Bias/Variance Trade-off, Some Practical Issues, Semi-supervised and Active Learning

Piyush Rai

Introduction to Machine Learning (CS771A)

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Plan for today

- Bias/Variance Trade-off of Learning Algorithms
- Some basic guidelines for debugging ML algorithms
- What if training data and test data distributions are NOT the same
- How to utilize unlabeled data: Semi-supervised Learning
- How to selectively ask for the most informative data: Active Learning

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- Approximation error: Error of best model f^* because of the model class $\mathcal{F}$ being too simple
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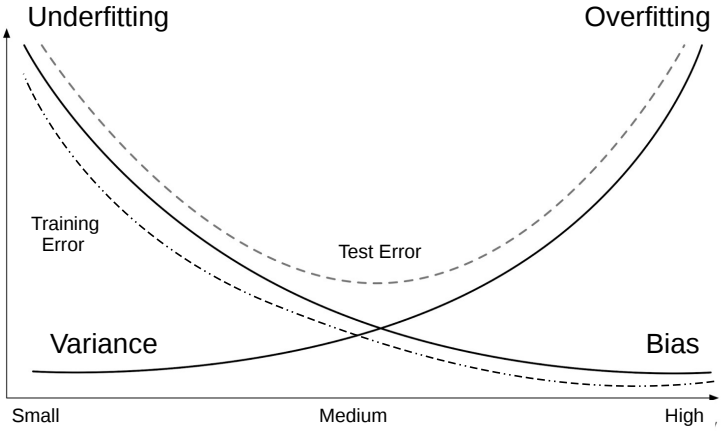
A Visual Illustration of the Trade-off



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- How to know what might be going wrong and how to debug?

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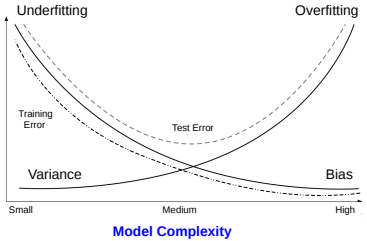
  - High Bias (Underfitting)
  - High Variance (Overfitting)
- Looking at the training and test error can tell which of the two is the case



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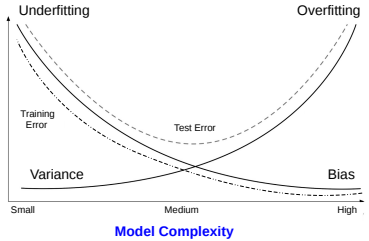

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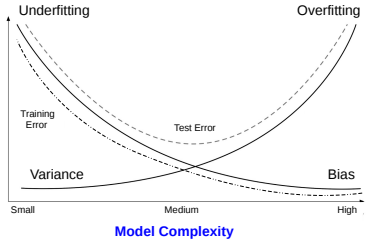

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- High Variance: Small training error, large test error (and huge gap)

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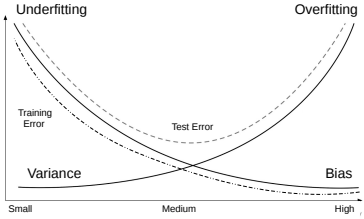

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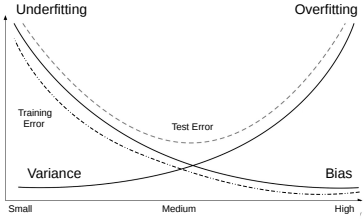

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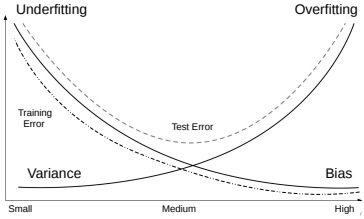

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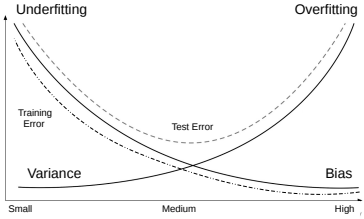

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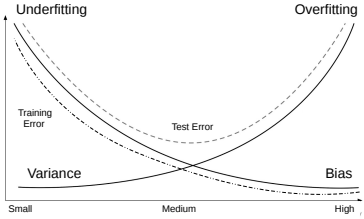

