IIT KHARAGPUR

NPTEL ONLINE CERTIFICATION COURSES

Data Mining

Week 8: Regression, Dimensionality Reduction

Pabitra Mitra

Computer Science and Engineering, IIT Kharagpur

Regression

- Predict real-valued output for given input – given a training set
- Examples:
- Predict rainfall in cm for month
- Predict stock prices in next day
- Predict number of users who will click on an internet advertisement

Linear Regression

- Task: predict real-valued Y, given real-valued vector X using a regression model f
- Error function, e.g., least squares is often used
-

$$S(\underline{\theta}) = \sum_i \left[y(i) - f\left(X(i) ; \underline{\theta}\right) \right]^2$$

target value

predicted value

- Model structure: e.g., linear $f(X ; \underline{\theta}) = \alpha_0 + \sum \alpha_j x_j$
- Model parameters = $\underline{\theta} = \{\alpha_0, \alpha_1, \ldots\ldots \alpha_p\}$

Estimating θ (having least error): we can write-

$$S(\theta) = \sum_i [y(i) - \sum \alpha_j x_j]^2$$

$$= \sum_i e_i^2$$

$$= e' e$$

$$= (y - X\theta)' (y - X\theta)$$

where $e = y - X\theta$

y = N x 1 vector of target values

N x (p+1) vector of input values

(p+1) x 1 vector of parameter values

$$S(\theta) = \Sigma e^2 = e' e = (y - X\theta)' (y - X\theta)$$

$$= y' y - \theta' X' y - y' X \theta + \theta' X' X \theta$$

$$= y' y - 2\theta' X' y + \theta' X' X \theta$$

Taking derivative of $S(\theta)$ with respect to the components of θ gives -

$$dS/d\theta = -2 X' y + 2 X' X \theta$$

Set this to 0 to find the minimum of S as a function of θ.

Set to 0 to find the minimum of S as a function of θ …

$\Rightarrow$ $-2 X' y + 2 X' X \theta = 0$

$\Rightarrow$ $X' X \theta = X' y$ (known in statistics as the Normal Equations)

Letting $X' X = C$, and $X' y = b$,

we have $C \theta = b$, i.e., a set of linear equations

We could solve this directly, e.g., by matrix inversion

$$\theta = C^{-1} b = (X' X)^{-1} X' y$$

Solving for the θ's

- Problem is equivalent to inverting X' X matrix
  - Inverse does not exist if matrix is not of full rank
    - E.g., if 1 column is a linear combination of another (collinearity)
    - Note that X'X is closely related to the covariance of the X data
      - So we are in trouble if 2 or more variables are perfectly correlated
    - Numerical problems can also occur if variables are almost collinear

- Equivalent to solving a system of p linear equations
  - Many good numerical methods for doing this, e.g.,
    - Gaussian elimination, LU decomposition, etc
  - These are numerically more stable than direct inversion

- Alternative: gradient descent
  - Compute gradient and move downhill

Multivariate Linear Regression

- Prediction model is a linear function of the parameters
- Score function: quadratic in predictions and parameters
  - $\Rightarrow$ Derivative of score is linear in the parameters
  - $\Rightarrow$ Leads to a linear algebra optimization problem, i.e., $C\,\theta = b$
- Model structure is simple….
  - p-1 dimensional hyperplane in p-dimensions
  - Linear weights => interpretability
- Often useful as a baseline model
  - e.g., to compare more complex models to
- Note: even if it's the wrong model for the data (e.g., a poor fit) it can still be useful for prediction

Limitations of Linear Regression

- True relationship of X and Y might be non-linear
  - Suggests generalizations to non-linear models
- Complexity:
  - $O(N p^2 + p^3)$ - problematic for large p
- Correlation/Collinearity among the X variables
  - Can cause numerical instability (C may be ill-conditioned)
  - Problems in interpretability (identifiability)
- Includes all variables in the model…
  - But what if p=1000 and only 3 variables are actually related to Y?

Non-linear Regression

- We can generalize further to models that are nonlinear:

$$f(\underline{x}\,;\,\underline{\theta}) = \alpha_0 + \Sigma\, \alpha_k\, g_k(\beta_{k0} + \Sigma\, \beta_{kj}\, x_j)$$

where the g's are *non-linear functions.*

- In statistics this is referred to as a generalized linear regression

- Closed form (analytical) solutions are rare.

- We have a multivariate non-linear optimization problem (which may be quite difficult!)

Optimization in the Non-Linear Case

- We seek the minimum of a function in d dimensions, where d is the number of parameters (d could be large!)

