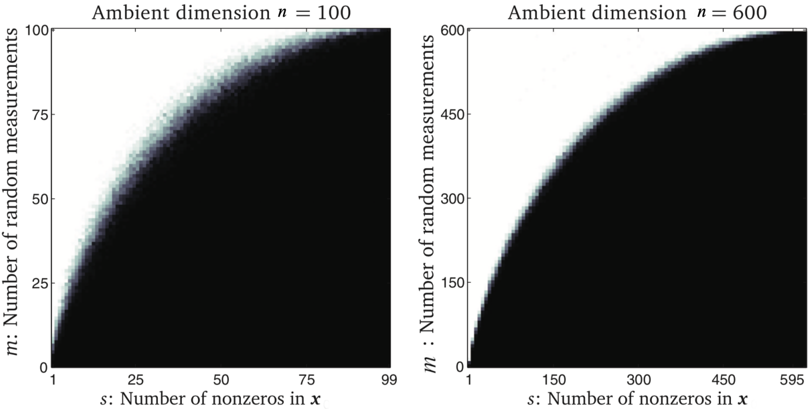


- $\hat{x}$ such that $A\hat{x} = b$ approximates x in ℓ_p norms
- $p = 1$ only convex case zeroing some components

From [Davenport et al., 2012]; again, this is not a proof!

Phase transition in sparse recovery

For $x \in \mathbb{R}^n$, $A \in \mathbb{R}^{m \times n}$: consider $P^1(A, Ax)$ and its opt. x^*



Pixel grayscale: avg density of x^* over many samplings of A; white = sparse, black = dense

Prob$(x^*$ has sparsity $s)$ undergoes a phase transition

For a given n, if m is too small P^1 fails to find the optimum of P^0

[Tropp et al., Information and Inference, 2014]

Subsection 3

Theoretical results

Main theorem and proof structure

Defn. (i) Given a small $\epsilon \geq 0$, a scalar α is *near-zero* if $|\alpha| < \epsilon$;
(ii) a vector is *s-sparse* if it has $\leq s$ nonzero components

- **Thm.** Let:

  1. $A \sim \mathsf{N}(0,1)^{mn}$ with $m < n$ but m "not too small"
  2. $\hat{x} \in \mathbb{R}^n$ have s nonzeros and $n - s$ zeros or near-zeros
  3. $\bar{x}$ be the best approx of $\hat{x}$ with exactly s nonzeros
  4. $\hat{b} = A\hat{x}$ and x^* be the unique s-sparse min of $P^1(A, \hat{b})$

  then x^* is a "good approximation" of $\bar{x}$ $\quad (\star)$

- Proof sketch:

  - **Prop.** A has the null space property (NSP) $\Rightarrow (\star)$
  - **Prop.** A has restricted isometry prop. (RIP) $\Rightarrow$ A has NSP
  - **Prop.** $A \sim \mathsf{N}(0,1)^{mn} \Rightarrow A$ has RIP
  - adapt to near-zeros by modifying NSP

Some notation

Defn. (i) For any $n \in \mathbb{N}$ define $[n] = \{1, \ldots, n\}$;
(ii) for $z \in \mathbb{R}^n$ and $S \subseteq [n]$ let $z[S] = ((z_j \text{ iff } j \in S) \text{ xor } 0 \mid j \leq n)$ be the *restriction* of z to S

- Consider $Ax = b$ where A is $m \times n$ with $m < n$
  $\Rightarrow$ *if feasible it has uncountably many solutions*
- Let $x \in \mathbb{R}^n$ s.t. $Ax = b$, $\mathsf{N}_A = \mathsf{null}(A)$, $\mathsf{N}^0_A = \mathsf{N}_A \smallsetminus \{0\}$
  $\Rightarrow \forall y \in \mathsf{N}_A$ we have $A(x + y) = Ax + Ay = Ax + 0 = b$
- For $S \subseteq [n]$ let $\bar{S} = [n] \smallsetminus S$
- Note that $\forall z \in \mathbb{R}^n$ we have $z = z[S] + z[\bar{S}]$

Null space property

Defn. For $x \in \mathbb{R}^n$ let $\mathsf{supp}(x) = \{j \leq n \mid x_j \neq 0\}$

- **Defn.** $\mathsf{NSP}_s(A) \equiv$
  $$\boxed{\forall S \subseteq [n] \ \big(|S| = s \ \rightarrow \ \forall y \in \mathsf{N}_A^0 \ \ \|y[S]\|_1 < \|y[\bar{S}]\|_1\big)}$$
  A has the *null space property of order s*

- A has the NSP of order s iff each s-sparse solution of $Ax = b$ is the unique optimun of $P^1(A, b)$

- **Prop.** $\forall x^* \in \mathbb{R}^n$ with $|\mathsf{supp}(x^*)| \leq s$ and $b = Ax^*$
  $$[x^* \text{ unique min of } P^1(A, b)] \quad \Leftrightarrow \quad \mathsf{NSP}_s(A)$$

the "NSP proposition"

Strength of NSP_t as t grows

NSP Prop. states $|\mathsf{supp}(x^*)| \le s$ *but* $\mathsf{NSP}_s(A)$ *assumes* $|S| = s$*: why?*

Lemma

$$\forall A \in \mathbb{R}^{m\times n}, t < s \le n \quad \mathsf{NSP}_s(A) \Rightarrow \mathsf{NSP}_t(A)$$

Proof

$\mathsf{NSP}_s(A) \equiv \forall S \subseteq [n]\ (|S| = s \to \forall y \in \mathsf{N}^0_A\ \|y[S]\|_1 < \|y[\bar{S}]\|_1)$, hence:

given $T, U \subseteq [n]$ with T, U nontrivial disjoint, $|T| = t$ and $|T \cup U| = s$,

- $\forall y \in \mathsf{N}^0_A\ \|y[T \cup U]\|_1 < \|y[\overline{T \cup U}]\|_1 = \|y[[n] \setminus (T \cup U)]\|_1 \Rightarrow$

(†) $\forall y \in \mathsf{N}^0_A\ \|y[T]\|_1 + \|y[U]\|_1 < \|y\|_1 - \|y[T]\|_1 - \|y[U]\|_1 \Rightarrow$

(‡) $\forall y \in \mathsf{N}^0_A\ \|y[T]\|_1 < \|y[\bar{T}]\|_1 - 2\|y[U]\|_1$

- whence $\forall T \subseteq [n]\ (|T| = t \ \to\ \forall y \in \mathsf{N}^0_A\ \|y[T]\|_1 < \|y[\bar{T}]\|_1)$

  since $\|y[U]\|_1 > 0$, and so $\mathsf{NSP}_t(A)$

(†) $\|y[T \cup U]\|_1 = \sum_{j \in T\cup U} |y_j| = \sum_{j\in T} |y_j| + \sum_{j \in U} |y_j| = \|y[T]\|_1 + \|y[U]\|_1$

$\|y[[n] \setminus V]\|_1 = \sum_{j \in [n]\setminus V} |y_j| = \sum_{j\in[n]} |y_j| - \sum_{j\in V} |y_j| = \|y\|_1 - \|y[V]\|_1$

(‡) $\|y\|_1 - \|y[T]\|_1 = \sum_{j \le n} |y_j| - \sum_{j \in T} |y_j| = \sum_{j \notin T} |y_j| = \sum_{j \in \bar{T}} |y_j| = \|y_j[\bar{T}]\|_1$

Proof of the NSP proposition ($\Rightarrow$)

$\forall x$ (x uniq min of $P^1(A, Ax) \wedge |\mathsf{supp}(x)| = s) \Rightarrow \mathsf{NSP}_s(A)$

- <u>*Claim*</u> $\forall y \in \mathsf{N}_A^0\ \exists S \subseteq [n]$ with $|S| = s$ such that $A\,y[S] \neq 0$
  Pf. $|\mathsf{supp}(y[S])| = |S| = s$ by definition
  $\Rightarrow$ by hypothesis $y[S]$ unique min of $P^1(A, A\,y[S])$
  $\Rightarrow$ by assumption (rhs vector $\neq 0$) $A\,y[S] \neq 0$
- $\forall y \in \mathbb{R}^n$ and $S \subseteq [n]$ we have $y = y[S] + y[\bar{S}]$
- $\Rightarrow$ for any $y \in \mathsf{N}_A^0$ we have $Ay = A\,y[S] + A\,y[\bar{S}] = 0$
  $\Rightarrow A(-y[\bar{S}]) = A\,y[S] \neq 0$ by claim
- Moreover, $-y[\bar{S}]$ is feasible in $P^1(A, A\,y[S])$
- $\boxed{y[S] \neq -y[\bar{S}]}$ othw by $y = y[S] + y[\bar{S}]$ both would be scalings of y and hence both in N_A^0, which cannot happen as $A\,y[S] \neq 0$
- $\|y[S]\|_1$ uniq min value and $-y[\bar{S}]$ feas in $P^1(A, Ay[S]) \Rightarrow$
  $\|-y[\bar{S}]\|_1 = \|y[\bar{S}]\|_1 > \|y[S]\|_1 \Rightarrow \mathsf{NSP}_s(A)$

Proof of the NSP proposition ($\Leftarrow$)

$\mathsf{NSP}_s(A) \Rightarrow \forall x^*\ (x^* \text{ uniq min } P^1(A, Ax^*) \wedge |\mathsf{supp}(x^*)| = s)$

- Let $x^* \in \mathbb{R}^n$, $b = Ax^*$, $S = \mathsf{supp}(x^*)$ and $|S| = s$
- Let $\bar{x}$ soln. of $Ax = b$, then $\bar{x} = x^* - y$ with $y \in \mathsf{N}_A^0$

$$
\begin{array}{rrcl}
\text{[add and subtract same qty]} & \|x^*\|_1 & = & \|(x^* - \bar{x}[S]) + \bar{x}[S]\|_1 \\
\text{[by triangle inequality]} & & \le & \|x^* - \bar{x}[S]\|_1 + \|\bar{x}[S]\|_1 \\
{[S = \mathsf{supp}(x^*) \Rightarrow x^* = x^*[S]]} & & = & \|x^*[S] - \bar{x}[S]\|_1 + \|\bar{x}[S]\|_1 \\
\text{[since } x^* - \bar{x} = y] & & = & \|y[S]\|_1 + \|\bar{x}[S]\|_1 \\
\text{[since } y \in \mathsf{N}_A^0 \text{ and } \mathsf{NSP}_s(A) \text{ holds]} & & < & \|y[\bar{S}]\|_1 + \|\bar{x}[S]\|_1 \\
\text{[since } y = x^* - \bar{x} \text{ and } x^*[\bar{S}] = 0] & & = & \|-\bar{x}[\bar{S}]\|_1 + \|\bar{x}[S]\|_1 \\
\text{[since } \|-z\|_1 = \|z\|_1 \wedge z[S] + z[\bar{S}] = z] & & = & \|\bar{x}\|_1 \\
\Rightarrow & \|x^*\|_1 & < & \|\bar{x}\|_1
\end{array}
$$

so x^* is a min of $P^1(A, Ax^*)$; ℓ_1 norm strictly convex $\Rightarrow x^*$ uniq min

A variant of the null space property

- **Motivation: "almost sparse solutions"**
  given $\hat{x}$ with $|\mathsf{supp}(\hat{x})| > s$ and $b = A\hat{x}$
  let $S = \underset{T \subseteq [n]:|T|=s}{\arg\max} \|\hat{x}[T]\|_1$ and $\bar{x} = \hat{x}[S]$ $(\Rightarrow |\mathsf{supp}(\bar{x})| = s)$

- Assume $\|\hat{x}[\bar{S}]\|_1 \ll \|\hat{x}[S]\|_1$ and $\epsilon = \max_{j \in \bar{S}} |\hat{x}_j|$ is small
  i.e. $\hat{x}$ "almost" has support size s (up to ϵ)

- Show min x^* of $P^1(A, A\hat{x})$ is s-sparse and close to $\hat{x}$

- Generalize NSP with $\rho \in (0,1)$: $\mathsf{NSP}_s^\rho(A) \Leftrightarrow$
  $\boxed{\forall S \subseteq [n]\ (|S| = s \to \forall y \in \mathsf{N}_A^0\ \|y[S]\|_1 \le \rho \|y[\bar{S}]\|_1)}$

- **Prop.** $\mathsf{NSP}_s^\rho(A) \Rightarrow$ if x^* min of $P^1(A, A\hat{x})$ then
  $$\|x^* - \hat{x}\|_1 \le 2\frac{1+\rho}{1-\rho}\|\bar{x} - \hat{x}\|_1 \le (n-s)\epsilon$$
  i.e. x^* is a good approximation of $\bar{x}$

- Moreover, if $|\mathsf{supp}(\hat{x})| = s$ then $x^* = \hat{x} = \bar{x}$

Proof of the NSP_s^ρ proposition

- x^* feasible in $Ax = A\hat{x}$ so $\exists! y \in \mathsf{N}_A$ $(x^* = \hat{x} + y)$
- $\Rightarrow \|x^*\|_1 = \|\hat{x} + y\|_1 \le \|\hat{x}\|_1$ since x^* min of $P^1(A, A\hat{x})$
- $\|\hat{x} + y\|_1 = \sum_{j\in S} |\hat{x}_j + y_j| + \sum_{j\in \bar{S}} |\hat{x}_j + y_j|$
  $\ge \sum_{j\in S}(|\hat{x}_j| - |y_j|) + \sum_{j\in \bar{S}}(|y_j| - |\hat{x}_j|)$ by triangle ineq
- $= \|\hat{x}[S]\|_1 - \|y[S]\|_1 + \|y[\bar{S}]\|_1 - \|\hat{x}[\bar{S}]\|_1$ (add and subtract $\|\hat{x}[\bar{S}]\|_1 \Rightarrow$)
  $= \|\hat{x}\|_1 + \|y[\bar{S}]\|_1 - 2\|\hat{x}[\bar{S}]\|_1 - \|y[S]\|_1$ (since $\bar{x} = \hat{x}[S] \Rightarrow$)
  $= \|x\|_1 - 2\|\hat{x} - \bar{x}\|_1 + \|y[\bar{S}]\|_1 - \|y[S]\|_1$ $(*)$
- Therefore $(*) \le \|\hat{x} + y\|_1 \le \|\hat{x}\|_1$, whence
  $\|\hat{x}\|_1 \ge \|\hat{x}\|_1 - 2\|\hat{x} - \bar{x}\|_1 + \|y[\bar{S}]\|_1 - \|y[S]\|_1$ (cancel $\|\hat{x}\|_1 \Rightarrow$)
  $2\|\hat{x} - \bar{x}\|_1 \ge \|y[\bar{S}]\|_1 - \|y[S]\|_1$
- By NSP_s^ρ, $-\|y[S]\|_1 \ge -\rho\|y[\bar{S}]\|_1$, so
  $2\|\hat{x} - \bar{x}\|_1 \ge (1-\rho)\|y[\bar{S}]\|_1$ whence $\|y[\bar{S}]\|_1 \le \frac{2}{1-\rho}\|\hat{x} - \bar{x}\|_1$ $(\dagger)$
- $x^* = \hat{x} + y \Rightarrow \|x^* - \hat{x}\|_1 = \|y\|_1 = \|y[S]\|_1 + \|y[\bar{S}]\|_1$
  by NSP_s^ρ $\|y[S]\|_1 \le \rho\|y[\bar{S}]\|_1$ hence $\|x^* - \hat{x}\|_1 \le (1+\rho)\|y[\bar{S}]\|_1$
  by $(\dagger)$ $\|x^* - \hat{x}\|_1 \le 2\frac{1+\rho}{1-\rho}\|\hat{x} - \bar{x}\|_1$
- Further, $\|\hat{x} - \bar{x}\|_1 = \|\hat{x} - \hat{x}[S]\|_1 = \|\hat{x}[\bar{S}]\| \le |\bar{S}|\epsilon = (n-s)\epsilon$

