Machine Learning
Lecture 2

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Reading list: Andrew's Lecure note 1, 《机器学习》第三章，PRML 3.1

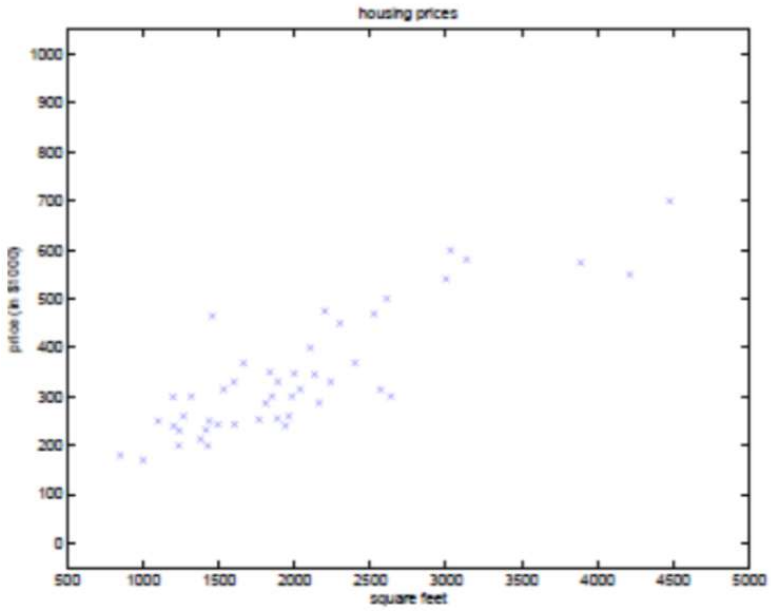
Linear Regression

Machine Learning for house hunting

- Suppose we have a dataset giving the living areas and prices of some houses :

Living area (feet^2)	Price(1000$s)
2014	400
1600	330
2400	369
1416	232
3000	540
…	
2005	?
3200	?
1280	?

We can plot this data set:



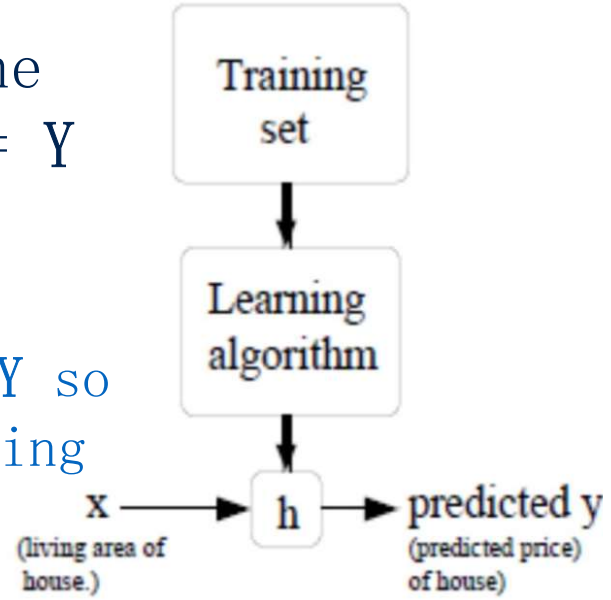
- How can we learn to predict the prices of other houses, as a function of the size of their living areas?

The learning problem

- $x^{(i)}$ denotes the "input" variables/features
- $y^{(i)}$ denotes the "output" or target variable that we are trying to predict (price)
- A pair ($x^{(i)}$, $y^{(i)}$) is called a training example
- A list of m training examples {($x^{(i)}$, $y^{(i)}$); i = 1, …, m}—is called a training set.
- X denote the space of input values, and Y the space of output values. In this example, X = Y = R.
- Our goal:

Given a training set, learn a function h : X —>Y so that h(x) is a "good" predictor for the corresponding value of y.

For historical reasons, this function h is called a hypothesis.



A slightly richer dataset

- If you want to find the most reasonably priced house satisfying your needs: square-ft, # of bedroom, distance to work place...

Living area (feet^2)	# bedrooms	Price(1000$s)
2014	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540
...		
2005	3	?
3200	4	?
1280	2	?

The learning problem

- Features:
  - Living area, #bedroom, distance to work place
    …
  - Denote as x = $[x_1, x_2, \ldots, x_n]^T$
- Target:
  - Price
  - Denoted as y
- Training set:

$$X=\begin{bmatrix} --(x^{(1)})^T-- \\ --(x^{(2)})^T-- \\ \vdots \\ --(x^{(m)})^T-- \end{bmatrix}=\begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_n^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_n^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(m)} & x_2^{(m)} & \cdots & x_n^{(m)} \end{bmatrix} \qquad Y=\begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

m: #examples/samples
n: #features

Linear Regression

- Assume that Y (target) is a linear function of X (features):

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

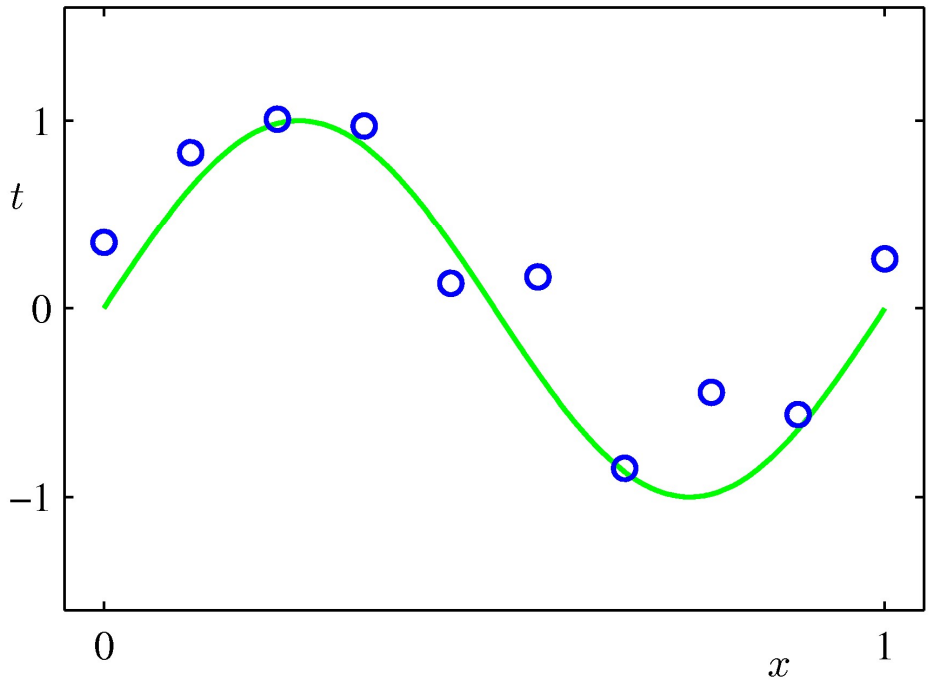
Here, the θ_i' s are the **parameters** (also called **weights**) parameterizing the space of linear functions mapping from $\mathcal{X}$ to $\mathcal{Y}$. When there is no risk of confusion, we will drop the θ subscript in $h_\theta(x)$ and write it more simply as $h(x)$. To simplify our notation, we also introduce the convention of letting $x_0 = 1$ (this is the **intercept term**), so that

$$h(x) = \sum_{i=0}^{n} \theta_i x_i = \theta^T \underbrace{x}_{\emptyset(x)}$$

Pre-processing of features or feature extraction

Linear Basis Function Models (1)

Example: Polynomial Curve Fitting



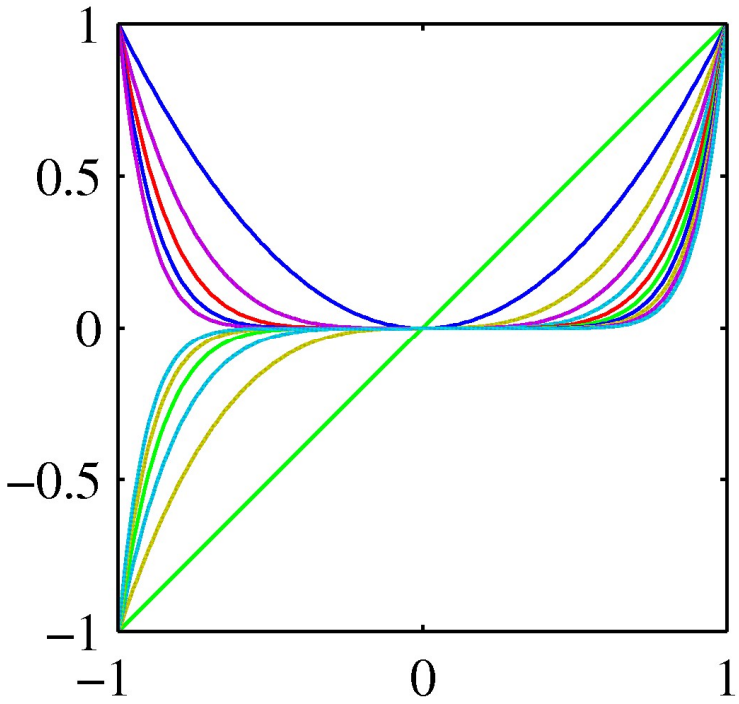
$$y(x,\theta) = \theta_0 + \theta_1 x + \theta_2 x^2 + \ldots + \theta_M x^M = \sum_{j=0}^{M} \theta_j x^j$$

Linear Basis Function Models (2)

Polynomial basis functions:

$$\phi_j(x) = x^j.$$

These are global; a small change in x affects all basis functions.



Linear Basis Function Models (4)

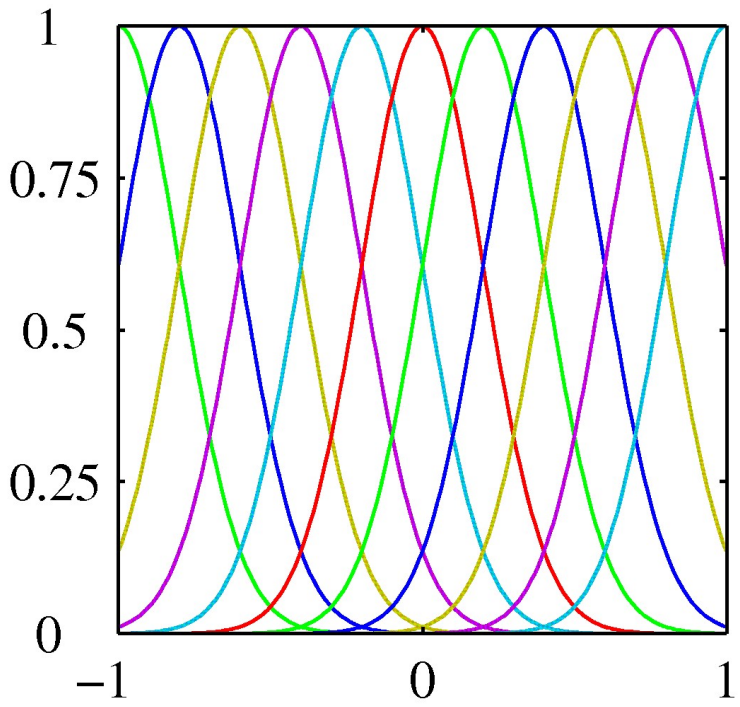
Sigmoidal basis functions:

$$\phi_j(x) = \sigma\left(\frac{x - \mu_j}{s}\right)$$

Where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$

Also these are local; a small change in **x** only affect nearby basis functions. μ_j and **s** control location and scale (slope).



