

# Machine Learning DSECL ZG565

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## innovate achieve lead

#### **Session Content**

- Decision Theory Bishop
- Probabilistic Generative Model versus Probabilistic Discriminative Model
- Logistic Regression –Bayesian Analysis (New chapter Tom Mitchell)
- Estimating Parameters Linear Regression: Closed form solution
- Linear basis function models (3.1 Bishop)
- Evaluation metrics

## **Decision Theory**

## **Decision Theory**

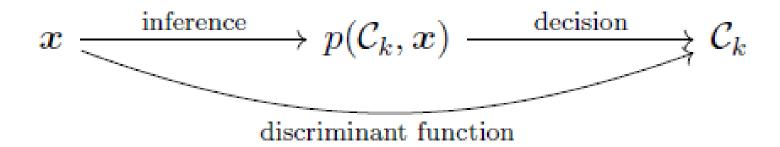
We have broken the classification problem down into two separate stages

• Inference step: Determine p(x, t) OR  $p(x|C_k)$  from training data. (For regression problems t is continuous variables, whereas for classification problems t represents class labels.)

 $t = \arg\max_{k} \{ \underbrace{p(x|\mathcal{C}_k)}$ 

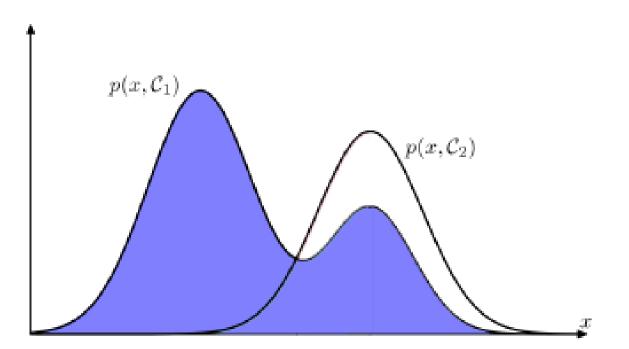
Likelihood

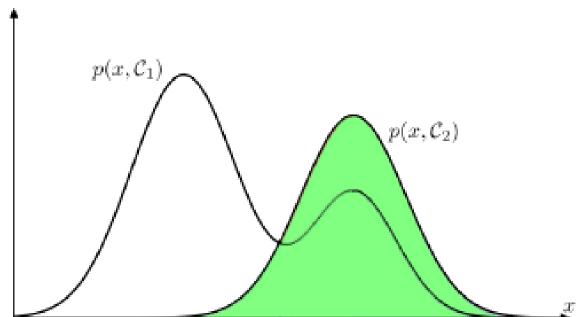
• **Decision step**: Determine optimal *t* for test input *x*: how to make optimal decisions given the appropriate probabilities.



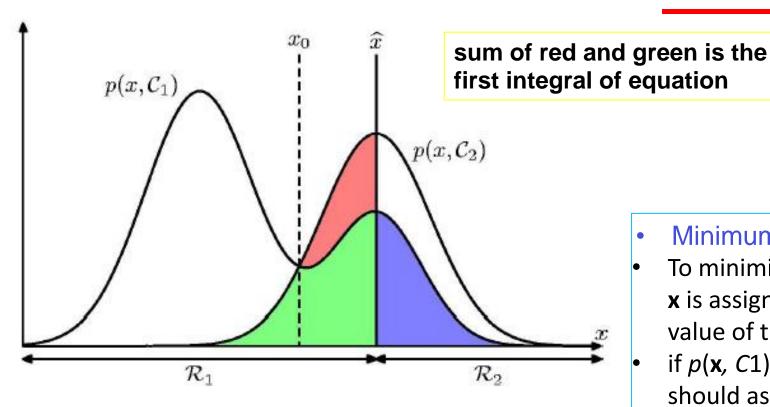
#### **Minimum Misclassification Rate**

- Divide the input space into regions Rk called decision regions, one for each class, such that all points
  in Rk are assigned to class Ck
- Boundaries between decision regions are called decision boundaries or decision surfaces
- A mistake occurs when an input vector belonging to class C1 is assigned to class C2 or vice versa.





## Minimum Misclassification Rate



$$p(\text{mistake}) = p(\mathbf{x} \in \mathcal{R}_1, \mathcal{C}_2) + p(\mathbf{x} \in \mathcal{R}_2, \mathcal{C}_1)$$
$$= \int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2) d\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1) d\mathbf{x}.$$

 $\hat{x}$ : decision boundary.

