- Simple matching coefficient  $\overline{(C_{00}+C_{01}+C_{10}+C_{11})}$ 
  - How many times the variables are the same
- $(C_{01} + C_{10} + C_{11})$ Jaccard coefficient
- $\bullet\,$  intersection divided by union of 1 values

# Fitting stumps using classification error

```
store this rule ifits the lowest error so far
                                                                                                                                            classify all examples based on threshold
                                                                          find mode of y when X(:,j) > threshold
                                                                                                              find mode of y when X(:,j) < threshold
                    for every object i
threshold = X(i,j)
                                                                                                                                                                        sum(yhat ~= y)
for every feature j
```

# Classifying a new example

```
if X(i,model.splitVariable) > model.splitValue
function [y] = predict(model,X)
                                                        if isempty(model.splitVariable)
                                                                                     y = model.splitSat*ones(t,1);
                                                                                                                                                                                                                           y(i,1) = model.splitSat;
                                                                                                                                                                                                                                                                            y(i,1) = model.splitNot;
                                                                                                                                   y = zeros(t, 1);
                             [t,d] = size(X);
                                                                                                                                                                      for i = 1:t
```

#### Big O notation

- Computing one rule costs O(n)
- Compute scores for dt rules (where t = thresholds) is O(ndt)
- If we use at most n thresholds for each feature its now  $O(n^2d)$
- If we sort the features it costs O(nlogn) per feature and you do at most O(n) updates per feature
- This gives us runtime O(ndlogn) down from  $O(n^d)$
- For trees of depth m,
- the number of stumps to fit is  $2^{m-1}$  naive approach would be to say  $O(2^{m-1}ndlogn)$
- · However at each depth we split the n examples across the stumps. this means that each depth will only need to look at n examples and the cost for each layer is O(ndlogn)
- This gives us total cost O(mndlogn) to go through all m layers

### Effect of depth

- Depth will usually lead to more complicated and longer models that will also decrease the training error this usually means you are
  - over fitting to your training set. • It usually best to choose the depth based on cross validation to see where the model has begun to over fit the data.

## Learning theory

Training vs Test error

- Memorization vs Learning
- Can do well on training data by memorizing it, only learned if you do well in new situations Most common assumption: independent and identically distributed

- all objects come from the same distribution
- the objects are sampled independently (order doesn't matter)

# Validation Sets and Cross Validation - train on your training data, predict on your validation data

- Validation error initially decreases, eventually increases (overfits), its only unbiased if you use it once
  - if you minimize it to choose between models it introduces optimization bias
    - Optimization bias is:
- small if you compare a few models ie. best decision tree on training set depths 1 to 10 validation likely still approximates error, overfitting risk is low
- comparing a ton of models some that may likely have low validation error by chance, overfitting is likely - large if you compare a lot of models - ie. all decision trees of depth 10 or less
  - Cross Validation ie 10 fold cross-validation
- Train on 90% of the data, validate on the other 10%, repeat this 10 times where each fold (10% of the data) gets to be the validation set once, average the score, this is a likely test error approximation
  - Usually want to retrain based on the results learned from the CV (ie. after picking the best depth), and if data is ordered then folds should be random splits

# Fundamental Tradeoff

- How small can you make the training error vs. (complex models small training error, sensitive to the training data)
- · How well training error approximates the test error (simple models good approximation of test error but doesn't fit the training
- Irreducible Error that you cannot lower
- Golden Rule Test data cannot influence the training phase at all
- No Free Lunch theorem nothing works the best on every dataset etc.

#### Naive Bayes

#### Bayes Rule

$$p(A|B) = \frac{p(B|A)p(A)}{p(B)} = \frac{p(B|A)p(A)}{p(B) = \sum_{j=1}^{n} p(B|A_j)p(B_j)}$$

Because we want to know if  $p(y_i = "spam" x_i) > p(y_i = "not spam" | x_i)$ , This lets us drop the denominator

$$\frac{p(x_i|y_i = "spam")p(y_i = "spam")}{p(x_i)} > \frac{p(x_i|y_i = "notspam")p(y_i = "notspam")}{p(x_i)}$$

$$p(x_i|y_i = "spam")p(y_i = "spam") > p(x_i|y_i = "notspam")p(y_i = "notspam")$$

- For Naive Bayes we assume each variables in  $x_i$  is independent of the others in  $x_i$  given  $y_i$
- works well with tons of features compared to number of objects
- needs to know the probability of the features given the class
- Naive bayes model assumption showed in line 2-3 all the features are conditionally independent given their label  $(y_i)$  this is not true but a good approximation

$$p(spam|hello,vicodin,CPSC340) = \frac{p(hello,vicodin,CPSC340|spam)p(spam)}{p(hello,vicodin,CPSC340)} \\ \propto p(hello,vicodin,CPSC340|spam)p(spam) \\ \approx p(hello|spam)p(vicodin|spam)p(CPSC340|spam)p(spam)p(spam)p(or counts = zeros ( k , 1 ) ; \\ \text{for c} = 1 : k$$

