Caltech

Machine Learning & Data Mining

CS/CNS/EE 155

Lecture 3:

SVM, Logistic Regression, Neural Nets, Evaluation Metrics

Announcements

- HW1 Due Tomorrow
  - Will be graded in about a week
- HW2 Released Tonight/Tomorrow
  - Due Jan 23^{rd} at 9pm
- Recitation Thursday
  - Linear Algebra (& Vector Calculus)
  - Annenberg 105

Recap: Basic Recipe

- Training Data: $S = \{(x_i, y_i)\}_{i=1}^{N}$ $\quad x \in R^D$ $\quad y \in \{-1,+1\}$

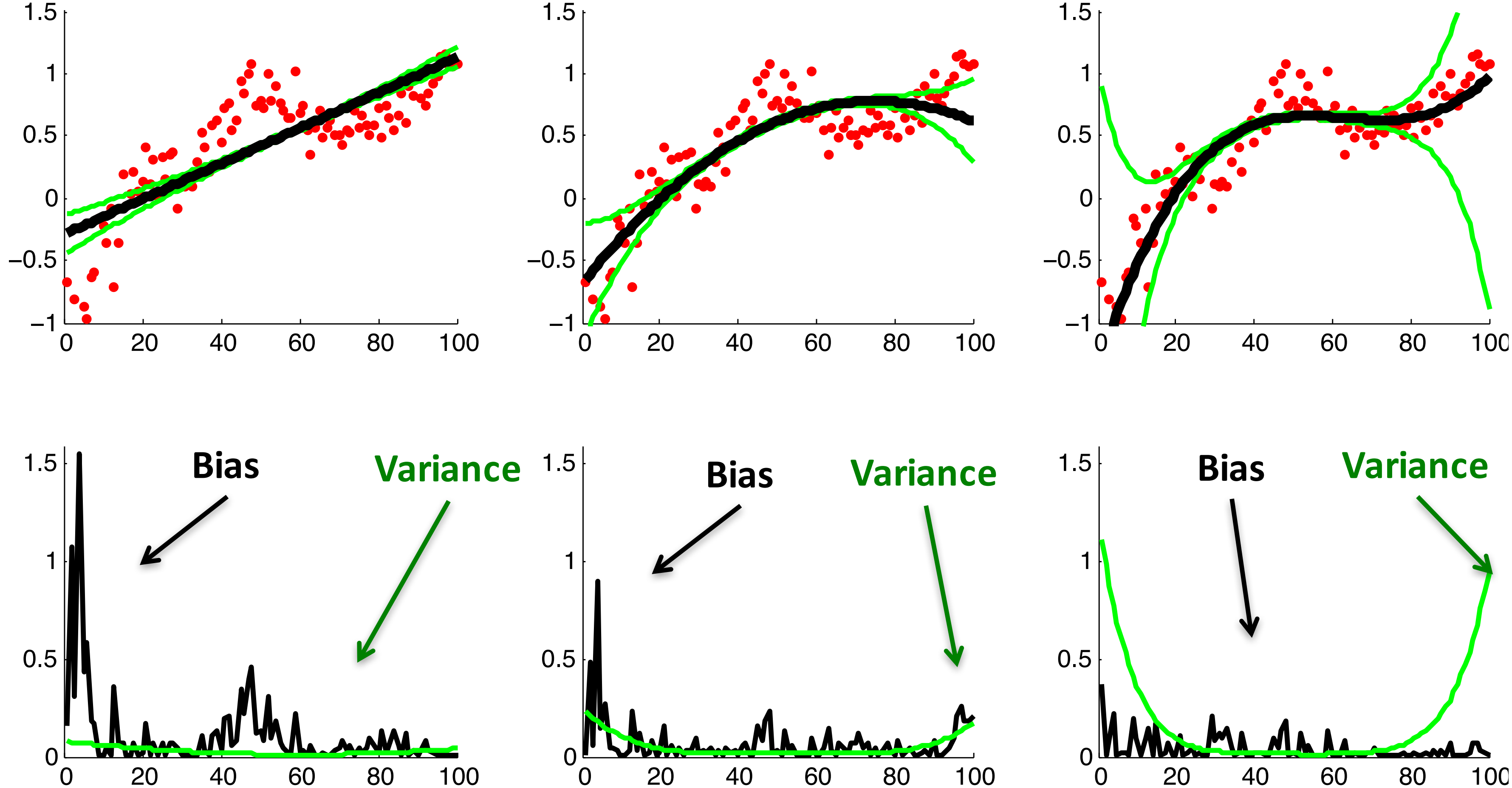
- Model Class: $f(x \mid w, b) = w^T x - b$ **Linear Models**

- Loss Function: $L(a,b) = (a-b)^2$ **Squared Loss**

- Learning Objective: $\underset{w,b}{\operatorname{argmin}} \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$

Optimization Problem

Recap: Bias-Variance Trade-off



Recap: Complete Pipeline

$$S = \{(x_i, y_i)\}_{i=1}^{N}$$

Training Data

$$f(x \mid w, b) = w^T x - b$$

Model Class(es)

$$L(a,b) = (a-b)^2$$

Loss Function

$$\underset{w,b}{\operatorname{argmin}} \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$$

SGD!

Cross Validation & Model Selection

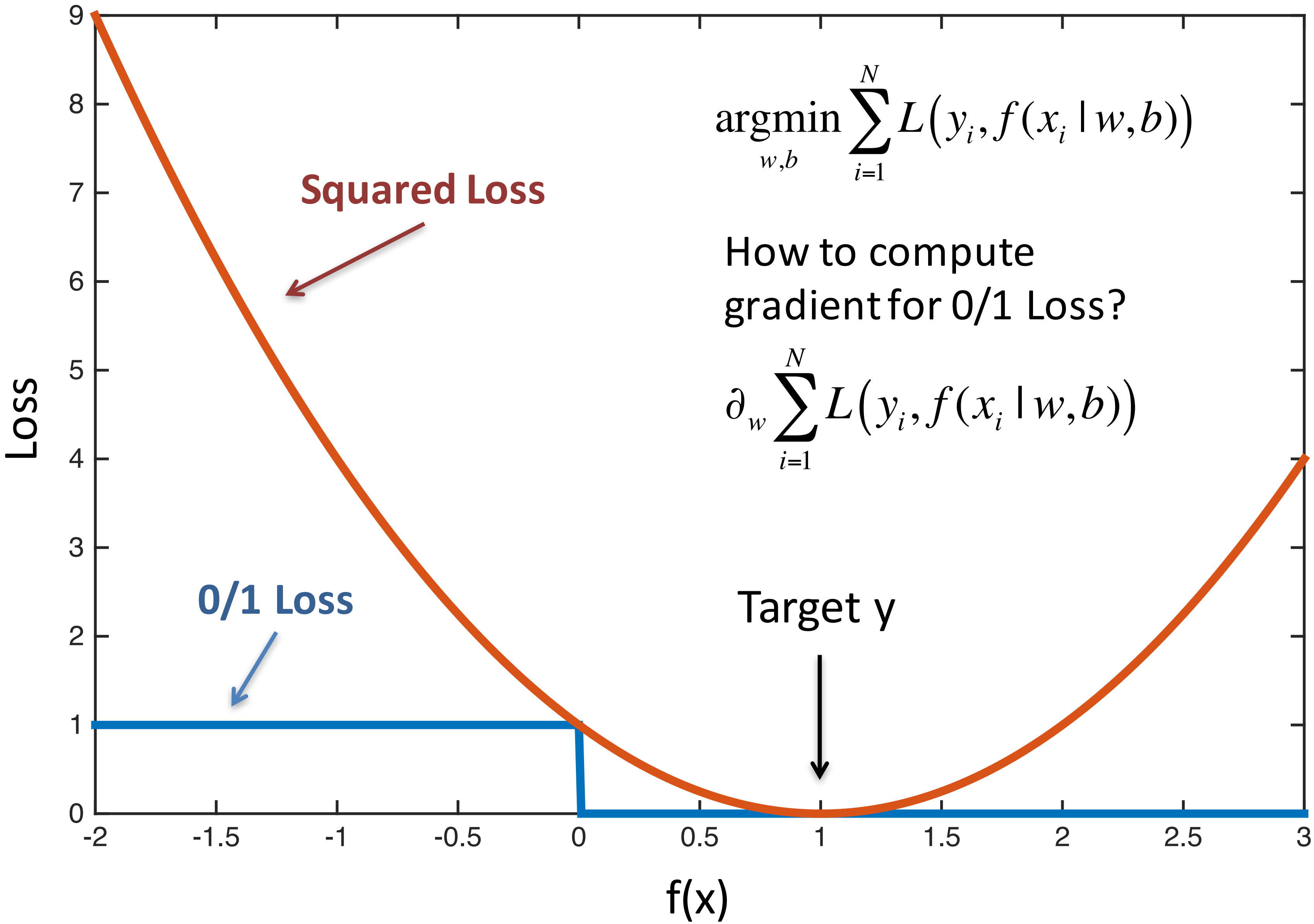
Profit!

Today

- Beyond Basic Linear Models
  - Support Vector Machines
  - Logistic Regression
  - Feed-forward Neural Networks
  - Different ways to interpret models
- Different Evaluation Metrics

Today

- **Beyond Basic Linear Models**
  - **Support Vector Machines**
  - **Logistic Regression**
  - **Feed-forward Neural Networks**
  - **Different ways to interpret models**
- Different Evaluation Metrics



$$\underset{w,b}{\operatorname{argmin}} \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$$
How to compute
gradient for 0/1 Loss?
$$\partial_w \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$$
Squared Loss
0/1 Loss
Target y
Loss
f(x)
0
1
2
3
4
5
6
7
8
9
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
2.5
3