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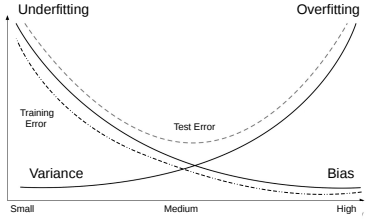

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  - Using a simpler model class or fewer features or regularization can help

When Train and Test Distributions Differ

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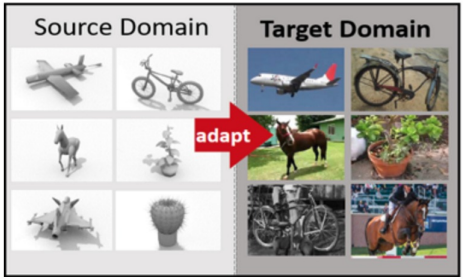

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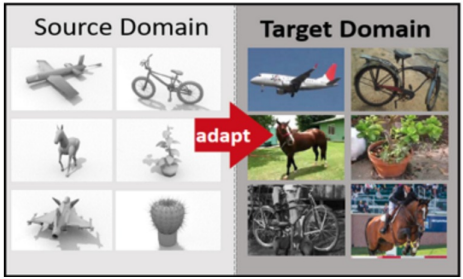

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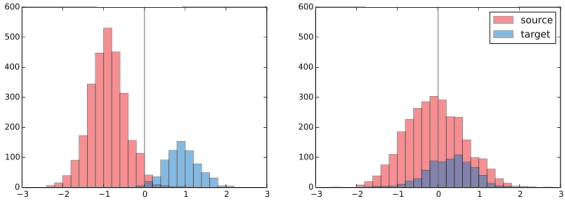
- Known as "domain adaptation" (also "covariate-shift", since features $\boldsymbol{x}$ are also called covariates)

Handling Domain Differences: Some Approaches

- Learning a transformation that makes the training and test data distributions "close"



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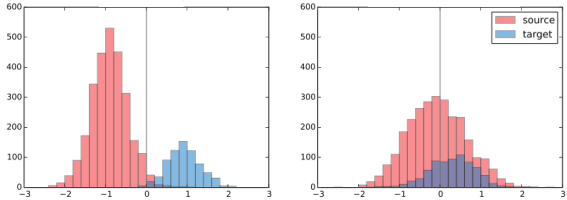

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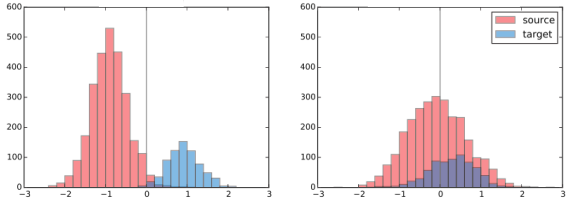

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.. basically, assign a weight to each term of the loss function, depending on how "close" the training example $(\boldsymbol{x}_n, y_n)$ is from the test distribution

Importance-Weighted Correction: A Closer Look

- Note that, since we care about test data, ideally, we would like to learn f by minimizing

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Importance-Weighted Correction: A Closer Look

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- In order to do this, we need to estimate the two densities $p_{tr}(\boldsymbol{x})$ and $p_{te}(\boldsymbol{x})$ (can assume some form for these and estimate them using unlabeled data from both domains)

Semi-supervised Learning

Labeled vs Unlabeled Data

- Supervised Learning models require labeled data
- Learning a reliable model usually requires plenty of labeled data
- Labeled Data: Expensive and Scarce (someone has to do the labeling)
  - Often labeling is very difficult too (e.g., in speech analysis or NLP problems)
- Unlabeled Data: Abundant and Free/Cheap
  - E.g., can easily crawl the web and download webpages/images

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- Here, we will focus on Semi-supervised Learning (SSL)

Why/How Might Unlabeled Data Help?