- There are a multitude of heuristic search techniques
  - Steepest descent (follow the gradient)
  - Newton methods (use 2nd derivative information)
  - Conjugate gradient
  - Line search
  - Stochastic search
  - Genetic algorithms
- Two cases:
  - Convex (nice -> means a single global optimum)
  - Non-convex (multiple local optima => need multiple starts)

Other non-linear models

- Splines
  - "patch" together different low-order polynomials over different parts of the x-space
  - Works well in 1 dimension, less well in higher dimensions

- Memory-based models

  $y' = \sum w_{(x',x)}\, y,$ where y's are from the training data

  $w_{(x',x)}$ = function of distance of x from x'

- Local linear regression

  $y' = \alpha_0 + \sum \alpha_j x_j$, where the alpha's are fit at prediction time just to the (y,x) pairs that are close to x'

Overfitting

- Squared Error score (as an example: we could use other scores)

$$S(\underline{\theta}) = \sum_i \left[y(i) - f\left(\underline{x}(i) ; \underline{\theta}\right) \right]^2$$

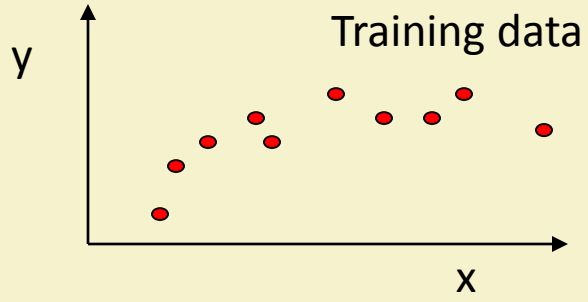
where $S(\underline{\theta})$ is defined on the training data D

- We are really interested in finding the $f(x; \underline{\theta})$ that best predicts y on **future** data, i.e., minimizing

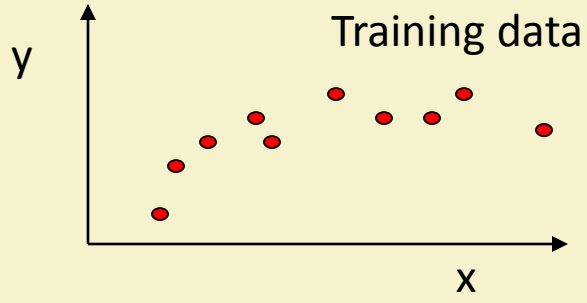
$$E[S] = E\left[y - f\left(\underline{x} ; \underline{\theta}\right) \right]^2$$ (where the expectation is over future data)

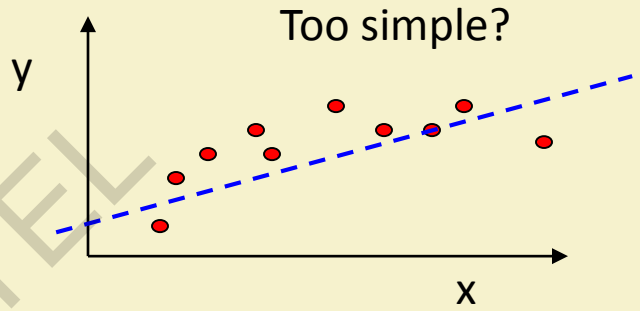
- Empirical learning
  - Minimize $S(\underline{\theta})$ on the training data D_{train}
  - If D_{train} is large and model is simple we are assuming that the best f on training data is also the best predictor f on future test data D_{test}

Complexity versus Goodness of Fit



Complexity versus Goodness of Fit





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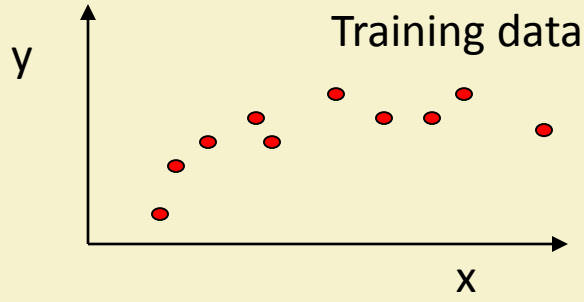