 $p_y = counts/n$ ; % This is the probability of each class, p(y(i) = c)

% We will store

sum( y==c )

counts(c) =

end

```
p_xy = zeros (d, 2, k);
```

```
p_xy(j,2,c) = sum(X(y==c,j)==0)/counts(c)
                                                     p_xy(j,1,c) = sum(X(y==c,j)==1)/ counts(c)
                         for j = 1 : d
for c = 1: k
```

end

# Parametric vs Non-Parametric

- Parametric models: fixed number of parameters size of 'model' is O(n) in terms of 'n'
- Non-Parametric models: number of parameters grows with 'n': size of model depends on 'n' model gets more complicated with more

# K-nearest neighbours

# Classification for KNN

```
find k training examples x_i that are most similar to x
                                                                                classify using their mode
For every object x:
```

## Condensed Version

```
go through examples in order if incorrectly classified by KNN, add example to training set if correctly classified do not add it to the training set
inital subset is the first k examples
```

#### KNN details

- non-parametric (grows with data)
- assumes objects with similar features have similar labels no training phase (lazy learning)
- define nearest via 11 norm absolute, 12 norm euclidean distance, etc.
  - with a fixed k it has consistency properties

- with binary labels and mild assumptions as n goes to infinity KNN test error is less than twice the irreducible error
  - if k/n goes to zero and k goes to infinity:
- KNN is universally consistent = test error converges to irreducible error

# Big O - O(nd) to classify one test object (compute the similarities)

# Random forests - average a set of deep decision trees, with bootstrap aggregation and random trees

# Bootstrapping (bagging)

- Take a set of n objects chosen independently with replacement
- Generate several bootstrap samples of the objects  $(x_i, y_i)$ , fit a classifier to each sample at test time, average the predictions

#### Random trees

- When fitting each decision stump to construct deep decision tree
- do not consider all the features, each split looks at small number of randomly chosen features
- Each tree will tend to be very different from each other: they will still overfit but in different ways

```
model.subModel{m} = randomTree(X(randoms,:),y(randoms),depth);
function [model] = decisionForest(X, y, depth, nBootstraps)
                                                                        \% Fit model to each bootstrap sample of data
                                                                                                                                           randoms = randi(n,n,1);
                                                                                                             for m = 1:nBootstraps
                                 [n,d] = size(X);
```

```
y(:,m) = model.subModel{m}.predict(model.subModel{m},X);
                                                                   for m = 1:length(model.subModel)
function [y] = predict(model,X)
                                                                                                                                                                       % Take the most common label
                                    % Predict using each model
                                                                                                                                                                                                            y = mode(y, 2);
                                                                                                                                                                                                                                             end
```

model.predict = Opredict;

end

# Effect of number of trees/random-features

· When it comes to increasing the number of trees/submodels then the performance with bootstrapping converges to the performance without it

#### K-Means

#### Initialization

- Start with k initial means (usually random points), sensitive to outliers
- · try several different random starting points, choose best one (minimizes average squared distance of data to means)

### Error functions

- Functions that determine how 'right' we are and can improve the model (even to be convergent)
  - $L_2$  norm -> euclidean distance -> bigger values are more important.  $L_1$  norm -> absolute value -> all values are equal
- L∞ norm -> max(r) -> only biggest value important

# Big O - Total is O(ndk)

- Calculating distance from each  $x_i$  to each mean  $w_c$  is bottleneck each time is O(d) for all features For each n objects we compute the distance to k clusters
  - Updating means is easier O(nd) sum objects in cluster divide by num objects in cluster

How to cluster new example

```
% Compute Euclidean distance between each data point and each mean
                                                                                                                                                                                                                                                    distances = sqrt(X2 + ones(t,d)*(W').^2 - 2*X*W');
function [y] = predict(model,X)
                                                                                                                                                                                                                 X2 = X.^2 \text{ ones}(d,k);
                                      [t,d] = size(X);
                                                                                                        k = size(W, 1);
                                                                        W = model.W;
```

```
% Assign each data point to closest
               [~,y] = min(distances,[],2);
end
```

Elbow method - choosing the k in which the the sharpest elbow (biggest change in slope) for minimum error vs k.

