Welcome to CME 250 Introduction to Machine Learning!

Spring 2020 – Online version

April 28th 2020

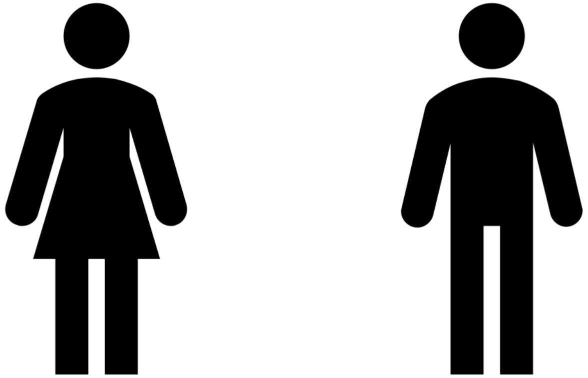
Stanford | Institute for Computational & Mathematical Engineering

Today's schedule: Classification

- Why does the distinction between regression and classification matters?
- Classification looking at Y as a random variable:
  - Logistic regression as a Generalized linear model
- Classification finding boundaries:
  - Support Vector Machines
- How to measure classification success?
  - Confusion Matrix

Let's get to know each other…

Breakout room



You

Another student

Name

Location

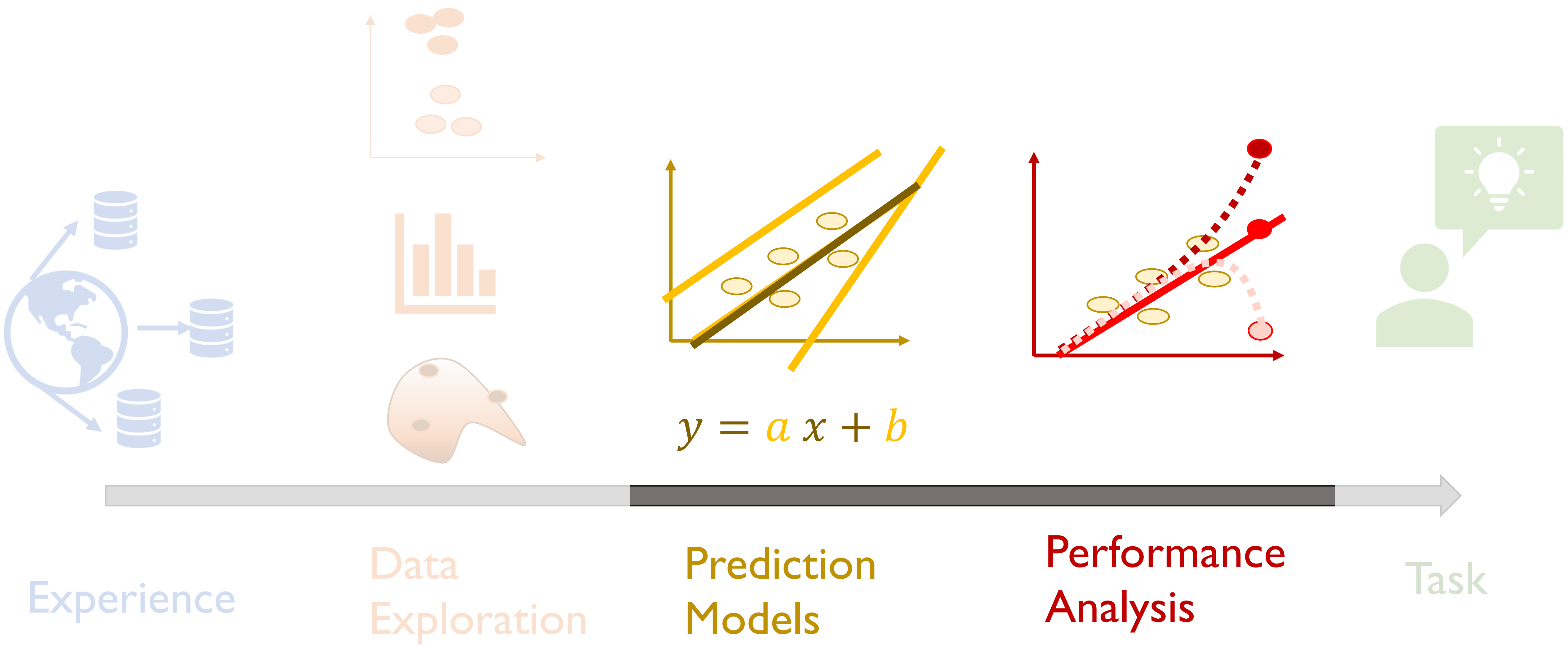
Department

Year

How was Part I Project? Interesting/unexpected/ unforgettable lessons or insights.

3 mins

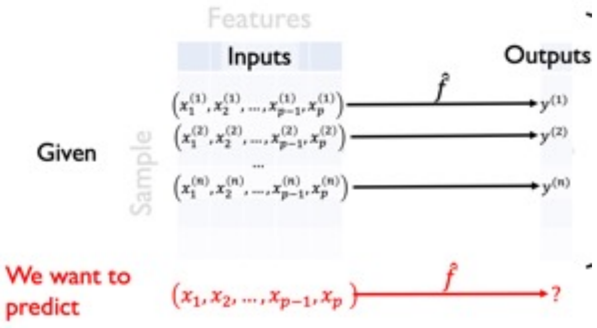
Chat/Audio/Video


$y = a\,x + b$
Experience
Data Exploration
Prediction Models
Performance Analysis
Task

Last week recap

Supervised Learning

Learn from examples



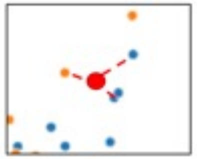
Regression

Y is quantitative

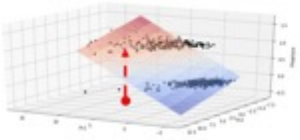
Classification

Y is categorical

KNN

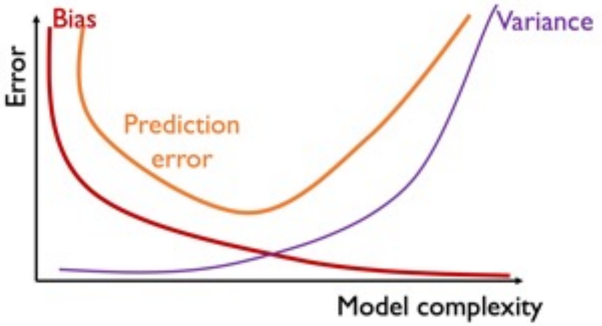


Linear Regression



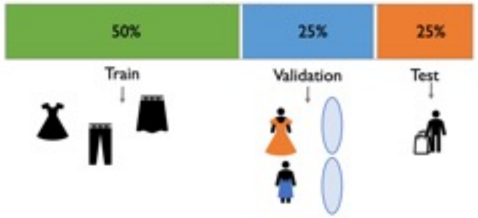
Using dummy variables?

Model Selection



Cross-Validation

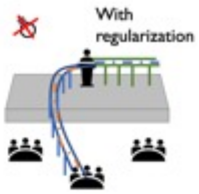
Estimate prediction error



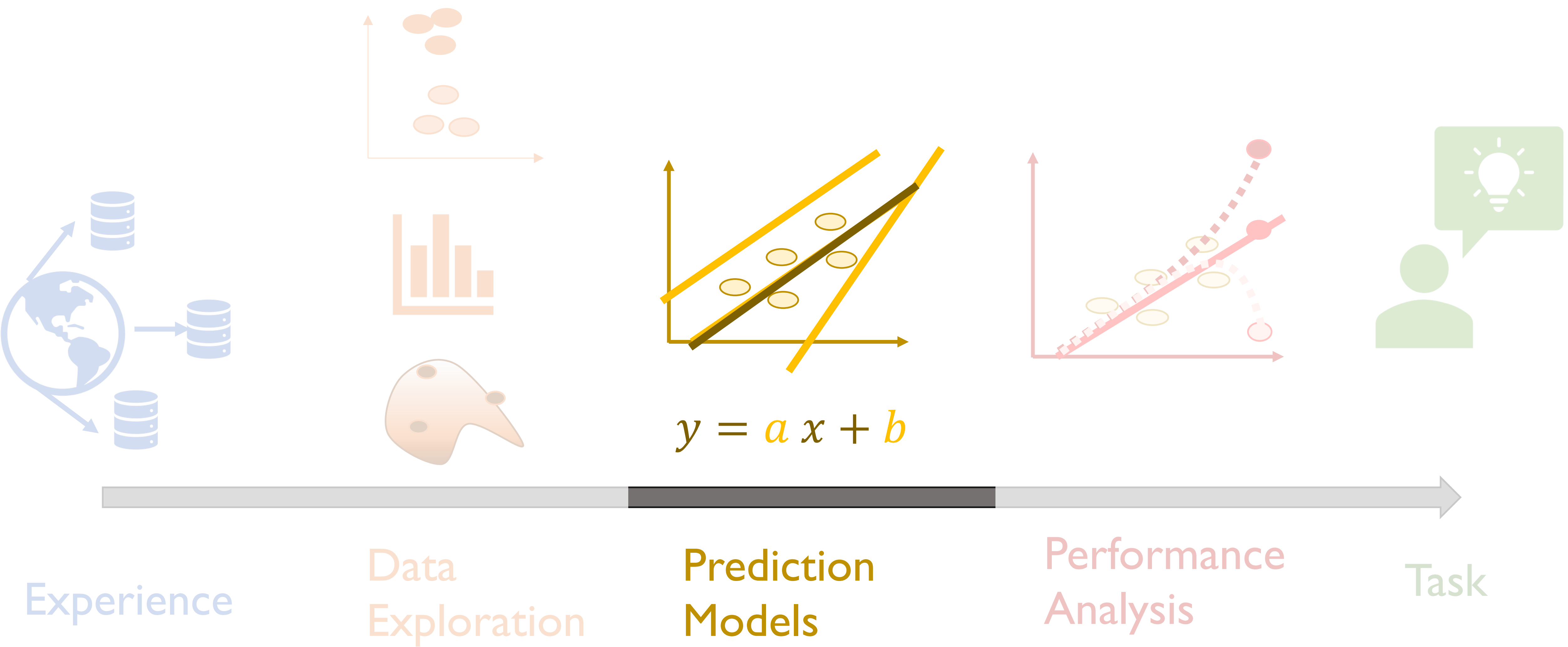
K-fold CV, LOOCV

Regularization

Control complexity: Hyperparameters



Ridge, Lasso


$y = a\,x + b$
Experience
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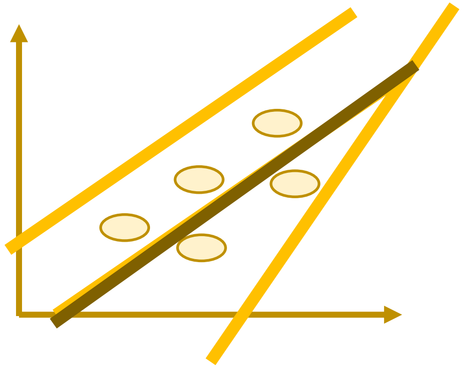


$$y = a\,x + b$$

Prediction Models

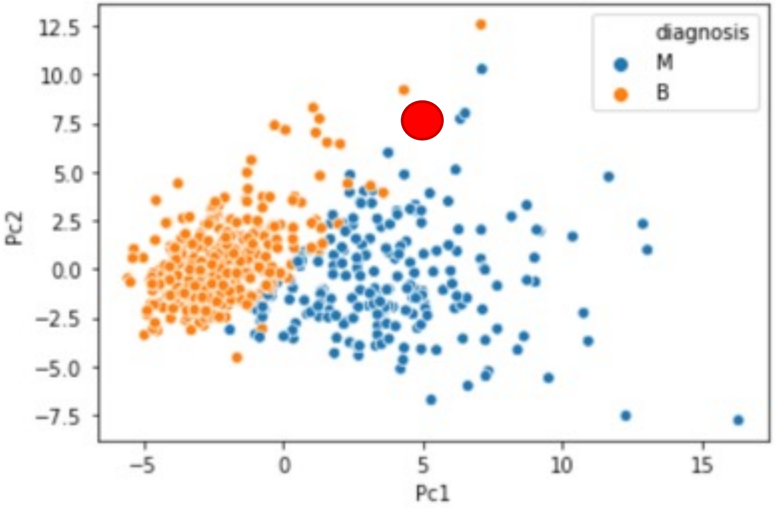
Supervised Learning Part II: Prediction Models for Classification

Introduction to Statistical Learning
Chapter 4: Classification
Chapter 9: Support Vector Machines

Elements Statistical Learning
Chapter 3.2: Linear Methods for Classification
Chapter 12: Support Vector Machines

More on Generalized Linear Models
Bayesian and Frequentist Regression Methods.
Jon Wakefield, 2013
Chapter 6.3: Generalized Linear Models

Breast Cancer Wisconsin (Diagnostic) Dataset



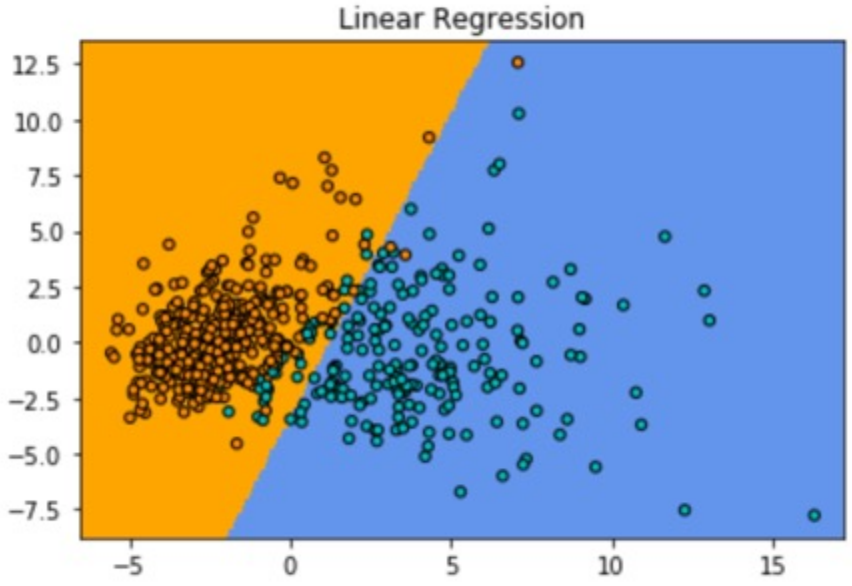
What is the diagnosis for this sample?

