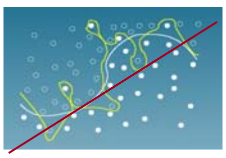
Machine Learning

10-701/15-781, Spring 2008

Overfitting and Model Selection



Eric Xing

Lecture 13, February 27, 2008

Reading: Chap. 1&2, CB & Chap 5,6, TM

Outline

- Overfitting
  - Instance-based learning
  - Regression
- Bias-variance decomposition
- The battle against overfitting:

  each learning algorithm has some "free knobs" that one can "tune" (i.e., heck) to make the algorithm generalizes better to test data.

  But is there a more principled way?
  - Cross validation
  - Regularization
  - Model selection --- Occam's razor
  - Model averaging
    - The Bayesian-frequentist debate
    - Bayesian learning (weight models by their posterior probabilities)

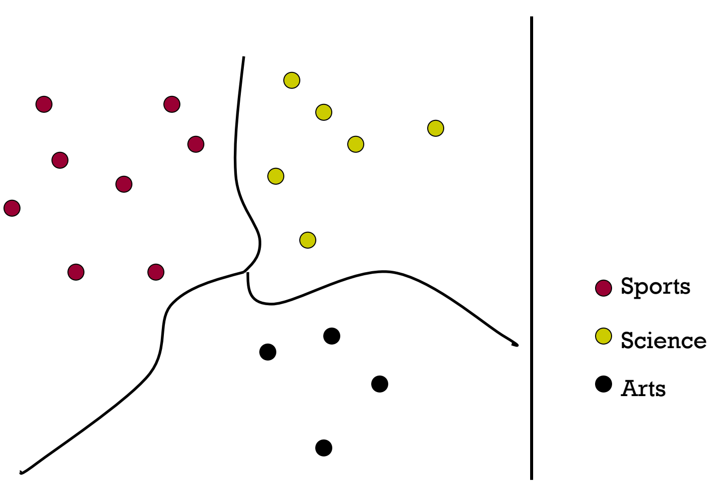
Recall: Vector Space Representation

- Each document is a vector, one component for each term (= word).

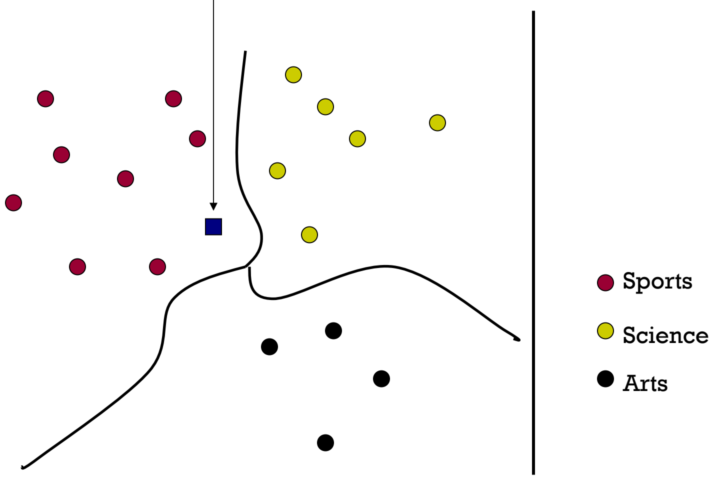
	Doc 1	Doc 2	Doc 3	...
Word 1	3	0	0	...
Word 2	0	8	1	...
Word 3	12	1	10	...
...	0	1	3	...
...	0	0	0	...

