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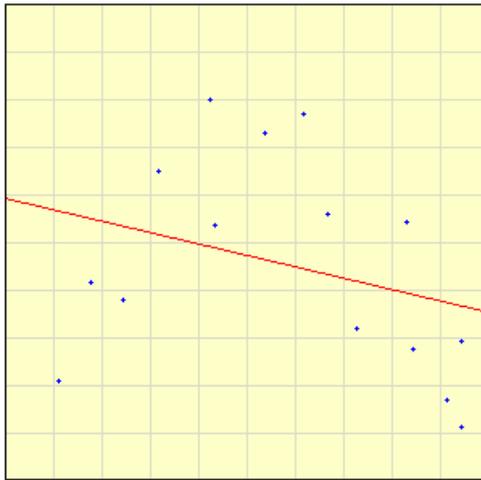
# Machine Learning

## 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
    - Naïve Bayes, linear and logistic regression
  - Decision trees
    - depth, number of leaves
  - Boosting
    - Number of rounds
- More generally, these are called **Model Selection Problems**

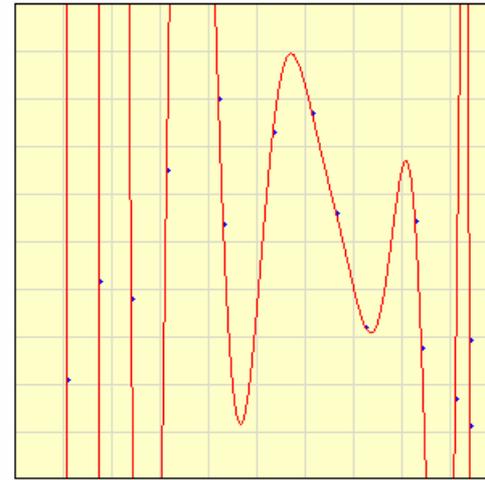
# Training and test set error as a function of model complexity



Select points by clicking on the graph or press [Example](#)

Degree of polynomial:   Fit Y to X  
 Fit X to Y

[Calculate](#) [View Polynomial](#) [Reset](#)



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# 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  $F_0 = \emptyset$
  - Run learning algorithm for current set of features  $F_t$ 
    - Obtain  $h_t$
  - 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

# 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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  - Recurse

When do you stop???

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

# Validation set

- Thus far: Given a dataset, **randomly** split it into two parts:
  - Training data –  $\{\mathbf{x}_1, \dots, \mathbf{x}_{N_{\text{train}}}\}$
  - Test data –  $\{\mathbf{x}_1, \dots, \mathbf{x}_{N_{\text{test}}}\}$
- But **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 –  $\{\mathbf{x}_1, \dots, \mathbf{x}_{N_{\text{train}}}\}$
  - Validation data –  $\{\mathbf{x}_1, \dots, \mathbf{x}_{N_{\text{valid}}}\}$
  - Test data –  $\{\mathbf{x}_1, \dots, \mathbf{x}_{N_{\text{test}}}\}$
- 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**  $X_i^*$ 
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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, get to estimate error of 1 hypothesis on 1 dataset
  - e.g. Should I use a polynomial of degree 3 or 4
- Need to estimate error of learner over multiple datasets to select parameters  $E_{\{x,y\}}[h_t]$

Expected error over all  
datasets

# (LOO) Leave-one-out cross validation

- Consider a **validation set with 1 example**:
  - $D$  – training data
  - $D \setminus i$  – training data with  $i$ th data point moved to validation set
- **Learn classifier  $h_{D \setminus i}$  with  $D \setminus i$  dataset**
- **Estimate true error** as:
  - 0 if  $h_{D \setminus i}$  classifies  $i$ th data point correctly
  - 1 if  $h_{D \setminus i}$  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  $h_{D \setminus i}$**
  - **Estimate error** as:

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

# 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 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!!!**

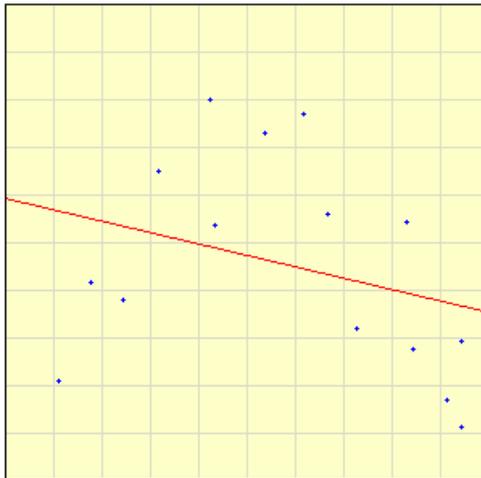
# Simple greedy model selection algorithm

- 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<sub>LOO</sub> IS LOW!!!**

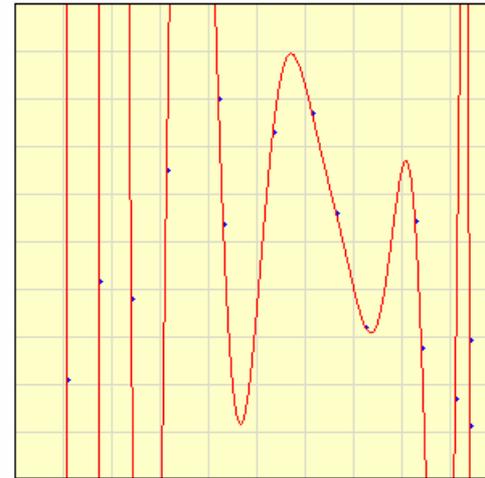
# LOO cross validation error



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# 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**

- $D_1, \dots, D_k$

- For each  $i$

- **Learn classifier  $h_{D \setminus D_i}$  using data point not in  $D_i$**

- **Estimate error of  $h_{D \setminus D_i}$  on validation set  $D_i$ :**

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

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

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

- $k$ -fold cross validation properties:

- **Much faster to compute** than LOO

- **More (pessimistically) biased** – using much less data, only  $m(k-1)/k$

# Regularization

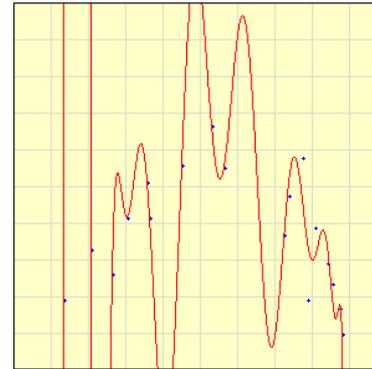
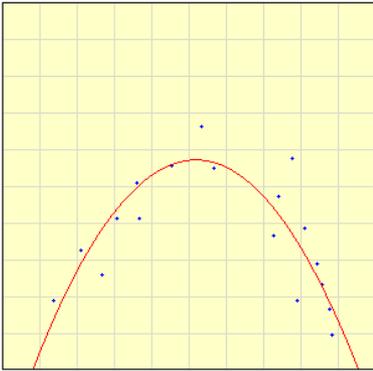
- Model selection 1 (using CV): **Greedy**
  - Pick subset of features that have yield low LOO error
- Model selection 2: **Regularization**
  - Include **all possible features!**
  - **Penalize “complicated” hypothesis**

# Regularization in linear regression

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

$$-2.2 + 3.1 X - 0.30 X^2$$

$$-1.1 + 4,700,910.7 X - 8,585,638.4 X^2 + \dots$$



- 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**

For example, the Beta distribution we discussed

- **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.:**

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

How do we pick magic parameter  $\lambda$ ?

