Weighted word collector

Jérémie du Boisberranger* Danièle Gardy* Yann Ponty•

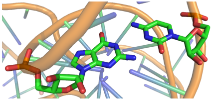
* PRiSM, CNRS/Université de Versailles, France

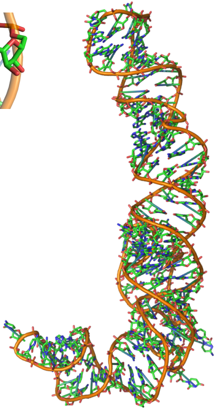
• LIX, CNRS/Ecole Polytechnique, France

Motivation: RNA folding prediction through statistical sampling

- RNA Structure

  RNA = Sequence over $\{A, C, G, U\}$.
  RNA folds, establishing hydrogen bonds.
  Such base-pairs stabilize structure.
  Free-energy E_S assigned to each structure S.





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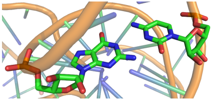

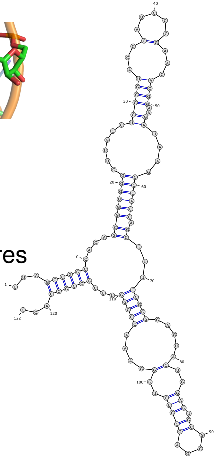

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  Only non-crossing base-pairs allowed $\rightarrow$ Secondary Structures
  Free-Energy = $-\#$ Base-pairs

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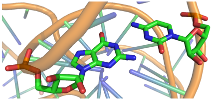

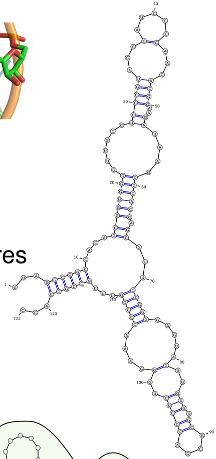

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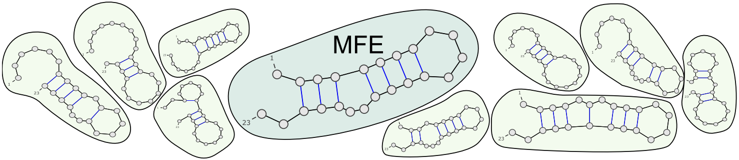
- Boltzmann equilibrium [McCaskill, 90]

  Any structure S exists w.p. $p_S \propto e^{-\#E_S/RT}$.



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RNA *in silico* search: sequence $\rightarrow$ functional secondary structure

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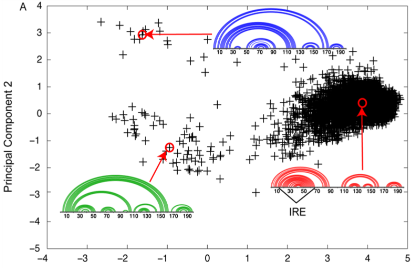

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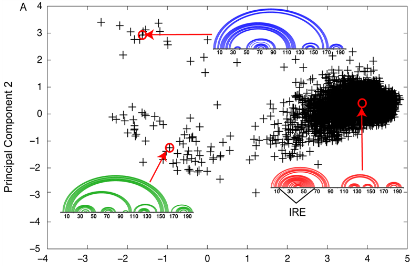

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(Meta)-Algorithm:

1. Draw k sec. str. at random at Boltzmann equilibrium ($\neq$ Boltzmann sampling)
2. Cluster samples using your favorite machine learning method
3. Return centroid of most probable cluster

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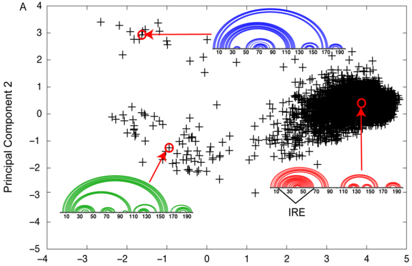

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$\Rightarrow$ This simple idea greatly improved specificity of predictions.

