

# INDEPENDENT MODELS

- The most naive way to make multi-target predictions: learning a model for each target independently.

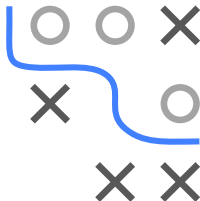
		Mol1	Mol2	Mol3	Mol4	Mol5	Mol6
01101	❌	1,3	0,2	1,4	1,7	3,5	1,3
00111	❌	2	1,7	1,5	7,5	8,2	7,6
01110	❌	0,2	0	0,3	0,4	1,2	2,2
10001	❌	3,1	1,1	1,3	1,1	1,7	5,2
01011	❌	4,7	2,1	2,5	1,5	2,3	8,5
11110	❌	?	?	?	?	?	?

...

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- In multi-label classification this approach is also known as *binary relevance learning*.
- Advantage: easy to realize, as for single-target prediction we have a wealth of methods available.

## INDEPENDENT MODELS

- Assume a linear basis function model for the  $m$ -th target:

$$f_k(\mathbf{x}) = \boldsymbol{\theta}_k^\top \phi(\mathbf{x}),$$

$\theta_k$  is target-specific parameter and  $\phi$  some feature mapping.

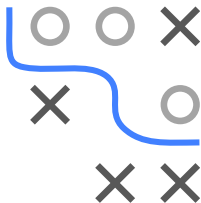
- Use this with with large nr of targets.
- We optimize jointly:

$$\min_{\Theta} \|Y - \Phi\Theta\|_F^2 + \sum_{m=1}^l \lambda_m \|\theta_m\|^2,$$

$$\|B\|_F^2 = \sqrt{\sum_{i=1}^n \sum_{m=1}^l B_{i,m}^2}$$
 is Frobenius norm for  $B \in \mathbb{R}^{n \times l}$  and

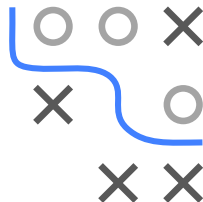
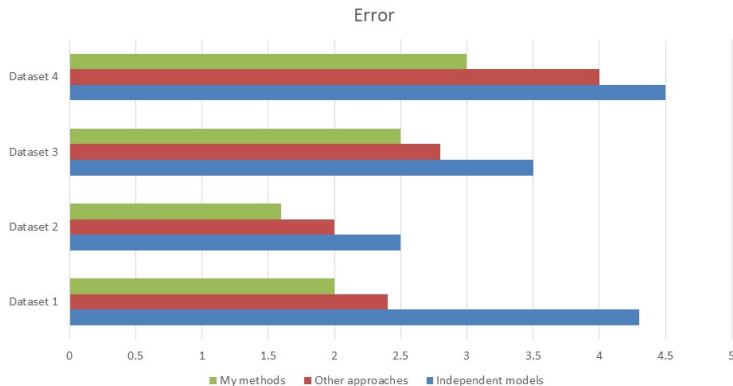
$$\Phi = \begin{bmatrix} \phi(\mathbf{x}^{(1)})^\top \\ \vdots \\ \phi(\mathbf{x}^{(n)})^\top \end{bmatrix} \quad \Theta = [\theta_1 \quad \cdots \quad \theta_l].$$

Frobenius norm = sum of SSE-s of all targets



# INDEPENDENT MODELS

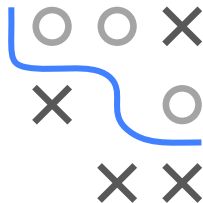
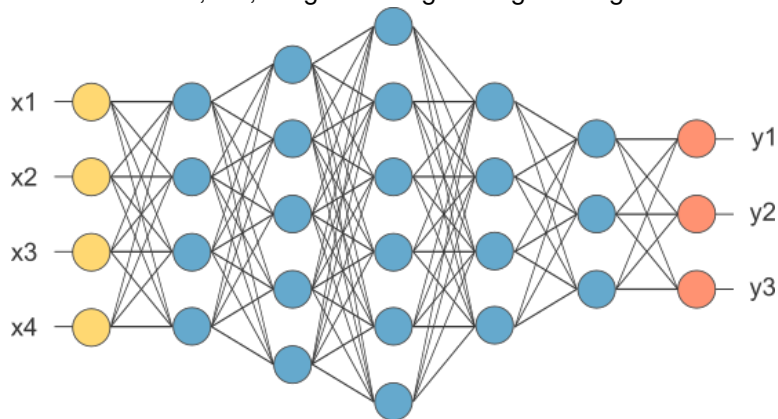
The experimental results section of a typical MTP paper:



→ Independent models don't exploit target deps, compared to more sophisticated methods, seems to be key for better performance.