- Normalize to unit length.
- High-dimensional vector space:
  - Terms are axes, 10,000+ dimensions, or even 100,000+
  - Docs are vectors in this space

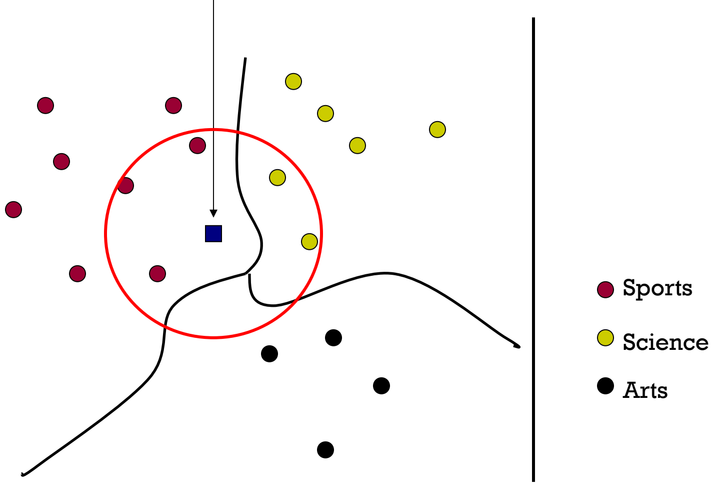
Classes in a Vector Space



Test Document = ?



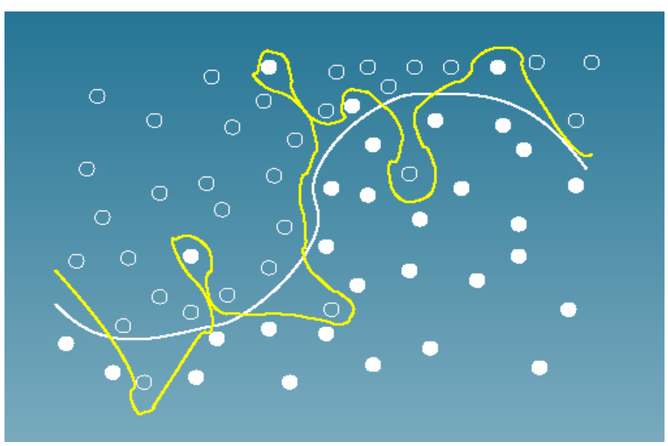
K-Nearest Neighbor (kNN) classifier



Nearest-Neighbor Learning Algorithm

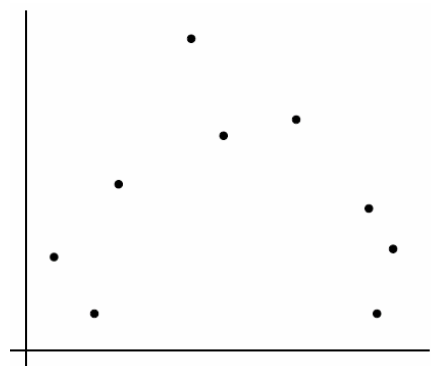
- Learning is just storing the representations of the training examples in *D*.
- Testing instance *x*:
  - Compute similarity between *x* and all examples in *D*.
  - Assign *x* the category of the most similar example in *D*.
- Does not explicitly compute a generalization or category prototypes.
- Also called:
  - Case-based learning
  - Memory-based learning
  - Lazy learning

Overfitting



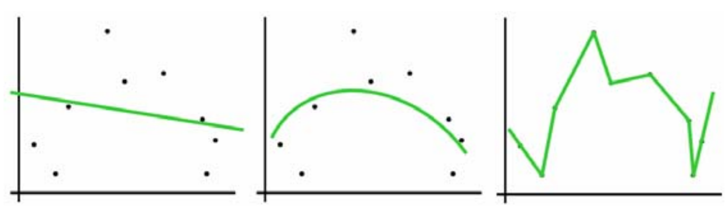
Another example:

- Regression

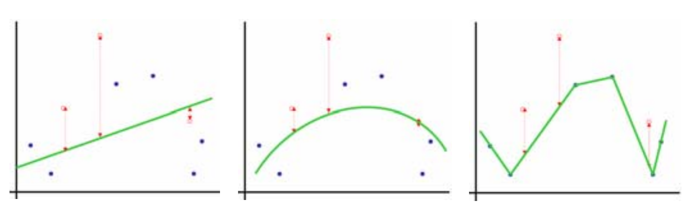


Overfitting, con'd

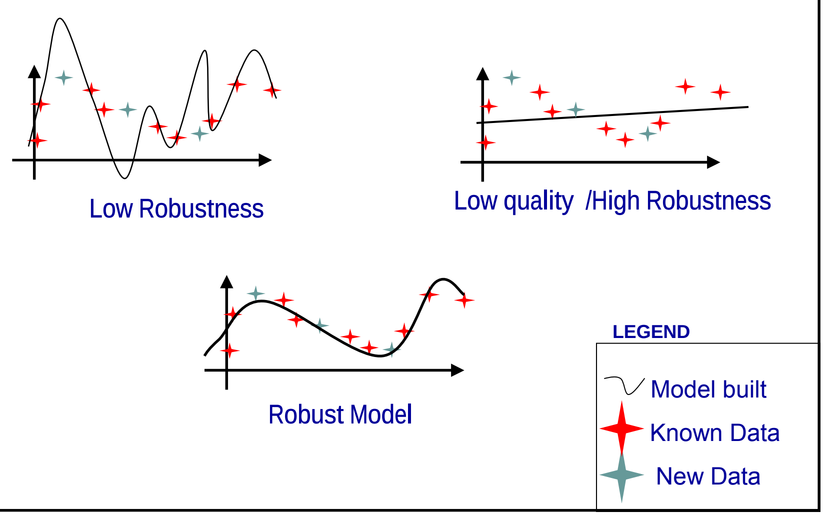
- The models:



- Test errors:

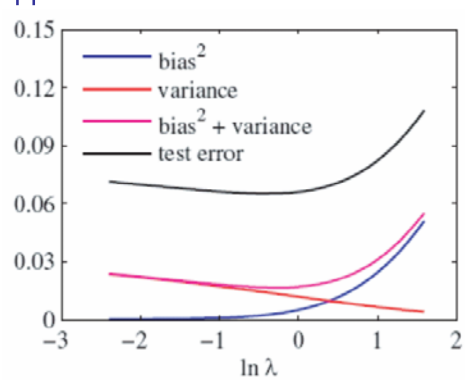


What is a good model?



Bias-variance decomposition

- Now let's look more closely into two sources of errors in an functional approximator:



- In the following we show the Bias-variance decomposition using LR as an example.

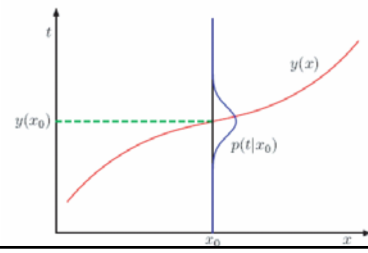
Loss functions for regression

- Let t be the true (target) output and $y(x)$ be our estimate. The expected squared loss is

$$E(L) = \iint L(t, y(x)) p(x,t) dxdt$$
$$= \iint (t - y(x))^2 p(x,t) dxdt$$

- Out goal is to choose $y(x)$ that minimize $E(L)$:
  - Calculus of variations:

$$\frac{\partial E(L)}{\partial y(x)} = 2\int (t - y(x)) p(x,t) dt = 0$$
$$\int y(x) p(x,t) dt = \int t p(x,t) dt$$
$$y^*(x) = \int \frac{tp(x,t)}{p(x)} dt = \int tp(t \mid x) dt = E_{t|x}[t] = E[t \mid x]$$



Expected loss

- Let $h(x) = E[t|x]$ be the **optimal** predictor, and $y(x)$ our actual predictor, which will incur the following expected loss

$$E(y(x) - t)^2 = \int (y(x) - h(x) + h(x) - t)^2 p(x,t) dxdt$$
$$= \int (y(x) - h(x))^2 + 2(y(x) - h(x))(h(x) - t) + (h(x) - t)^2 p(x,t) dxdt$$
$$= \int (y(x) - h(x))^2 p(x) dx + \int (h(x) - t)^2 p(x,t) dxdt$$

