CS 6375
Midterm Review: Part I

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Topics for the Midterm Exam

- Linear Regression
- Perceptron
- Support Vector Machines
- Nearest Neighbor Methods
- Decision Trees
- Bayesian Methods
- Naïve Bayes
- Logistic Regression

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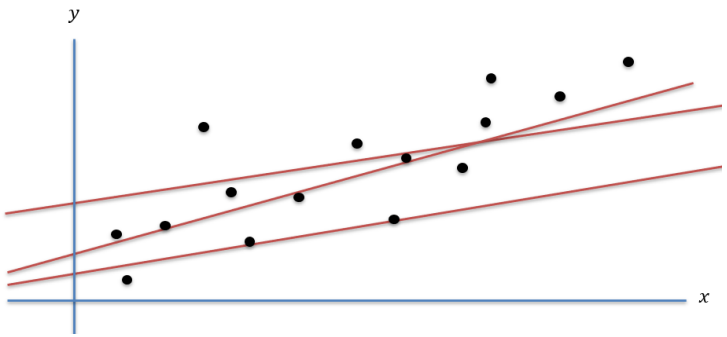
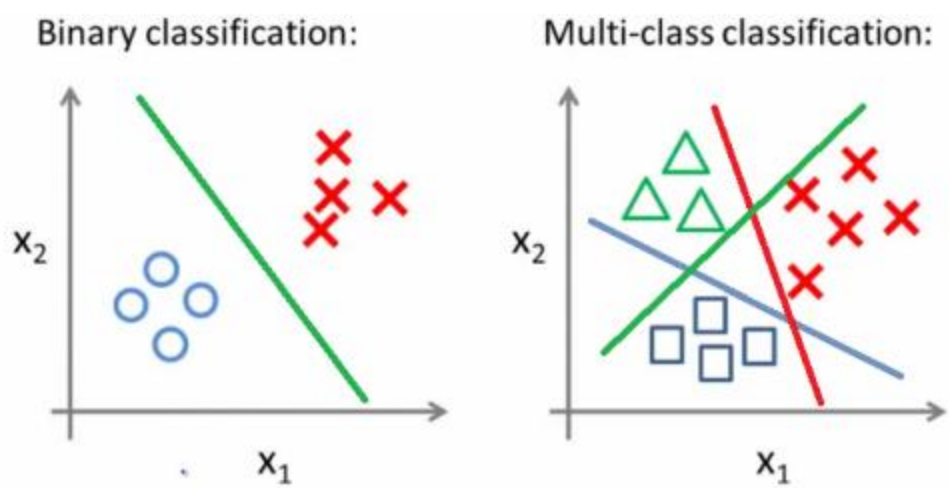
Classification vs Regression

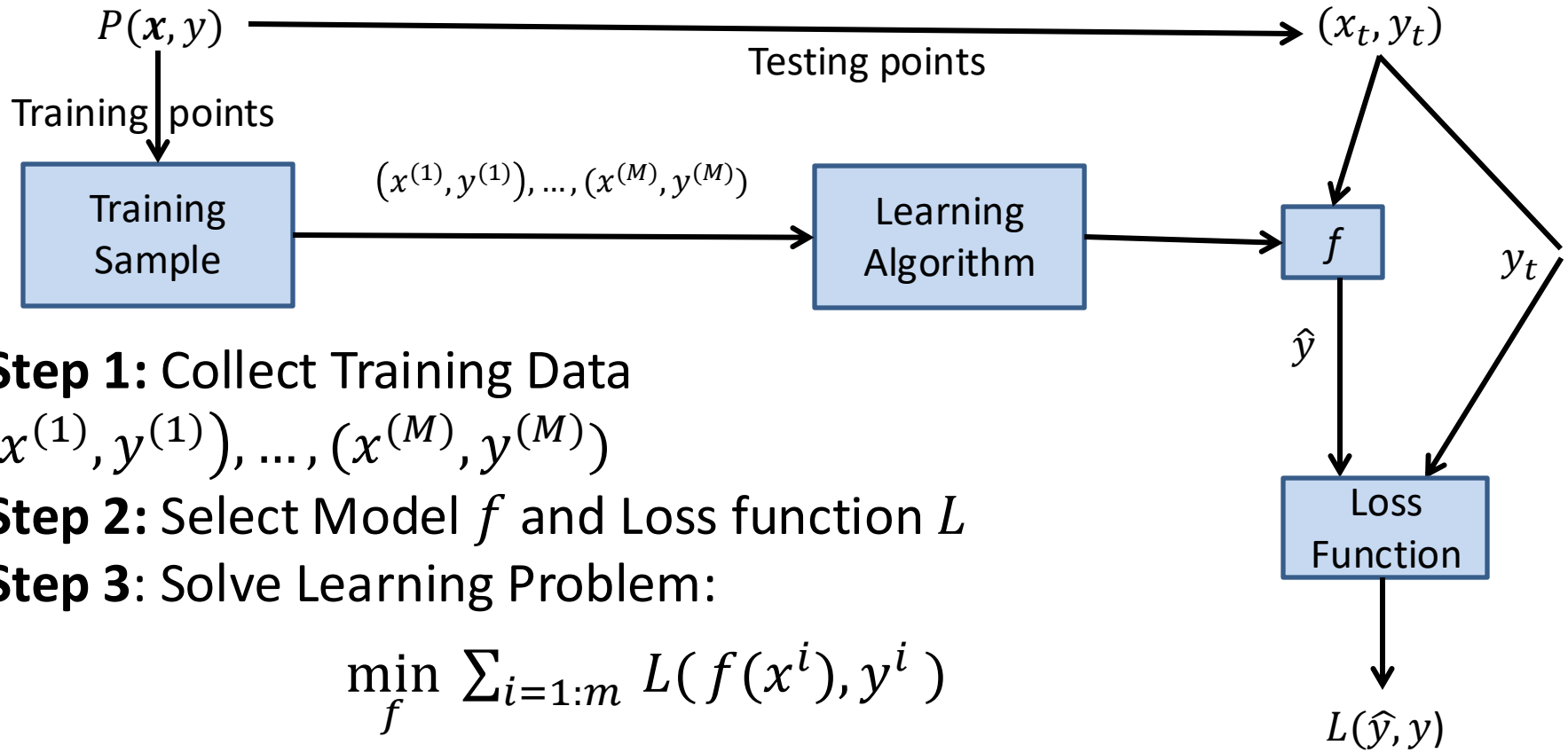
Classification vs Regression

- Input: pairs of points $\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(M)}, y^{(M)}\right)$ with $x^{(m)} \in \mathbb{R}^n$
- Regression case: $y^{(m)} \in \mathbb{R}$
- Classification case: $y^{(m)} \in [0, k-1]$ [k-class classification]
- If k = 2, we get Binary classification





Recap: Supervised Learning Workflow



- **Step 1:** Collect Training Data $(x^{(1)}, y^{(1)}), \ldots, (x^{(M)}, y^{(M)})$
- **Step 2:** Select Model f and Loss function L
- **Step 3**: Solve Learning Problem:

$$\min_{f} \sum_{i=1:m} L(f(x^i), y^i)$$

- **Step 4:** Obtain Predictions $\hat{y}_t = f(x_t)$ on all **Test Data**
- **Step 5:** Evaluation -- Measure the error $Err(\hat{y}_t, y_t)$

Linear Regression: Loss Function

- For any data point, x, the learning algorithm predicts $f(x)$
- In typical regression applications, measure the fit using a squared loss function

$$L(f) = \frac{1}{M}\sum_{m}\left(f\left(x^{(m)}\right) - y^{(m)}\right)^2$$

- Want to minimize the average loss on the training data
- The optimal linear hypothesis is then given by

$$\min_{a,b}\frac{1}{M}\sum_{m}\left(ax^{(m)} + b - y^{(m)}\right)^2$$

Linear Regression Optimization: Gradient Descent

Iterative method to minimize a (convex) differentiable function L

- Pick an initial point w_0
- Iterate until convergence

$$w_{t+1} = w_t - \gamma_t \nabla L(w_t)$$

where γ_t is the tth step size (sometimes called learning rate)

- w in this case is (a, b)

Gradients for Linear Regression

- The Loss Function for Linear Regression is:

$$L(a,b) = \frac{1}{M}\sum_{m}\left(ax^{(m)} + b - y^{(m)}\right)^2$$

- The gradients with respect to a and b are:

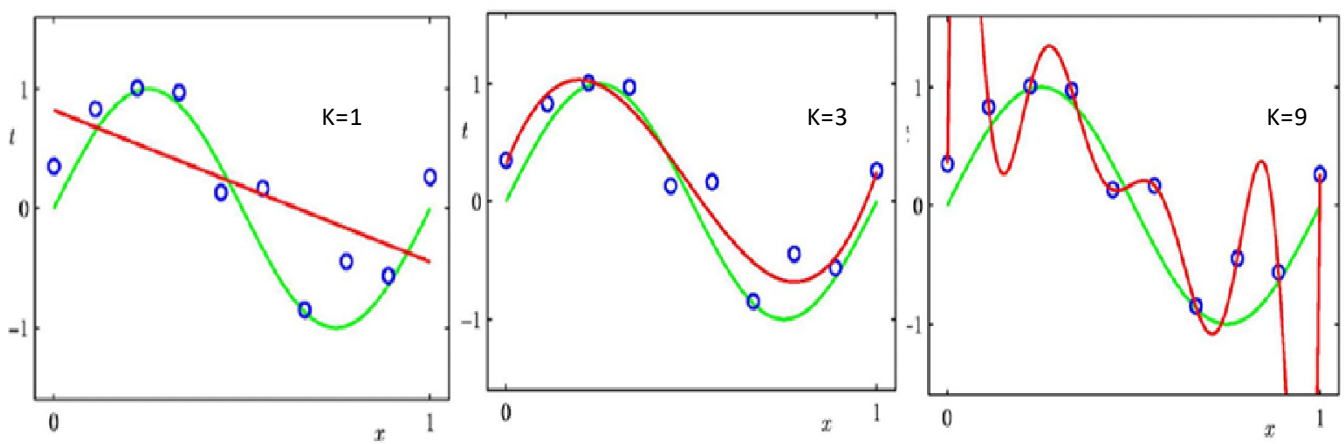
$$\nabla L_a(a,b) = \frac{1}{M}\sum_m 2(ax^{(m)} + b - y^m)\, x^{(m)}$$

$$\nabla L_b(a,b) = \frac{1}{M}\sum_m 2(ax^{(m)} + b - y^m)$$

- The gradients can be obtained by using the chain rule

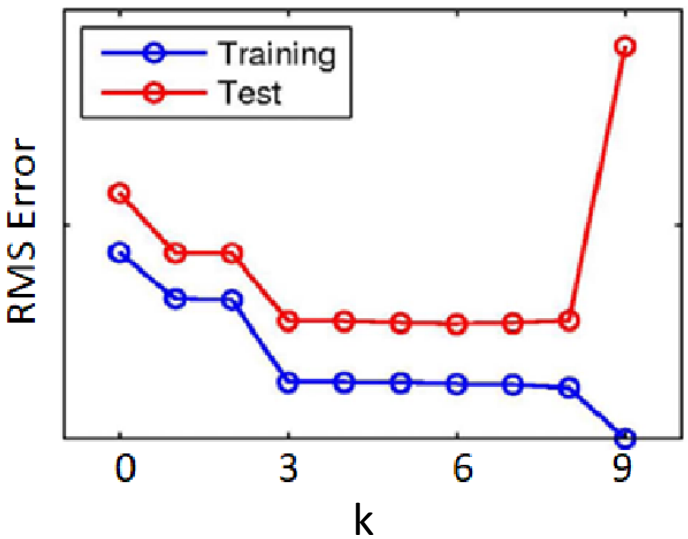
Polynomial Regression

- What if we enlarge the hypothesis class?
  - Quadratic functions: $ax^2 + bx + c$
  - k-degree polynomials: $a_k x^k + a_{k-1} x^{k-1} + \cdots + a_1 x + a_0$
- Can we always learn "better" with a larger hypothesis class?