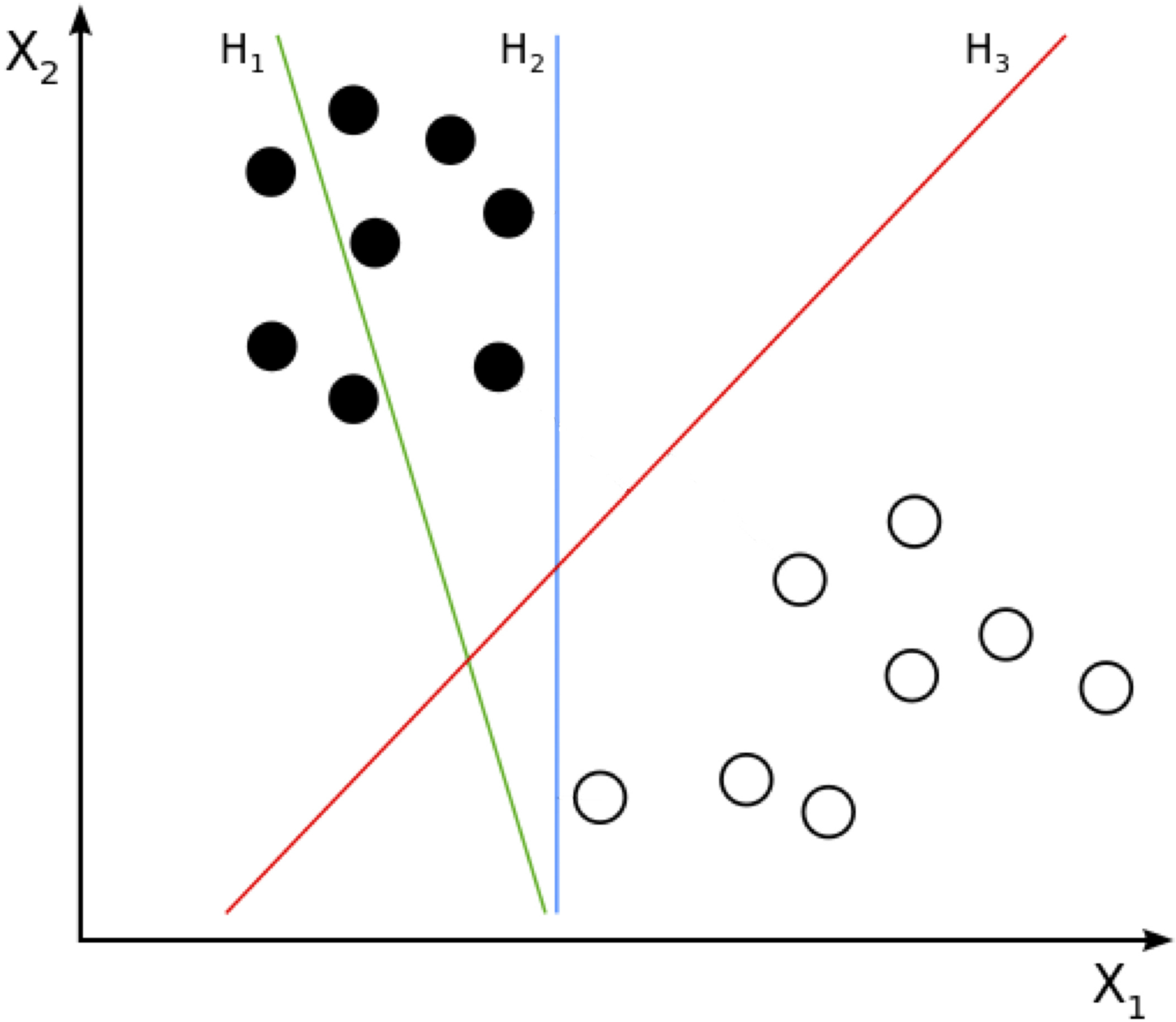
Recap: 0/1 Loss is Intractable

- 0/1 Loss is flat or discontinuous everywhere
- VERY difficult to optimize using gradient descent
- **Solution:** Optimize surrogate Loss
  - **Today: Hinge Loss (…eventually)**

Support Vector Machines

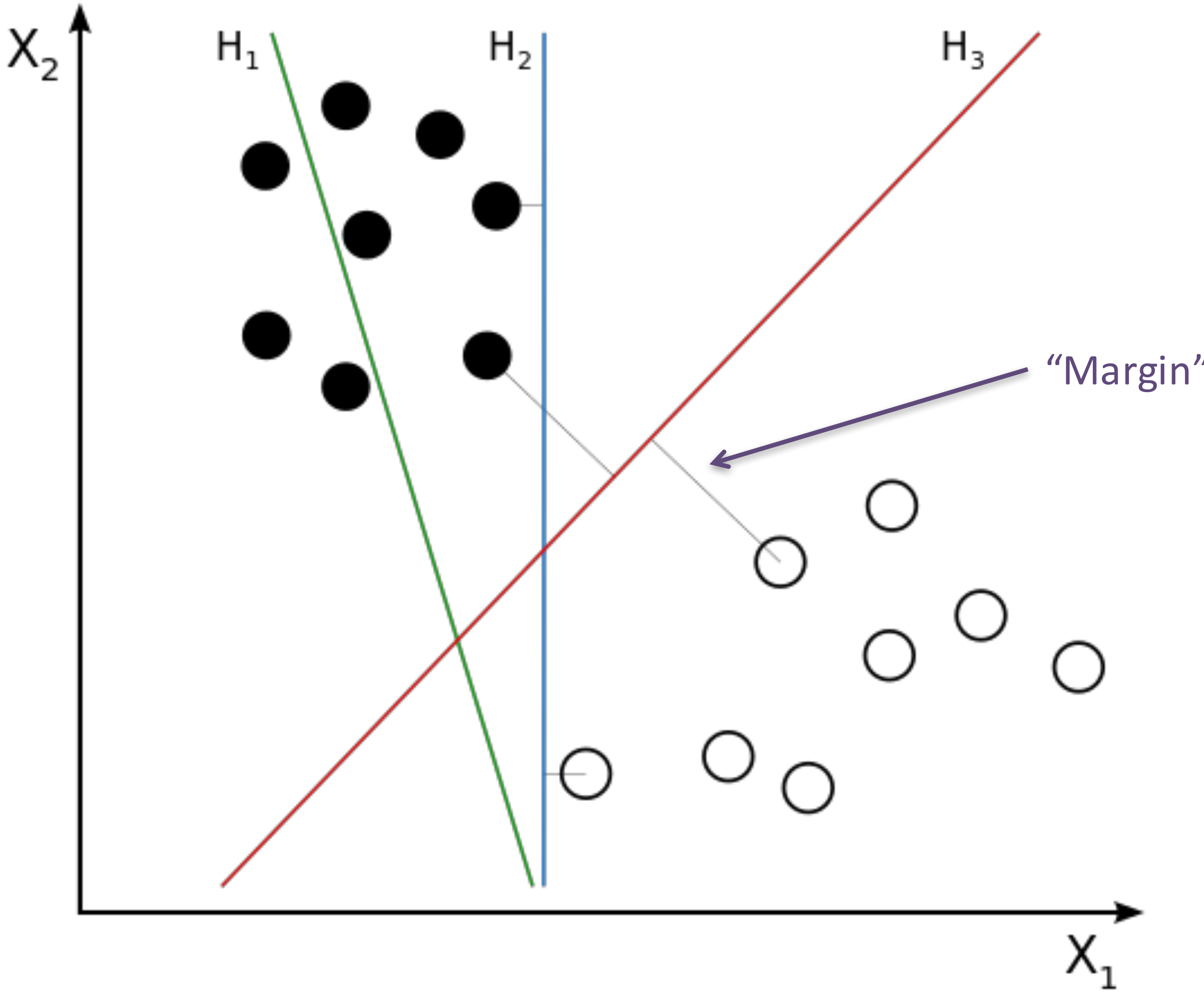
aka Max-Margin Classifiers

Which Line is the Best Classifier?



Source: http://en.wikipedia.org/wiki/Support_vector_machine

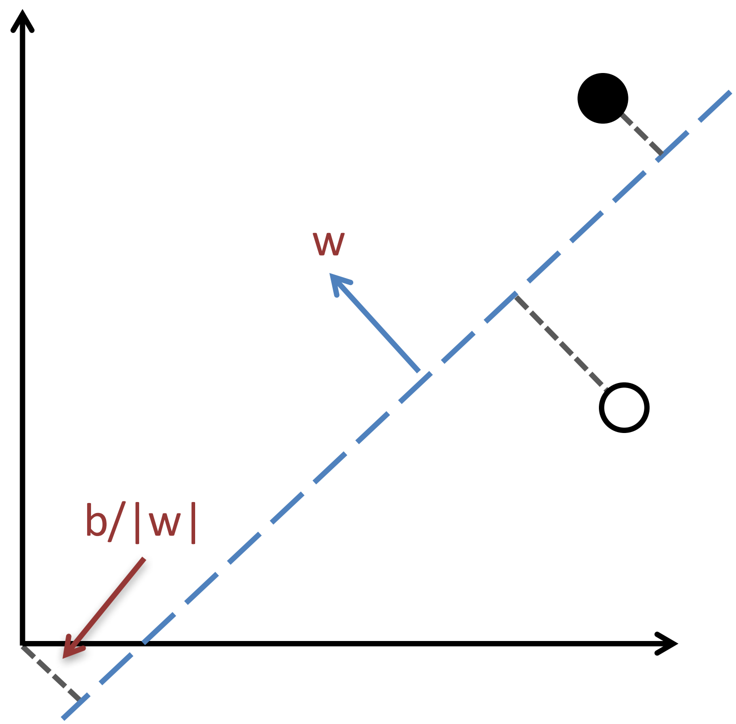
Which Line is the Best Classifier?