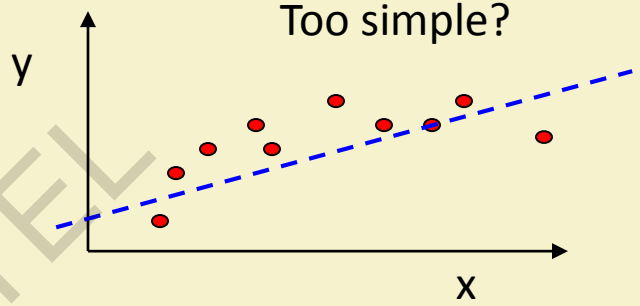

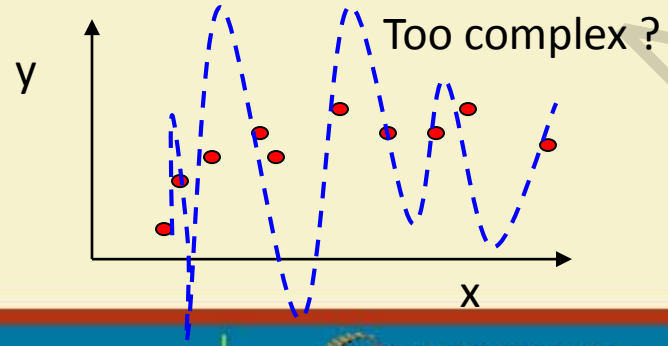

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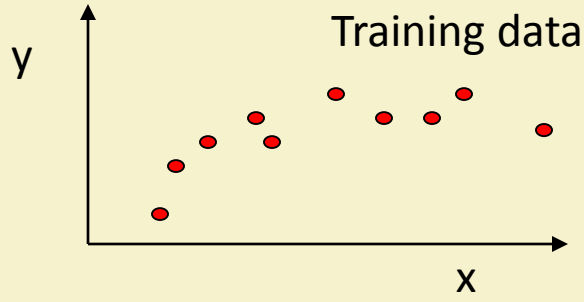