- Red: + 1, Dark Blue: -1

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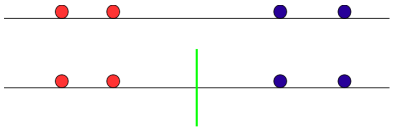

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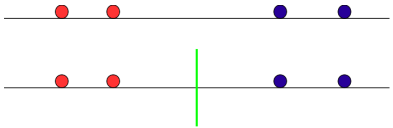

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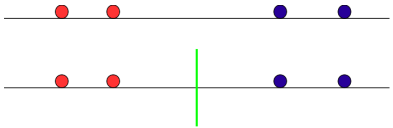

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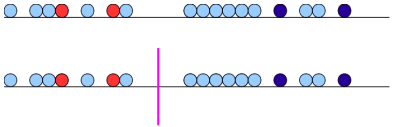

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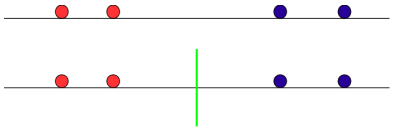

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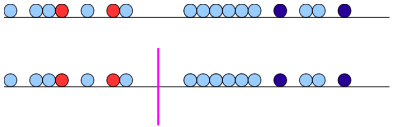

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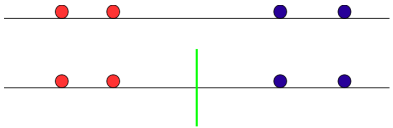

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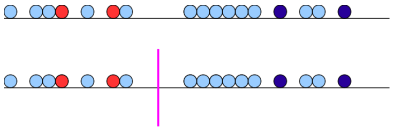

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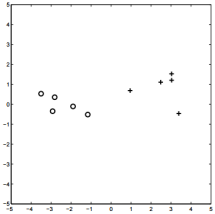

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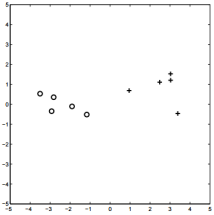

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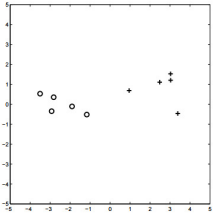

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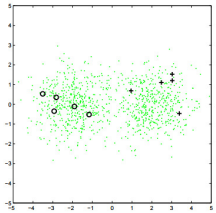
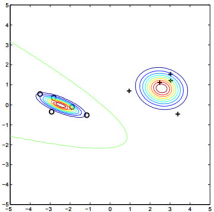


labeled and unlabeled data (small dots)



model learned from labeled data

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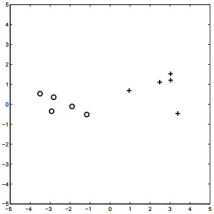

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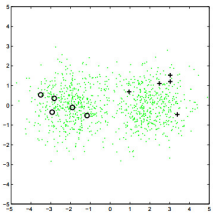

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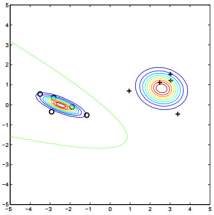

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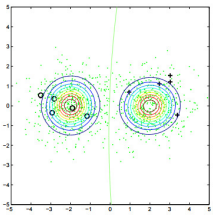

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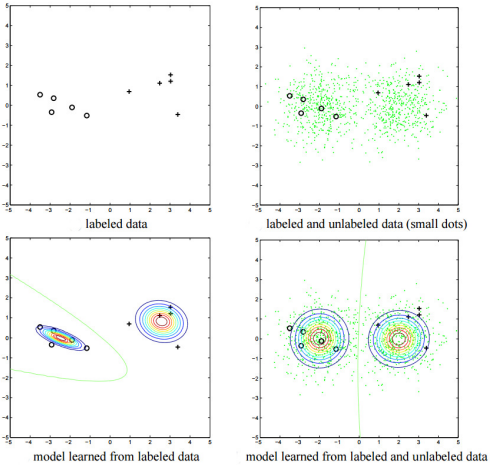

Knowledge of the input distribution helps even if the data is unlabeled

Some Basic Assumptions used in SSL

- Nearby points (may) have the same label
  - Smoothness assumption

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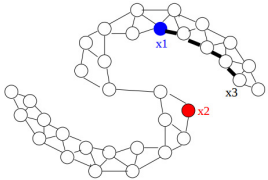
- Note: Generative models already take some of these assumptions into account (recall HW3 problem on semi-supervised learning using EM)

SSL using Graph-based Regularization

- Based on smoothness assumption
- Requires constructing a graph between all the examples (labeled/unlabeled)



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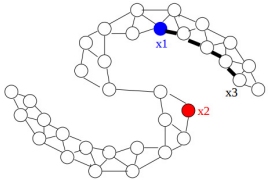