Use dummy variable for Y

M → 1

- - - - - - 0.5

B → 0



$Y \approx f(x) = \beta_0 + \beta_1 X_{PC1} + \beta_2 X_{PC2}$

What if we have more than 2 categories?

Linear regression with more than 2 categories

Option 1)

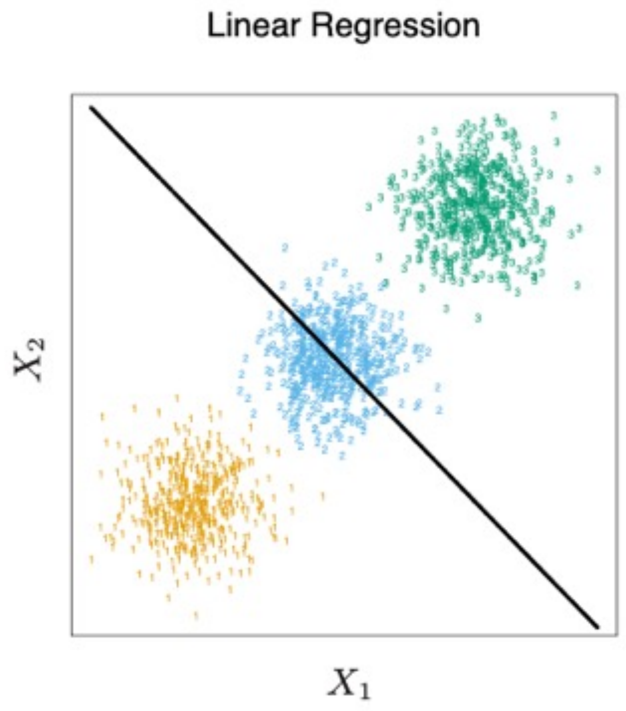
	Y
Cat. 1	0
	- - - - - 0.5
Cat.2	1
	- - - - - 1.5
Cat. 3	2

✗ Imposes order in categories

Option 2)

	Y_1	Y_2	Y_3
Cat. 1	1	0	0
Cat.2	0	1	0
Cat. 3	0	0	1

✗ Ignores category 2

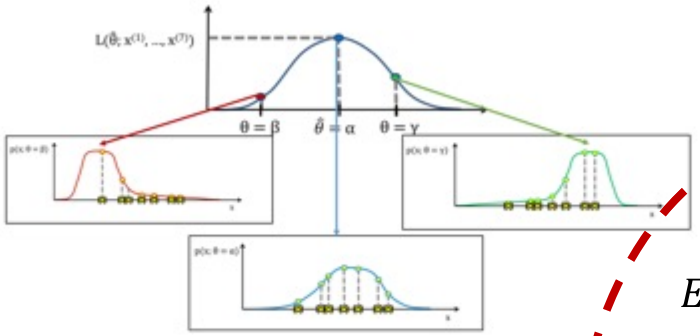


ESL Fig 4.2

We need a different approach!

How can we extend Linear Regression?

LR is Maximum Likelihood estimator



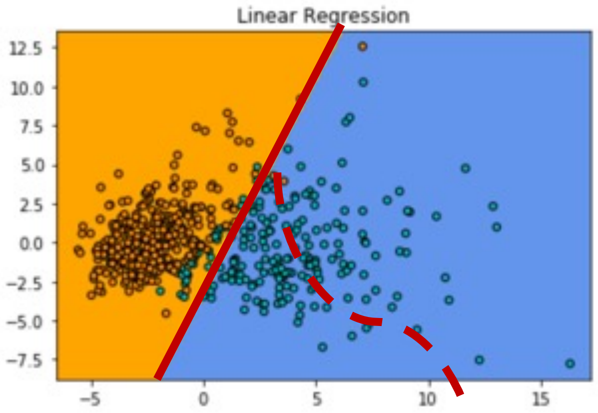
$$\boxed{Y \sim Normal}$$

$$E[Y|X] = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$$

Find a better distribution for Y
categorical

Logistic Regression

LR creates separating hyperplanes



Y

M $\longrightarrow$ 1

- - - - - - 0.5

B $\longrightarrow$ 0

Optimize the hyperplane

Support Vector Machines

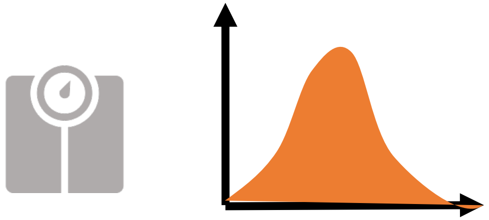
Extend LR: Generalized Linear Models

Exponential Family

$$\boxed{p(y|\,\theta,\alpha) = \exp\left(\frac{y\theta - b(\theta)}{\alpha} + c(y,\alpha)\right)}$$

Normal distribution

$N(\mu,\sigma^2)$



$$\boxed{p(y|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(\frac{(y-\mu)^2}{2\sigma^2}\right)}$$

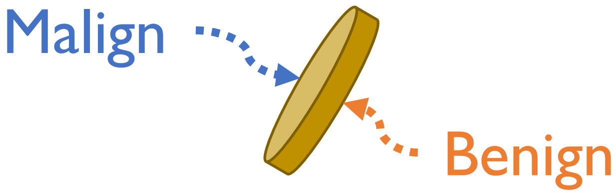
Poisson distribution

$Poisson(\lambda)$

$$\boxed{p(y|\lambda\,) = \frac{\lambda^y \exp(-\lambda)}{y!}}$$

Bernoulli distribution

$Bernoulli(p)$



$$\boxed{p(y|\lambda\,) = p^y(1-p)^{1-y}}$$

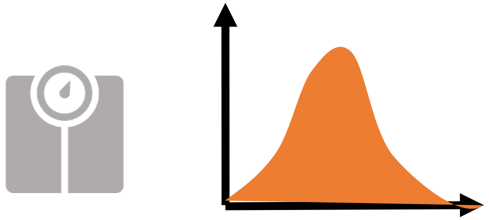
Extend LR: Generalized Linear Models

Exponential Family

$\boxed{E(y|\ \theta, \alpha) = b'(\theta)}$

Normal distribution

$N(\mu, \sigma^2)$



$b(\theta) = \theta^2/2$

$\mu = E[Y|\theta, \alpha] = \theta$

Poisson distribution

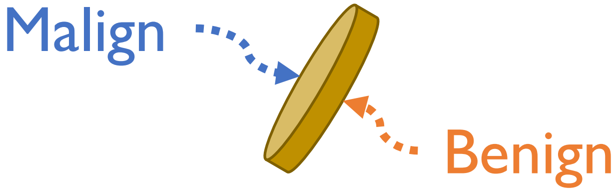
$Poisson(\lambda)$

$b(\theta) = \exp(\theta)$

$\lambda = E[Y|\theta, \alpha] = \exp(\theta)$

Bernoulli distribution

$Bernoulli(p)$



$b(\theta) = \log(1 + \exp(\theta))$

$p = E[Y|\theta, \alpha] = \dfrac{\exp(\theta)}{1 + \exp(\theta)}$

Calculate a linear regression of $\theta = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$

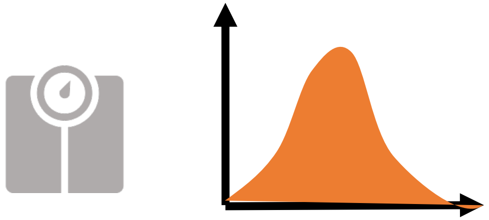
Extend LR: Generalized Linear Models

Exponential Family

$\boxed{E(y|\,\theta,\alpha) = b'(\theta)}$

Normal distribution

$N(\mu,\sigma^2)$



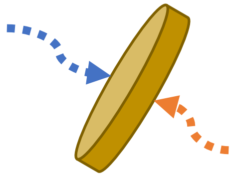
Poisson distribution

$Poisson(\lambda)$

Bernoulli distribution

$Bernoulli(p)$

Malign



Benign

Linear Regression

$y \approx \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$

Log-Linear Regression

$\log(y) \approx \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$

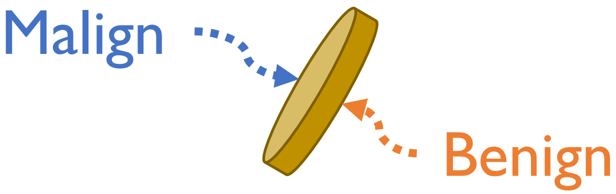
Logistic Regression

$\log\left(\frac{p}{1-p}\right) \approx \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$

Logistic Regression

Bernoulli distribution

$Bernoulli(p)$

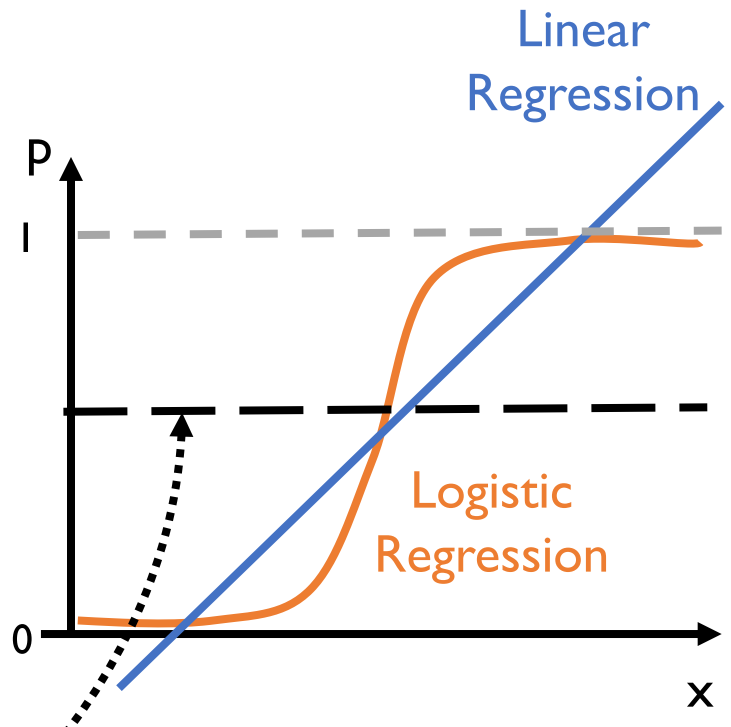


Log-odds / Logit

$$\boxed{\log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p}$$

$$\boxed{p = \frac{\exp(\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p\ )}{1 + \exp(\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p\ )}}$$

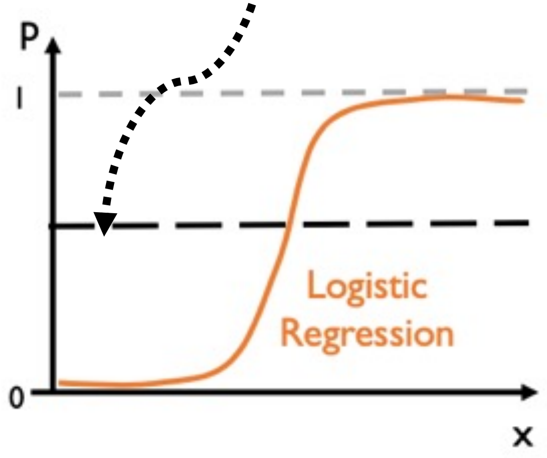
Sigmoid



To classify, we specify probability threshold

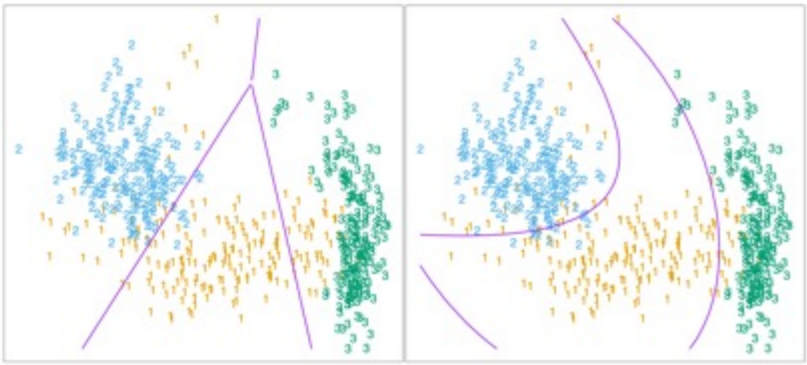
Challenges of Logistic Regression

Probability Threshold



Hyperparameter
Usually 0.5 (not always)

Linear Decision Boundary



ESL Fig 4.1

As in Linear regression:
Add additional features
$X_1, X_2, X_1X_2, X_1^2, X_2^2$

Multiple Categories

$$p_1 = \frac{\exp(\beta_{01} + \beta_1^T X)}{1 + \sum_{l=1}^{K-1} \exp\left(\beta_{0l} + \beta_l^T X\right)}$$