The Least Mean Square (LMS) method

- The Cost Function:

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

- Consider a gradient descent algorithm:

$$\theta_j := \theta_j - \alpha\frac{\partial}{\partial\theta_j}J(\theta)$$

The Least Mean Square (LMS) method

- For a single training example, this gives the update rule:

$$\theta_j := \theta_j + \alpha(y^{(i)} - h_\theta(x^{(i)}))x_j^{(i)}$$

- This is known as the LMS update rule, or the Widrow-Hoff learning rule
- If the training set has more than one example

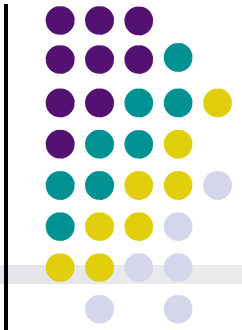
Repeat until convergence {

$$\theta_j := \theta_j + \alpha \sum_{i=1}^{m} \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)} \qquad \text{(for every } j\text{)}$$

}

Batch gradient descent

Stochastic gradient descent



- The above results were obtained with batch gradient descent. There is an alternative to batch gradient descent that also works very well. Consider the following algorithm:

Loop {

for i=1 to m, {

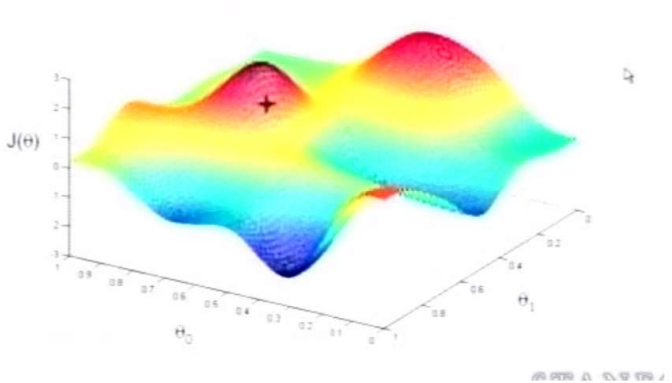
$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)} \qquad \text{(for every } j\text{)}$$

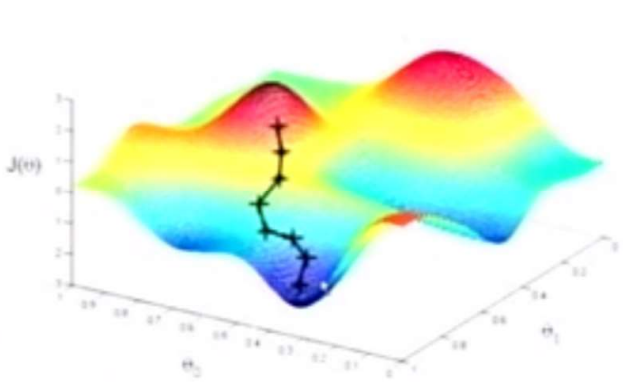
}

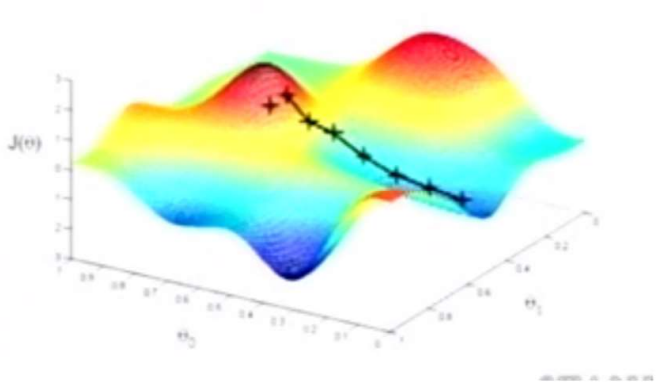
}

- When the training set is large, stochastic gradient descent is often preferred over batch gradient descent.

Gradient descent







The normal equations

- Given a training set, define the design matrix X to be the m-by-n matrix that contains the training examples' input values in its rows:

$$X=\begin{bmatrix} --(x^{(1)})^T-- \\ --(x^{(2)})^T-- \\ \vdots \\ --(x^{(m)})^T-- \end{bmatrix}=\begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_n^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_n^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(m)} & x_2^{(m)} & \cdots & x_n^{(m)} \end{bmatrix} \qquad Y=\begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

m: #samples

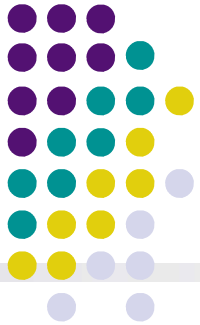
n: #features

The normal equations

- Write the cost function in matrix form:

$$
\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(X\theta - \vec{y})^T (X\theta - \vec{y}) \\
&= \frac{1}{2}\nabla_\theta \left(\theta^T X^T X\theta - \theta^T X^T \vec{y} - \vec{y}^T X\theta + \vec{y}^T \vec{y}\right) \\
&= \frac{1}{2}\nabla_\theta \operatorname{tr} \left(\theta^T X^T X\theta - \theta^T X^T \vec{y} - \vec{y}^T X\theta + \vec{y}^T \vec{y}\right) \\
&= \frac{1}{2}\nabla_\theta \left(\operatorname{tr} \theta^T X^T X\theta - 2\operatorname{tr} \vec{y}^T X\theta\right) \\
&= \frac{1}{2}\left(X^T X\theta + X^T X\theta - 2X^T \vec{y}\right) \\
&= X^T X\theta - X^T \vec{y}
\end{aligned}
$$

The normal equations



- To minimize J, we set its derivatives to zero, and obtain the normal equations:

$$X^T X\theta = X^T \vec{y}$$

- Thus, the value of θ that minimizes J is given in closed form by the equation:

$$\theta = (X^T X)^{-1} X^T \vec{y}$$

Comments on the normal equation

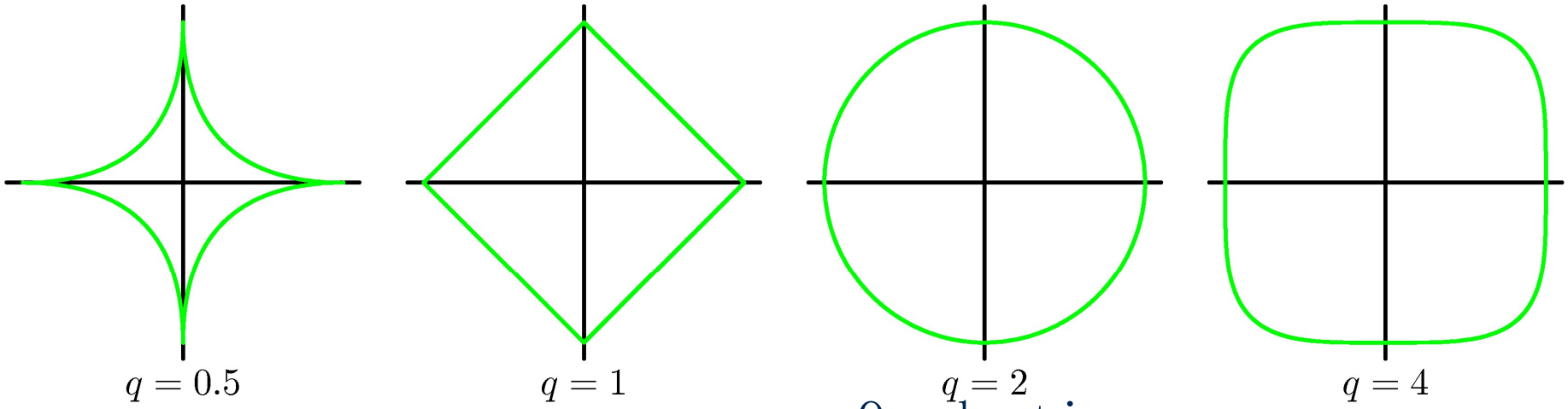
- In most situations of practical interest, the number of data points N is larger than the dimensionality k of the input space and the matrix X is of full column rank. If this condition holds, then it is easy to verify that $X^T X$ is necessarily invertible.
- The assumption that $X^T X$ is invertible implies that it is positive definite, thus at the critical point we have found is a minimum.
- What if X has less than full column rank

  Regularization

Regularized Least Squares

- With a more general regularizer, we have

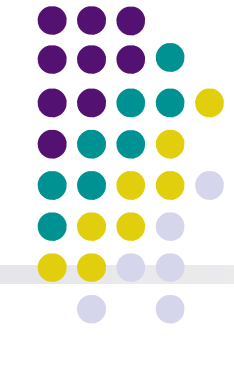
$$\frac{1}{2}\sum_{i=1}^{m}\{h_\theta(x^{(i)}) - y^{(i)}\}^2 + \frac{\lambda}{2}\sum_{j=1}^{n}|\theta_j|^q$$



Lasso

Quadratic ridge regression

Regularized Least Squares



No regularization: $\hat{\theta} = (X^T X)^{-1} X^T Y$

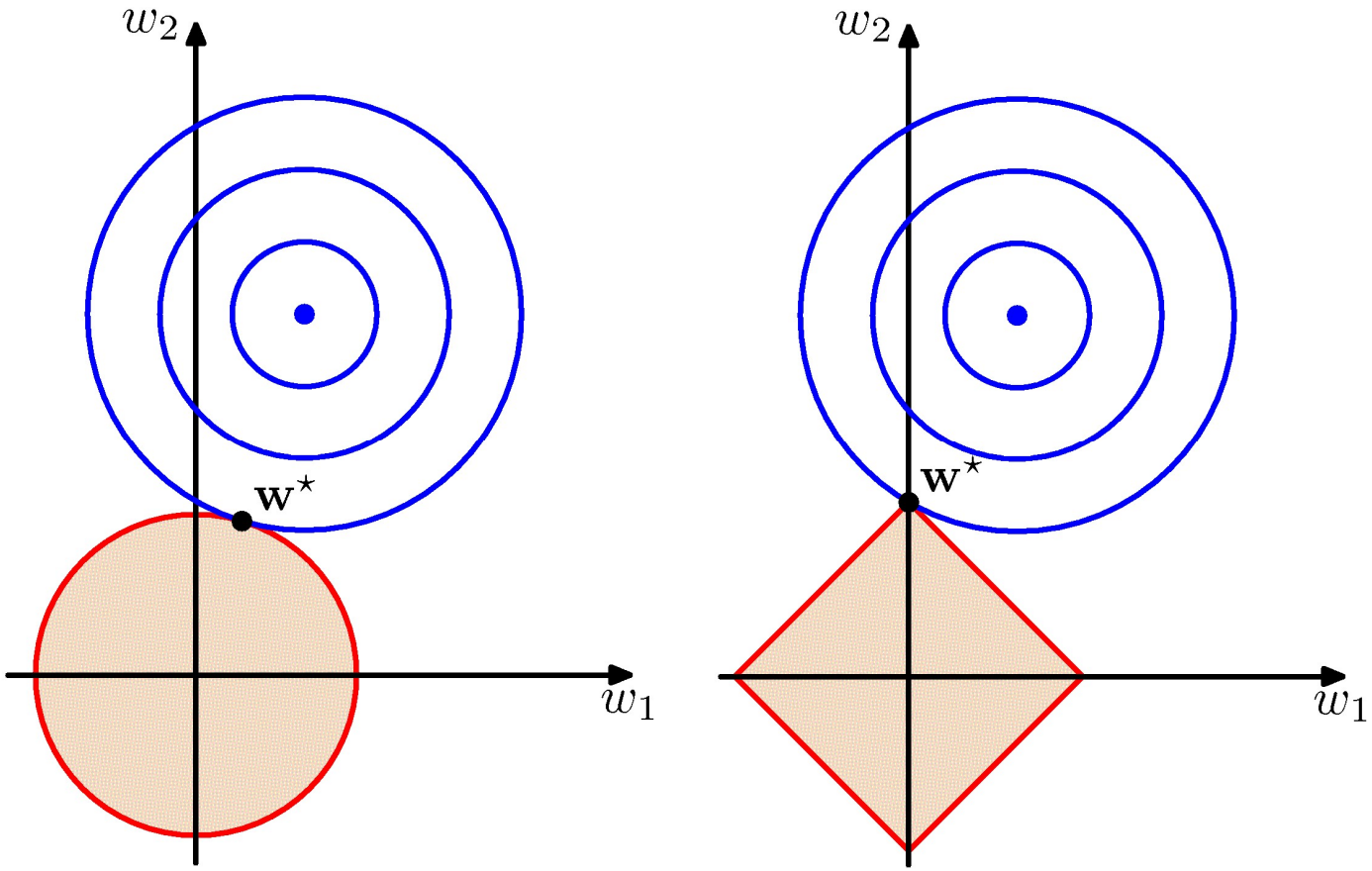
L_2 norm (q=2) regularization:

$$\nabla_\theta J = 2X^T (Y - X\theta) - 2\lambda\theta$$

$$\hat{\theta} = (X^T X + \lambda I)^{-1} X^T Y$$

Regularized Least Squares

- Lasso tends to generate sparser solutions than a quadratic regularizer.