Motivation: RNA folding prediction through statistical sampling

A closer look at the (meta)-algorithm:

1. Draw k sec. str. at random (with replacement!) in the Boltzmann distribution

Redundancy is uninformative, one should aim for k distinct secondary structures.

Which additional cost is induced by the redundant generation?

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Coupon collector problem!

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10¢ per sticker
$m = 539$ stickers

$\Rightarrow$ 339 €!!!

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- One must then buy, on the average, $\frac{m}{m-k}$ coupons to get the $k+1$-th coupon...

$$E[C_m] = 1 + \frac{m}{m-1} + \frac{m}{m-2} + \ldots + \frac{m}{m-k} + \ldots = m \cdot \mathcal{H}_m \underset{m\to\infty}{\sim} m \ln m.$$

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Each sticker v_i is now drawn with probability p_i, $\sum_{i=1}^{m} p_i = 1$.

Theorem (Flajolet-Gardy-Thimonier,92)

$$E[C_m] = \int_0^\infty \left(1 - \prod_{i=1}^{m} \left(1 - e^{-p_i t}\right)\right) dt.$$

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(i) [David-Barton,62] $\quad p_i = \dfrac{2i}{m(m+1)} \quad \Rightarrow \quad E[C_m] \underset{m\to\infty}{\sim} \left(\frac{2\pi}{\sqrt{3}} - 3\right) \cdot m \cdot (m+1).$

(ii) [Hildebrand,93] $\quad p_i = \dfrac{1}{iH_m} \quad \Rightarrow \quad E[C_m] \underset{m\to\infty}{\sim} m \cdot H_m \cdot \log m.$

A more general result

- Distribution defined by a sequence of positive numbers $\{a_1, ..., a_m\}$:

$$p_i = \frac{a_i}{\mu_m}, \qquad \text{with} \qquad \mu_m = \sum_{i=1}^{m} a_i.$$

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Theorem (Boneh-Papanicolaou,94)

If $f(i) := 1/a_i$ satisfies:

$$\textit{(i)}\ f(x) \nearrow \infty, \qquad \textit{(ii)}\ \frac{f'(x)}{f(x)} \searrow, \qquad \textit{and} \qquad \textit{(iii)}\ \frac{f''(x)/f'(x)}{(f'(x)/f(x))\log(f'(x)/f)(x)} \to 0,$$

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What about sequences whose weights appear with multiplicities?
(e.g. unbounded #occurrences of some a_i as $m \to \infty$)

Random generation of words

Word collector?

Random generation of words

+

Coupon Collector

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=

Word collector

Which probability distribution on words?

Definition (Weighted language)

- **i** $\mathcal{L}$ *is a language over* $\Sigma = (a_1, ..., a_k)$*, and* $\mathcal{L}_n$ *its restriction to words of length* n*.*
- **ii** *Weight of a letter* $a_i \to \pi_{a_i} \in \mathbb{R}^+$.
- **iii** *Weight of a word* $\omega \in \mathcal{L}_n \to \pi(\omega) = \prod_{a \in \omega} \pi_a$
- **iv** *Weighted probability distribution, defined on* $\mathcal{L}_n$ *by:*

$$\forall \omega \in \mathcal{L}_n : \ \mathbb{P}[\omega] = \frac{\pi(\omega)}{\mu_n}, \qquad \text{with} \qquad \mu_n = \sum_{\omega \in \mathcal{L}_n} \pi(\omega).$$

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Remark: Words having equal composition have equal probability:

$$\mathbb{P}[ababbabaaa] = \mathbb{P}[aababbbaaa] = \mathbb{P}[aaaaaabbbb] = \frac{\pi_a^6 \pi_b^4}{\mu_{10}}.$$

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Many coupons share equal weight, i.e. equal probability! $\Rightarrow$ Large multiplicities
$\Rightarrow$ None of existing results applies…