Restricted isometry property

- A is an $m \times n$ matrix, $\delta \in (0,1)$, $s \in \mathbb{N}$
- $\mathsf{RIP}_s^\delta(A) \quad \Leftrightarrow \quad \forall x \in \mathbb{R}^n$ s.t. $|\mathsf{supp}(x)| = s$ we have

$$(1-\delta)\,\|x\|_2^2 \quad \leq \quad \|Ax\|_2^2 \quad \leq \quad (1+\delta)\,\|x\|_2^2$$

- **Prop.** $\mathsf{RIP}_{2s}^\delta(A) \ \wedge \ \rho = \frac{\sqrt{2}\delta}{1-\delta} < 1 \quad \Rightarrow \quad \mathsf{NSP}_s^\rho(A)$

  See Thm. 5.12 in [Damelin & Miller 2012] for a proof
- It suffices that $\delta < \sqrt{2} - 1 \approx 0.4142$

RIP and $P^0(A, b)$

- Recall $P^0(A, b) \equiv \min\{\|x\|_0 \mid Ax = b\}$ is **NP**-hard
  find solution to $Ax = b$ with smallest support size

- **Thm.** Let $\hat{x} \in \mathbb{R}^n$ with $|\mathsf{supp}(\hat{x})| = s$, $\delta < 1$, A a matrix s.t. $\mathsf{RIP}^{\delta}_{2s}(A)$, $x^* = \mathsf{arg}P^0(A, A\hat{x})$; then $x^* = \hat{x}$

  Pf. Suppose false, let $y = x^* - \hat{x} \neq 0$; by defn of x^* we have $\|x^*\|_0 \leq \|\hat{x}\|_0 \leq s$, hence $\|y\|_0 \leq 2s$; since A has RIP get $\|Ay\|_2^2 \in (1 \pm \delta)\|y\|_2^2$, but $Ay = Ax^* - A\hat{x} = 0$ while $y \neq 0$, and $\delta \in (0, 1) \to 1 \pm \delta > 0$, hence $0 \in (\alpha, \beta)$ where $\alpha, \beta > 0$, contradiction

  Thm. 23.6 [Shwartz & Ben-David, 2014]

- Result of limited scope, since we don't know if $P^0(A, b)$ can be solved efficiently if A has the RIP

Sufficient eigenvalue conditions for RIP

- Recall $\mathsf{RIP}_s^\delta(A)$: $\forall x$ with $S = \mathsf{supp}(x)$ and $|S| = s$
$$(1-\delta)\|x\|_2^2 \le \|Ax\|_2^2 \le (1+\delta)\|x\|_2^2$$
- Let $A^J = (A^j \mid j \in J)$, where A^j is the j-th col. of A
- $\|Ax\|_2^2 = \langle Ax, Ax\rangle = \langle A^S x[S], A^S x[S]\rangle = \langle B_S x[S], x[S]\rangle$
where $B_S = (A^S)^\top A^S$ is $s \times s$ and PSD, and consider $x[S]$ as a vector in $\mathbb{R}^s$
- $\Rightarrow 0 \le \lambda_{\mathsf{min}}(B_S)\|x\|_2^2 \le \langle B_S x, x\rangle \le \lambda_{\mathsf{max}}(B_S)\|x\|_2^2$
replace B_S by its spectral decomp $P\Lambda P^\top$, note $\Lambda = \mathsf{diag}(\lambda_{\mathsf{min}}, \ldots, \lambda_{\mathsf{max}})$
- Let $\lambda^L = \min\limits_{|S|=s} \lambda_{\mathsf{min}}(B_S)$, $\lambda^U = \max\limits_{|S|=s} \lambda_{\mathsf{max}}(B_S)$
- $\Leftarrow \exists\delta > 0$ s.t. $1-\delta \le \lambda^L \le \lambda^U \le 1+\delta$
i.e. all eigenvalues of $B(S)$ close to 1 for all $S \subset [n]$ with $|S| = s$

Construction of A s.t. $\mathsf{RIP}_s^\delta(A)$

- Need $\lambda \approx 1$ for each eigenvalue λ of B_S
- $\Rightarrow$ Need $\quad \forall S \subseteq N \quad |S| = s \;\rightarrow\; (A^S)^\top A^S \approx I_s$
- $\Rightarrow$ Need

$$\begin{array}{rcl} \forall i < j \le n \quad (A^i)^\top A^j & \approx & 0 \\ \forall i \le n \quad (A^i)^\top A^i = \|A^i\|_2^2 & \approx & 1 \end{array}$$

- **Sufficient condition:** A sampled from $\mathsf{N}\big(0, \frac{1}{\sqrt{m}}\big)^{mn}$
- *Difference with JLL*
  RIP holds for uncountably many vectors x with $|\mathsf{supp}(x)| = s$
  JLL holds for given sets of finitely many vectors with any support

Project idea 8: What other types of rectangular matrices M have the property $M^\top M = I$ or $\approx I$? Can they be used to prove the main theorem? How do they work, computationally, compared with matrices sampled from normal distributions? Compare on at least 50 random instances of $P^1(A, b)$

Isotropic vectors

1. **Defn.** Rnd vect $a \in \mathbb{R}^m$ is *isotropic* iff $\mathsf{cov}(a) = I_m$
   remark: (a) $\mathsf{cov}(a) = \mathsf{E}(aa^\top)$; (b) if $a \sim \mathsf{N}(0,1)^m$ then a isotropic
2. If rnd vect a isotropic, then $\forall x \in \mathbb{R}^m\ \mathsf{E}(\langle a, x\rangle^2) = \|x\|_2^2$
   For two sq. symm. matrices B, C we have $B = C$ iff $\forall x\ (x^\top B x = x^\top C x)$;
   hence $\mathsf{E}(\langle a, x\rangle^2) = x^\top \mathsf{E}(aa^\top) x = x^\top I_m x = \|x\|_2^2$
3. If rnd vect $a \in \mathbb{R}^m$ isotropic, then $\mathsf{E}(\|a\|_2^2) = m$
   $\mathsf{E}(\|a\|_2^2) = \mathsf{E}(a^\top a) = \mathsf{E}(\mathsf{tr}(a^\top a)) = \mathsf{E}(\mathsf{tr}(aa^\top)) = \mathsf{tr}(\mathsf{E}(aa^\top)) = \mathsf{tr}(I_m) = m$
4. If rnd vect $a, c \in \mathbb{R}^m$ indep. isotropic, then $\mathsf{E}(\langle a, c\rangle^2) = m$
   By conditional expectation $\mathsf{E}(\langle a, c\rangle^2) = \mathsf{E}_c(\mathsf{E}_a(\langle a, c\rangle^2 \mid c))$; by Item 2 inner expectation is $\|c\|_2^2$, by Item 3 outer is m
5. If $a \sim \mathsf{N}(0,1)^m$, $\|a\|_2 = O(\sqrt{m})$ wahp
   by Thm. 3.1.1 in [Vershynin, 2018]
6. Independent rnd vectors are almost orthogonal
   Results above $\Rightarrow \|a\|_2, \|c\|_2, \langle a, c\rangle = O(\sqrt{m})$, normalize a, c to $\bar{a}, \bar{c}$ to get $\langle \bar{a}, \bar{c}\rangle = O(1/\sqrt{m}) \Rightarrow$ for m large $\langle \bar{a}, \bar{c}\rangle \approx 0$

Construction of A s.t. $\mathsf{RIP}_s^\delta(A)$

- **Thm.** For $A \sim \mathsf{N}(0,1)^{m\times n}$ and $\delta \in (0,1)$ $\exists C_1, C_2 > 0$ depending on δ s.t.

$$\forall s < m \left(m \geq \frac{s \ln(n/s)}{C_1} \to \mathsf{Prob}(\mathsf{RIP}_s^\delta(A)) \geq 1 - e^{-C_2 m} \right)$$

  Pf. see Thm. 5.17 in [Damelin & Miller, 2012]

  Remark: extra $\sqrt{m}$ factor in A comes from $\|\cdot\|_2 \leq \|\cdot\|_1 \leq \sqrt{m}\|\cdot\|_2$

- In practice:
  - $\mathsf{Prob}(\mathsf{RIP}_s^\delta(A)) = 0$ for m too small w.r.t. s fixed
  - as m increases $\mathsf{Prob}(\mathsf{RIP}_s^\delta(A)) > 0$
  - as m increases even more $\mathsf{Prob}(\mathsf{RIP}_s^\delta(A)) \to 1$ wahp
  - achieve logarithmic compression for large n and fixed s
  - $A \sim \mathsf{N}(0,1)^{mn} \wedge m \geq 10 s \ln \frac{n}{s} \Rightarrow \mathsf{RIP}_s^{1/3}(A)$ wahp, Lem. 5.5.2 [Moitra 2018]
  - works better than worst case bounds ensured by theory

Some literature

1. Damelin & Miller, The mathematics of signal processing, CUP, 2012
2. Vershynin, High-dimensional probability, CUP, 2018
3. Moitra, Algorithmic aspects of machine learning, CUP, 2018
4. Shwartz & Ben-David, Understanding machine learning, CUP, 2014
5. Hand & Voroninski, `arxiv.org/pdf/1611.03935v1.pdf`
6. Candès & Tao
   `statweb.stanford.edu/~candes/papers/DecodingLP.pdf`
7. Candès
   `statweb.stanford.edu/~candes/papers/ICM2014.pdf`
8. Davenport *et al.*, `statweb.stanford.edu/~markad/publications/ddek-chapter1-2011.pdf`
9. Lustig *et al.*, `people.eecs.berkeley.edu/~mlustig/CS/CSMRI.pdf`

and many more (look for "compressed sensing")

Subsection 4

Application to noisy channel encoding

Noisy channel encoding procedure

Algorithm:

1. message: *character string* μ
2. $w = \mathsf{string2bitlist}(\mu) \in \{0,1\}^d$
3. send $z = Qw$, receive $\bar{z} = z + \hat{x}$, let $b = A\bar{z}$

   $\Delta = s/n =$ *density of* $\hat{x}$, $\quad Q$ *is* $n \times d$ *full rank with* $n > d$
4. $x^* =$ optimum of $P^1(A, b)$
5. $z^* = \bar{z} - x^*$
6. $w^* = \mathsf{cap}(\mathsf{round}(\,(Q^\top Q)^{-1} Q^\top z^*), [0,1])$

   $\mathsf{cap}(t, [\alpha, \beta]) = (\alpha \text{ if } t < \alpha)$ xor $(\beta \text{ if } t > \beta)$ xor $(t \text{ othw})$
7. $\mu^* = \mathsf{bitlist2string}(w^*)$
8. evaluate $\mu_{\mathsf{err}} = \|\mu - \mu^*\|$

Parameter choice [Matousek]:

- noise $\Delta = 0.08$
- redundancy $n = R\,d$, where $R = 4$

Finding orthogonal A, Q

- [Matousek, Gärtner 2007]:
  - sample A componentwise from $\mathsf{N}(0,1)$
  - then "find Q s.t. $QA = 0$"
  - *Gaussian elim. on underdet. system $AQ = 0$*
- Faster:
  - sample $n \times n$ matrix M from uniform distr
    full rank with probability 1
  - find eigenvector matrix of $M^\top M$ (orthonormal basis)
    random rotation of standard basis (used in original JLL proof)
  - Concatenate d eigenvectors to make Q
    Concatenate $m = n - d$ eigenvectors to make A
    $AQ = 0$ by construction!

Subsection 5

Improvements

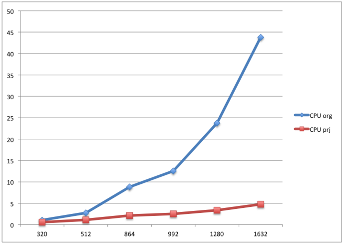
LP size reduction

- Motivation
  - Reduce CPU time spent on LP
  - $R = 4$ redundancy for $\Delta = 0.08$ noise seems excessive
- Size of basis pursuit LP
  - $Ax = b$ is an $m \times n$ system where $m = n - d$
  - If $n = Rd \gg d$, m "relatively close" to n
  - *Recall random projections for LP: use them!*

Computational results

d	n	Δ	ϵ	α	$\mu_{\text{err}}^{\text{org}}$	$\mu_{\text{err}}^{\text{prj}}$	CPU$^{\text{org}}$	CPU$^{\text{prj}}$
80	320	0.08	0.20	0.02	0	0	1.05	0.56
128	512	0.08	0.20	0.02	0	0	2.72	1.10
216	864	0.08	0.20	0.02	0	0	8.83	2.12
248	992	0.08	0.20	0.02	0	0	12.53	2.53
320	1280	0.08	0.20	0.02	0	0	23.70	3.35
408	1632	0.08	0.20	0.02	0	0	43.80	4.75

- $d = |\mu|$, $n = 4d$, $\Delta = 0.08$, $\epsilon = 0.2$
- $\alpha =$ Achlioptas density
  $\mathsf{P}(T_{ij} = -1) = \mathsf{P}(T_{ij} = 1) = \frac{\alpha}{2}$
  $\mathsf{P}(T_{ij} = 0) = 1 - \alpha$
- $\mu_{\text{err}} =$ number of different characters
- CPU: seconds of elapsed time
- *1 sampling of A, Q, T*



Sentence: *Conticuere omnes intentique ora tenebant, inde toro* [...]

Reducing redundancy in n

- *How about taking $n = (1+\Delta)d$?*
- $m = n - d \approx \Delta d$ is very small
- Makes $Ax = b$ very short and fat
- Prevents compressed sensing from working correctly
  not enough constraints
- Would need both m and d to be $\approx n$ and $AQ = 0$: impossible
  $\mathbb{R}^n$ too small to host $m + d \approx 2n$ orthogonal vectors
- Relax to $AQ \approx 0$?

