CS4442/9542b
Artificial Intelligence II
Prof. Olga Veksler

Lecture 2

Introduction to ML

Basic Linear Algebra

Matlab

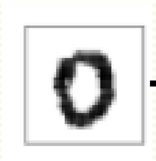
Some slides on Linear Algebra are from Patrick Nichols

Outline

- Introduction to Machine Learning
- Basic Linear Algebra
- Matlab Intro

Intro: What is Machine Learning?

- Difficult to come up with explicit program for some tasks
- Digit Recognition, a classic example

 $\longrightarrow$ 0

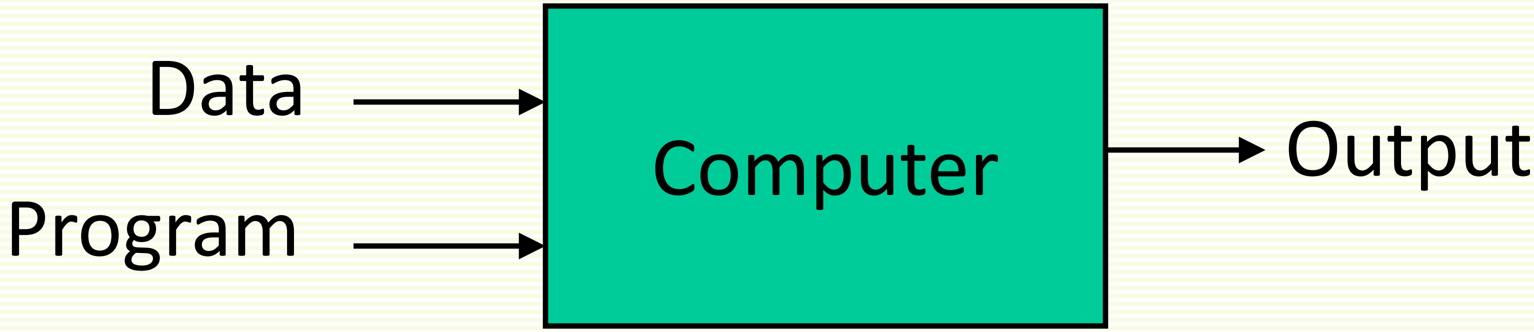
 $\longrightarrow$ 4

- Easy to collect images of digits with their correct labels

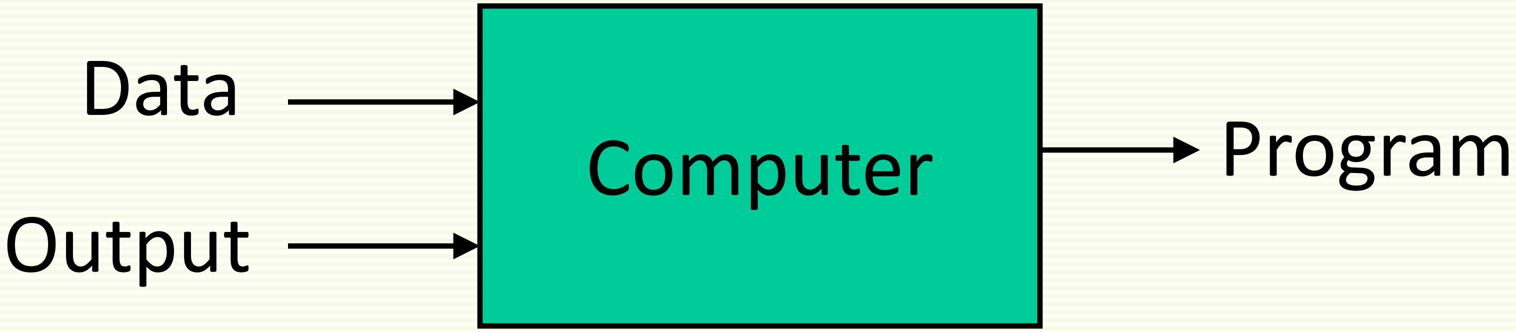
- Machine Learning Algorithm takes collected data and produces program for recognizing digits
  - done right, program will recognize correctly new images it has never seen

Intro: What is Machine Learning?