Asymptotics

Reminder: $$E[C_m] = \int_0^\infty \Phi(t)dt \qquad with \qquad \Phi(t) = 1 - \prod_{i=1}^{m}\left(1 - e^{-p_i t}\right).$$

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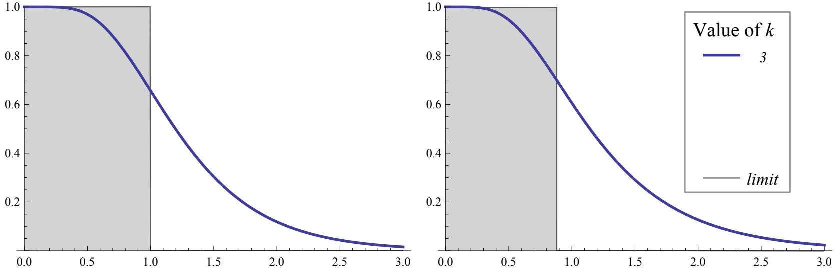

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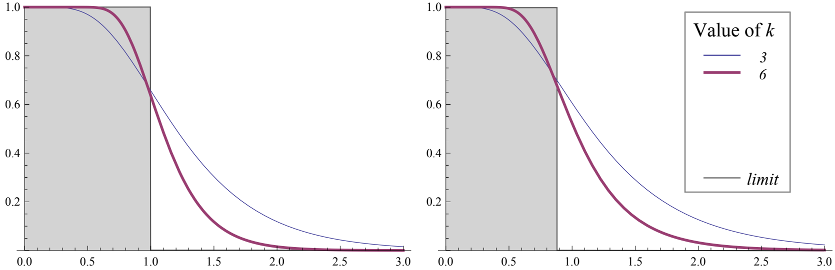

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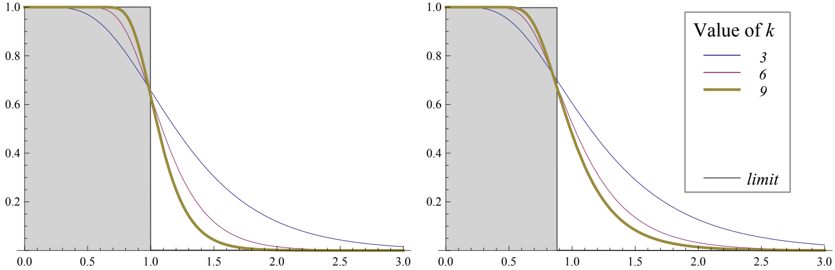

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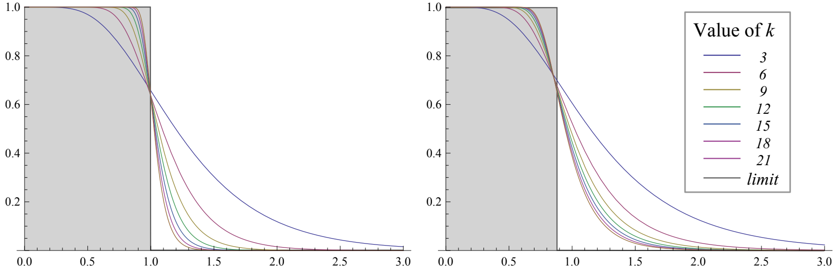

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Theorem (du Boisberranger-Gardy-P,2012)

If weight distribution satisfies hypotheses ***H1****,* ***H2*** *et* ***H3****, then*

$$E[C_m] \underset{m\to\infty}{\sim} \kappa \cdot \frac{\mu_m}{\omega(m)} \cdot g(m)$$

where κ*: explicit constant,*

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H2. *Regularity*. For large values of m, smallest weights of $\mathbf{W}_m$ no longer depend on m.
H3. *Growth*. Weight growth dominates multiplicity growth.

Theorem (du Boisberranger-Gardy-P,2012)

*If weight distribution satisfies hypotheses **H1**, **H2** et **H3**, then*

$$E[C_m] \underset{m\to\infty}{\sim} \kappa \cdot \frac{\mu_m}{\omega(m)} \cdot g(m)$$

where κ: explicit constant, $\omega(m)$: smallest weight in collection

Asymptotics (continued)

Evaluating the integral? $\rightarrow$ **for distributions featuring large multiplicities**.