Polynomial Regression: Overfitting

- As *the degree of the polynomial (k)* increases, training error decreases monotonically
- As *k* increases test error can increase
- Test error can decrease at first, but increases
- Overfitting can occur
  - When the model is too complex and trivially fits the data (i.e., too many parameters)
  - When the data is not enough to estimate the parameters
  - Model captures the noise (or the chance)



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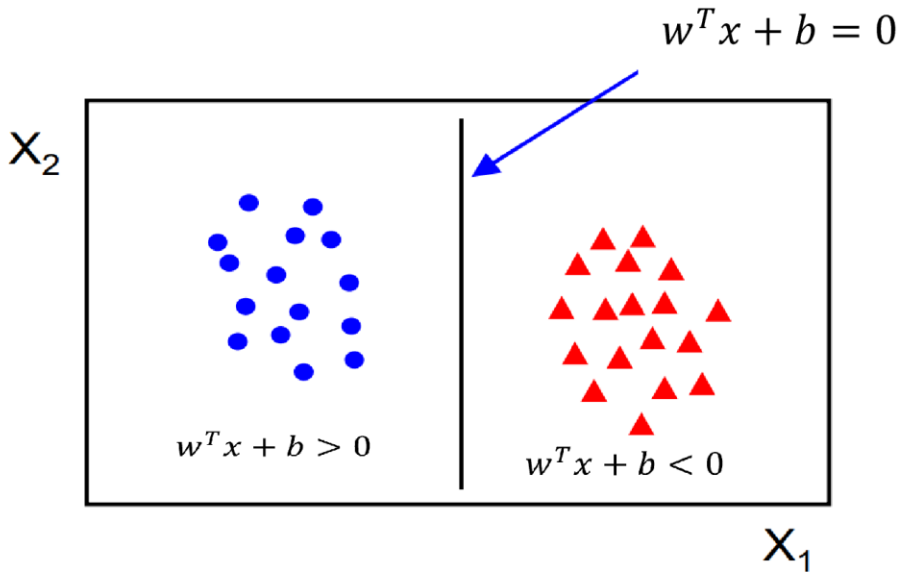
Linear Separators and Hyperplanes

- In n dimensions, a hyperplane is a solution to the equation

$$w^T x + b = 0$$

with $w \in \mathbb{R}^n, b \in \mathbb{R}$

- Hyperplanes divide $\mathbb{R}^n$ into two distinct sets of points (called open halfspaces)
  - Half Space 1: $w^T x + b > 0$
  - Half Space 2: $w^T x + b < 0$



The 0/1 Loss (Seperable Case)

- Input $\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(M)}, y^{(M)}\right)$ with $x^{(m)} \in \mathbb{R}^n$ and $y^{(m)} \in \{-1, +1\}$
- Hypothesis space: separating hyperplanes

$$f(x) = sign\,(w^T x + b)$$

- How should we choose the loss function?
  - Count the number of misclassifications

$$zero/one\ loss = \frac{1}{2}\sum_m \left|y^{(m)} - sign(w^T x^{(m)} + b)\right|$$

    - Tough to optimize, gradient contains no information

The Perceptron Loss (Seperable Case)

- Input $\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(M)}, y^{(M)}\right)$ with $x^{(m)} \in \mathbb{R}^n$ and $y^{(m)} \in \{-1, +1\}$
- Hypothesis space: separating hyperplanes

$$f(x) = sign\,(w^T x + b)$$

- How should we choose the loss function?
  - Penalize misclassification linearly by the size of the violation

$$perceptron\ loss = \sum_m \max\{0, -y^{(m)}(w^T x^{(m)} + b)\}$$

    - Modified hinge loss (this loss is convex, but not differentiable)

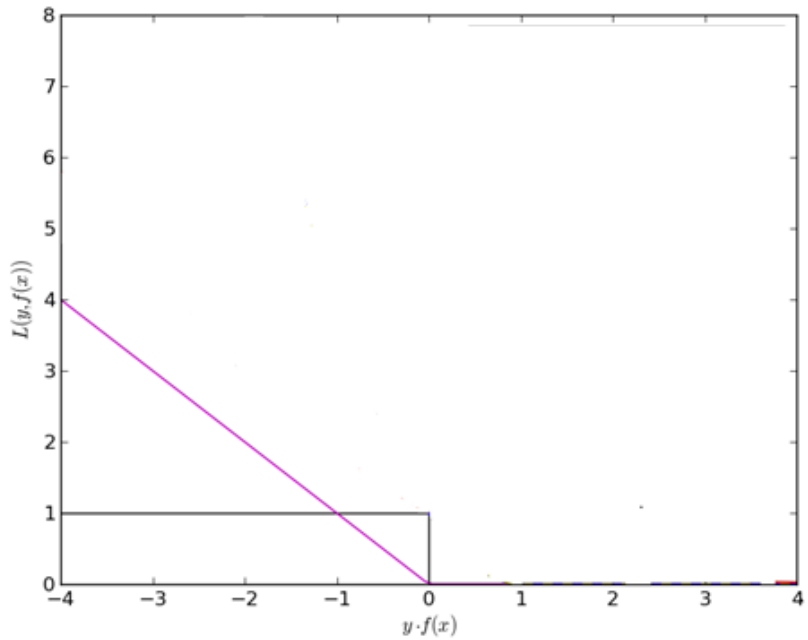
0/1 Loss Vs Perceptron Loss

- Zero/One Loss which counts the number of mis-classifications:

$$zero/one\ loss = \frac{1}{2}\sum_{m}\left|y^{(m)} - sign(w^T x^{(m)} + b)\right|$$

- Perceptron Loss:

$$perceptron\ loss = \sum_{m} \max\{0, -y^{(m)}(w^T x^{(m)} + b)\}$$



The Perceptron Algorithm

- Try to minimize the perceptron loss using (sub)gradient descent

$$\nabla_w(perceptron\ loss) = -\sum_{m=1}^{M}\left(y^{(m)}x^{(m)} \cdot 1_{-y^{(m)}f_{w,b}(x^{(m)})\geq 0}\right)$$

$$\nabla_b(perceptron\ loss) = -\sum_{m=1}^{M}\left(y^{(m)} \cdot 1_{-y^{(m)}f_{w,b}(x^{(m)})\geq 0}\right)$$

Is equal to zero if the mth data point is correctly classified and one otherwise

The Perceptron Algorithm

- Try to minimize the perceptron loss using (sub)gradient descent

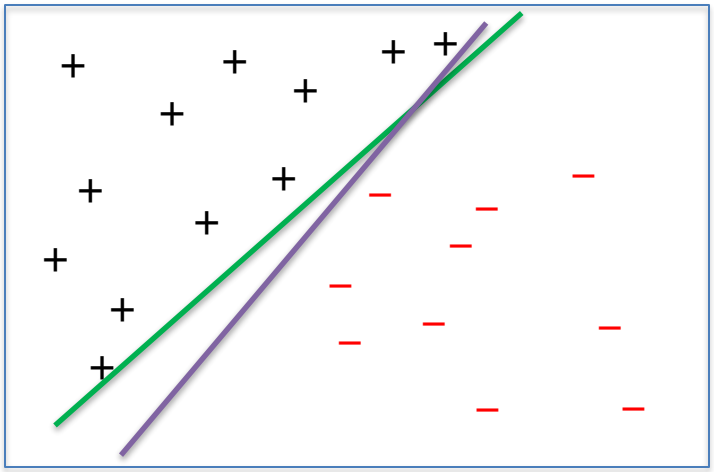
$$w^{(t+1)} = w^{(t)} + \gamma_t \sum_{m=1}^{M} \left(y^{(m)} x^{(m)} \cdot 1_{-y^{(m)} f_{w,b}(x^{(m)}) \geq 0} \right)$$

$$b^{(t+1)} = b^{(t)} + \gamma_t \sum_{m=1}^{M} \left(y^{(m)} \cdot 1_{-y^{(m)} f_{w,b}(x^{(m)}) \geq 0} \right)$$

- With step size γ_t (also called the learning rate)
- Note that, for convergence of subgradient methods, a diminishing step size, e.g., $\gamma_t = \frac{1}{1+t}$ is required

Perceptron Drawbacks

- No convergence guarantees if the observations are not linearly separable
- Can overfit
  - There can be a number of perfect classifiers, but the perceptron algorithm doesn't have any mechanism for choosing between them



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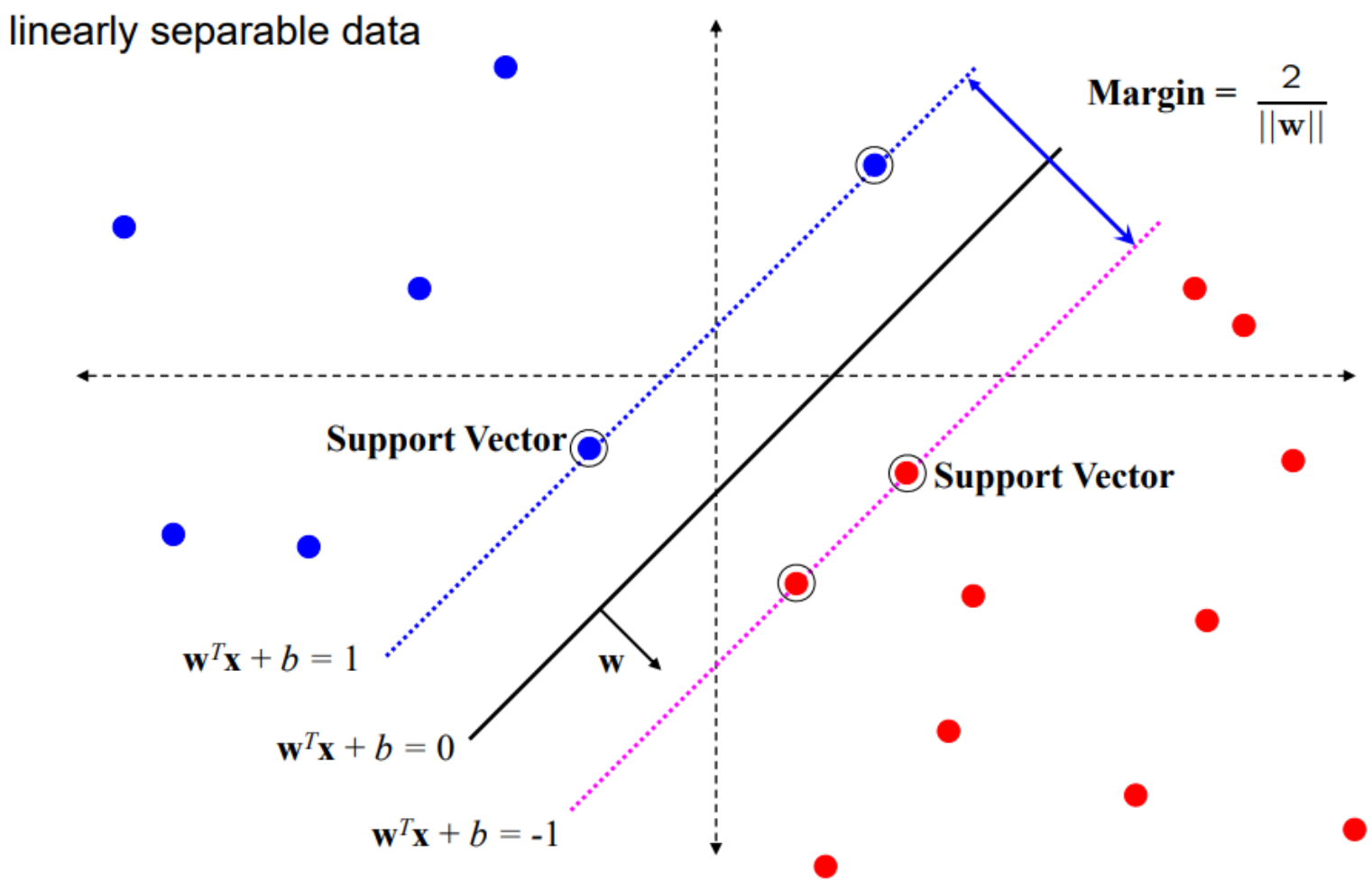
Support Vector Machines