#### k-medians

- change objective function to  $L_1$  norm (absolute value) from  $L_2$  norm
- this is much more robust to outliers update medians as median value of each cluster

## Vector Quantization

essentially replace vectors with a set of means

function [Iquant] = quantizeImage(I,b)
[n,m,d] = size(I);

% number of clusters can represent with a b-bit number is 2°b % reshape the image to [n\*m,3] pixels = reshape(I,n\*m,3);

clusters = model.predict(model, pixels); model = clusterKmeans(pixels,k,0);

% replace each pixels color with the quantized one pixels(i,:) = model.W(clusters(i),:); for i = 1:t

Iquant = reshape(pixels,n,m,d);
end

Density-based clustering

• clusters are defined by objects in dense regions

 $\bullet$  non-parametric - clusters can become complicated the more data, no fixed # of clusters

not sensitive to initialization (except boundaries)

· Curse of dimensionality: problems with high-dimen spaces - volume of space grows exponentially with dimension

Effect of parameters

 $\bullet$  radius - minimum distance between points considered close or reachable  $\bullet$  minpoints - # of reachable points needed to define a cluster, if you have enough considered core

• merge core points if reachable from each other

Sometimes may miss overarching or hierarchical clusters so we may need to play with parameters
 fix minpoints, record clusters as you vary radius, much more information than using a fixed radius

## Shape of clusters

• can find non-convex clusters unlike kmeans/medians, doesn't cluster all the points

• computing distance between two examples is O(d)• n training examples so  $O(n^2)$  examples • Computing distance between all examples is  $O(n^2d)$ 

summation and vector/matrix/norm notation

 $\max_{e_1, 2, \dots, n} |w^T x_i - y_i| + \frac{\lambda}{2} \sum_{i=1}^n |w_j| = ||Xw - y||_{\infty} + \frac{\lambda}{2} w^T w$  $\sum_{i=1}^{n} |w^{T} x_{i} - y_{i}| = ||Xw - y||_{1}$ 

 $\sum_{i=1}^n z_i (w^T x_i - y_i)^2 + \lambda \sum_{j=1}^d |u_j| = (Xw - y)^T Z(Xw - y) + \lambda ||w|| 1$ 

Absolute value -> L<sub>1</sub> norm

- Max ->  $L_{\infty}$ norm Distance (or  $x^Tx)$  ->  $L_2$ norm (distance squared ->  $L_2$ norm squared)

# minimizing quadratic functions as linear systems

$$\nabla[c] = 0$$

$$\nabla[w^{T}b] = b$$

$$\nabla[\frac{1}{2}w^{T}Aw] = Aw$$

function

gradient

 $\nabla f(w) = w - v = 0$ 

$$f(w) = \frac{1}{2} |||w - v||||^2$$

$$= \frac{1}{2} ((w - v)^T (w - v))$$

$$= \frac{1}{2} (w^T w - w^T v - v^T w + v^T v)$$

$$= \frac{1}{2} (w^T w - 2w^T v + v^T v)$$

$$= \frac{1}{2} w^T w - w^T v + \frac{1}{2} v^T v$$

$$f(w) = \frac{1}{2} |||w||||^2 + w^T X^T y$$
$$= \frac{1}{2} w^T w + w^T X^T y$$

$$\nabla f(w) = w + X^T y = 0$$
$$w = X^T y$$

$$\begin{split} f(w) &= \frac{1}{2} \| \| Xw - y \| \|^2 + \frac{1}{2} w^T Aw \\ &= \frac{1}{2} (Xw - y)^T (Xw - y) + \frac{1}{2} w^T Aw \\ &= \frac{1}{2} (Xw - y)^T (Xw - y) + \frac{1}{2} w^T Aw \\ &= \frac{1}{2} (w^T X^T Xw - w^T X^T y - y^T Xw + y^T y) + \frac{1}{2} w^T Aw \\ &= \frac{1}{2} (w^T X^T Xw - x^T X^T y + y^T y) + \frac{1}{2} w^T Aw \\ &= \frac{1}{2} (w^T X^T Xw - 2w^T X^T y + y^T y) + \frac{1}{2} w^T Aw \end{split}$$

$$f(w) = \frac{1}{2} \sum_{i=1}^{n} z_i(w^T x_i - y_i)^2$$

$$= \frac{1}{2} (Xw - y)^T Z(Xw - x^T Zy - x^T$$

Linear regression - Least Squares Objective =  $f(w) = \sum_{i=1}^{n} (wx_i - y_i)^2$ 