 $x_0$ : optimal decision boundary

 $x_0$ : arg min $\{p \text{ (mistake)}\}$ 

- Minimum error decision rule
- To minimize p(mistake) we should arrange that each
   x is assigned to whichever class has the smaller
   value of the integrand
- if  $p(\mathbf{x}, C1) > p(\mathbf{x}, C2)$  for a given value of  $\mathbf{x}$ , then we should assign that  $\mathbf{x}$  to class C1.
- Since  $p(x,C_k)=p(C_k/x)p(x)$ , choose class for which a posteriori probability is highest
  - Called Bayes Classifier

#### Minimum Misclassification Rate

#### General case of K classes

$$p(\text{correct}) = \sum_{k=1}^{K} p(\mathbf{x} \in \mathcal{R}_k, \mathcal{C}_k)$$
$$= \sum_{k=1}^{K} \int_{\mathcal{R}_k} p(\mathbf{x}, \mathcal{C}_k) d\mathbf{x}$$

#### Three distinct approaches to Decision Problems

- 1.Generative
- 2. Discriminative
- 3. Discriminant Function

#### 1. Generative Models



- Model class-conditional pdfs and prior probabilities
- First solve inference problem of determining class-conditional densities P(X|Y), for each class separately
- Then use Bayes theorem to determine posterior probabilities
- Then use decision theory to determine class membership
- "Generative" since sampling can generate synthetic data points
- Use the capacity of the model to characterize how the data is generated (both inputs and outputs)
- explicitly models the actual distribution of each class.
- Gaussians, Naïve Bayes, Mixtures of multinomials, Mixtures of Gaussians, Bayesian networks,

#### 2. Discriminative Models

- Directly estimate posterior probabilities P(Y|X) directly from training data and use decision theory to assign each new x to one of the classes
- No attempt to model underlying probability distributions
- models the decision boundary between the classes
- Logistic regression, SVMs, tree based classifiers (e.g. decision tree) Traditional neural networks, Nearest neighbor

#### 3. Discriminant Functions

- Find a function f (x) that maps each input x
- directly to class label
  - In two-class problem, f (.) is binary valued
    - f =0 represents class C1 and f =1 represents class C2
- Probabilities play no role
  - No access to posterior probabilities p(Y|X)
  - Linear discriminant, Fisher Linear Disc, Perceptron

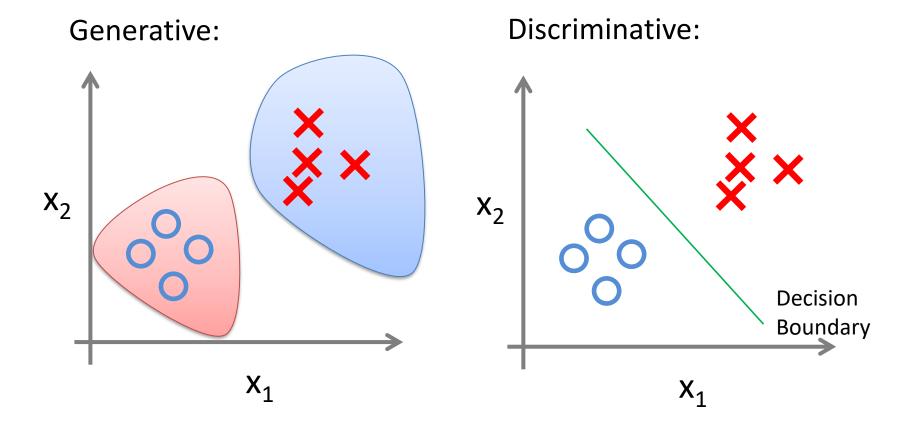
#### Spam classification problem

#### First Strategy: discriminative (e.g., logistic regression)

- Use training set to find a decision boundary in the feature space that separates spam and non-spam emails
- Given a test point, predict its label based on which side of the boundary it is on.

#### Second Strategy: generative (e.g., naive bayes)

- Look at spam emails and build a model of what they look like.
- Similarly, build a model of what non-spam emails look like.
- To classify a new email, match it against both the spam and non-spam models to see which is the better fit.