Direct and Iterative methods

- Direct methods: we can achieve the solution in a single step by solving the normal equation
  - Using Gaussian elimination or QR decomposition, we converge in a finite number of steps
  - It can be infeasible when data are streaming in in real time, or of very large amount
- Iterative methods: stochastic or steepest gradient
  - Converging in a limiting sense
  - But more attractive in large practical problems
  - Caution is needed for deciding the learning rate α

Probabilistic Interpretation of LMS

- Let us assume that the target variables and the inputs are related via the equation

$$y^{(i)} = \theta^T x^{(i)} + \epsilon^{(i)}$$

Where $\epsilon^{(i)}$ is an error term of unmodeled effects or random noise, and distributed i.i.d.

- Now assume that follows a Gaussian $N(0, \sigma^2)$, then we have:

$$p(y^{(i)}|x^{(i)};\theta) = \frac{1}{\sqrt{2\pi}\sigma} exp(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2})$$

Probabilistic Interpretation of LMS

- When we wish to explicitly view this as a function of , we will instead call it the likelihood function:

$$L(\theta) = L(\theta; X, \vec{y}) = p(\vec{y}|X;\theta)$$

- By independence assumption:

$$L(\theta) = \prod_{i=1}^{m} p(y^{(i)}|x^{(i)};\theta)$$

$$= \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} exp(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2})$$

Probabilistic Interpretation of LMS

- Hence the log-likelihood is:

$$\begin{aligned}\iota(\theta) &= \log L(\theta) \\ &= \log \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} exp(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}) \\ &= \sum_{i=1}^{m} \log \frac{1}{\sqrt{2\pi}\sigma} exp(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}) \\ &= m \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{\sigma^2} \times \frac{1}{2} \sum_{i=1}^{m} (y^{(i)} - \theta^T x^{(i)})^2\end{aligned}$$

- Do you recognize the last term? maximizing $\iota(\theta)$ gives the same answer as minimizing $J(\theta)$
- Thus under independence assumption, LMS is equivalent to MLE of θ !

Locally weighted linear regression (LWR)

- The algorithm:
- Instead of minimizing $\sum_i (y^{(i)} - \theta^T x^{(i)})^2$
- Now we fit θ to minimize $\sum_i w^{(i)} (y^{(i)} - \theta^T x^{(i)})^2$
- Where do $w^{(i)}$' s come from $w^{(i)} = exp(-\frac{(x^{(i)} - x)^2}{2\tau^2})$
- Where x is the query point for which we'd like to know its corresponding y
- Essentially we put higher weights on (errors on) training examples that are close to the query point (than those that are further away from the query)

Parametric vs. non-parametric

- LWR is a **non-parametric** algorithm.
- The (unweighted) linear regression algorithm that we saw earlier is known as a **parametric** learning algorithm because it has a fixed, finite number of parameters (θ), which are fit to the data;
- Once we've fit the θ and stored them away, we no longer need to keep the training data around to make future predictions.
- In contrast, to make predictions using locally weighted linear regression, we need to keep the entire training set around.
- The term "non-parametric" (roughly) refers to the fact that the amount of stuff we need to keep in order to represent the hypothesis grows linearly with the size of the training set.

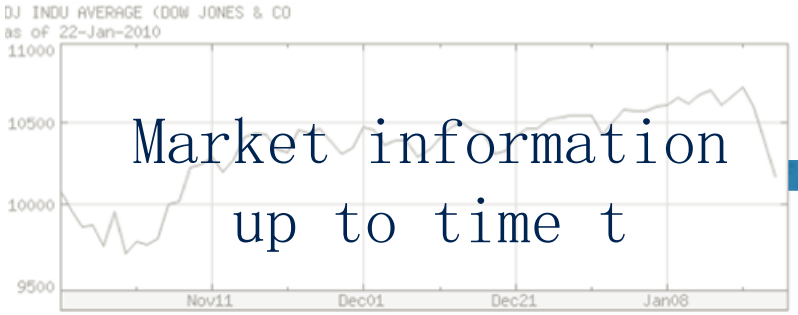
Another nonparametric learning algorithm: KNN

- In k-NN classification, the output is a class membership
- An object is classified by a majority vote of its neighbors, with the object being assigned to the class most common among its k nearest neighbors
- If k = 1, then the object is simply assigned to the class of that single nearest neighbor.
- k-NN is a type of instance-based learning, or lazy learning

Classification and Logistic Regression

Supervised Learning

- Regression



Market information up to time t → Share Price "$ 24.50" Continuous Labels Regression

- Classification

Feature Space $\mathcal{X}$ → Label Space $\mathcal{Y}$

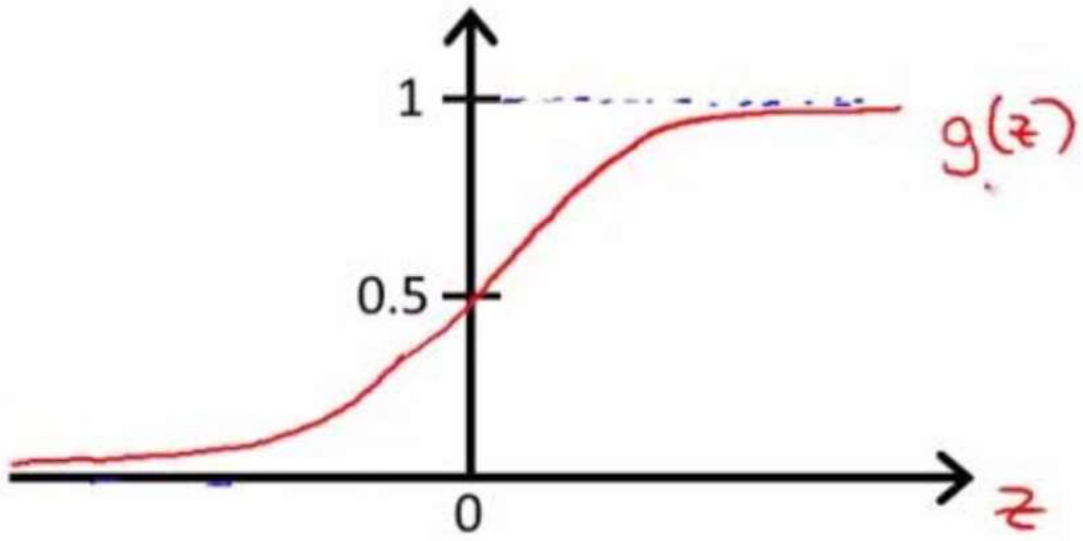
Words in a document →

"Sports"
"News"
"Science"
...

Discrete Labels Classification

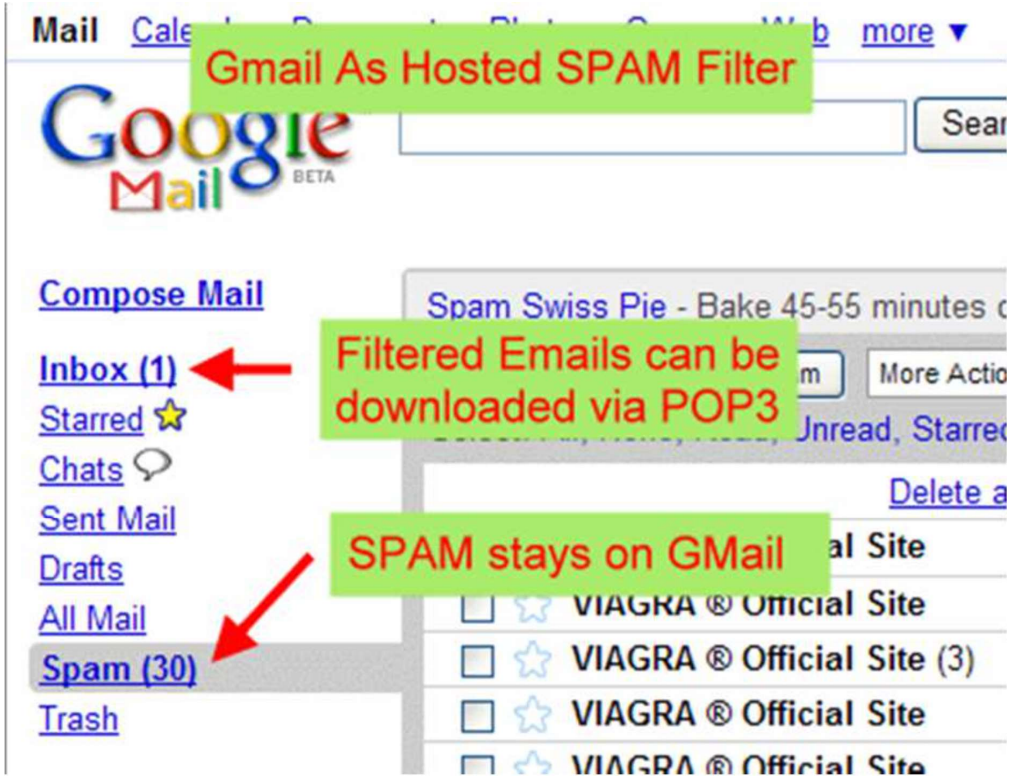
The logistic function

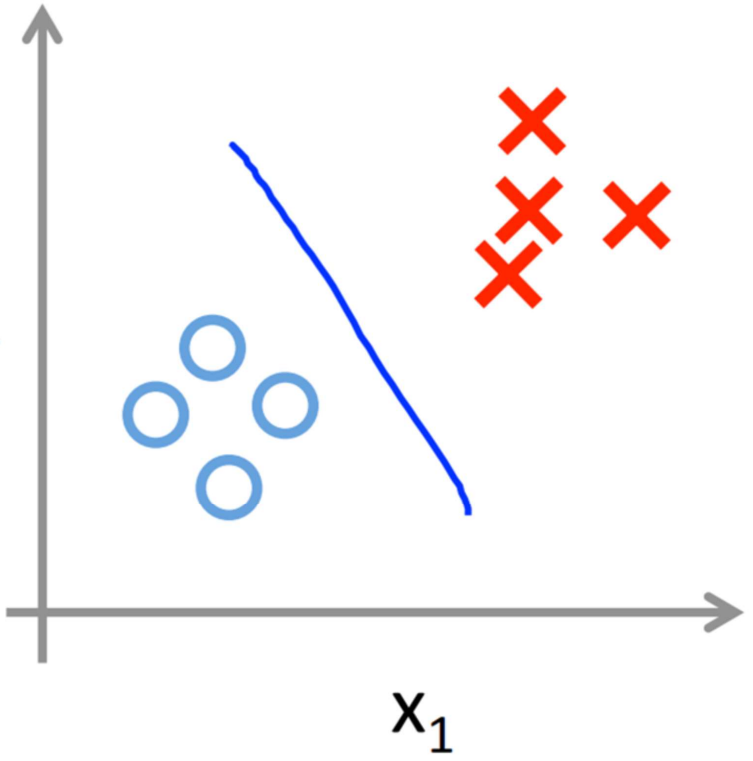
$$g(z) = \frac{1}{1 + e^{-z}}$$



Logistic Regression

- Logistic Regression is a classification model, although it is called "regression"
- It is a binary classification model
- It is a linear classification model