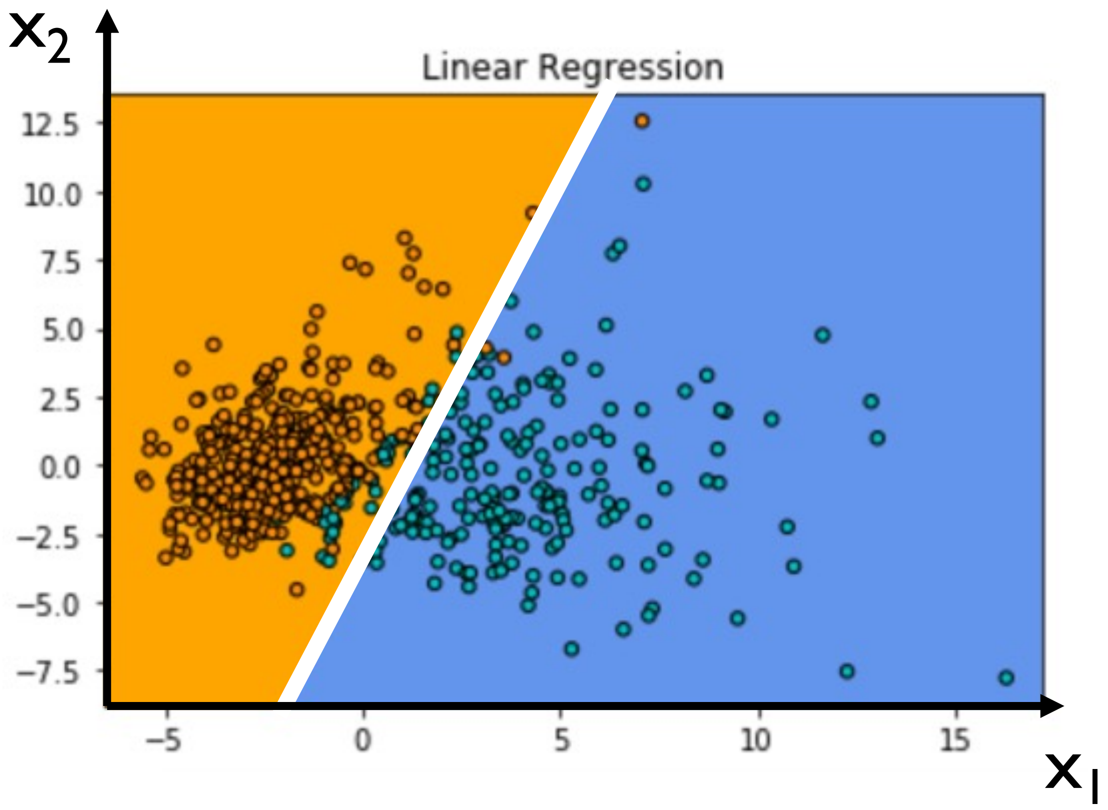
…

$$p_{K-1} = \frac{\exp(\beta_{0K-1} + \beta_K^T X)}{1 + \sum_{l=1}^{K-1} \exp\left(\beta_{0l} + \beta_l^T X\right)}$$

$$p_K = \frac{1}{1 + \sum_{l=1}^{K-1} \exp\left(\beta_{0l} + \beta_l^T X\right)}$$

Do we need probabilities or decision boundaries?

Find “optimal” boundary to separate classes



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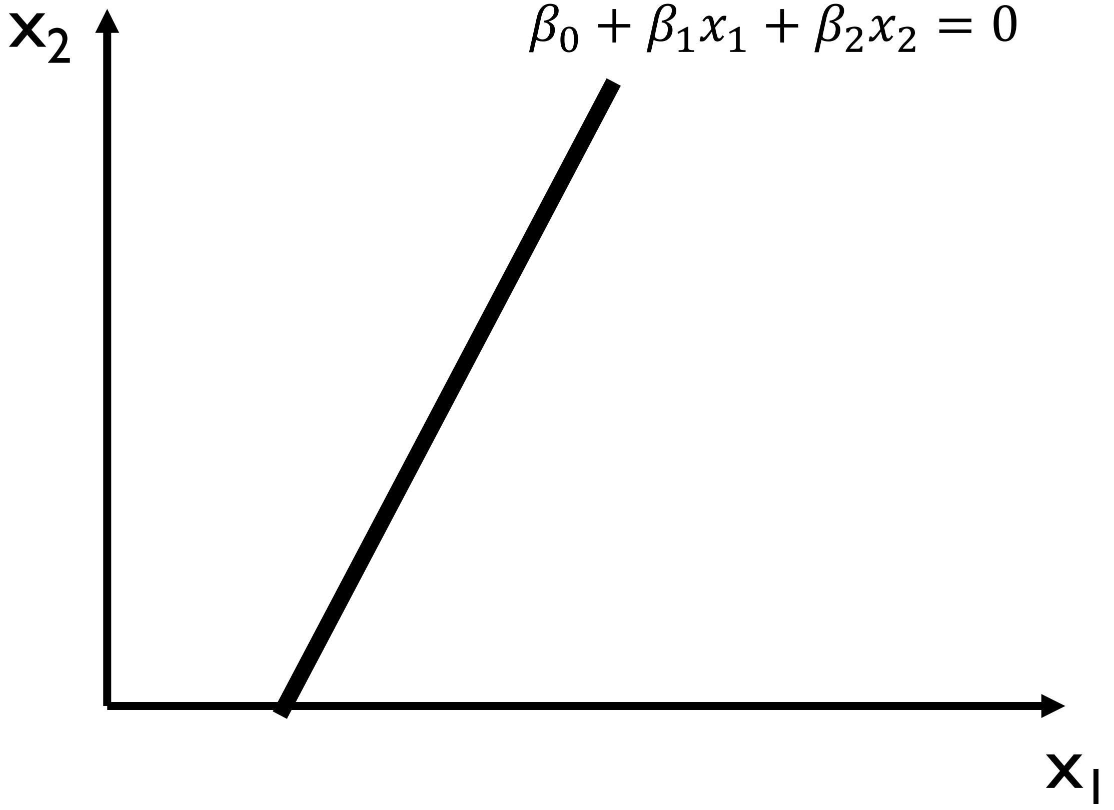

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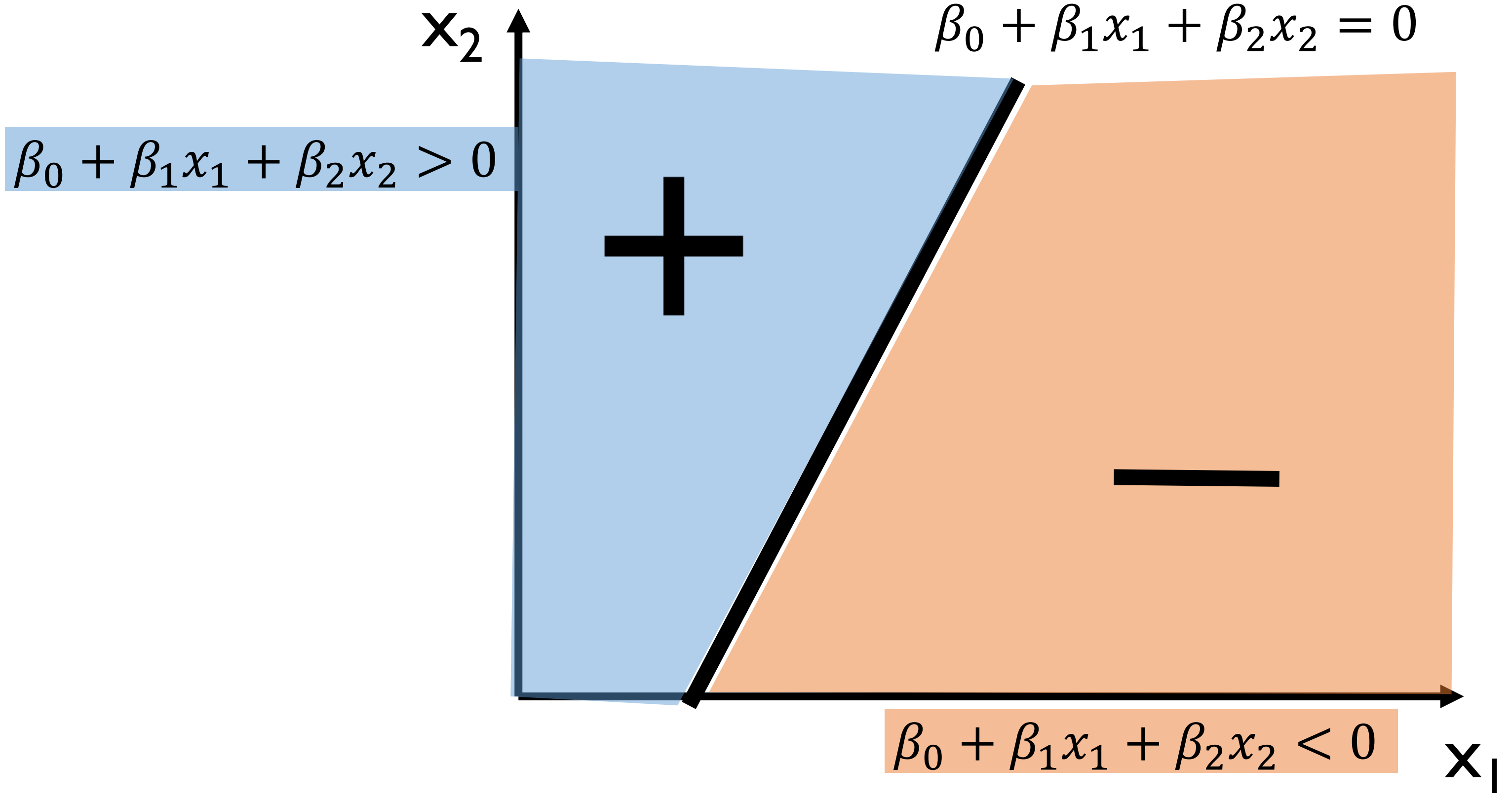

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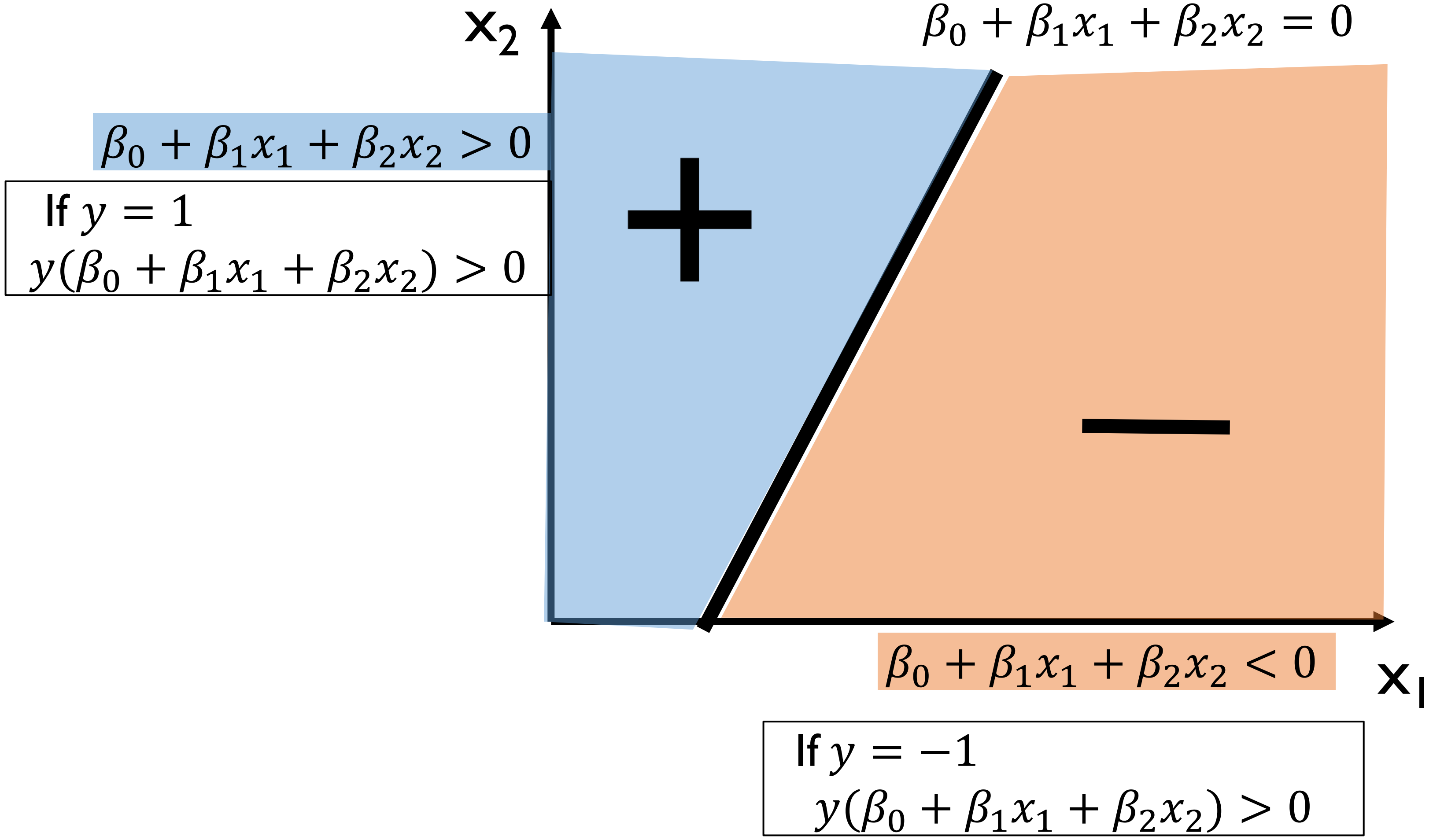
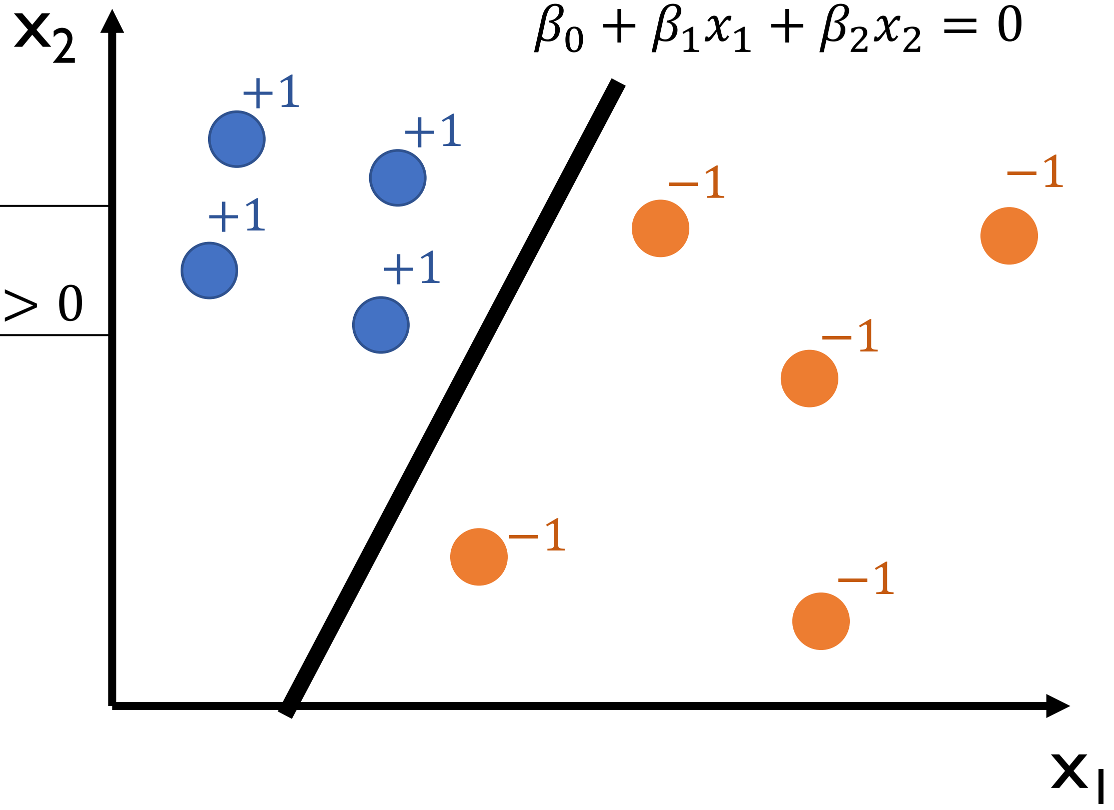


