

# Multi-label Learning: An Update

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June 9, 2023 @ BCAM. Bilbao.

**5th BIDAS Workshop**

# Outline

- 1 Introduction: Multi-Label Learning
- 2 Issues with the Standard Approach/Assumptions
- 3 Label Dependence: A Fresh Investigation and Update
- 4 Cross-Domain Transfer Learning: Lessons from MLL
- 5 Summary (and Recent Advances and Open Questions)

# Introduction: Multi-Label Learning

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# Multi-label Classification

**Multi-label classification:** a subset/vector of labels is be assigned to each input instance.



$x =$

$y = [1, 0, 1, 0] \Leftrightarrow$  labels {Beach, Foliage} are relevant to  $x$ .

Input	Beach	Sunset	Foliage	Urban
	1	0	1	0
	0	1	0	0
	0	1	0	1
	0	1	1	0
	0	0	1	1
	?	?	?	?

Task:

$$\hat{\mathbf{y}} = [?, ?, ?, ?] = h(\mathbf{x}) \quad \hat{\mathbf{y}} \in \{0, 1\}^m$$

Also,

- text categorization
- missing-value imputation
- recommender systems
- time-series forecasting
- network inference
- tracking and localization
- image segmentation
- molecule design
- audio labelling
- ...



The Lord of the Rings: The Fellowship of the Ring (2001)

PG-13 | 125 min | Adventure, Fantasy | 21 (based on 2011 215K)

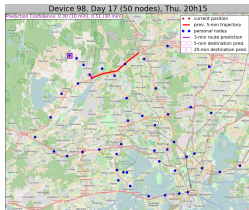
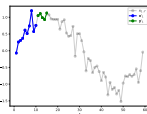
Your rating: 0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0

★ **3.8** Perhaps 4.8 (1) from 1,118,940 users | Metascore: 82/100  
 Reviews: 4,980 user | 284 critic | 34 from Metacritic.com

A week holiday of the Shire and night comparisons set out on a journey to Mount Doom to destroy the One Ring and the dark lord Sauron.

Director: Peter Jackson  
 Writers: J.R.R. Tolkien (novel), Fran Walsh (screenplay), Elizabeth Magill  
 Stars: Elijah Wood, Ian McKellen, Orlando Bloom

See full cast and crew »



Mol1 Mol2 Mol3 Mol4 Mol5 Mol6

🧩	1,3	0,2	1,4	1,7	3,5	1,3
🧩	2	1,7	1,5	7,5	8,2	7,6
🧩	0,2	0	0,3	0,4	1,2	2,2
🧩	3,1	1,1	1,3	1,1	1,7	5,2
🧩	4,7	2,1	2,5	1,5	2,3	8,5
🧩	?	?	?	?	?	?

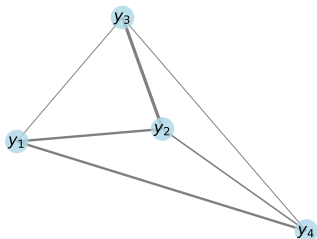
# Label Dependence: The 'Why' of Multi-Label Learning



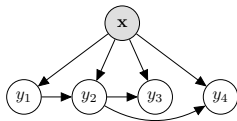
Graph of correlation among the labels of the *Music-Emotions* data

# Standard 'Recipe' / Traditional Approach

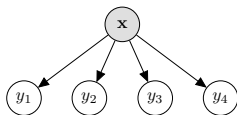
- 1 'We measure label dependence using  $\langle xxx \rangle$ '



- 2 'We construct a model called  $\langle yyy \rangle$ '
- 3 'We show  $\langle zzz \rangle$  %-improvement vs independent models'



vs



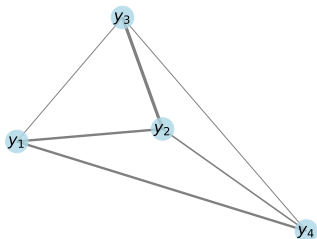
vs ... ?

Implication: **Predictive performance**  $\Leftrightarrow$  **label dependence**.