Almost orthogonality by the JLL

Aim at $A^\top, Q$ with $m + d \approx 2n$ and $AQ \approx 0$

- **JLL Corollary:** $\exists O(e^k)$ *approx orthog vectors in* $\mathbb{R}^k$

  Pf. Let T be a $k \times p$ RP, use concentration of measure on $\|z\|_2^2$

  $$\mathsf{Prob}(\,(1-\varepsilon)\|z\|_2^2 \le \|Tz\|_2^2 \le (1+\varepsilon)\|z\|_2^2\,) \ge 1 - 2e^{-\mathcal{C}(\varepsilon^2-\varepsilon^3)k}$$

  given $x, y \in \mathbb{R}^p$ apply to $x+y$, $x-y$ and union bound:

  $$\begin{aligned} |\langle Tx, Ty\rangle - \langle x, y\rangle| &= \tfrac{1}{4}\left|\|T(x+y)\|^2 - \|T(x-y)\|^2 - \|x+y\|^2 + \|x-y\|^2\right| \\ &\le \tfrac{1}{4}\left|\|T(x+y)\|^2 - \|x+y\|^2\right| + \tfrac{1}{4}\left|\|T(x-y)\|^2 - \|x-y\|^2\right| \\ &\le \tfrac{\varepsilon}{4}(\|x+y\|^2 + \|x-y\|^2) = \tfrac{\varepsilon}{2}(\|x\|^2 + \|y\|^2) \end{aligned}$$

  with prob $\ge 1 - 4e^{-\mathcal{C}(\varepsilon^2-\varepsilon^3)k}$; apply to std basis matrix I_p, get

  $$-\varepsilon \le \langle T\mathbf{e}_i, T\mathbf{e}_j\rangle - \langle \mathbf{e}_i, \mathbf{e}_j\rangle \le \varepsilon$$

  $\Rightarrow \exists p$ almost orthogonal vectors in $\mathbb{R}^k$, and $k = O(\frac{1}{\varepsilon^2}\ln p) \Rightarrow p = O(e^k)$

- **Algorithm:** $k = n, p = \lceil e^n \rceil$, get $2k$ columns from $T\,I_p$

Also see [https://terrytao.wordpress.com/2013/07/18/a-cheap-version-of-the-kabatjanskii-levenstein-bound-for-almost-orthogonal-vectors/]

Almost orthogonality by the JLL

- Aim at $m \times n$ A and $n \times m$ Q s.t. $AQ \approx 0$
  with $n = (1 + \Delta')m$ and Δ' "small" (say $\Delta' < 1$)
- Need $2m$ approx orthog vectors in $\mathbb{R}^n$ with $n < 2m$
- Computationally: get large errors on $\|AQ\|_2$
  JLL theory requires exceedingly large sizes

- In fact, we only need $AQ = 0$!
  can accept non-orthogonality in rows of A & cols of Q

Almost orthogonality by LP

- Sample Q and compute A using an LP
- $\max \sum_{\substack{i\le m\\ j\le n}} \mathsf{Uniform}(-1,1)A_{ij}$
- subject to $AQ = 0$ and $A \in [-1,1]$
- for $m = 328$ and $n = 590$ (i.e. $\Delta' = 0.8$):
  - error: $\sum A_i Q^j = O(10^{-10})$
  - rank: full up to error precision (*not really though*)
  - CPU: 688s (*meh*)
- for $m = 328$ and $n = 492$ (i.e. $\Delta' = 0.5$): *the same*
- for $m = 328$ and $n = 426$ (i.e. $\Delta' = 0.3$): *CPU 470s*
- Reduce CPU time by solving m LPs deciding A_i for all $i \le m$

Computational results

m	n	Δ'	$\mu_{\mathsf{err}}^{\mathsf{org}}$	$\mu_{\mathsf{err}}^{\mathsf{prj}}$	$\mathrm{CPU}^{\mathsf{org}}$	$\mathrm{CPU}^{\mathsf{prj}}$
328	426	0.3	182	15	2.45	1.87
328	426	0.3	154	0	2.20	1.49
328	459	0.4	0	1	4.47	2.45
328	459	0.4	5	17	2.86	1.46
328	492	0.5	60	0	4.53	1.18
328	492	0.5	34	0	5.38	1.18
328	590	0.8	14	0	8.30	1.41
328	590	0.8	107	4	6.76	1.43

- CPU for computing A, Q not counted: *precomputation is possible*
- Approximate beats precise!

In summary

- If μ is short, set $\Delta' = \Delta$ and use compressed sensing (CS)
- If μ is longer, try increasing Δ' and use CS
- If μ is very long, use *JLL-projected CS*
- Can use approximately orthogonal A, Q too

Conticuere omnes, intentique ora tenebant.
Inde toro pater Aeneas sic orsus ab alto:
Infandum, regina, iubes renovare dolorem.
Troianas ut opes et lamentabile regnum eruerint Danai
Quaequae ipse miserrima vidi et quorum pars magna fui.
[Virgil, *Aeneid*, Cantus II]

$m = 1896$, $n = 2465$
$\Delta' = 0.3$: min s.t. CS is accurate

method	*error*	*CPU*
CS	0	29.67s
JLL-CS	2	17.13s

These results are consistent over 3 samplings

Project idea 9: Implement and test RPs applied to CS, as described in the last slides. Aim at setting the redundancy n equal to the noise $(1+\Delta)d$, and use CPLEX to compute A such that $AQ \approx 0$. Test your code on at least 10 different texts of various lengths, up to around 500 characters. How does decoding quality depend on $\|AQ\|_2$?

Outline

Definition

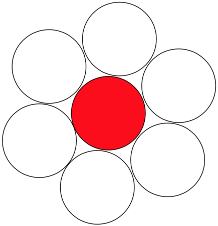
- *Optimization version.* Given $K \in \mathbb{N}$, determine the maximum number $\mathsf{kn}(K)$ of unit spheres that can be placed adjacent to a central unit sphere so their interiors do not overlap
- *Decision version.* Given $n, K \in \mathbb{N}$, is $\mathsf{kn}(K) \leq n$?

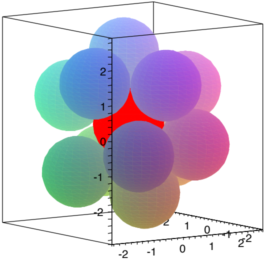
  in other words, determine whether n unit spheres can be placed adjacent to a central unit sphere so that their interiors do not overlap

Funny story: *Newton and Gregory went down the pub. . .*

Some examples

$n = 6,\ K = 2$ $\qquad$ $n = 12,\ K = 3$ $\qquad$ *more dimensions*



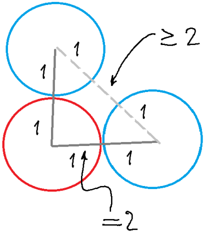


n	τ (lattice)	τ (nonlattice)
0	0	
1	2	
2	6	
3	12	
4	24	
5	40	
6	72	
7	126	
8	240	
9	272	(306)*
10	336	(500)*
11	438	(582)*
12	756	(840)*
13	918	(1130)*
14	1422	(1582)*
15	2340	
16	4320	
17	5346	
18	7398	
19	10668	
20	17400	
21	27720	
22	49896	

Radius formulation

Given $n, K \in \mathbb{N}$, determine whether there exist n vectors $x_1, \ldots, x_n \in \mathbb{R}^K$ such that:

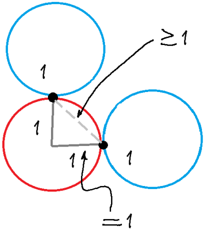
$$\begin{array}{rrcl} \forall i \le n & \|x_i\|_2^2 & = & 4 \\ \forall i < j \le n & \|x_i - x_j\|_2^2 & \ge & 4 \end{array}$$



Contact point formulation

Given $n, K \in \mathbb{N}$, determine whether there exist n vectors $x_1, \ldots, x_n \in \mathbb{R}^K$ such that:

$$\begin{array}{rrcl} \forall i \leq n & \|x_i\|_2^2 & = & 1 \\ \forall i < j \leq n & \|x_i - x_j\|_2^2 & \geq & 1 \end{array}$$



Spherical codes

- $S^{K-1} \subset \mathbb{R}^K$ unit sphere centered at origin
- *K-dimensional spherical z-code*:
  - (finite) subset $\mathcal{C} \subset S^{K-1}$
  - $\forall x \neq y \in \mathcal{C} \qquad x \cdot y \leq z$
- non-overlapping interiors:

$$\begin{array}{rcl} \forall i < j \quad \|x_i - x_j\|_2^2 & \geq & 1 \\ \Leftrightarrow \quad \|x_i\|_2^2 + \|x_j\|_2^2 - 2\,x_i \cdot x_j & \geq & 1 \\ \Leftrightarrow \quad 1 + 1 - 2\,x_i \cdot x_j & \geq & 1 \\ \Leftrightarrow \quad 2\,x_i \cdot x_j & \leq & 1 \\ \Leftrightarrow \quad x_i \cdot x_j & \leq & \frac{1}{2} = \cos\left(\frac{\pi}{3}\right) = z \end{array}$$

- we aim at maximizing $\mathsf{kn}_z(K) \triangleq |\mathcal{C}|$

  let $\mathsf{kn}(K) = \mathsf{kn}_{\frac{1}{2}}(K)$

Subsection 1

Lower bounds

Lower bounds

- Construct spherical $\frac{1}{2}$-code $\mathcal{C}$ with $|\mathcal{C}|$ large
- Nonconvex NLP formulations
- SDP relaxations
- Combination of the two techniques

MINLP formulation

Maculan, Michelon, Smith 1995

Parameters:

- K: space dimension
- n: upper bound to $\mathsf{kn}(K)$

Variables:

- $x_i \in \mathbb{R}^K$: contact pt. of i-th surrounding sphere
- $\alpha_i = 1$ iff sphere i in configuration

$$\left.\begin{array}{rrcl} \max & \sum\limits_{i=1}^{n} \alpha_i & & \\ \forall i \le n & ||x_i||^2 & = & \alpha_i \\ \forall i < j \le n & ||x_i - x_j||^2 & \ge & \alpha_i \alpha_j \\ \forall i \le n & x_i & \in & [-1,1]^K \\ \forall i \le n & \alpha_i & \in & \{0,1\} \end{array}\right\}$$

Reformulating the binary products

- **Additional variables**: $\beta_{ij} = 1$ iff vectors i, j in configuration
- Linearize $\alpha_i \alpha_j$ by β_{ij}
- Add constraints:

$$
\begin{array}{llcl}
\forall i < j \le n & \beta_{ij} & \le & \alpha_i \\
\forall i < j \le n & \beta_{ij} & \le & \alpha_j \\
\forall i < j \le n & \beta_{ij} & \ge & \alpha_i + \alpha_j - 1
\end{array}
$$

Computational experiments

AMPL and Baron

- **Certifying** YES
  - $n = 6, K = 2$: OK, 0.60s
  - $n = 12, K = 3$: OK, 0.07s
  - $n = 24, K = 4$: FAIL, CPU time limit (100s)
- **Certifying** NO
  - $n = 7, K = 2$: FAIL, CPU time limit (100s)
  - $n = 13, K = 3$: FAIL, CPU time limit (100s)
  - $n = 25, K = 4$: FAIL, CPU time limit (100s)

Almost useless

Modelling the decision problem

$$\left.\begin{array}{rrcl}
\max\limits_{x,\alpha} & \alpha & & \\
\forall i \le n & \|x_i\|^2 & = & 1 \\
\forall i < j \le n & \|x_i - x_j\|^2 & \ge & \alpha \\
\forall i \le n & x_i & \in & [-1,1]^K \\
 & \alpha & \ge & 0
\end{array}\right\}$$

- Feasible solution (x^*, α^*)
- *KNP instance is* YES *iff* $\alpha^* \ge 1$

[Kucherenko, Belotti, Liberti, Maculan, *Discr. Appl. Math.* 2007]

Computational experiments

AMPL and Baron

- **Certifying** YES
  - $n = 6, K = 2$: FAIL, CPU time limit (100s)
  - $n = 12, K = 3$: FAIL, CPU time limit (100s)
  - $n = 24, K = 4$: FAIL, CPU time limit (100s)
- **Certifying** NO
  - $n = 7, K = 2$: FAIL, CPU time limit (100s)
  - $n = 13, K = 3$: FAIL, CPU time limit (100s)
  - $n = 25, K = 4$: FAIL, CPU time limit (100s)

Apparently even more useless

But more informative ($\arccos \alpha$ = min. angular sep)

Certifying YES **by** $\alpha \geq 1$

- $n = 6, K = 2$: OK, 0.06s
- $n = 12, K = 3$: OK, 0.05s
- $n = 24, K = 4$: OK, 1.48s
- $n = 40, K = 5$: FAIL, CPU time limit (100s)

What about polar coordinates?

- $\forall i \le n \quad x_i = (x_{i1}, \ldots, x_{iK}) \mapsto (\vartheta_{i1}, \ldots, \vartheta_{i,K-1})$
- Formulation

$$\begin{array}{rrcl}
(\dagger) \quad \forall k \le K & \rho \sin \vartheta_{i,k-1} \prod_{h=k}^{K-1} \cos \vartheta_{ih} & = & x_{ik} \\
(\ddagger) \qquad \forall i < j \le n & \|x_i - x_j\|_2^2 & \ge & \rho^2 \\
\forall i \le n, k \le K & (\sin(\vartheta_{ik}))^2 + (\cos(\vartheta_{ik}))^2 & = & 1 \\
 & \textit{(optional)} \qquad \rho & = & 1
\end{array}$$

- Only need to decide $s_{ik} = \sin \vartheta_{ik}$ and $c_{ik} = \cos \vartheta_{ik}$
- Replace x in ($\ddagger$) using ($\dagger$): get polyprog in s, c
- *Numerically more challenging to solve (polydeg $2K$)*
- OPEN QUESTION: useful for bounds?

Subsection 2

Upper bounds from SDP?

SDP relaxation of Euclidean distances

- Linearization of scalar products

$$\forall i, j \le n \qquad x_i \cdot x_j \longrightarrow X_{ij}$$

  where X is an $n \times n$ symmetric matrix
- $\|x_i\|_2^2 = x_i \cdot x_i = X_{ii}$
- $\|x_i - x_j\|_2^2 = \|x_i\|_2^2 + \|x_j\|_2^2 - 2x_i \cdot x_j = X_{ii} + X_{jj} - 2X_{ij}$
- $X = xx^\top \Rightarrow X - xx^\top = 0$ makes linearization exact
- Relaxation:

$$X - xx^\top \succeq 0 \Rightarrow \mathsf{Schur}(X, x) = \begin{pmatrix} I_K & x^\top \\ x & X \end{pmatrix} \succeq 0$$

SDP relaxation of binary constraints

- $\forall i \le n \qquad \alpha_i \in \{0,1\} \Leftrightarrow \alpha_i^2 = \alpha_i$
- Let A be an $n \times n$ symmetric matrix
- Linearize $\alpha_i \alpha_j$ by A_{ij} (hence α_i^2 by A_{ii})
- $A = \alpha\alpha^\top$ makes linearization exact
- Relaxation: $\mathsf{Schur}(A, \alpha) \succeq 0$

SDP relaxation of [MMS95]

$$\left.\begin{array}{rrcl}
\max & \displaystyle\sum_{i=1}^{n} \alpha_i & & \\
\forall i \le n & X_{ii} & = & \alpha_i \\
\forall i < j \le n & X_{ii} + X_{jj} - 2X_{ij} & \ge & A_{ij} \\
\forall i \le n & A_{ii} & = & \alpha_i \\
\forall i < j \le n & A_{ij} & \le & \alpha_j \\
\forall i < j \le n & A_{ij} & \le & \alpha_i \\
\forall i < j \le n & A_{ij} & \ge & \alpha_i + \alpha_j - 1 \\
 & \mathsf{Schur}(X, x) & \succeq & 0 \\
 & \mathsf{Schur}(A, \alpha) & \succeq & 0 \\
\forall i \le n & x_i & \in & [-1, 1]^K \\
 & \alpha & \in & [0, 1]^n \\
 & X & \in & [-1, 1]^{n^2} \\
 & A & \in & [0, 1]^{n^2}
\end{array}\right\}$$