Do we need probabilities or decision boundaries?

Find "optimal" boundary to separate classes

If $y = 1$
$y(\beta_0 + \beta_1 x_1 + \beta_2 x_2) > 0$

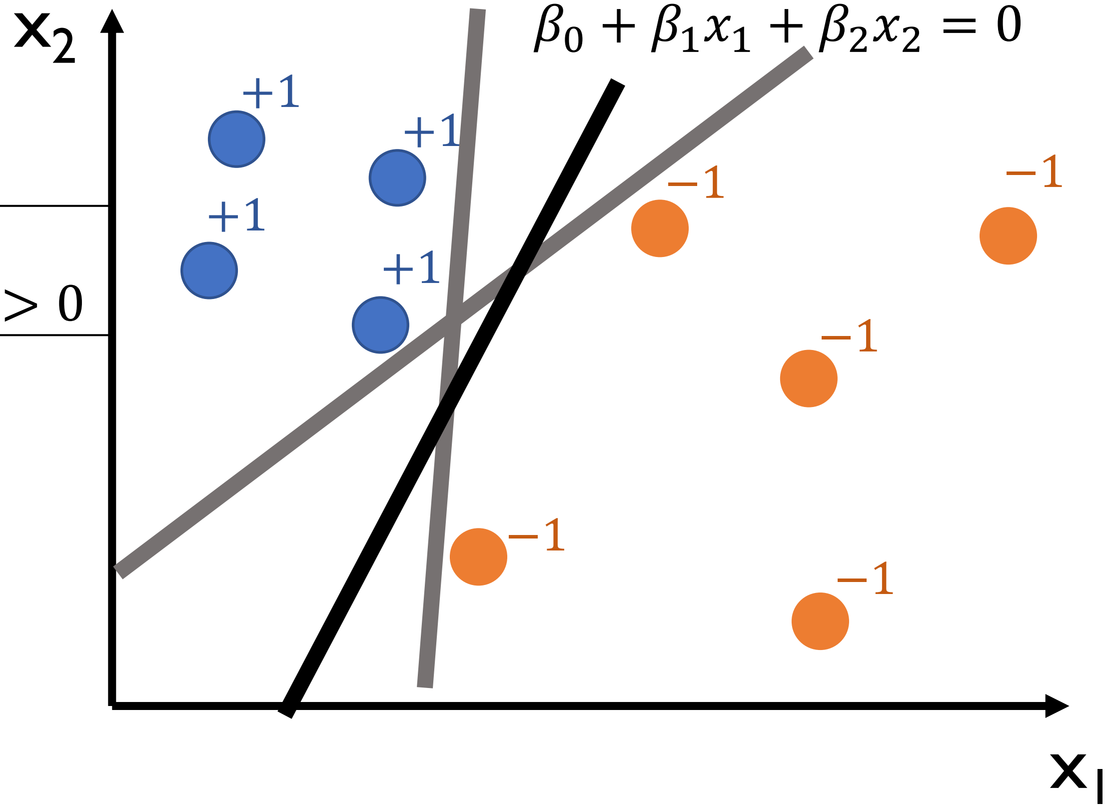


If $y = -1$
$y(\beta_0 + \beta_1 x_1 + \beta_2 x_2) > 0$

Do we need probabilities or decision boundaries?

Find **"optimal"** boundary to separate classes

If $y = 1$
$y(\beta_0 + \beta_1 x_1 + \beta_2 x_2) > 0$

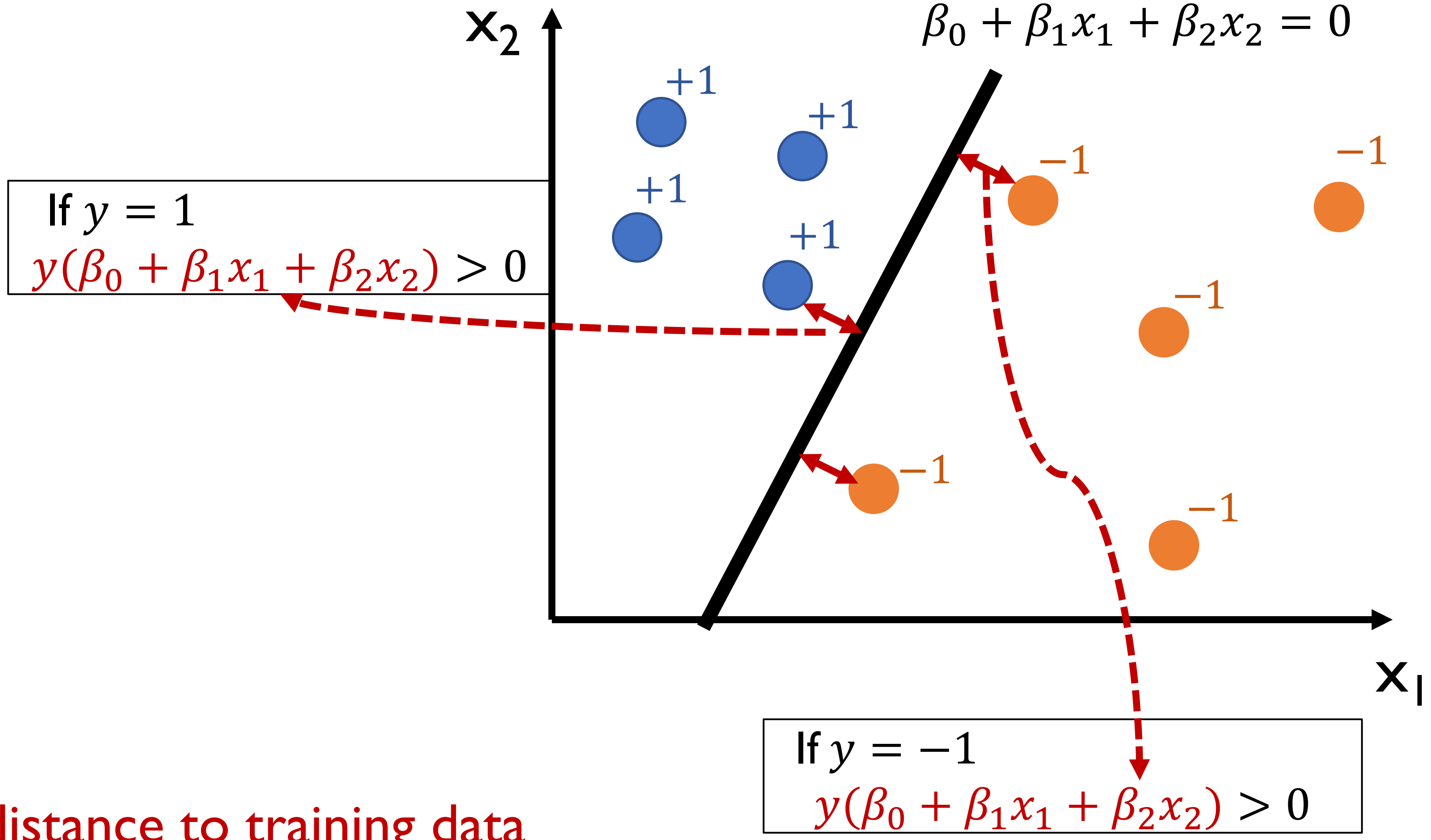


If $y = -1$
$y(\beta_0 + \beta_1 x_1 + \beta_2 x_2) > 0$

Optimal: Farthest distance to training data

Maximal Margin Classifier

Find **“optimal”** boundary to separate classes



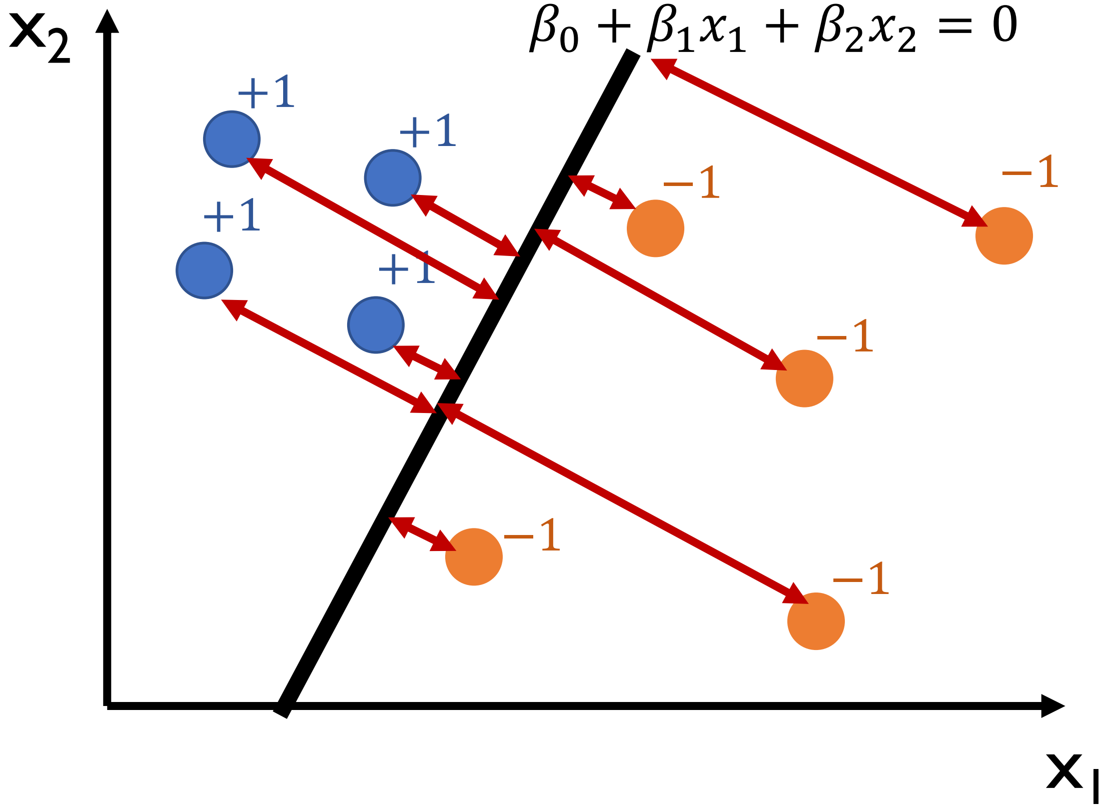
Optimal: Farthest distance to training data

Maximal Margin Classifier

$$\max_{\beta_0,\beta_1,\beta_2} M$$

such that $\beta_0^2 + \beta_1^2 + \beta_2^2 = 1$

For all training data
$$y^{(i)}\left(\beta_0 + \beta_1 x_1^{(i)} + \beta_2 x_2^{(i)}\right) \geq M$$