Support Vector Machines Formulation

- This analysis yields the following optimization problem

$$\max_{w,b} \frac{1}{\|w\|}$$

such that

$$y^{(i)}\left(w^T x^{(i)} + b\right) \geq 1, \text{for all } i$$

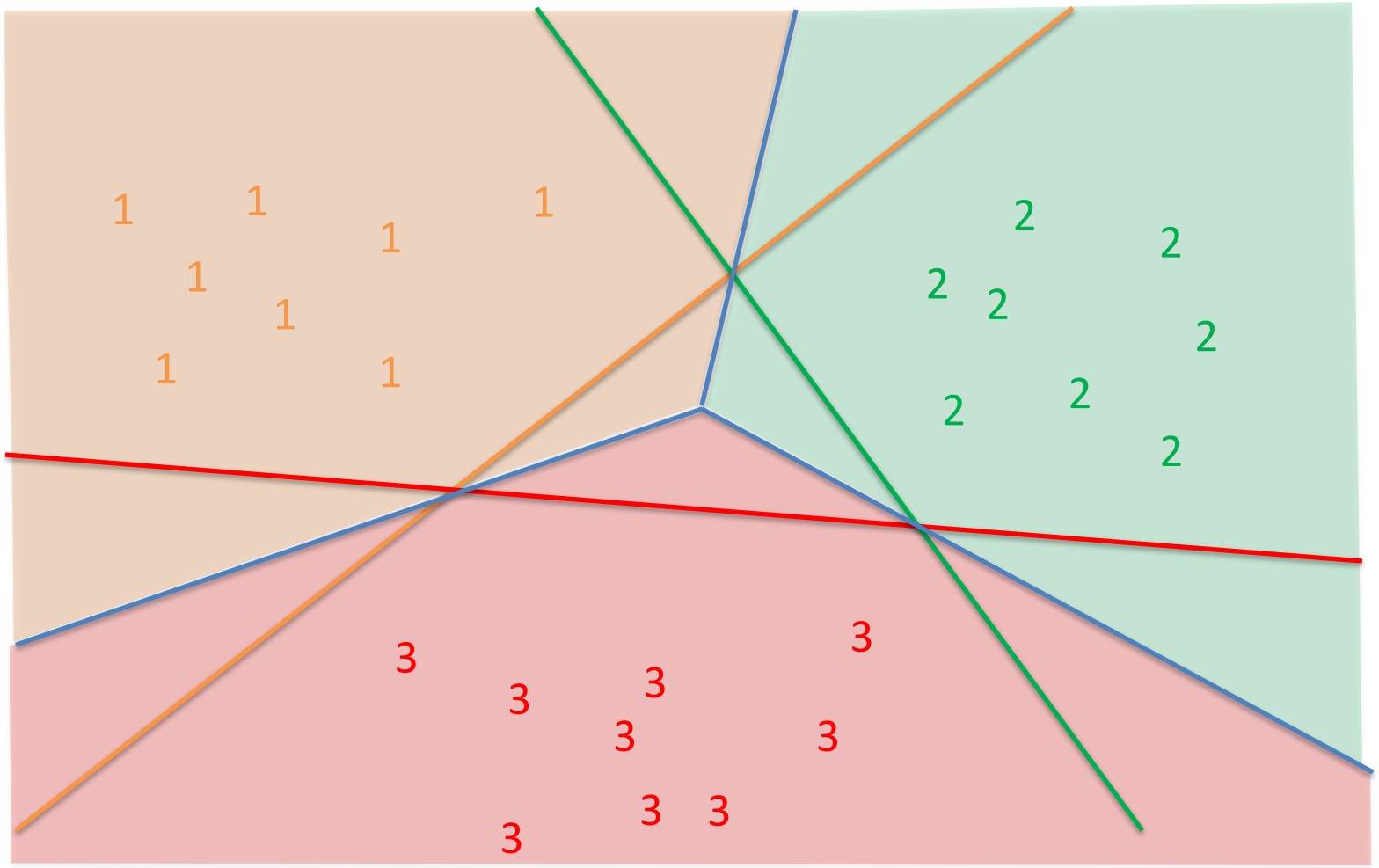
- Or, equivalently,

$$\min_{w,b} \|w\|^2$$

such that

$$y^{(i)}\left(w^T x^{(i)} + b\right) \geq 1, \text{for all } i$$

One-Versus-All SVMs



Regions in which points are classified by highest value of $w^T x + b$

SVM and Slack Variables

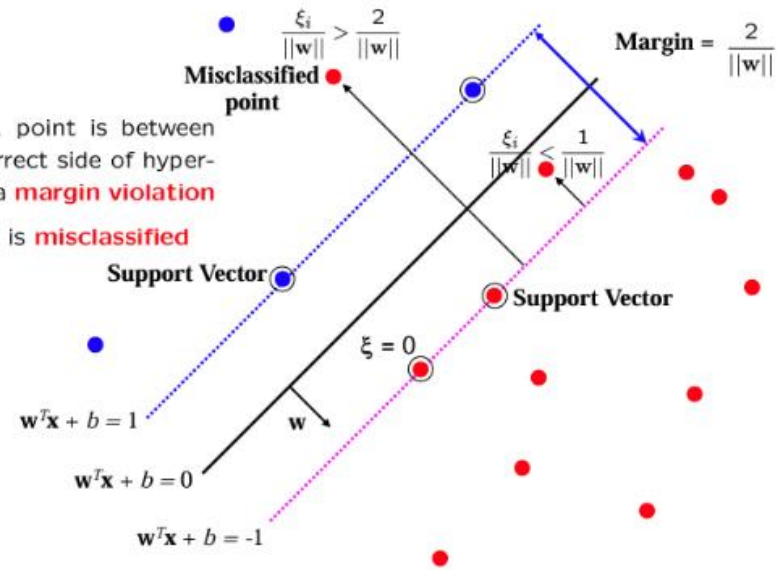
$$\min_{w,b,\xi} \frac{1}{2}||w||^2 + C\sum_{i=1}^{M} \xi_i$$

subject to $y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$ for all i.

$\xi_i \geq 0$

for $0 < \xi \leq 1$ point is between margin and correct side of hyper-plane. This is a margin violation

for $\xi > 1$ point is misclassified



Hinge Loss Formulation

- Obtain a new objective by substituting in for ξ

$$\min_{w,b} \underbrace{\frac{1}{2}\|w\|^2}_{\text{Penalty to prevent overfitting}} + \underbrace{c\sum_i \max\{0, 1 - y_i(w^T x^{(i)} + b)\}}_{\text{Hinge loss}}$$

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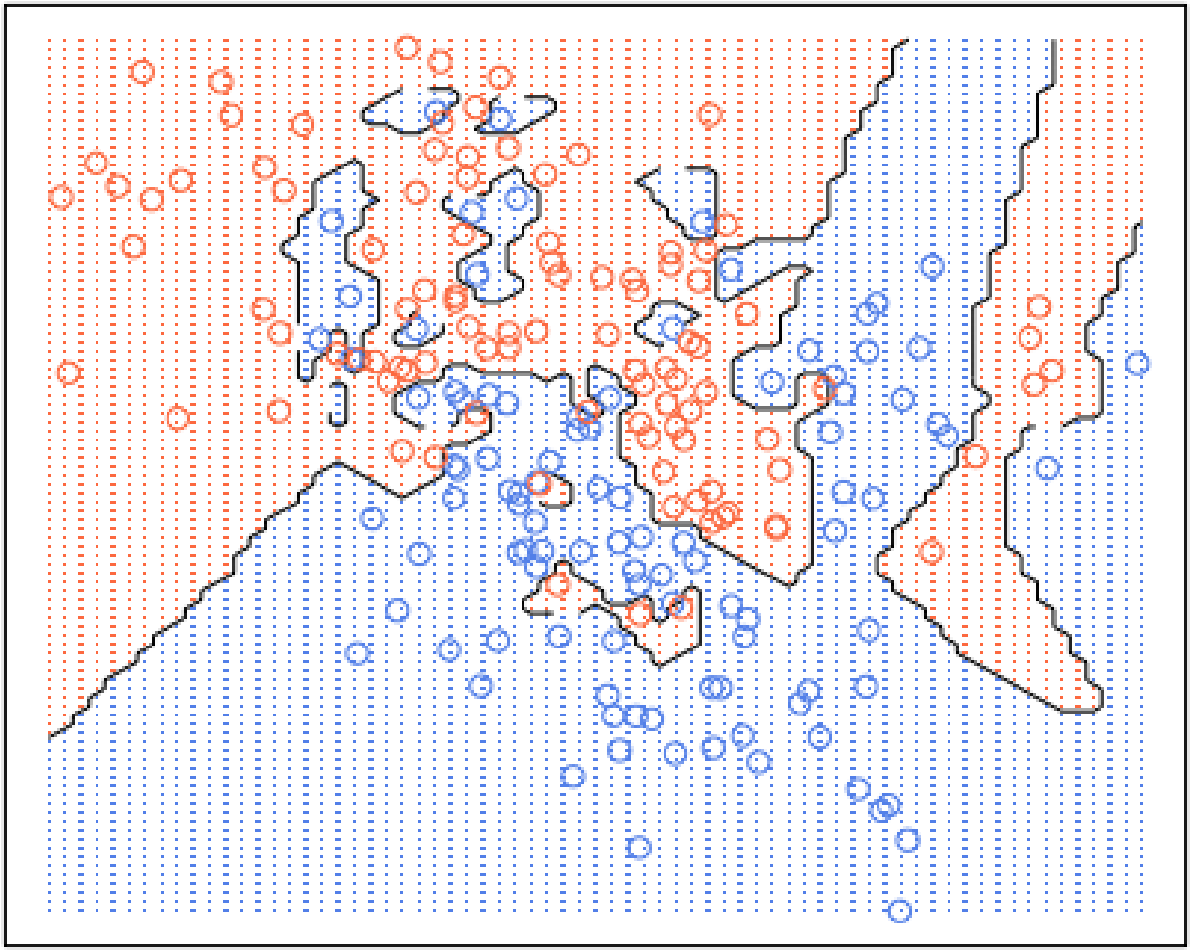
Nearest Neighbor Methods

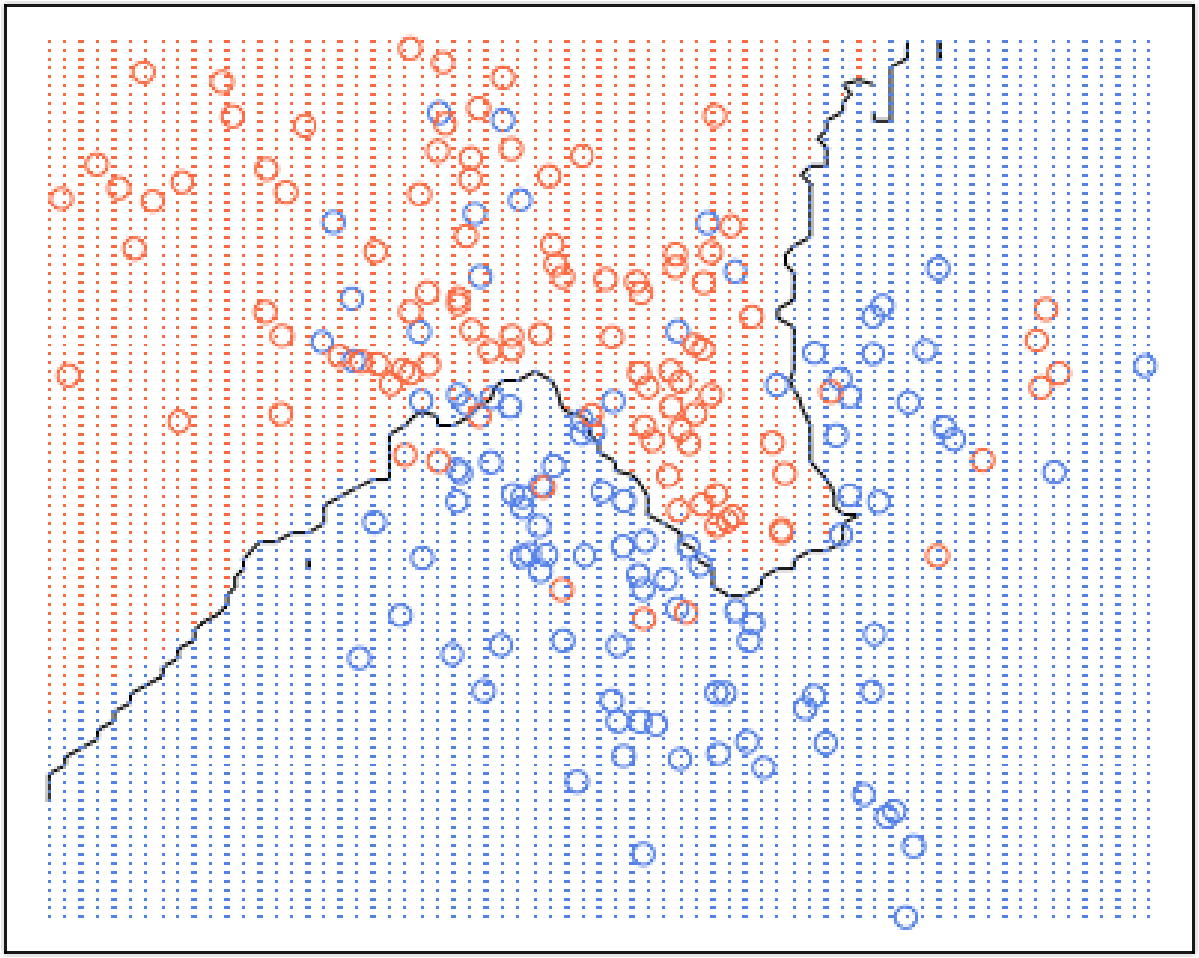
- Learning
  - Store all training examples
- Classifying a new point x'
  - Find the training example $(x^{(i)}, y^{(i)})$ such that $x^{(i)}$is closest (for some notion of close) to x'
  - Classify x' with the label $y^{(i)}$