Model Description

- Hypothesis

$$P(y=1|x;\theta) = h_\theta(x) = g(\theta^T x) = \frac{1}{1+e^{-\theta^T x}}$$

$$P(y=0|x;\theta) = 1 - h_\theta(x)$$

- Compact Form

$$P(y|x;\theta) = (h_\theta(x))^y (1-h_\theta(x))^{1-y}$$

- Parameters θ

Maximum Likelihood Estimation

- (Conditional) Likelihood

$$
\begin{aligned}
L(\theta) &= p(\vec{y}|X;\theta) \\
&= \prod_{i=1}^{m} p(y^{(i)}|x^{(i)};\theta) \\
&= \prod_{i=1}^{m} (h_\theta(x^{(i)}))^{y^{(i)}} (1 - h_\theta(x^{(i)}))^{1-y^{(i)}}
\end{aligned}
$$

- Log-likelihood

$$
\begin{aligned}
\iota(\theta) &= \log L(\theta) \\
&= \sum_{i=1}^{m} y^{(i)} \log h(x^{(i)}) + (1 - y^{(i)}) \log(1 - h(x^{(i)}))
\end{aligned}
$$

Cross-Entropy

Unconstraint Optimization Methods

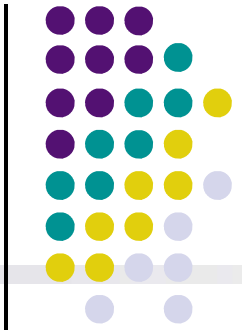
- Problem

$$argmax_\theta \sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))$$

$$where \quad h(x) = \frac{1}{1 + exp^{-\theta^T x}}$$

- Optimization Methods
  - Gradient Descent
  - Stochastic Gradient Descent
  - Newton Method
  - Quasi-Newton Method
  - Conjugate Gradient
  - …

Gradient Ascent



- Property of sigmoid function:

$$
\begin{aligned}
g'(z) &= \frac{d}{dz}\frac{1}{1+e^{-z}} \\
&= \frac{1}{(1+e^{-z})^2}(e^{-z}) \\
&= \frac{1}{(1+e^{-z})}(1-\frac{1}{(1+e^{-z})}) \\
&= g(z)(1-g(z))
\end{aligned}
$$

Gradient Ascent

- Gradient

$$\begin{aligned}
\frac{\partial \iota(\theta)}{\partial \theta_j} &= \sum_{i=1}^{m} (y^{(i)} \frac{1}{h_\theta(x^{(i)})} - (1-y^{(i)}) \frac{1}{1-h_\theta(x^{(i)})}) \frac{\partial}{\partial \theta_j} h_\theta(x^{(i)}) \\
&= \sum_{i=1}^{m} (y^{(i)} \frac{1}{h_\theta(x^{(i)})} - (1-y^{(i)}) \frac{1}{1-h_\theta(x(i))}) h_\theta(x^{(i)})(1-h_\theta(x^{(i)})) \frac{\partial}{\partial \theta_j} \theta^T x^{(i)} \\
&= \sum_{i=1}^{m} (y^{(i)}(1-h_\theta(x^{(i)})) - (1-y^{(i)}) h_\theta(x^{(i)})) x_j \\
&= \sum_{i=1}^{m} (y - h_\theta(x^{(i)})) x_j
\end{aligned}$$

- Batch Gradient Ascent Method

$$\theta_j := \theta_j + \alpha \sum_{i=1}^{m} (y^{(i)} - h_\theta(x^{(i)})) x_j^{(i)}$$

Stochastic Gradient Ascent

- Randomly choose a training sample (x, y)
- Compute gradient

$$(y - h_\theta(x))x_j$$

- Updating weights

$$\theta_j := \theta_j + \alpha(y - h_\theta(x))x_j$$

- Repeat …

Batch Gradient Ascent -- batch updating

Stochastic Gradient Ascent—online updating

The Newton's method

- A method for finding successively better approximations to the zeroes of a real-valued function.

$$x : f(x) = 0$$

- Start from an initial guess x_0

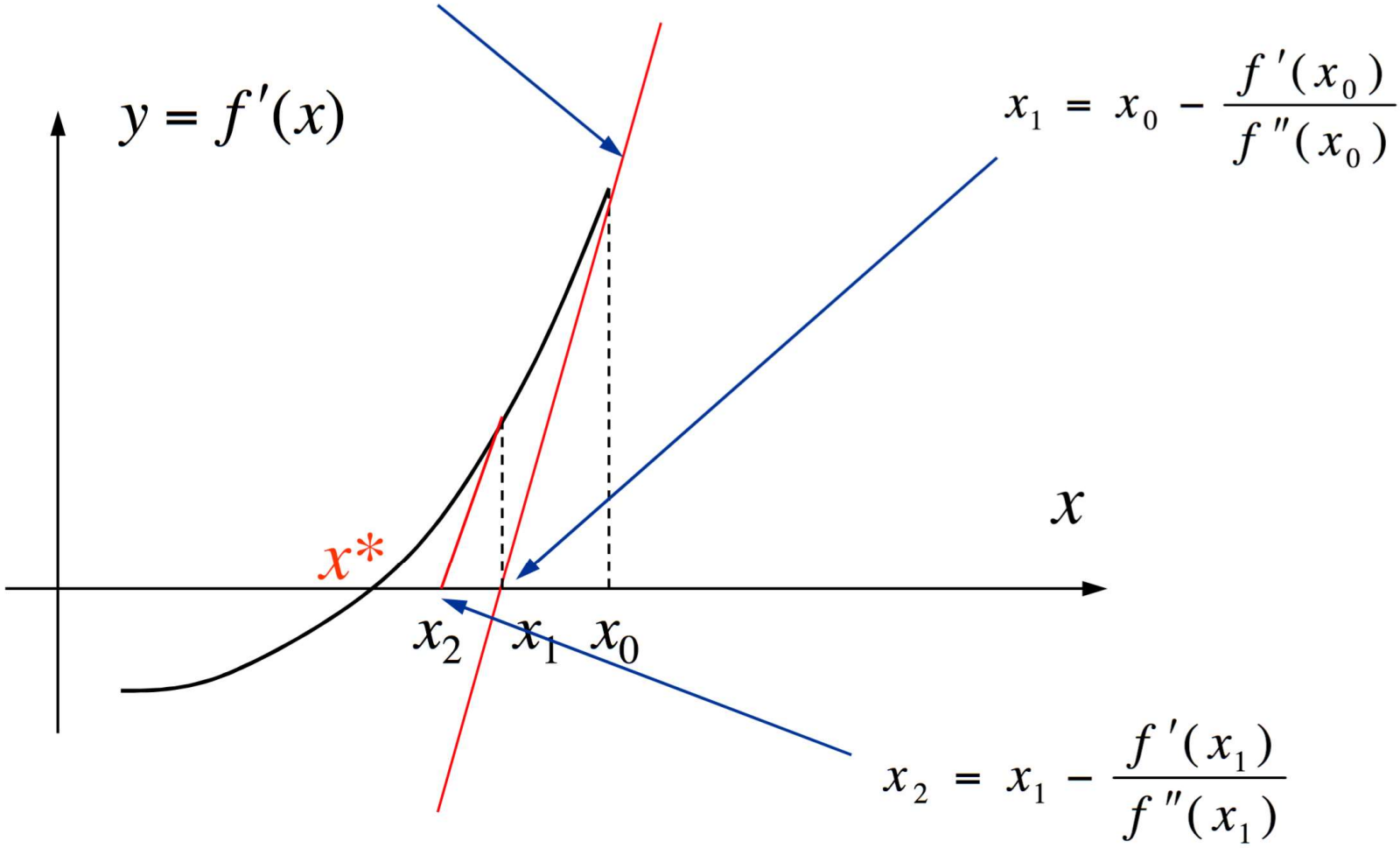
$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

- Geometrically, $(x_1, 0)$ is the intersection of the x-axis and the tangent of the graph of f at $(x_0, f(x_0))$.
- The process is repeated as

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Illustration of Newton's Method

- Tangent line: $y = f'(x_0) + f''(x_0)(x - x_0)$



Newton's Method

- Problem

$$\arg\min f(x) \iff solve : \nabla f(x) = 0$$

- Second-order Taylor expansion

$$\phi(x) = f(x^{(k)}) + \nabla f(x^{(k)})(x - x^{(k)}) + \frac{1}{2}\nabla^2 f(x^{(k)})(x - x^{(k)})^2 \approx f(x)$$

$$\nabla\phi(x) = 0 \Rightarrow x = x^{(k)} - \nabla^2 f(x^{(k)})^{-1}\nabla f(x^{(k)})$$

- Newton's method (also called Newton-Raphson method)

$$x^{(k+1)} = x^{(k)} - \nabla^2 f(x^{(k)})^{-1}\nabla f(x^{(k)})$$

The Newton-Raphson method

- In LR the θ is vector-valued, thus we need the following generalization:

$$\theta := \theta - H^{-1}\nabla_\theta \iota(\theta)$$

Here, $\nabla_\theta \iota(\theta)$ is, as usual, the vector of partial derivatives of $\iota(\theta)$ with respect to the θ_i's; and H is an n-by-n matrix (actually, n+1-by-n+1, assuming that we include the intercept term) called the Hessian, whose entries are given by

$$H_{ij} = \frac{\partial^2 \iota(\theta)}{\partial \theta_i \partial \theta_j}$$

Newton's Method for Logistic Regression

- Problem

$$\arg\min_{\theta} J(\theta) = \frac{1}{m}\sum_{i=1}^{m} -y^{(i)} \log h_\theta(x^{(i)}) - (1-y^{(i)}) \log(1-h_\theta(x^{(i)}))$$

- Gradient and Hessian Matrix

$$\nabla J(\theta) = \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j$$

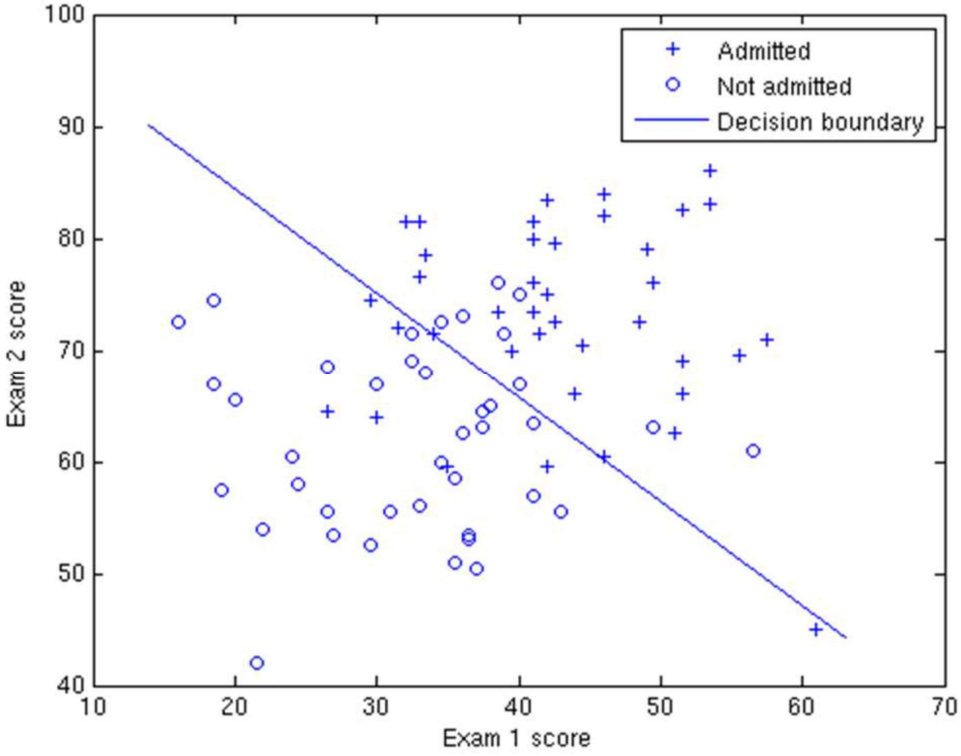
$$H = \frac{1}{m}\sum_{i=1}^{m} h_\theta(x^{(i)})(1-h_\theta(x^{(i)}))x^{(i)}(x^{(i)})^T$$