Optimal: Farthest distance to training data

Maximal Margin Classifier

$$\max_{\beta_0,\beta_1,\beta_2} \; M$$

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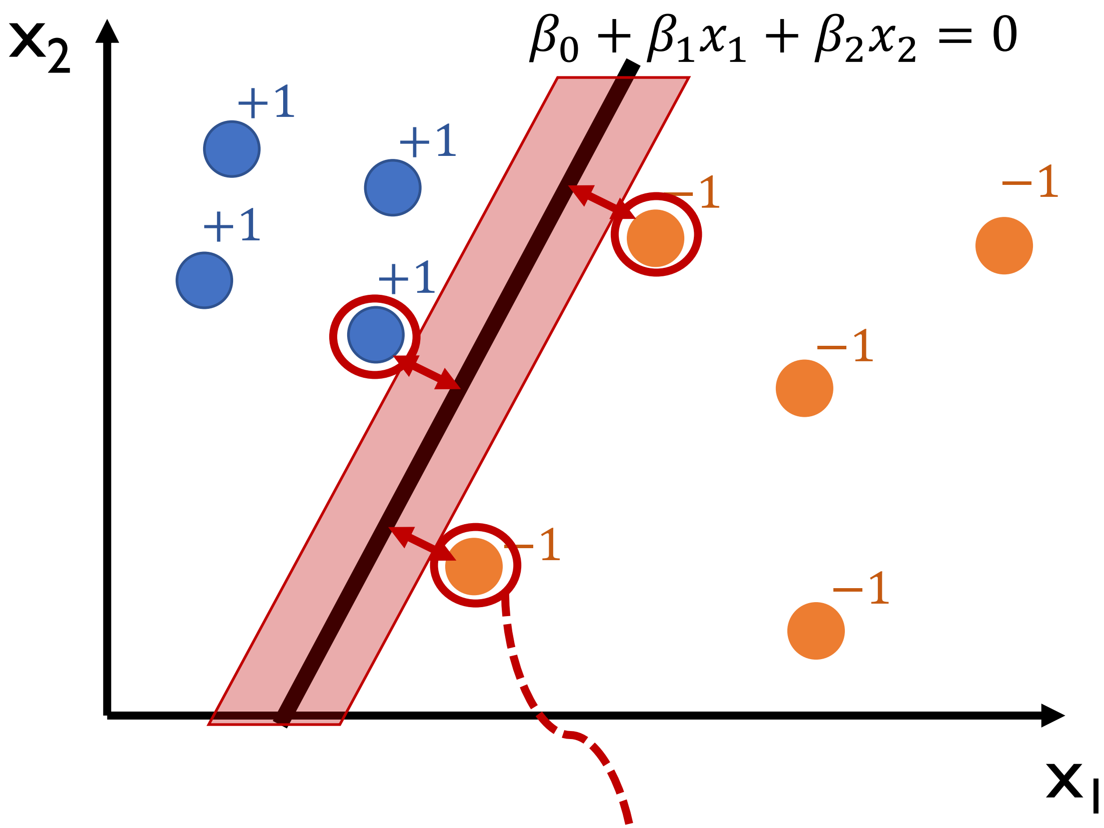
For all training data

$$y^{(i)}\left(\beta_0 + \beta_1 x_1^{(i)} + \beta_2 x_2^{(i)}\right) \geq M$$

Only points with equality matter



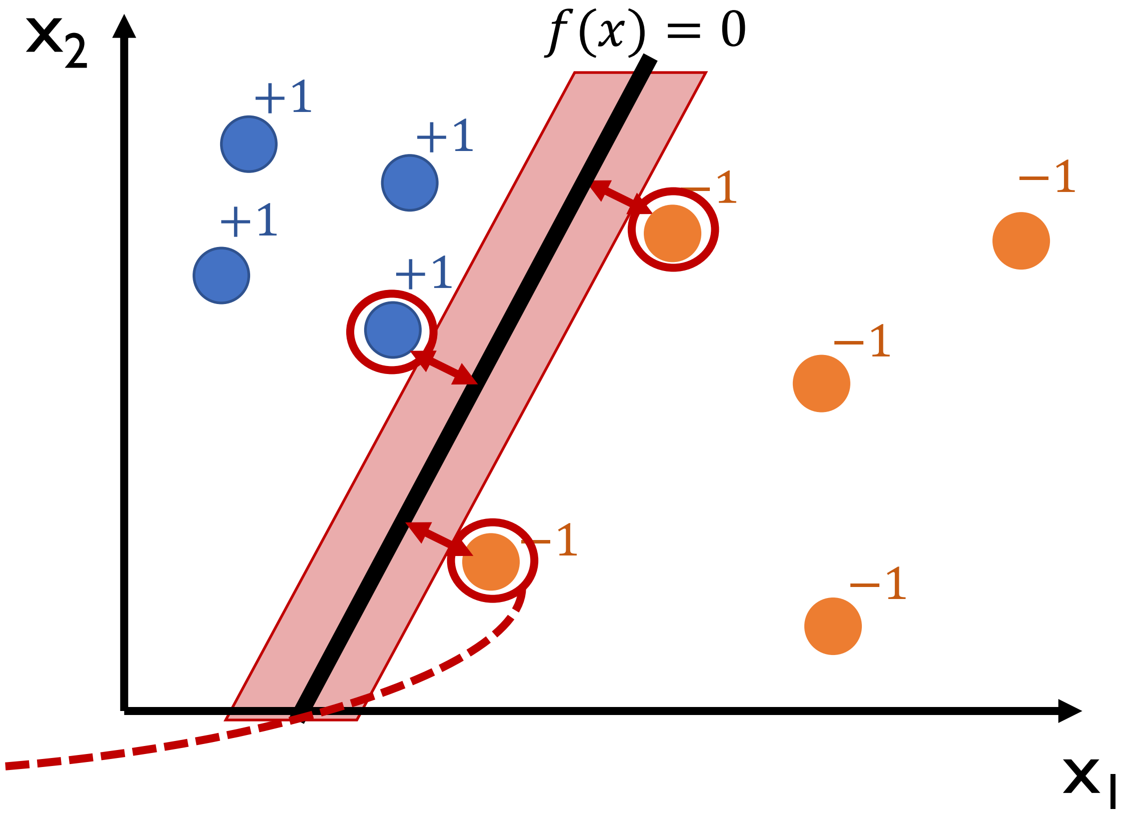
Support Vectors

Maximal Margin Classifier

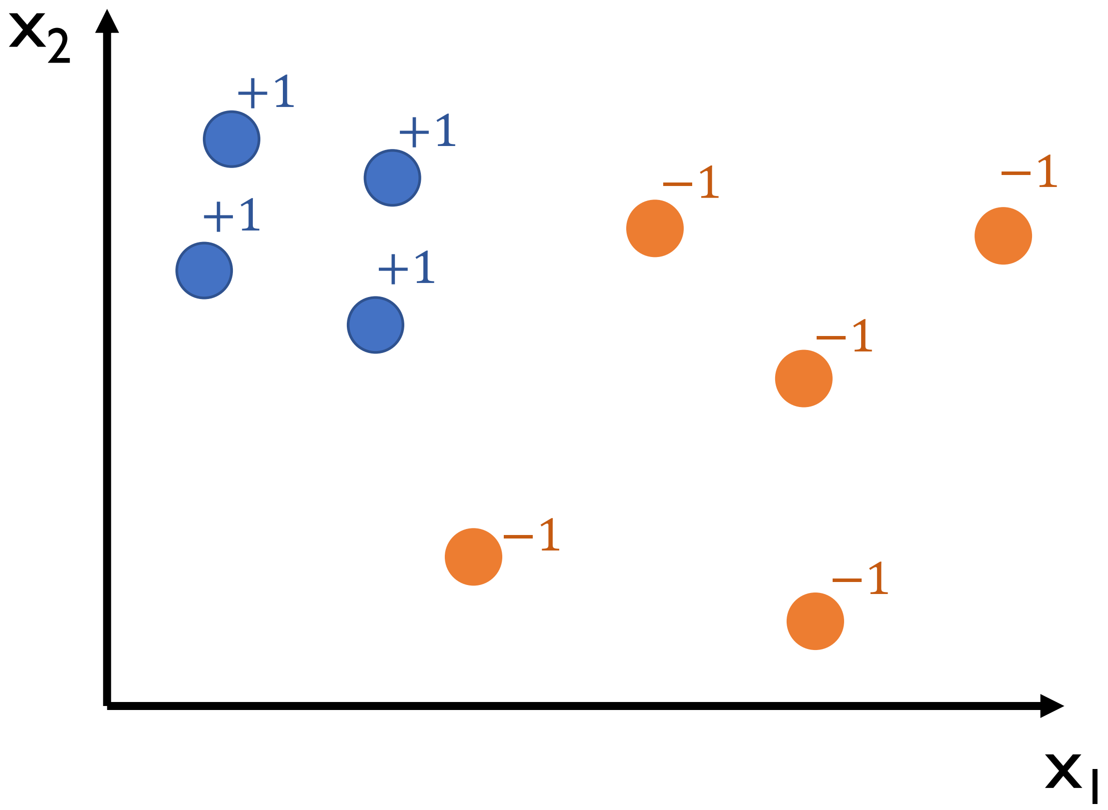
Solving optimization problem we find $\beta_0, \alpha_1, \ldots, \alpha_N$ such that hyperplane:

$$f(x) = \beta_0 + \sum_{i \in S} \alpha_i \, x^T x^{(i)}$$

Support Vectors



What if there is no separating hyperplane?



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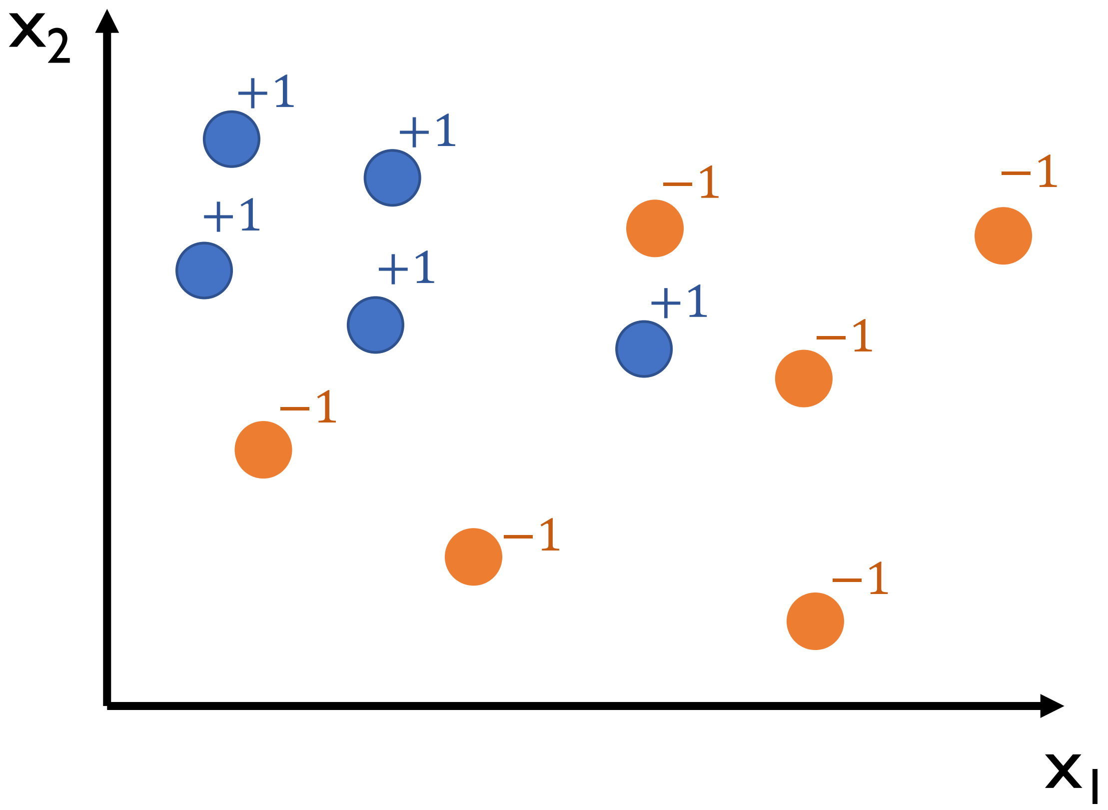
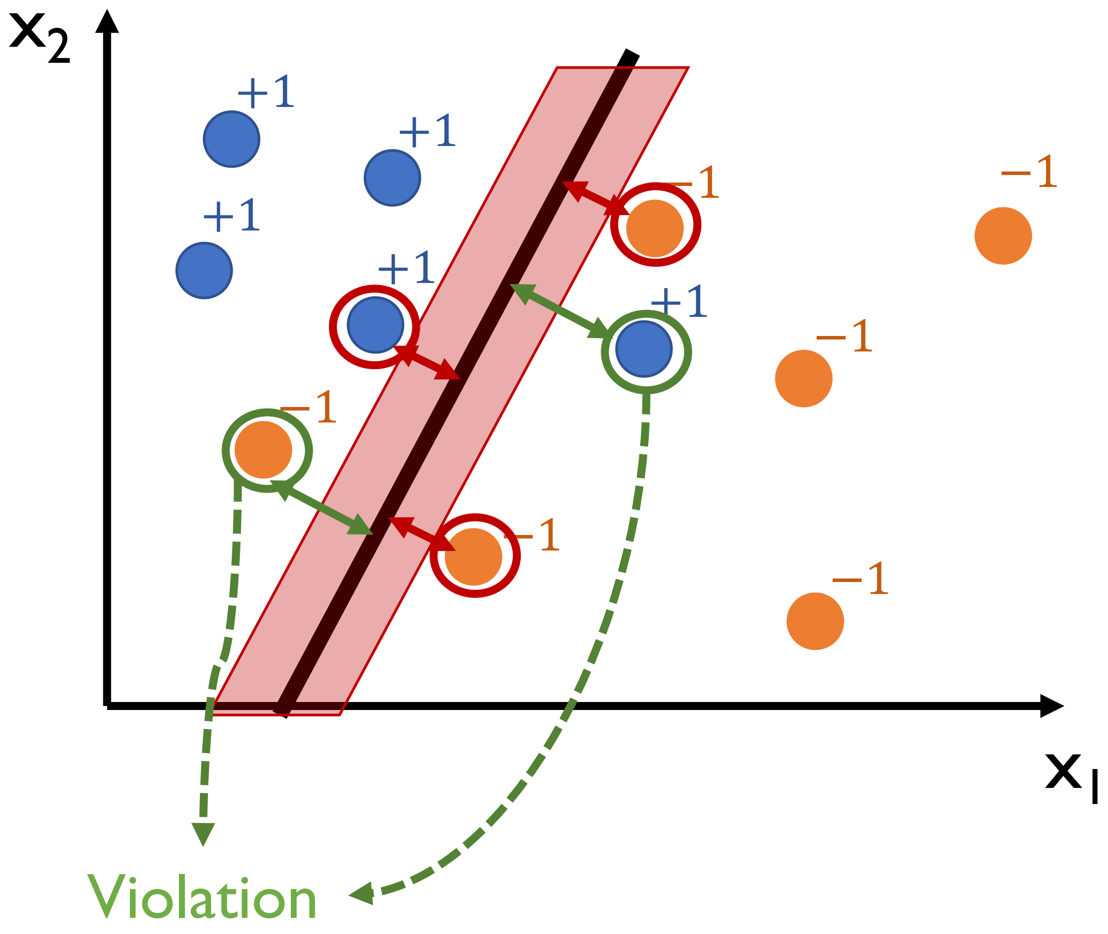