1-NN Example



[Kevin Zakka]

20-NN Example



[Kevin Zakka]

Nearest Neighbor Methods

- Applies to data sets with points in $\mathbb{R}^d$
  - Best for large data sets with only a few (< 20) attributes
- Advantages
  - Learning is easy
  - Can learn complicated decision boundaries
- Disadvantages
  - Classification is slow (need to keep the entire training set around)
  - Easily fooled by irrelevant attributes

Secret to Getting Nearest Neighbors to Work

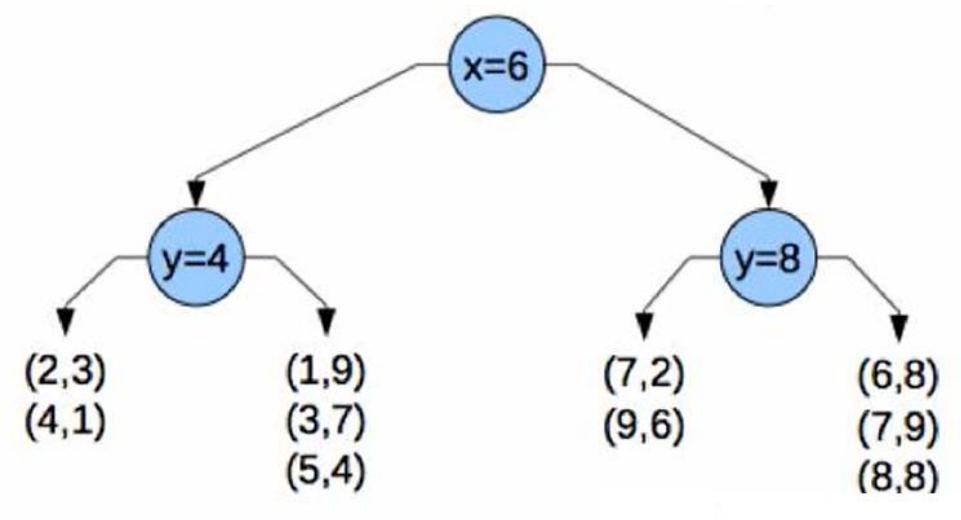
- Make sure there are no Irrelevant Attributes
  - Clean up features and remove features with low correlation with labels
- Make sure all features are normalized!
  - Feature normalization is key in KNN
- Make sure to tune k
- For large datasets use approximate nearest neighbor methods like kD trees

K-Dimensional Trees

- k-d trees provide a data structure that can help simplify the classification task by constructing a tree that partitions the search space
  - Starting with the entire training set, choose some dimension, i
  - Select an element of the training data whose i^{th} dimension has the median value among all elements of the training set
  - Divide the training set into two pieces: depending on whether their i^{th} attribute is smaller or larger than the median
  - Repeat this partitioning process on each of the two new pieces separately

K-Dimensional Trees

- Building a K-D tree from training data:
  - {(1,9), (2,3), (4,1), (3,7), (5,4), (6,8), (7,2), (8,8), (7,9), (9,6)}
  - pick random dimension, find median, split data, repeat



Adapted from Victor Lavrenko

K-Dimensional Trees

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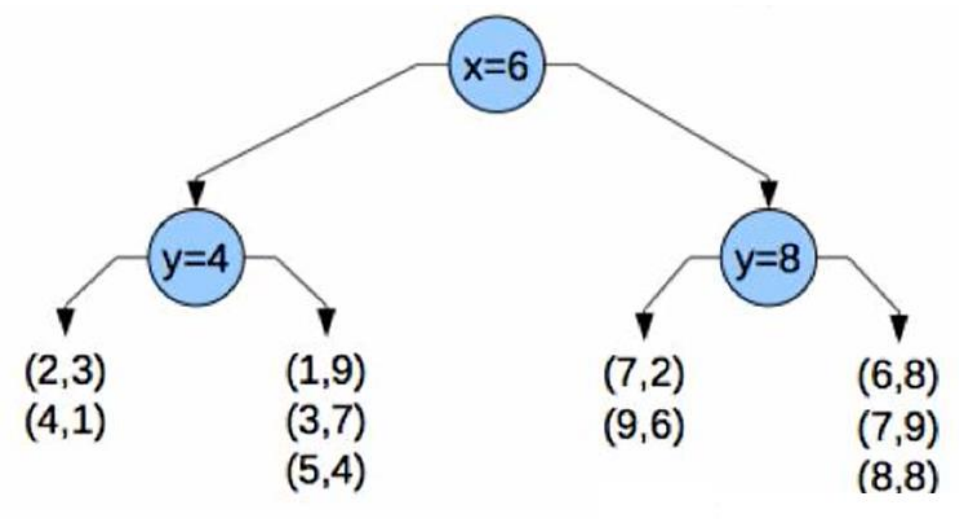

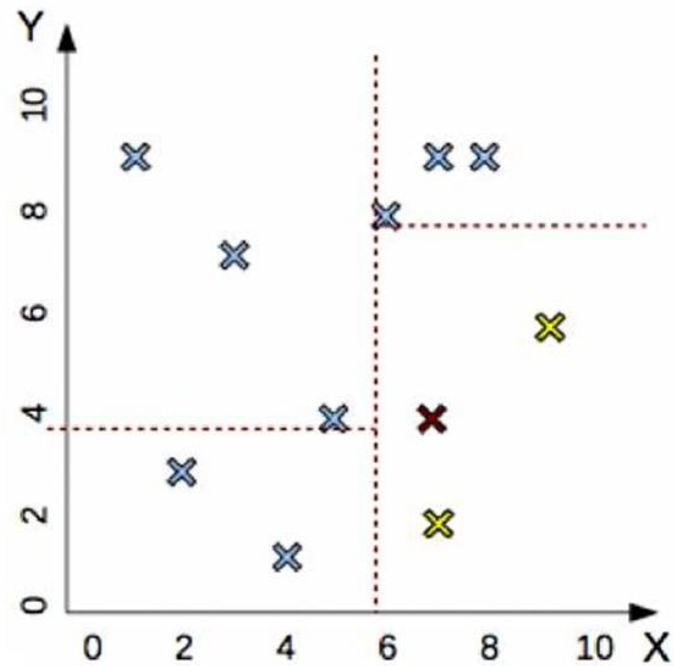

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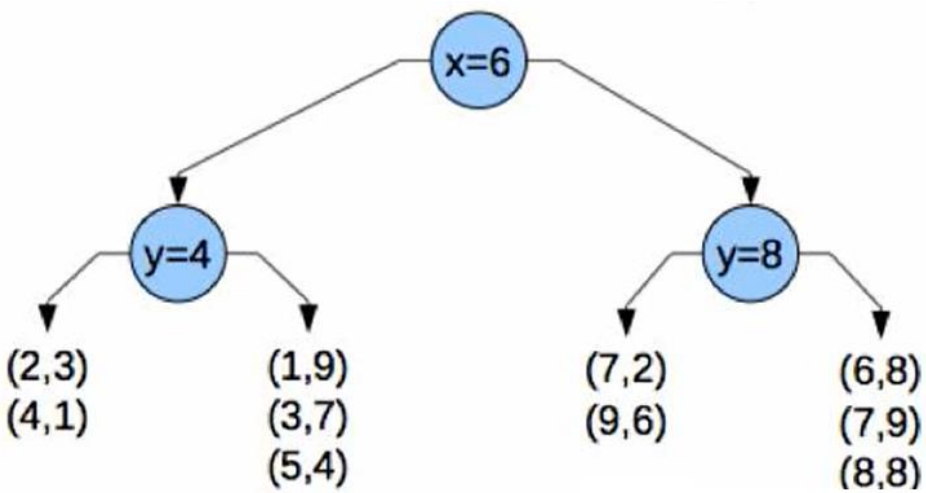
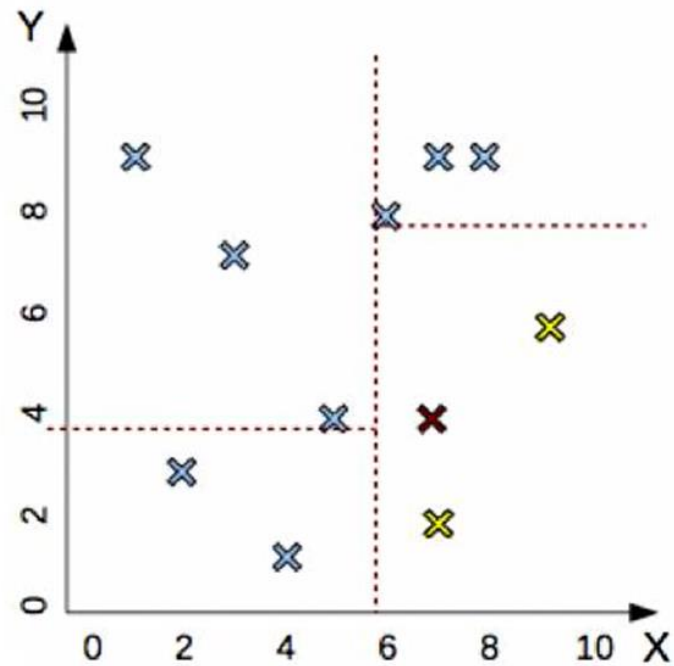
K-Dimensional Trees: Inference

- Find NNs for new point (7,4)
  - find region containing (7,4)
  - compare to all points in region