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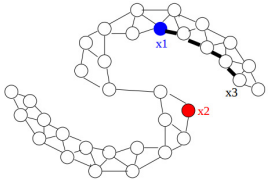

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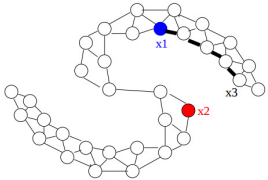

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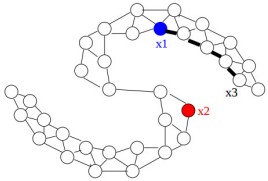

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  - Weighted case: weight of edge connecting examples $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$

$$a_{ij} = \exp(-||\boldsymbol{x}_i - \boldsymbol{x}_j||^2/\sigma^2)$$

.. where $\mathbf{A}$ is the $(L+U) \times (L+U)$ matrix of pairwise similarities

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  - Graph-based regularization optimizes the following objective:

$$\min_{\boldsymbol{f}} \underbrace{\sum_{i \in \mathcal{L}} \ell(y_i, f_i)}_{\text{loss term}} + \underbrace{\lambda R(f)}_{\text{usual regularizer}} + \underbrace{\gamma \sum_{i,j \in \mathcal{L},\mathcal{U}} a_{ij}(f_i - f_j)^2}_{\text{graph-based regularizer}}$$

SSL using EM based Generative Classification

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$$\mathbb{E}[y_j] = +1 \times P(y_j = +1|\hat{\theta}, \boldsymbol{x}_j) + (-1) \times P(y_j = -1|\hat{\theta}, \boldsymbol{x}_j)$$

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$$\mathbb{E}[y_j] = +1 \times P(y_j = +1|\hat{\theta}, \boldsymbol{x}_j) + (-1) \times P(y_j = -1|\hat{\theta}, \boldsymbol{x}_j)$$

  - M step can then perform standard MLE for re-estimating the parameters θ

SSL using EM based Generative Classification

- Suppose data $\mathcal{D}$ is labeled $\mathcal{L} = \{\boldsymbol{x}_i, y_i\}_{i=1}^{L}$ and unlabeled $\mathcal{U} = \{\boldsymbol{x}_j\}_{j=L+1}^{L+U}$
- Assume the following model

$$p(\mathcal{D}|\theta) = \underbrace{\prod_{i=1}^{L} p(\boldsymbol{x}_i, y_i|\theta)}_{\text{labeled}} \underbrace{\prod_{j=L+1}^{L+U} p(\boldsymbol{x}_j|\theta)}_{\text{unlabeled}} = \prod_{i=1}^{L} p(\boldsymbol{x}_i, y_i|\theta) \prod_{j=L+1}^{L+U} \sum_{y_j} p(\boldsymbol{x}_j, y_j|\theta)$$

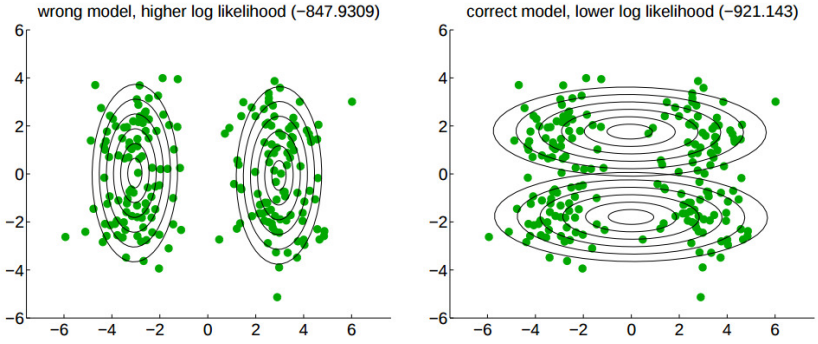
- The unknowns are $\{y_j\}_{j=L+1}^{L+U}$ (latent variables) and θ (parameters)
- We can use EM to estimate the unknowns
  - Given $\theta = \hat{\theta}$, E step will compute expected labels for unlabeled examples

$$\mathbb{E}[y_j] = +1 \times P(y_j = +1|\hat{\theta}, \boldsymbol{x}_j) + (-1) \times P(y_j = -1|\hat{\theta}, \boldsymbol{x}_j)$$

  - M step can then perform standard MLE for re-estimating the parameters θ
- A fairly general framework for semi-supervised learning. Can be used for different types of data (by choosing the appropriate $p(\boldsymbol{x}|y)$ distribution)

Things can go wrong..