Computational experiments

- Python, PICOS and Mosek
  or Octave and SDPT3
- bound always equal to n
- prominent failure :-(
- **Why?**
  - *can combine inequalities to remove A from SDP*

$$\begin{aligned} \forall i < j \; X_{ii} + X_{jj} - 2X_{ij} &\geq A_{ij} \geq \alpha_i + \alpha_i - 1 \\ \Rightarrow X_{ii} + X_{jj} - 2X_{ij} &\geq \alpha_i + \alpha_i - 1 \end{aligned}$$

    (then eliminate all constraints in A)
  - *integrality of α completely lost*

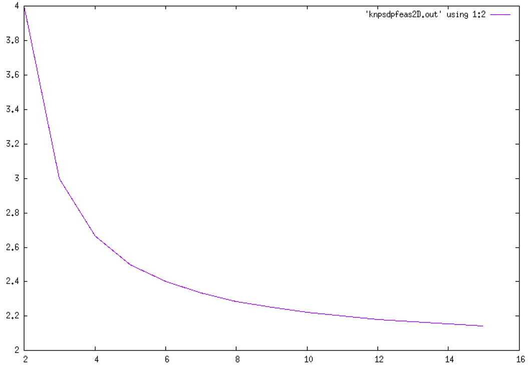
SDP relaxation of [KBLM07]

$$\left.\begin{array}{rrcl}
\max & \alpha & & \\
\forall i \le n & X_{ii} & = & 1 \\
\forall i < j \le n & X_{ii} + X_{jj} - 2X_{ij} & \ge & \alpha \\
 & X & \in & [-1,1]^{n^2} \\
 & X & \succeq & 0 \\
 & \alpha & \ge & 0
\end{array}\right\}$$

Computational experiments

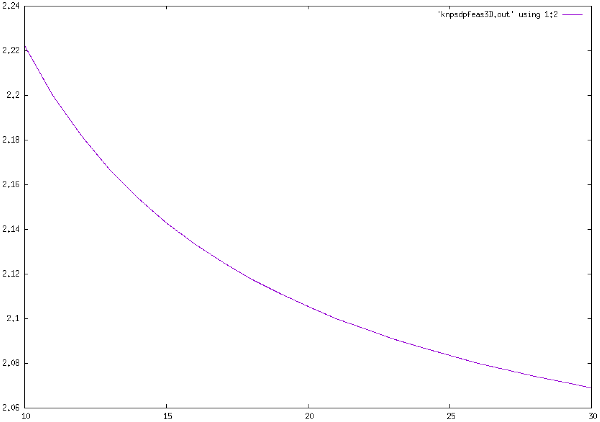
With $K = 2$

n	α^*
2	4.00
3	3.00
4	2.66
5	2.50
6	2.40
7	2.33
8	2.28
9	2.25
10	2.22
11	2.20
12	2.18
13	2.16
14	2.15
15	2.14



Computational experiments

With $K = 3$



Always $\longrightarrow 2$*?*

An SDP-based heuristic?

1. $X^* \in \mathbb{R}^{n^2}$: SDP relaxation solution of [KBLM07]
2. Perform PCA, get $\bar{x} \in \mathbb{R}^{nK}$
3. Local NLP solver on [KBLM07] with starting point $\bar{x}$

However...

The *Uselessness Theorem*

Thm.

1. The SDP relaxation of [KBLM07] is useless
2. In fact, it is *extremely* useless

1. Part 1: Uselessness
   - *Independent of K:*
     no useful bounds in function of K
2. Part 2: Extreme uselessness
   (a) *For all n, the bound is* $\frac{2n}{n-1}$
   (b) $\exists$ *opt.* X^* *with eigenvalues* $0, \frac{n}{n-1}, \dots, \frac{n}{n-1}$

By 2(b), applying MDS/PCA makes no sense

Proof of extreme uselessness

Strategy:

- Pull a simple matrix solution out of a hat
- Write primal and dual SDP of [KBLM07]
- Show it is feasible in both
- Hence it is optimal
- Analyse solution:
  - all $n-1$ positive eigenvalues are equal
  - its objective function value is $2n/(n-1)$

Primal SDP

$$\boxed{\forall 1 \le i \le j \le n \text{ let } B_{ij} = (1_{ij}) \text{ and } 0 \text{ elsewhere}}$$

quantifier	*natural form*	*standard form*	*dual var*
	$\max \alpha$	$\max \alpha$	
$\forall i \le n$	$X_{ii} = 1$	$E_{ii} \bullet X = 1$	u_i
$\forall i < j \le n$	$X_{ii} + X_{jj} - 2X_{ij} \ge \alpha$	$A_{ij} \bullet X + \alpha \le 0$	w_{ij}
		$A_{ij} = -E_{ii} - E_{jj} + E_{ij} + E_{ji}$	
$\forall i < j \le n$	$X_{ij} \le 1$	$(E_{ij} + E_{ji}) \bullet X \le 2$	y_{ij}
$\forall i < j \le n$	$X_{ij} \ge -1$	$(-E_{ij} - E_{ji}) \bullet X \le 2$	z_{ij}
	$X \succeq 0$	$X \succeq 0$	
	$\alpha \ge 0$	$\alpha \ge 0$	

Dual SDP

$$\min \sum_i u_i + 2\sum_{i<j}(y_{ij} + z_{ij})$$

$$\begin{aligned}\sum_i u_i E_{ii} + \sum_{i<j}\big((y_{ij} - z_{ij})(E_{ij} - E_{ji}) + w_{ij}A_{ij}\big) &\succeq 0\\ \sum_{i<j} w_{ij} &\geq 1\\ w, y, z \geq 0\end{aligned}$$

Simplify $|v| = y + z$, $v = y - z$:

$$\min \sum_i u_i + 2\sum_{i<j}|v_{ij}|$$

$$\begin{aligned}\sum_i u_i E_{ii} + \sum_{i<j}\big(v_{ij}(E_{ij} - E_{ji}) + w_{ij}A_{ij}\big) &\succeq 0\\ \sum_{i<j} w_{ij} &\geq 1\\ w, v \geq 0\end{aligned}$$

Pulling a solution out of a hat

$$
\begin{aligned}
\alpha^* &= \frac{2n}{n-1} \\
X^* &= \frac{n}{n-1} I_n - \frac{1}{n-1} \mathbf{1}_n \\
u^* &= \frac{2}{n-1} \\
w^* &= \frac{1}{n(n-1)} \\
v^* &= 0
\end{aligned}
$$

where $\mathbf{1}_n =$ *all-one* $n \times n$ *matrix*

Solution verification

- linear constraints: *by inspection*
- $X \succeq 0$: *eigenvalues of* X^* *are* $0, \frac{n}{n-1}, \ldots, \frac{n}{n-1}$
- $\sum_i u_i E_{ii} + \sum_{i<j}(v_{ij}(E_{ij} - E_{ji}) + w_{ij} A_{ij}) \succeq 0$:

$$\begin{aligned}
&\sum_i u_i^* E_{ii} + \sum_{i<j} w_{ij}^* A_{ij} \\
=\ & \frac{2}{n-1} \sum_i E_{ii} + \frac{1}{n(n-1)} \sum_{i<j} A_{ij} \\
=\ & \frac{2}{n-1} I_n + \frac{1}{n(n-1)} \big(-(n-1) I_n + (\mathbf{1}_n - I_n) \big) \\
=\ & \frac{1}{n(n-1)} \mathbf{1}_n \succeq 0
\end{aligned}$$

Corollary

$$\lim_{n\to\infty} \mathsf{v}(n, [\text{KBLM07}]) = \lim_{n\to\infty} \frac{2n}{n-1} = 2$$

as observed in computational experiments

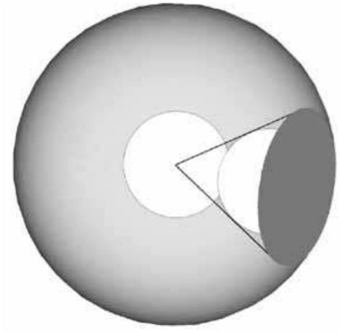
Subsection 3

Gregory's upper bound

Surface upper bound

Gregory 1694, Szpiro 2003

Consider a $\mathsf{kn}(3)$ configuration inscribed into a super-sphere of radius 3. Imagine a lamp at the centre of the central sphere that casts shadows of the surrounding balls onto the inside surface of the super-sphere. Each shadow has a surface area of 7.6; the total surface of the super-ball is 113.1. So $\frac{113.1}{7.6} = 14.9$ is an upper bound to $\mathsf{kn}(3)$.



At end of XVII century, yielded Newton/Gregory dispute

Subsection 4

Delsarte's upper bound

Pair distribution on sphere surface

- Spherical z-code $\mathcal{C}$ has $x_i \cdot x_j \leq z$ $(i < j \leq n = |\mathcal{C}|)$

$$\forall t \in [-1,1] \quad \sigma_t = \frac{1}{n}\Big|\{(i,j) \mid i,j \leq n \wedge x_i \cdot x_j = t\}\Big|$$

- z-code: let $\sigma_t = 0$ for $t \in (z,1)$ *($z = 1/2$ for KNP)*
- $|\mathcal{C}| = n < \infty$: only finitely many $\sigma_t \neq 0$

$$\int_{[-1,1]} \sigma_t dt = \sum_{\substack{t\in[-1,1] \\ \sigma_t \neq 0}} \sigma_t = \frac{1}{n}|\text{all pairs}| = \frac{n^2}{n} \quad = \quad n$$

$$\begin{aligned} \sigma_1 = \frac{1}{n} n \quad &= \quad 1 \\ \forall t \in (z,1) \quad \sigma_t \quad &= \quad 0 \\ \forall t \in [-1,1] \quad \sigma_t \quad &\geq \quad 0 \\ |\{\sigma_t > 0 \mid t \in [-1,1]\}| \quad &< \quad \infty \end{aligned}$$

Growing Delsarte's LP

- Decision variables: σ_t, for $t \in [-1, 1]$
- Objective function:

$$\max |\mathcal{C}| = \max n = \max_{\sigma} \sum_{\substack{t \in [-1,1] \\ \sigma_t \neq 0}} \sigma_t$$

$$= \sigma_1 + \max_{\sigma} \sum_{\substack{t \in [-1,z] \\ \sigma_t \neq 0}} \sigma_t = 1 + \max_{\sigma} \sum_{\substack{t \in [-1,z] \\ \sigma_t \neq 0}} \sigma_t$$

Note n not a parameter in this formulation

- Constraints:

$$\forall t \in [-1, z] \quad \sigma_t \geq 0$$

- LP unbounded! — need more constraints

The general approach

- We need σ to encode the fact that

$$\forall t \in [-1,1] \quad \sigma_t = \frac{1}{n}\left|\{(i,j) \mid i,j \leq n \wedge x_i \cdot x_j = t\}\right|$$

- We use the algebraic theory in [Delsarte et al., "Spherical codes and designs", *Geometriæ Dedicata* 6:363-388, 1977]
- It involves the expression of a non-negative polynomial by means of a linear combination of Gegenbauer polynomials weighted by the σ_t

  I will skip over the details
- You can also see the proof in [Odlyzko, Sloane, "New bounds on the number of unit spheres that can touch a unit sphere in n dimensions", *J. of Comb. Theory A*, 26:210-214, 1979]

Gegenbauer cuts

- Look for function family $\mathscr{F} : [-1,1] \to \mathbb{R}$ s.t.

$$\forall \phi \in \mathscr{F} \qquad \sum_{\substack{t\in[-1,z]\\ \sigma_t\neq 0}} \phi(t)\sigma_t \geq 0$$

- Most popular $\mathscr{F}$: *Gegenbauer polynomials* G_h^K
- Special case $G_h^K = P_h^{\gamma,\gamma}$ of *Jacobi polynomials* (where $\gamma = (K-2)/2$)

$$P_h^{\alpha,\beta}(t) = \frac{1}{2^h}\sum_{i=0}^{h}\binom{h+\alpha}{i}\binom{h+\beta}{h-1}(t+1)^i(t-1)^{h-i}$$

- Matlab knows them: $G_h^K(t) = \texttt{gegenbauerC}(h,(K-2)/2,t)$
- Octave knows them: $G_h^K(t) = \texttt{gsl\_sf\_gegenpoly\_n}(h,\frac{K-2}{2},t)$

  need command `pkg load gsl` *before function call*
- **They encode dependence on K**

Delsarte's LP

- Primal: (given some Gegenbauer polynomial index set H)

$$\left.\begin{array}{rrcl} 1 + \max & \sum\limits_{t\in[-1,\frac{1}{2}]} \sigma_t & & \\ \forall h \in H & \sum\limits_{\substack{t\in[-1,\frac{1}{2}] \\ \sigma_t\neq 0}} G_h^K(t)\sigma_t & \geq & -G_h^K(1) \\ \forall t \in [-1, z] & \sigma_t & \geq & 0. \end{array}\right\} [\text{DelP}]$$

MP syntax error: decision variables σ in sum quantifier!

- Dual:

$$\left.\begin{array}{rrcl} 1 + \min & \sum\limits_{h\in H} (-G_h^K(1))d_h & & \\ \forall t \in [-1, z] & \sum\limits_{h\in H} G_h^K(t)d_h & \geq & 1 \\ \forall h \in H & d_h & \leq & 0. \end{array}\right\} [\text{DelD}]$$

Delsarte's theorem

- [Delsarte *et al.*, 1977; Odlyzko & Sloane, 1979]

> **Theorem**
> *Let* $d_0 > 0$ *and* $F : [-1,1] \to \mathbb{R}$ *such that:*
>
> (i) $\exists H \subseteq (\mathbb{N} \cup \{0\})$ *and* $d \in \mathbb{R}_+^{|H|} \geq 0$
> *s.t.* $F(t) = \sum_{h \in H} d_h G_h^K(t)$
>
> (ii) $\forall t \in [-1, z]\ F(t) \leq 0$
>
> *Then* $\mathsf{kn}_z(K) \leq \frac{F(1)}{d_0}$

- *Proof based on properties of Gegenbauer polynomials*
- Best upper bound: $\min F(1)/d_0 \Rightarrow \min\limits_{d_0=1} F(1) \Rightarrow$ [DelD]
- [DelD] "models" Delsarte's theorem

Delsarte's normalized LP ($G_h^K(1) = 1$)

- Primal:

$$\left.\begin{array}{rrcc} 1 + \max & \displaystyle\sum_{\substack{t \in [-1, \frac{1}{2}] \\ \sigma_t \neq 0}} \sigma_t & & \\ \forall h \in H & \displaystyle\sum_{\substack{t \in [-1, \frac{1}{2}] \\ \sigma_t \neq 0}} G_h^K(t)\sigma_t & \geq & -1 \\ \forall t \in [-1, \frac{1}{2}] & \sigma_t & \geq & 0 \end{array}\right\} \text{[DelP]}$$

- Dual:

$$\left.\begin{array}{rrcc} 1 + \min & \displaystyle\sum_{h \in H} (-1) d_h & & \\ \forall t \in [-1, \frac{1}{2}] & \displaystyle\sum_{h \in H} G_h^K(t) d_h & \geq & 1 \\ \forall h \in H & d_h & \leq & 0 \end{array}\right\} \text{[DelD]}$$

- $d_0 = 1 \Rightarrow$ *remove* 0 *from* H

Focus on normalized [DelD]

Rewrite $-d_h$ as d_h:

$$\left.\begin{array}{rrcl} 1+\min & \displaystyle\sum_{h\in H} d_h & & \\ \forall t\in[-1,\frac{1}{2}] & \displaystyle\sum_{h\in H} G_h^K(t)d_h & \leq & -1 \\ \forall h\in H & d_h & \geq & 0 \end{array}\right\}\text{[DelD]}$$

Issue: *semi-infinite LP* (SILP) (how do we solve it?)

