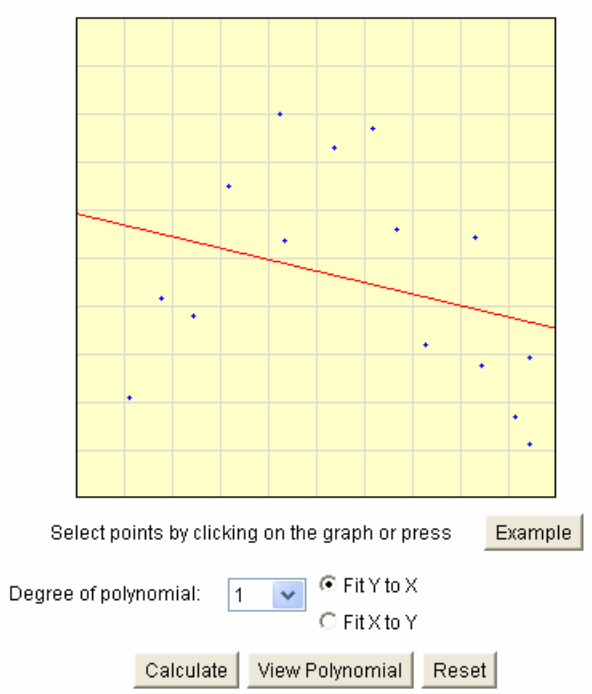
10601
Machine Learning

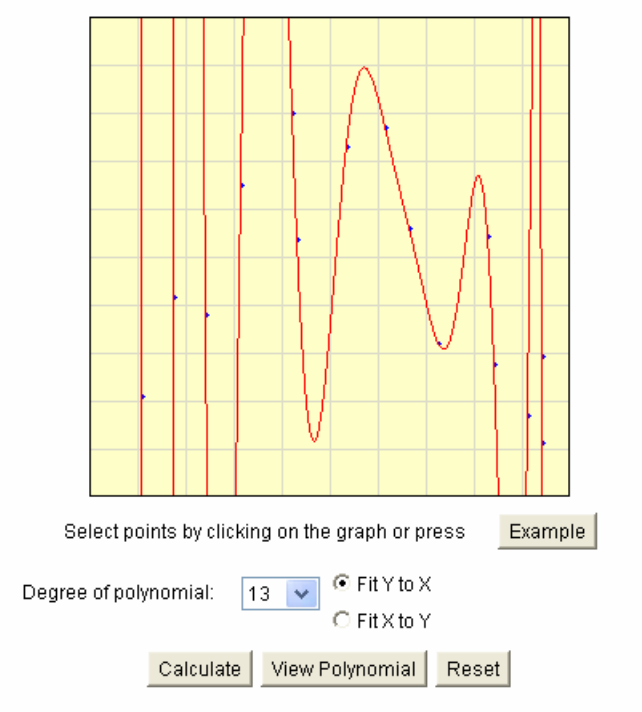
Evaluating classifiers: Model and feature selection

Model selection issues

- **We have seen some of this before …**
- **Selecting features (or basis functions)**
  - Linear regression
  - Logistic regression
  - SVMs
- **Selecting parameter value**
  - Prior strength
    - Naïve Bayes, linear and logistic regression
  - Regularization strength
    - Linear and logistic regression
  - Decision trees
    - depth, number of leaves
  - Clustering
    - Number of clusters
- More generally, these are called **Model Selection** Problems

Training and test set error as a function of model complexity





Simple greedy model selection algorithm

- Pick a dictionary of features
  - e.g., polynomials for linear regression
- Greedy heuristic:
  - Start from empty (or simple) set of features $F_0 = \varnothing$
  - Run learning algorithm for current set of features F_t
    - Obtain h_t
  - Select **next best feature $\mathbf{X_i^*}$**
    - e.g., X_j that results in lowest training error learner when learning with $F_t \cup \{X_j\}$
  - $F_{t+1} \leftarrow F_t \cup \{X_i^*\}$
  - Recurse

Greedy model selection

- Applicable in many settings:
  - Linear regression: Selecting basis functions
  - Naïve Bayes: Selecting (independent) features $P(X_i|Y)$
  - Logistic regression: Selecting features (basis functions)
  - Decision trees: Selecting leaves to expand
- Only a heuristic!
  - But, sometimes you can prove something cool about it

Simple greedy model selection algorithm

- Greedy heuristic:
  - …
  - Select **next best feature X_i^***
    - e.g., X_j that results in lowest training error learner when learning with $F_t \cup \{X_j\}$
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When do you stop???

