Fundamentals of Learning

MIT 15.097 Course Notes

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Important Problems in Data Mining

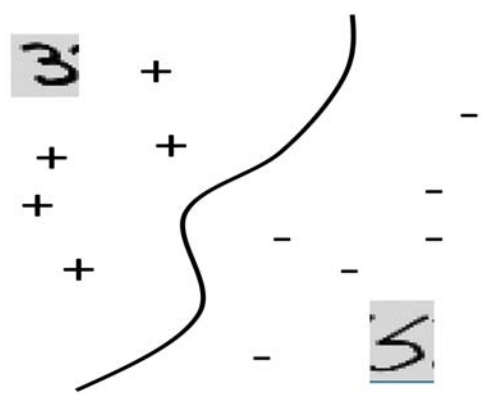
1. Finding patterns (correlations) in large datasets
   -e.g. (Diapers $\rightarrow$ Beer). Use Apriori!

2. Clustering - grouping data into clusters that "belong" together - objects within a cluster are more similar to each other than to those in other clusters.

   - Kmeans, Kmedians
   - Input: $\{x_i\}_{i=1}^m, x_i \in \mathcal{X} \subset \mathbf{R}^n$
   - Output: $f : \mathcal{X} \rightarrow \{1, \ldots, K\}$ (K clusters)
   - clustering consumers for market research, clustering genes into families, image segmentation (medical imaging)

3. Classification

   - Input: $\{(x_i, y_i)\}_{i=1}^m$ "examples," "instances with labels," "observations"
   - $x_i \in \mathcal{X}, y_i \in \{-1, 1\}$ "binary"



   - Output: $f : \mathcal{X} \rightarrow \mathbf{R}$ and use $sign(f)$ to classify.
   - automatic handwriting recognition, speech recognition, biometrics, document classification
   - "LeNet"

4. Regression

- Input: $\{(x_i, y_i)\}_{i=1}^m$, $x_i \in \mathcal{X}, y_i \in \mathbf{R}$
- Output: $f : \mathcal{X} \to \mathbf{R}$
- predicting an individual's income, predict house prices, predict stock prices, predict test scores

5. Ranking (later) - in between classification and regression. Search engines use ranking methods

6. Density Estimation - predict conditional probabilities

   - $\{(x_i, y_i)\}_{i=1}^m$, $x_i \in \mathcal{X}, y_i \in \{-1, 1\}$
   - Output: $f : \mathcal{X} \to [0, 1]$ as "close" to $P(y = 1|x)$ as possible.
   - estimate probability of failure, probability to default on loan

Rule mining and clustering are **unsupervised methods** (no ground truth), and classification, ranking, and density estimation are **supervised methods** (there is ground truth). In all of these problems, we do not assume we know the distribution that the data are drawn from!

Training and Testing (in-sample and out-of-sample) for supervised learning

Training: training data are input, and model f is the output.

$$\{(x_i, y_i)\}_{i=1}^m \Longrightarrow \boxed{\text{Algorithm}} \Longrightarrow f.$$

Testing: You want to predict y for a new x, where (x, y) comes from the same distribution as $\{(x_i, y_i)\}_{i=1}^m$.

That is, $(x, y) \sim D(\mathcal{X}, \mathcal{Y})$ and each $(x_i, y_i) \sim D(\mathcal{X}, \mathcal{Y})$.

Compute $f(x)$ and compare it to y. How well does $f(x)$ match y? Measure goodness of f using a loss function $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbf{R}$:

$$\begin{aligned} R^{\text{test}}(f) &= \mathbf{E}_{(x,y)\sim D}\ell(f(x), y) \\ &= \int_{(x,y)\sim D} \ell(f(x), y)dD(x, y). \end{aligned}$$

R^{test} is also called the **true risk** or the **test error**.

Can we calculate R^{test}?

We want R^{test} to be small, to indicate that $f(x)$ would be a good predictor ("estimator") of y.

For instance

$$\begin{aligned} \ell(f(x), y) &= (f(x) - y)^2 \quad \text{least squares loss, or} \\ \ell(f(x), y) &= \mathbf{1}_{[\text{sign}(f(x)) \neq y]} \quad \text{(mis)classification error} \end{aligned}$$

Which problems might these loss functions correspond to?

How can we ensure $R^{\text{test}}(f)$ is small?

Look at how well f performs (on average) on $\{(x_i, y_i)\}_i$.

$$R^{\text{train}}(f) = \frac{1}{m} \sum_{i=1}^{m} \ell(f(x_i), y_i).$$

R^{train} is also called the **empirical risk** or **training error**. For example,

$$R^{\text{train}}(f) = \frac{1}{m} \sum_{i=1}^{m} \mathbf{1}_{[\text{sign}(f(x_i)) \neq y_i]}.$$

(How many handwritten digits did f classify incorrectly?)

Say our algorithm constructs f so that $R^{\text{train}}(f)$ is small. If $R^{\text{train}}(f)$ is small, hopefully $R^{\text{test}}(f)$ is too.

We would like a guarantee on how close R^{train} is to R^{test}. When would it be close to R^{test}?