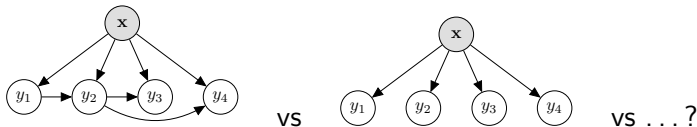


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Implication: **Predictive performance**  $\Leftrightarrow$  **label dependence**.

This talk: A fresh investigation, and an updated view.

# A Timeline of Multi-label Learning in Academia

- < 2000s Just use independent models.
- ... 2010 Model labels together; label dependence/co-occurrences.
- ... 2015 Using label dependence in a more sophisticated/efficient way.
- ... 2015 Multi-label learning for image, text, forecasting, recommendation, audio, health applications, distilling wine ...
- 2020 [... and for covid19].
- ... 2020 Just use independent models
- ... 2020 Must use deep [convolution / recurrent] neural networks.
- 2020... ... deep [graph-embedding / residual / generative adversarial / transformer/...] neural networks with [missing / weak / incremental / evolving / imbalanced / millions of/...] labels.
- 2023 Still persistent in the literature<sup>1</sup>

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<sup>1</sup> Mylonas et al., "On the Persistence of Multilabel Learning, Its Recent Trends, and Its Open Issues", 2023

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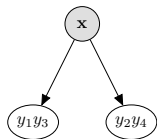
2023 Still persistent in the literature<sup>1</sup>

Multi-target regression? < 1/10-th volume of literature.

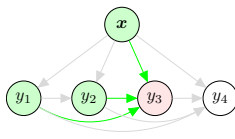
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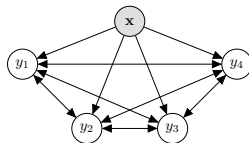
# Multi-label Classifiers: Examples



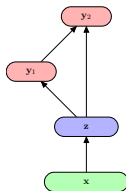
Random  $k$ -Label Sets and Meta Labels



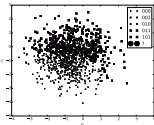
Classifier Chains and Bayesian Networks



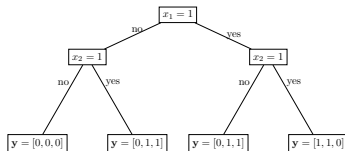
Conditional Dependency Networks



Neural Networks



$k$ -Nearest Neighbours



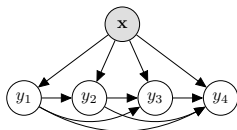
Decision Trees and Random Forests

## Algorithm Adaptation vs Task Adaptation / Problem Transformation

# Classifier Chains: An Example of 'Problem Transformation'

A chain (**structure**) over the output variables;

- Cascaded prediction across a chain/graph
- Motivation: Model label dependence



$X$	$Y_1$	$Y_2$	$Y_3$	$Y_4$
$x^{(1)}$	0	1	1	1
$x^{(2)}$	1	0	0	0
$x^{(3)}$	0	1	0	1
$x^{(4)}$	1	0	0	0
$x^{(5)}$	0	0	0	0

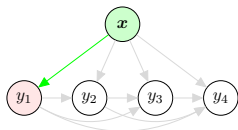
  

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-------------	-------------	-------------	-------------	-------------

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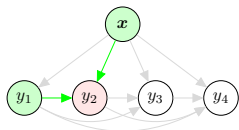
  

$\tilde{x}$	$\hat{y}_1$			
-------------	-------------	--	--	--

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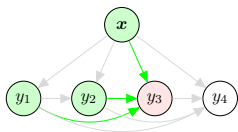
  

$\tilde{x}$	$\hat{y}_1$	$\hat{y}_2$		
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$\tilde{x}$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_3$	

For example,  $\hat{y}_3 = h_3(x, \hat{y}_1, \hat{y}_2)$  with **base classifier** (or regressor)  $h_3$  (e.g., decision tree, logistic regression, ...).