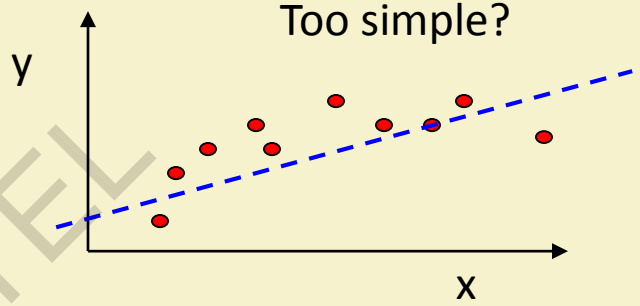
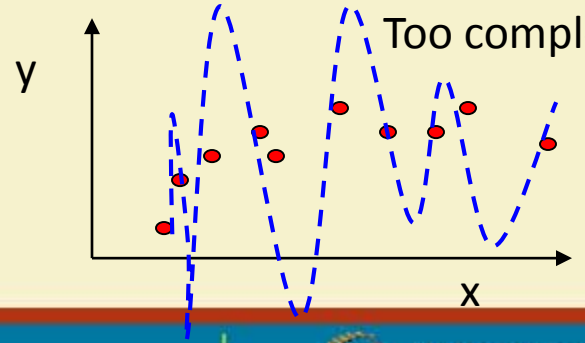
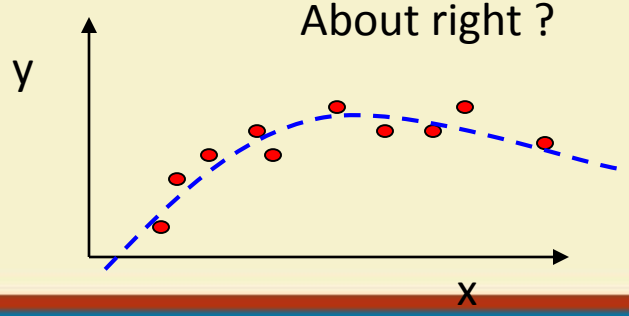
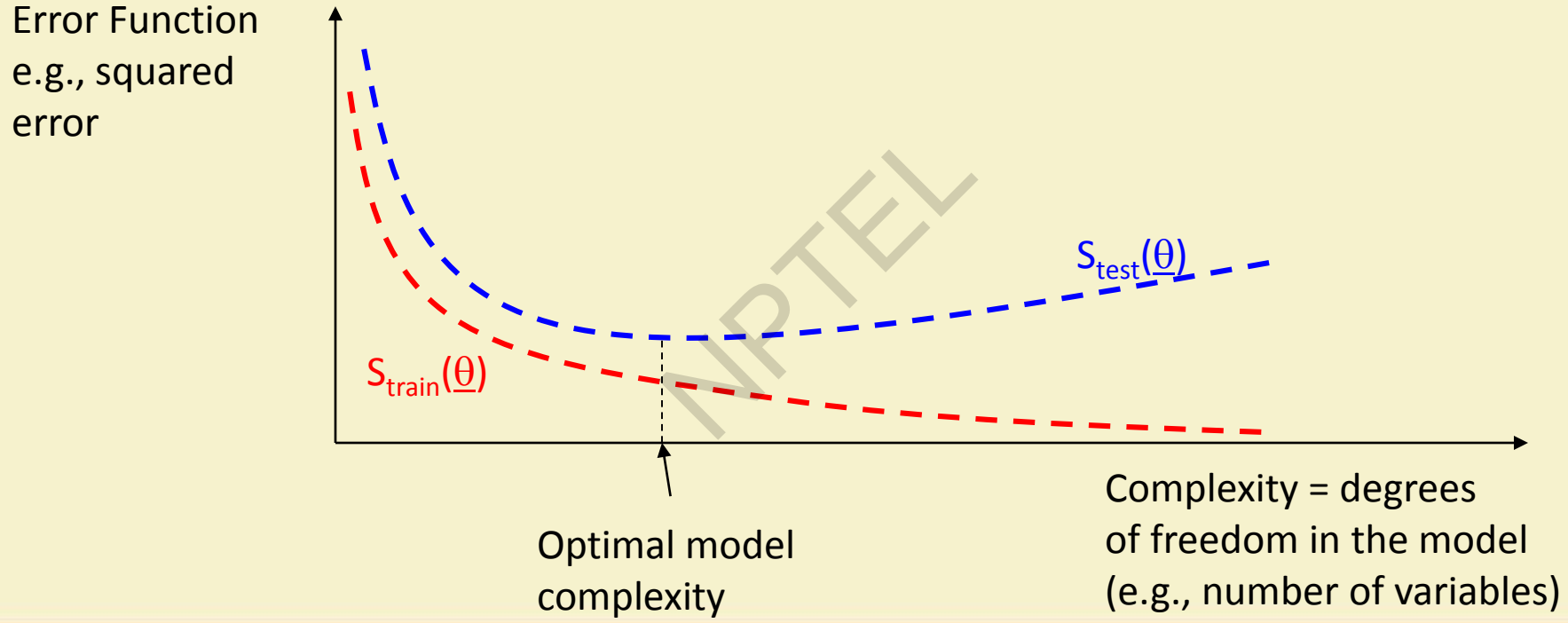