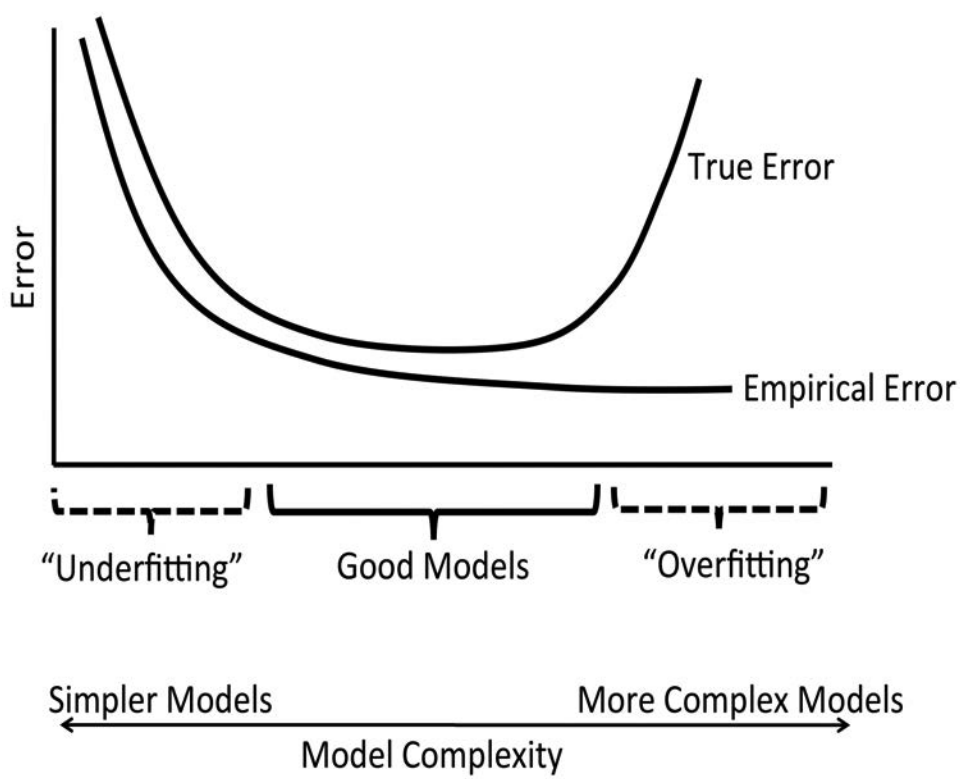
- If m is large.
- If f is "simple."

Illustration

In one of the figures in the illustration, f:

- was overfitted to the data
- modeled the noise
- "memorized" the examples, but didn't give us much other useful information
- doesn't "generalize," i.e., predict. We didn't "learn" anything!

Computational Learning Theory, a.k.a. Statistical Learning Theory, a.k.a., learning theory, and in particular, Vapnik's **Structural Risk Minimization** (SRM) addresses generalization. Here's SRM's classic picture:



Which is harder to check for, overfitting or underfitting?

Computational learning theory addresses how to construct probabilistic guarantees on the true risk. In order to do this, it quantifies the class of "simple models."

Bias/Variance Tradeoff is related to learning theory (actually, bias is related to learning theory).

Inference Notes - Bias/Variance Tradeoff

Regularized Learning Expression

Structural Risk Minimization says that we need some bias in order to learn/generalize (avoid overfitting). Bias can take many forms:

- "simple" models $f(x) = \sum_j \lambda_j x^{(j)}$ where $\|\lambda\|_2^2 = \sum_j \lambda_j^2 < C$
- "prior" in Bayesian statistics
- connectivity of neurons in the brain

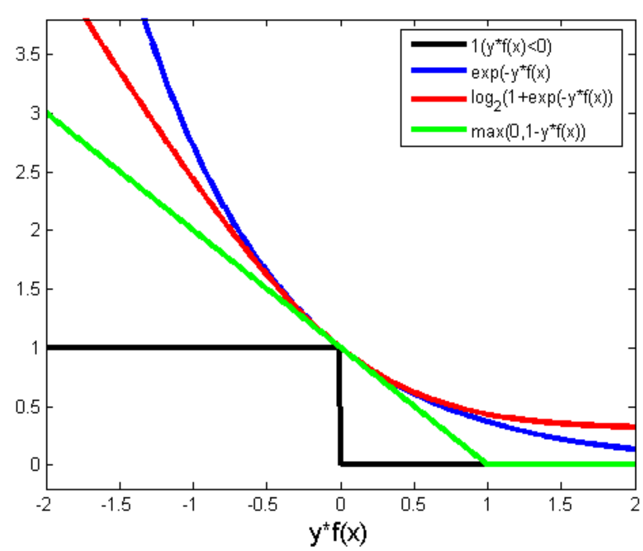
Regularized Learning Expression:

$$\sum_i \ell(f(x_i), y_i) + C R^{\text{reg}}(f)$$

This expression is kind of omnipresent. This form captures many algorithms: SVM, boosting, ridge regression, LASSO, and logistic regression.

In the regularized learning expression, the loss $\ell(f(x_i), y_i)$ could be:

- "least squares loss" $(f(x_i) - y_i)^2$
- "misclassification error" $\mathbf{1}_{[y_i \neq \text{sign}(f(x_i))]} = \mathbf{1}_{[y_i f(x_i) \leq 0]}$
  - Note that minimizing $\sum_i \mathbf{1}_{[y_i f(x_i) \leq 0]}$ is computationally hard.



- "logistic loss" $\log_2\left(1 + e^{-y_i f(x_i)}\right) \Longleftarrow$ logistic regression

- "hinge loss" $\max(0, 1 - y_i f(x_i)) \Longleftarrow$ SVM
- "exponential loss" $e^{-y_i f(x_i)} \Longleftarrow$ AdaBoost

In the regularized learning expression, we define a couple of options for $R^{\text{reg}}(f)$. Usually f is linear, $f(x) = \sum_j \lambda_j x^{(j)}$. We choose $R^{\text{reg}}(f)$ to be either:

- $\|\lambda\|_2^2 = \sum_j \lambda_j^2 \Longleftarrow$ ridge regression, SVM
- $\|\lambda\|_1 = \sum_j |\lambda_j| \Longleftarrow$ LASSO, approximately AdaBoost