Generative	Discriminative		
Ex: Naïve Bayes	Ex: Logistic Regression		
Estimate $P(Y)$ and $P(X Y)$	Finds class label directly $P(Y X)$		
Prediction $\hat{y} = \operatorname{argmax}_{y} P(Y = y)P(X = x   Y = y)$	Prediction $\hat{y} = P(Y = y   X = x) = \frac{1}{1 + e^{-\theta^{T} x}}$		
Decision boundary	Probability distributions of the data		

## Logistic Regression —Bayesian Analysis

# Logistic Regression and Gaussian Naïve Bayes Classifier

- Interestingly, the parametric form of P(Y|X) used by Logistic Regression is precisely the form implied by the assumptions of a Gaussian Naive Bayes classifier.
- Therefore, we can view Logistic Regression as a closely related alternative to GNB, though the two can produce different results in many cases

- Estimation of n+1 parameters say,  $\theta = (\theta_0, \theta_1, \dots, \theta_n)$  for which the probability of the observed data is the maximum on the training data set.
  - generative learning
    - the Gaussian Naive Bayes assumptions
  - discriminative learning
    - maximize the conditional data likelihood ( or minimizing negative likelihood)
    - Uses gradient descent optimization

#### Bayesian inference

Bayesian inference for logistic analyses follows the usual pattern for all Bayesian analyses:

- 1. Write down the likelihood function of the data
- 2. Form a prior distribution over all unknown parameters.
- 3. Use Bayes theorem to find the posterior distribution over all parameters.

#### Where does the **hypothesis function** come from?

Logistic regression hypothesis representation

$$P(Y=1|X) = h_{\theta}(x) = \frac{1}{1 + e^{-\theta^{\top}x}} = \frac{1}{1 + e^{-(\theta_{0} + \theta_{1}x_{1} + \theta_{2}x_{2} + \dots + \theta_{n}x_{n})}}$$

- Consider learning f:  $X \rightarrow Y$ , where
  - X is a vector of real-valued features  $[X_1, \dots, X_n]^{\mathsf{T}}$
  - Y is Boolean
  - Assume all  $X_i$  are conditionally independent given Y
  - Model <u>likelihood</u>  $P(X_i|Y=y_k)$  as Gaussian  $N(\mu_{ik},\sigma_i)$  and assume variance is independent of class, i.e.  $\sigma_{i0} = \sigma_{i1} = \sigma_{i}$

$$P(X_i|Y = y_k) = \frac{1}{\sqrt{2\pi\sigma_{ik}^2}} e^{-\frac{1}{2}\left(\frac{X_i - \mu_{ik}}{\sigma_{ik}}\right)^2}$$

$$P(x|y_k) = \frac{1}{\sqrt{2\pi}\sigma_i} e^{-\frac{(x - \mu_{ik})^2}{2\sigma_i^2}}$$

$$P(x|y_k) = \frac{1}{\sqrt{2\pi}\sigma_i} e^{-\frac{(x-\mu_{ik})^2}{2\sigma_i^2}}$$

Model prior P(Y) as Bernoulli  $\pi : P(Y=1) = \pi$  and  $P(Y=0) = 1-\pi$ 

What is  $P(Y|X_1, X_2, \cdots, X_n)$ ?

## Logistic Regression –Bayesian Analysis

$$P(Y = 1|X) = \frac{P(Y = 1)P(X|Y = 1)}{P(Y = 1)P(X|Y = 1) + P(Y = 0)P(X|Y = 0)}$$

**Applying Bayes rule** 

$$P(Y = 1|X) = \frac{1}{1 + \frac{P(Y=0)P(X|Y=0)}{P(Y=1)P(X|Y=1)}}$$

Divide by P(Y = 1)P(X|Y = 1)

$$P(Y = 1|X) = \frac{1}{1 + \exp(\ln \frac{P(Y=0)P(X|Y=0)}{P(Y=1)P(X|Y=1)})}$$

Apply  $\exp(\ln(\cdot))$ 

By independence assumption:

$$\frac{P(X|Y=0)}{P(X|Y=1)} = \prod_{i} \frac{P(X_{i}|Y=0)}{P(X_{i}|Y=1)}$$

 $P(Y=1)=\pi$  and  $P(Y=0)=1-\pi$ by modelling P(Y) as Bernoulli

$$P(Y = 1|X) = \frac{1}{1 + \exp\left(\ln\frac{P(Y = 0)}{P(Y = 1)} + \ln\frac{P(X|Y = 0)}{P(X|Y = 1)}\right)}$$

$$P(Y = 1|X) = \frac{1}{1 + \exp\left(\ln\frac{1-\pi}{\pi} + \sum_{i}\ln\frac{P(X_{i}|Y = 0)}{P(X_{i}|Y = 1)}\right)}$$

$$P(Y = 1|X) = \frac{1}{1 + \exp\left(\ln\frac{1-\pi}{\pi} + \ln\prod_{i}\frac{P(X_{i}|Y = 0)}{P(X_{i}|Y = 1)}\right)}$$