There is an error on pp47

  - $\int (h(x) - t)^2 p(x,t) dxdt$ is a noisy term, and we can do no better than this. Thus it is a lower bound of the expected loss.
  - The other part of the error come from $\int (y(x) - h(x))^2 p(x) dx$, and let's take a close look of it.
  - We will assume $y(x) = y(x|w)$ is a parametric model and the parameters w are fit to a training set D. (thus we write $y(x;D)$)

Bias-variance decomposition

- For one data set D and one test point x
  - since the predictor y depend on the data training data D, write $E_D[y(x,D)]$ for the expected predictor over the ensemble of datasets, then (using the same trick) we have:

$$\begin{aligned}(y(x;D)-h(x))^2 &= (y(x;D)-E_D[y(x;D)]+E_D[y(x;D)]-h(x))^2\\ &= (y(x;D)-E_D[y(x;D)])^2+(E_D[y(x;D)]-h(x))^2\\ &\quad +2(y(x;D)-E_D[y(x;D)])(E_D[y(x;D)]-h(x))\end{aligned}$$

  - Surely this error term depends on the training data, so we take an expectation over them:

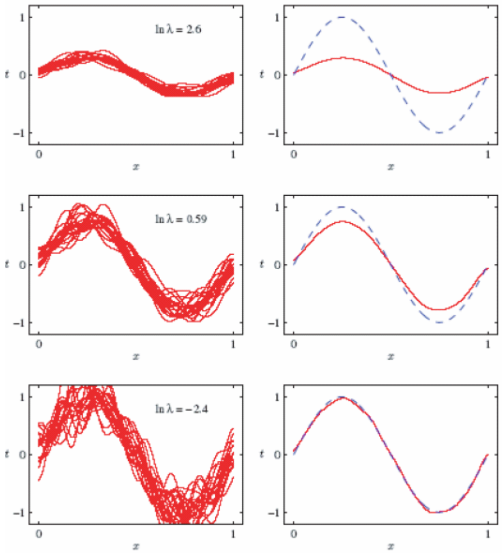
$$E_D\left[(y(x;D)-h(x))^2\right]=(E_D[y(x;D)]-h(x))^2+E_D\left[(y(x;D)-E_D[y(x;D)])^2\right]$$

- Putting things together:

expected loss = $(\text{bias})^2$ + variance + noise

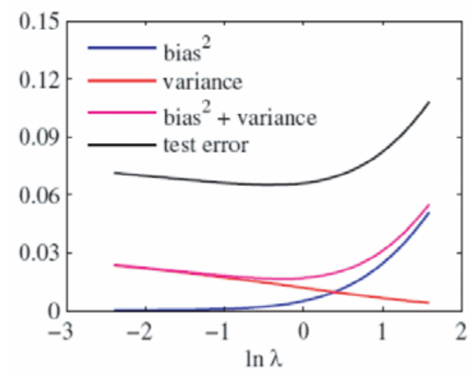
Regularized Regression

Bias-variance tradeoff



- λ is a "regularization" terms in LR, the smaller the λ, is more complex the model (why?)
  - Simple (highly regularized) models have low variance but high bias.
  - Complex models have low bias but high variance.
- You are inspecting an empirical average over 100 training set.
- The actual E_D can not be computed

Bias2+variance vs regularizer



- Bias^2+variance predicts (shape of) test error quite well.
- However, bias and variance cannot be computed since it relies on knowing the true distribution of x and t (and hence $h(x) = E[t|x]$).

The battle against overfitting

Model Selection

- Suppose we are trying select among several different models for a learning problem.
- Examples:
  1. polynomial regression

     $$h(x;\theta) = g(\theta_0 + \theta_1 x + \theta_2 x^2 + \ldots + \theta_k x^k)$$

     - Model selection: we wish to **automatically** and **objectively** decide if k should be, say, 0, 1, . . . , or 10.
  2. locally weighted regression,
     - Model selection: we want to automatically choose the bandwidth parameter τ.
  3. Mixture models and hidden Markov model,
     - Model selection: we want to decide the number of hidden states
- The Problem:
  - Given model family $\mathcal{F} = \{M_1, M_2, \ldots, M_I\}$, find $M_i \in \mathcal{F}$ s.t.