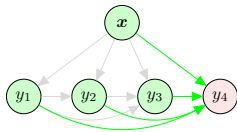
Typical example of a "problem transformation" (or model agnostic) meta method that **works well** vs independent models



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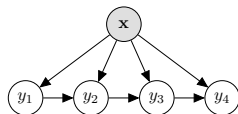
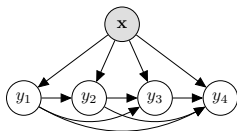
Typical example of a "**problem transformation**" (or model agnostic) meta method that **works well** vs independent models – **but why?**

# Issues with the Standard Approach/Assumptions

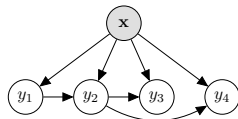
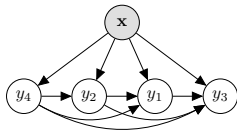
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# War Story 1 (Initial Intuition Fails)

These models perform well:



These ones perform not so well:

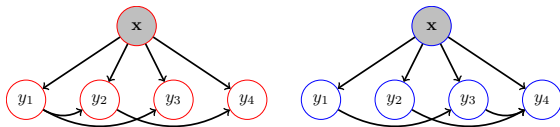


Yet it is difficult to associate accuracy to a particular [type of] structure based on dependence, time order, or 'inherent' hierarchy.

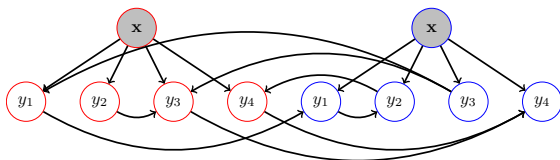
## War Story 2 (Sanity Check Fails)

Take two **totally unrelated datasets**; stick them together; search for inherent structure.

Hypothesis: Find something like this,

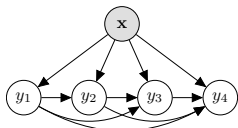


Outcome: Found something like this,

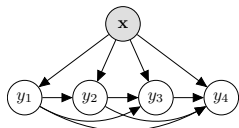


Remark: It's not [only] a small data problem!

## War Story 3 (More Weirdness)



outperforms



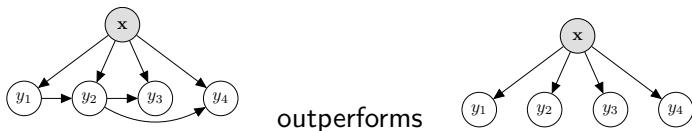
Average accuracy over 100 random train/test splits:

(Left) 0.47 > 0.41 (Right)

and the left wins 100/100 times! Yet, it's the

- **same model** (classifier chains)!
- **same base classifier** (SGD)
- **same structure!**
- **same data** (Scene dataset; **same splits**)  
**except:**  $\mathbf{Y}_{\text{Right}} = \mathbf{1} - \mathbf{Y}_{\text{Left}}$  (all bits are flipped).

## War Story 4 (Theory $\neq$ Practice?)

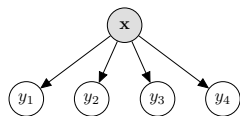


(significantly) *under Hamming loss* metric which **does not require joint modelling** to optimize<sup>2</sup>!

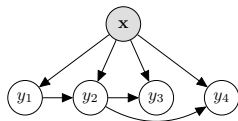
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<sup>2</sup>Neither do ranking-based metrics, by the way; Dembczyński et al., "On Label Dependence and Loss Minimization in Multi-label Classification", 2012

## War Story 5 (Back to Square One?)



*equals* performance of



under **0/1-Loss**/exact-match metric which **requires joint modelling** to optimize, and even though we know **there is label dependence**. (By the way: especially common in multi-target regression<sup>3</sup>).

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<sup>3</sup>Borchani et al., "A Survey on Multi-output Regression", 2015

# Label Dependence: A Fresh Investigation and Update

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## Suggestion 1: Because Label Dependence

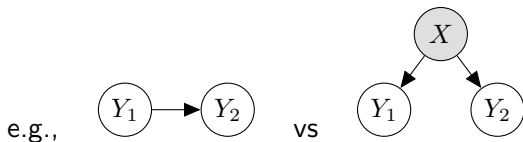
**Argument:** If label variables are correlated/interdependent, we should model/predict them together; accuracy will better.