Approximate SILP solution

- *Only keep finitely many constraints*
- Discretize $[-1, 1]$ with a finite $T \subset [-1, 1]$
- *Obtain <u>relaxation</u>* $[\mathrm{DelD}]_T$*:*

$$\mathsf{val}([\mathrm{DelD}]_T) \le \mathsf{val}([\mathrm{DelD}])$$

- **Risk:** $\mathsf{val}([\mathrm{DelD}]_T) < \min F(1)/d_0$
  not a valid upper bound to $\mathsf{kn}_z(K)$
- Happens if soln. of $[\mathrm{DelD}]_T$ infeasible in $[\mathrm{DelD}]$
  i.e. infeasible w.r.t. some of the ∞ly many removed constraints

SILP feasibility

- Given SILP $\bar{S} \equiv \min\{c^\top x \mid \forall t \in \bar{T}\ a^\top(t)x \leq b(t)\}$
- Relax to LP $S \equiv \min\{c^\top x \mid \forall t \in T\ a^\top(t)x \leq b(t)\}$
  with $T \subsetneq \bar{T}$ and $|T| < \infty$
- Solve S, get solution x^*
- Let $\epsilon = \max_t\{a^\top(t)x^* - b(t) \mid t \in \bar{T}\}$
  $\boxed{\textit{continuous optimization w.r.t. single var. } t}$
- If $\epsilon \leq 0$ then x^* feasible in $\bar{S}$
  $\Rightarrow \mathsf{val}(\bar{S}) \leq c^\top x^*$
- If $\epsilon > 0$ refine S and repeat
- Apply to $[\mathrm{DelD}]_T$, get solution d^* feasible in $[\mathrm{DelD}]$

[DelD] feasibility

1. Choose discretization T of $[-1, z]$
2. Solve
$$\left.\begin{array}{rrcl} 1 + \min & \sum\limits_{h \in H} d_h & & \\ \forall t \in T & \sum\limits_{h \in H} G_h^K(t) d_h & \leq & -1 \\ \forall h \in H & d_h & \geq & 0 \end{array}\right\} [\text{DelD}]_T$$
   get solution d^*
3. Solve PP $\quad \epsilon = \max_t \{1 + \sum\limits_{h \in H} G_h^K(t) d_h^* \mid t \in [-1, z]\}$
4. If $\epsilon \leq 0$ then d^* feasible in [DelD]
$$\boxed{\Rightarrow \mathsf{kn}_z(K) \leq 1 + \sum_{h \in H} d_h^*}$$
5. *Else refine T and repeat from Step 2*

Subsection 5

Pfender's upper bound

Pfender's upper bound theorem

Thm.

Let $\mathcal{C}_z = \{x_i \in \mathbb{S}^{K-1} \mid i \le n \wedge \forall j \ne i\ (x_i \cdot x_j \le z)\}$; $c_0 > 0$; $f : [-1,1] \to \mathbb{R}$ s.t.:
(i) $\sum_{i,j \le n} f(x_i \cdot x_j) \ge 0$ (ii) $f(t) + c_0 \le 0$ for $t \in [-1, z]$ (iii) $f(1) + c_0 \le 1$

Then $\mathsf{kn}_z(K) = n \le \frac{1}{c_0}$

([Pfender 2006])

Let $g(t) = f(t) + c_0$

$$
\begin{aligned}
n^2 c_0 &\le n^2 c_0 + \sum_{i,j \le n} f(x_i \cdot x_j) && \text{by (i)} \\
&= \sum_{i,j \le n} (f(x_i \cdot x_j) + c_0) = \sum_{i,j \le n} g(x_i \cdot x_j) \\
&\le \sum_{i \le n} g(x_i \cdot x_i) && \text{since } g(t) \le 0 \text{ for } t \le z \text{ and } x_i \in \mathcal{C}_z \text{ for } i \le n \\
&= n g(1) && \text{since } \|x_i\|_2 = 1 \text{ for } i \le n \\
&\le n && \text{since } g(1) \le 1.
\end{aligned}
$$

Pfender's LP

- Condition (i) of Theorem valid for conic combinations of suitable functions $\mathcal{F}$:

$$f(t) = \sum_{h \in H} c_h f_h(t) \quad \text{for some } c_h \geq 0,$$

  e.g. $\mathcal{F}$ = Gegenbauer polynomials (again)

- Get SILP

$$\left.\begin{array}{rrcll}
\max\limits_{c \in \mathbb{R}^{|H|}} & c_0 & & & \text{(minimize } 1/c_0 \geq n) \\
\forall\, t \in [-1, z] & \sum\limits_{h \in H} c_h G_h^K(t) + c_0 & \leq & 0 & \text{(ii)} \\
& \sum\limits_{h \in H} c_h G_h^K(1) + c_0 & \leq & 1 & \text{(iii)} \\
\forall\, h \in H & c_h & \geq & 0 & \text{(conic comb.)}
\end{array}\right\}$$

- *Discretize $[-1, z]$ by finite T, solve LP, check validity (again)*

Delsarte's and Pfender's theorem compared

- Delsarte & Pfender's theorem look similar:

Delsarte	**Pfender**
(i) $F(t)$ G. poly comb	(i) $f(t)$ G. poly comb
(ii) $\forall t \in [-1, z]$ $F(t) \le 0$	(ii) $\forall t \in [-1, z]$ $f(t) + c_0 \le 0$
	(iii) $f(1) + c_0 \le 1$
$\Rightarrow \mathsf{kn}_z(K) \le \frac{F(1)}{d_0}$	$\Rightarrow \mathsf{kn}_z(K) \le \frac{1}{c_0}$

- **Try setting** $F(t) = f(t) + c_0$**:** condition (ii) is the same
- By condition (iii) in Pfender's theorem

$$\mathsf{kn}_z(K) \le \frac{F(1)}{d_0} = \frac{f(1) + c_0}{c_0} \le \frac{1}{c_0}$$

$\Rightarrow$ *Delsarte bound at least as tight as Pfender's*

- Delsarte (i) $\Rightarrow \int_{[-1,1]} F(t)dt \ge 0 \Rightarrow \int_{[-1,1]} (f(t) + c_0)dt \ge 0$
  Pfender (i) $\Rightarrow \int_{[-1,1]} f(t)dt \ge 0$ more stringent

If $\mathcal{F}$ are Gegenbauer polynomials, Delsarte requires weaker condition and yields tighter bound; but Pfender allows for more general $\mathcal{F}$, can get improved results
see [Pfender, "Improved Delsarte bounds for spherical codes in small dimensions", *J. Comb. Theory A*, 114:1133-1147, 2007]

The final, easy improvement

- However you compute your upper bound B:
- The number of surrounding balls is *integer*
- If $\mathsf{kn}_z(K) \leq B$, then in fact $\mathsf{kn}_z(K) \leq \lfloor B \rfloor$

Outline

Job offers

Optimisation / Operations Senior Manager
VINCI Airports
Rueil-Malmaison, Île-de-France, France
...for the delivery of the various **optimization** projects... to the success of each **optimization** project...

Pricing Data Scientist/Actuary - Price **Optimization** Specialist(H-F)
AXA Global Direct
Région de Paris, France
...**optimization**. The senior price **optimization**... **Optimization** and Innovation team, and will be part...

Growth Data scientist - Product Features Team
Deezer
Paris, FR
OverviewPress play on your next adventure! Music... to join the Product Performance & **Optimization** team... www.deezer.com

Analystes et Consultants - Banque -Optimisation des opérations financières...
Accenture
Région de Paris, France
Nous recherchons des analystes jeunes diplômés et des consultants H/F désireux de travailler sur des problématiques d'optimisation des opérations bancaires (optimisation des modèles opérationnels et des processus) en France et au Benelux. Les postes sont à pourvoir en CDI, sur base d'un rattachement...

Electronic Health Record (EHR) Coordinator (Remote)
Aledade, Inc. - Bethesda, MD
Must have previous implementation or optimization experience with ambulatory EHRs and practice management software, preferably with expertise in Greenway,...

Operations Research Scientist
Ford Motor Company - ★★★★☆ 2,381 reviews - Dearborn, MI
Strong knowledge of optimization techniques (e.g. Develop optimization frameworks to support models related to mobility solution, routing problem, pricing and...

IS&T Controller
Alstom
Saint-Ouen, FR
The Railway industry today is characterized... reviews, software deployment **optimization**, running... jobsearch.alstom.com

Fares Specialist / Spécialiste Optimisation des Tarifs Aériens
Egencia, an Expedia company
Courbevoie - FR
EgenciaChaque année, Egencia accompagne des milliers de sociétés réparties dans plus de 60 pays à mieux gérer leurs programmes de voyage. Nous proposons des solutions modernes et des services d'exception à des millions de voyageurs, de la planification à la finalisation de leur voyage. Nous répondons...

Automotive HMI Software Experts or Software Engineers
Elektrobit (EB)
Paris Area, France
Elektrobit Automotive offers in Paris interesting... performances and **optimization** area, and/or software...

Deployment Engineer, Professional Services, Google Cloud
Google
Paris, France
Note: By applying to this position your... migration, network **optimization**, security best...

Operations Research Scientist
Marriott International, Inc - ★★★★☆ 4,694 reviews - Bethesda, MD 20817
Analyzes data and builds optimization,. Programming models and familiarity with optimization software (CPLEX, Gurobi)....

Research Scientist - AWS New Artificial Intelligence Team!
A Research Scientist - AWS New Artificial Intelligence Team! eviews - Palo Alto, CA
We are pioneers in areas such as recommendation engines, product search, eCommerce fraud detection, and large-scale optimization of fulfillment center...

A typical job offer

Under the responsibility of the Commercial Director, the Optimisation / Operations Senior Manager will have the responsibility to optimise and develop operational aspects for VINCI Airports current and future portfolio of airports. They will also be responsible for driving forward and managing key optimisation projects that assist the Commercial Director in delivering the objectives of the Technical Services Agreements activities of VINCI Airports. The Optimisation Manager will support the Commercial Director in the development and implementation of plans, strategies and reporting processes. As part of the exercise of its function, the Optimisation Manager will undertake the following: Identification and development of cross asset synergies with a specific focus on the operations and processing functions of the airport. Definition and implementation of the Optimisation Strategy in line with the objectives of the various technical services agreements, the strategy of the individual airports and the Group. This function will include: Participation in the definition of airport strategy. Definition of this airport strategy into the Optimisation Strategy. Regularly evaluate the impact of the Optimisation Strategy. Ensure accurate implementation of this strategy at all airports. Management of the various technical services agreements with our airports by developing specific technical competences from the Head Office level. Oversee the management and definition of all optimisation projects. Identification, overview and management of the project managers responsible for the delivery of the various optimization projects at each asset. Construction of good relationships with the key stakeholders, in order to contribute to the success of each optimization project. Development and implementation of the Group optimisation plan. Definition of economic and quality of service criteria, in order to define performance goals. Evaluation of the performance of the Group operations in terms of processing efficiency, service levels, passenger convenience and harmonization of the non-aeronautical activities. Monitoring the strategies, trends and best practices of the airport industry and other reference industries in terms of the applicability to the optimization plan. Study of the needs and preferences of the passengers, through a continuous process of marketing research at all of the airports within the VINCI Airports portfolio. Development of benchmarking studies in order to evaluate the trends, in international airports or in the local market. Development and participation in the expansion or refurbishment projects of the airports, to assure a correct configuration and positioning of the operational and commercial area that can allow the optimization of the revenues and operational efficiency. Support the Director Business Development through the analysis and opportunity assessment of areas of optimization for all target assets in all bids and the preparation and implementation of the strategic plan once the assets are acquired. Maintain up to date knowledge of market trends and key initiatives related to the operational and commercial aspects of international airports [...]

...and blah blah blah: *IS THIS APPROPRIATE FOR MY CV?*

Rationalizing the application process

- You collect many offers
- Don't have time to tailor application to each offer
- Partition offers into groups: clustering
- *Need a similarity relation*
  given two offers, do they describe "similar jobs"?
- Try Natural Language Processing (NatLangProc):
  - *Automated summary*
  - *Relation Extraction*
  - *Named Entity Recognition* (NER)
  - *Keywords*

Automated summary

```
./summarize.py job01.txt
```

```
They will also be responsible for driving forward and managing key
optimisation projects that assist the Commercial Director in delivering
the objectives of the Technical Services Agreements activities of VINCI
Airports. The Optimisation Manager will support the Commercial Director
in the development and implementation of plans, strategies and reporting
processes. Identification and development of cross asset synergies with
a specific focus on the operations and processing functions of the airport.
Construction of good relationships with the key stakeholders, in order to
contribute to the success of each optimization project. Definition of
economic and quality of service criteria, in order to define performance
goals. Evaluation of the performance of the Group operations in terms of
processing efficiency, service levels, passenger convenience and
harmonization of the non-aeronautical activities. Development of
benchmarking studies in order to evaluate the trends, in international
airports or in the local market. Maintain up to date knowledge of market
trends and key initiatives related to the operational and commercial
aspects of international airports. You have a diverse range of
experiences working at or with airports across various disciplines such
as operations, ground handling, commercial, etc. Demonstrated high
level conceptual thinking, creativity and analytical skills.
```

Does it help? hard to say

Relation Extraction

```
./relextr-mitie.py job01.txt
```

```
======= RELATIONS =======
Optimisation Strategy [ INCLUDES_EVENT ] VINCI Airports
Self [ INCLUDES_EVENT ] Head Office
Head Office [ INFLUENCED_BY ] Self
Head Office [ INTERRED_HERE ] Self
VINCI Airports [ INTERRED_HERE ] Optimisation Strategy
Head Office [ INVENTIONS ] Self
Optimisation Strategy [ LOCATIONS ] VINCI Airports
Self [ LOCATIONS ] Head Office
Self [ ORGANIZATIONS_WITH_THIS_SCOPE ] Head Office
Self [ PEOPLE_INVOLVED ] Head Office
Self [ PLACE_OF_DEATH ] Head Office
Head Office [ RELIGION ] Self
VINCI Airports [ RELIGION ] Optimisation Strategy
```

Does it help? hardly

Named Entity Recognition

```
./ner-mitie.py job01.txt
```

```
==== NAMED ENTITIES =====
English MISC
French MISC
Head Office ORGANIZATION
Optimisation / Operations ORGANIZATION
Optimisation Strategy ORGANIZATION
Self PERSON
Technical Services Agreements MISC
VINCI Airports ORGANIZATION
```

Does it help? …maybe

For a document D, let $\mathsf{NER}(D)$ = named entity words

Subsection 1

Clustering on graphs

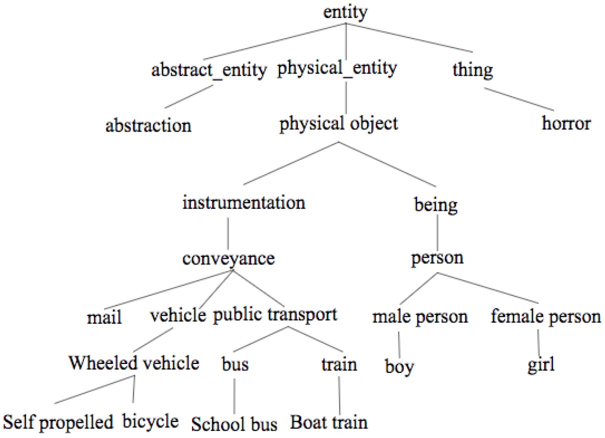
Constructing the graph

1. Recognize named entities from all documents
2. Use them to compute similarities among documents
3. Use modularity clustering