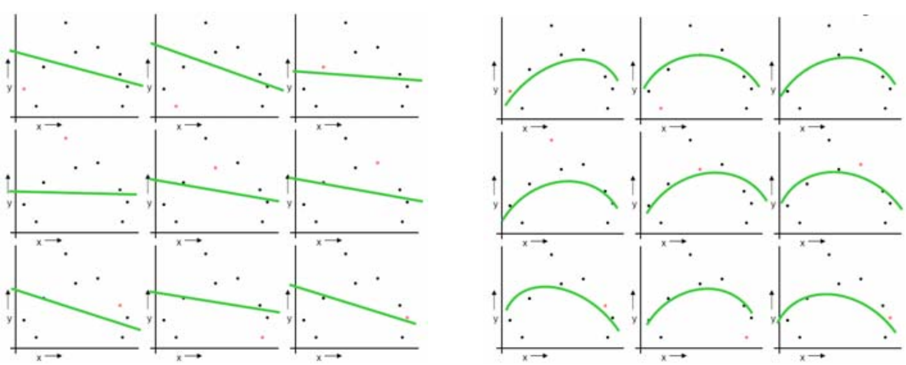
    $$M_i = \arg\max_{M \in \mathcal{F}} J(D, M)$$

Cross Validation

- We are given training data D and test data D_{test}, and we would like to fit this data with a model $p_i(x;\theta)$ from the family $\mathcal{F}$ (e.g, an LR), which is indexed by i and parameterized by θ.
- K-fold cross-validation (CV)
  - Set aside αN samples of D (where $N = |D|$). This is known as the held-out data and will be used to evaluate different values of i.
  - For each candidate model i, fit the optimal hypothesis $p_i(x;\theta^*)$ to the remaining $(1-\alpha)N$ samples in D (i.e., hold i fixed and find the best θ).
  - Evaluate each model $p_i(x|\theta*)$ on the held-out data using some pre-specified risk function.
  - Repeat the above ***K* times**, choosing a **different** held-out data set each time, and the scores are averaged for each model $p_i(.)$ over all held-out data set. This gives an estimate of the risk curve of models over different i.
  - For the model with the lowest rish, say $p_{i^*}(.)$, we use all of D to find the parameter values for $p_{i^*}(x;\theta^*)$.

Example:

- When $\alpha=1/N$, the algorithm is known as Leave-One-Out-Cross-Validation (LOOCV)



MSELOOCV(M$_1$)=2.12 *MSELOOCV(M$_2$)=0.962*

Practical issues for CV

- How to decide the values for K and α
  - Commonly used K = 10 and α = 0.1.
  - when data sets are small relative to the number of models that are being evaluated, we need to decrease α and increase K
  - K needs to be large for the variance to be small enough, but this makes it time-consuming.
- Bias-variance trade-off
  - Small α usually lead to low bias. In principle, *LOOCV* provides an almost unbiased estimate of the generalization ability of a classifier, especially when the number of the available training samples is severely limited; but it can also have high variance.
  - Large α can reduce variance, but will lead to under-use of data, and causing high-bias.
- One important point is that the test data D_{test} is never used in CV, because doing so would result in overly (indeed dishonest) optimistic accuracy rates during the testing phase.

Regularization

- Maximum-likelihood estimates are not always the best (James and Stein showed a counter example in the early 60's)
- Alternative: we "regularize" the likelihood objective (also known as penalized likelihood, shrinkage, smoothing, etc.), by adding to it a penalty term:

$$\hat{\theta}_{\text{shrinkage}} = \arg\max_{\theta}\left[l(\theta; D) - \lambda\|\theta\|\right]$$

  where λ>0 and $||\theta||$ might be the L_1 or L_2 norm.