Label **dependence**:

$$P(Y_1, Y_2) \neq P(Y_1)P(Y_2)$$

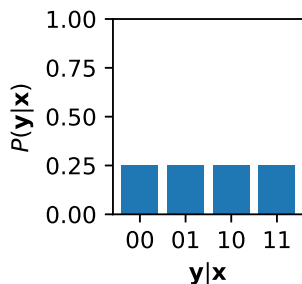
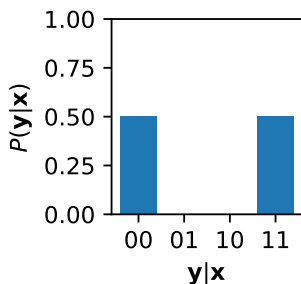
Actually, we should be interested in **conditional dependence**:

$$P(Y_1, Y_2|\mathbf{x}) \neq P(Y_1|\mathbf{x})P(Y_2|\mathbf{x})$$



# Label Dependence and Loss Metrics

Posterior of two multi-label classifiers (2 labels, test instance  $\mathbf{x}$ ):

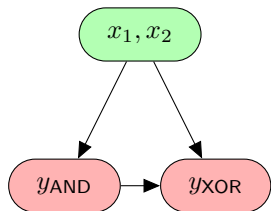


$\mathbb{E}[\text{Hamming loss}]$  the same;  $\mathbb{E}[\text{0/1-loss}]$ : twice as large!

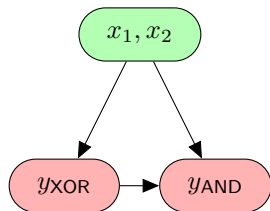
Not only a question of dependence, but of loss metrics and uncertainty; modelling together  $\neq$  predicting together.

## A 'Logical' Problem: The 'Wrong' Dependence

$X_1$	$X_2$	$Y_{\text{XOR}}$	$Y_{\text{AND}}$
0	0	0	0
0	1	1	1
1	0	1	1
1	1	0	1



outperforms  
(sometimes<sup>†</sup>)



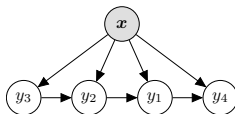
<sup>†</sup>when

$$P_{\star}(y_1, y_2 | \mathbf{x}) \neq \hat{P}(y_1, y_2 | \mathbf{x})$$

where  $\hat{P}$  depends on **base classifier**, **inference**, etc. We measured the 'wrong' dependence; but got extra **capacity** from it!

## Suggestion 2: Put Easy Labels First

**Argument:** There may be **error propagation** across the structure, so we should, e.g., **put easy labels first**.



But

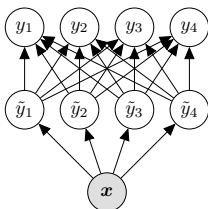
- Empirically: *Incorrect* label predictions may also *increase* the accuracy of *other* label predictions!
- Observation  $x$  is available at each step; error should *not* propagate!<sup>4</sup>

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<sup>4</sup> A more complete discussion in Senge, Coz, and Hüllermeier, "On the Problem of Error Propagation in Classifier Chains for Multi-label Classification", 2014 (probabilistic/probability-tree view)

## Suggestion 3: Error Correction

**Argument:** We can ‘correct’ errors at prediction time, e.g., via **stacking**.



Maybe we can<sup>5</sup>; but

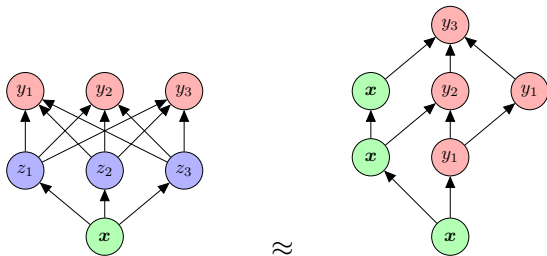
- $P(y_1 | \tilde{y}_1, \tilde{y}_2, \tilde{y}_3, \tilde{y}_4) \neq P(y_1, y_2, y_3, y_4 | x)$ , i.e., this is **not label dependence modelling**, we only correct bias of individual models;
- Empirical results: Not much improvement (esp. in 0/1 loss)
- involves a separate training mechanism for each layer.