- Weight updating using Newton's method

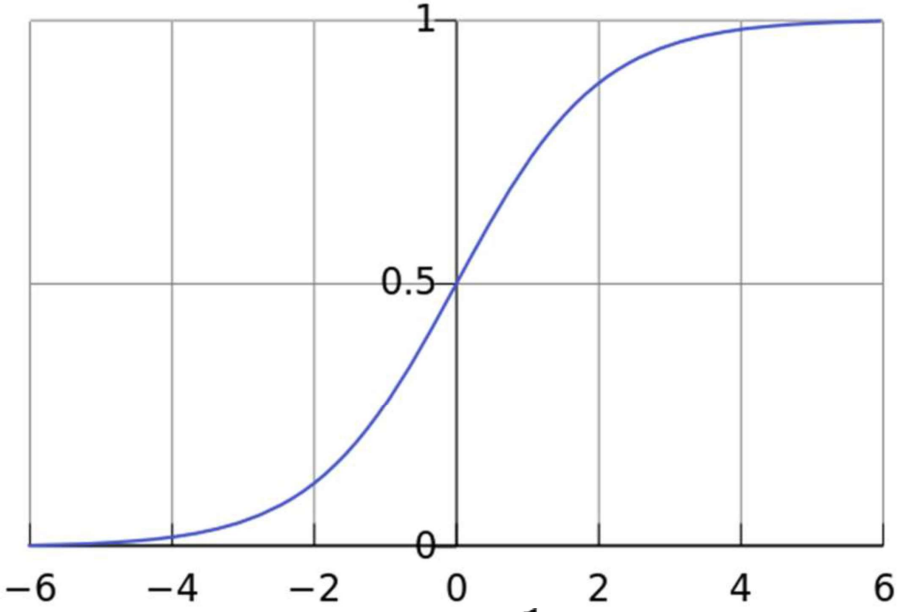
$$\theta^{(t+1)} = \theta^{(t)} - H^{-1}\nabla J(\theta^{(t)})$$

A Linear Classification Model

- Logistic regression has a linear decision boundary (hyperplane)



- But with a nonlinear activation function (Sigmoid function) to model the posterior probability

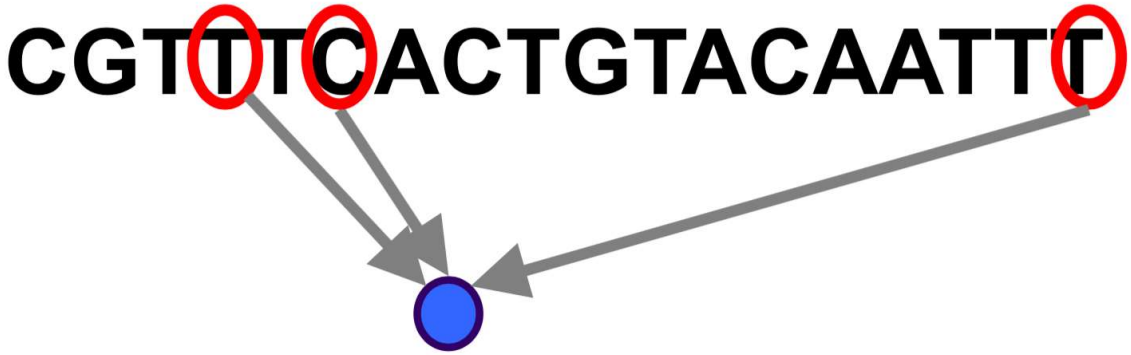


$$h(x) = \frac{1}{1 + exp^{-\theta^T x}}$$

Case Study: Gene Association Study

The genetic picture

causal SNPs

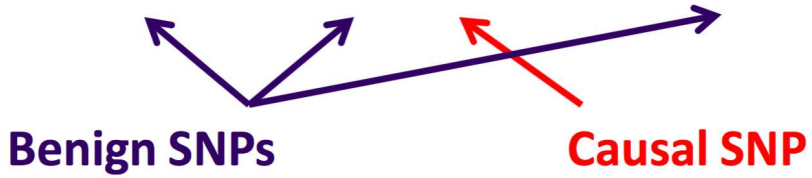


a univariate phenotype:

i.e., the expression intensity of a gene

Association Mapping as Regression

	Phenotype (BMI)	Genotype
Individual 1	2.5	..C.....T..C.....T... ..C.....A..C.....T...
Individual 2	4.8	..G.....A..G.....A... ..C.....T..C.....T...
⋮		
Individual N	4.7	..G.....T..C.....T... ..G.....T..G.....T...



Association Mapping as Regression

	Phenotype (BMI)	Genotype
Individual 1	2.5	..0..... 1..0.......0...
Individual 2	4.8	..1 .....1..1.......1...
⋮		
Individual N	4.7	..2 .....2..1.......0...

$$y_i = \sum_{j=1}^{J} x_{ij}\beta_j$$

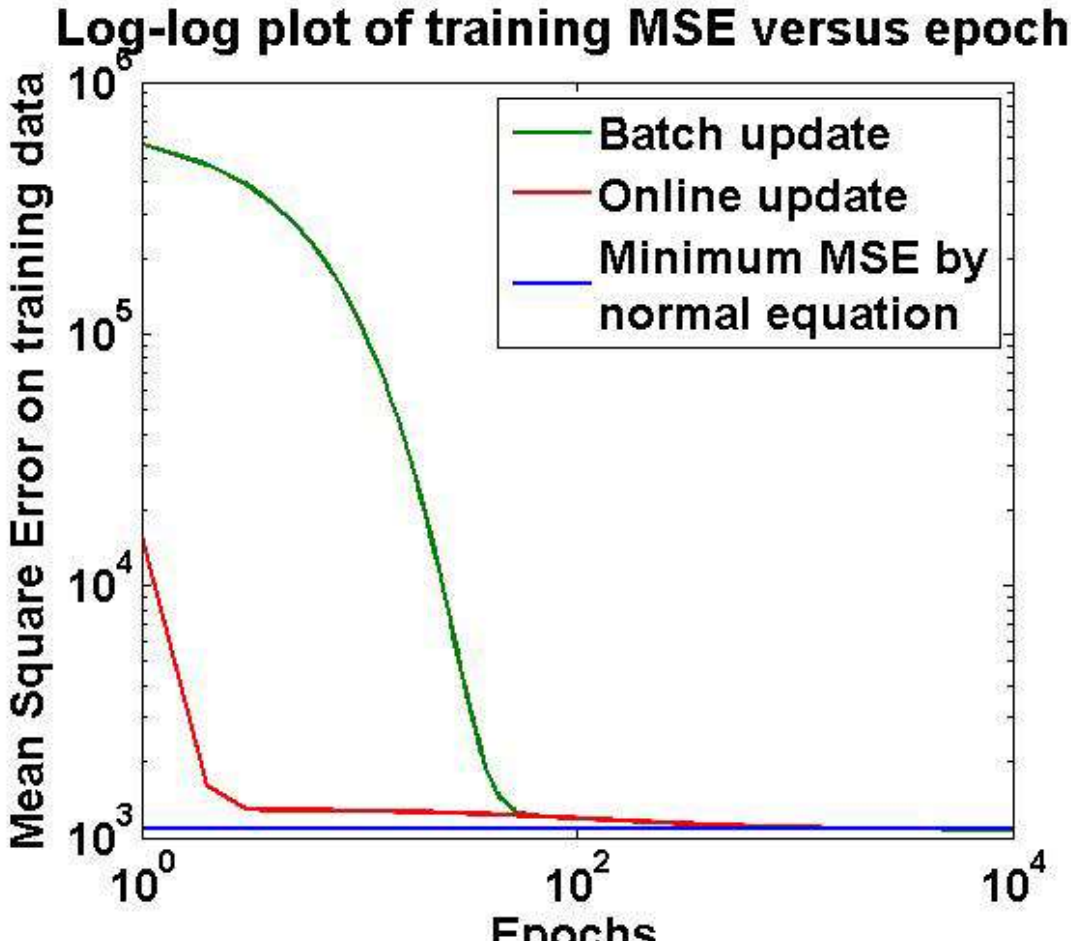
SNPs with large $|\beta_j|$ are relevant

Experimental setup

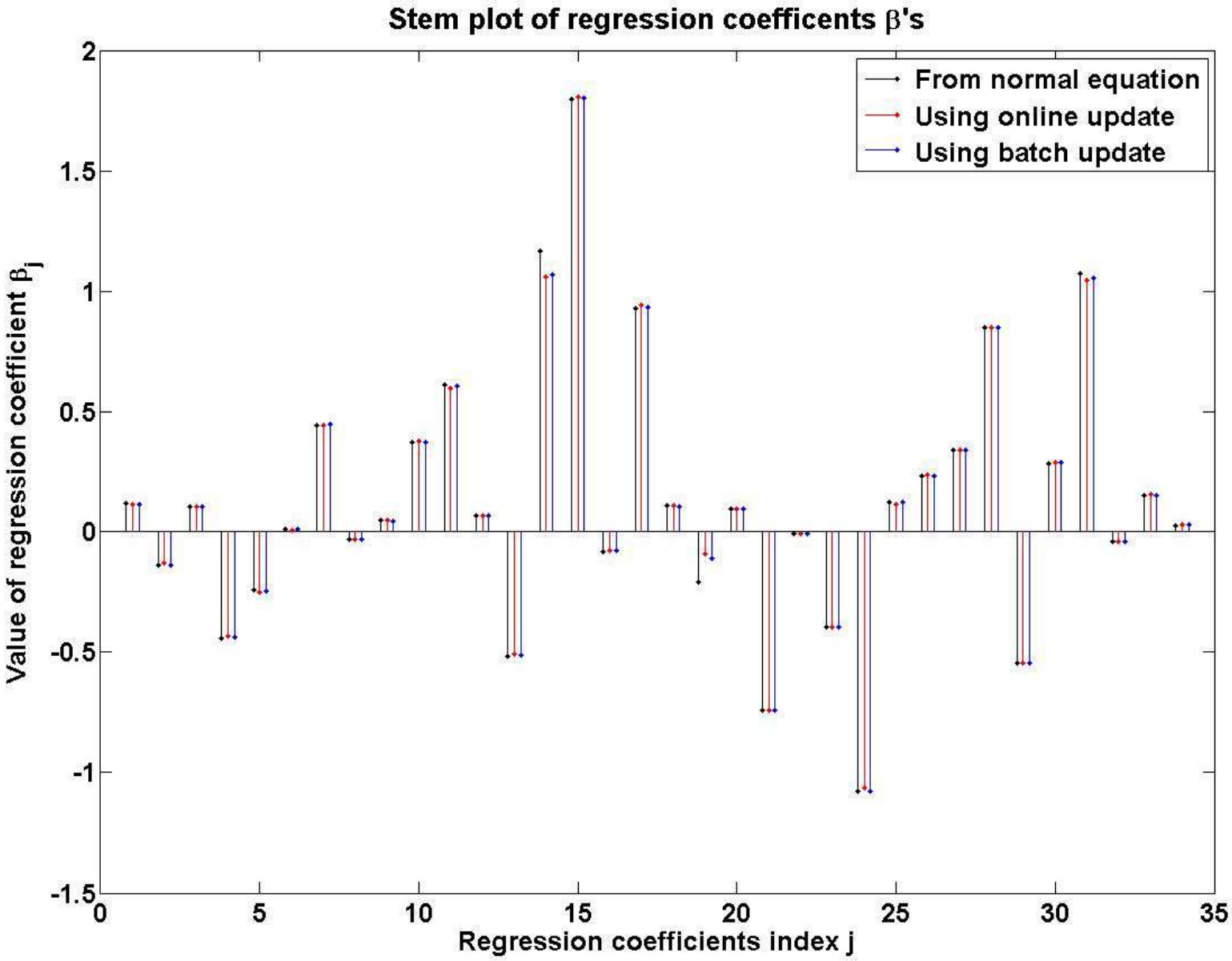
- Asthama dataset
  - 543 individuals, genotyped at 34 SNPs
  - Diploid data was transformed into 0/1 (for homozygotes) or 2 (for heterozygotes)
  - X=543x34 matrix
  - Y=Phenotype variable (continuous)
- A single phenotype was used for regression
- Implementation details
  - Iterative methods: Batch update and online update implemented.
  - For both methods, step size α is chosen to be a small fixed value (10^{-6}). This choice is based on the data used for experiments.
  - Both methods are only run to a maximum of 2000 epochs or until the change in training MSE is less than 10^{-4}