Definition (Distribution description)

- **i** *Smallest weight of a letter set to* 1*.*
- **ii** $\mathbf{W}_m$*: Vector of distinct weights, ordered increasingly.*
- **iii** $M_{m,i}$*: Multiplicity of weight* $W_{m,i}$*.*

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Application: Σ^*

Description: Language $(a_1, ..., a_k)^*$ with $1 = \pi_{a_1} = ... = \pi_{a_j} < \pi_{a_{j+1}} \leq ... \leq \pi_{a_k}$.

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. . . Verify Hypotheses H1, H2 and H3 (ouch!). . .

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Reminder: $E[C_m] \sim \kappa \cdot \frac{\mu_m}{\omega(m)} \cdot g(m)$.

i $m \equiv$ #coupons $\equiv$ #words of length $n = k^n$.

ii $\omega(m) \equiv$ smallest weight $=$ weight of word $a_1^n = \pi_{a_1}^n \to 1$.

iii $\mu_m = (\pi_{a_1} + ... + \pi_{a_k})^n = m^{\log_k(\pi_{a_1}+\cdots+\pi_{a_k})}$.

iv $g(m) \sim \log\log m$ if $j = 1$, or $g(m) \sim \log m$ otherwise.

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Proposition (Waiting time – Full collection – Σ^*)

$$E[C_m] \sim \begin{cases} \kappa_1 \cdot m^p \cdot \log\log m & \text{if } j = 1, \\ \kappa_2 \cdot m^p \cdot \log m & \text{otherwise.} \end{cases}$$

where $p = \log_k(\pi_{a_1} + \cdots + \pi_{a_k}) > 1$.

Asymptotic waiting time differs from the uniform case.

Application: RNA Secondary Structures

Description: RNA sec. str. unambiguously generated by context-free grammar

$$S \to (\, S_{\geq\theta}\,)\, S \mid \bullet\; S \mid \varepsilon \qquad \text{and} \qquad S_{\geq\theta} \to (\, S_{\geq\theta}\,)\, S \mid \bullet\; S_{\geq\theta} \mid \bullet^{\theta}\,.$$

where θ: minimal distance between matching parentheses ($\theta = 1$ or 3).

Boltzmann probability distribution $\Rightarrow \pi_{\bullet} = 1$ and $\pi_{(} \times \pi_{)} = e^{1/RT}$ ($\pi_{(} < \pi_{)}$).

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Properties:

- **i** Gen. fun. + Singularity analysis $\Rightarrow \mu_m \sim \kappa \cdot m \cdot (\log m)^{-3/2}$
- **ii** Smallest weight = Weight of unpaired structure $\bullet^n = 1$
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Proposition (Waiting time – Full collection – Boltzmann weighted Sec. Struct.)

$$E[C_m] \sim \kappa \cdot m^p \cdot (\log m)^{3p/2} \cdot \log\log m$$

where $p > 1$ depends on the dom. sing. of the cardinality and cumulated weight.

Again, asymptotic waiting time differs from the uniform case.

Corollary: On average, a sec. str. is generated $\Theta(m^{p-1}) = \mathcal{O}(\alpha^n)$ times, $\alpha > 1$.

Conclusion

- Words collector: new instance of the coupon collector.
- Original probability distribution: Large multiplicities.
- Asymptotic behaviors differ from uniform ones. . .
- . . . and arise as a trade-off between multiplicity and weight.
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- Tighten and explain intuitively hypotheses.
- Variants: Partial collections? Waiting time before *k* distinct objects (alt. cumulated probability of $1 - \varepsilon$) are obtained.
- Language classes adopting ubiquitous asymptotic behaviors (regular/algebraic/strongly connected $\rightarrow$ Drmota/Lalley/Woods theorem...)
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Thanks for listening
Questions?

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