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<sup>5</sup> e.g., (among many others) Loza Mencía and Janssen, “Learning rules for multi-label classification: a stacking and a separate-and-conquer approach”, 2016

## Suggestion 4: Build (Deep) Neural Networks

**Argument:** Structure among labels  $\Rightarrow$  'deep' 'neural' network.  
Classifiers as activation/[transfer functions](#), labels as [hidden nodes](#).  
A bit like ResNets.

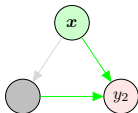


OK (depth works). But, note in 'deep chains' (right):

- No back propagation (this is deep *prediction*, but **not deep learning**);
- the hidden nodes are not 'hidden'.

Consider prediction task

$$\tilde{x} \mapsto \hat{y}_2$$



and the data available at training time (left) vs test time (right):

	$X_1$		$Y_2$		$X_1$		$Y_2$
Basis expansion	$x$	$\phi_1$	$y_2$		$\tilde{x}$	$\phi_2$	$\hat{y}_2$
Stacking	$x$	$\tilde{y}_2$	$y_2$		$\tilde{x}$	$\tilde{y}_2$	$\hat{y}_2$
Classifier chain	$x$	$y_1$	$y_2$		$\tilde{x}$	$\hat{y}_1$	$\hat{y}_2$
Neural network	$x$		$y_2$		$\tilde{x}$	$z$	$\hat{y}_2$

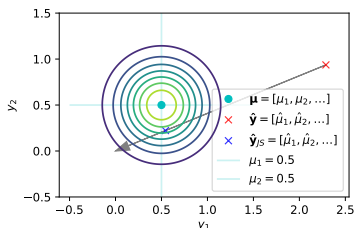
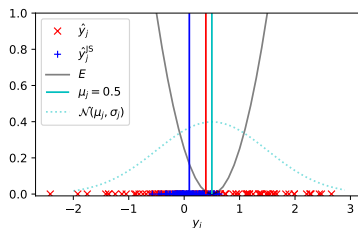
## Suggestion 5: Structure Provides Regularisation

**Argument:** Modelling labels together provides better results **even if they are independent**, because of regularization.

For example the **James Stein estimator**

$$\hat{y}_{JS} = \frac{1 - (m - 2)\hat{\sigma}^2}{\|\hat{y}\|^2} \hat{y} = \lambda \cdot \hat{y}$$

where  $\lambda$  *shrinks* (regularises) the max.-likelihood estimate  $\hat{y}$ .

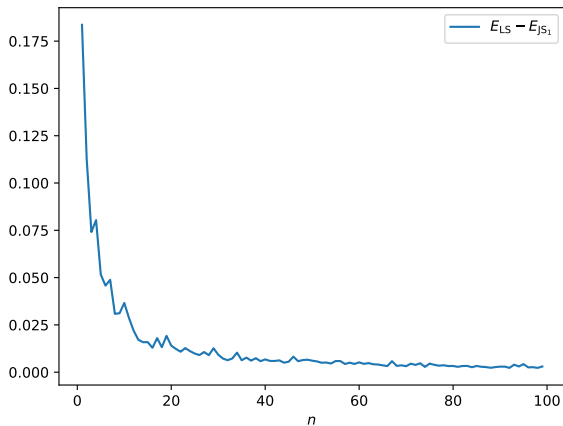


This helps explain the bit-inversion story!

Good discussion by Waegeman, Dembczyński, and Hüllermeier, "Multi-target prediction: a unifying view on problems and methods", 2019



Benefit from modelling **non-existent** label dependence (shown where **blue**  $> 0$ ):



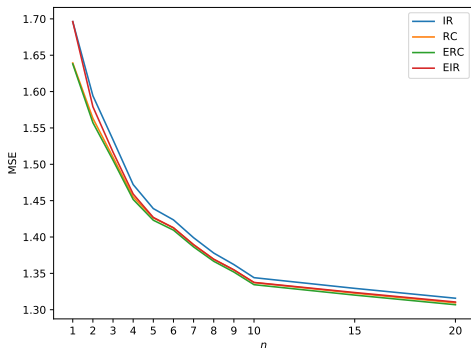
But: gains are minimal when  $n \gg m$  (many examples, few labels).