Convergence Curves

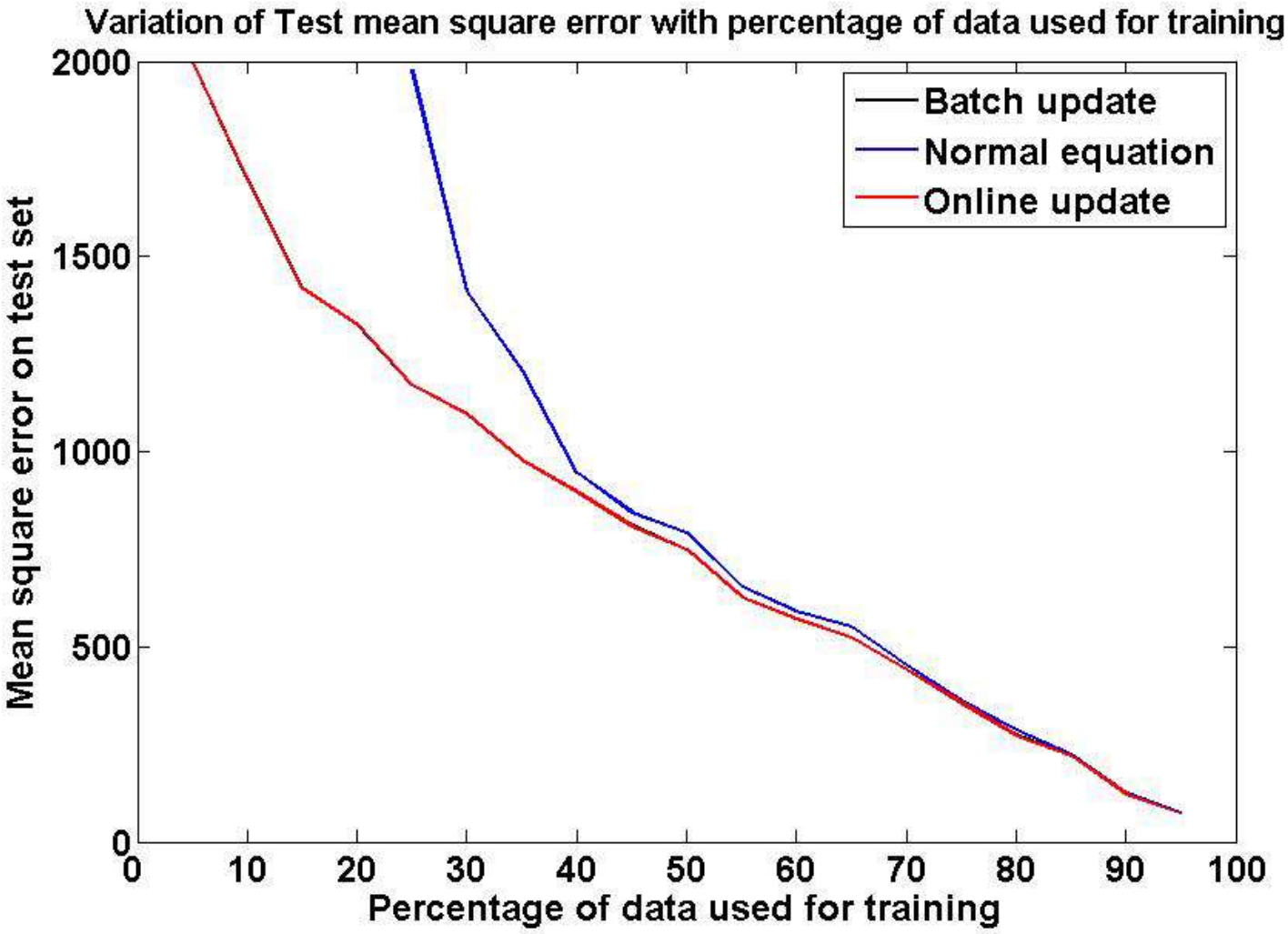
- For the batch method, the training MSE is initially large due to uninformed initialization
- In the online update, N updates for every epoch reduces MSE to a much smaller value



The Learned Coefficients



Performance vs. Training Size



- The results from B and O update are almost identical. So the plots coincide.
- The test MSE from the normal equation is more than that of B and O during small training. This is probably due to overfitting.
- In B and O, since only 2000 iterations are allowed at most. This roughly acts as a mechanism that avoids overfitting.

Linear discriminant analysis

- One way to view a linear classification model is in terms of dimensionality reduction.
  - Consider first the case of two classes, and suppose we take the n dimensional input vector x and project it down to one dimension

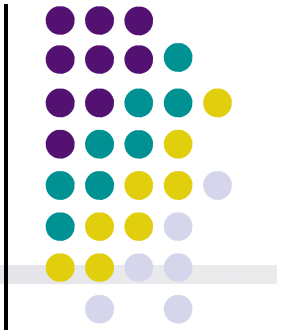
$$y = \mathbf{w}^{\mathrm{T}}\mathbf{x}$$

  - We can place a threshold on y and classify y as class C_1/C_2
- In general, the projection onto one dimension leads to a considerable loss of information, and classes that are well separated in the original n-dimensional space may become strongly overlapping in one dimension
- However, by adjusting the components of the weight vector **w**, we can select a projection that maximizes the class separation

Linear discriminant analysis

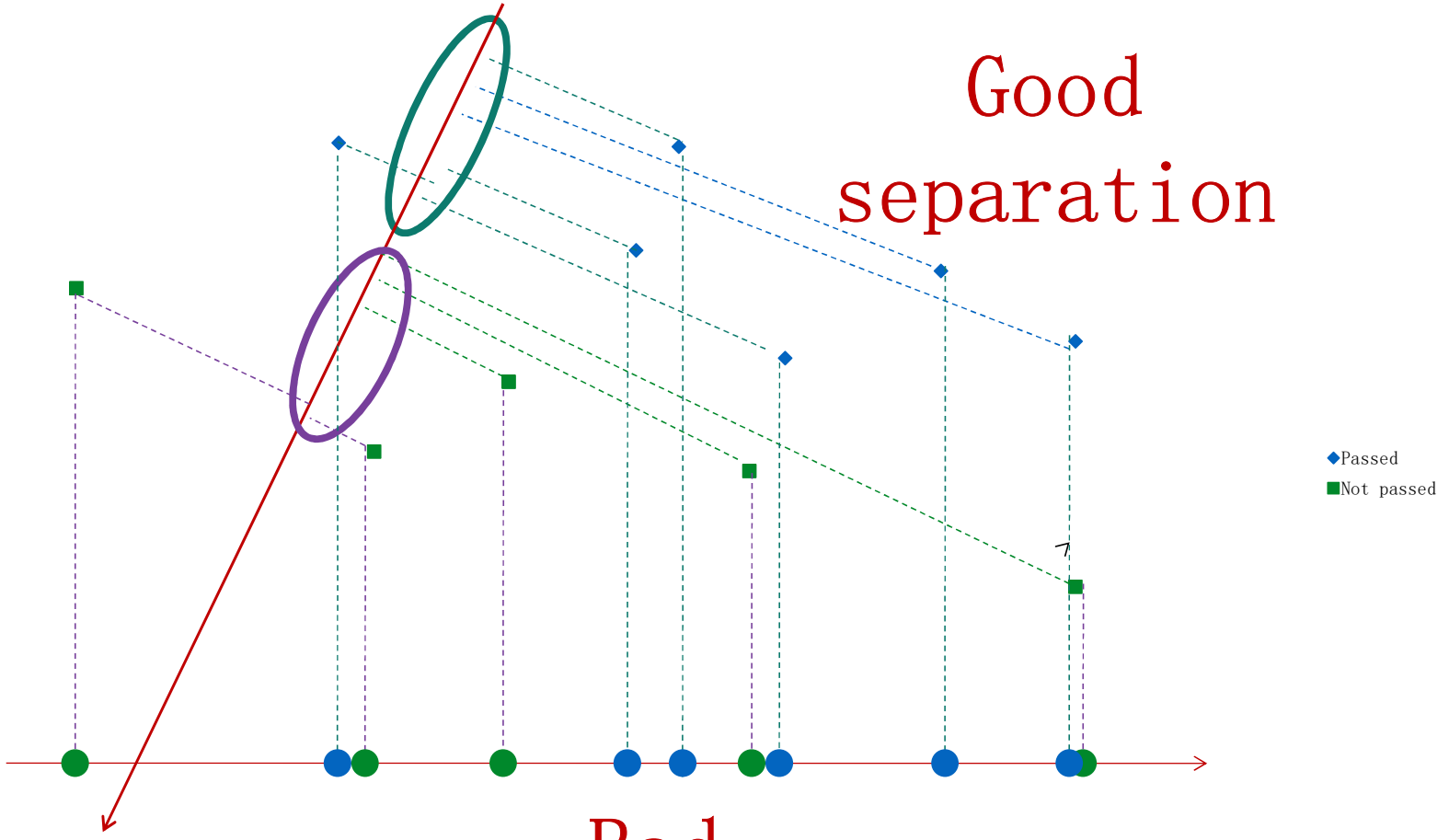
- Linear discriminant analysis is another way of finding a linear transformation that reduces the number of dimensions
- Unlike PCA or ICA it uses labeled data: it is a supervised technique, but designed for classification
- Often used for dimensionality reduction prior to classification, but can be used as a classification technique itself
- When used for dimensionality reduction, it yields (k-1) dimensions for a k-class classification problem