Support Vector Classifier



Support Vector Classifier

$$\max_{\beta_0,\beta_1,\beta_2} M$$

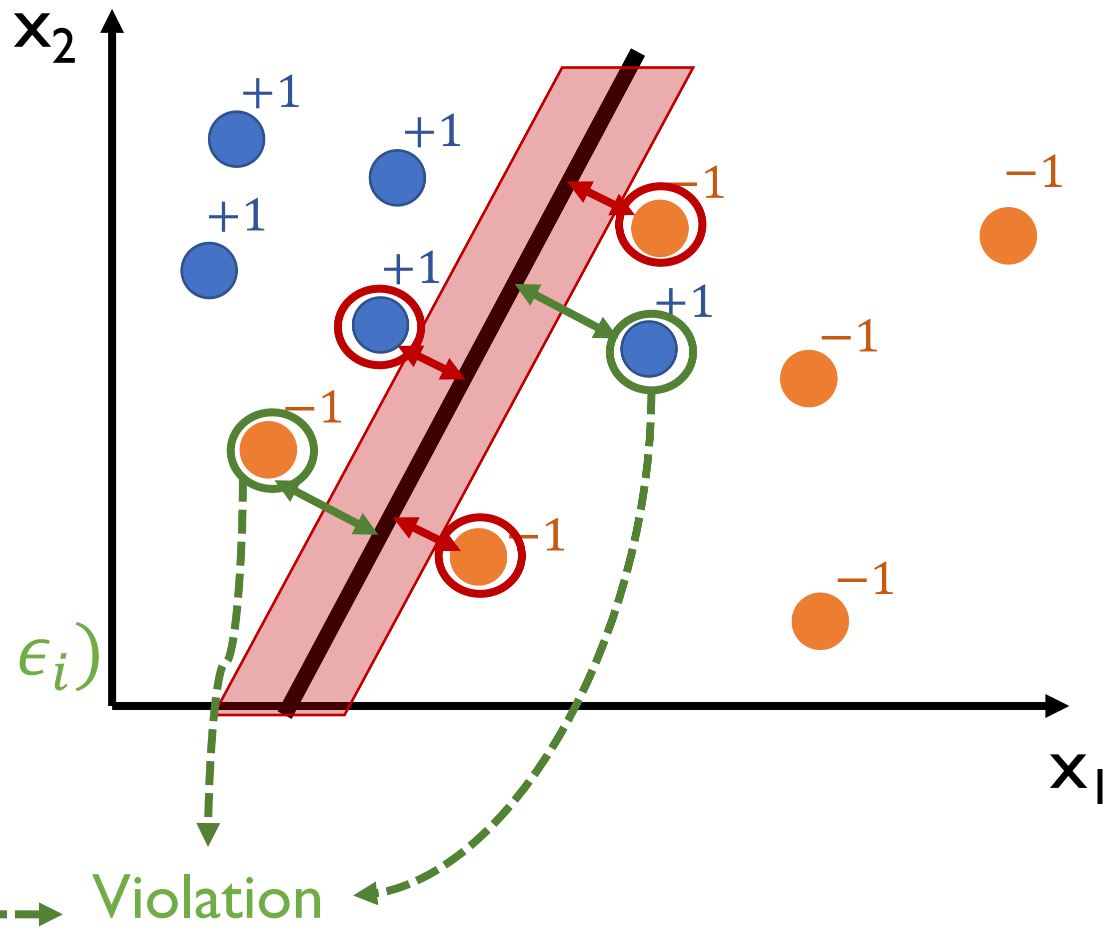
such that $\beta_0^2 + \beta_1^2 + \beta_2^2 = 1$

For all training data

$$y^{(i)}\left(\beta_0 + \beta_1 x_1^{(i)} + \beta_2 x_2^{(i)}\right) \geq M(1 - \epsilon_i)$$