- The choice of norm has an effect
  - using the L_2 norm pulls directly towards the origin,
  - while using the L1 norm pulls towards the coordinate axes, i.e it tries to set some of the coordinates to 0.
  - This second approach can be useful in a feature-selection setting.

Bayesian and Frequentist

- Frequentist interpretation of probability
  - Probabilities are objective properties of the real world, and refer to limiting relative frequencies (e.g., number of times I have observed heads). Hence one cannot write *P*(Katrina could have been prevented|*D*), since the event will never repeat.
  - Parameters of models are *fixed, unknown constants*. Hence one cannot write $P(\theta|D)$ since θ does not have a probability distribution. Instead one can only write $P(D|\theta)$.
  - One computes point estimates of parameters using various *estimators*, $\theta^* = f(D)$, which are designed to have various desirable qualities when *averaged over future data D* (assumed to be drawn from the "true" distribution).
- Bayesian interpretation of probability
  - Probability describes degrees of belief, not limiting frequencies.
  - Parameters of models are *hidden variables*, so one can compute $P(\theta|D)$ or $P(f(\theta)|D)$ for some function *f*.
  - One estimates parameters by computing $P(\theta|D)$ using Bayes rule:

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)}$$

Bayesian interpretation of regulation

- Regularized Linear Regression
  - Recall that using squared error as the cost function results in the LMS estimate
  - And assume iid data and Gaussian noise, LMS is equivalent to MLE of θ

$$l(\theta) = n\log\frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{\sigma^2}\frac{1}{2}\sum_{i=1}^{n}(y_i - \theta^T\mathbf{x}_i)^2$$

  - Now assume that vector θ follows a normal prior with 0-mean and a diagonal covariance matrix

$$\theta \sim N(0, \tau^2 I)$$

  - What is the posterior distribution of θ?

$$p(\theta|D) \propto p(D,\theta)$$

$$= p(D|\theta)p(\theta) = \left(2\pi\sigma^2\right)^{-n/2}\exp\left\{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}\left(y_n - \theta^T x_i\right)^2\right\} \times C\exp\left\{-(\theta^T\theta/2\tau^2\right\}$$

Bayesian interpretation of regulation, con'd

- The posterior distribution of θ

$$p(\theta|D) \propto \exp\left\{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}\left(y_n - \theta^T x_i\right)^2\right\} \times \exp\left\{-\theta^T\theta/2\tau^2\right\}$$

- This leads to a now objective

$$l_{MAP}(\theta; D) = -\frac{1}{2\sigma^2}\frac{1}{2}\sum_{i=1}^{n}(y_i - \theta^T \mathbf{x}_i)^2 - \frac{1}{\tau^2}\frac{1}{2}\sum_{k=1}^{K}\theta_k^2$$
$$= l(\theta; D) - \lambda\|\theta\|$$

  - This is L_2 regularized LR! --- a MAP estimation of θ
  - What about L_1 regularized LR! (homework)
- How to choose λ.
  - cross-validation!

Feature Selection

- Imagine that you have a supervised learning problem where the number of features n is very large (perhaps n >>#samples), but you suspect that there is only a small number of features that are "**relevant**" to the learning task.

- Later lecture on VC-theory will tell you that this scenario is likely to lead to high generalization error – the learned model will potentially overfit unless the training set is fairly large.

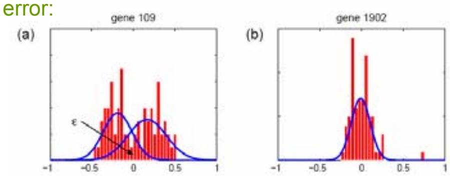
- So lets get rid of useless parameters!