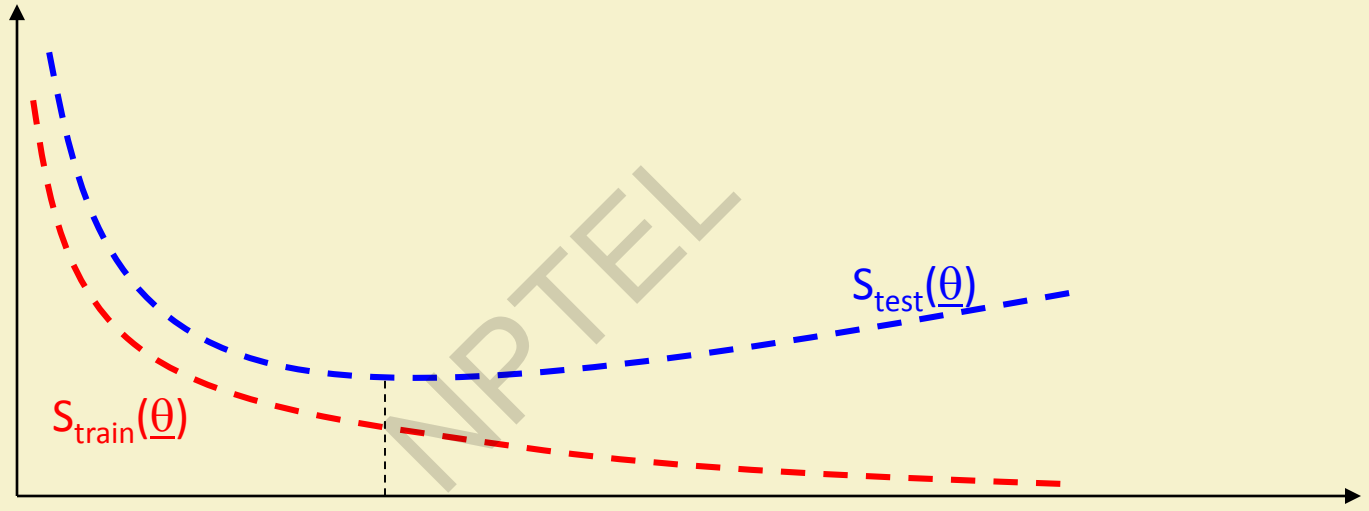


Model Complexity and Generalization



Complexity and Generalization

Score Function
e.g., squared
error



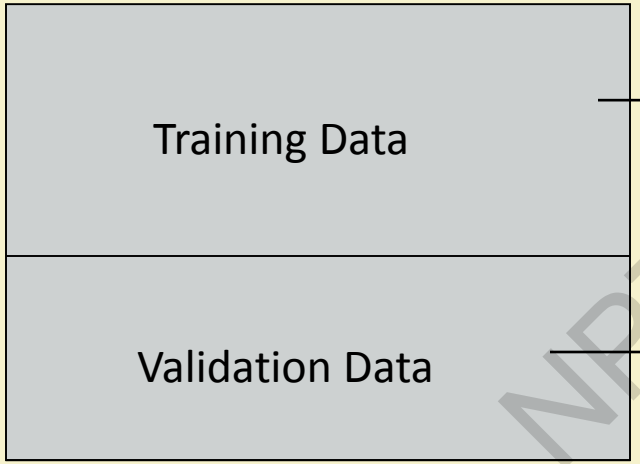
High bias
Low variance

Low bias
High variance

Training Data

Use this data to find the best $\underline{\theta}$ for each model $f_k(\underline{x} ; \underline{\theta})$

Validation Data



Use this data to find the best $\underline{\theta}$ for each model $f_k(\underline{x} ; \underline{\theta})$

Use this data to

(1) calculate an estimate of $S_k(\underline{\theta})$ for each $f_k(\underline{x} ; \underline{\theta})$ and

(2) select $k^* = \arg\min_k S_k(\underline{\theta})$

Validation Data

can generalize to **cross-validation….**

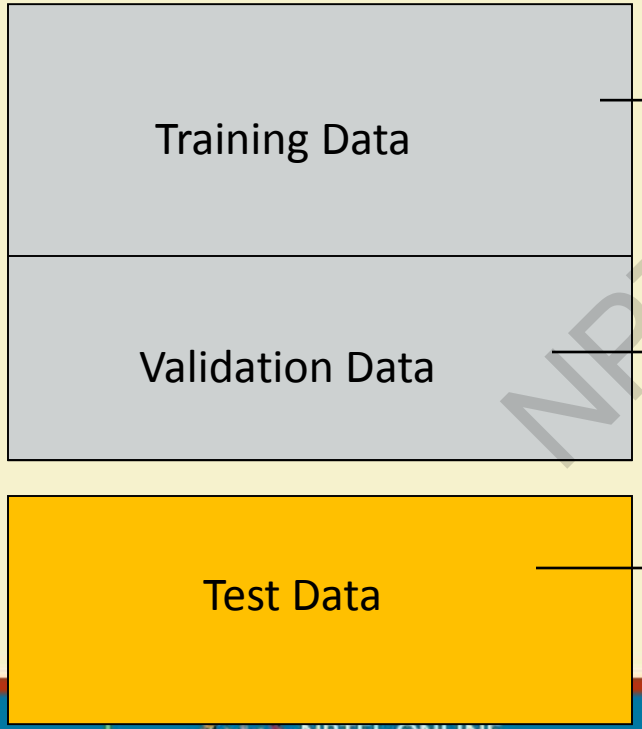
Use this data to find the best $\underline{\theta}$ for each model $f_k(\underline{x} ; \underline{\theta})$

Use this data to

(1) calculate an estimate of $S_k(\underline{\theta})$ for each $f_k(\underline{x} ; \underline{\theta})$ and

(2) select $k^* = \arg\min_k S_k(\underline{\theta})$

Test Data



Use this data to find the best $\underline{\theta}$ for each model $f_k(\underline{x} ; \underline{\theta})$

Use this data to
(1) calculate an estimate of $S_k(\underline{\theta})$ for each $f_k(\underline{x} ; \underline{\theta})$ and
(2) select $k^* = \arg\min_k S_k(\underline{\theta})$

Use this data to calculate an unbiased estimate of $S_{k^*}(\underline{\theta})$ for the selected model

Time-series prediction as regression

- Measurements over time $x_1, \ldots\ldots x_t$
- We want to predict x_{t+1} given $x_1, \ldots\ldots x_t$
- Autoregressive model

$$x_{t+1} = f(x_1, \ldots\ldots x_t ; \underline{\theta}) = \sum \alpha_k x_{t-k}$$

  - Number of coefficients K = memory of the model
  - Can take advantage of regression techniques in general to solve this problem (e.g., linear in parameters, score function = squared error, etc)

- Generalizations
  - Vector x
  - Non-linear function instead of linear
  - Add in terms for time-trend (linear, seasonal), for “jumps”, etc

Generalized Linear Models (GLMs)

- $g(y) = u(x) = \alpha_0 + \sum \alpha_j x_j$
  - Where g [ ] is a "link" function
  - u(x) is a linear function of the vector x