## Logistic Regression –Bayesian Analysis

#### Plug in $P(X_i|Y)$

$$P(Y = 1|X) = \frac{1}{1 + \exp(\ln\frac{1-\pi}{\pi} + \sum_{i} \left(\frac{\mu_{i0} - \mu_{i1}}{\sigma_{i}^{2}} X_{i} + \frac{\mu_{i1}^{2} - \mu_{i0}^{2}}{2\sigma_{i}^{2}}\right))}$$

$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_{i=1}^{n} w_i X_i)} = \frac{1}{1 + \exp(\theta_0 + \sum_{i=1}^{n} \theta_i X_i)}$$

$$w_0 = \ln \frac{1-\pi}{\pi} + \sum_i \frac{\mu_{i1}^2 - \mu_{i0}^2}{2\sigma_i^2} \qquad w_i = \frac{\mu_{i0} - \mu_{i1}}{\sigma_i^2}$$

$$w_i = \frac{\mu_{i0} - \mu_{i1}}{\sigma_i^2}$$

$$P(Y = 0|X) = 1 - P(Y = 1|X) = \frac{\exp(w_0 + \sum_{i=1}^n w_i X_i)}{1 + \exp(w_0 + \sum_{i=1}^n w_i X_i)}$$

#### linear classification rule

$$\frac{P(Y = 0|X)}{P(Y = 1|X)} = \exp(w_0 + \sum_i w_i X_i)$$

$$\ln \frac{P(Y = 0|X)}{P(Y = 1|X)} = w_0 + \sum_{i} w_i X_i$$

## $P(X_i|Y)$ derivation

$$\begin{split} \sum_{i} \ln \frac{P(X_{i}|Y=0)}{P(X_{i}|Y=1)} &= \sum_{i} \ln \frac{\frac{1}{\sqrt{2\pi\sigma_{i}^{2}}} \exp\left(\frac{-(X_{i}-\mu_{i0})^{2}}{2\sigma_{i}^{2}}\right)}{\frac{1}{\sqrt{2\pi\sigma_{i}^{2}}} \exp\left(\frac{-(X_{i}-\mu_{i1})^{2}}{2\sigma_{i}^{2}}\right)} \\ &= \sum_{i} \ln \exp\left(\frac{(X_{i}-\mu_{i1})^{2} - (X_{i}-\mu_{i0})^{2}}{2\sigma_{i}^{2}}\right) \\ &= \sum_{i} \left(\frac{(X_{i}-\mu_{i1})^{2} - (X_{i}-\mu_{i0})^{2}}{2\sigma_{i}^{2}}\right) \\ &= \sum_{i} \left(\frac{(X_{i}^{2}-2X_{i}\mu_{i1}+\mu_{i1}^{2}) - (X_{i}^{2}-2X_{i}\mu_{i0}+\mu_{i0}^{2})}{2\sigma_{i}^{2}}\right) \\ &= \sum_{i} \left(\frac{2X_{i}(\mu_{i0}-\mu_{i1}) + \mu_{i1}^{2} - \mu_{i0}^{2}}{2\sigma_{i}^{2}}\right) \\ &= \sum_{i} \left(\frac{\mu_{i0}-\mu_{i1}}{\sigma_{i}^{2}}X_{i} + \frac{\mu_{i1}^{2}-\mu_{i0}^{2}}{2\sigma_{i}^{2}}\right) \end{split}$$

$$P(Y = 1|X) = \frac{1}{1 + \exp(\ln\frac{1-\pi}{\pi} + \sum_{i} \left(\frac{\mu_{i0} - \mu_{i1}}{\sigma_{i}^{2}} X_{i} + \frac{\mu_{i1}^{2} - \mu_{i0}^{2}}{2\sigma_{i}^{2}}\right))}$$

lead

#### Where does the cost come from? - Logistic regression

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \text{Cost}(h_{\theta}(x^{(i)}), y^{(i)}))$$

$$= -\frac{1}{m} \left[ \sum_{i=1}^{m} y^{(i)} \log \left( h_{\theta}(x^{(i)}) \right) + (1 - y^{(i)}) \log \left( 1 - h_{\theta}(x^{(i)}) \right) \right]$$