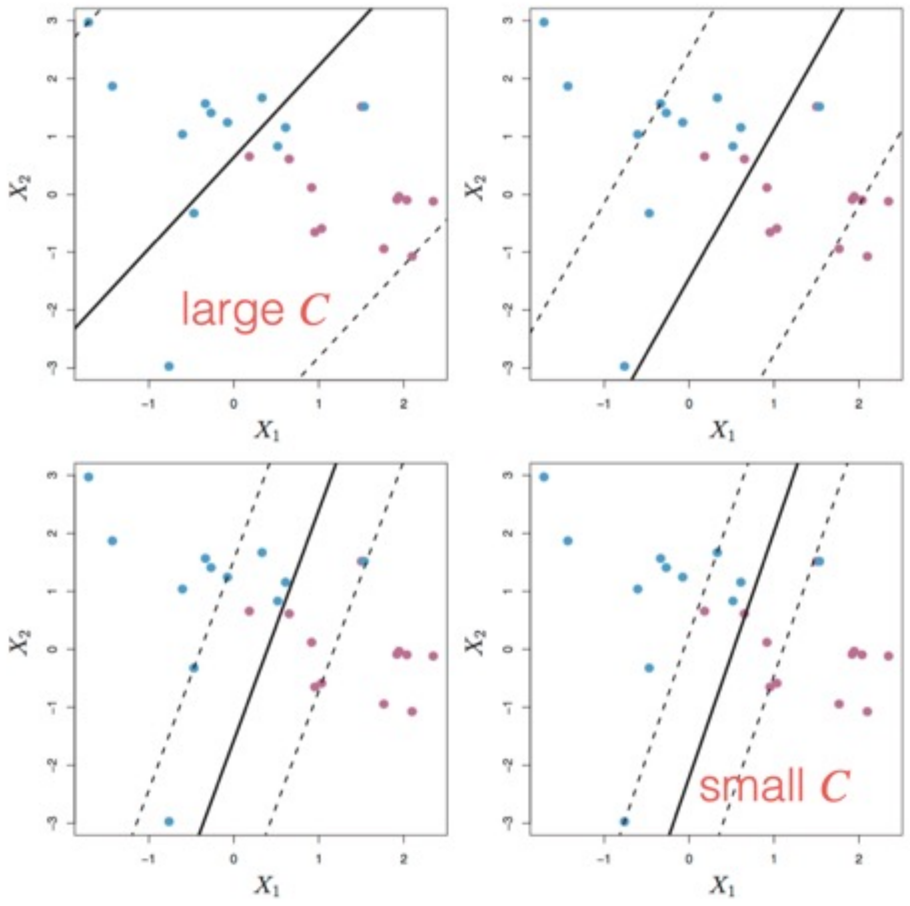
such that

$$\sum_{i=1}^{N} \epsilon_i \leq C\,, \qquad \epsilon_i \geq 0$$



Support Vector Classifier

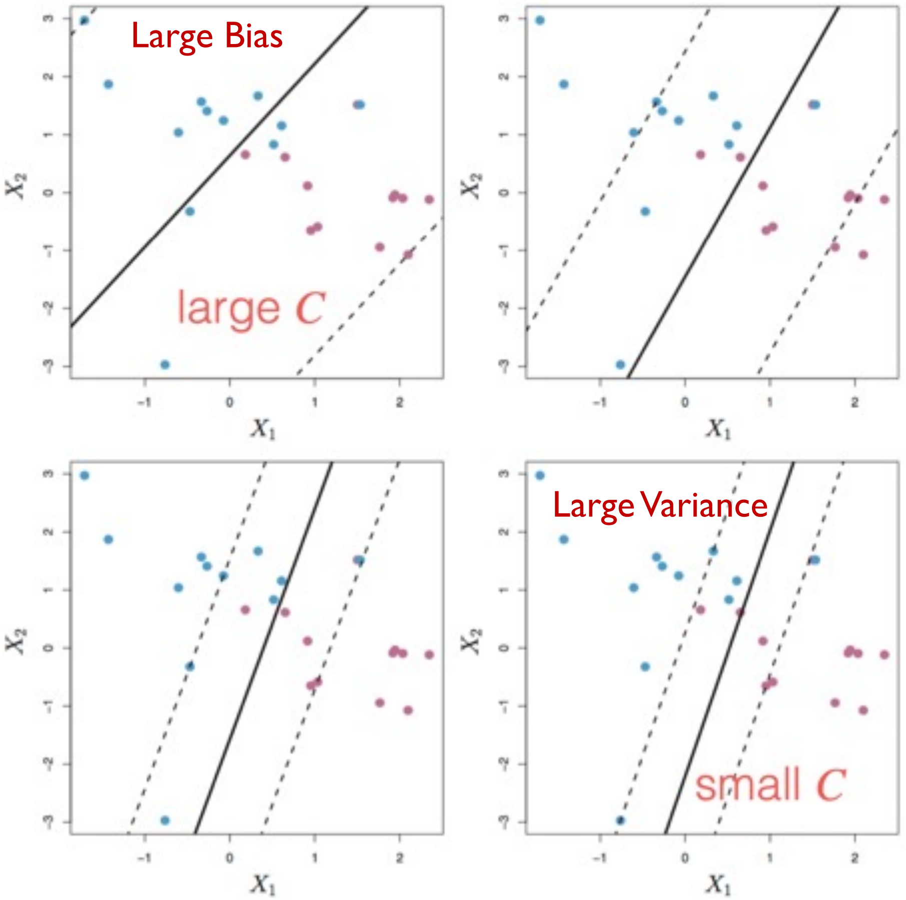
C is the "budget" for violations



ISL Fig 9.7

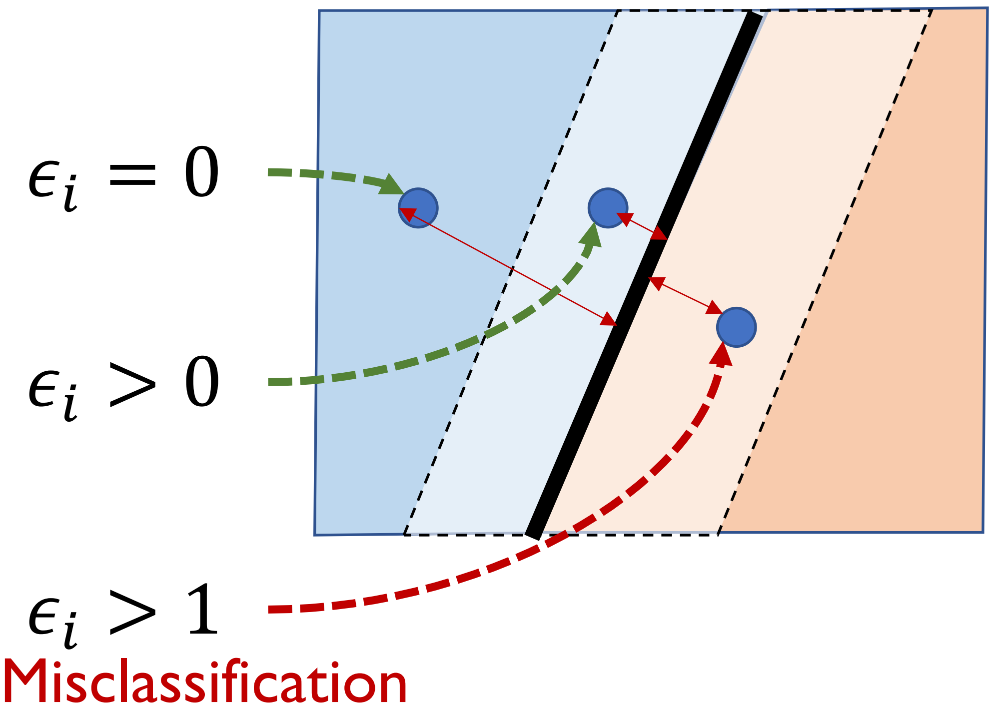
Support Vector Classifier

C is the "budget" for violations



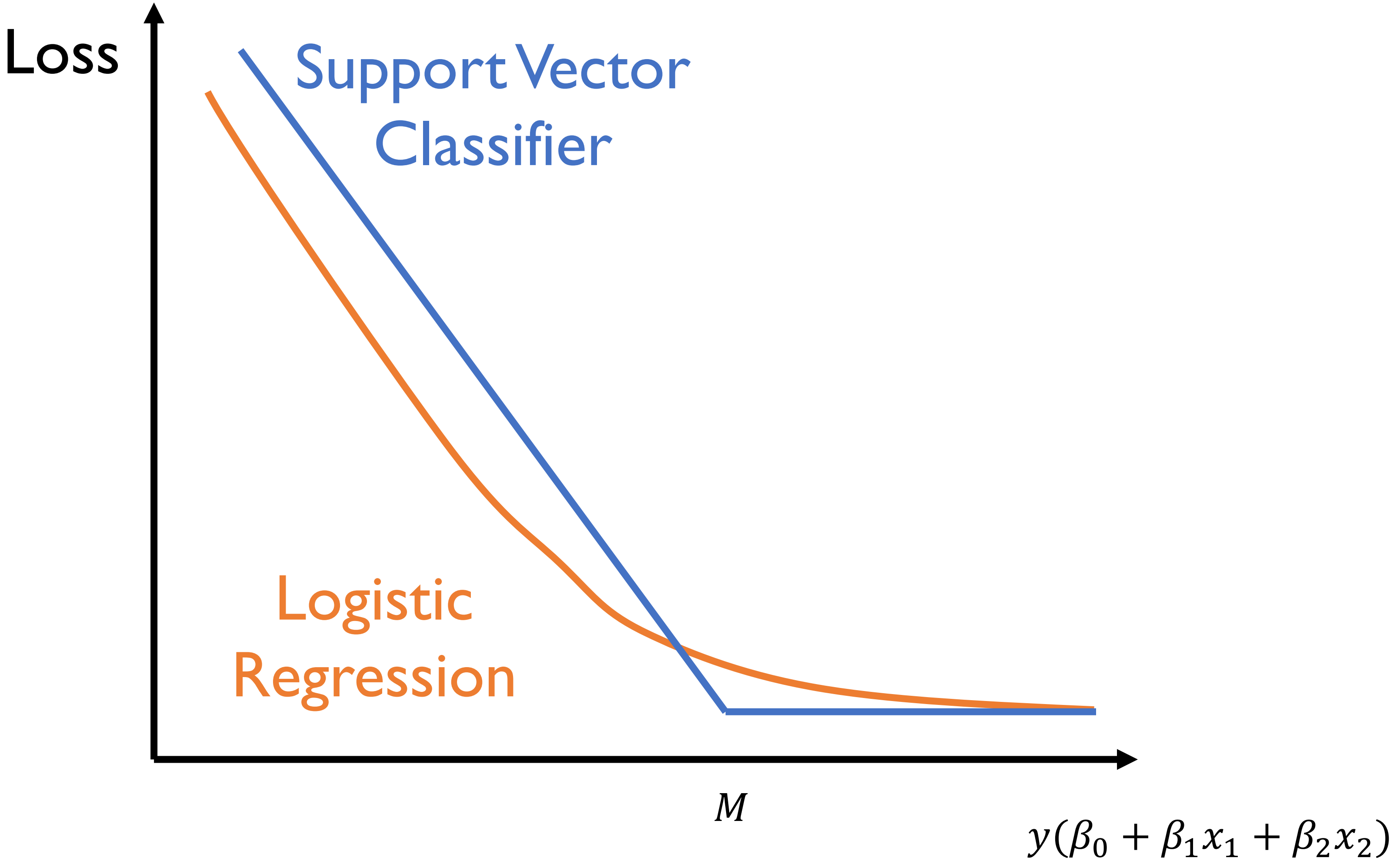
ISL Fig 9.7

Slack variables ϵ_i



Support Vector Classifier vs Logistic Regression

Similar Behavior

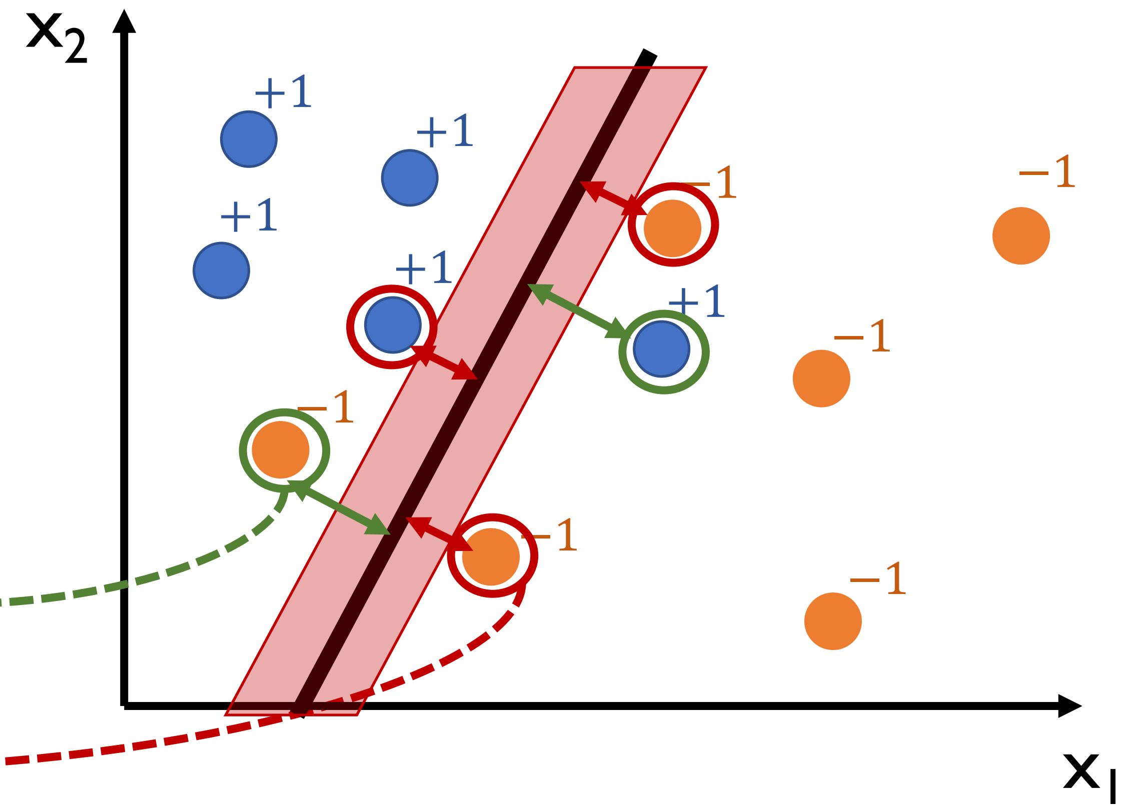


Support Vector Classifier

Solving optimization problem we find $\beta_0, \alpha_1, \ldots, \alpha_N$ such that hyperplane:

$$f(x) = \beta_0 + \sum_{i \in S} \alpha_i \, x^T x^{(i)}$$

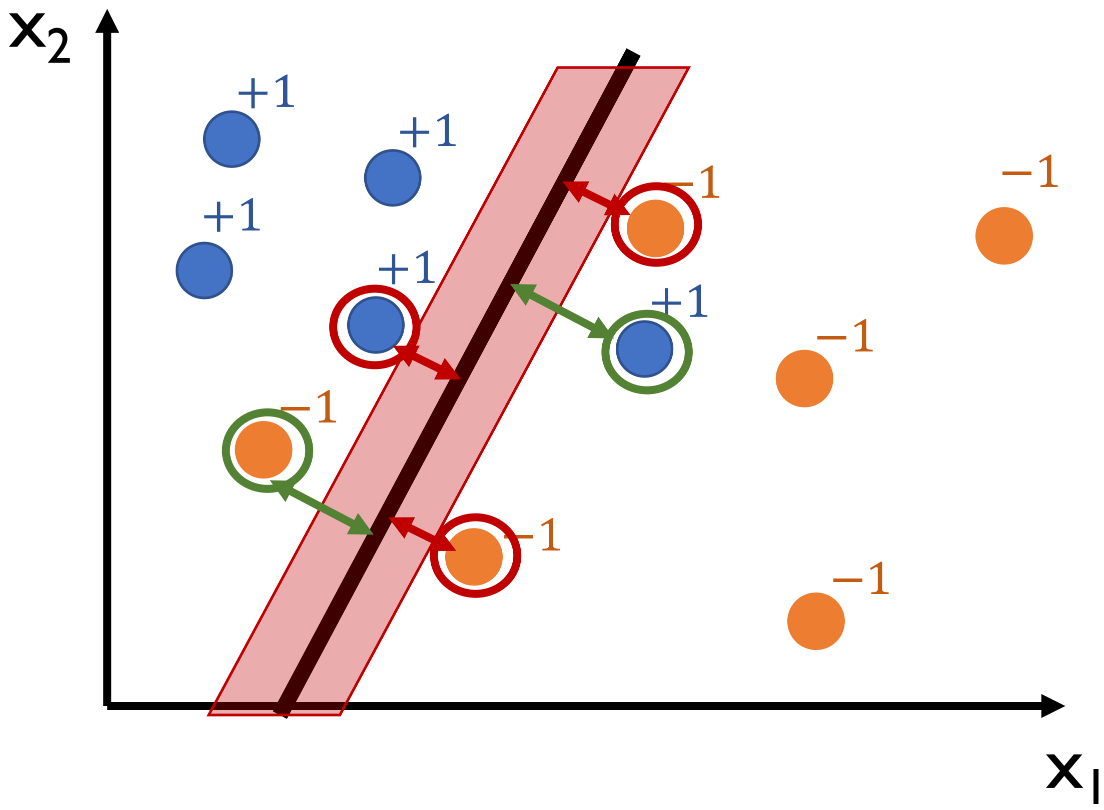
Support Vectors



Support Vector Classifier

Solving optimization problem we find $\beta_0, \alpha_1, \ldots, \alpha_N$ such that hyperplane:

$$f(x) = \beta_0 + \sum_{i \in S} \alpha_i \boxed{x^T x^{(i)}}$$



We only get linear boundaries

Beyond linear decision boundaries

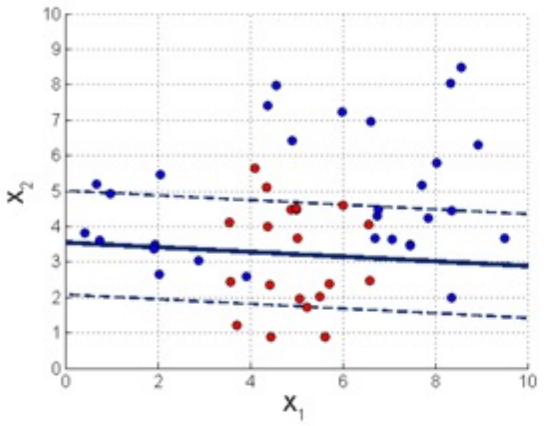
$$f(x) = \beta_0 + \sum_{i \in S} \alpha_i \boxed{x^T x^{(i)}}$$

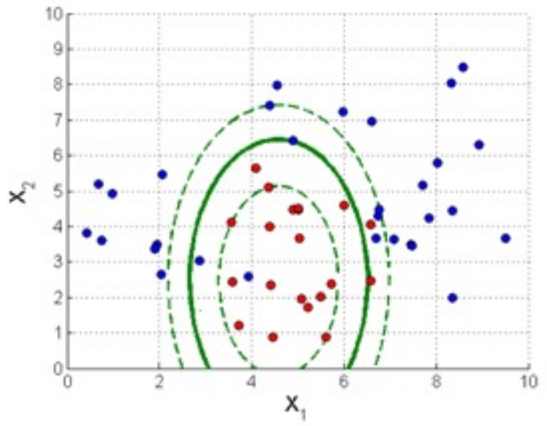
Option 1)
Add additional features

$$X_1, X_2, X_1X_2, X_1^2, X_2^2, \ldots$$

Option 2)
Generalize inner product

Kernels $\quad x^T x^{(i)} \rightarrow K(x, x^{(i)})$





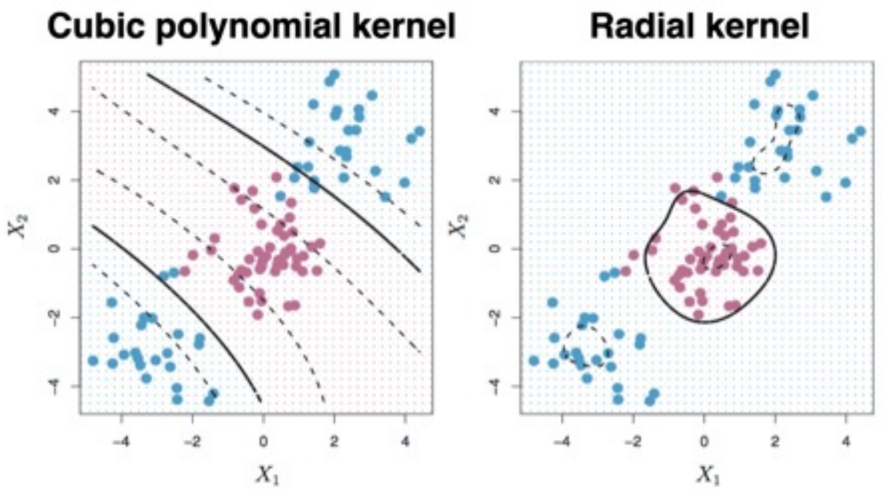


FIGURE 9.9, ISL (8th printing 2017)

Support Vector Machines

$$f(x) = \beta_0 + \sum_{i \in S} \alpha_i \boxed{K(x, x^{(i)})}$$

Linear Kernel $K\left(x, x^{(i)}\right) = x^T x^{(i)}$

Polynomial Kernel $K\left(x, x^{(i)}\right) = \left(1 + x^T x^{(i)}\right)^p$ Includes $x_1^k x_2^l$, $k + l \le p$

Radial Basis Kernel $K\left(x, x^{(i)}\right) = \exp\left(-\gamma \|x - x^{(i)}\|^2\right)$ Includes infinite # features

Kernel ≈ Similarity Measure

Challenges Support Vector Machines

Hyperparameters: C and Kernel

✓ Flexibility

✗ Delicate tuning

✗ Difficult to Interpret

✓ Convex Optimization (easy)

Extend to more than 2 classes

One vs one
1 SVM per pair

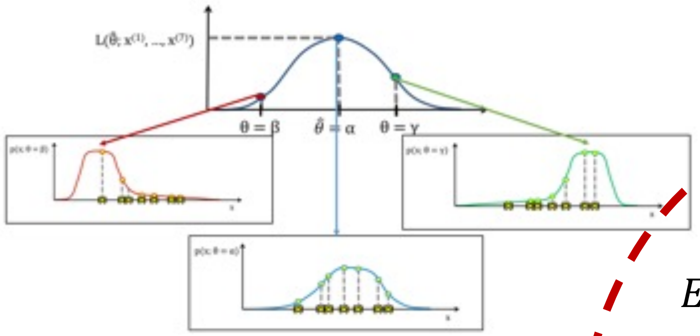
	C1	C2	C3	C4
C1				
C2				
C3				
C4				

One vs all
1 SVM per class

C1	C2 C3 C4
C2	C1 C3 C4
C3	C1 C2 C4
C4	C1 C2 C3

How can we extend Linear Regression?