- Examples:
  - g = identity function -> linear regression
  - Logistic regression: $g(y) = \log(y / 1\text{-}y) = \alpha_0 + \sum \alpha_j x_j$
  - Logarithmic link: $g(y) = \log(y) = \alpha_0 + \sum \alpha_j x_j$
  - GLMs are widely used in statistics
  - Details of learning/fitting algorithm depend on the specifics of the link function

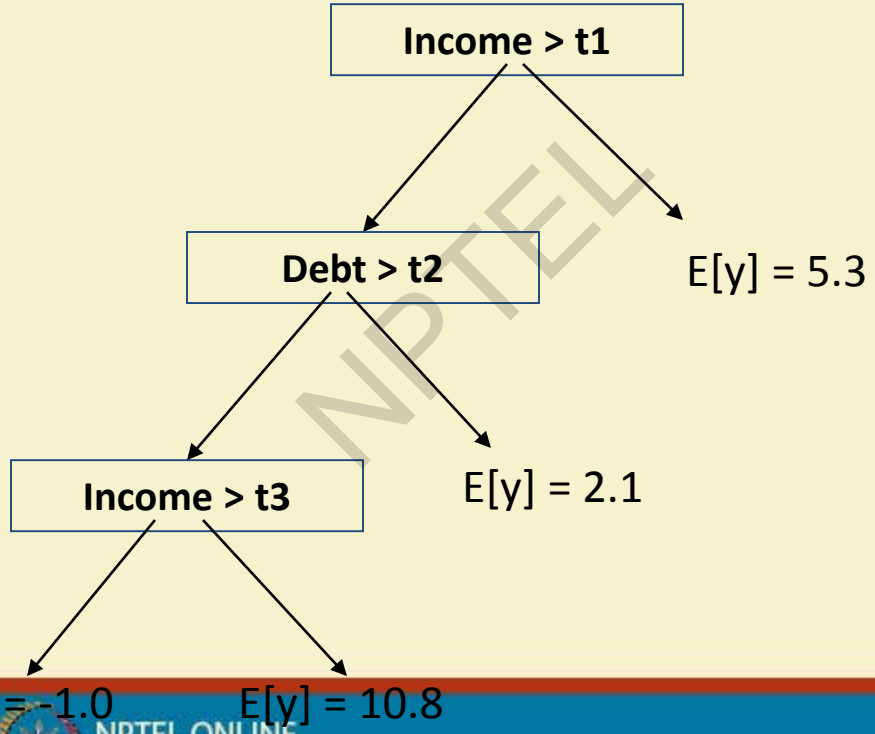
Tree-Structured Regression

- Functional form of model is a “regression tree”
  - Univariate thresholds at internal nodes
  - Constant or linear surfaces at the leaf nodes
  - Yields piecewise constant (or linear) surface
  - (like classification tree, but for regression)

- Very crude functional form…. but
  - Can be very useful in high-dimensional problems
  - Can useful for interpretation
  - Can handle combinations of real and categorical variables

- Search problem
  - Finding the optimal tree is intractable
  - Practice: greedy algorithms

Simple example of Tree Model



Greedy Search for Learning Regression Trees

- Binary_node_splitting, real-valued variables
  - For each variable x_j
    - For each possible threshold t_{jk} , compute

$$MSE(y; t_{jk}) = P(x \leq t_{jk})MSE(y|x \leq t_{jk}) + P(x > t_{jk})MSE(y|x > t_{jk})$$

MSE in left branch MSE in right branch

    - Select t_{jk} with the lowest MSE for that variable
  - Select variable x_j and t_{jk} with the lowest MSE
  - Split the training data into the 2 branches
  - For each branch
    - If leaf-node: prediction at this leaf node = mean value of y data points
    - If not: call binary_node_splitting recursively
- Time complexity?

Model Averaging/Ensembles

- Can average over parameters and models
  - E.g., weighted linear combination of predictions from multiple models

$$y = \sum w_k \, y_k$$

  - Why? Any predictions from a point estimate of parameters or a single model has only a small chance of the being the best

  - Averaging makes our predictions more stable and less sensitive to random variations in a particular data set (good for less stable models like trees)

Components of Data Mining Algorithms

- Model Representation:
  - Determining the nature and structure of the representation to be used
- Score function
  - Measuring how well different representations fit the data
- Search/Optimization method
  - An algorithm to optimize the score function
- Data Management
  - Deciding what principles of data management are required to implement the algorithms efficiently.