How to score features

- How do you know which features can be pruned?
  - Given labeled data, we can compute some simple score $S(i)$ that measures how informative each feature x_i is about the class labels y.
  - Ranking criteria:
    - Mutual Information: score each feature by its mutual information with respect to the class labels

$$MI(x_i, y) = \sum_{x_i \in \{0,1\}} \sum_{y \in \{0,1\}} p(x_i, y) \log \frac{p(x_i, y)}{p(x_i) p(y)}$$

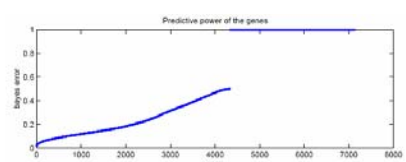
    - Bayes error:



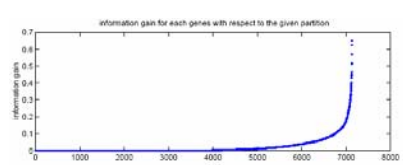
    - Redundancy (Markov-blank score) …
  - We need estimate the relevant p()'s from data, e.g., using MLE

Feature Ranking

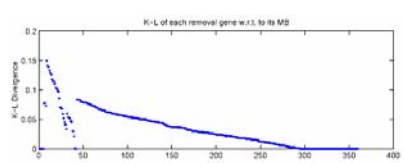
- Bayes error of each gene



- information gain for each genes with respect to the given partition



- KL of each removal gene w.r.t. to its MB



Feature selection schemes

- Given n features, there are 2^n possible feature subsets (why?)
- Thus feature selection can be posed as a model selection problem over 2^n possible models.
- For large values of n, it's usually too expensive to explicitly enumerate over and compare all 2^n models. Some heuristic search procedure is used to find a good feature subset.
- Three general approaches:
  - Filter: i.e., direct feature ranking, but taking no consideration of the subsequent learning algorithm
    - add (from empty set) or remove (from the full set) features one by one based on $S(i)$
    - Cheap, but is subject to local optimality and may be unrobust under different classifiers
  - Wrapper: determine the (inclusion or removal of) features based on performance under the learning algorithms to be used. See next slide
  - Simultaneous learning and feature selection.
    - E.x. L_1 regularized LR, Bayesian feature selection (will not cover in this class), etc.

Wrapper

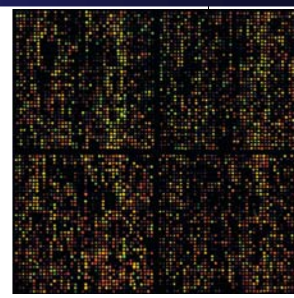
- Forward:
  1. Initialize $\mathcal{F} = \emptyset$
  2. Repeat
     - For $i = 1, \ldots, n$

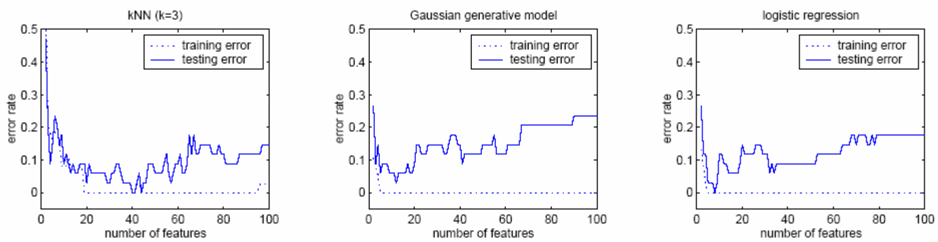
       if $i \notin \mathcal{F}$, let $\mathcal{F}_i = \mathcal{F} \cup \{i\}$, and use some version of cross validation to evaluate features $\mathcal{F}_i$. (I.e., train your learning algorithm using only the features in $\mathcal{F}_i$, and estimate its generalization error.)
     - Set $\mathcal{F}$ to be the best feature subset found on the last step step.
  3. Select and output the best feature subset that was evaluated during the entire search procedure.