If assumptions are not appropriate for the data (e.g., incorrectly specified class conditional distributions)

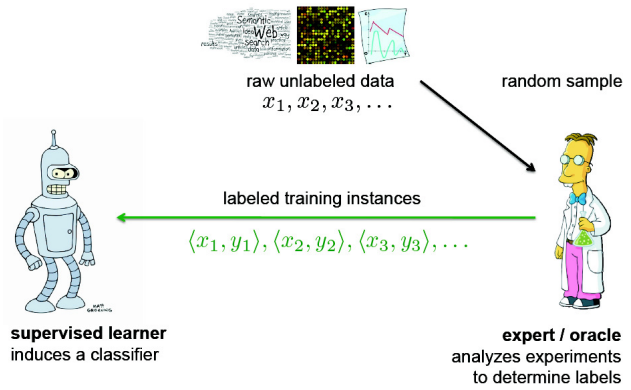


Thus need to be careful/flexible about the choice of class conditional distributions

Active Learning

Passive vs Active Learning

Standard supervised learning assumes a "passive" learner



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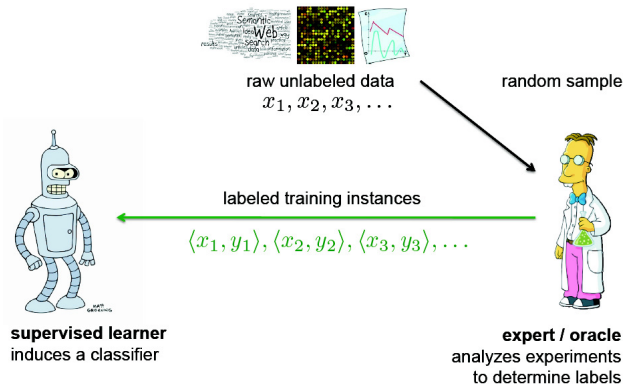
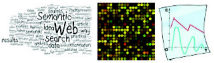


Called "passive" because the learner doesn't have any control over the labeled data it gets to learn

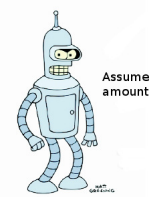
Active Learning

An "active" learner can specifically request labels of "hard" examples that are most useful for learning



raw unlabeled data

$x_1, x_2, x_3, \ldots$



Assumes some small amount of initial labeled training data

active learner
induces a classifier

expert / oracle
analyzes experiments to determine labels

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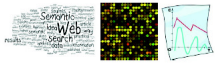
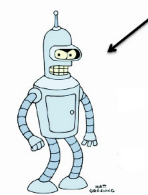


inspect the unlabeled data

raw unlabeled data
$x_1, x_2, x_3, \ldots$



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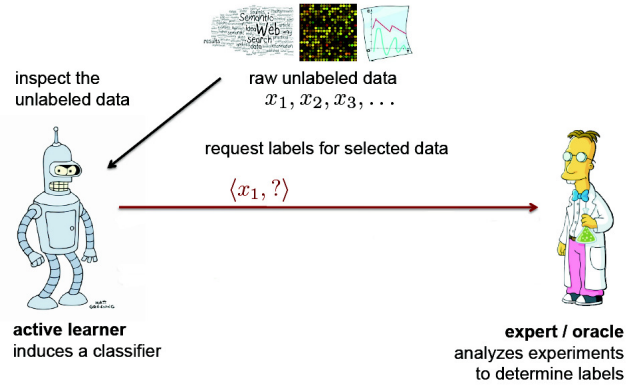

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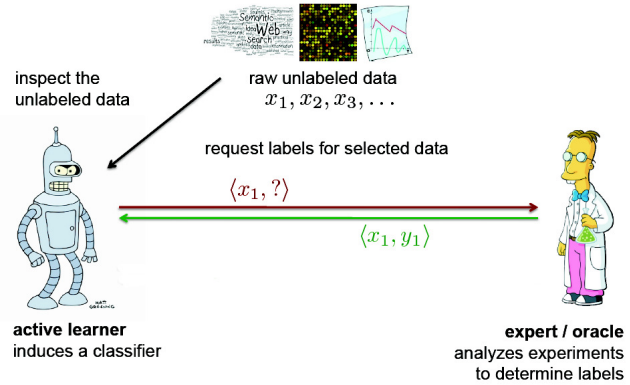