Steps of Data Mining Algorithm

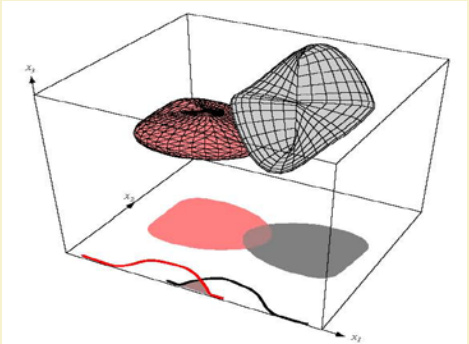
Dimensionality Reduction

- Purpose:
  - Avoid curse of dimensionality
  - Reduce amount of time and memory required by data mining algorithms
  - Allow data to be more easily visualized
  - May help to eliminate irrelevant features or reduce noise
- Techniques
  - Principle Component Analysis
  - Singular Value Decomposition
  - Others: supervised and non-linear techniques

Data Dimensionality

- From a theoretical point of view, increasing the number of features should lead to better performance.

- In practice, the inclusion of more features leads to worse performance (i.e., curse of dimensionality).



- The number of training examples required increases exponentially with dimensionality.

Dimensionality Reduction

- Significant improvements can be achieved by first mapping the data into a *lower-dimensional* space.

$$x = \begin{bmatrix} a_1 \\ a_2 \\ \dots \\ a_N \end{bmatrix} \text{ --> reduce dimensionality --> } y = \begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_K \end{bmatrix} \quad (K << N)$$

- Dimensionality can be reduced by:
  - Combining features using a linear or non-linear
  - Selecting a subset of features (i.e., feature selection).

Dimensionality Reduction (cont'd)

- Linear combinations are particularly attractive because they are simple to compute and analytically tractable.

- Given $x \in R^N$, the goal is to find an N x K matrix U such that:

$$y = U^T x \in R^K \text{ where } K << N$$

U^T

$$x = \begin{bmatrix} a_1 \\ a_2 \\ \dots \\ a_N \end{bmatrix} \text{ --> reduce dimensionality --> } y = \begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_K \end{bmatrix} \quad (K << N)$$

Dimensionality Reduction (cont'd)

- Idea: represent data in terms of basis vectors in a lower dimensional space (embedded within the original space)

(1) Higher-dimensional space representation:

$$x = a_1 v_1 + a_2 v_2 + \cdots + a_N v_N$$

$v_1, v_2, \ldots, v_N$ is a basis of the N-dimensional space

$$x = \begin{bmatrix} a_1 \\ a_2 \\ \cdots \\ a_N \end{bmatrix}$$

(2) Lower-dimensional sub-space representation:

$$\hat{x} = b_1 u_1 + b_2 u_2 + \cdots + b_K u_K$$

$u_1, u_2, \ldots, u_K$ is a basis of the K-dimensional space

$$y = \begin{bmatrix} b_1 \\ b_2 \\ \cdots \\ b_K \end{bmatrix}$$

Dimensionality Reduction (cont'd)

- Classical approaches for finding an optimal linear transformation:
  - Principal Components Analysis (PCA): Seeks a projection that preserves as much **information** in the data as possible (in a least-squares sense).
  - Linear Discriminant Analysis (LDA): Seeks a projection that best **separates** the data (in a least-squares sense).

Principal Component Analysis (PCA)

- Dimensionality reduction implies information loss; PCA preserves as much information as possible by minimizing the reconstruction error:

$$\|x - \hat{x}\|$$

$$x = a_1 v_1 + a_2 v_2 + \cdots + a_N v_N$$

$$\hat{x} = b_1 u_1 + b_2 u_2 + \cdots + b_K u_K$$

- How should we determine the "best" lower dimensional space?

The "best" low-dimensional space can be determined by the "best" eigenvectors of the covariance matrix of the data (i.e., the eigenvectors corresponding to the "largest" eigenvalues – also called "principal components").

PCA - Steps

- Suppose $x_1, x_2, ..., x_M$ are N x 1 vectors

Step 1: $\bar{x} = \frac{1}{M}\sum_{i=1}^{M} x_i$

Step 2: subtract the mean: $\Phi_i = x_i - \bar{x}$ (i.e., center at zero)

Step 3: form the matrix $A = [\Phi_1 \; \Phi_2 \; \cdots \; \Phi_M]$ ($N \times M$ matrix), then compute:

$$C = \frac{1}{M}\sum_{n=1}^{M} \Phi_n \Phi_n^T = AA^T$$

(sample **covariance** matrix, $N \times N$, characterizes the *scatter* of the data)

Step 4: compute the eigenvalues of C: $\lambda_1 > \lambda_2 > \cdots > \lambda_N$