Traditional Programming



Machine Learning



Intro: What is Machine Learning?

- General definition (Tom Mitchell):
  - Based on experience **E**, improve performance on task **T** as measured by performance measure **P**
- Digit Recognition Example
  - **T** = recognize character in the image
  - **P** = percentage of correctly classified images
  - **E** = dataset of human-labeled images of characters

Different Types of Machine Learning

- **Supervised Learning**
  - given training examples with corresponding outputs
  - learn to produces correct labels for new examples
- **Unsupervised Learning**
  - given training examples only
  - discover good data representation
    - e.g. “natural” clusters
  - not covered
- **Reinforcement Learning**
  - learn to select action that maximizes payoff
  - not covered

Two Types of Supervised Machine Learning

- Classification
  - output belongs to a finite set
  - example: age $\in$ {baby, child, adult, elder}
  - output is also called *class* or *label*

- Regression
  - output is continuous
  - example: age $\in [0,130]$

Supervised Machine Learning

- We are given examples with corresponding outputs
- Fish classification example (*salmon* or sea *bass*)

$$\mathbf{x}^1 = \begin{bmatrix} 3.3 \\ 5.7 \end{bmatrix} \quad \mathbf{x}^2 = \begin{bmatrix} 6.3 \\ 8.7 \end{bmatrix} \quad \mathbf{x}^3 = \begin{bmatrix} 2.3 \\ 1.7 \end{bmatrix} \quad \mathbf{x}^4 = \begin{bmatrix} 6.4 \\ 7.0 \end{bmatrix}$$

salmon

$\mathbf{y}^1=0$

sea bass

$\mathbf{y}^2=1$

salmon

$\mathbf{y}^3 = 0$

sea bass

$\mathbf{y}^4=1$

- Each example is represented in vector form
  - data may be given in vector form from the start
  - if not, for each example **i**, extract useful features and put them in a vector $\mathbf{x}^\mathbf{i}$
  - fish classification example
    - extract two features, *fish length* and *average fish brightness*
    - can extract as many other features
    - can also use raw pixel values as features (for images)
  - An example is often called *feature vector*
- Each output is represented with integer $\mathbf{y}^\mathbf{i}$