## Suggestion 6: The 'Ensemble Effect'

**Argument:** Modelling labels *appears* to provide better results but actually **the ensemble deserves the credit**, by providing

- More predictive power
- More regularisation

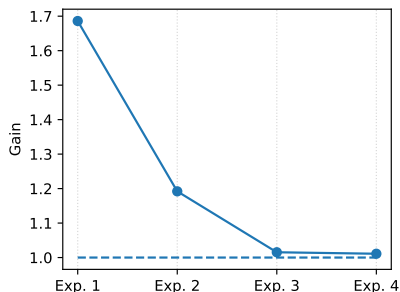
Here, reg. **only** (task is fully linear/independent models/concept):



E = Ensemble, I = Independent, C = Chain

## So Which Is It Then?

Classifier chains vs independent models (Music-Emotions data):



- Experiment 1: All effects confounded (logistic reg., 0/1 loss)
- Experiment 2: Remove motiv. of label dependence ( $\rightarrow$ h.loss)
- Experiment 3: Remove influence of capacity (+ depth)
- Experiment 4: Remove influence of regularisation (+ reg.)

interesting result: **20% higher accuracy by modelling label dependence, even when theoretically pointless!**

# A First Update

We can offer a minor rephrasing:

*We should model and predict labels together **mainly** because of label dependence (i.e., **if our loss metric suggests that we need to learn it**), but we can also get **benefits from additional capacity and regularisation** brought by additional structure inherent to modelling labels together.*

*With enough data/computational power, regularised deep neural network architectures likely to overpower traditional methods of multi-label learning.*

*But (to say it again): this is not because of label dependence modelling!*

# Reasons to Retain Interest

Modelling labels together with model-agnostic/base-classifier approaches (and other algorithm-adaptations):

- still work well especially **on fewer training examples** (important for, e.g., small data and recovery from concept drift in data streams)
- require **no hidden units**; depth/non-linearity comes 'for free'
- requires **no back propagation**
- more choice (decision trees, including a mixture of different models, ...) – for reasons of **interpretability** or reliability; and

And we have seen **improvement from modelling totally unrelated tasks together**

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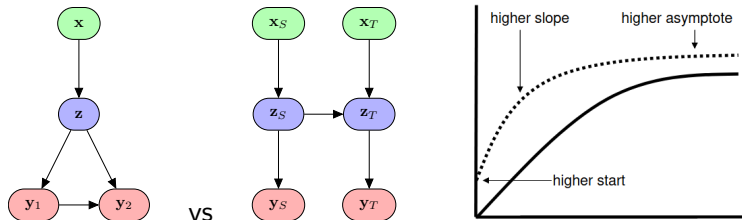
And we have seen **improvement from modelling totally unrelated tasks together** ← **very interesting!?**

# Cross-Domain Transfer Learning: Lessons from MLL

- 1 Introduction: Multi-Label Learning
- 2 Issues with the Standard Approach/Assumptions
- 3 Label Dependence: A Fresh Investigation and Update
- 4 Cross-Domain Transfer Learning: Lessons from MLL**
- 5 Summary (and Recent Advances and Open Questions)

# Transfer Learning: A Quick Intro

- 1 Find related source task ( $S$ )
- 2 Use it to improve the model you deploy on target task ( $T$ )

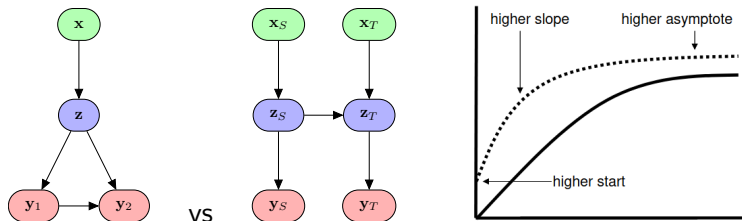


Plot (right) from Torrey and Shavlik, "Transfer learning", 2010.



# Transfer Learning: A Quick Intro

- 1 Find related source task ( $S$ )
- 2 Use it to improve the model you deploy on target task ( $T$ )



Plot (right) from Torrey and Shavlik, "Transfer learning", 2010.

A key word was: *related*. But what if related-ness is not a requirement?

In other words: we go back to where our sanity check failed (multi-label learning with no label dependence).