Step 5: compute the eigenvectors of C: $u_1, u_2, \ldots, u_N$

PCA – Steps (cont'd)

- Since C is symmetric, $u_1, u_2, \ldots, u_N$ form a basis, (i.e., any vector x or actually $(x - \bar{x})$, can be written as a linear combination of the eigenvectors):

$$x - \bar{x} = b_1 u_1 + b_2 u_2 + \cdots + b_N u_N = \sum_{i=1}^{N} b_i u_i \qquad \text{where } b_i = \frac{(x - \bar{x}).u_i}{(u_i.u_i)}$$

Step 6: (**dimensionality reduction step**) keep only the terms corresponding to the K largest eigenvalues:

$$\hat{x} - \bar{x} = \sum_{i=1}^{K} b_i u_i \text{ where } K << N$$

- The representation of $\hat{x} - \bar{x}$ into the basis $u_1, u_2, \ldots, u_K$ is thus

$$\begin{bmatrix} b_1 \\ b_2 \\ \ldots \\ b_K \end{bmatrix}$$

PCA – Linear Transformation

If u_i has unit length:

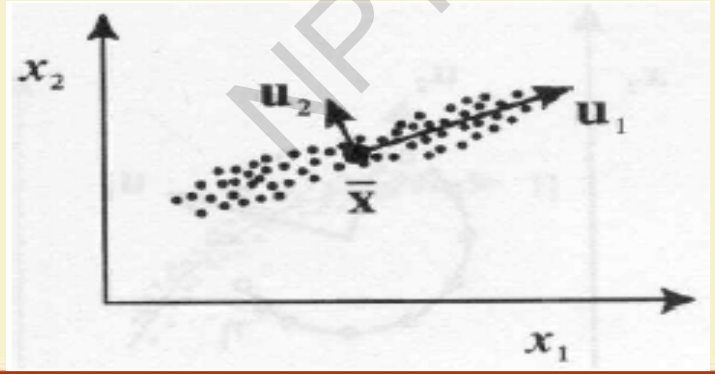
$$b_i = \frac{(x - \bar{x}).u_i}{(u_i.u_i)} = (x - \bar{x}).u_i$$

- The linear transformation $R^N \rightarrow R^K$ that performs the dimensionality reduction is:

$$\begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_K \end{bmatrix} = \begin{bmatrix} u_1^T \\ u_2^T \\ \dots \\ u_K^T \end{bmatrix} (x - \bar{x}) = U^T (x - \bar{x})$$

Geometric interpretation

- PCA projects the data along the directions where the data varies most.
- These directions are determined by the eigenvectors of the covariance matrix corresponding to the largest eigenvalues.
- The magnitude of the eigenvalues corresponds to the variance of the data along the eigenvector directions.



Error due to dimensionality reduction

- The original vector x can be reconstructed using its principal components:

$$\hat{x} - \bar{x} = \sum_{i=1}^{K} b_i u_i \text{ or } \hat{x} = \sum_{i=1}^{K} b_i u_i + \bar{x}$$

- PCA minimizes the reconstruction error:

$$e = \|x - \hat{x}\|$$

- It can be shown that the reconstruction error is:

$$e = 1/2 \sum_{i=K+1}^{N} \lambda_i$$

Feature Subset Selection

- Another way to reduce dimensionality of data
- Redundant features
  - duplicate much or all of the information contained in one or more other attributes
  - Example: purchase price of a product and the amount of sales tax paid
- Irrelevant features
  - contain no information that is useful for the data mining task at hand
  - Example: students' ID is often irrelevant to the task of predicting students' GPA

Feature Subset Selection

- Evaluate a subset of feature
- Search for the best subset

Feature Subset Selection

- Techniques:
  - Brute-force approch:
    - Try all possible feature subsets as input to data mining algorithm
  - Embedded approaches:
    - Feature selection occurs naturally as part of the data mining algorithm
  - Filter approaches:
    - Features are selected before data mining algorithm is run
  - Wrapper approaches:
    - Use the data mining algorithm as a black box to find best subset of attributes

Software

- MATLAB
  - Many free “toolboxes” on the Web for regression and prediction
  - e.g., see http://lib.stat.cmu.edu/matlab/
    and in particular the CompStats toolbox
- R
  - General purpose statistical computing environment (successor to S)
  - Free (!)
  - Widely used by statisticians, has a huge library of functions and visualization tools
- Commercial tools
  - SAS, Salford Systems, other statistical packages
  - Various data mining packages
  - Often are not progammable: offer a fixed menu of items

Useful References

T. Hastie, R. Tibshirani, and J. Friedman,
Elements of Statistical Learning, 2nd edition,
Springer Verlag, 2009