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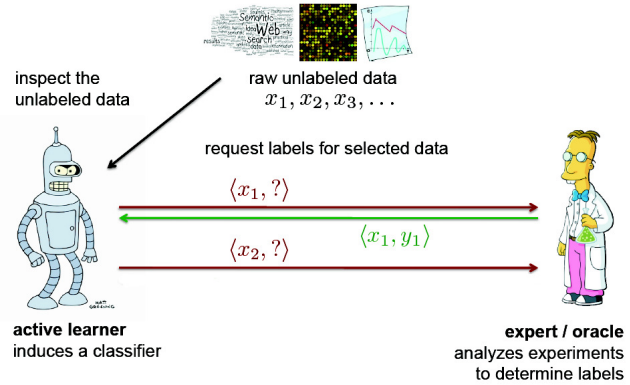

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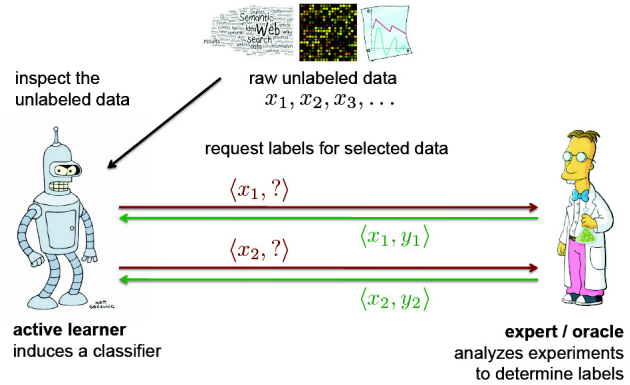

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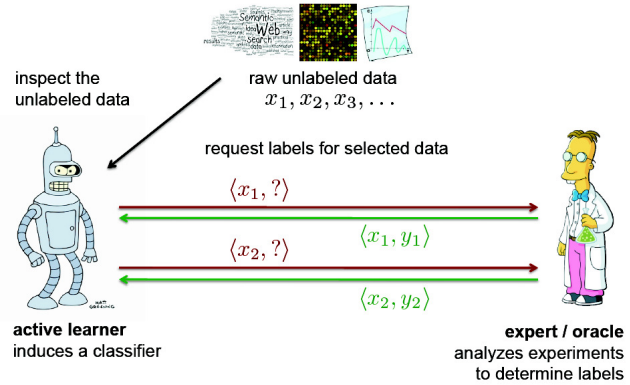

How to quantify the "hardness" or "usefulness" of an unlabeled example?

Active Learning

- Various ways to define the usefulness/hardness of an unlabeled example $\boldsymbol{x}$
- A probabilistic approach can use distribution of y given $\boldsymbol{x}$ to quantify usefulness of $\boldsymbol{x}$

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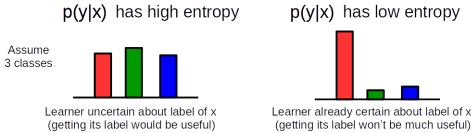

.. and choose example(s) for which the distribution of y given $\boldsymbol{x}$ has the largest entropy

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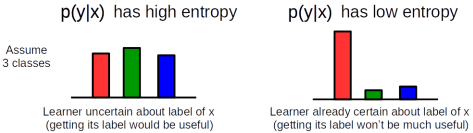
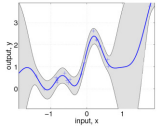


  .. and choose example(s) for which the distribution of y given $\boldsymbol{x}$ has the largest entropy
  - Look at the variance of the posterior predictive $p(y|\boldsymbol{x})$. E.g. for regression,



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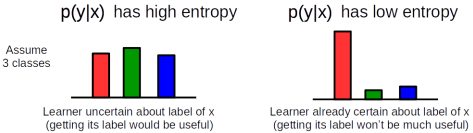

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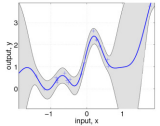

  .. and choose choose example(s) for which variance of posterior predictive is the largest
  - .. many other ways to utilize the information in $p(y|\boldsymbol{x})$