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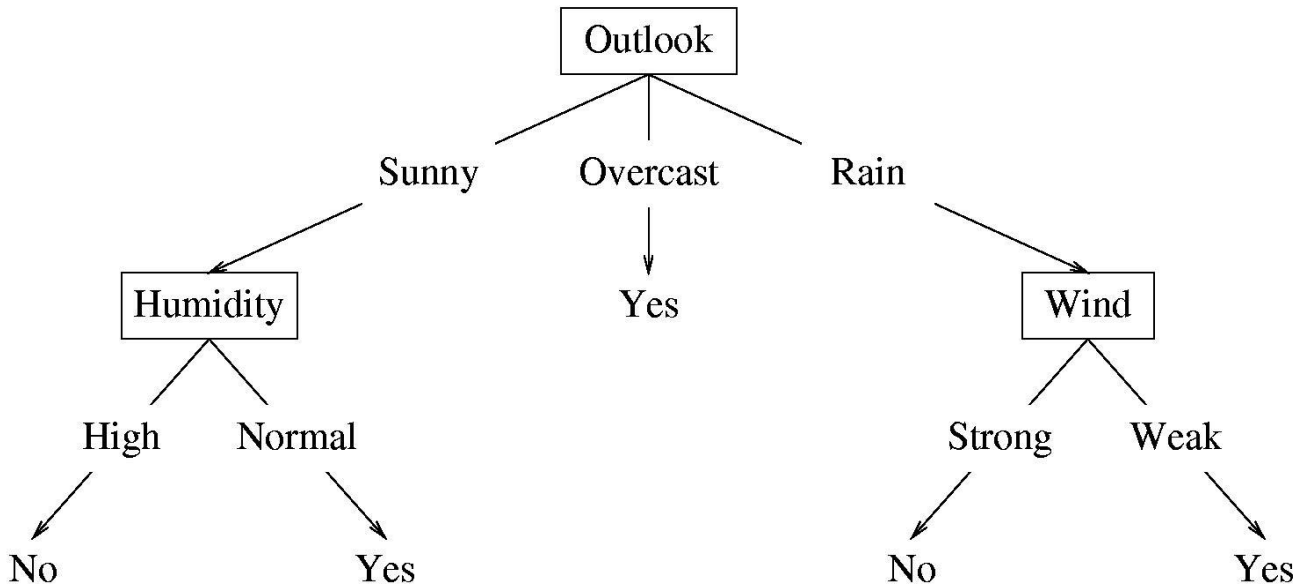
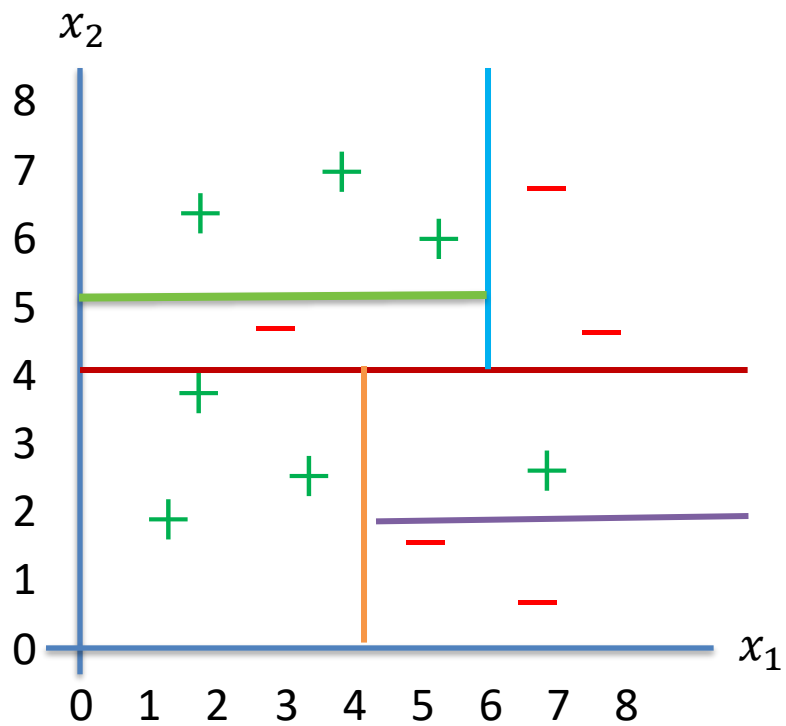
Decision Trees

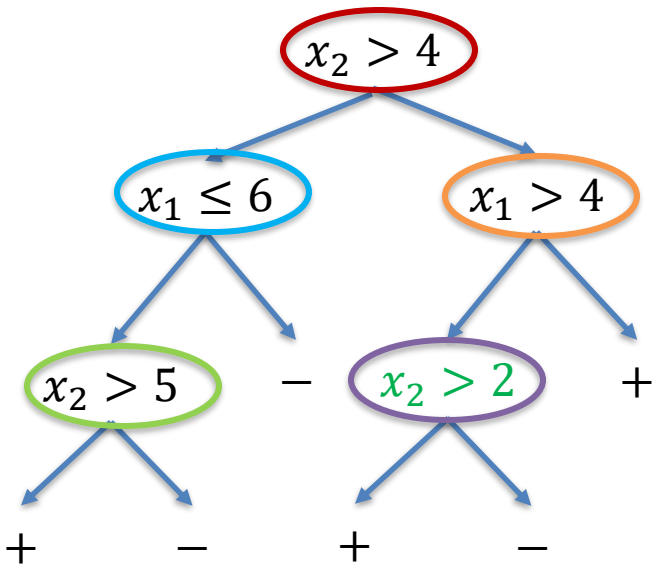


- A tree in which each internal (non-leaf) node tests the value of a particular feature
- Each leaf node specifies a class label (in this case whether or not you should play tennis)

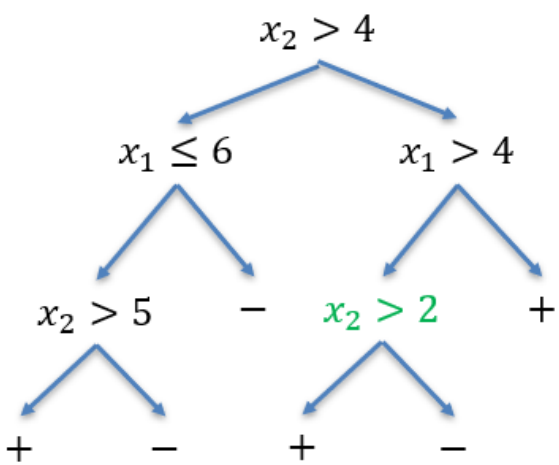
Decision Trees

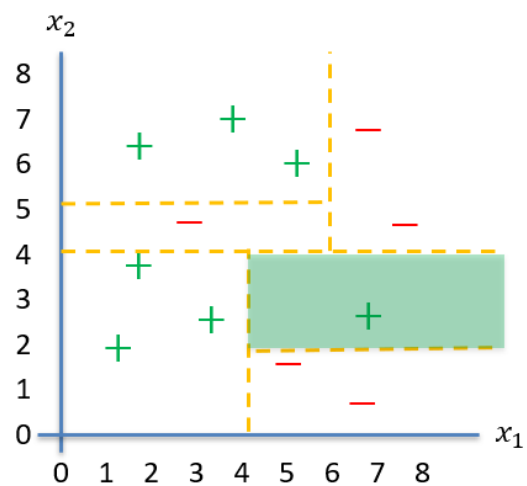
- Decision trees divide the feature space into axis parallel rectangles





Decision Tree Learning



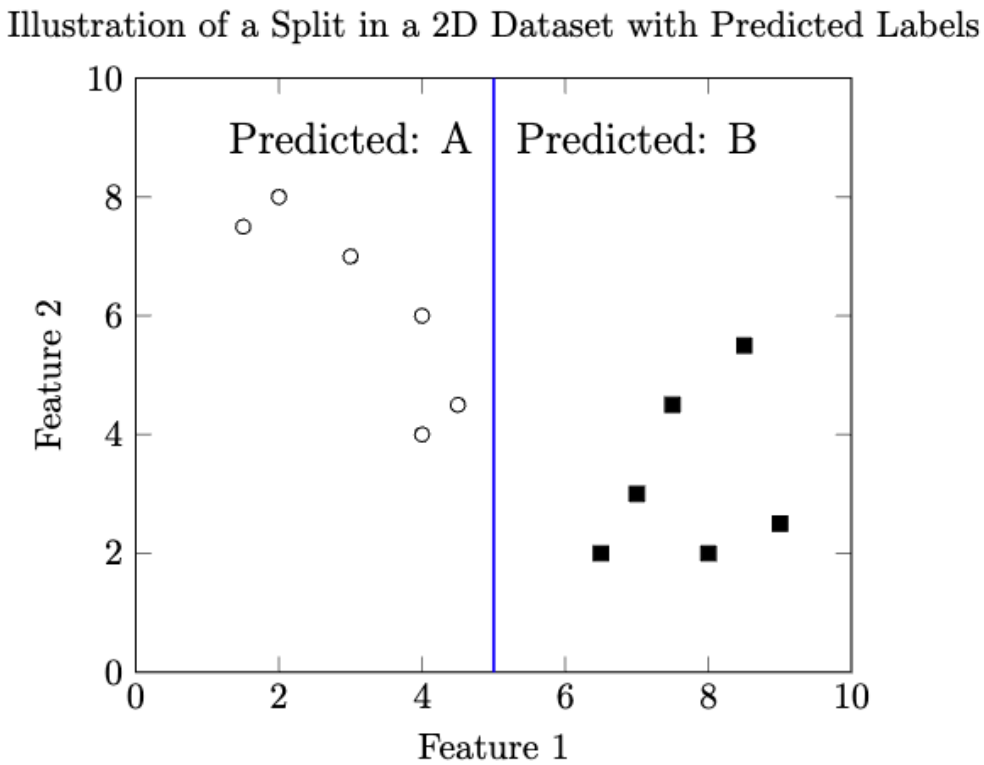


Basic decision tree building algorithm:

Pick some feature/attribute (how to pick the "best"?)	Partition the data based on the value of this attribute	Recurse over each new partition (when to stop?)

We'll focus on the discrete case first (i.e., each feature takes a value in some finite set)

Choosing the Best Attribute to Split



- Splitting on Feature 1 results in homogeneous datasets (i.e., the same label in the two child datasets after the split).
- No split on Feature 2 would achieve this!

Recap: Information Gain

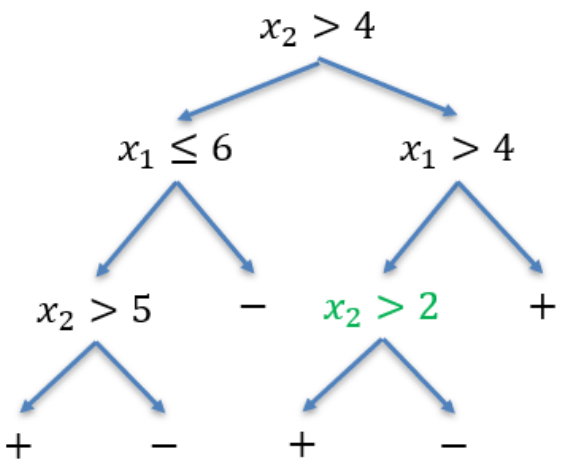
- Using entropy to measure uncertainty, we can greedily select an attribute that guarantees the largest expected decrease in entropy (with respect to the empirical partitions)

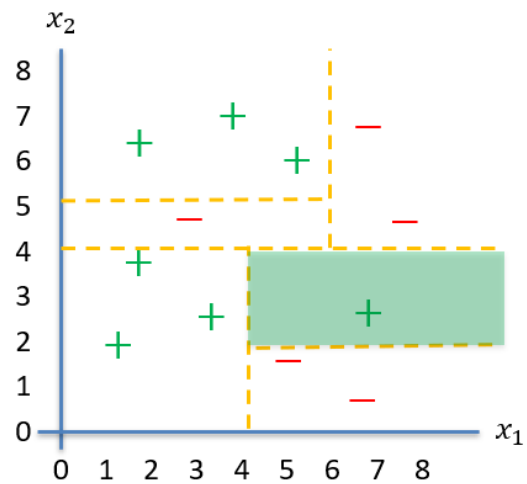
$$IG(X) = H(Y) - H(Y|X)$$

  - Called information gain
  - Larger information gain corresponds to less uncertainty about Y given X
    - Note that $H(Y|X) \leq H(Y)$

Decision Tree Learning

- Basic decision tree building algorithm:
  - Pick the feature/attribute with the highest information gain (or lowest conditional entropy)
  - Partition the data based on the value of this attribute
  - Recurse over each new partition





The Gini Coefficient

- The Gini coefficient is another popular measure used to evaluate splits, focusing on minimizing the probability of misclassification. It is defined for a set S as:

$$Gini(S) = 1 - \sum_{i=1:N} p_i^2$$

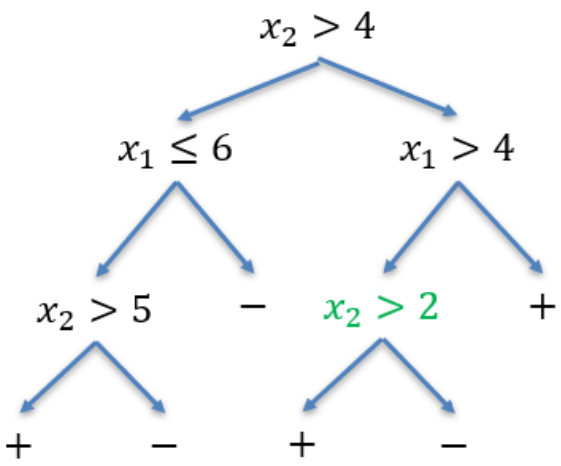
- Once a dataset is split into two sets S_1 and S_2, the Gini-split is defined as:

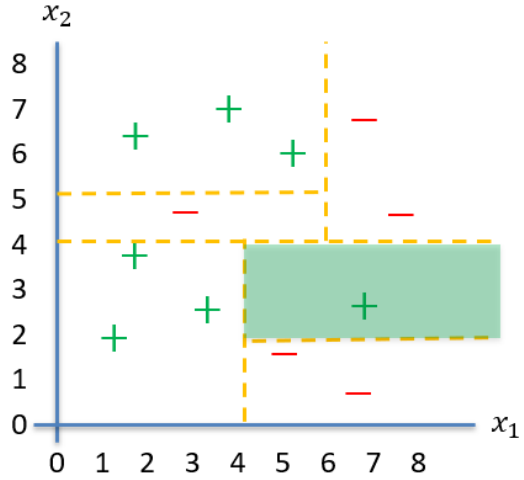
$$GiniSplit = \frac{|S_1|}{|S|} Gini(S_1) + \frac{|S_2|}{|S|} Gini(S_2)$$

- The goal is to find the split that **minimizes the Gini Split.**

Decision Tree Learning

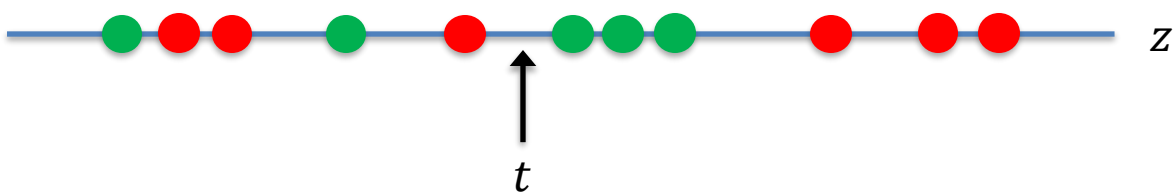
- Basic decision tree building algorithm:
  - Pick the feature/attribute with the lowest gini-split
  - Partition the data based on the value of this attribute
  - Recurse over each new partition





Handling Real-Valued Attributes

- Sort the data according to the kth attribute: $z_1 > z_2 > \cdots > z_n$



- Only a finite number of thresholds make sense
  - Just split in between each consecutive pair of data points (e.g., splits of the form $t = \frac{z_i + z_{i+1}}{2}$)

Regression Decision Trees

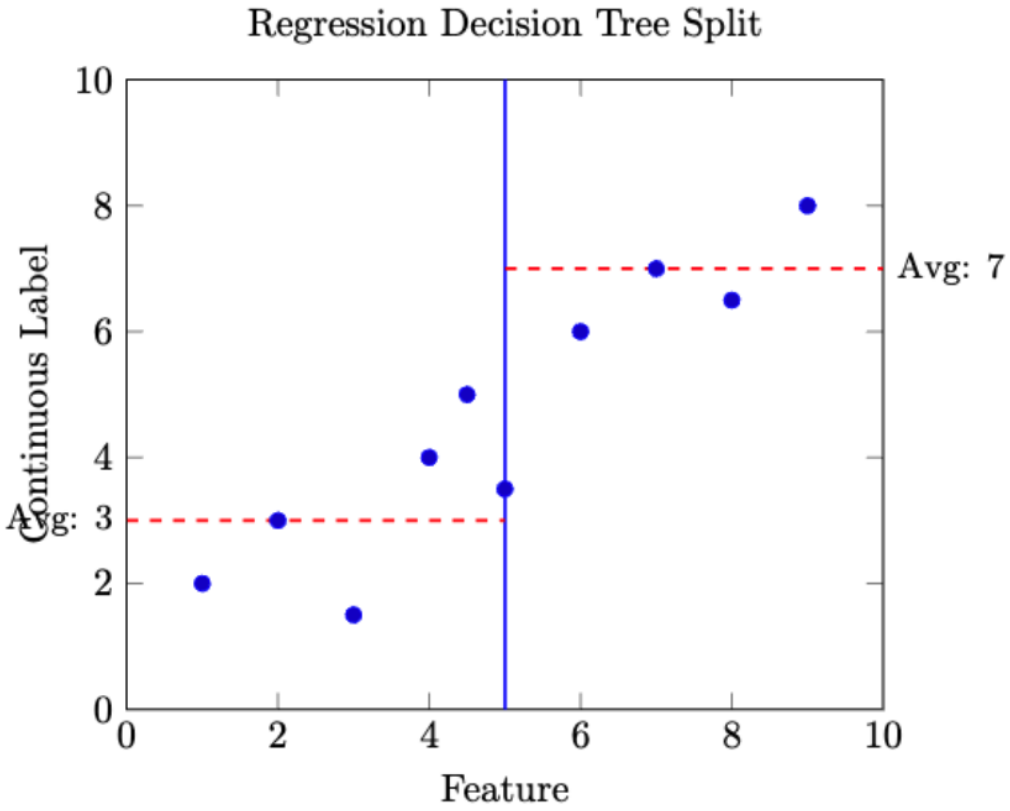


Figure 5: Illustration of a regression decision tree split with a single feature. The dataset is split at Feature = 5, with horizontal dashed lines representing the average label value for each partition.

Regression Splitting Criteria

- MSE Reduction: Calculate the Mean Squared Error of each dataset (i.e. parent dataset and the two children dataset)
- Given a dataset S, the predicted label y_S is the mean of the labels in that set.
- The MSE is then defined as:

$$MSE(S) = \frac{1}{|S|}\sum_{i \in S}(y_i - y_S)^2$$

- We can then define the MSE Reduction as:

$$MSERed = MSE(S) - \frac{|S_1|}{|S|}MSE(S_1) - \frac{|S_2|}{|S|}MSE(S_2)$$

- The goal is to find the split that maximize the MSE Reduction.

CS 6375
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Rishabh Iyer
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- Logistic Regression

Topics for the Midterm Exam

- Linear Regression
- Perceptron
- Support Vector Machines
- Nearest Neighbor Methods
- Decision Trees
- **Bayesian Methods and Parameter Estimation**
- Naïve Bayes
- Logistic Regression

Maximum Likelihood Estimation (MLE)

- **Data:** Observed set of α_H heads and α_T tails
- **Hypothesis:** Coin flips follow a Bernoulli distribution
- **Learning:** Find the "best" θ
- **MLE:** Choose θ to maximize probability of D given θ

$$\begin{aligned}\widehat{\theta} &= \arg\max_{\theta} \quad P(\mathcal{D} \mid \theta) \\ &= \arg\max_{\theta} \quad \ln P(\mathcal{D} \mid \theta)\end{aligned}$$

Coin Flipping – Binomial Distribution

- $P(Heads) = \theta,\ P(Tails) = 1 - \theta$
- Flips are i.i.d.
  - Independent events
  - Identically distributed according to Binomial distribution
- Our training data consists of α_H heads and α_T tails

$$p(D|\theta) = \theta^{\alpha_H} \cdot (1-\theta)^{\alpha_T}$$

First Parameter Learning Algorithm

$$\begin{aligned}\widehat{\theta} &= \arg\max_{\theta} \quad \ln P(\mathcal{D} \mid \theta) \\ &= \arg\max_{\theta} \quad \ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}\end{aligned}$$

Set derivative to zero, and solve!

$$\begin{aligned}\frac{d}{d\theta} \ln P(\mathcal{D} \mid \theta) &= \frac{d}{d\theta}\left[\ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}\right] \\ &= \frac{d}{d\theta}\left[\alpha_H \ln \theta + \alpha_T \ln(1-\theta)\right] \\ &= \alpha_H \frac{d}{d\theta} \ln \theta + \alpha_T \frac{d}{d\theta} \ln(1-\theta) \\ &= \frac{\alpha_H}{\theta} - \frac{\alpha_T}{1-\theta} \quad = 0\end{aligned}$$

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$$\begin{aligned}\widehat{\theta} &= \arg\max_{\theta} \quad \ln P(\mathcal{D} \mid \theta) \\ &= \arg\max_{\theta} \quad \ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}\end{aligned}$$

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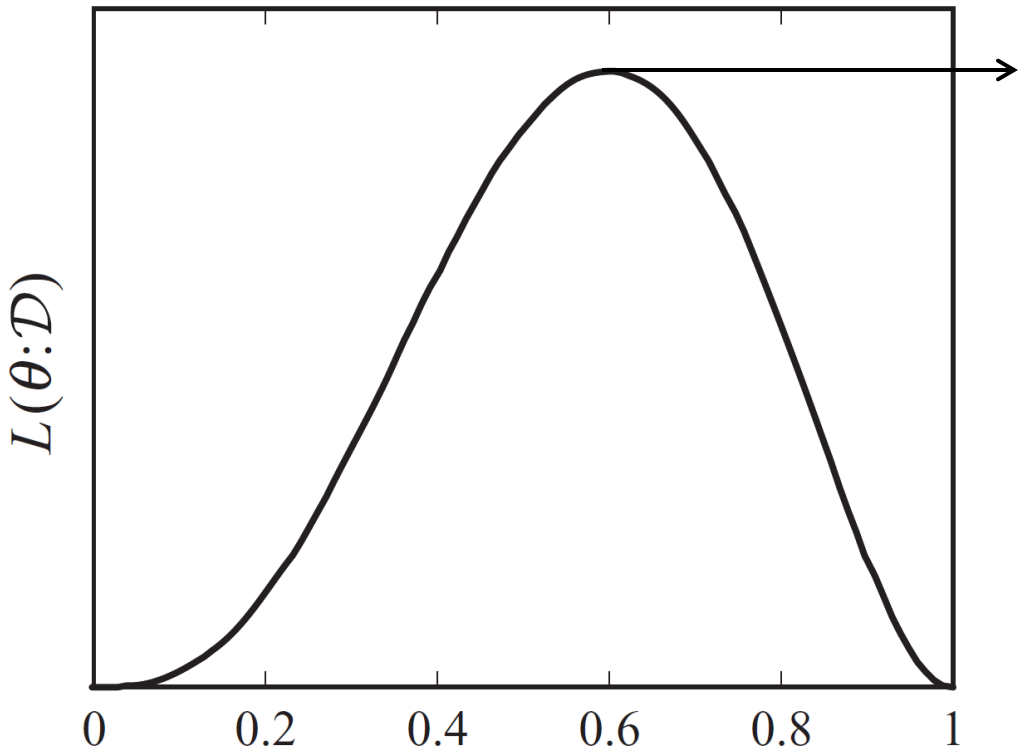
$$\boxed{\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}}$$

Coin Flip MLE

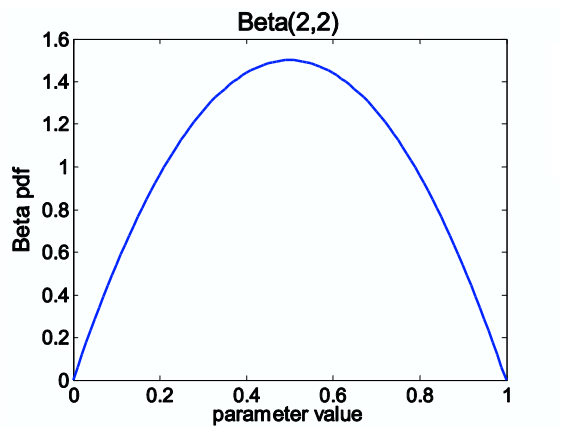


$$\hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

Priors

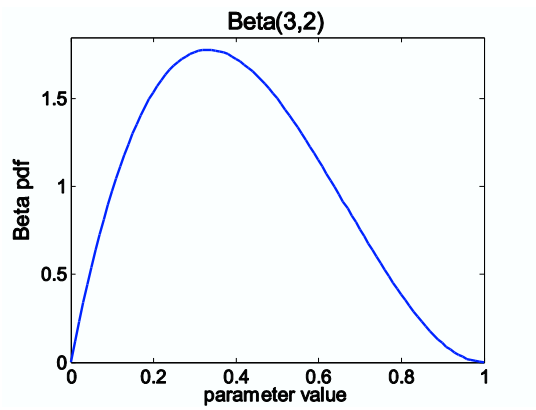
- Priors are a Bayesian mechanism that allow us to take into account "prior" knowledge about our belief in the outcome
- Rather than estimating a single θ, consider a distribution over possible values of θ given the data
  - Update our prior after seeing data