Source: http://en.wikipedia.org/wiki/Support_vector_machine

Recall: Hyperplane Distance

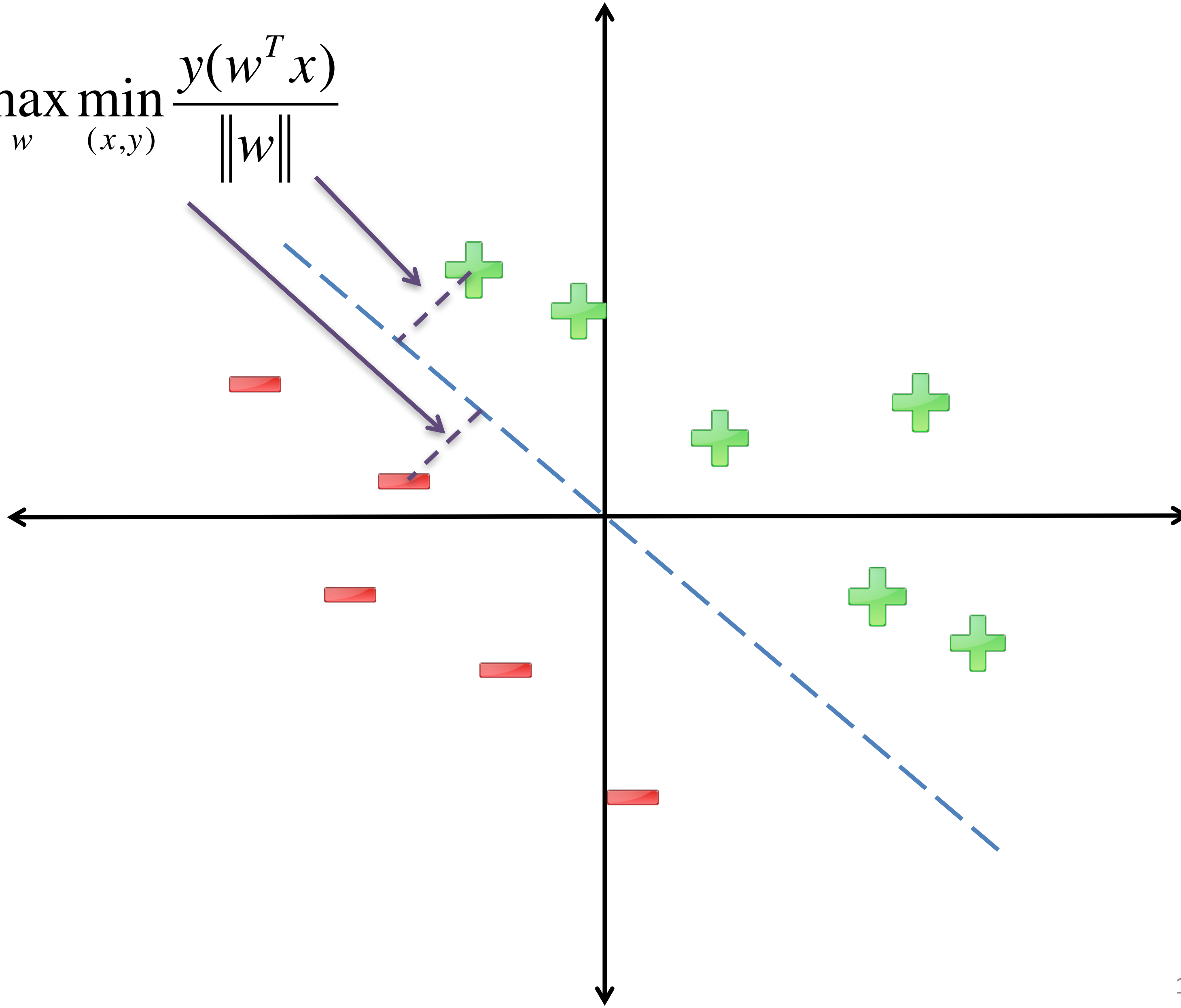
- Line is a 1D, Plane is 2D
- Hyperplane is many D
  - Includes Line and Plane
- Defined by (w,b)
- Distance: $$\frac{|w^T x - b|}{\|w\|}$$
- Signed Distance: $$\frac{w^T x - b}{\|w\|}$$



Linear Model = un-normalized signed distance!

Recall: Margin

$$\gamma = \max_{w} \min_{(x,y)} \frac{y(w^T x)}{\|w\|}$$

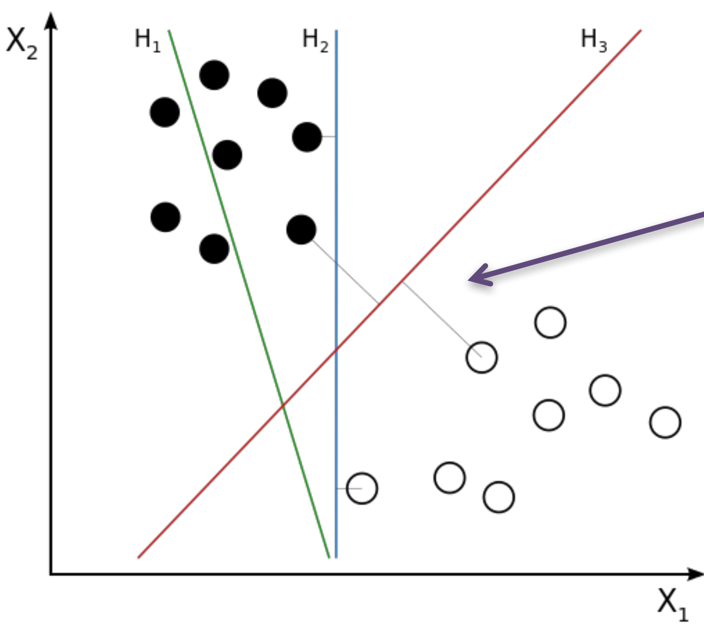


How to Maximize Margin?
(Assume Linearly Separable)

Choose w that maximizes:

$$\operatorname*{argmax}_{w,b}\left[\underbrace{\min_{(x,y)} \frac{y\left(w^T x - b\right)}{\|w\|}}\right]$$

Margin



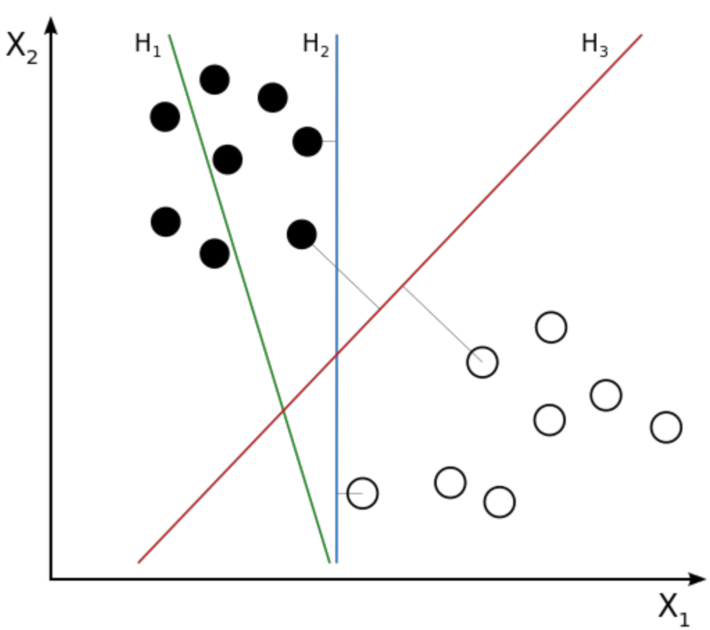
How to Maximize Margin?

(Assume Linearly Separable)

$$\underset{w,b}{\operatorname{argmax}}\left[\min_{(x,y)} \frac{y\left(w^T x - b\right)}{\|w\|}\right]$$

$$\equiv \underset{w,b:\ \|w\|=1}{\operatorname{argmax}}\left[\min_{(x,y)} y\left(w^T x - b\right)\right]$$

Hold Denominator Fixed



Suppose we instead enforce:

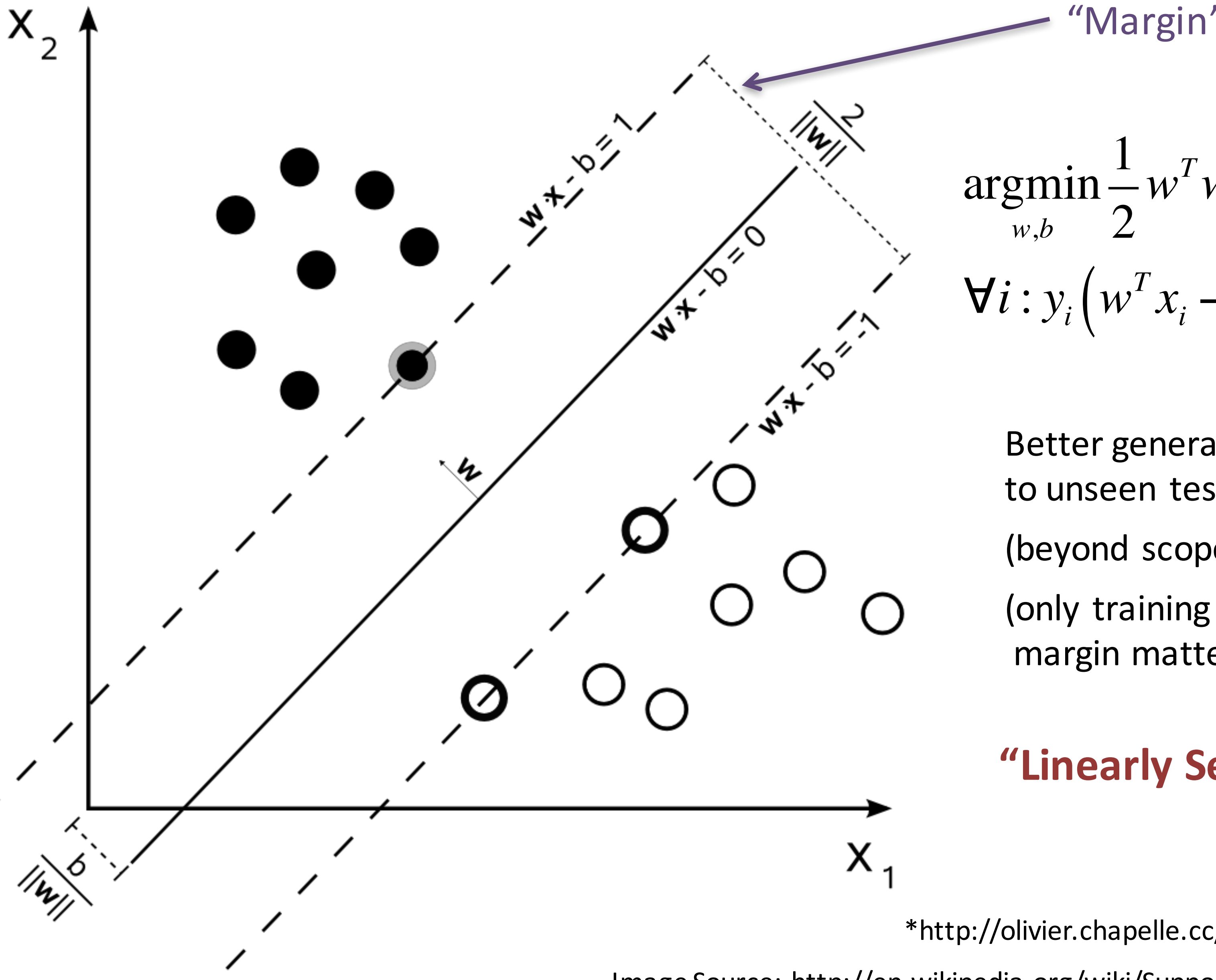
$$\min_{(x,y)} y\left(w^T x - b\right) = 1$$

Hold Numerator Fixed

Then:

$$= \underset{w,b}{\operatorname{argmin}} \|w\| \equiv \underset{w,b}{\operatorname{argmin}} \|w\|^2$$

Max Margin Classifier (Support Vector Machine)



$$\underset{w,b}{\operatorname{argmin}} \frac{1}{2} w^T w \equiv \frac{1}{2} \|w\|^2$$

$$\forall i : y_i \left(w^T x_i - b \right) \geq 1$$

Better generalization
to unseen test examples

(beyond scope of course*)

(only training data on
margin matter)