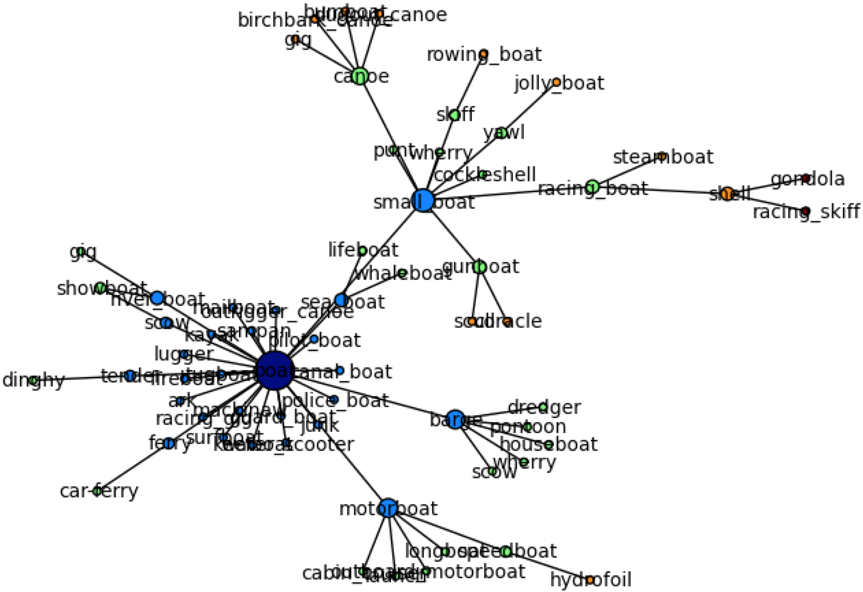
The named entities

1. *Operations Head Airports Office VINCI Technical Self French / Strategy Agreements English Services Optimisation*
2. *Europe and P&C Work Optimization Head He/she of Price Global PhDs Direct Asia Earnix AGD AXA Innovation Coordinate International English*
3. *Scientist Product Analyze Java Features & Statistics Science PHP Pig/Hive/Spark Optimization Crunch/analyze Team Press Performance Deezer Data Computer*
4. *Lean6Sigma Lean-type Office Banking Paris CDI France RPA Middle Accenture English Front Benelux*
5. *Partners Management Monitor BC Provide Support Sites Regions Mtiers Program Performance market develop Finance & IS&T Saint-Ouen Region Control Followings VP Sourcing external Corporate Sector and Alstom Tax Directors Strategic Committee*
6. *Customer Specialist Expedia Service Interact Paris Travel Airline French France Management Egencia English Fares with Company Inc*
7. *Paris Integration France Automation Automotive French . Linux/Genivi HMI UI Software EB Architecture Elektrobit technologies GUIDE Engineers German Technology SW well-structured Experts Tools*
8. *Product Google Managers Python JavaScript AWS JSON BigQuery Java Platform Engineering HTML MySQL Services Professional Googles Ruby Cloud OAuth*
9. *EHR Aledades Provide Wellness Perform ACO Visits EHR-system-specific Coordinator Aledade Medicare Greenway Allscripts*
10. *Global Java EXCEL Research Statistics Mathematics Analyze Smart Teradata & Python Company GDIA Ford Visa SPARK Data Applied Science Work C++ R Unix/Linux Physics Microsoft Operations Monte JAVA Mobility Insight Analytics Engineering Computer Motor SQL Operation Carlo PowerPoint*
11. *Management Java CANDIDATE Application Statistics Gurobi Provides Provider Mathematics Service Maintains Deliver SM&G SAS/HPF SAS Data Science Economics Marriott PROFILE Providers OR Engineering Computer SQL Education*
12. *Alto Statistics Java Sunnyvale Research ML Learning Science Operational Machine Amazon Computer C++ Palo Internet R Seattle*
13. *LLamasoft Work Fortune Chain Supply C# Top Guru What Impactful Team LLamasofts Makes Gartner Gain*
14. *Worldwide Customer Java Mosel Service Python Energy Familiarity CPLEX Research Partnering Amazon R SQL CS Operations*
15. *Operations Science Research Engineering Computer Systems or Build*
16. *Statistics Italy Broad Coins France Australia Python Amazon Germany SAS Appstore Spain Economics Experience R Research US Scientist UK SQL Japan Economist*
17. *Competency Statistics Knowledge Employer communication Research Machine EEO United ORMA Way OFCCP Corporation Mining & C# Python Visual Studio Opportunity Excellent Modeling Data Jacksonville Arena Talent Skills Science Florida Life Equal AnyLogic Facebook CSX Oracle The Strategy Vision Operations Industrial Stream of States Analytics Engineering Computer Framework*

Word similarity: WordNet



WordNet: hyponyms of “boat”



Wu-Palmer word similarity

Semantic WordNet similarity between words w_1, w_2:

$$\mathsf{wup}(w_1, w_2) = \frac{2\,\mathsf{depth}(\mathsf{lca}(w_1, w_2))}{\mathsf{len}(\mathsf{shpath}(w_1, w_2)) + 2\,\mathsf{depth}(\mathsf{lca}(w_1, w_2))}$$

- lca: *lowest common ancestor*

  earliest common word in paths from both words to WordNet root

- depth: *length of path from root to word*

Example: wup(dog, boat)?

```
lca( dog, boat ) = whole; depth( whole ) = 4

18 -> dog -> canine -> carnivore -> placental -> mammal -> vertebrate
   -> chordate -> animal -> organism -> living_thing -> whole -> artifact
   -> instrumentality -> conveyance -> vehicle -> craft -> vessel -> boat

13 -> dog -> domestic_animal -> animal -> organism -> living_thing
   -> whole -> artifact -> instrumentality -> conveyance -> vehicle
   -> craft -> vessel -> boat
```

$$\mathsf{wup}(\text{dog}, \text{boat}) = 8/21 = 0.380952380952$$

Extensions of Wu-Palmer similarity

- to lists of words H, L:

$$\mathsf{wup}(H, L) = \frac{1}{|H|\,|L|} \sum_{v \in H} \sum_{w \in L} \mathsf{wup}(v, w)$$

- to pairs of documents D_1, D_2:

$$\mathsf{wup}(D_1, D_2) = \mathsf{wup}(\mathsf{NER}(D_1), \mathsf{NER}(D_2))$$

- wup and its extensions are always in $[0, 1]$

The Wu-Palmer similarity matrix

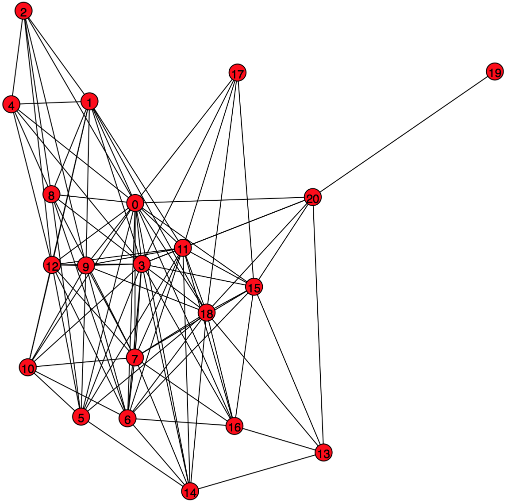
$$\begin{pmatrix}
1.00 & 0.63 & 0.51 & 0.51 & 0.66 & 0.45 & 0.46 & 0.47 & 0.72 & 0.58 & 0.54 & 0.50 & 0.72 & 0.38 & 0.49 & 0.47 & 0.47 & 0.44 & 0.54 & 0.31 & 0.44 \\
0.63 & 1.00 & 0.45 & 0.45 & 0.54 & 0.40 & 0.42 & 0.42 & 0.57 & 0.49 & 0.46 & 0.45 & 0.59 & 0.35 & 0.43 & 0.42 & 0.42 & 0.41 & 0.47 & 0.32 & 0.40 \\
0.51 & 0.45 & 1.00 & 0.40 & 0.53 & 0.35 & 0.37 & 0.37 & 0.58 & 0.47 & 0.43 & 0.40 & 0.59 & 0.28 & 0.39 & 0.37 & 0.38 & 0.35 & 0.43 & 0.24 & 0.35 \\
0.51 & 0.45 & 0.40 & 1.00 & 0.63 & 0.45 & 0.46 & 0.46 & 0.67 & 0.56 & 0.52 & 0.49 & 0.68 & 0.38 & 0.48 & 0.47 & 0.47 & 0.45 & 0.53 & 0.33 & 0.44 \\
0.66 & 0.54 & 0.53 & 0.63 & 1.00 & 0.34 & 0.35 & 0.35 & 0.49 & 0.42 & 0.39 & 0.37 & 0.50 & 0.29 & 0.36 & 0.35 & 0.35 & 0.34 & 0.40 & 0.26 & 0.34 \\
0.45 & 0.40 & 0.35 & 0.45 & 0.34 & 1.00 & 0.42 & 0.43 & 0.66 & 0.54 & 0.49 & 0.45 & 0.67 & 0.34 & 0.44 & 0.43 & 0.43 & 0.40 & 0.49 & 0.28 & 0.40 \\
0.46 & 0.42 & 0.37 & 0.46 & 0.35 & 0.42 & 1.00 & 0.44 & 0.66 & 0.54 & 0.49 & 0.47 & 0.67 & 0.34 & 0.45 & 0.45 & 0.44 & 0.42 & 0.50 & 0.28 & 0.40 \\
0.47 & 0.42 & 0.37 & 0.46 & 0.35 & 0.43 & 0.44 & 1.00 & 0.67 & 0.55 & 0.51 & 0.48 & 0.68 & 0.36 & 0.47 & 0.45 & 0.45 & 0.43 & 0.51 & 0.30 & 0.42 \\
0.72 & 0.57 & 0.58 & 0.67 & 0.49 & 0.66 & 0.66 & 0.67 & 1.00 & 0.33 & 0.31 & 0.29 & 0.40 & 0.23 & 0.28 & 0.27 & 0.28 & 0.26 & 0.31 & 0.21 & 0.26 \\
0.58 & 0.49 & 0.47 & 0.56 & 0.42 & 0.54 & 0.54 & 0.55 & 0.33 & 1.00 & 0.46 & 0.43 & 0.59 & 0.34 & 0.42 & 0.41 & 0.41 & 0.39 & 0.46 & 0.31 & 0.39 \\
0.54 & 0.46 & 0.43 & 0.52 & 0.39 & 0.49 & 0.49 & 0.51 & 0.31 & 0.46 & 1.00 & 0.39 & 0.56 & 0.29 & 0.38 & 0.36 & 0.36 & 0.34 & 0.41 & 0.24 & 0.35 \\
0.50 & 0.45 & 0.40 & 0.49 & 0.37 & 0.45 & 0.47 & 0.48 & 0.29 & 0.43 & 0.39 & 1.00 & 0.70 & 0.40 & 0.50 & 0.49 & 0.48 & 0.46 & 0.54 & 0.35 & 0.46 \\
0.72 & 0.59 & 0.59 & 0.68 & 0.50 & 0.67 & 0.67 & 0.68 & 0.40 & 0.59 & 0.56 & 0.70 & 1.00 & 0.23 & 0.29 & 0.29 & 0.29 & 0.28 & 0.33 & 0.20 & 0.27 \\
0.38 & 0.35 & 0.28 & 0.38 & 0.29 & 0.34 & 0.34 & 0.36 & 0.23 & 0.34 & 0.29 & 0.40 & 0.23 & 1.00 & 0.48 & 0.45 & 0.46 & 0.42 & 0.52 & 0.30 & 0.43 \\
0.49 & 0.43 & 0.39 & 0.48 & 0.36 & 0.44 & 0.45 & 0.47 & 0.28 & 0.42 & 0.38 & 0.50 & 0.29 & 0.48 & 1.00 & 0.39 & 0.39 & 0.36 & 0.45 & 0.26 & 0.37 \\
0.47 & 0.42 & 0.37 & 0.47 & 0.35 & 0.43 & 0.45 & 0.45 & 0.27 & 0.41 & 0.36 & 0.49 & 0.29 & 0.45 & 0.39 & 1.00 & 0.48 & 0.46 & 0.54 & 0.33 & 0.44 \\
0.47 & 0.42 & 0.38 & 0.47 & 0.35 & 0.43 & 0.44 & 0.45 & 0.28 & 0.41 & 0.36 & 0.48 & 0.29 & 0.46 & 0.39 & 0.48 & 1.00 & 0.43 & 0.51 & 0.32 & 0.43 \\
0.44 & 0.41 & 0.35 & 0.45 & 0.34 & 0.40 & 0.42 & 0.43 & 0.26 & 0.39 & 0.34 & 0.46 & 0.28 & 0.42 & 0.36 & 0.46 & 0.43 & 1.00 & 0.53 & 0.31 & 0.43 \\
0.54 & 0.47 & 0.43 & 0.53 & 0.40 & 0.49 & 0.50 & 0.51 & 0.31 & 0.46 & 0.41 & 0.54 & 0.33 & 0.52 & 0.45 & 0.54 & 0.51 & 0.53 & 1.00 & 0.36 & 0.46 \\
0.31 & 0.32 & 0.24 & 0.33 & 0.26 & 0.28 & 0.28 & 0.30 & 0.21 & 0.31 & 0.24 & 0.35 & 0.20 & 0.30 & 0.26 & 0.33 & 0.32 & 0.31 & 0.36 & 1.00 & 0.47 \\
0.44 & 0.40 & 0.35 & 0.44 & 0.34 & 0.40 & 0.40 & 0.42 & 0.26 & 0.39 & 0.35 & 0.46 & 0.27 & 0.43 & 0.37 & 0.44 & 0.43 & 0.43 & 0.46 & 0.47 & 1.00
\end{pmatrix}$$