**Learning**: fit parameter  $\theta$  $\min_{\theta} J(\theta)$ 

**Prediction**: given new xOutput  $h_{\theta}(x) = \frac{1}{1 + e^{-\theta^{\mathsf{T}}x}}$ 

Slide credit: Andrew Ng

• **Goal**: choose  $\theta$  to maximize conditional likelihood of training data

$$-P_{\theta}(Y=1|X=x) = h_{\theta}(x) = \frac{1}{1+e^{-\theta^{T}x}}$$

$$-P_{\theta}(Y=0|X=x) = 1 - h_{\theta}(x) = \frac{e^{-\theta^{T}x}}{1+e^{-\theta^{T}x}}$$
conditional likelihood

- Training data  $D = \{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(m)}, y^{(m)})\}$
- Data likelihood =  $\prod_{i=1}^{m} P_{\theta}\left(\left(x^{(i)}, y^{(i)}\right)\right)$
- Data conditional likelihood =  $\prod_{i=1}^{m} P_{\theta}(y^{(i)}|x^{(i)})$

$$\theta_{\text{MCLE}} = \underset{\theta}{\operatorname{argmax}} \prod_{i=1}^{m} P_{\theta}(y^{(i)}|x^{(i)})$$

Slide credit: Tom Mitchell

#### Expressing conditional log-likelihood

$$L(\theta) = \log \prod_{i=1}^{m} P_{\theta}(y^{(i)}|x^{(i)}) = \sum_{i=1}^{m} \log P_{\theta}(y^{(i)}|x^{(i)})$$

Recall, each label  $y^{(i)}$  is binary with prob.  $P_{\theta}(y^{(i)}|x^{(i)})$ : Assume Bernoulli likelihood: (use PMF of Bernoulli dist.)

$$= \sum_{i=1}^{m} y^{(i)} \log P_{\theta} (y^{(i)} = 1 | x^{(i)}) (1 - y^{(i)}) \log P_{\theta} (y^{(i)} = 0 | x^{(i)})$$

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

#### To turn Logliklihood into loss function flip the sign

$$\theta_{MCLE} = \underset{\theta}{argmax} \prod_{i=1}^{m} P_{\theta}(y^{(i)}|x^{(i)}) = -\underset{\theta}{argmin} \prod_{i=1}^{m} P_{\theta}(y^{(i)}|x^{(i)})$$

$$\theta_{MCLE} = -\underset{\theta}{argmin} \sum_{i=1}^{m} y^{(i)} \log (h_{\theta}(x^{(i)})) + (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)}))$$

## Learning Model Parameters – Closed Form Solution (using vectorization)

#### Vectorization

- Benefits of vectorization
  - More compact equations
  - Faster code (using optimized matrix libraries)
- Consider our model:

$$h(\boldsymbol{x}) = \sum_{j=0}^{n} \theta_j x_j$$

Let

Can write the model in vectorized form as  $h(m{x}) = m{ heta}^\intercal m{x}$ 

#### Vectorization

Consider our model for n instances:

$$h\left(\boldsymbol{x}^{(i)}\right) = \sum_{j=0}^{d} \theta_j x_j^{(i)}$$

Let

$$oldsymbol{\mathcal{H}} oldsymbol{ heta} oldsymbol{ heta} = egin{bmatrix} heta_0 \ heta_1 \ heta_1 \ heta_2 \ heta_d \end{bmatrix} \quad oldsymbol{X} = egin{bmatrix} 1 & x_1^{(1)} & \dots & x_d^{(1)} \ heta_1 & \dots & x_d^{(i)} \ heta_1 & \dots & x_d^{(i)} \ heta_2 & \dots & \dots & \dots \ heta_d \ heta_1 & \dots & x_d^{(n)} \ heta_2 & \dots & x_d^{(n)} \ heta_3 & \dots & x_d^{(n)} \ heta_4 & \dots & x_d^{(n)} \ heta_4$$