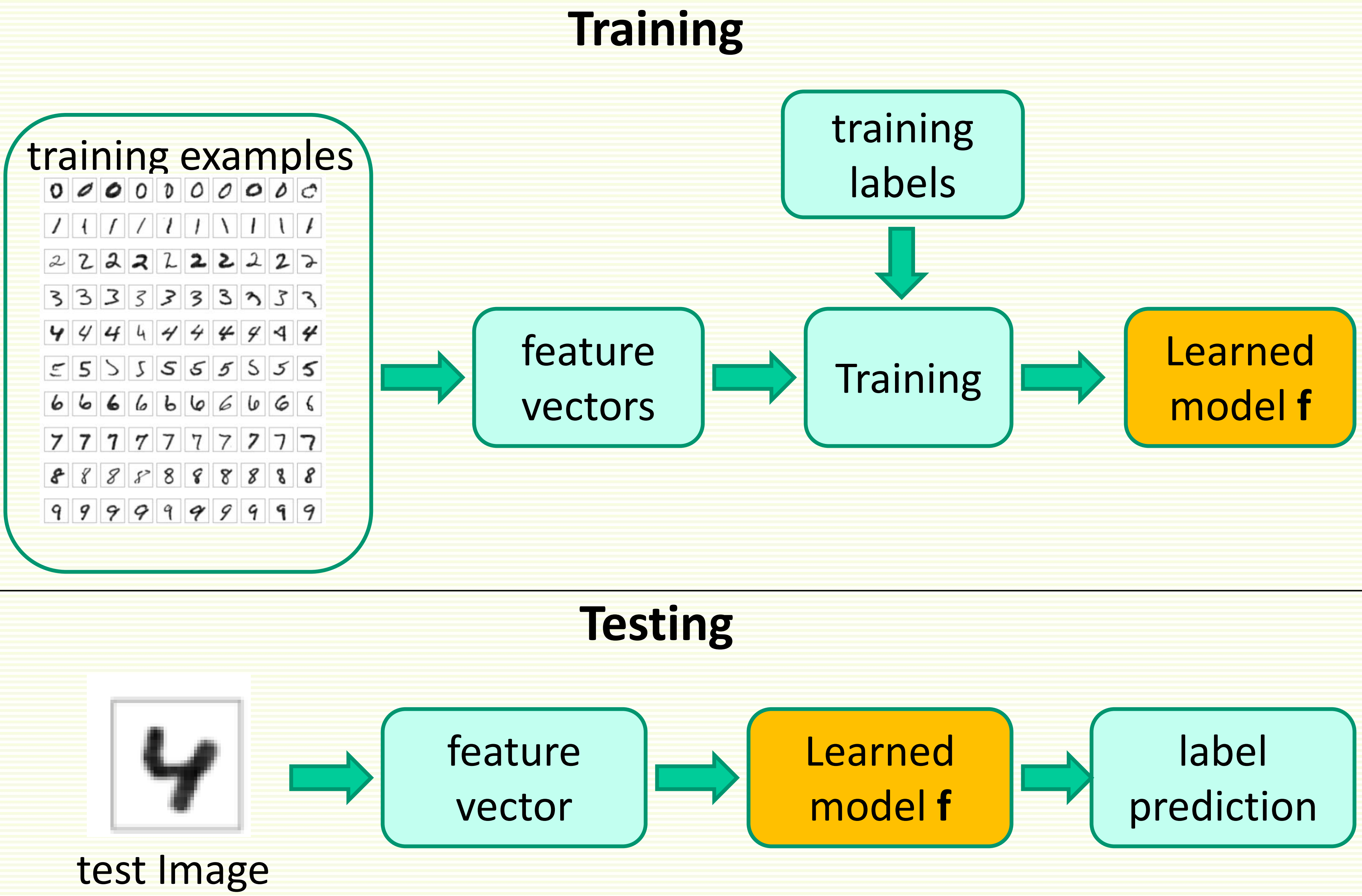
Supervised Machine Learning

- We are given
  1. Training examples $\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^n$
  2. Target output for each sample $\mathbf{y}^1, \mathbf{y}^2, \ldots \mathbf{y}^n$

  $\Big\}$ *labeled data*

- **Training phase**
  - estimate function $\mathbf{y} = \mathbf{f}(\mathbf{x})$ from labeled data
    - **f** is called *classifier*, *learning machine*, *prediction function*, etc.
- **Testing phase** (deployment)
  - predict label $\mathbf{f}(\mathbf{x})$ for a new (unseen) sample $\mathbf{x}$

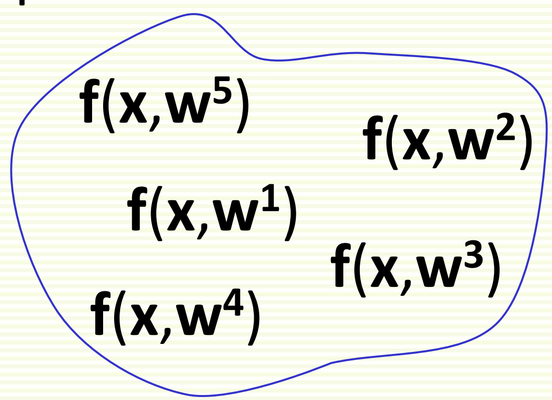
Training/Testing Phases Illustrated



More on Training Phase

- Estimate prediction function **y** = **f**(**x**) from labeled data
- Choose *hypothesis space* **f**(**x**) belongs to
  - hypothesis space **f**(**x**,**w**) is parameterized by vector of *weights* **w**
  - each setting of **w** corresponds to a different hypothesis