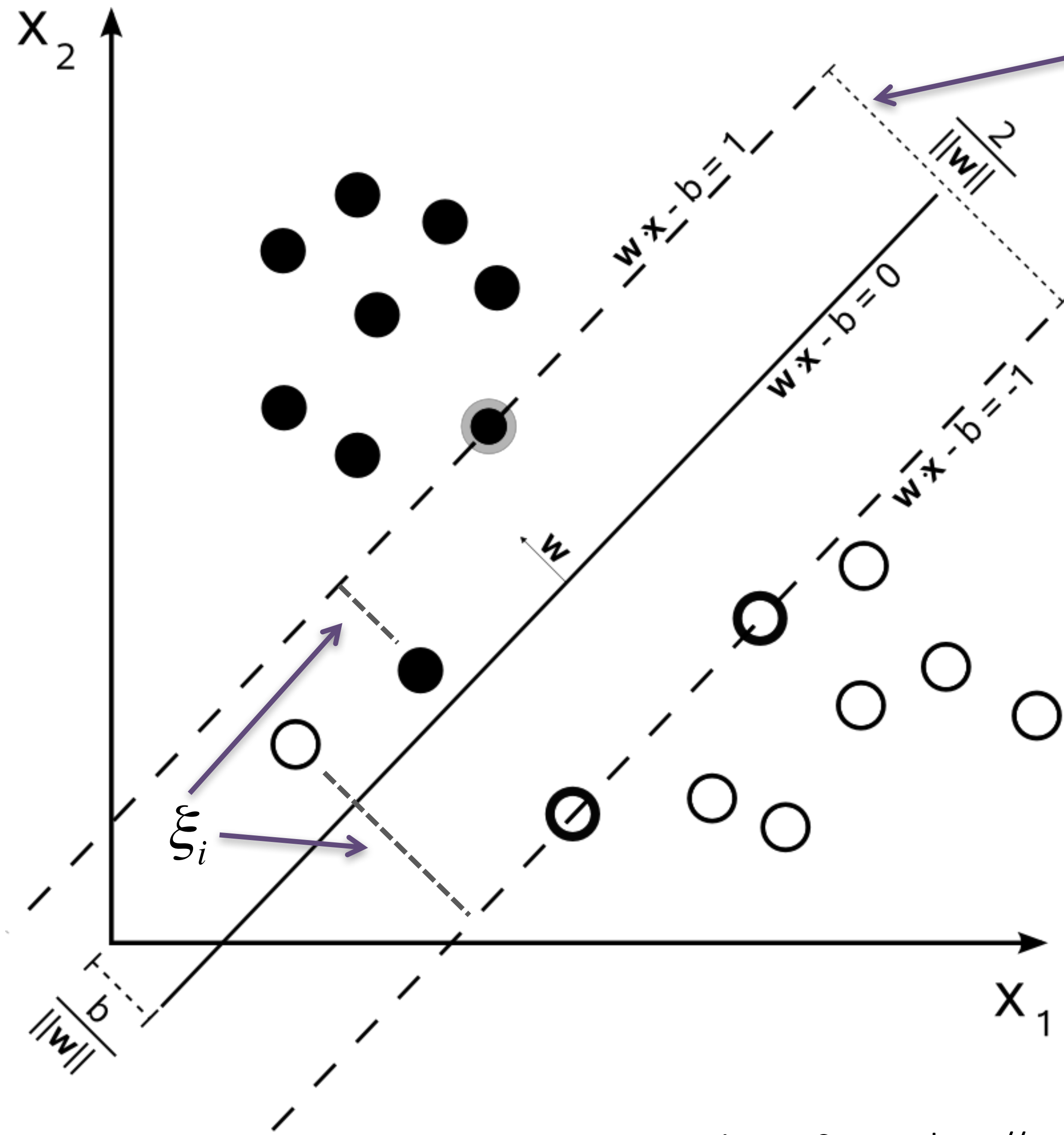
"Linearly Separable"

*http://olivier.chapelle.cc/pub/span_lmc.pdf

Image Source: http://en.wikipedia.org/wiki/Support_vector_machine

Soft-Margin Support Vector Machine

“Margin”



$$\underset{w,b,\xi}{\operatorname{argmin}} \frac{1}{2} w^T w + \frac{C}{N} \sum_i \xi_i$$

$$\forall i : y_i \left(w^T x_i - b \right) \geq 1 - \xi_i$$

$$\forall i : \xi_i \geq 0$$

“Slack”

Size of Margin

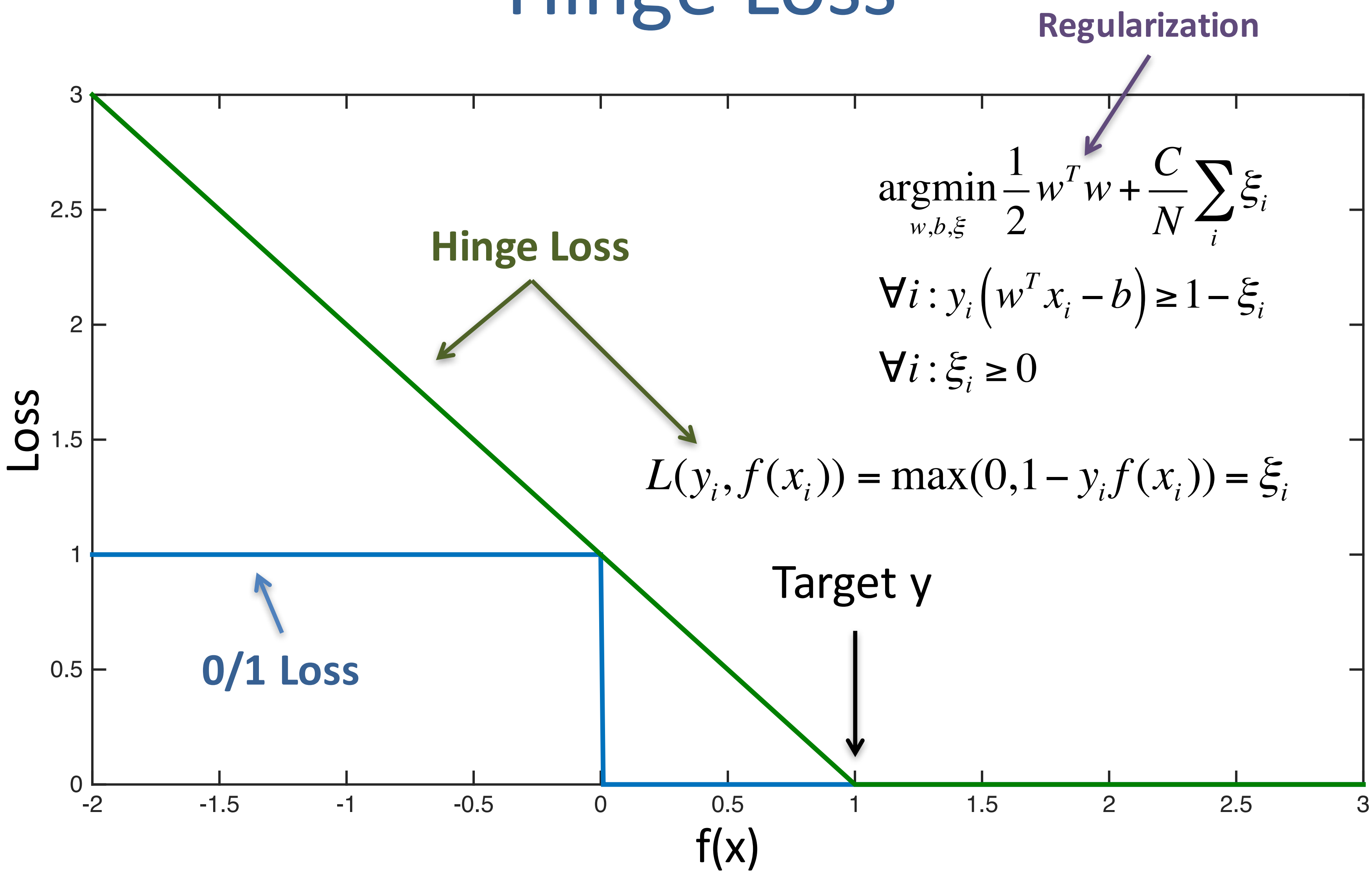
vs

Size of Margin Violations

(C controls trade-off)

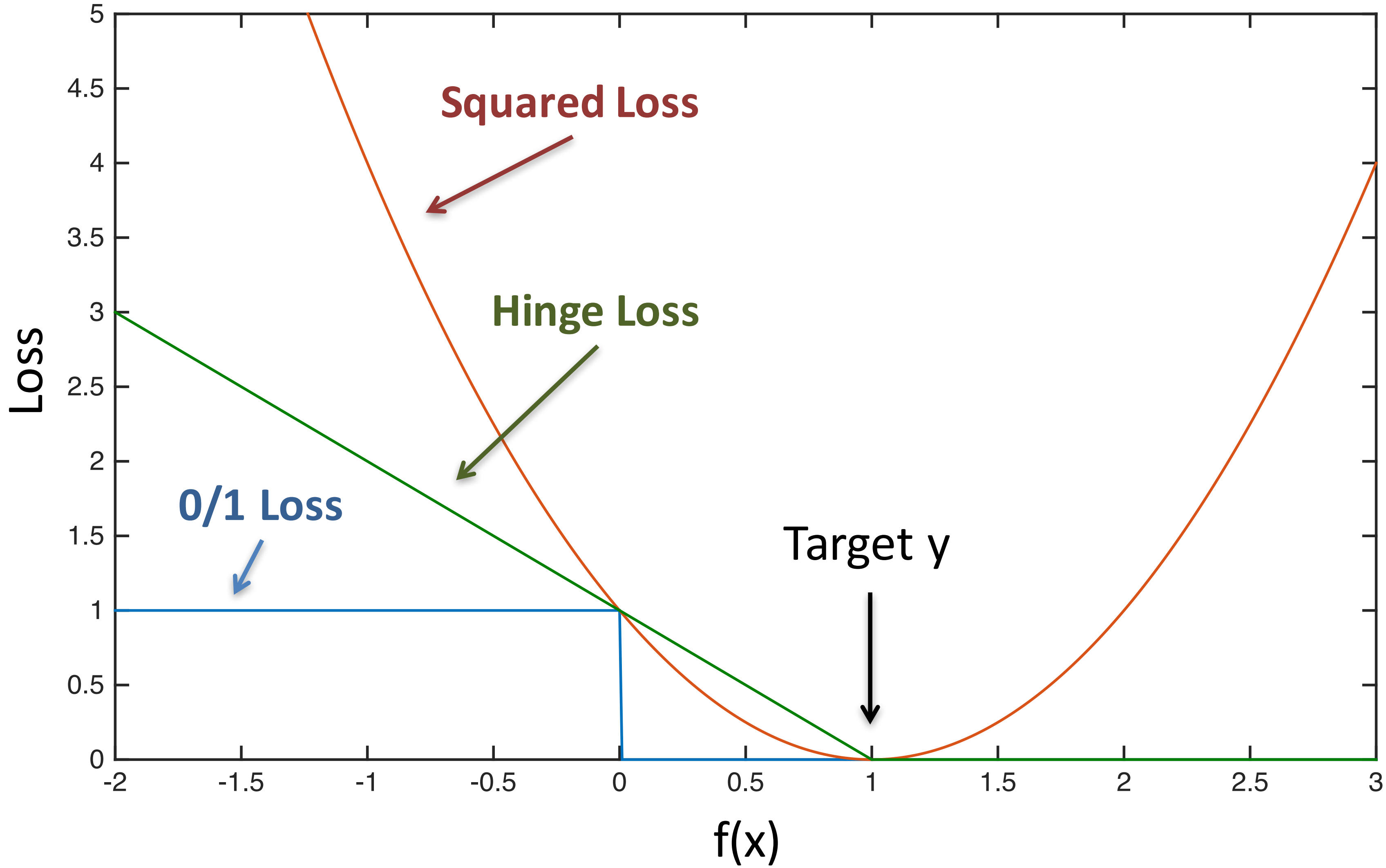
Image Source: http://en.wikipedia.org/wiki/Support_vector_machine