# ENFORCING SIMILARITY IN DEEP LEARNING

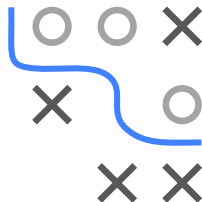
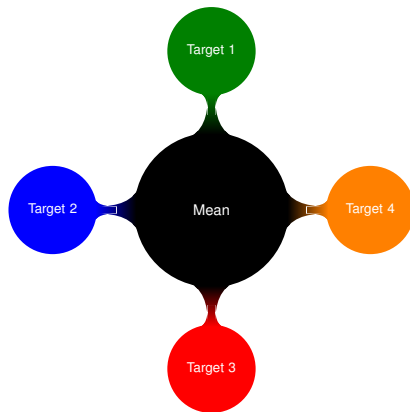
Commonly-used architecture: weight sharing in the final layer with  $m$  nodes, i.e., weight sharing among the targets



► Caruana, 1997

# MEAN-REGULARIZED MULTI-TASK LEARNING

- Models for similar targets should behave similarly
- So params should be similar

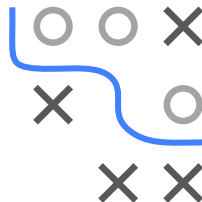
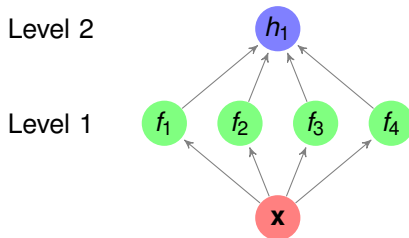


- Approach: Bias parameter vectors towards mean vector:

$$\min_{\Theta} \|Y - \Phi\Theta\|_F^2 + \lambda \sum_{m=1}^l \|\theta_m - \frac{1}{l} \sum_{m'=1}^l \theta_{m'}\|^2$$

# STACKING

- Originally, general ensemble learning technique.
- Level 1: apply series of ML methods on the same dataset
- Level 2: apply ML method to a new dataset consisting of the predictions obtained at level 1



► Wolpert, 1992

# STACKING APPLIED TO MTP

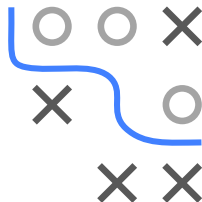
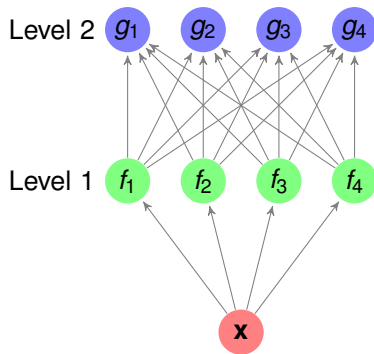
- Level 1: learn all  $f_k(\mathbf{x})$  independently
- Level 2: learn model for each target independently, using predictions of level 1  $\rightsquigarrow$

$$f(\mathbf{x}) = g(f_1(\mathbf{x}), \dots, f_l(\mathbf{x}))$$

Or:

$$f(\mathbf{x}) = g(f_1(\mathbf{x}), \dots, f_l(\mathbf{x}), \mathbf{x})$$

- Advantages: easy to implement and general
- Has been shown to avoid overfitting in multivariate regression
- If level 2 learner uses regularization  $\rightsquigarrow$  models are forced to learn similar parameters for different targets.



► Cheng and Hüllermeier, 2009

# STACKING VS BINARY RELEVANCE: EXAMPLE

- Compare F1-Score of random forest with stacking vs random forest with binary relevance on different multilabel datasets:

	birds	emotions	enron	genbase	image	langLog	reuters	scene	slashdot	yeast
BR(rf) F1-Score	0.637	0.620	0.578	0.989	0.431	0.319	0.671	0.616	0.441	0.615
STA(rf) F1-Score	0.646	0.634	0.583	0.986	0.446	0.317	0.685	0.633	0.453	0.624

- F1-Score is decomposed over targets.
- NB: Stacking slightly outperforms binary relevance on average.
- For more details, please refer to [Probst et al., 2017](#).