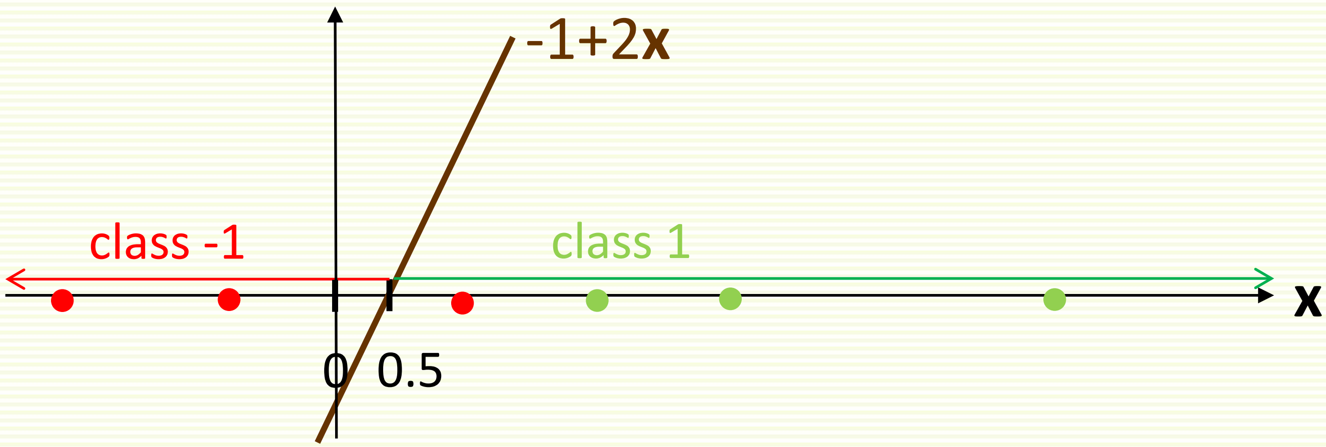
hypothesis space



- find **f**(**x**,**w**) in the hypothesis space s.t. **f**($\mathbf{x}^i$,**w**) = $\mathbf{y}^i$ "as much as possible" for training examples
  - "as much as possible" can be defined with loss function **L**(**f**(**x**,**w**),**y**)

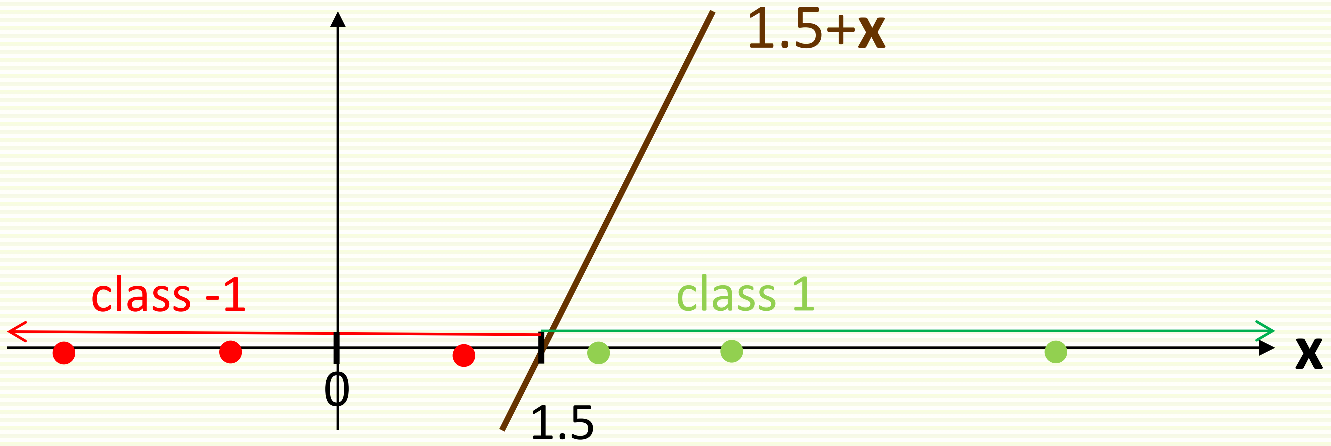
Training Phase Example in 1D

- 2 class classification problem
  - $y^i \in \{-1,1\}$
- Examples are one dimensional feature vectors
  - examples in class -1: {-2, -1, 1}
  - examples in class 1: {2, 3, 5}
- Hypothesis space $\mathbf{f}(\mathbf{x},\mathbf{w}) = \text{sign}(\mathbf{w}_0 + \mathbf{w}_1\mathbf{x})$
  - $\mathbf{w} = \begin{bmatrix} \mathbf{w}_0 \\ \mathbf{w}_1 \end{bmatrix}$
  - one member is $\mathbf{f}(\mathbf{x}) = \text{sign}(-1 + 2\mathbf{x})$, i.e. $\mathbf{w}_0 = -1$, $\mathbf{w}_1 = 2$