Hinge Loss



Regularization
$\underset{w,b,\xi}{\operatorname{argmin}} \frac{1}{2} w^T w + \frac{C}{N} \sum_i \xi_i$
$\forall i : y_i \left(w^T x_i - b \right) \geq 1 - \xi_i$
$\forall i : \xi_i \geq 0$
Hinge Loss
$L(y_i, f(x_i)) = \max(0, 1 - y_i f(x_i)) = \xi_i$
Target y
0/1 Loss
Loss
f(x)
3
2.5
2
1.5
1
0.5
0
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
2.5
3

Hinge Loss vs Squared Loss



Recall: Perceptron Learning Algorithm
(Linear Classification Model)

$$f(x \mid w) = sign(w^T x - b)$$

- $w^1 = 0$, $b^1 = 0$
- For t = 1 ….
  - Receive example (x,y)
  - If $f(x|w^t,b^t) = y$
    - $[w^{t+1}, b^{t+1}] = [w^t, b^t]$
  - Else
    - $w^{t+1} = w^t + yx$
    - $b^{t+1} = b^t - y$

Training Set:

$$S = \{(x_i, y_i)\}_{i=1}^N$$

$$y \in \{+1, -1\}$$

Go through training set in arbitrary order (e.g., randomly)

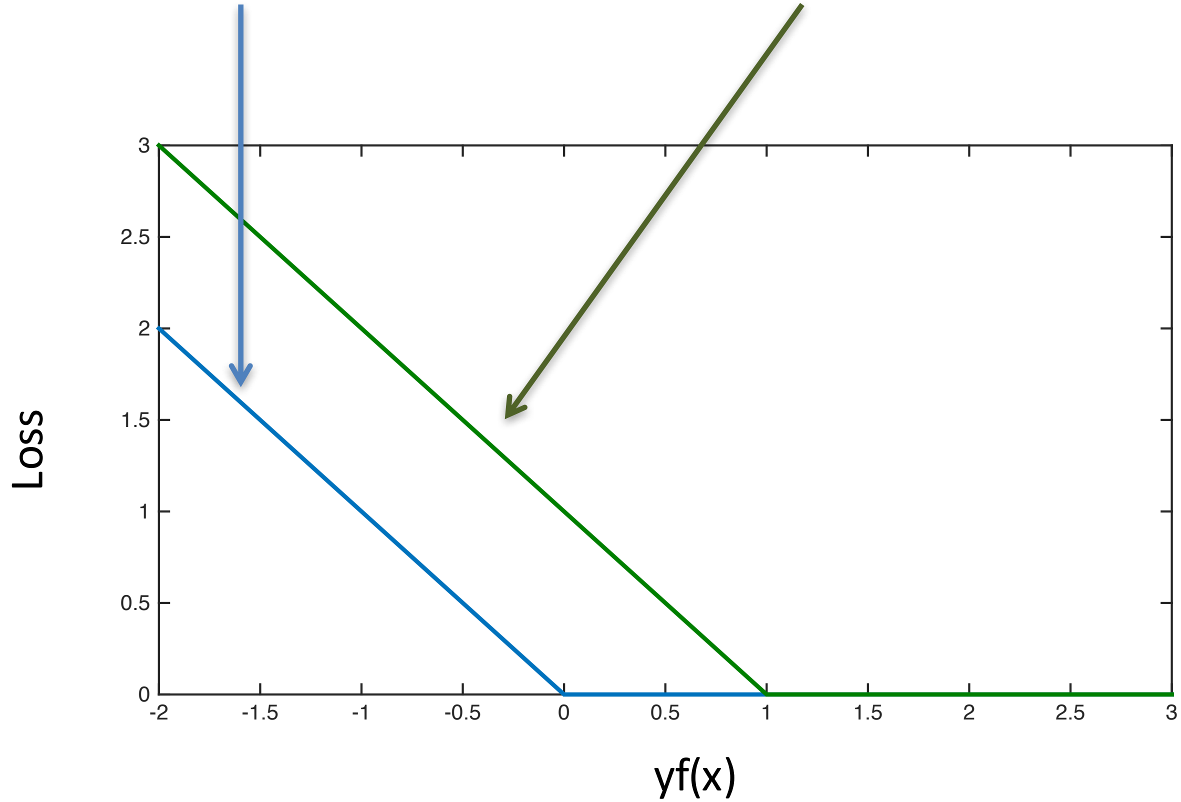
Comparison with Perceptron "Loss"

Perceptron

$$\max\left\{0, -y_i f(x_i \mid w, b)\right\}$$

SVM/Hinge

$$\max\left\{0, 1 - y_i f(x_i \mid w, b)\right\}$$



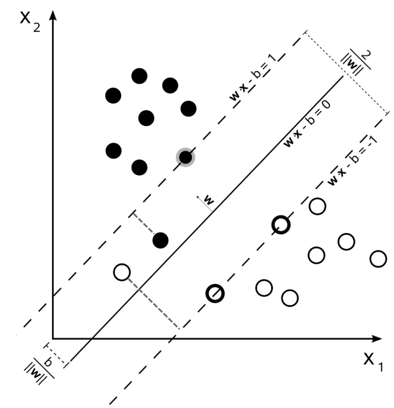
Support Vector Machine

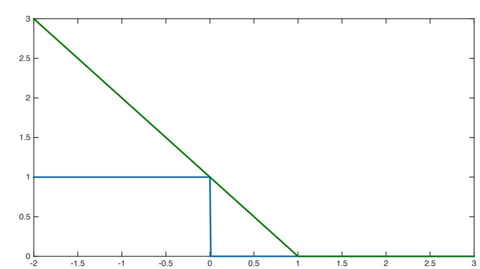
- 2 Interpretations
- Geometric
  - Margin vs Margin Violations
- Loss Minimization
  - Model complexity vs Hinge Loss
  - (Will discuss in depth next lecture)
- **Equivalent!**

$$\underset{w,b,\xi}{\operatorname{argmin}} \frac{1}{2} w^T w + \frac{C}{N} \sum_i \xi_i$$

$$\forall i : y_i \left(w^T x_i - b \right) \geq 1 - \xi_i$$

$$\forall i : \xi_i \geq 0$$





Comment on Optimization

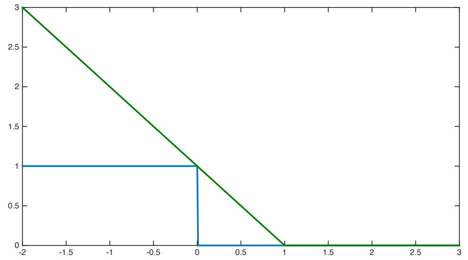
- Hinge Loss is not smooth
  - Not differentiable

$$\underset{w,b,\xi}{\operatorname{argmin}} \frac{1}{2} w^T w + \frac{C}{N} \sum_i \xi_i$$

$$\forall i : y_i \left(w^T x_i - b \right) \geq 1 - \xi_i$$

$$\forall i : \xi_i \geq 0$$

- How to optimize?



- **Stochastic (Sub-)Gradient Descent still works!**
  - Sub-gradients discussed next lecture

https://en.wikipedia.org/wiki/Subgradient_method

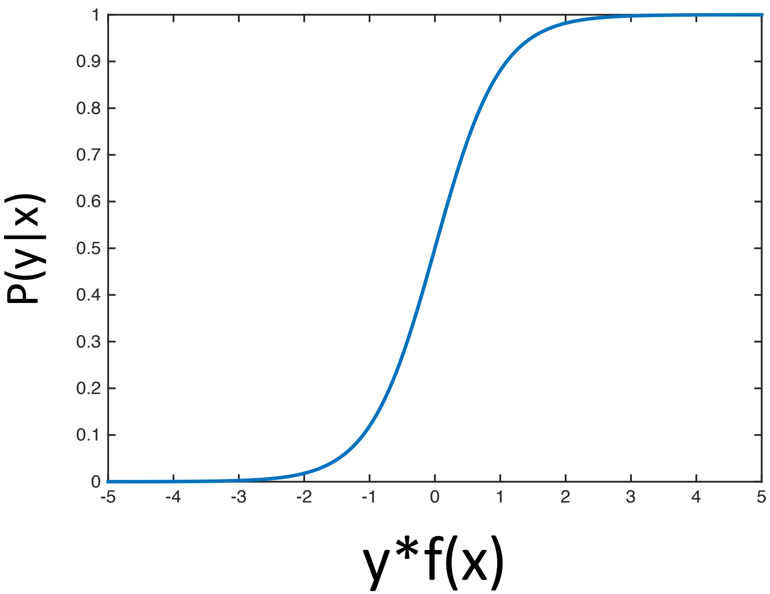
Logistic Regression

aka “Log-Linear” Models

Logistic Regression

$$P(y \mid x, w, b) = \frac{e^{\frac{1}{2}y\left(w^T x - b\right)}}{e^{\frac{1}{2}y\left(w^T x - b\right)} + e^{-\frac{1}{2}y\left(w^T x - b\right)}}$$

$$P(y \mid x, w, b) = \frac{1}{1 + e^{-y(w^T x - b)}}$$



"Log-Linear" Model

Also known as sigmoid function: $\sigma(a) = \frac{e^a}{1 + e^a}$

$y \in \{-1, +1\}$

Maximum Likelihood Training

- Training set: $$S = \{(x_i, y_i)\}_{i=1}^{N} \qquad \begin{array}{l} x \in R^D \\ y \in \{-1,+1\} \end{array}$$

- Maximum Likelihood: $$\underset{w,b}{\operatorname{argmax}} \prod_i P(y_i \mid x_i, w, b)$$
  - **(Why?)**

- Each (x,y) in S sampled independently!
  - Discussed further in Probably Recitation

Why Use Logistic Regression?