- When training error is low enough?
- When test set error is low enough?

But how can we tell what is the test error?

Validation set

- In general, for evaluating a classifier we **randomly** split a dataset into two parts:
  - Training data – $\{\mathbf{x}_1,\ldots, \mathbf{x}_{\text{Ntrain}}\}$
  - Test data – $\{\mathbf{x}_1,\ldots, \mathbf{x}_{\text{Ntest}}\}$
- Why not use the test data to determine the correct model? Or when to stop?
- **Test data must always remain independent**!
  - Never ever ever ever learn on test data, including for model selection
- Given a dataset, **randomly** split it into three parts:
  - Training data – $\{\mathbf{x}_1,\ldots, \mathbf{x}_{\text{Ntrain}}\}$
  - Validation data – $\{\mathbf{x}_1,\ldots, \mathbf{x}_{\text{Nvalid}}\}$
  - Test data – $\{\mathbf{x}_1,\ldots, \mathbf{x}_{\text{Ntest}}\}$
- Use validation data for tuning learning algorithm, e.g., model selection
  - Save test data for very final evaluation

Simple greedy model selection algorithm

- Greedy heuristic:
  - …
  - Select **next best feature $\mathbf{X_i^*}$**
    - e.g., X_j that results in lowest training error learner when learning with $F_t \cup \{X_j\}$
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When do you stop???

- When training error is low enough?
- When test set error is low enough?
- When validation set error is low enough?

Sometimes, but there is an even better option …

Validating a learner, not a hypothesis (intuition only, not proof)

- With a validation set, we can estimate the error of 1 hypothesis on 1 dataset

  - e.g. Should I use a polynomial of degree 3 or 4

- However, what we really want is to estimate the error of learner over multiple datasets

$$E_{\{x,y\}}[h_t]$$

Expected error over all datasets

Our current model / classifier

(LOO) Leave-one-out cross validation

- Consider a **validation set with 1 example**:
  - D – training data
  - D\i – training data with i th data point moved to validation set
- **Learn classifier $h_{D\backslash i}$ with the $D\backslash i$ dataset**
- **Estimate true error** as:
  - 0 if $h_{D\backslash i}$ classifies i th data point correctly
  - 1 if $h_{D\backslash i}$ is wrong about i th data point
  - Seems really bad estimator, but wait!
- **LOO cross validation**: Average over all data points i:
  - **For each data point you leave out, learn a new classifier $h_{D\backslash i}$**
  - **Estimate error** as:

$$error_{LOO} = \frac{1}{m} \sum_{i=1}^{m} \mathbb{1}\left(h_{\mathcal{D}\backslash i}(\mathbf{x}^i) \neq y^i\right)$$

LOO cross validation is (almost) unbiased estimate of true error!

- When computing **LOOCV error, we only use *m-1* data points**
  - So it's not an estimate of true error of learning with *m* data points
  - Usually pessimistic, though – learning with less data typically gives worse answer

- **LOO is almost unbiased**!
  - Let $error_{true,m-1}$ be true error of learner when you only get *m-1* data points
  - LOO is unbiased estimate of $error_{true,m-1}$:

$$E_{\mathcal{D}}[error_{LOO}] = error_{true,m-1}$$

- **Great news!**
  - **Use LOO error for model selection!!!**

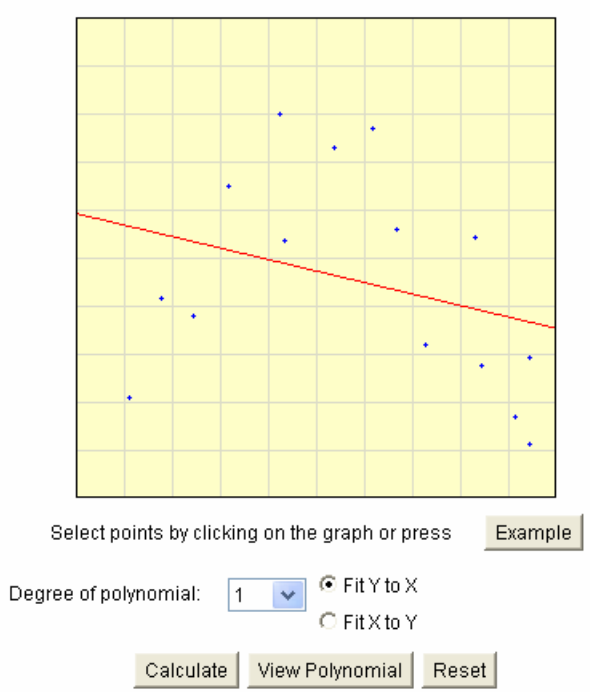
Simple greedy model selection algorithm

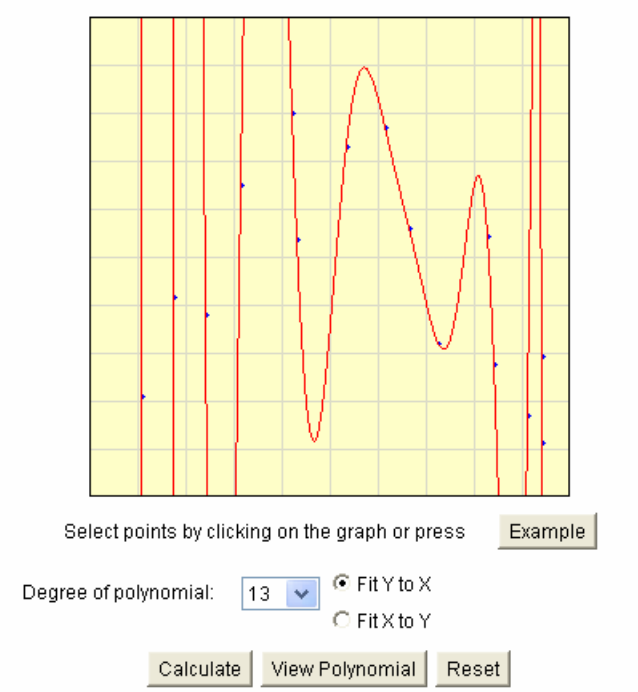
- Greedy heuristic:
  - …
  - Select **next best feature X_i^***
    - e.g., X_j that results in lowest training error learner when learning with $F_t \cup \{X_j\}$
  - $F_{t+1} \leftarrow F_t \cup \{X_i^*\}$
  - Recurse

When do you stop???

- When training error is low enough?
- When test set error is low enough?
- When validation set error is low enough?
- **STOP WHEN $error_{LOO}$ IS LOW!!!**

LOO cross validation error





Computational cost of LOO

- Suppose you have 100,000 data points
- You implemented a great version of your learning algorithm
  - Learns in only 1 second
- Computing LOO will take about 1 day!!!
  - If you have to do for each choice of basis functions, it will take forever!

Solution: Use *k*-fold cross validation

- Randomly **divide training data into *k* equal parts**
  - $D_1,\ldots,D_k$
- For each *i*
  - **Learn classifier $h_{D\setminus Di}$ using data point not in D_i**
  - **Estimate error of $h_{D\setminus Di}$ on validation set D_i:**

$$error_{\mathcal{D}_i} = \frac{k}{m} \sum_{(\mathbf{x}^j, y^j) \in \mathcal{D}_i} \mathbb{1}\left(h_{\mathcal{D}\setminus\mathcal{D}_i}(\mathbf{x}^j) \neq y^j\right)$$

- ***k*-fold cross validation error is average** over data splits:

$$error_{k-fold} = \frac{1}{k} \sum_{i=1}^{k} error_{\mathcal{D}_i}$$

- *k*-fold cross validation properties:
  - **Much faster to compute** than LOO
  - **More (pessimistically) biased** – using much less data, only *m(k-1)/k*