Our best guess in the absence of any data



Observe flips
e.g.: {tails, tails}

Our estimate after we see some data

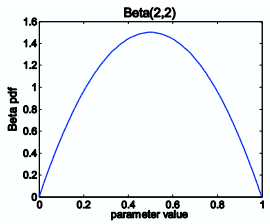


Bayesian Learning

Apply Bayes rule:

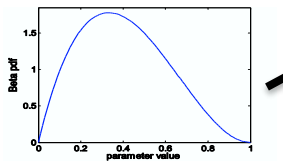
Data Likelihood

Prior



$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)}$$

Posterior



Normalization

- Or equivalently: $p(\theta|D) \propto p(D|\theta)p(\theta)$
- For uniform priors this reduces to the MLE objective

$$p(\theta) \propto 1 \qquad \Rightarrow \qquad p(\theta|D) \propto p(D|\theta)$$

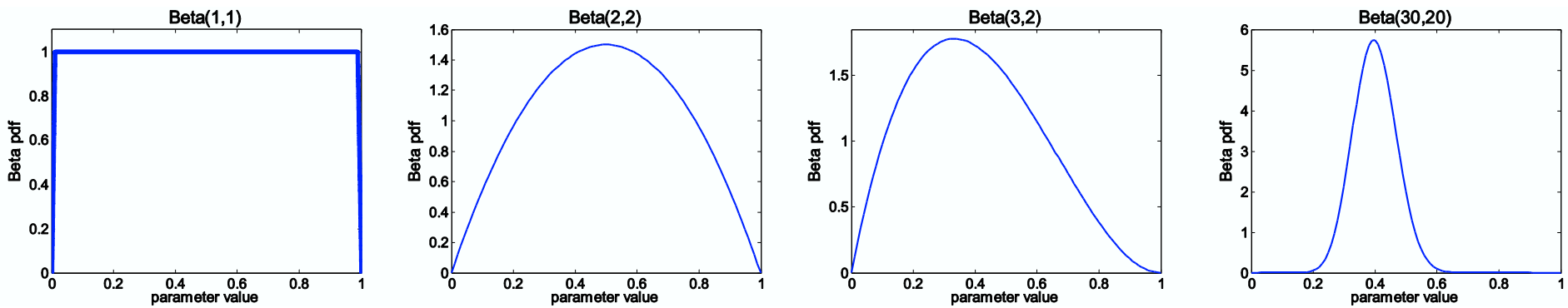
Coin Flips with Beta Distribution

Likelihood function:

$$P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

Prior:

$$P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)} \sim Beta(\beta_H, \beta_T)$$



$$\begin{aligned} P(\theta \mid \mathcal{D}) &\propto \theta^{\alpha_H}(1-\theta)^{\alpha_T}\ \theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1} \\ &= \theta^{\alpha_H + \beta_H - 1}(1-\theta)^{\alpha_T + \beta_T - 1} \\ &= Beta(\alpha_H + \beta_H, \alpha_T + \beta_T) \end{aligned}$$

MAP Estimation

- Choosing θ to maximize the posterior distribution is called maximum a posteriori (MAP) estimation

$$\theta_{MAP} = \arg\max_{\theta} p(\theta|D)$$

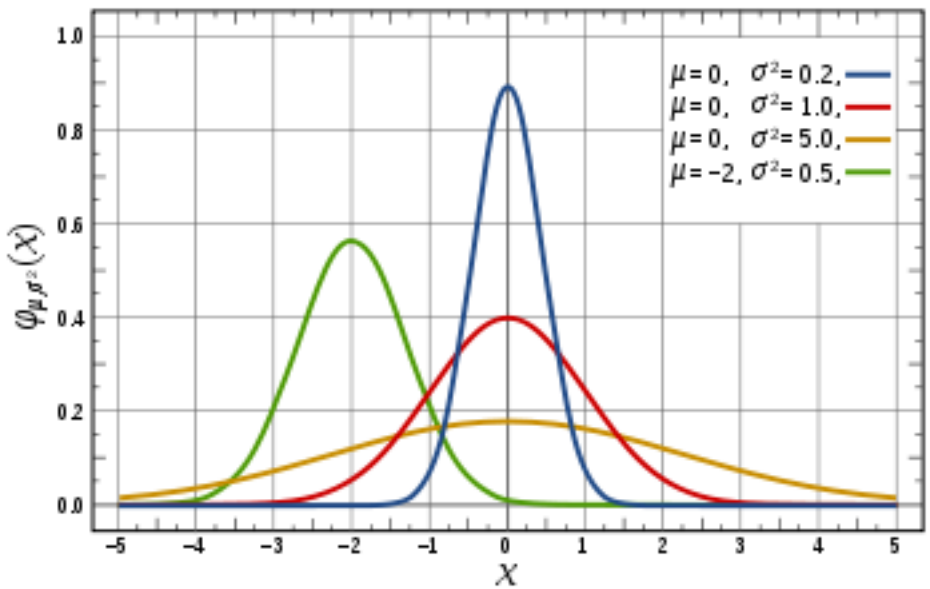
- The only difference between θ_{MLE} and θ_{MAP} is that one assumes a uniform prior (MLE) and the other allows an arbitrary prior

MAP for the Coin Flip Model

- Suppose we have 5 coin flips all of which are heads
  - MLE would give $\theta_{MLE} = 1$
  - MLE with a $Beta(2,2)$ prior gives $\theta_{MAP} = \frac{6}{7} \approx .857$
  - As we see more data, the effect of the prior diminishes
    - $\theta_{MAP} = \frac{\alpha_H + \beta_H - 1}{\alpha_H + \beta_H + \alpha_T + \beta_T - 2} \approx \frac{\alpha_H}{\alpha_H + \alpha_T}$ for large # of observations

MLE for Gaussian Distributions

- Two parameter distribution characterized by a mean and a variance



$$P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

Learning a Gaussian

- Collect data
  - Hopefully, i.i.d. samples
  - e.g., exam scores
- Learn parameters
  - Mean: μ
  - Variance: σ

i	Exam Score
0	85
1	95
2	100
3	12
…	…
99	89

$$P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

MLE for Gaussian:

- Probability of N i.i.d. samples $D = x^{(1)}, \dots, x^{(N)}$

$$p(D|\mu,\sigma) = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^N \prod_{i=1}^{N} e^{-\frac{\left(x^{(i)}-\mu\right)^2}{2\sigma^2}}$$

$$\mu_{MLE}, \sigma_{MLE} = \arg\max_{\mu,\sigma} P(\mathcal{D} \mid \mu, \sigma)$$

- Log-likelihood of the data

$$\ln p(D|\mu,\sigma) = -\frac{N}{2}\ln 2\pi\sigma^2 - \sum_{i=1}^{N}\frac{\left(x^{(i)}-\mu\right)^2}{2\sigma^2}$$

MLE for the Mean of a Gaussian

$$\frac{\partial}{\partial \mu} \ln p(D|\mu,\sigma) = \frac{\partial}{\partial \mu}\left[-\frac{N}{2}\ln 2\pi\sigma^2 - \sum_{i=1}^{N}\frac{\left(x^{(i)}-\mu\right)^2}{2\sigma^2}\right]$$

$$= \frac{\partial}{\partial \mu}\left[-\sum_{i=1}^{N}\frac{\left(x^{(i)}-\mu\right)^2}{2\sigma^2}\right]$$

$$= \sum_{i=1}^{N}\frac{\left(x^{(i)}-\mu\right)}{\sigma^2}$$

$$= \frac{\left[N\mu - \sum_{i=1}^{N} x^{(i)}\right]}{\sigma^2} = 0$$

$$\boxed{\mu_{MLE} = \frac{1}{N}\sum_{i=1}^{N} x^{(i)}}$$

MLE for Variance

$$\frac{\partial}{\partial\sigma}\ln p(D|\mu,\sigma) = \frac{\partial}{\partial\sigma}\left[-\frac{N}{2}\ln 2\pi\sigma^2 - \sum_{i=1}^{N}\frac{\left(x^{(i)}-\mu\right)^2}{2\sigma^2}\right]$$

$$= -\frac{N}{\sigma} + \frac{\partial}{\partial\sigma}\left[-\sum_{i=1}^{N}\frac{\left(x^{(i)}-\mu\right)^2}{2\sigma^2}\right]$$

$$= -\frac{N}{\sigma} + \sum_{i=1}^{N}\frac{\left(x^{(i)}-\mu\right)^2}{\sigma^3} = 0$$

$$\boxed{\sigma_{MLE}^2 = \frac{1}{N}\sum_{i=1}^{N}\left(x^{(i)}-\mu_{MLE}\right)^2}$$

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Bayesian Categorization/Classification

- Given features $x = (x_1, \dots, x_m)$ predict a label y
- If we had a joint distribution over x and y, given x we could find the label using MAP inference

$$\arg\max_y p(y|x_1, \dots, x_m)$$

- Can compute this in exactly the same way that we did before using Bayes rule:

$$p(y|x_1, \dots, x_m) = \frac{p(x_1, \dots, x_m|y)p(y)}{p(x_1, \dots, x_m)}$$

Bag of Words

aardvark	0
about	2
all	2
Africa	1
apple	0
anxious	0
...	
gas	1
...	
oil	1
…	
Zaire	0

Naïve Bayes

- Naïve Bayes assumption
  - Features are independent given class label

$$p(x_1, x_2|y) = p(x_1|y)\, p(x_2|y)$$

  - More generally

$$p(x_1, \dots, x_m|y) = \prod_{i=1}^{m} p(x_i|y)$$

- How many parameters now?
  - Suppose x is composed of d binary features

Naïve Bayes

- Naïve Bayes assumption
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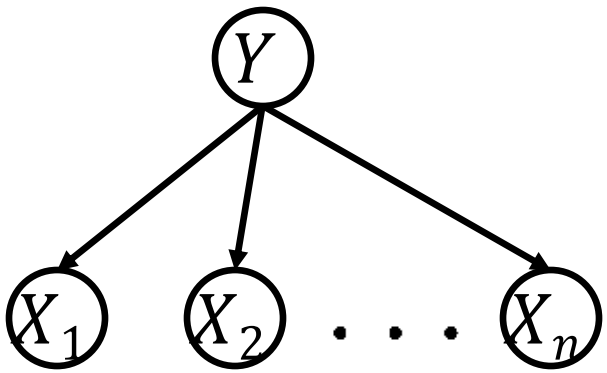
  - More generally

$$p(x_1, \dots, x_m|y) = \prod_{i=1}^{m} p(x_i|y)$$

- How many parameters now?
  - Suppose x composed of d binary features $\Rightarrow O(d \cdot L)$ where L is the number of class labels

The Naïve Bayes Classifier

- **Given**
  - Prior $p(y)$
  - m conditionally independent features X given the class Y
  - For each X_i, we have likelihood $P(X_i|Y)$



- Classify via

$$y^* = h_{NB}(x) = \arg\max_y p(y)p(x_1, \dots, x_m|y)$$
$$= \arg\max_y p(y) \prod_i^m p(x_i|y)$$

MLE for the Parameters of NB

- Given dataset, count occurrences for all pairs
  - $Count(X_i = x_i, Y = y)$ is the number of samples in which $X_i = x_i$ and $Y = y$
- MLE for discrete NB

$$p(Y = y) = \frac{Count(Y = y)}{\sum_{y'} Count(Y = y')}$$

$$p(X_i = x_i | Y = y) = \frac{Count(X_i = x_i, Y = y)}{\sum_{x_i'} Count\,(X_i = x_i', Y = y)}$$

See this link for more insights: http://www.datasciencecourse.org/notes/mle/

NB and MAP: Laplace Smoothing

- To fix this, use a prior!
  - Already saw how to do this in the coin-flipping example using the Beta distribution
  - For NB over discrete spaces, can use the Dirichlet prior
  - The Dirichlet distribution is a distribution over $z_1, \dots, z_k \in (0,1)$ such that $z_1 + \cdots + z_k = 1$ characterized by k parameters $\alpha_1, \dots, \alpha_k$

$$f(z_1, \dots, z_k; \alpha_1, \dots, \alpha_k) \propto \prod_{i=1}^{k} z_i^{\alpha_i - 1}$$

    - Called smoothing, what are the MLE estimates under these kinds of priors?