- SVMs often better at classification
  - Assuming margin exists…
- Calibrated Probabilities?
- Increase in SVM score….
  - …similar increase in P(y=+1|x)?
  - **Not well calibrated!**
- **Logistic Regression!**

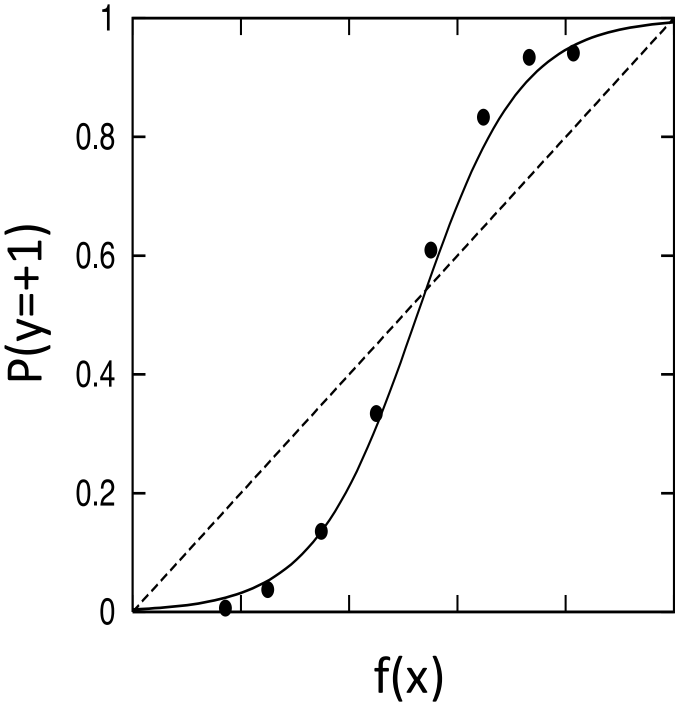


*Figure above is for Boosted Decision Trees (SVMs have similar effect)

Image Source: http://machinelearning.org/proceedings/icml2005/papers/079_GoodProbabilities_NiculescuMizilCaruana.pdf

Log Loss

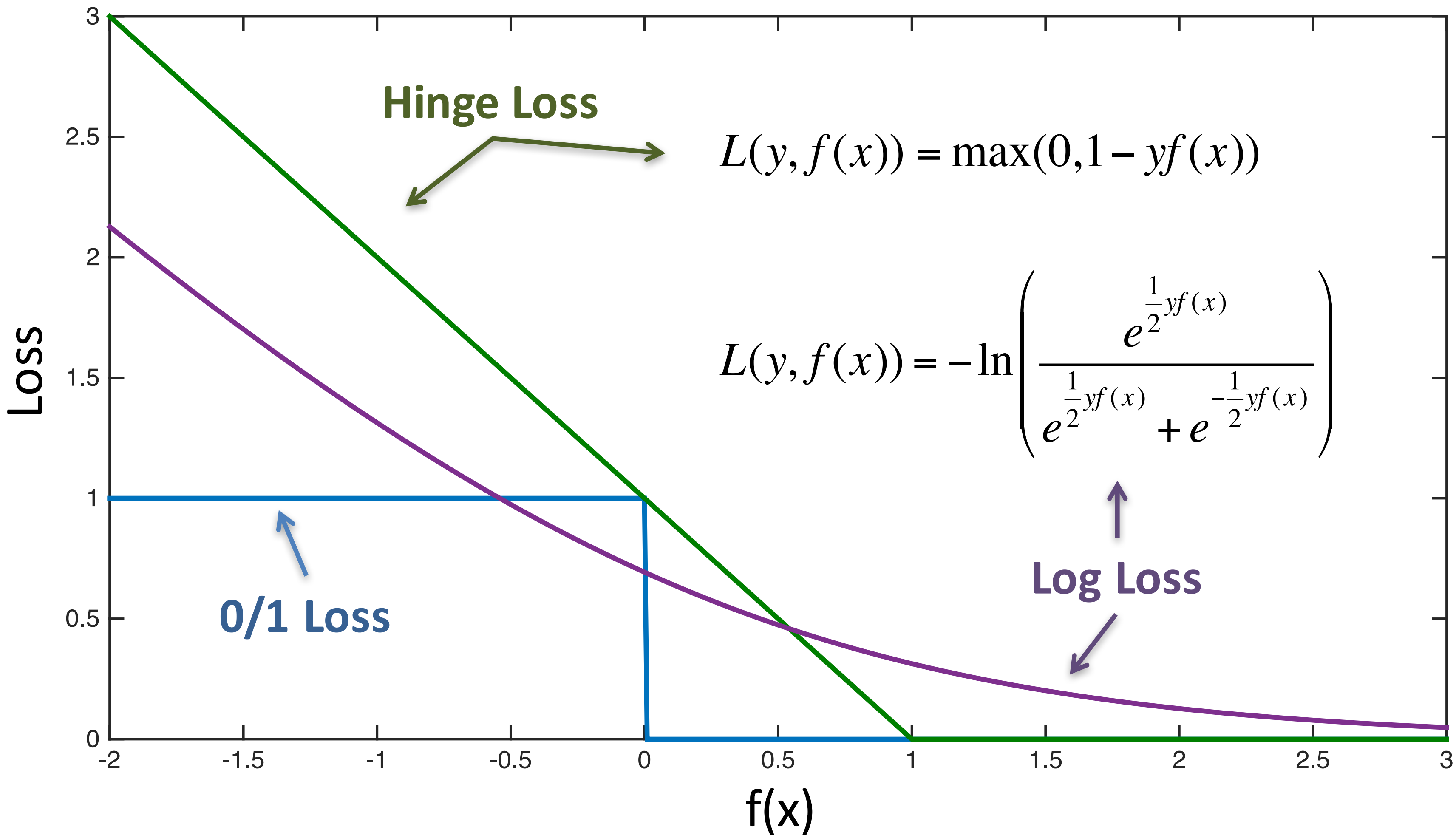
$$P(y \mid x, w, b) = \frac{e^{\frac{1}{2}y\left(w^T x - b\right)}}{e^{\frac{1}{2}y\left(w^T x - b\right)} + e^{-\frac{1}{2}y\left(w^T x - b\right)}} = \frac{e^{\frac{1}{2}yf(x|w,b)}}{e^{\frac{1}{2}yf(x|w,b)} + e^{-\frac{1}{2}yf(x|w,b)}}$$

$$\operatorname*{argmax}_{w,b} \prod_i P(y_i \mid x_i, w, b) = \operatorname*{argmin}_{w,b} \sum_i \underbrace{-\ln P(y_i \mid x_i, w, b)}_{\text{Log Loss}}$$

$$L(y, f(x)) = -\ln\left(\frac{e^{\frac{1}{2}yf(x)}}{e^{\frac{1}{2}yf(x)} + e^{-\frac{1}{2}yf(x)}} \right)$$

Solve using
(Stoch.) Gradient Descent

Log Loss vs Hinge Loss



Log-Loss Gradient

(For One Example)

$$\partial_w - \ln P(y_i \mid x_i) = -\partial_w \left(\frac{1}{2} y_i f(x_i \mid w,b) - \ln\left(e^{\frac{1}{2} y_i f(x_i \mid w,b)} + e^{-\frac{1}{2} y_i f(x_i \mid w,b)} \right) \right)$$

$$= -\frac{1}{2} y_i x_i + \partial_w \ln\left(e^{\frac{1}{2} y_i f(x_i \mid w,b)} + e^{-\frac{1}{2} y_i f(x_i \mid w,b)} \right)$$

$$= -\frac{1}{2} y_i x_i + \frac{1}{e^{\frac{1}{2} y_i f(x_i \mid w,b)} + e^{-\frac{1}{2} y_i f(x_i \mid w,b)}} \partial_w \left(e^{\frac{1}{2} y_i f(x_i \mid w,b)} + e^{-\frac{1}{2} y_i f(x_i \mid w,b)} \right)$$

$$= \left(-1 + \frac{1}{e^{\frac{1}{2} y_i f(x_i \mid w,b)} + e^{-\frac{1}{2} y_i f(x_i \mid w,b)}} \left(e^{\frac{1}{2} y_i f(x_i \mid w,b)} - e^{-\frac{1}{2} y_i f(x_i \mid w,b)} \right) \right) \frac{1}{2} y_i x_i$$

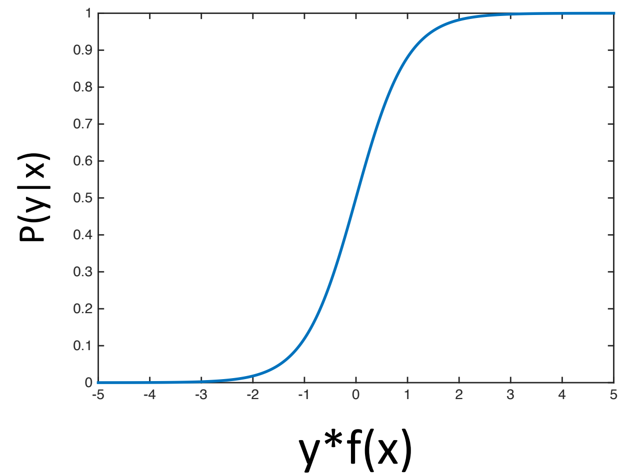
$$= \left(-1 + P(y_i \mid x_i) - P(-y_i \mid x_i) \right) \frac{1}{2} y_i x_i$$

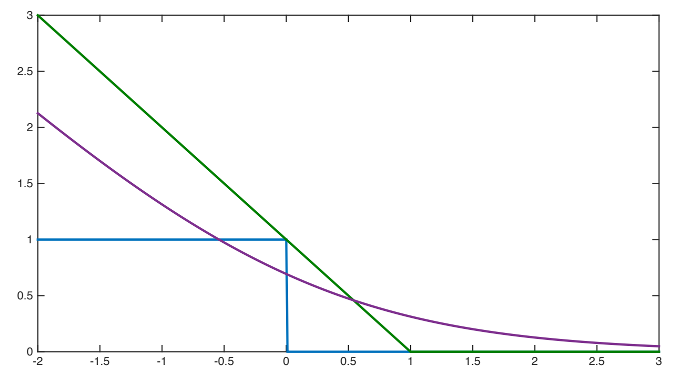
$$= -P(-y_i \mid x_i) y_i x_i = -\left(1 - P(y_i \mid x_i) \right) y_i x_i$$

$$P(y \mid x,w,b) = \frac{e^{\frac{1}{2} y f(x \mid w,b)}}{e^{\frac{1}{2} y f(x \mid w,b)} + e^{-\frac{1}{2} y f(x \mid w,b)}}$$