Can write the model in vectorized form as  $h_{m{ heta}}(m{x}) = m{X}m{ heta}$ 

#### Vectorization

For the linear regression cost function:

$$J(\boldsymbol{\theta}) = \frac{1}{2n} \sum_{i=1}^{n} \left( h_{\boldsymbol{\theta}} \left( \boldsymbol{x}^{(i)} \right) - y^{(i)} \right)^{2}$$

$$= \frac{1}{2n} \sum_{i=1}^{n} \left( \boldsymbol{\theta}^{\mathsf{T}} \boldsymbol{x}^{(i)} - y^{(i)} \right)^{2}$$

$$= \frac{1}{2n} \left( \boldsymbol{X} \boldsymbol{\theta} - \boldsymbol{y} \right)^{\mathsf{T}} \left( \boldsymbol{X} \boldsymbol{\theta} - \boldsymbol{y} \right)$$

$$\mathbb{R}^{n \times (d+1)}$$

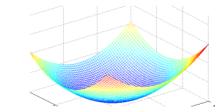
$$= \frac{1}{2n} \left( \boldsymbol{X} \boldsymbol{\theta} - \boldsymbol{y} \right)^{\mathsf{T}} \left( \boldsymbol{X} \boldsymbol{\theta} - \boldsymbol{y} \right)$$

Let:

#### Closed Form Solution



- Instead of using GD, solve for optimal heta analytically
  - Notice that the solution is when  $\frac{\partial}{\partial \boldsymbol{\theta}}J(\boldsymbol{\theta})=0$



Derivation:

$$\mathcal{J}(oldsymbol{ heta}) = rac{1}{2n} \left( oldsymbol{X} oldsymbol{ heta} - oldsymbol{y} 
ight)^{\intercal} \left( oldsymbol{X} oldsymbol{ heta} - oldsymbol{y} 
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Take derivative and set equal to 0, then solve for  $\theta$ :

$$\frac{\partial}{\partial \boldsymbol{\theta}} \left( \boldsymbol{\theta}^{\mathsf{T}} \boldsymbol{X}^{\mathsf{T}} \boldsymbol{X} \boldsymbol{\theta} - 2 \boldsymbol{\theta}^{\mathsf{T}} \boldsymbol{X}^{\mathsf{T}} \boldsymbol{y} + \boldsymbol{y} \boldsymbol{y} \boldsymbol{y} \right) = 0$$

$$(\boldsymbol{X}^{\mathsf{T}} \boldsymbol{X}) \boldsymbol{\theta} - \boldsymbol{X}^{\mathsf{T}} \boldsymbol{y} = 0$$

$$(\boldsymbol{X}^{\mathsf{T}} \boldsymbol{X}) \boldsymbol{\theta} = \boldsymbol{X}^{\mathsf{T}} \boldsymbol{y}$$

$$\boldsymbol{\theta} = (\boldsymbol{X}^{\intercal} \boldsymbol{X})^{-1} \boldsymbol{X}^{\intercal} \boldsymbol{y}$$

#### Closed Form Solution

Can obtain  $\theta$  by simply plugging X and y into

$$\boldsymbol{\theta} = (\boldsymbol{X}^{\intercal}\boldsymbol{X})^{-1}\boldsymbol{X}^{\intercal}\boldsymbol{y}$$

$$oldsymbol{y} = \left[egin{array}{c} y^{(1)} \ y^{(2)} \ dots \ y^{(n)} \end{array}
ight]$$

- If  $X^TX$  is not invertible (i.e., singular), may need to:
  - Use pseudo-inverse instead of the inverse
    - In python, numpy.linalg.pinv(a)
  - Remove redundant (not linearly independent) features
  - Remove extra features to ensure that  $d \le n$

#### Gradient Descent vs Closed Form

#### **Gradient Descent**

#### **Closed Form Solution**

- Requires multiple iterations
- Need to choose  $\alpha$
- Works well when n is large
- Can support incremental learning

- Non-iterative
- No need for  $\alpha$
- Slow if n is large
  - Computing  $(X^TX)^{-1}$  is roughly  $O(n^3)$

# Extending Linear Regression to More Complex Models

- The inputs X for linear regression can be:
  - Original quantitative inputs
  - Transformation of quantitative inputs
    - e.g. log, exp, square root, square, etc.
  - Polynomial transformation
    - example:  $y = \beta_0 + \beta_1 \cdot x + \beta_2 \cdot x^2 + \beta_3 \cdot x^3$
  - Basis expansions
  - Dummy coding of categorical inputs
  - Interactions between variables
    - example:  $x_3 = x_1 \cdot x_2$

This allows use of linear regression techniques to fit non-linear datasets.