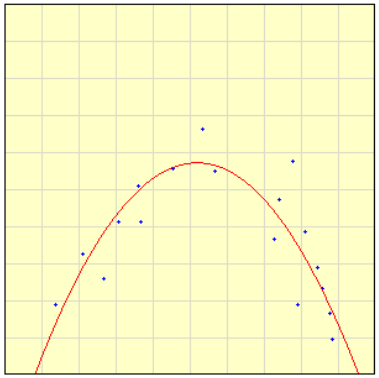
Regularization

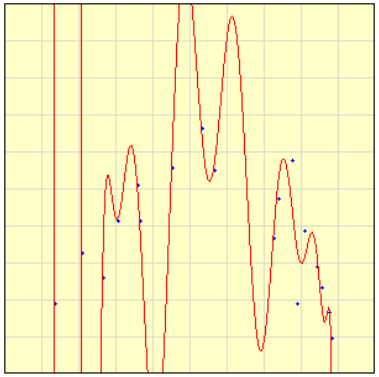
- Model selection 1 (using CV): **Greedy**
  - Pick subset of features that have yield low LOO error
- Model selection 2: **Regularization**
  - Include **all possible features!**
  - **Penalize "complicated" hypothesis**

Regularization in linear regression

- Overfitting usually leads to very large parameter choices, e.g.:

$-2.2 + 3.1\ X - 0.30\ X^2$ $\qquad$ $-1.1 + 4{,}700{,}910.7\ X - 8{,}585{,}638.4\ X^2 + \ldots$





- Regularized least-squares (a.k.a. ridge regression):

$$w^* = \arg\min_w \sum_j (w^T x_j - y_j)^2 + \lambda \sum_i w_i^2$$

Other regularization examples

- **Logistic regression** regularization
  - Maximize data likelihood minus **penalty for large parameters**

$$\arg\max_{\mathbf{w}} \sum_j \ln P(y^j|\mathbf{x}^j, \mathbf{w}) - \lambda \sum_i w_i^2$$

  - **Biases towards small parameter values**

- **Naïve Bayes** regularization
  - **Prior** over likelihood of features
  - **Biases away from zero probability** outcomes

- **Decision tree** regularization
  - Many possibilities, e.g., **Chi-Square test**
  - **Biases towards smaller trees**

- **Sparsity:** find good solution with few basis functions, e.g.:
  - **Simple greedy model selection from earlier in the lecture**
  - **L1 regularization, e.g.:**

$$w^* = \arg\min_w \sum_j (\mathbf{w}^T x_j - y_j)^2 + \lambda \sum_i |w_i|$$

Regularization and Bayesian learning

$$p(\mathbf{w} \mid Y, \mathbf{X}) \propto P(Y \mid \mathbf{X}, \mathbf{w}) p(\mathbf{w})$$

- For example, if we assume a zero mean, Gaussian prior for *w* in a logistic regression classification we would end up with an L2 regularization
  - Why?
  - Board …
  - What is λ?

- Similar interpretation for other learning approaches:
  - **Linear regression**: Also zero mean, Gaussian prior for **w**
  - **Naïve Bayes**: Directly defined as prior over parameters

How do we pick magic parameter λ?

Cross Validation!!!

Occam's Razor

- William of Ockham (1285-1349) *Principle of Parsimony*:
  - "One should not increase, beyond what is necessary, the number of entities required to explain anything."
- Regularization penalizes for *"complex explanations"*

- Alternatively (but pretty much the same), use *Minimum Description Length (MDL) Principle*:
  - minimize *length*(misclassifications) + *length*(hypothesis)

- *length*(misclassifications) – e.g., #wrong training examples
- *length*(hypothesis) – e.g., size of decision tree

Minimum Description Length Principle

- MDL prefers small hypothesis that fit data well:

$$h_{MDL} = \arg\min_h L_{C_1}(\mathcal{D} \mid h) + L_{C_2}(h)$$

  - $L_{C1}(D|h)$ – description length of data under code C_1 given h
    - Only need to describe points that h doesn't explain (classify correctly)
  - $L_{C2}(h)$ – description length of hypothesis h
- Decision tree example
  - $L_{C1}(D|h)$ – #bits required to describe data given h
    - If all points correctly classified, $L_{C1}(D|h) = 0$
  - $L_{C2}(h)$ – #bits necessary to encode tree
  - Trade off quality of classification with tree size