Logistic Regression

- Two Interpretations
- Maximizing Likelihood
- Minimizing Log Loss
- **Equivalent!**



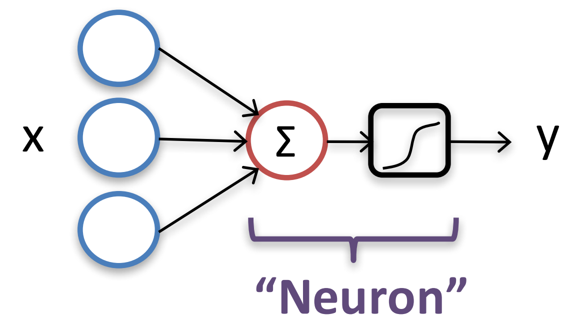


Feed-Forward Neural Networks

aka Not Quite Deep Learning

1 Layer Neural Network

- 1 Neuron
  - Takes input x
  - Outputs y

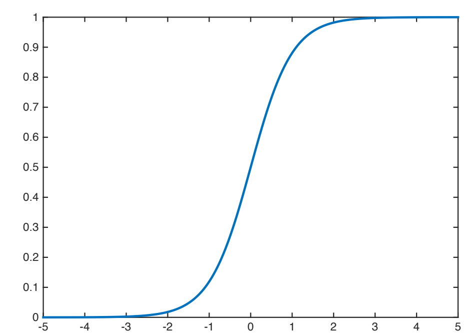


$f(x|w,b) = w^T x - b$

$= w_1 * x_1 + w_2 * x_2 + w_3 * x_3 - b$

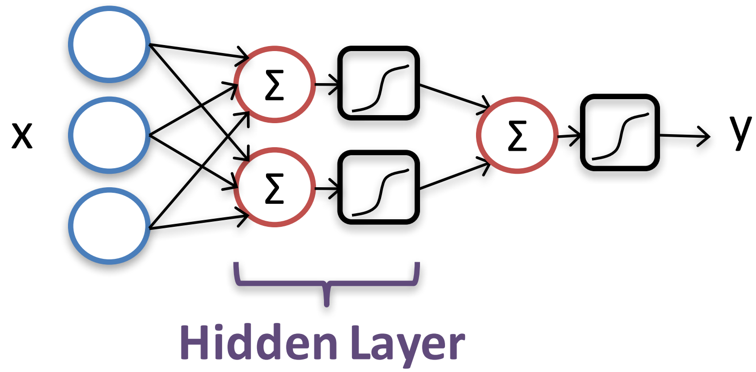
$\longrightarrow y = \sigma(f(x))$

- **~Logistic Regression!**
  - Solve via Gradient Descent



sigmoid
tanh
rectilinear

2 Layer Neural Network

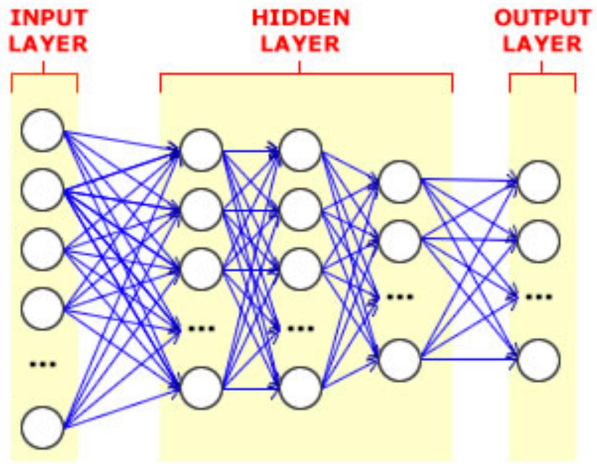


- 2 Layers of Neurons
  - 1st Layer takes input x
  - 2nd Layer takes output of 1st layer

Non-Linear!

- Can approximate arbitrary functions
  - Provided hidden layer is large enough
  - "fat" 2-Layer Network

Aside: Deep Neural Networks

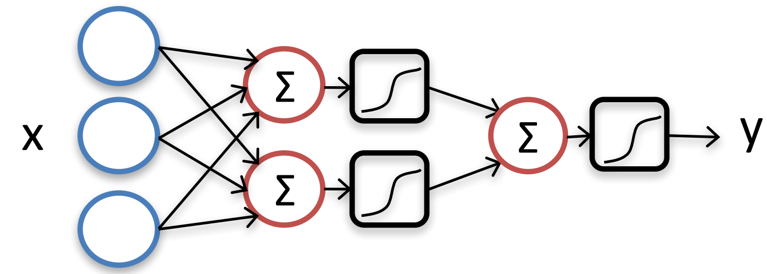


- Why prefer Deep over a “Fat” 2-Layer?
  – Compact model
    - (exponentially large “fat” model)
  – Easier to train?
  – Discussed further in deep learning lectures

Image Source: http://blog.peltarion.com/2014/06/22/deep-learning-and-deep-neural-networks-in-synapse/

Training Neural Networks

- Gradient Descent!
  - Even for Deep Networks*
- Parameters:
  - $(w_{11},b_{11},w_{12},b_{12},w_2,b_2)$



$f(x|w,b) = w^T x - b \qquad y = \sigma(\ f(x)\ )$

$$\partial_{w_2} \sum_{i=1}^{N} L(y_i,\sigma_2) = \sum_{i=1}^{N} \partial_{w_2} L(y_i,\sigma_2) = \sum_{i=1}^{N} \partial_{\sigma_2} L(y_i,\sigma_2)\partial_{w_2}\sigma_2 = \sum_{i=1}^{N} \partial_{\sigma_2} L(y_i,\sigma_2)\partial_{f_2}\sigma_2 \partial_{w_2} f_2$$

$$\partial_{w_{1m}} \sum_{i=1}^{N} L(y_i,\sigma_2) = \sum_{i=1}^{N} \partial_{\sigma_2} L(y_i,\sigma_2)\partial_{f_2}\sigma_2 \partial_{w_1} f_2 = \sum_{i=1}^{N} \partial_{\sigma_2} L(y_i,\sigma_2)\partial_{f_2}\sigma_2 \partial_{\sigma_{1m}} f_2 \partial_{f_{1m}} \sigma_{1m} \partial_{w_{1m}} f_{1m}$$

*more complicated

Backpropagation = Gradient Descent
(lots of chain rules)

Story So Far

- Different Loss Functions
  - Hinge Loss
  - Log Loss
  - Can be derived from different interpretations
- Non-Linear Model Classes
  - Neural Nets
  - Composable with different loss functions
- No closed-form solution for training
  - Must use some form of gradient descent

Today

- Beyond Basic Linear Models
  - Support Vector Machines
  - Logistic Regression
  - Feed-forward Neural Networks
  - Different ways to interpret models
- **Different Evaluation Metrics**

Evaluation

- 0/1 Loss (Classification)
- Squared Loss (Regression)
- Anything Else?

Example: Cancer Prediction

		Patient	
	Loss Function	Has Cancer	Doesn't Have Cancer
Model	Predicts Cancer	Low	Medium
	Predicts No Cancer	**OMG Panic!**	Low

- Value Positives & Negatives Differently
  - Care much more about positives
- "Cost Matrix"
  - 0/1 Loss is Special Case

Optimizing for Cost-Sensitive Loss

- There is no universally accepted way.

Simplest Approach (Cost Balancing):

$$\operatorname*{argmin}_{w,b}\left(1000\sum_{i:y_i=1} L\big(y_i, f(x_i \mid w,b)\big) + \sum_{i:y_i=-1} L\big(y_i, f(x_i \mid w,b)\big)\right)$$

Loss Function	Has Cancer	Doesn't Have Cancer
Predicts Cancer	0	1
Predicts No Cancer	1000	0

Precision & Recall

- **Precision** = TP/(TP + FP)
- **Recall** = TP/(TP + FN)

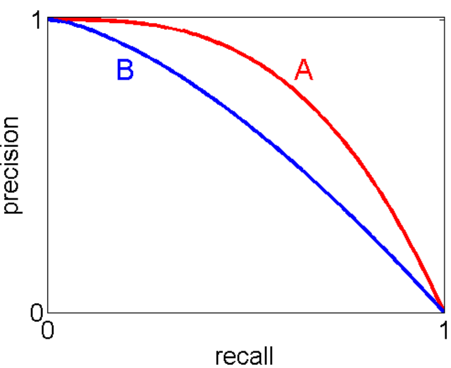
F1 = 2/(1/P+ 1/R)

Care More About Positives!

Patient

Model

Counts	Has Cancer	Doesn't Have Cancer
Predicts Cancer	20 (TP)	30 (FP)
Predicts No Cancer	5 (FN)	70 (TN)