- Backward search
  1. Initialize $\mathcal{F}$ = full set
  2. …

Case study [Xing et al, 2001]

- The case:
  - 7130 genes from a microarray dataset
  - 72 samples
  - 47 type I Leukemias (called ALL) and 25 type II Leukemias (called AML)
- Three classifier:
  - kNN
  - Gaussian classifier
  - Logistic regression

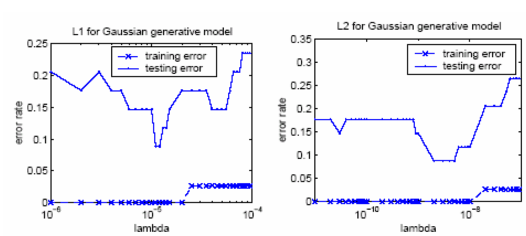




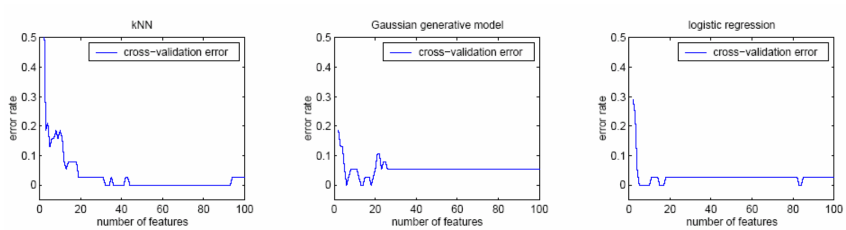
Regularization vs. Feature Selection

- Explicit feature selection often outperform regularization

regression



Feature Selection



Model Selection via Information Criteria

- How can we compare the closeness of a learned hypothesis and the true model?
- The relative entropy (also known as the ***Kullback-Leibler divergence***) is a measure of how different two probability distributions (over the same event space) are.
  - For 2 pdfs, $p(x)$ and $q(x)$, their ***KL-devergence*** is:

$$D(p \| q) = \sum_{x \in X} p(x) \log \frac{p(x)}{q(x)})$$

- The KL divergence between p and q can also be seen as the average number of bits that are wasted by encoding events from a distribution p with a code based on a not-quite-right distribution q .

An information criterion

- Let $f(x)$ denote the truth, the underlying distribution of the data
- Let $g(x,\theta)$ denote the model family we are evaluating
  - $f(x)$ does not necessarily reside in the model family
  - $\theta_{ML}(y)$ denote the MLE of model parameter from data y
- Among early attempts to move beyond Fisher's *Maliximum Likelihood* framework, **Akaike** proposed the following information criterion:

$$E_y\left[D\left(f \| g(x \mid \theta_{ML}(y)\right)\right]$$

which is, of course, intractable (because $f(x)$ is unknown)

AIC and TIC

- AIC (A information criterion, not **Akaike** information criterion)

$$A = \log g(x \mid \hat{\theta}(y)) - k$$

where k is the number of parameters in the model

- TIC (Takeuchi information criterion)

$$A = \log g(x \mid \hat{\theta}(y)) - \mathrm{tr}(I(\theta_0)\Sigma)$$

where

$$\theta_0 = \arg\min D(f \,\|\, g(\cdot \mid \theta)) \qquad I(\theta_0) = -E_x\left[\frac{\partial^2 \log g(x \mid \theta)}{\partial\theta\partial\theta^T}\right]\Bigg|_{\theta=\theta_0} \qquad \Sigma = E_y\left(\hat{\theta}(y) - \theta_0\right)\left(\hat{\theta}(y) - \theta_0\right)^T$$

  - We can approximate these terms in various ways (e.g., using the bootstrap)
  - $\mathrm{tr}(I(\theta_0)\Sigma) \approx k$

Bayesian Model Selection

- Recall the Bayesian Theory: (e.g., for date D and model M)

$$P(M|D) = P(D|M)P(M)/P(D)$$

  - the **posterior** equals to the **likelihood** times the **prior**, up to a constant.

- Assume that $P(M)$ is uniform and notice that $P(D)$ is constant, we have the following criteria:

$$P(D \mid M) = \int_\theta P(D \mid \theta, M) P(\theta \mid M) d\theta$$

- A few steps of approximations (you will see this in advanced ML class in later semesters) give you this:

$$P(D \mid M) \approx \log P(D \mid \hat{\theta}_{ML}) - \frac{k}{2}\log N$$

where N is the number of data points in D.