• Basic Linear Model:

- $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j x_j$
- Generalized Linear Model:  $h_{m{ heta}}(m{x}) = \sum heta_j \phi_j(m{x})$
- Once we have replaced the data by the outputs of the basis functions, fitting the generalized model is exactly the same problem as fitting the basic model
  - Unless we use the kernel trick more on that when we cover support vector machines
  - Therefore, there is no point in cluttering the math with basis functions

Generally,

$$h_{m{ heta}}(m{x}) = \sum_{j=0}^d heta_j \phi_j(m{x})$$

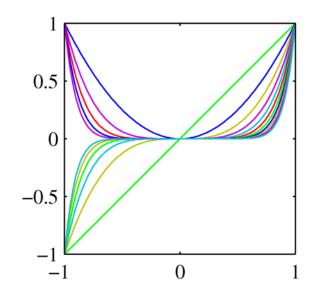
- Typically,  $\phi_0({m x})=1$  so that  $\,\, heta_0\,$  acts as a bias
- In the simplest case, we use linear basis functions:

$$\phi_j(\boldsymbol{x}) = x_j$$

#### Polynomial basis functions:

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

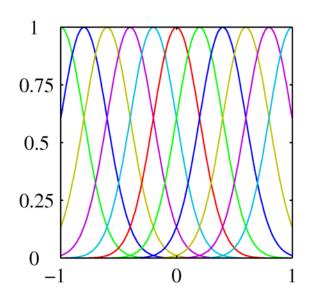
 These are global; a small change in x affects all basis functions



#### Gaussian basis functions:

$$\phi_j(x) = \exp\left\{-\frac{(x-\mu_j)^2}{2s^2}\right\}$$

- These are local; a small change in x only affect nearby basis functions.  $\mu_j$  and s control location and scale (width).



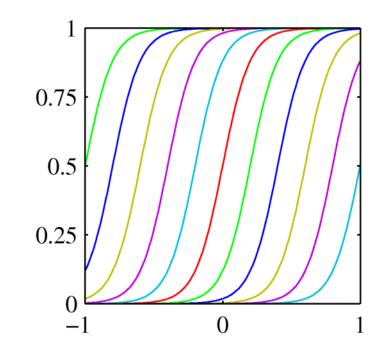
Sigmoidal basis functions:

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

where

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

- These are also local; a small change in x only affects nearby basis functions.  $\mu_j$  and s control location and scale (slope).



By using nonlinear basis functions, we allow the function  $y(\mathbf{x}, \mathbf{w})$  to be a nonlinear function of the input vector  $\mathbf{x}$ . They are called linear models because this function is linear in  $\mathbf{w}$ .

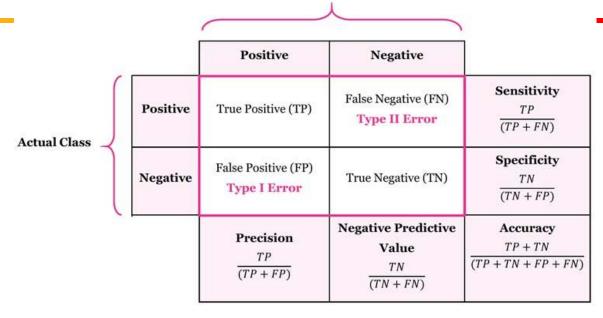
### **Evaluation**

- Accuracy
- Precision and recall
- Squared error
- Likelihood
- Posterior probability
- Cost / Utility
- Margin
- Entropy
- etc.

## **Evaluating Performance**

- If *y* is discrete:
  - Accuracy: # correctly classified / # all test examples
    - Good for class balanced dataset
- Want evaluation metric to be in some range, e.g. [0 1]
  - 0 = worst possible classifier, 1 = best possible classifier

#### **Predicted Class**



n=165	Predicted: NO	Predicted: YES	
Actual: NO	TN = 50	FP = 10	60
Actual: YES	FN = 5	TP = 100	105
	55	110	

## **Thanks**