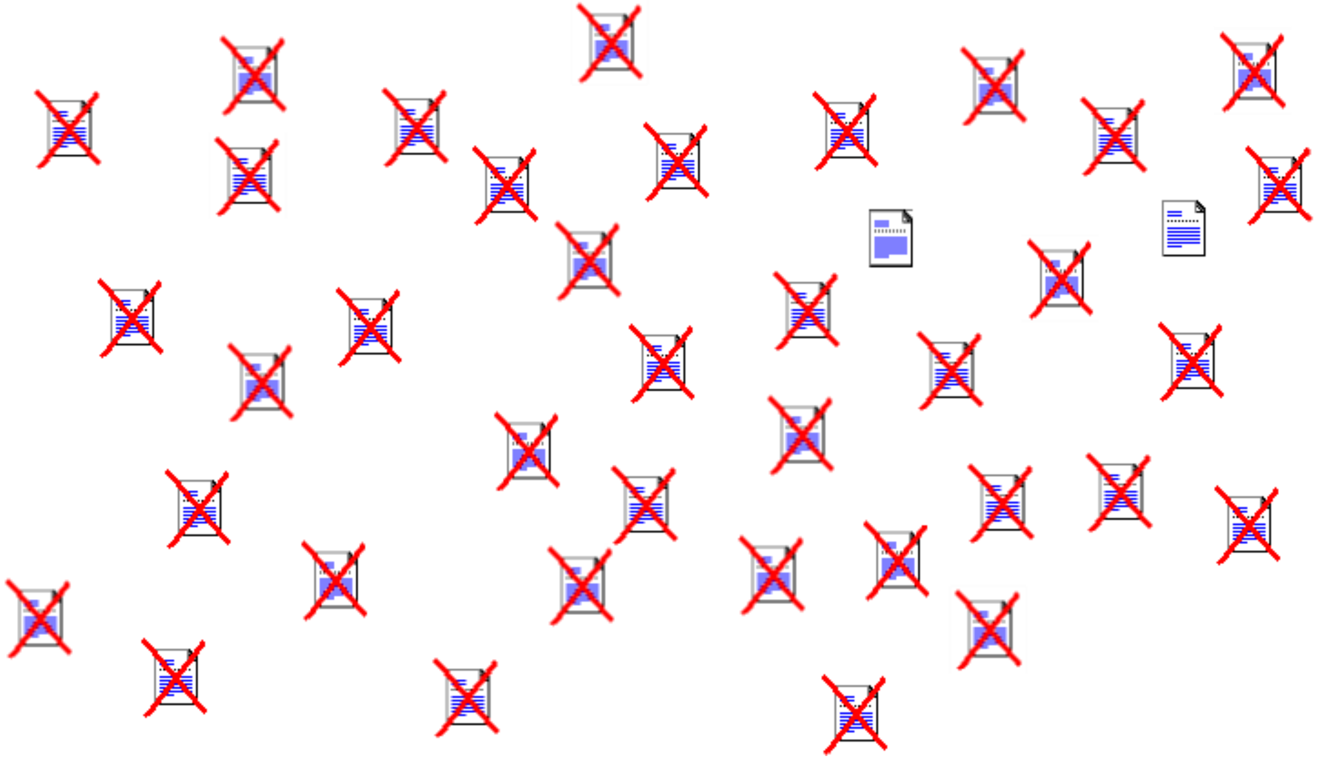


- TP = True Positive, TN = True Negative
- FP = False Positive, FN = False Negative

Image Source: http://pmtk3.googlecode.com/svn-history/r785/trunk/docs/demos/Decision_theory/PRhand.html

Example: Search Query

- Rank webpages by relevance

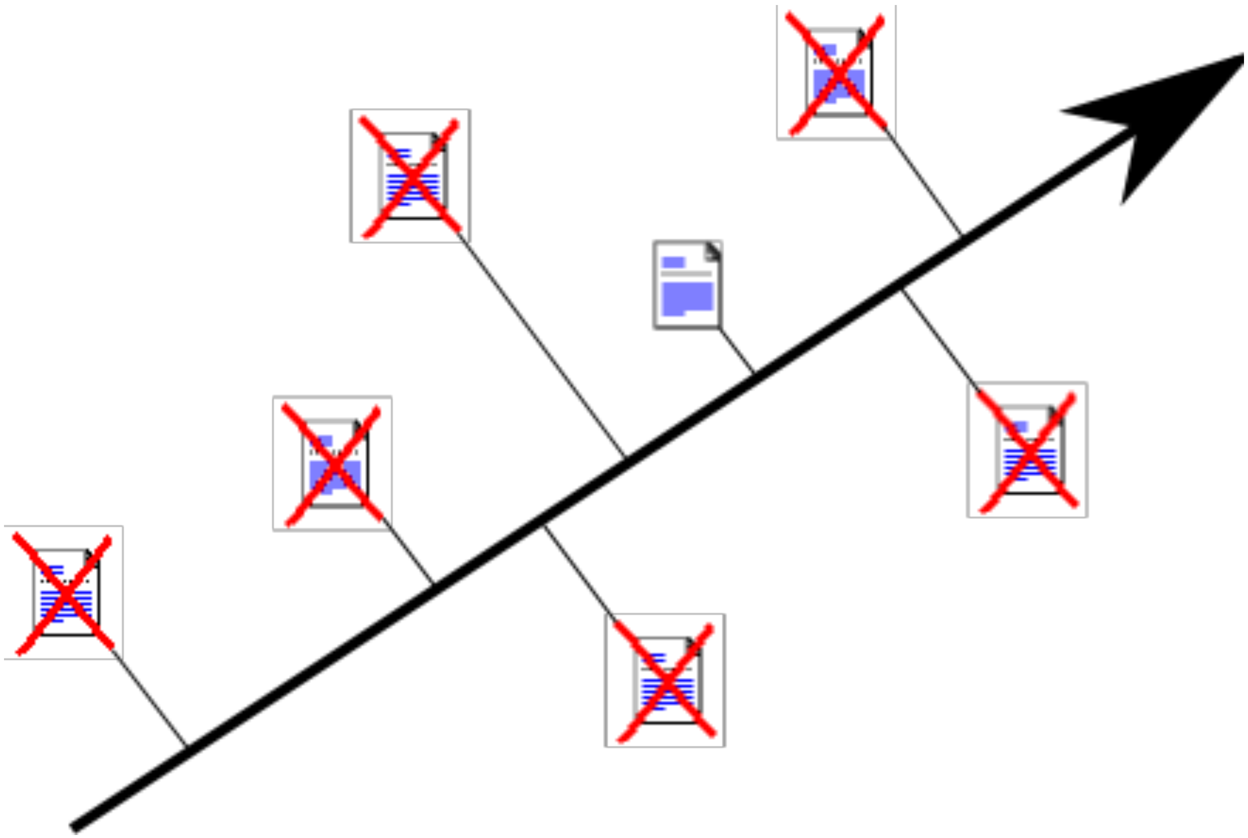


Ranking Measures

- Predict a Ranking (of webpages)
  - Users only look at top 4
  - Sort by f(x|w,b)
- Precision @4 =1/2
  - Fraction of top 4 relevant
- Recall @4 =2/3
  - Fraction of relevant in top 4
- Top of Ranking Only!

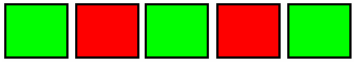
Image Source: http://pmtk3.googlecode.com/svn-history/r785/trunk/docs/demos/Decision_theory/PRhand.html

Pairwise Preferences



2 Pairwise Disagreements
4 Pairwise Agreements

ROC-Area

- ROC-Area
  - Area under ROC Curve
  - Fraction pairwise agreements
- Example: 

ROC-Area: 0.5
#Pairwise Preferences = 6
#Agreements = 3

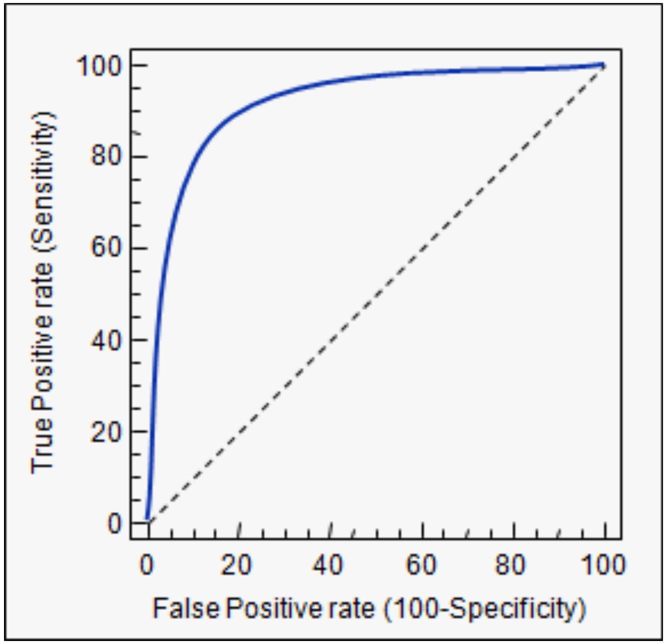
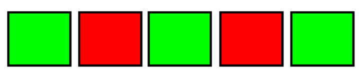


Image Source: http://www.medcalc.org/manual/roc-curves.php

Average Precision

- Average Precision
  - Area under P-R Curve
  - P@K for each positive

- Example: 

AP: $$\frac{1}{3}\cdot\left(\frac{1}{1}+\frac{2}{3}+\frac{3}{5}\right)\approx 0.76$$

Precision at Rank Location of Each Positive Example

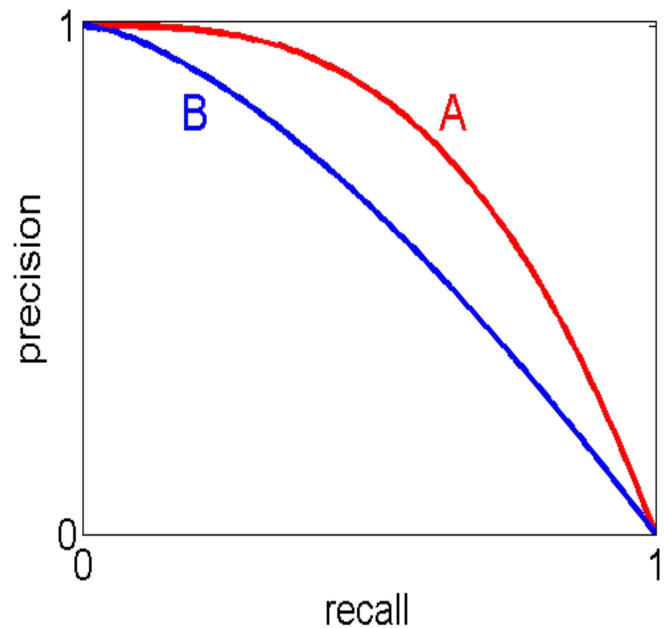
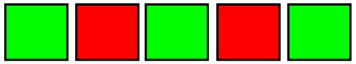


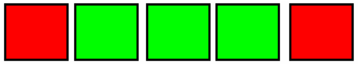
Image Source: http://pmtk3.googlecode.com/svn-history/r785/trunk/docs/demos/Decision_theory/PRhand.html

ROC-Area versus Average Precision

- ROC-Area Cares about every pairwise preference equally
- Average Precision cares more about top of ranking



ROC-Area: 0.5 Average Precision: 0.76



ROC-Area: 0.5 Average Precision: 0.64

Other Challenges

- "Correct" if overlap is large enough
- How to define large enough?
- Duplicate detections?
- What is learning objective?

- Similar challenges in videos:
  - E.g., temporal bounding box around "running" activity
  - Duplicate predictions: break into two separate running activities
- Other examples: heart-rate monitoring

http://slazebni.cs.illinois.edu/publications/iccv15_active.pdf

Summary: Evaluation Measures

- Different Evaluations Measures
  - Different Scenarios
- Large focus on getting positives
  - Large cost of mis-predicting cancer
  - Relevant webpages are rare
    - Aka “Class Imbalance”
- Other challenges:
  - localization in continuous domain

Next Lecture

- Regularization

- Lasso

- **Thursday:**
  - **Recitation on Matrix Linear Algebra (& Calculus)**