LR is Maximum Likelihood estimator



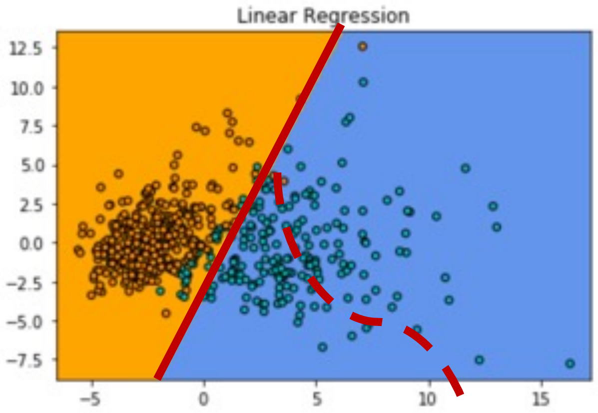
$$\boxed{Y \sim Normal}$$

$$E[Y|X] = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$$

Find a better distribution for Y categorical

Logistic Regression

LR creates separating hyperplanes



Y

M $\longrightarrow$ 1

0.5

B $\longrightarrow$ 0

Optimize the hyperplane

Support Vector Machines

How do we measure the error?

Most common approach: Error rate

$$error = \frac{1}{N}\sum_{i=1}^{N} I\left(\hat{y}^{(i)} \neq y^{(i)}\right)$$

1 if $\hat{y}^{(i)} \neq y^{(i)}$
0 if $\hat{y}^{(i)} = y^{(i)}$

Most common approach: Error rate

$$error = \frac{1}{N}\sum_{i=1}^{N} I\left(\hat{y}^{(i)} \neq y^{(i)}\right)$$

1 if $\hat{y}^{(i)} \neq y^{(i)}$
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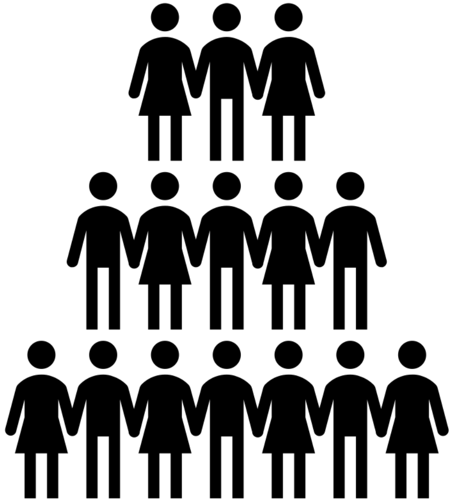
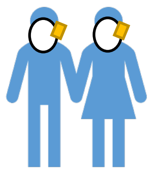


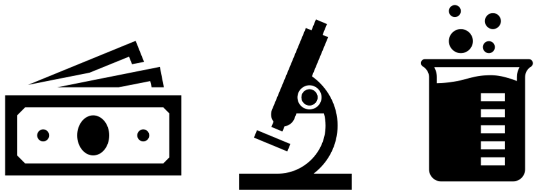
998 healthy

+



2 sick

Design test with
$error \leq 0.2\%$

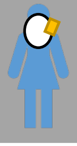
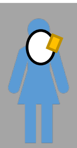
Option 1 

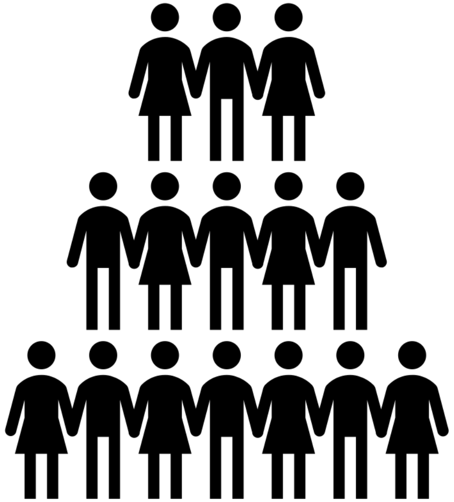
Option 2 Assign healthy to everyone

Useful approach: Confusion Matrix

Predicted Labels

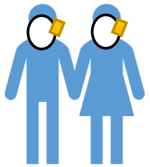
True Labels

		
	0	2
	0	998



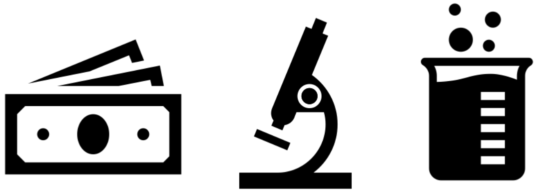
998 healthy

\+



2 sick

Design test with
$error \leq 0.2\%$

Option 1 

Option 2 Assign healthy to everyone

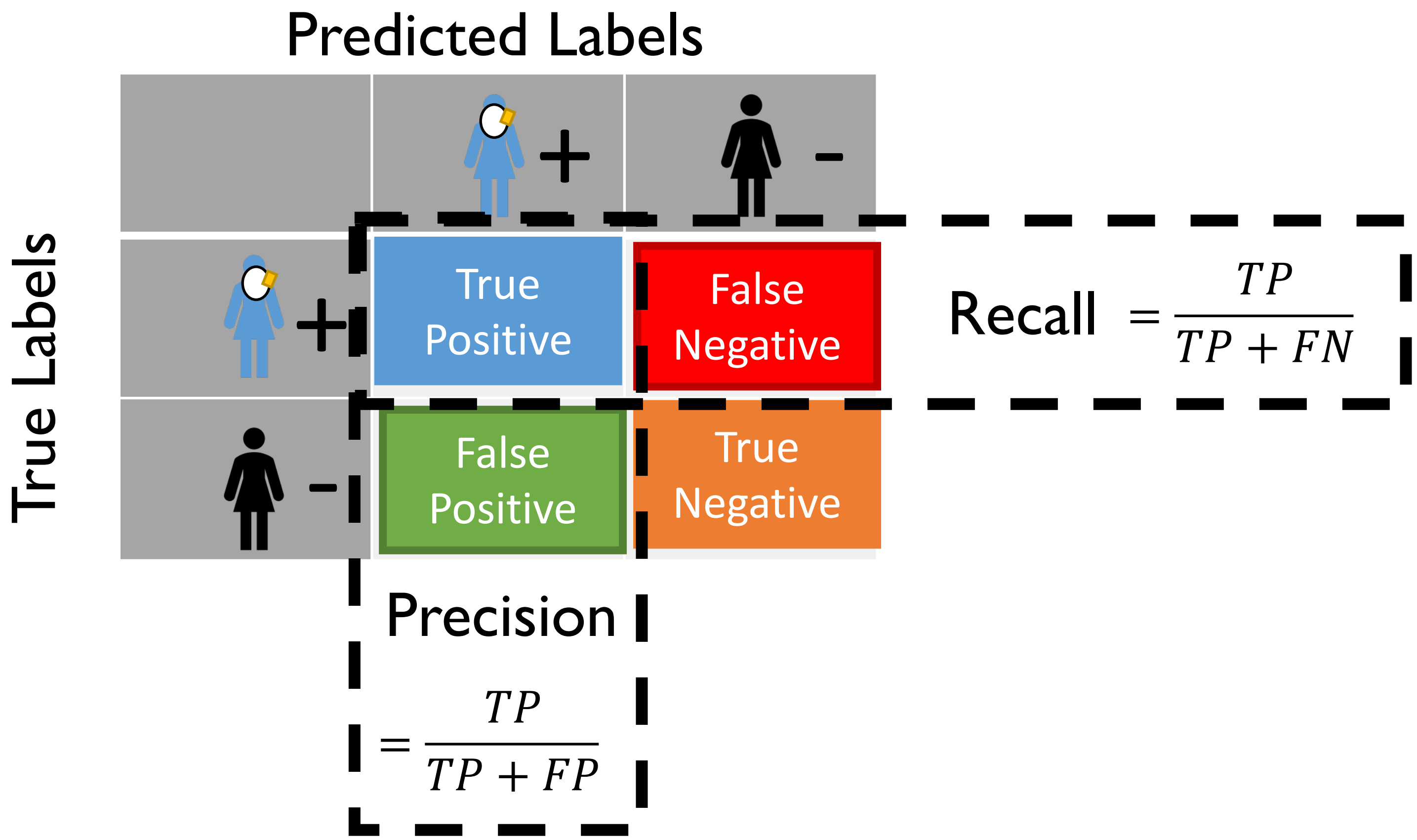
Useful approach: Confusion Matrix

Predicted Labels

True Labels

	+	-
+	True Positive	False Negative
-	False Positive	True Negative

Useful approach: Precision vs Recall



(+) samples correctly classified

(+) predictions that are truly(+)

Useful approach: Precision vs Recall

Predicted Labels

True Labels	+	-
+	0	2
-	0	998

Recall $= 0$

(+) samples correctly classified

Precision

$=?$

(+) predictions that are truly(+)

Useful approach: Precision vs Recall

Predicted Labels

True Labels	+	-
+	2	0
-	0	998

Recall $= 1$

(+) samples correctly classified

Precision $= 1$

(+) predictions that are truly(+)

Perfect Classifier

Useful approach: Precision vs Recall

Predicted Labels

True Labels	+	-
+	1	1
-	499	499

Recall $= 0.5$

(+) samples correctly classified

Precision $= 0.002$

(+) predictions that are truly(+)

Random Guessing 50/50

Useful approach: ROC curve

Predicted Labels

True Labels	+	-
+	True Positive	False Negative
-	False Positive	True Negative

$$\text{TP Rate} = \frac{TP}{TP + FN}$$

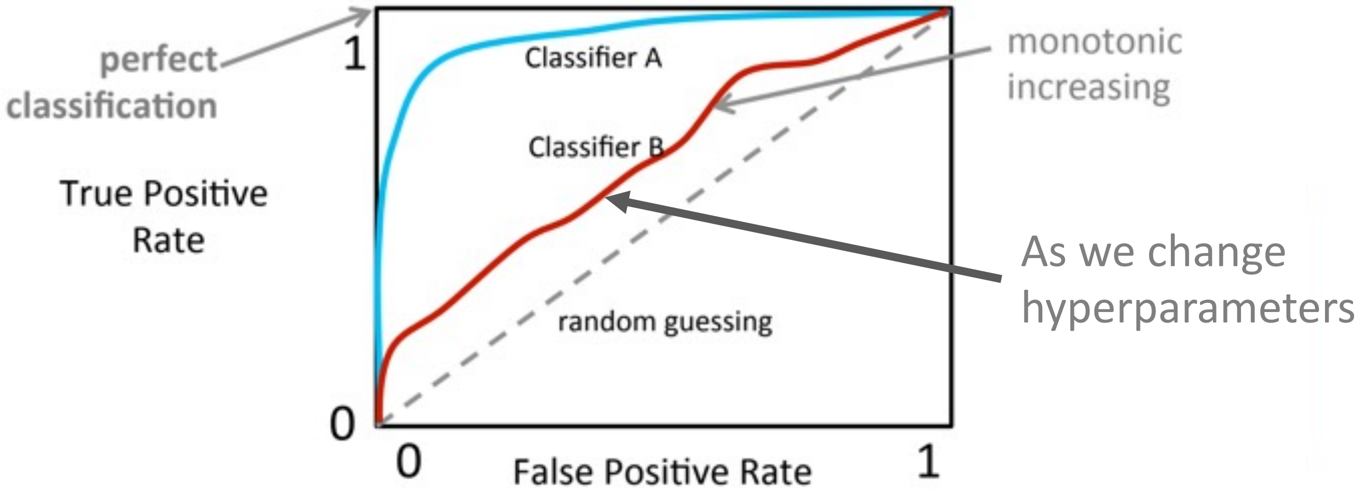
$$\text{FP Rate} = \frac{FP}{FP + TN}$$

Useful approach: ROC curve

True Labels \ Predicted Labels	+	-
+	True Positive	False Negative
-	False Positive	True Negative

$$\text{TP Rate} = \frac{TP}{TP + FN}$$

$$\text{FP Rate} = \frac{FP}{FP + TN}$$

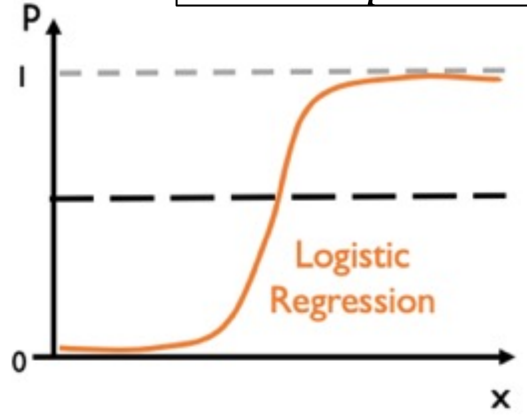


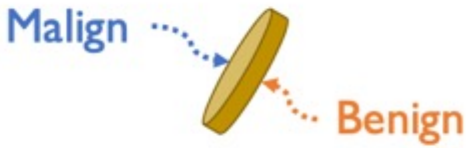
Today's Recap

Classification

Logistic Regression

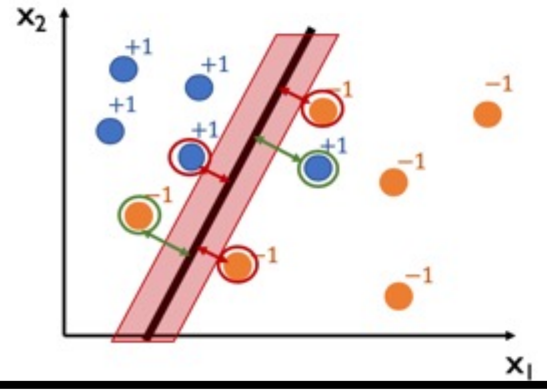
$$\boxed{\log\left(\frac{p}{1-p}\right) \approx \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p}$$





Support Vector Machines

$$f(x) = \beta_0 + \sum_{i \in S} \alpha_i K(x, x^{(i)})$$



Evaluation:
Confusion Matrix