The Wu-Palmer similarity matrix

Too uniform! Try zeroing values below median

$$
\left(\begin{array}{ccccccccccccccccccccc}
1.00 & 0.63 & 0.51 & 0.51 & 0.66 & 0.45 & 0.46 & 0.47 & 0.72 & 0.58 & 0.54 & 0.50 & 0.72 & 0.00 & 0.49 & 0.47 & 0.47 & 0.44 & 0.54 & 0.00 & 0.44 \\
0.63 & 1.00 & 0.45 & 0.45 & 0.54 & 0.00 & 0.00 & 0.00 & 0.57 & 0.49 & 0.46 & 0.45 & 0.59 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.47 & 0.00 & 0.00 \\
0.51 & 0.45 & 1.00 & 0.00 & 0.53 & 0.00 & 0.00 & 0.00 & 0.58 & 0.47 & 0.00 & 0.00 & 0.59 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.51 & 0.45 & 0.00 & 1.00 & 0.63 & 0.45 & 0.46 & 0.46 & 0.67 & 0.56 & 0.52 & 0.49 & 0.68 & 0.00 & 0.48 & 0.47 & 0.47 & 0.45 & 0.53 & 0.00 & 0.44 \\
0.66 & 0.54 & 0.53 & 0.63 & 1.00 & 0.00 & 0.00 & 0.00 & 0.49 & 0.00 & 0.00 & 0.00 & 0.50 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.45 & 0.00 & 0.00 & 0.45 & 0.00 & 1.00 & 0.00 & 0.00 & 0.66 & 0.54 & 0.49 & 0.45 & 0.67 & 0.00 & 0.44 & 0.00 & 0.00 & 0.00 & 0.49 & 0.00 & 0.00 \\
0.46 & 0.00 & 0.00 & 0.46 & 0.00 & 0.00 & 1.00 & 0.44 & 0.66 & 0.54 & 0.49 & 0.47 & 0.67 & 0.00 & 0.45 & 0.45 & 0.44 & 0.00 & 0.50 & 0.00 & 0.00 \\
0.47 & 0.00 & 0.00 & 0.46 & 0.00 & 0.00 & 0.44 & 1.00 & 0.67 & 0.55 & 0.51 & 0.48 & 0.68 & 0.00 & 0.47 & 0.45 & 0.45 & 0.00 & 0.51 & 0.00 & 0.00 \\
0.72 & 0.57 & 0.58 & 0.67 & 0.49 & 0.66 & 0.66 & 0.67 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.58 & 0.49 & 0.47 & 0.56 & 0.00 & 0.54 & 0.54 & 0.55 & 0.00 & 1.00 & 0.46 & 0.43 & 0.59 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.46 & 0.00 & 0.00 \\
0.54 & 0.46 & 0.00 & 0.52 & 0.00 & 0.49 & 0.49 & 0.51 & 0.00 & 0.46 & 1.00 & 0.00 & 0.56 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.50 & 0.45 & 0.00 & 0.49 & 0.00 & 0.45 & 0.47 & 0.48 & 0.00 & 0.43 & 0.00 & 1.00 & 0.70 & 0.00 & 0.50 & 0.49 & 0.48 & 0.46 & 0.54 & 0.00 & 0.46 \\
0.72 & 0.59 & 0.59 & 0.68 & 0.50 & 0.67 & 0.67 & 0.68 & 0.00 & 0.59 & 0.56 & 0.70 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 & 0.48 & 0.45 & 0.46 & 0.00 & 0.52 & 0.00 & 0.43 \\
0.49 & 0.00 & 0.00 & 0.48 & 0.00 & 0.44 & 0.45 & 0.47 & 0.00 & 0.00 & 0.00 & 0.50 & 0.00 & 0.48 & 1.00 & 0.00 & 0.00 & 0.00 & 0.45 & 0.00 & 0.00 \\
0.47 & 0.00 & 0.00 & 0.47 & 0.00 & 0.00 & 0.45 & 0.45 & 0.00 & 0.00 & 0.00 & 0.49 & 0.00 & 0.45 & 0.00 & 1.00 & 0.48 & 0.46 & 0.54 & 0.00 & 0.44 \\
0.47 & 0.00 & 0.00 & 0.47 & 0.00 & 0.00 & 0.44 & 0.45 & 0.00 & 0.00 & 0.00 & 0.48 & 0.00 & 0.46 & 0.00 & 0.48 & 1.00 & 0.00 & 0.51 & 0.00 & 0.00 \\
0.44 & 0.00 & 0.00 & 0.45 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.46 & 0.00 & 0.00 & 0.00 & 0.46 & 0.00 & 1.00 & 0.53 & 0.00 & 0.00 \\
0.54 & 0.47 & 0.00 & 0.53 & 0.00 & 0.49 & 0.50 & 0.51 & 0.00 & 0.46 & 0.00 & 0.54 & 0.00 & 0.52 & 0.45 & 0.54 & 0.51 & 0.53 & 1.00 & 0.00 & 0.46 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 & 0.47 \\
0.44 & 0.00 & 0.00 & 0.44 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.46 & 0.00 & 0.43 & 0.00 & 0.44 & 0.00 & 0.00 & 0.46 & 0.47 & 1.00
\end{array}\right)
$$

The similarity graph



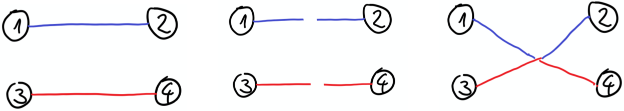
$G = (V, E)$, weighted adjacency matrix A

Modularity clustering

"Modularity is the fraction of the edges that fall within a cluster minus the expected fraction if edges were distributed at random."

- *"at random"* = random graphs over same degree sequence
- *degree sequence* = $(k_1, \ldots, k_n)$ where $k_i = |N(i)|$
- *"expected"* = over all possible "half-edge" recombinations

  degree sequence invariant operation



- expected edges between u, v: $k_u k_v/(2m)$ where $m = |E|$
- $\mathsf{mod}(u, v) = \frac{1}{2m}(A_{uv} - k_u k_v/(2m))$ `param`
- $\mathsf{mod}(G) = \sum_{\{u,v\}\in E} \mathsf{mod}(u, v) x_{uv}$

  $x_{uv} = 1$ if u, v in the same cluster and 0 otherwise `var`
- *"Natural extension" to weighted graphs:* $k_u = \sum_v A_{uv}$, $m = \sum_{uv} A_{uv}$

Use modularity to define clustering

- What is the "best clustering"?
- *Maximize discrepancy between actual and expected*
  "as far away as possible from average"

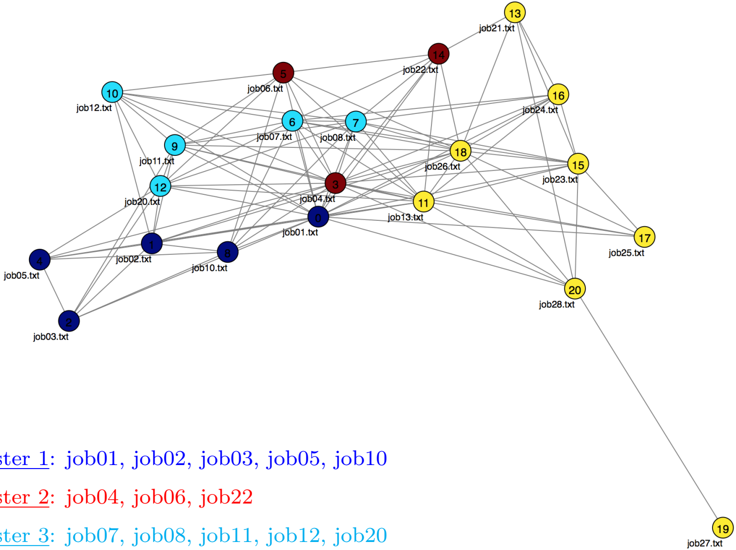
$$\left.\begin{array}{rl} \max & \sum_{\{u,v\}\in E} \mathsf{mod}(u,v)x_{uv} \\ \forall u \in V, v \in V & x_{uv} \in \{0,1\} \end{array}\right\}$$

- Issue: optimum could be intransitive
- Idea: *treat clusters as cliques (even if zero weight)*
  $\Rightarrow$ *clique partitioning constraints for transitivity*

$$\begin{array}{rrcl} \forall i<j<k & x_{ij}+x_{jk}-x_{ik} & \le & 1 \\ \forall i<j<k & x_{ij}-x_{jk}+x_{ik} & \le & 1 \\ \forall i<j<k & -x_{ij}+x_{jk}+x_{ik} & \le & 1 \end{array}$$

if $i,j \in C$ and $j,k \in C$ then $i,k \in C$

The resulting clustering



cluster 1: job01, job02, job03, job05, job10

cluster 2: job04, job06, job22

cluster 3: job07, job08, job11, job12, job20

cluster 4: job13, job21, job23, job24, job25, job26, job27, job28

Is it good?

Vinci	Accenture	Elektrobit	Amazon 1-3
Axa	Expedia	Google	CSX
Deezer	fragment1	Ford	Westrock
Alstom		Marriott	Mitre
Aledade		Llamasoft	Clarity
			fragment2

- ? — *named entities rarely appear in WordNet*
- Desirable property: *chooses number of clusters*

Subsection 2

Clustering in Euclidean spaces

Clustering vectors

Most frequent words $\boxed{w}$ *over collection* $\boxed{C}$ *of documents* $\boxed{d}$

`./keywords.py`

```
global environment customers strategic processes teams sql job industry use
java developing project process engineering field models opportunity drive
results statistical based operational performance using mathematical computer
new technical highly market company science role dynamic background products
level methods design looking modeling manage learning service customer
effectively technology requirements build mathematics problems plan services
time scientist implementation large analytical techniques lead available plus
technologies sas provide machine product functions organization algorithms
position model order identify activities innovation key appropriate different
complex best decision simulation strategy meet client assist quantitative
finance commercial language mining travel chain amazon pricing practices
cloud supply
```

$$
\begin{aligned}
\mathsf{tfidf}_C(w,d) &= \frac{|(t \in d \mid t = w)|\,|C|}{|\{h \in C \mid w \in h\}|} \\
\mathsf{keyword}_C(i,d) &= \textit{word } w \textit{ having } i^{th} \textit{ best } \mathsf{tfidf}_C(w,d) \textit{value} \\
\mathsf{vec}_C^m(d) &= (\mathsf{tfidf}_C(\mathsf{keyword}_C(i,d),d) \mid i \le m)
\end{aligned}
$$

Transforms documents to vectors

tfidf: text frequency inverse document frequency

Minimum sum-of-squares clustering

- MSSC, a.k.a. the *k-means problem*
- Given points $p_1, \ldots, p_n \in \mathbb{R}^m$, find clusters $C_1, \ldots, C_k$

$$\min \sum_{j \le k} \sum_{i \in C_j} \| p_i - \mathsf{centroid}(C_j) \|_2^2$$

where $\mathsf{centroid}(C_j) = \frac{1}{|C_j|} \sum_{i \in C_j} p_i$

- k-means alg.: given initial clustering $C_1, \ldots, C_k$

1: $\forall j \le k$ compute $y_j = \mathsf{centroid}(C_j)$
2: $\forall i \le n, j \le k$ if y_j is the closest centr. to p_i let $x_{ij} = 1$ else 0
3: $\forall j \le k$ update $C_j \leftarrow \{p_i \mid x_{ij} = 1 \wedge i \le n\}$
4: repeat until stability

k-means with $k = 2$

Vinci	AXA
Deezer	Alstom
Accenture	Elektrobit
Expedia	Ford
Google	Marriott
Aledade	Amazon 1-3
Llamasoft	CSX
	WestRock
	MITRE
	Clarity
	fragments 1-2

k-means with $k = 2$: *another run*

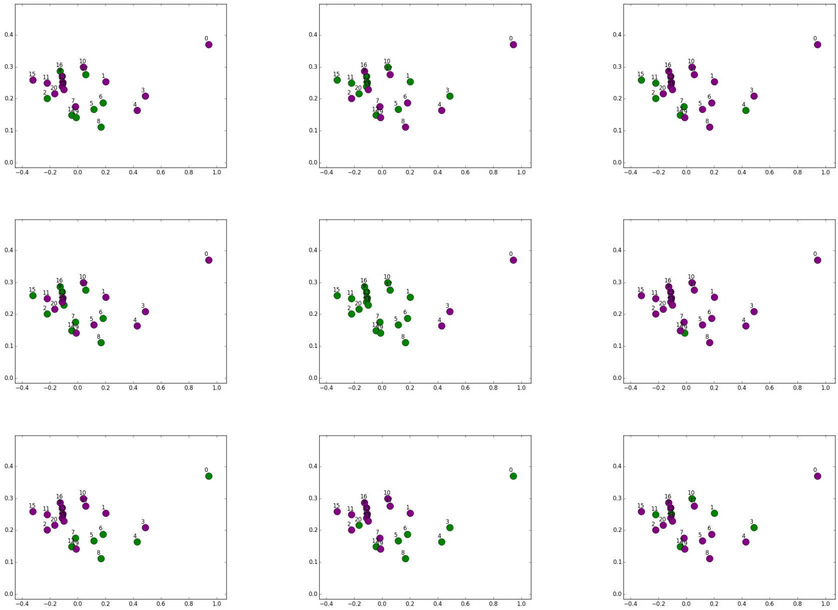
Deezer	Vinci
Elektrobit	AXA
Google	Accenture
Aledade	Alstom
	Expedia
	Ford
	Marriott
	Llamasoft
	Amazon 1-3
	CSX
	WestRock
	MITRE
	Clarity
	fragments 1-2

k-means with $k = 2$: *third run!*

AXA	Vinci
Deezer	Accenture
Expedia	Alstom
Ford	Elektrobit
Marriott	Google
Llamasoft	Aledade
Amazon 1-3	
CSX	
WestRock	
MITRE	
Clarity	
fragments 1-2	

A fickle algorithm

We can't trust k-means: why?



Subsection 3

Distance instability

Nearest Neighbours

k-NEAREST NEIGHBOURS (k-NN).

Given:

- $k \in \mathbb{N}$
- *a distance function* $d : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}_+$
- *a set* $\mathcal{X} \subset \mathbb{R}^n$
- *a point* $z \in \mathbb{R}^n \setminus \mathcal{X}$,

find the subset $\mathcal{Y} \subset \mathcal{X}$ *such that:*

(a) $|\mathcal{Y}| = k$

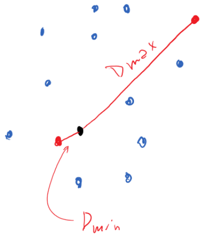
(b) $\forall y \in \mathcal{Y}, x \in \mathcal{X} \quad (d(z, y) \leq d(z, x))$

- basic problem in data science
- pattern recognition, computational geometry, machine learning, data compression, robotics, recommender systems, information retrieval, natural language processing and more
- Example: Used in Step 2 of k-means:

  assign points to closest centroid

[Cover & Hart 1967]

With random variables



- Consider 1-NN
- Let $\ell = |\mathcal{X}|$
- Distance function family $\{d^m : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}_+\}_m$
- For each m:
  - random variable Z^m with some distribution over $\mathbb{R}^n$
  - for $i \leq \ell$, random variable X_i^m with some distrib. over $\mathbb{R}^n$
  - X_i^m iid w.r.t. i, Z^m independent of all X_i^m
  - $D_{\min}^m = \min\limits_{i \leq \ell} d^m(Z^m, X_i^m)$
  - $D_{\max}^m = \max\limits_{i \leq \ell} d^m(Z^m, X_i^m)$

Distance Instability Theorem

- Let $p > 0$ be a constant
- If

$$\exists i \leq \ell \quad (d^m(Z^m, X_i^m))^p \textit{ converges as } m \to \infty$$

then, for any $\varepsilon > 0$,

closest and furthest point are at about the same distance

Note "$\exists i$" suffices since $\forall m$ we have X_i^m iid w.r.t. i

[Beyer et al. 1999]

Distance Instability Theorem

- Let $p > 0$ be a constant
- If

$$\forall i \le \ell \lim_{m\to\infty} \mathsf{Var}\left(\frac{(d^m(Z^m, X_i^m))^p}{\mathbb{E}((d^m(Z^m, X_i^m))^p)}\right) = 0$$

then, for any $\varepsilon > 0$,

$$\lim_{m\to\infty} \mathbb{P}(D^m_{\max} \le (1+\varepsilon) D^m_{\min}) = 1$$

Note "$\exists i$" suffices since $\forall m$ we have X_i^m iid w.r.t. i

[Beyer et al. 1999]