Purpose



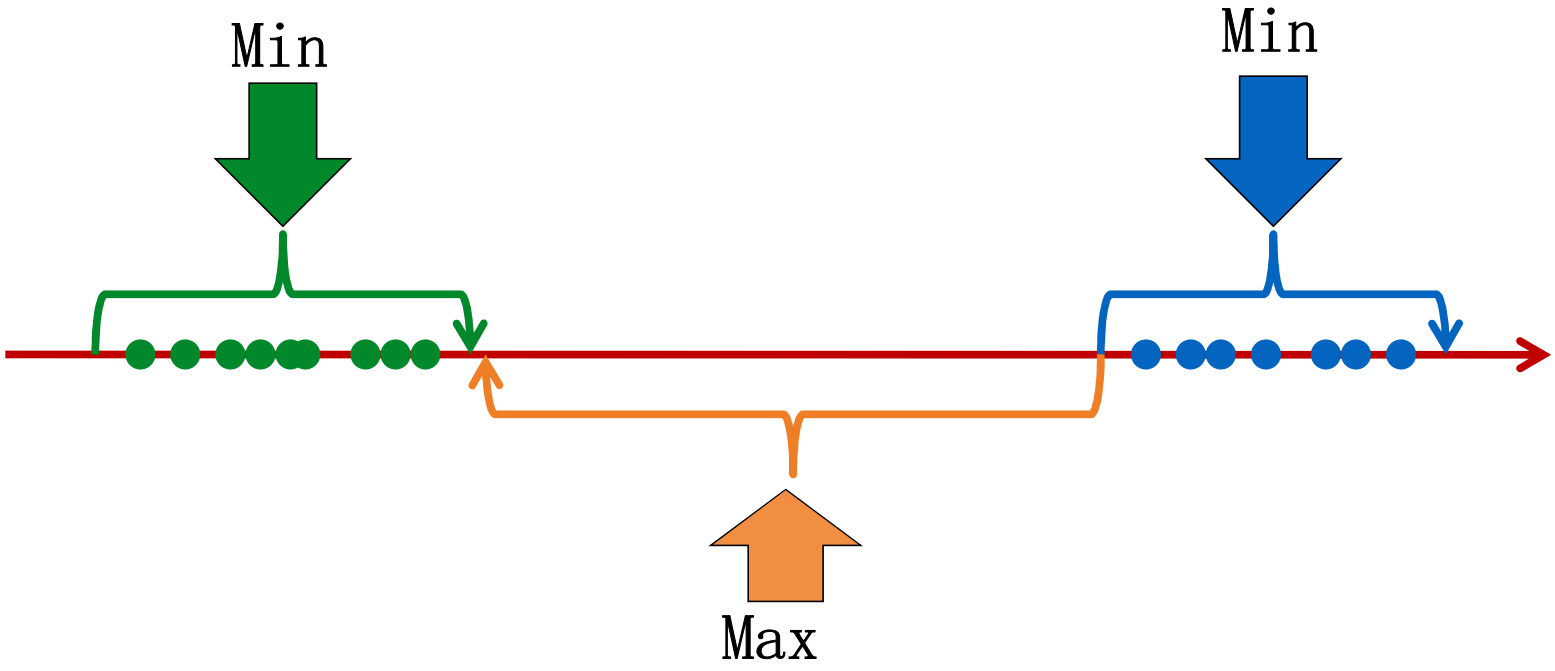
- Discriminant Analysis classifies objects in two or more groups according to linear combination of features
- Dimensionality reduction
  - Which set of features can best determine group membership of the object?
- Classification
  - What is the classification rule or model to best separate those groups?

Method (1)



Method (2)

- Maximize the between-class scatter
  - Difference of mean values (m_1-m_2)
- Minimize the within-class scatter
  - Covariance



Fisher's linear discriminant analysis

- Let us now consider Fisher's LDA projection for dimensionality reduction, considering the two-class case first
- We seek a projection vector $\mathbf{a}$ that can be used to compute scalar projections $y = \mathbf{a}^T\mathbf{x}$ for input vectors $\mathbf{x}$
- This vector is obtained by computing the means of each class, μ_1 and μ_2, and then computing two special matrices
- The between-class scatter matrix is calculated as

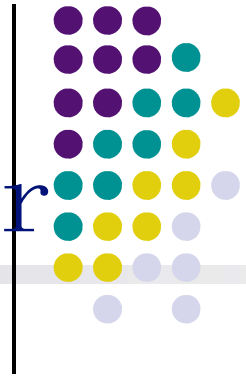
$$\mathbf{S}_B = (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^{\mathrm{T}}$$

(note the use of the outer product of two vectors here, which gives a matrix)

- The within-class scatter matrix is

$$\mathbf{S}_W = \sum_{i:c_i=1} (\mathbf{x}_i - \boldsymbol{\mu}_1)(\mathbf{x}_i - \boldsymbol{\mu}_1)^{\mathrm{T}} + \sum_{i:c_i=2} (\mathbf{x}_i - \boldsymbol{\mu}_2)(\mathbf{x}_i - \boldsymbol{\mu}_2)^{\mathrm{T}}$$

Fisher's LDA: the solution vector



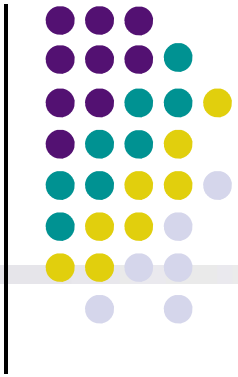
- The solution vector a for FLDA is found by maximizing the "Rayleigh quotient"

$$J(\mathbf{a}) = \frac{\mathbf{a}^{\mathrm{T}}\mathbf{S}_B\mathbf{a}}{\mathbf{a}^{\mathrm{T}}\mathbf{S}_W\mathbf{a}}$$

- This leads to the solution

$$\mathbf{a} = \mathbf{S}_W^{-1}(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)$$

Multi-class FLDA



- FLDA can be generalized to multi-class problems
- Aim: projection A so that $y = A^T x$ yields points that are close when they are in the same class relative to the overall spread
- To do this, first compute both the means for each class and the global mean, and then compute the scatter matrices

$$\mathbf{S}_B = \sum_{c=1}^{C} n_c(\boldsymbol{\mu}_c - \boldsymbol{\mu})(\boldsymbol{\mu}_c - \boldsymbol{\mu})^{\mathrm{T}} \qquad \mathbf{S}_W = \sum_{j=1}^{C} \sum_{i:c_i=j} (\mathbf{x}_i - \boldsymbol{\mu}_{c=j})(\mathbf{x}_i - \boldsymbol{\mu}_{c=j})^{\mathrm{T}}$$

- Then, find the projection matrix A that maximizes $J(\mathbf{A}) = \dfrac{\left|A^{\mathrm{T}}\mathbf{S}_B A\right|}{\left|A^{\mathrm{T}}\mathbf{S}_W A\right|}$

  Determinants are analogs of variances computed in multiple dimensions, along the principal directions of the scatter matrices, and multiplied together
- Solutions for finding A are based on solving a "generalized eigenvalue problem" for each column of the matrix A.

From Two-Class to Multiple-Class

Model:

- Binary: One-vs-Rest
- Binary: One-vs-One
- Binary: ECOC

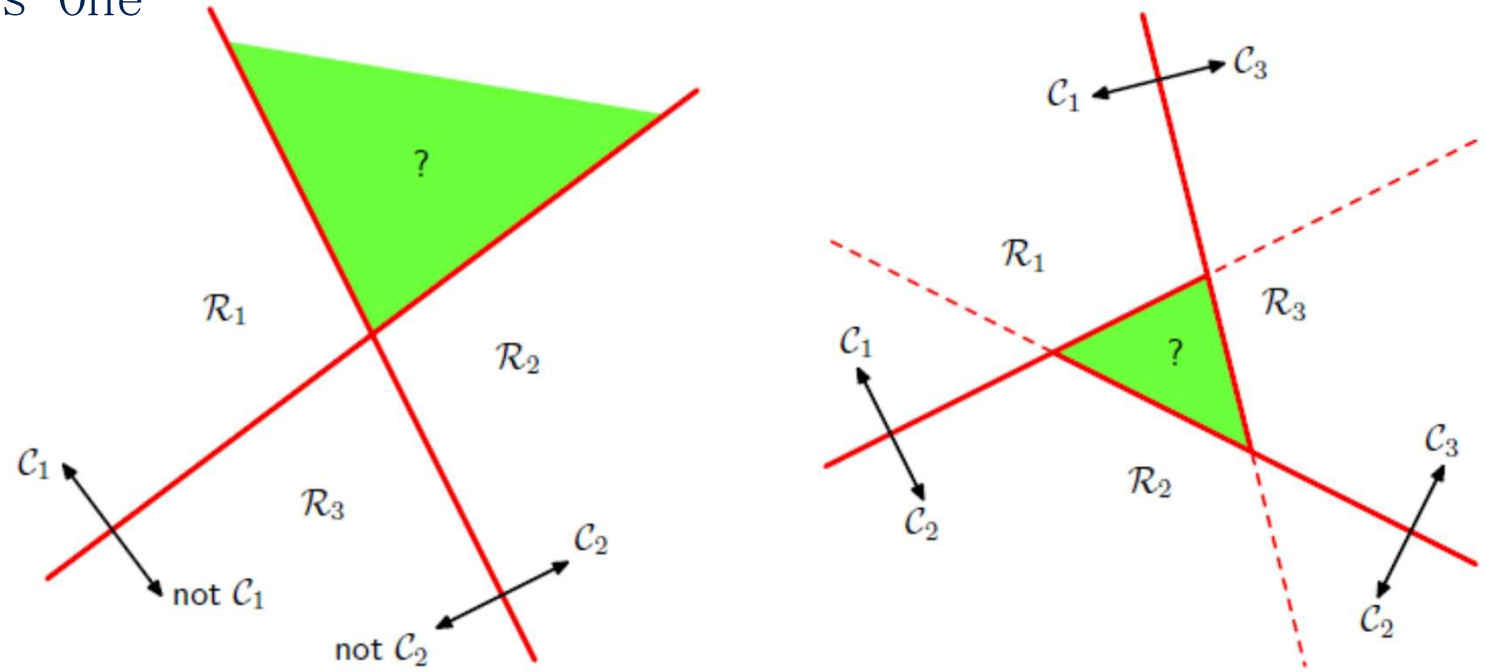


Figure 4.2 Attempting to construct a K class discriminant from a set of two class discriminants leads to ambiguous regions, shown in green. On the left is an example involving the use of two discriminants designed to distinguish points in class $\mathcal{C}_k$ from points not in class $\mathcal{C}_k$. On the right is an example involving three discriminant functions each of which is used to separate a pair of classes $\mathcal{C}_k$ and $\mathcal{C}_j$.

From Two-Class to Multiple-Class

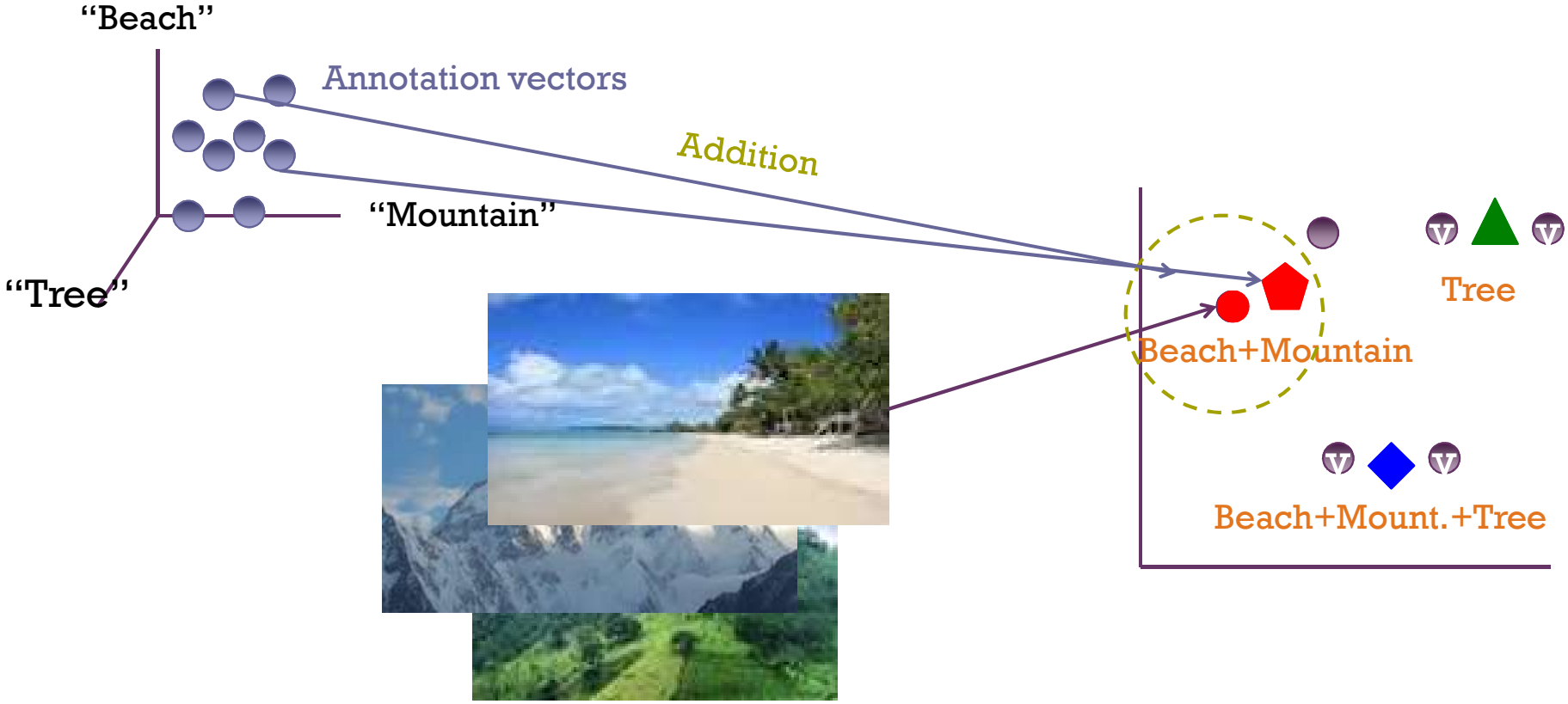
- Decompose a n-class problem into several two-classes problems:
- One-vs-Rest: Use n - 1 binary classifiers each of which solves a two-class problem of separating points in a particular class from points not in that class.
- Pros: small storing cost and short test time
- Cons: long training time, imbalanced Samples