Training Phase Example in 1D

- 2 class classification problem
  - $\mathbf{y}^i \in \{-1,1\}$
- Examples are one dimensional feature vectors
  - examples in class -1: {-2, -1, 1}
  - examples in class 1: {2, 3, 5}
- Let classifier be $\mathbf{f}(\mathbf{x},\mathbf{w}) = \text{sign}(\mathbf{w}_0+\mathbf{w}_1\mathbf{x})$
  - another member is $\mathbf{f}(\mathbf{x}) = \text{sign}(-1.5 + \mathbf{x})$, i.e. $\mathbf{w_0} = -1.5$, $\mathbf{w_1} = 1$

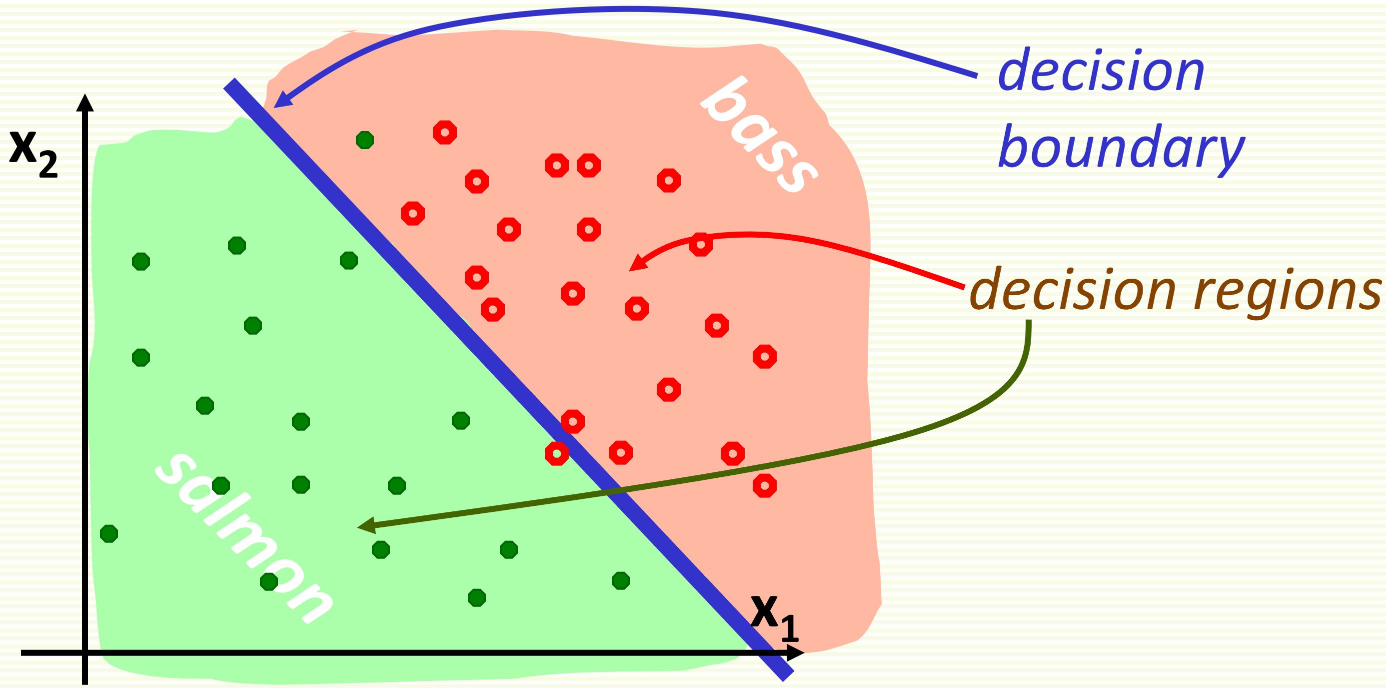


- Often say $\mathbf{f}(\mathbf{x},\mathbf{w})$ is a classifier, and the process of finding good $\mathbf{w}$ is *weight tuning*