# Thoughts on That

Transfer learning by connecting the model from an unrelated source task; This is similar to connecting the first layer of a neural network randomly.

*"[C]onnecting the first layer randomly is just about the stupidest thing you could do" – Yann LeCun*

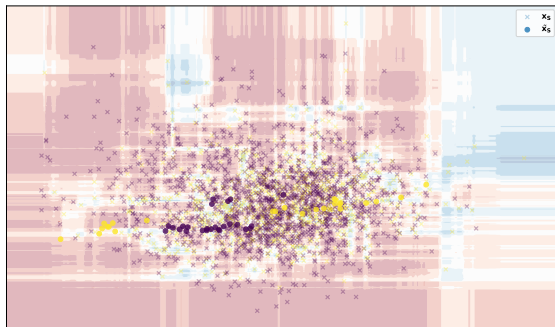
Remarks:

- He said "just about"
- He didn't say it didn't work
- There's a minor difference: We mean, not randomly drawn from all possible models, rather randomly drawn from all [a collection of] existing *trained* models

So let's try it anyway. . .

## Insomniac Fungi

A model (random forest) for classifying patients<sup>6</sup>: suffering **insomnia** (red) or not (blue), based on sleep measurements  $x_S = [x_1, x_2]$ :

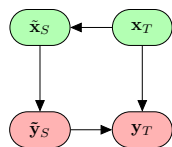
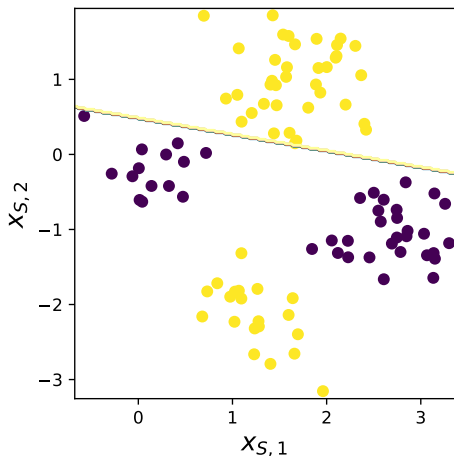


A **yeast genome** vector is cast into  $\tilde{x}_S$ , and given an insomnia diagnosis  $\hat{y}_S$ ; which, when used as new feature, boosts +2% accuracy when predicting genome function.

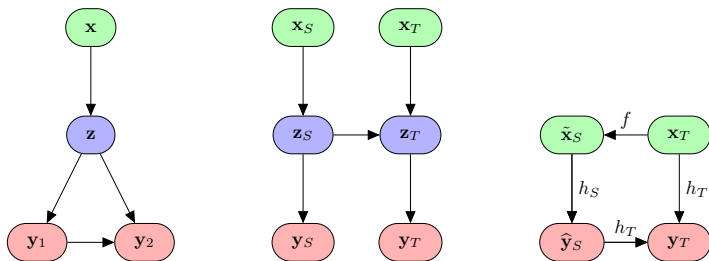
<sup>6</sup>Medical data thanks to Olivier Pallanca

## Replicating on Synthetic Data

A target task XOR (data shown, some noise added) is solved via predictions from AND-function (decision boundary shown) as an additional feature:

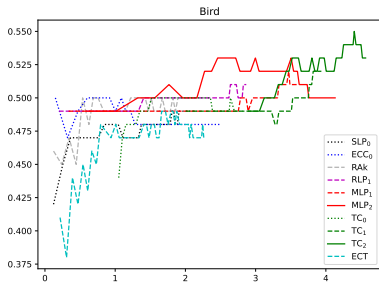
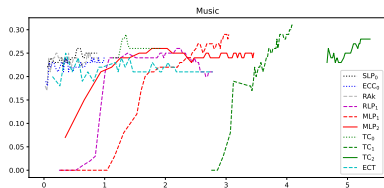


# Multi-Label Chain vs Deep Transfer vs Chain Transfer



Main difference from standard Deep Transfer: A **model agnostic** approach; **require only outputs** (as per chained multi-label models).

# Results (Did it Work?)



Well, it, 'shows promise' (green line gets higher).