- One-vs-One: Use (n - 1)n/2 binary classifiers, one for every possible pairs of classes. Each point is classified according to a majority vote amongst the discriminant functions.
- Pros: short training time
- Cons: Too many classifiers; large storing cost and long test time

Multi-Label Zero-Shot

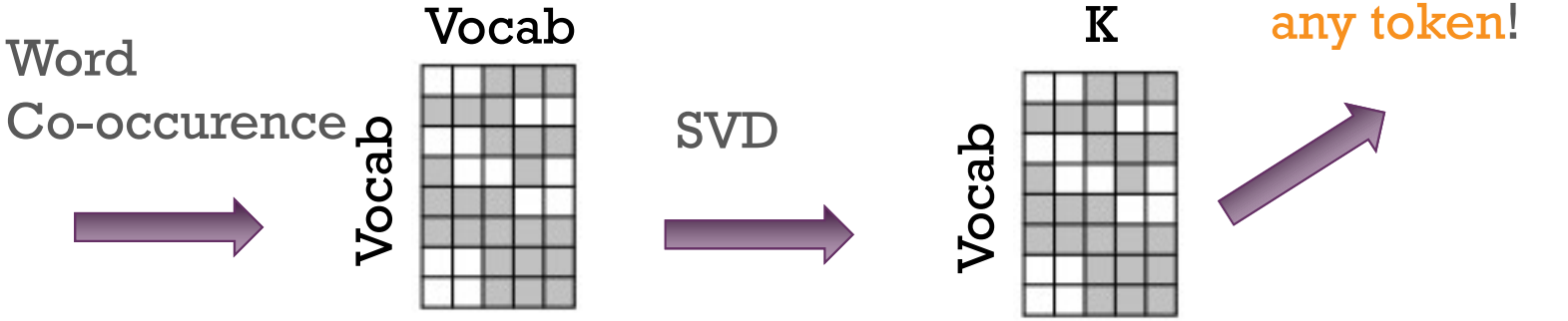
From Dr. Timothy Hospedales's slides
Queen Mary University of London
@ Yandex School of Data Analysis Conference 2015

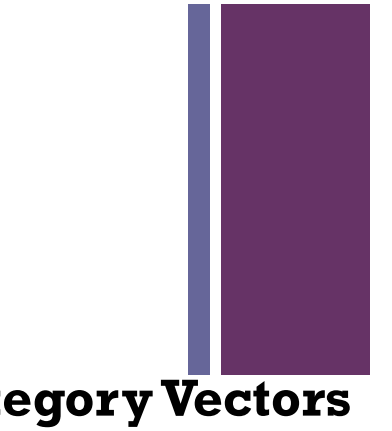
- Sometimes we want to annotate (multi-label), rather than classify (single-label).
  - Solution: Rely on class vector aggregation (e.g., addition) to generate all possible multi-label class prototypes. [Hospedales BMVC'14]



Where to get Category Vectors?

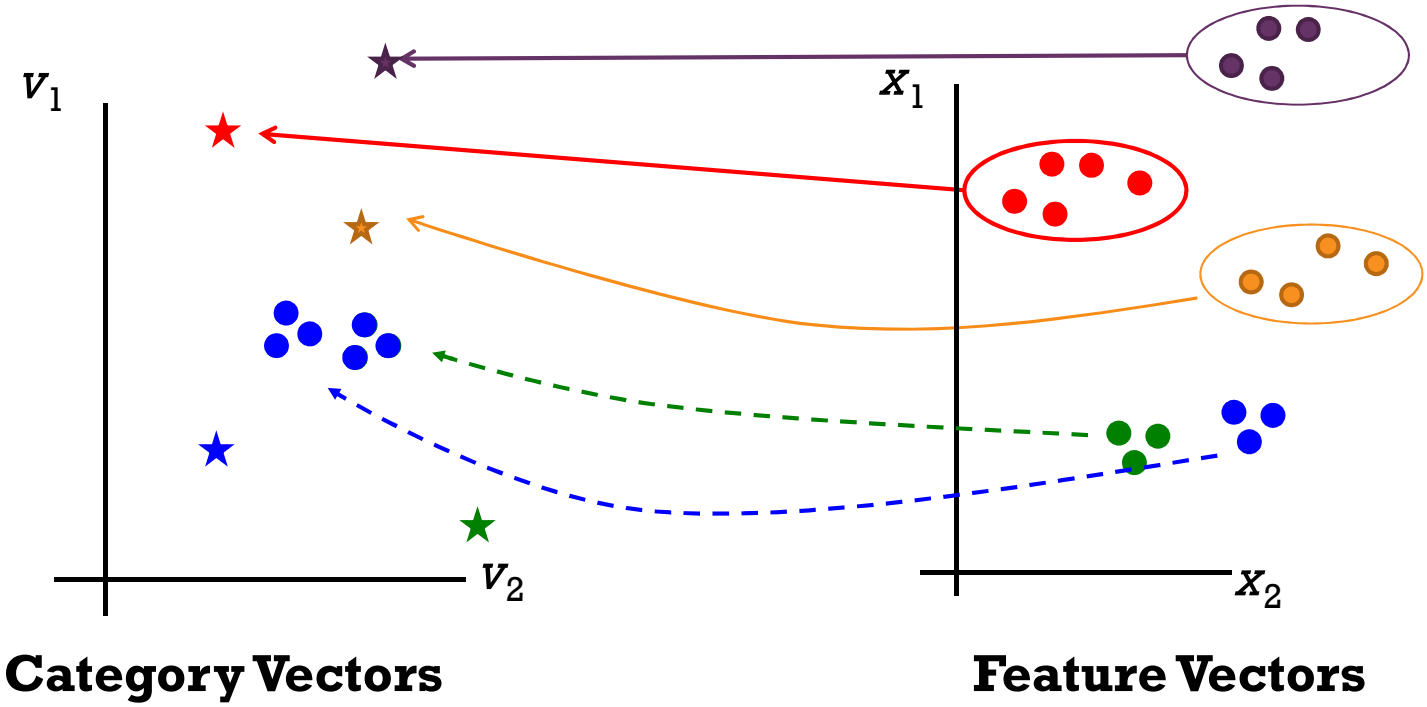
- "Supervised" sources:
  - Manual annotation of class properties
  - Vector encoding of a taxonomic class hierarchy
- "Unsupervised" sources: Existing unstructured data
  - Word (token) co-occurrence.
    - OR: word2vec: Representation of word prediction neural net.
  - => Automatic+Free word vector for any "nameable" category.

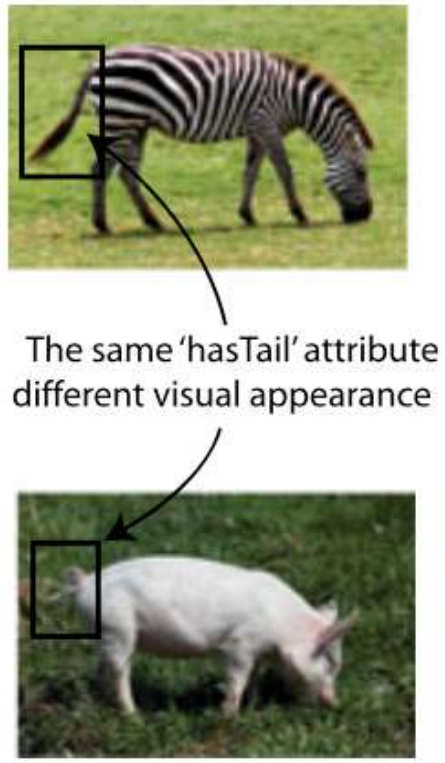




Domain Shift

- ZSL necessarily entails a train/test domain shift.

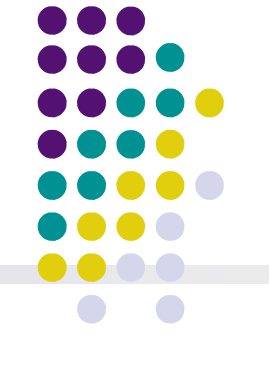




Application to Video Recognition

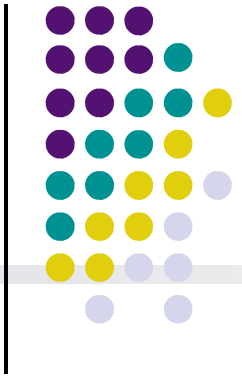
- Also video recognition: UCF101/HMDB51/etc.

A case study



Classification (Discrimination, Supervised Learning) Using Microarray Data

Gene expression data



mRNA samples

Genes		Normal sample1	Normal sample2	Normal sample3	Cancer sample4	Cancer sample5	…
	1	0.46	0.30	0.80	1.51	0.90	...
	2	-0.10	0.49	0.24	0.06	0.46	...
	3	0.15	0.74	0.04	0.10	0.20	...
	4	-0.45	-1.03	-0.79	-0.56	-0.32	...
	5	-0.06	1.06	1.35	1.09	-1.09	...

Gene expression level of gene *i* in mRNA sample *j*

Tumor Classification Using Gene Expression Data

- Three main types of statistical problems associated with the microarray data:
  - Identification of "marker" genes that characterize the different tumor classes (feature or variable selection).
  - Identification of new/unknown tumor classes using gene expression profiles (unsupervised learning – clustering)
  - Classification of sample into known classes (supervised learning – classification)

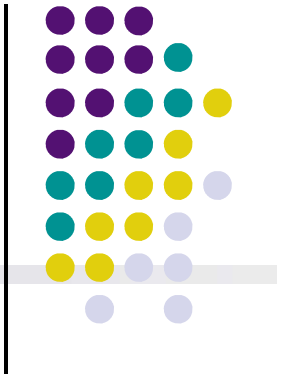
Classification

Y	Normal	Normal	Normal	Cancer	Cancer		unknown =Y_new
	sample1	**sample2**	**sample3**	**sample4**	**sample5**	**…**	**New sample**
1	0.46	0.30	0.80	1.51	0.90	...	0.34
2	-0.10	0.49	0.24	0.06	0.46	...	0.43
3	0.15	0.74	0.04	0.10	0.20	...	-0.23
4	-0.45	-1.03	-0.79	-0.56	-0.32	...	-0.91
5	-0.06	1.06	1.35	1.09	-1.09	...	1.23
	X						X_new

Each object (e.g. arrays or columns)associated with a class label (or response) $Y \in \{1, 2, \ldots, K\}$ and a feature vector (vector of predictor variables) of G measurements: $X = (X_1, \ldots, X_G)$

Aim: predict Y_new from X_new.

Methods



- Linear Regression
- Logistic Regression
- Fisher Linear Discriminant Analysis
- Nearest Neighbor Classification
- ...