Continuous Naïve Bayes

- Continuous Naïve Bayes, also known as Guassian Naïve Bayes is where the features are continuous
- The distribution $p(X_i = x_i \mid Y = y) = N\left(x_i, \mu_y, \sigma_y^2\right)$
- In other words, the conditional distribution of each feature given the class is a Guassian distribution with mean μ_y and variance σ_y^2
- We can use the Naïve Bayes assumption and assume:

$$p(x_1, \dots, x_m | y) = \prod_{i=1}^{m} p(x_i | y)$$

- The distribution of labels is the same as the multinomial case

Parameter Estimation of Cont. NB

- The parameter estimation can similarly be obtained using the Maximum Likelihood Estimation
- The mean and variance can be estimated as the standard Gaussian distribution except that we restrict to each label

$$\mu_y = \frac{\sum_{j=1}^{m} x_i^{(j)} 1\{y^{(j)} = y\}}{\sum_{j=1}^{m} 1\{y^{(j)} = y\}},$$

$$\sigma_y^2 = \frac{\sum_{j=1}^{m} (x_i^{(j)} - \mu_y)^2 1\{y^{(j)} = y\}}{\sum_{j=1}^{m} 1\{y^{(j)} = y\}}$$

Parameter Estimation of Cont. NB

- Finally, we need to estimate $p(y)$
- This is like the discrete Naïve Bayes case:

$$p(Y = y) = \frac{Count(Y = y)}{\sum_{y'} Count(Y = y')}$$

- We can classify a test example in a similar way to discrete NB:

$$y^* = h_{NB}(x) = \arg\max_y p(y) p(x_1, \dots, x_m | y)$$
$$= \arg\max_y p(y) \prod_i^m p(x_i | y)$$

- Here $p(x_i \,|y) = \mathrm{N}\left(\mathrm{x_i}, \mu_y, \sigma_y^2\right)$

Summary of Naïve Bayes Models

- Two kinds of Naïve Bayes: Discrete and Continuous
- Learning is often very simple
  - Using counts (discrete NB) or mean/variance (cont. NB), obtain estimates for $p(x_i \mid y)$
  - Using counts, obtain estimates for $p(y)$
- At inference time, we classify based on:

$$y^* = h_{NB}(x) = \arg\max_y p(y) p(x_1, \dots, x_m \mid y)$$
$$= \arg\max_y p(y) \prod_i^m p(x_i \mid y)$$

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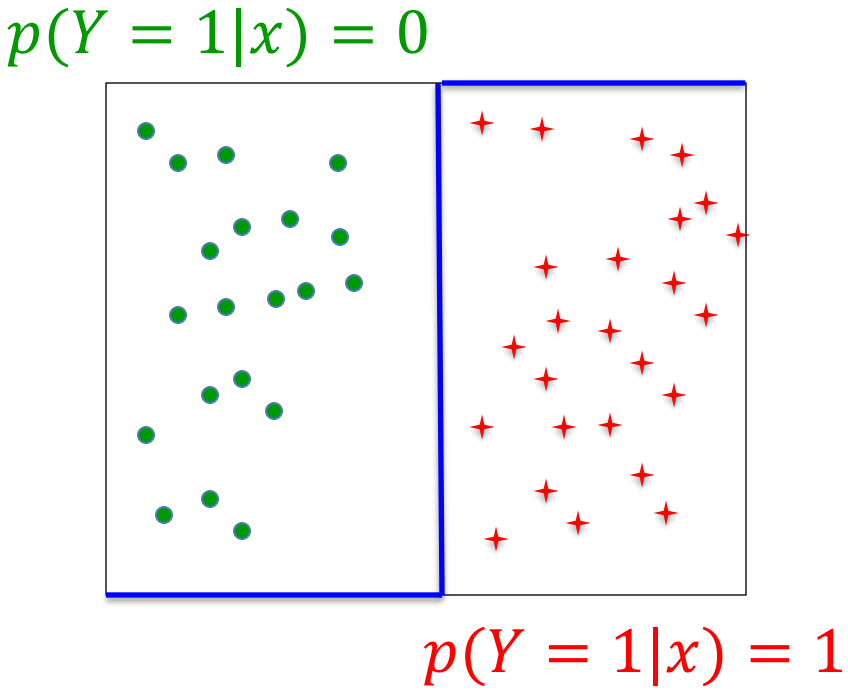
Ideal 0/1 Probability

- Learn $p(Y|X)$ directly from the data
  - Assume a particular functional form, e.g., a linear classifier $p(Y = 1|x) = 1$ on one side and 0 on the other
  - Not differentiable…
    - Makes it difficult to learn
    - Can't handle noisy labels

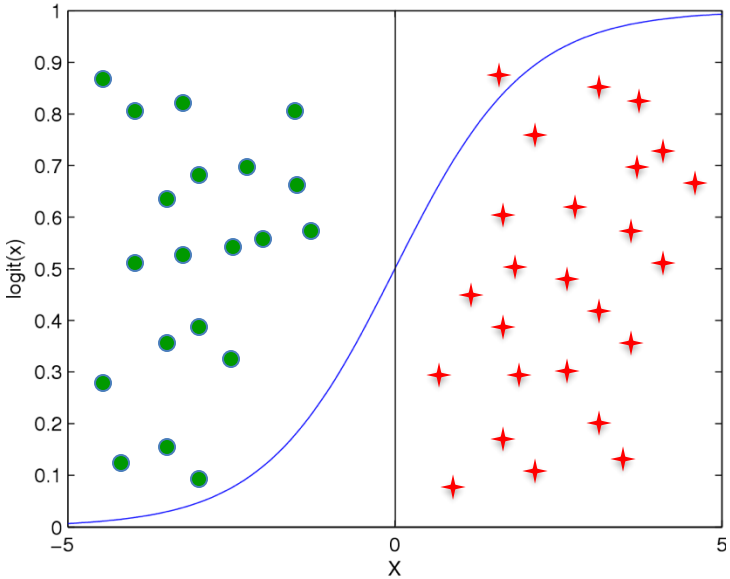


Logistic Regression

- Learn $p(y|x)$ directly from the data
  - Assume a particular functional form

$$p(Y=-1|x) = \frac{1}{1+\exp(w^T x + b)}$$

$$p(Y=1|x) = \frac{\exp(w^T x + b)}{1+\exp(w^T x + b)}$$



Functional Form: Two classes

- Given some w and b, we can classify a new point x by assigning the label 1 if $p(Y = 1|x) > p(Y = -1|x)$ and -1 otherwise
  - This leads to a linear classification rule:
    - Classify as a 1 if $w^T x + b > 0$
    - Classify as a -1 if $w^T x + b < 0$

Learning the Weights

- To learn the weights, we maximize the conditional likelihood

$$(w^*, b^*) = \arg\max_{w,b} \prod_{i=1}^{N} p(y^{(i)} | x^{(i)}, w, b)$$

- This is the not the same strategy that we used in the case of naive Bayes
  - For naive Bayes, we maximized the log-likelihood

Learning the Weights

$$
\begin{aligned}
\ell(w,b) &= \ln \prod_{i=1}^{N} p(y^{(i)}|x^{(i)},w,b) \\
&= \sum_{i=1}^{N} \ln p(y^{(i)}|x^{(i)},w,b) \\
&= \sum_{i=1}^{N} \frac{y^{(i)}+1}{2} \ln p(Y=1|x^{(i)},w,b) + \left(1-\frac{y^{(i)}+1}{2}\right) \ln p(Y=-1|x^{(i)},w,b) \\
&= \sum_{i=1}^{N} \frac{y^{(i)}+1}{2} \ln \frac{p\left(Y=1\middle|x^{(i)},w,b\right)}{p\left(Y=-1\middle|x^{(i)},w,b\right)} + \ln p(Y=-1|x^{(i)},w,b) \\
&= \sum_{i=1}^{N} \frac{y^{(i)}+1}{2} \left(w^T x^{(i)} + b\right) - \ln\left(1+\exp\left(w^T x^{(i)} + b\right)\right)
\end{aligned}
$$

Learning the Weights

$$
\begin{aligned}
\ell(w,b) &= \ln \prod_{i=1}^{N} p(y^{(i)}|x^{(i)},w,b) \\
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&= \sum_{i=1}^{N} \frac{y^{(i)}+1}{2} \left(w^T x^{(i)} + b\right) - \ln\left(1+\exp\left(w^T x^{(i)} + b\right)\right)
\end{aligned}
$$

This is concave in w and b: take derivatives and solve!

Learning the Weights

$$
\begin{aligned}
\ell(w,b) &= \ln \prod_{i=1}^{N} p(y^{(i)}|x^{(i)},w,b) \\
&= \sum_{i=1}^{N} \ln p(y^{(i)}|x^{(i)},w,b) \\
&= \sum_{i=1}^{N} \frac{y^{(i)}+1}{2} \ln p(Y=1|x^{(i)},w,b) + \left(1-\frac{y^{(i)}+1}{2}\right) \ln p(Y=-1|x^{(i)},w,b) \\
&= \sum_{i=1}^{N} \frac{y^{(i)}+1}{2} \ln \frac{p\left(Y=1\middle|x^{(i)},w,b\right)}{p\left(Y=-1\middle|x^{(i)},w,b\right)} + \ln p(Y=-1|x^{(i)},w,b) \\
&= \sum_{i=1}^{N} \frac{y^{(i)}+1}{2} \left(w^T x^{(i)} + b\right) - \ln\left(1+\exp\left(w^T x^{(i)} + b\right)\right)
\end{aligned}
$$

No closed form solution ☹

Learning the Weights

- Can apply gradient ascent to maximize the conditional likelihood

$$\frac{\partial \ell}{\partial b} = \sum_{i=1}^{N} \left[\frac{y^{(i)} + 1}{2} - p(Y = 1 | x^{(i)}, w, b) \right]$$

$$\frac{\partial \ell}{\partial w_j} = \sum_{i=1}^{N} x_j^{(i)} \left[\frac{y^{(i)} + 1}{2} - p(Y = 1 | x^{(i)}, w, b) \right]$$

Priors

- Can define priors on the weights to prevent overfitting
  - Normal distribution, zero mean, identity covariance

$$p(w) = \prod_j \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{w_j^2}{2\sigma^2}\right)$$

  - "Pushes" parameters towards zero
- Regularization
  - Helps avoid very large weights and overfitting

Priors as Regularization

- The log-MAP objective with this Gaussian prior is then

$$\ln \prod_{i=1}^{N} p\left(y^{(i)} \middle| x^{(i)}, w, b\right) p(w) p(b) = \left[\sum_{i}^{N} \ln p\left(y^{(i)} \middle| x^{(i)}, w, b\right)\right] - \frac{\lambda}{2} \|w\|_2^2$$

  - Quadratic penalty: drives weights towards zero
  - Adds a negative linear term to the gradients
  - Different priors can produce different kinds of regularization

Somtimes called an ℓ_2 regularizer

Generative vs. Discriminative Classifiers

Generative classifier:
(e.g., Naïve Bayes)

- Assume some **functional form** for $p(x|y), p(y)$
- Estimate parameters of $p(x|y)$, $p(y)$ directly from training data
- Use Bayes rule to calculate $p(y|x)$
- This is a **generative model**
  - **Indirect** computation of $p(Y|X)$ through Bayes rule
  - As a result, **can also generate a sample of the data**, $p(x) = \sum_y p(y)p(x|y)$

Discriminative classifiers:
(e.g., Logistic Regression)

- Assume some **functional form for** $p(y|x)$
- Estimate parameters of $p(y|x)$ directly from training data
- This is a discriminative model
  - Directly learn $p(y|x)$
  - But **cannot obtain a sample of the data** as $p(x)$ is not available
  - Useful for discriminating labels