- Not a state-of-the-art method.
- But it works!
- Reminder: extremely difficult transfer setting: no model introspection, no source data, **no label/task dependence**
- Advantages: depth without the deep learning; use 'any' source model

# Discussion Points

- Intersection with *multi-task learning*, *deep transfer learning*, *lifelong learning*, *concept drift adaptation*; 'pretrained', 'frozen' layers, 'parameter isolation', 'universal computation', ...
- Interest of multi-label models: larger  $\hat{y}$  (more information)
- What does it mean for a label/task to be related to another?
- Transfer learning vs **reduction/reuse/recycling** of models?
- **Model-driven learning** rather than [raw] data-driven learning
- Example implication: When **adapting to concept shift in data streams**; keep using the 'irrelevant' models!

# Summary (and Recent Advances and Open Questions)

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# Multi-label Learning: An Update

Take-away points (so far):

- Many methods, many applications; **still relevant!**
- But **not** just '*model label dependence*  $\Rightarrow$  good accuracy'
- You may model labels/tasks together **even if there is 'none'!**  
**Label dependence, model capacity, regularization**
- You may ignore label dependence and still perform optimally
- Big data + deep learning  $\Rightarrow$  good accuracy
- But extreme multi-label classification can imply extreme cost

And let's not forget about

- **Interpretability**: *how* methods work; *why* labels together; different contexts of **uncertainty**
- Ever larger/more complex problems via data-driven learning 'from scratch' – increasingly challenging/wasteful!  
(sparse learning is interesting) **Reduce/Reuse/Recycle** models!

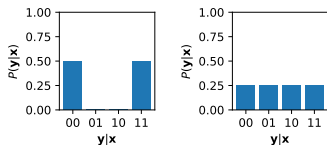
But many current trends do not need to be considered separately.

## Current Work: Missing Value Imputatation

- Missing values are common
- Problem: Often, too many to ignore  
e.g., in high- $d$  data (many attributes, few instances)
- Missing inputs  $\approx$  noisy labels
- 'Structured missing-ness' and predicting modes
- Proposed: Auto-replicative Random Forests:  $f : \mathbf{X} \mapsto \mathbf{X}$
- Connection to Denoising Auto-Encoder

$X_1$	$X_2$	$X_3$	$X_4$		$Y_1$	$Y_2$	$Y_3$	$Y_4$
0	1	1	0		0	1	1	0
1	?	0	?	$\Rightarrow$	1	-	0	-
0	1	0	0		0	1	0	0
1	?	0	1		1	-	0	1
0	0	?	?		0	0	-	-

& repeat (impute). We produce multi-mode estimates  $\mathbf{x} \sim P(\mathbf{x})$ .



# Current Work: Multi-label ECG Classification and Transfer

- Multi-label classification of ECG signals (multiple heart issues)
- A pre-trained deep neural network works well, but
- Problem: Multiple datasets, **partial**[ly-overlapping] **labels**
- Problem: **Poor** domain **transfer**

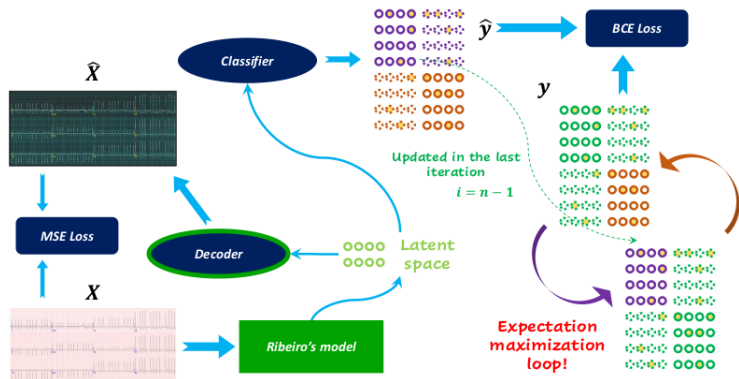


Image credit: Eran Zvuloni

# Multi-label Learning: An Update

Jesse Read



Thank you!


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`http://www.lix.polytechnique.fr/~jread/`


# References I

This talk is based on (many more references within): *From Multi-label Learning to Cross-Domain Transfer: A Model-Agnostic Approach*, J. Read, 2022.

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