**Cross Validation!!!**

# 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  $\lambda$ ?
- Similar interpretation for other learning approaches:
  - **Linear regression**: Also zero mean, Gaussian prior for  $\mathbf{w}$
  - **Naïve Bayes**: Directly defined as prior over parameters

# 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  $length(\text{misclassifications}) + length(\text{hypothesis})$
- $length(\text{misclassifications})$  – e.g., #wrong training examples
- $length(\text{hypothesis})$  – e.g., size of decision tree

# Minimum Description Length Principle

- MDL prefers small hypothesis that fit data well:

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

- $L_{C_1}(D|h)$  – description length of data under code  $C_1$  given  $h$ 
  - Only need to describe points that  $h$  doesn't explain (classify correctly)
- $L_{C_2}(h)$  – description length of hypothesis  $h$

- Decision tree example

- $L_{C_1}(D|h)$  – #bits required to describe data given  $h$ 
  - If all points correctly classified,  $L_{C_1}(D|h) = 0$
- $L_{C_2}(h)$  – #bits necessary to encode tree
- Trade off quality of classification with tree size

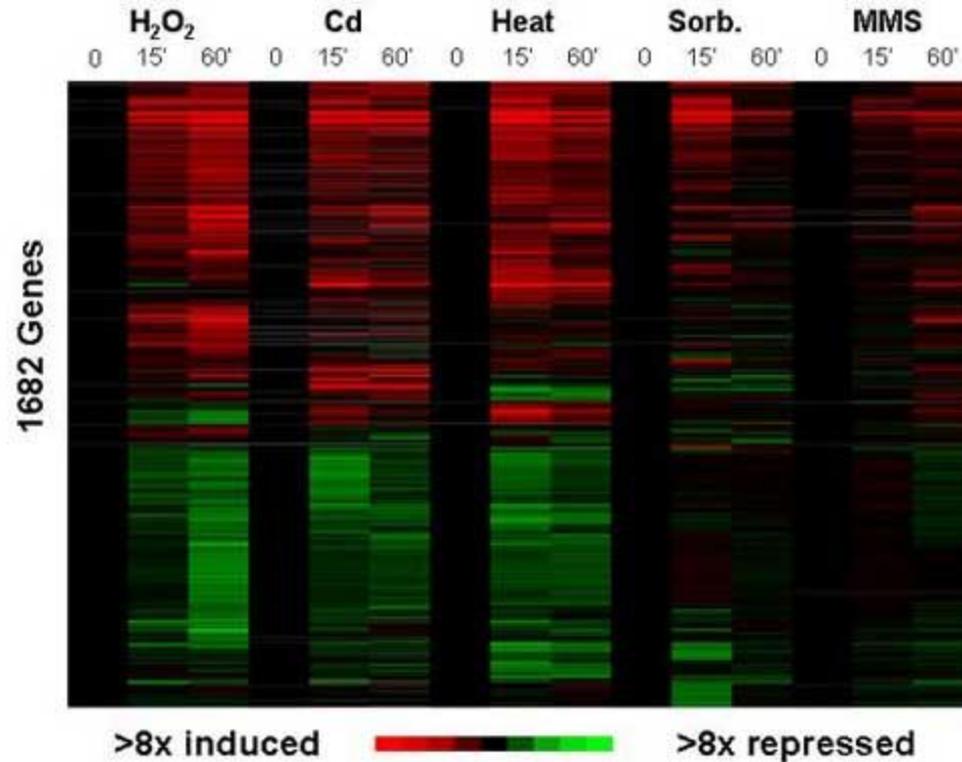
# What you need to know about Model Selection, Regularization and Cross Validation

- 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  $F = \text{null set}$ 
  - 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  $F + \text{new feature}$ ]
  - Add the chosen feature to the subset
- Repeat until no improvement to CV accuracy

# Midterm

- In class, 2 hours
- Open book, open notes
- You can bring a calculator
- No communication devices

Next week

The Google logo is displayed in its characteristic multi-colored font. The letters are: 'G' (blue), 'O' (red), 'O' (yellow), 'g' (blue), 'l' (green), and 'e' (red). Each letter has a slight 3D effect with a shadow underneath.

Google