#### change of basis

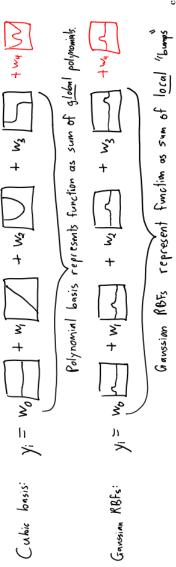
- Allows us to fit a quadratic model by changing the features
- $y_i = w_0 + w^T x_i$  becomes  $y_i = w_0 + \tilde{w}^T z_i$  where x > z, eg.  $x = \begin{bmatrix} 1 \\ 2 \end{bmatrix} > z = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} \begin{bmatrix} 2 \\ 2 \end{bmatrix}^2$  As polynomial degree increase, the training error goes down, but becomes a worse approximation of the test error usual approach for selecting the degree = cross validation
  - Can combine multiple bases to improve performance like linear/periodic
- Can fit better as n increases but eventually data doesn't help if basis isn't flexible enough
- Non-Parametric bases: size of basis (# of features) grows with 'n', model gets more complicated with more data

# RBFs - Radial Basis Functions

- Non-Parametric bases that depend on distances to training points
  - Most common is Gaussian RBF  $g(\alpha) = exp(-\frac{\alpha}{2\sigma^2})$
- Variance ( $\sigma^2$  stdev squared) controls influence of nearby points
- Replace X: n by d matrix with Z: n by n (distances of all points to each other)

$$X = \begin{bmatrix} x_{1,1} & \dots & x_{1,d} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \dots & x_{n,d} \end{bmatrix} becomes Z = \begin{bmatrix} g(||x_1 - x_1||) & \dots & g(||x_1 - x_n||) \\ \vdots & \ddots & \vdots \\ g(||x_n - x_1||) & \dots & g(||x_n - x_n||) \end{bmatrix}$$

- To predict your Xtest becomes t by d, and Z becomes t by n, so your features is the number of training examples Can add bias and linear basis to Z as well



#### regularization

- As we decrease variance we can make the training error go down
- the training error then becomes a worse approximation of the test error
- control this by using regularization: a penalty on complexity of the model  $\frac{\lambda}{2} w^T w$ 
  - large weight  $w_j$  leads to overfitting (cancel each other out)
- this gives objective function that minimize squared error + penalty on L2 norm of w
  - balances getting a low error with the complexity of the model, reduces overfitting regularization parameter λ controls strength of regularization
    - as n grows  $\lambda$  should be in the range from O(1) to  $O(n^{1/2})$

# cost of training/testing

- $X^TX$  costs  $O(nd^2)$  for  $O(d^2)$  inner products at O(n) each, and inverting  $X^TX$  costs  $O(d^3)$ • Linear Basis -  $O(nd^2 + d^3)$ 
  - Classification costs O(td) to compute t inner products at a cost of O(d) each

  - Gaussian RBF  $O(n^2d + n^3)$

- $Z \cos ts O(n^2d)$  to compute  $O(n^2)$  distances at a cost of O(d) each.
  - $Z^TZ$  costs  $O(n^3)$  while inverting costs the same
    - Classification costs O(tnd)

# effect of basis parameters

- if scales are different, penalizing the weight  $w_j$  means different things to different features
  - can standardize features by subtracting its mean and dividing by its stddev.

## Robust regression

# weighted least squares - weighted by distance = locally linear regression

- or can use mean y<sub>i</sub> among k-nearest neighbours put less focus on outliers
- use absolute error instead of squared error  $(L_1 \text{ norm instead of } L_2^2 \text{ norm })$ 
  - setback -> cannot take gradient at 0 of absolute value function

# smooth approximations

- harder to minimize non-smooth functions so we can use approximations to absolute value
- Huber loss: squared error near zero (within some  $|\mathbf{r}|$ ), absolute value otherwise
- setting the gradient to zero does not give a linear system
- Gradient Descent -> starts with guess weight and uses that iteratively to find better one have to minimize f using gradient descent
  - eventually the weight will converge of the gradient to zero, has some step size
    - finds a global minimum on convex functions
- Normal equations cost  $O(nd^2 + d^3)$  whereas GD costs O(ndt) for t iterations
- In case we care about getting outliers correctly ->  $L_{\infty}$  norm (max), sensitive to outliers but better worst case – faster if solution is good enough for t < d and  $t < d^2 / n$ 
  - convex but not smooth -> aka we can use GD
- log-sum-exp is a smooth approximation to max function
  - $\max_{i}(z_i) \approx log(\sum_{i} exp(z_i))$
- Robust Regression using L1-norm/Huber is less sensitive to outliers Gradient descent finds local minimum of differentiable functions
  - Convex functions do not have non-global local minima
    - Log-Sum-Exp function: smooth approx to maximum
      - function is convex iff  $f''(w) \ge 0$  for all w
- norms and squared norms are convex, sum/max of convex functions is convex, composition of linear and convex is convex

# computing gradients

• Usual inputs to a gradient method is a function that given w returns f(w) and  $\nabla f(w)$