Preliminary results

- *Lemma*. $\{B^m\}_m$ seq. of rnd. vars with finite variance and $\lim_{m\to\infty} \mathbb{E}(B^m) = b \wedge \lim_{m\to\infty} \mathsf{Var}(B^m) = 0$; then

  $$\forall \varepsilon > 0 \ \lim_{m\to\infty} \mathbb{P}(\|B^m - b\| \leq \varepsilon) = 1$$

  $\boxed{\text{denoted } B^m \to_{\mathbb{P}} b}$

- *Slutsky's theorem*. $\{B^m\}_m$ seq. of rnd. vars and g a continuous function; if $B^m \to_{\mathbb{P}} b$ and $g(b)$ exists, then $g(B^m) \to_{\mathbb{P}} g(b)$

- *Corollary*. If $\{A^m\}_m, \{B^m\}_m$ seq. of rnd. vars. s.t. $A^m \to_{\mathbb{P}} a$ and $B^m \to_{\mathbb{P}} b \neq 0$ then $\frac{A^m}{B^m} \to_{\mathbb{P}} \frac{a}{b}$

Proof

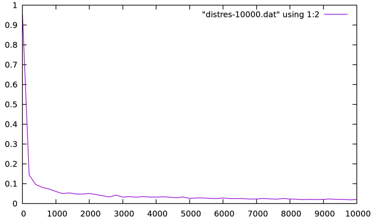
1. $\mu_m = \mathbb{E}((d^m(Z^m, X_i^m))^p)$ independent of i
   (since all X_i^m iid)
2. $V_m = \frac{(d^m(Z^m, X_i^m))^p}{\mu_m} \to_{\mathbb{P}} 1$:
   - $\mathbb{E}(V_m) = 1$ (rnd. var. over mean) $\Rightarrow \lim_m \mathbb{E}(V_m) = 1$
   - Hypothesis of thm. $\Rightarrow \lim_m \mathsf{Var}(V_m) = 0$
   - *Lemma* $\Rightarrow V_m \to_{\mathbb{P}} 1$
3. $\mathbf{V}^m = (V_m \mid i \leq \ell) \to_{\mathbb{P}} \mathbf{1}$ (by iid)
4. *Slutsky's thm.* $\Rightarrow \min(\mathbf{V}^m) \to_{\mathbb{P}} \min(\mathbf{1}) = 1$
   simy for max
5. *Corollary* $\Rightarrow \frac{\max(\mathbf{V}^m)}{\min(\mathbf{V}^m)} \to_{\mathbb{P}} 1$
6. $\frac{D^m_{\max}}{D^m_{\min}} = \frac{\mu_m \max(\mathbf{V}^m)}{\mu_m \min(\mathbf{V}^m)} \to_{\mathbb{P}} 1$
7. Result follows (defn. of $\to_{\mathbb{P}}$ and $D^m_{\max} \geq D^m_{\min}$)

A precision limit

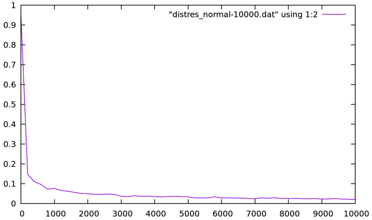
- Closest and farthest point from z:
  can't be told apart with precision $> \varepsilon$
- In real algorithms, often want "closest"
- Hope of telling apart closest from second-closest?

Loss of precision ε for $K \leq 10000$

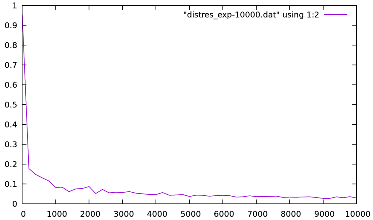
Uniform$(0, 1)$



Normal$(0, 1)$



Exponential(1)



- Precision falls exponentially fast
- Generates algorithmic instability

When it applies

- iid random variables from any distribution
- Particular forms of correlation
  e.g. $U_i \sim \mathsf{Uniform}(0, \sqrt{i})$, $X_1 = U_1$, $X_i = U_i + (X_{i-1}/2)$ for $i > 1$
- Variance tending to zero
  e.g. $X_i \sim \mathsf{N}(0, 1/i)$
- Discrete uniform distribution on m-dimensional hypercube
  for both data and query
- Computational experiments with k-means:
  instability already with $n > 15$

. . . and when it doesn't

- Complete linear dependence on all distributions
  can be reduced to NN in 1D
- Exact and approximate matching
  query point = (or ≈) data point
- Query point in a well-separated cluster in data
- Implicitly low dimensionality
  project; but NN must be stable in lower dim.

Subsection 4

MP formulations

Why?

- With k-means being so fast, why bother with MP?
- Principle:
  changing an MP is easier than changing an algorithm
- Side constraints
  e.g. clusters are spheres, or other shapes
- Clustering subproblems
  e.g. assign resources subject to optimal clustering
- MP delivers a bound
  "can't do better than bound" guarantee

MP formulation

$$\left.\begin{array}{rrcl}
\min\limits_{x,y,s} & \sum\limits_{i\le n}\sum\limits_{j\le k}\|p_i - y_j\|_2^2\, x_{ij} & & \\
\forall j\le k & \frac{1}{s_j}\sum\limits_{i\le n} p_i x_{ij} & = & y_j \\
\forall i\le n & \sum\limits_{j\le k} x_{ij} & = & 1 \\
\forall j\le k & \sum\limits_{i\le n} x_{ij} & = & s_j \\
\forall j\le k & y_j & \in & \mathbb{R}^m \\
 & x & \in & \{0,1\}^{nk} \\
 & s & \in & \mathbb{N}^k
\end{array}\right\} \quad \text{(MSSC)}$$

MINLP: nonconvex terms; continuous, binary and integer variables

Reformulation

The (MSSC) formulation has the same optima as:

$$\left.\begin{array}{rrcl}
\min\limits_{x,y,P} & \sum\limits_{i\le n}\sum\limits_{j\le k} P_{ij}\, x_{ij} & & \\
\forall i\le n, j\le k & \|p_i - y_j\|_2^2 & \le & P_{ij} \\
\forall j\le k & \sum\limits_{i\le n} p_i x_{ij} & = & \sum\limits_{i\le n} y_j x_{ij} \\
\forall i\le n & \sum\limits_{j\le k} x_{ij} & = & 1 \\
\forall j\le k & y_j & \in & ([\min\limits_{i\le n} p_{ih}, \max\limits_{i\le n} p_{ih}] \mid h\le k) \\
 & x & \in & \{0,1\}^{nk} \\
 & P & \in & [0, P^U]^{nk}
\end{array}\right\}$$

- The only nonconvexities are *products of binary by continuous* *__bounded__* *variables*

Products of binary and continuous vars.

- Suppose term xy appears in a formulation
- Assume $x \in \{0, 1\}$ and $\boxed{y \in [0, 1]}$ is bounded
- means "either $z = 0$ or $z = y$"
- *Replace xy by a new variable z*
- Adjoin the following constraints:

$$\begin{array}{rcl} & z \in & [0,1] \\ y-(1-x) \leq & z & \leq y+(1-x) \\ -x \leq & z & \leq x \end{array}$$

- $\Rightarrow$ Everything's linear now!

[Fortet 1959]

Products of binary and continuous vars.

- Suppose term xy appears in a formulation
- Assume $x \in \{0,1\}$ and $\boxed{y \in [y^L, y^U]}$ is <u>bounded</u>
- means "either $z = 0$ or $z = y$"
- *Replace xy by a new variable z*
- Adjoin the following constraints:

$$
\begin{aligned}
z &\in [\min(y^L, 0), \max(y^U, 0)] \\
y - (1-x)\max(|y^L|, |y^U|) \leq\ z &\leq y + (1-x)\max(|y^L|, |y^U|) \\
-x\max(|y^L|, |y^U|) \leq\ z &\leq x\max(|y^L|, |y^U|)
\end{aligned}
$$

- $\Rightarrow$ Everything's linear now!

[L. et al. 2009]

MSSC is a convex MINLP

$$
\begin{array}{rrcll}
 & \min\limits_{x,y,P,\chi,\xi} \sum\limits_{i\le n}\sum\limits_{j\le k} & \chi_{ij} & & \\
\forall i\le n, j\le k & 0 \le & \chi_{ij} & \le P_{ij} & \\
\forall i\le n, j\le k & P_{ij}-(1-x_{ij})P^U \le & \chi_{ij} & \le x_{ij}P^U & \\
\forall i\le n, j\le k & \|p_i-y_j\|_2^2 & \le & P_{ij} & \boxed{\Leftarrow \ \textbf{convex}} \\
\forall j\le k & \sum\limits_{i\le n} p_i x_{ij} & = & \sum\limits_{i\le n}\xi_{ij} & \\
\forall i\le n, j\le k & y_j-(1-x_{ij})\max(|y^L|,|y^U|) \le & \xi_{ij} & \le y_j+(1-x_{ij})\max(|y^L|,|y^U|) & \\
\forall i\le n, j\le k & -x_{ij}\max(|y^L|,|y^U|) \le & \xi_{ij} & \le x_{ij}\max(|y^L|,|y^U|) & \\
\forall i\le n & \sum\limits_{j\le k} x_{ij} & = & 1 & \\
\forall j\le k & y_j & \in & [y^L,y^U] & \\
 & x & \in & \{0,1\}^{nk} & \\
 & P & \in & [0,P^U]^{nk} & \\
 & \chi & \in & [0,P^U]^{nk} & \\
\forall i\le n, j\le k & \xi_{ij} & \in & [\min(y^L,0),\max(y^U,0)] &
\end{array}
$$

y_j, ξ_{ij}, y^L, y^U are vectors in $\mathbb{R}^m$

How to solve it

- cMINLP is **NP**-hard
- Algorithms:
  - *Outer Approximation* (OA)
  - *Branch-and-Bound* (BB)
- Best (open source) solver: BONMIN
- Another good (commercial) solver: KNITRO
- *With $k = 2$, unfortunately…*

  ```
  Cbc0010I After 8300 nodes, 3546 on tree, 14.864345 best solution,
    best possible 6.1855969 (32142.17 seconds)
  ```
- *Interesting feature: the bound*

  guarantees we can't do better than *bound*

  all BB algorithms provide it

Bonmin

Alstom	Vinci
Elektrobit	AXA
Ford	Deezer
Llamasoft	Accenture
Amazon 2	Expedia
CSX	Google
MITRE	Aledade
Clarity	Marriott
fragment 2	Amazon 1 & 3
	WestRock
	fragment 1

Couple of things left to try

- Approximate ℓ_2 by ℓ_1 norm
  ℓ_1 is a linearizable norm
- Randomly project the data
  lose dimensions but keep approximate shape

Linearizing convexity

- Replace $\|p_i - y_j\|_2^2$ by $\|p_i - y_j\|_1$
- Warning: optima will change

  but still within "clustering by distance" principle

$$\forall i \le n, j \le k \quad \|p_i - y_j\|_1 = \sum_{a \le d} |p_{ia} - y_{ja}|$$

- Replace each $|\cdot|$ term by new vars. $Q_{ija} \in [0, P^U]$

  Adjust P^U in terms of $\|\cdot\|_1$

- Adjoin constraints

$$\begin{aligned} \forall i \le n, j \le k \quad \sum_{a \le d} Q_{ija} &\le P_{ij} \\ \forall i \le n, j \le k, a \le d \quad -Q_{ija} &\le p_{ia} - y_{ja} \le Q_{ija} \end{aligned}$$

- Obtain a MILP

  Most advanced MILP solver: CPLEX

CPLEX

objective 112.24, bound 39.92, in 44.74s

AXA	Vinci
Deezer	Accenture
Ford	Alstom
Marriott	Expedia
Amazon 1-3	Elektrobit
Llamasoft	Google
CSX	Aledade
WestRock	
MITRE	
Clarity	
fragments 1-2	

Interrupted after 281s with bound 59.68

Subsection 5

Random projections again

Works on the MSSC MP formulation too!

$$\left.\begin{array}{rrcl}
\min\limits_{x,y,s} & \sum\limits_{i\le n}\sum\limits_{j\le d}\|Tp_i - Ty_j\|_2^2\, x_{ij} & & \\
\forall j \le d & \frac{1}{s_j}\sum\limits_{i\le n} Tp_i x_{ij} & = & Ty_j \\
\forall i \le n & \sum\limits_{j\le d} x_{ij} & = & 1 \\
\forall j \le d & \sum\limits_{i\le n} x_{ij} & = & s_j \\
\forall j \le d & y_j & \in & \mathbb{R}^m \\
 & x & \in & \{0,1\}^{nd} \\
 & s & \in & \mathbb{N}^d
\end{array}\right\}$$

where T *is a* $k \times m$ *random projector*

replace Ty by y'

Works on the MSSC MP formulation too!

$$
\left.
\begin{array}{lrcl}
\min\limits_{x,y',s} & \sum\limits_{i\le n}\sum\limits_{j\le d} \|Tp_i - y'_j\|_2^2\, x_{ij} & & \\
\forall j \le d & \frac{1}{s_j}\sum\limits_{i\le n} Tp_i x_{ij} & = & y'_j \\
\forall i \le n & \sum\limits_{j\le d} x_{ij} & = & 1 \\
\forall j \le d & \sum\limits_{i\le n} x_{ij} & = & s_j \\
\forall j \le d & y'_j & \in & \mathbb{R}^k \\
 & x & \in & \{0,1\}^{nd} \\
 & s & \in & \mathbb{N}^d
\end{array}
\right\} \quad (\text{MSSC}')
$$

- *where* $k = O(\frac{1}{\varepsilon^2}\ln n)$
- less data, $|y'| < |y| \Rightarrow$ get solutions faster
- Yields smaller cMINLP

BONMIN on randomly proj. data

objective 5.07, bound 0.48, stopped at 180s

Deezer	Vinci
Ford	AXA
Amazon 1-3	Accenture
CSX	Alstom
MITRE	Expedia
fragment 1	Elektrobit
	Google
	Aledade
	Marriott
	Llamasoft
	WestRock
	Clarity
	fragment 2

CPLEX on randomly proj. data

. . . although it doesn't make much sense for $\|\cdot\|_1$ norm. . .

objective 53.19, bound 20.68, stopped at 180s

Vinci	AXA
Deezer	Accenture
Expedia	Alstom
Google	Elektrobit
Aledade	Marriott
Ford	Llamasoft
Amazon 1-3	WestRock
CSX	MITRE
Clarity	fragment 1-2

Many clusterings?

Compare them with clustering measures
e.g. "adjusted mutual information score"

	bonmRP	bonmin	cplxRP	cplex	kmea1	kmea2	kmea3	modul
bonminRP	1.000	0.170	0.095	0.333	0.333	0.316	0.315	0.346
bonmin	0.170	1.000	0.021	0.079	0.179	0.179	0.086	0.178
cplexRP	0.095	0.021	1.000	0.044	0.095	0.185	0.069	0.055
cplex	0.333	0.079	0.044	1.000	0.317	0.316	0.775	0.271
kmeans2-1	0.333	0.179	0.095	0.317	1.000	0.316	0.249	0.271
kmeans2-2	0.316	0.179	0.185	0.316	0.316	1.000	0.381	0.286
kmeans2-3	0.315	0.086	0.069	0.775	0.249	0.381	1.000	0.252
modularity	0.346	0.178	0.055	0.271	0.271	0.286	0.252	1.000

THE END