Generalizing to a zero-data task: a linear model case study

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with Yoshua Bengio and Aaron Courville

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Plan

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- **Why do this ?**
  - this situation occurs in certain applications : drug discovery, song/movie recommandation, NLP tasks
  - gives us a worst case scenario in an inductive transfer model
  - hasn't been studied so much

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- I will compare different training settings for the linear model in a classification task :
  - discriminative (with 2 different cost functions)
  - generative
- I will present results for two problems :
  - classifi cation problem
  - ranking problem

First problem : classifi cation

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- **Test tasks :** we are given two class descriptors and we need to discriminate between these two classes for a given set of untagged instances

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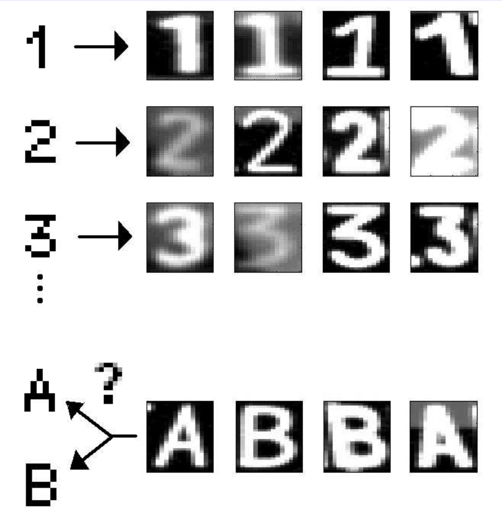

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- Here, we will have $g(d_y)$ be a linear transformation $A'd_y$, hence

$$f_y(x) = d_y A x$$

or, in the energy-based framework

$$E(x, y) = -d_y A x$$

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- We use standard regularisation techniques, such as early stopping, weight decay, etc.

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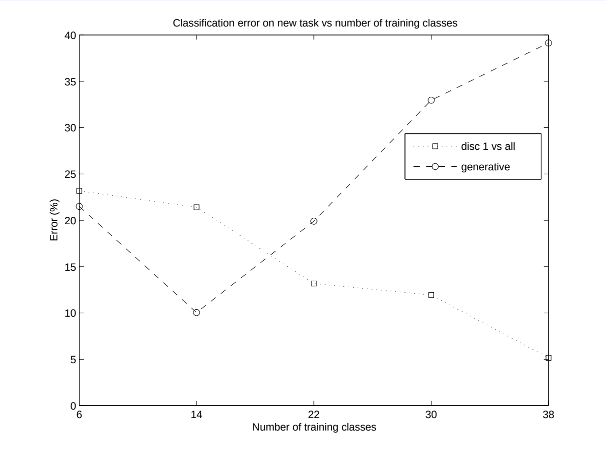
- We vary the number of classes present in the training set, but we keep the same test classes of the different folds

Results


Classification error on new task vs number of training classes
Error (%)
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- Discriminative model does better when many task examples are available
- More “examples” of tasks doesn’t imply better generalisation

Other model variation

- Discriminative 0-1 multi-task classification

$$\begin{aligned}\mathcal{L}(x,y) &= -log(sigmoid(-E(x,y))) \\ &\quad - \sum_{c \in \mathcal{Y}, c \neq y} log(1 - sigmoid(-E(x,c)))\end{aligned}$$

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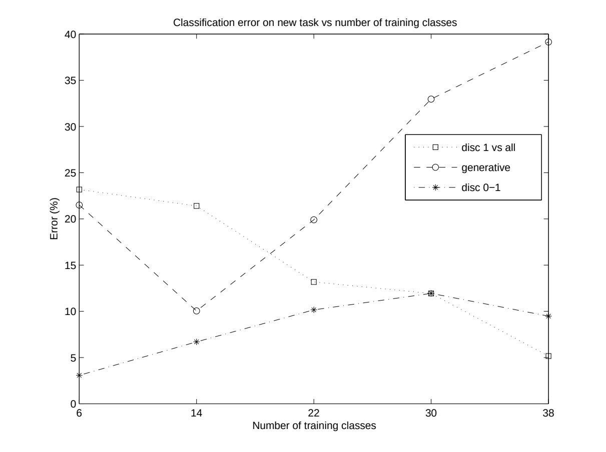
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- **Nature of descriptors d_y :** TOP SECRET !

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- The evaluation metric is the “lift” :

$$LIFT = 100 \cdot \frac{a_s}{a_{100}}$$

where a_s is the fraction of active compounds in the s first compounds, as ranked by the model. Here, we use $s = 30$, which is a standard size in computational chemistry.

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LIFT results for the different proteins.

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D	152.89
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- Do more experiments, on other datasets (any suggestion ?)
- Use a more complex model (Deep Belief Network ?)