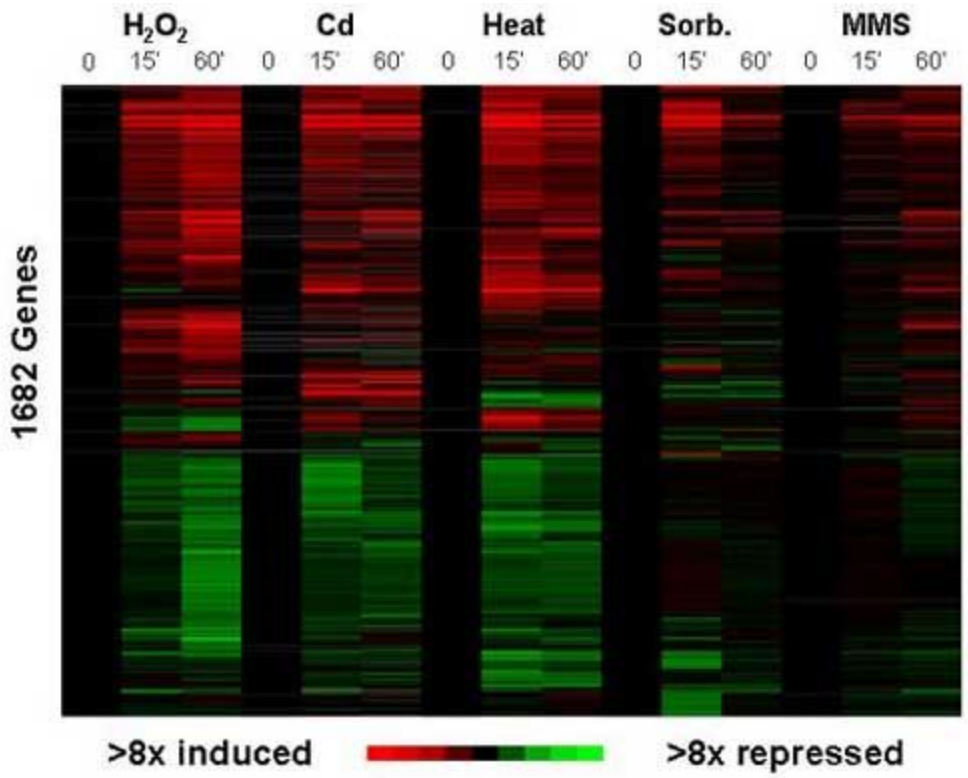
What you need to know about Model Selection, Regularization and Cross Validation

- Cross validation
  - (Mostly) Unbiased estimate of true error
  - LOOCV is great, but hard to compute
  - *k*-fold much more practical
  - Use for selecting parameter values!
- Model selection
  - Search for a model with low cross validation error
- Regularization
  - Penalizes for complex models
  - Select parameter with cross validation
  - Really a Bayesian approach
- Minimum description length
  - Information theoretic interpretation of regularization

Feature selection

- Choose an optimal subset from the set of all N features
  - Only use a subset of a possible words in a dictionary
  - Only use a subset of genes
- Why?
- Can we do model selection to solve this? – 2^n models

eg. Microarray data



Courtesy : Paterson Institute

Two approaches: 1. Filter

- Independent of classifier used
- Rank features using some criteria based on their relevance to the classification task
- For example, mutual information:

$$I(X;Y) = \sum_{y \in Y} \sum_{x \in X} p(x,y) \log \left(\frac{p(x,y)}{p_1(x)\, p_2(y)} \right),$$

- Choose a subset based on the sorted scores for the criteria used

2. Wrapper

- Classifier specific
- Greedy (large search space)
- Initialize F = null set
  - At each step, using cross validation or an information theoretic criteria, choose a feature to add to the subset [training should be done with only features in F + new feature]
  - Add the chosen feature to the subset
- Repeat until no improvement to CV accuracy