Training Phase Example in 2D

- For 2 class problem and 2 dimensional samples

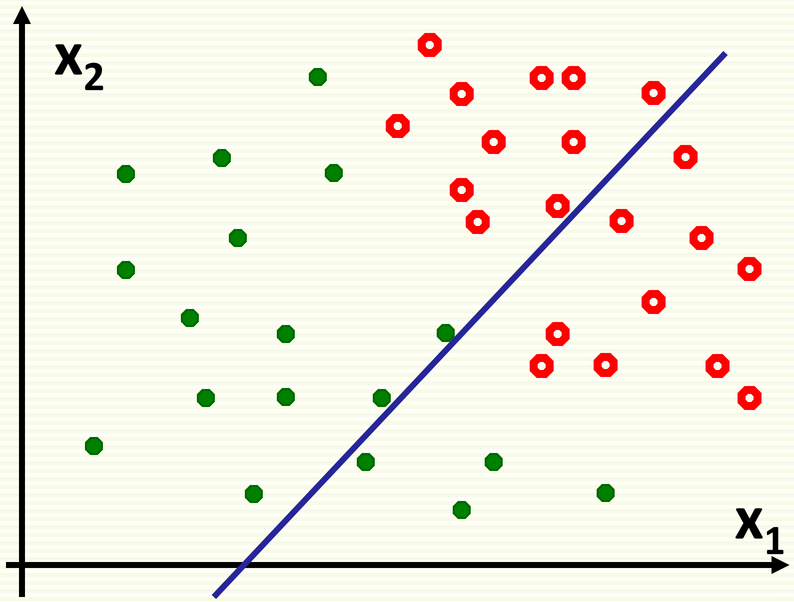
$$\mathbf{f}(\mathbf{x},\mathbf{w}) = \text{sign}(\mathbf{w}_0+\mathbf{w}_1\mathbf{x}_1+\mathbf{w}_2\mathbf{x}_2)$$



- Can be generalized to examples of arbitrary dimension
- Classifier that makes a decision based on linear combination of features is called a **linear classifier**

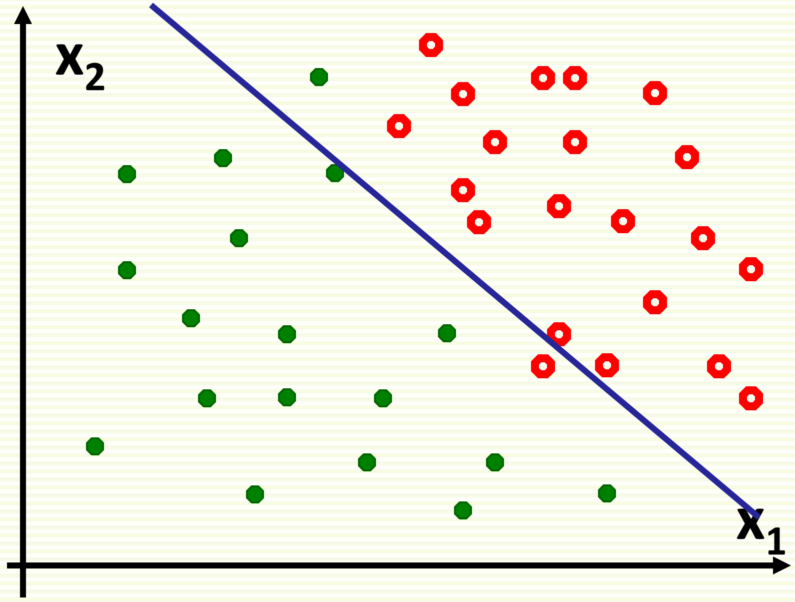
Training Phase: Linear Classifier

bad setting of **w**



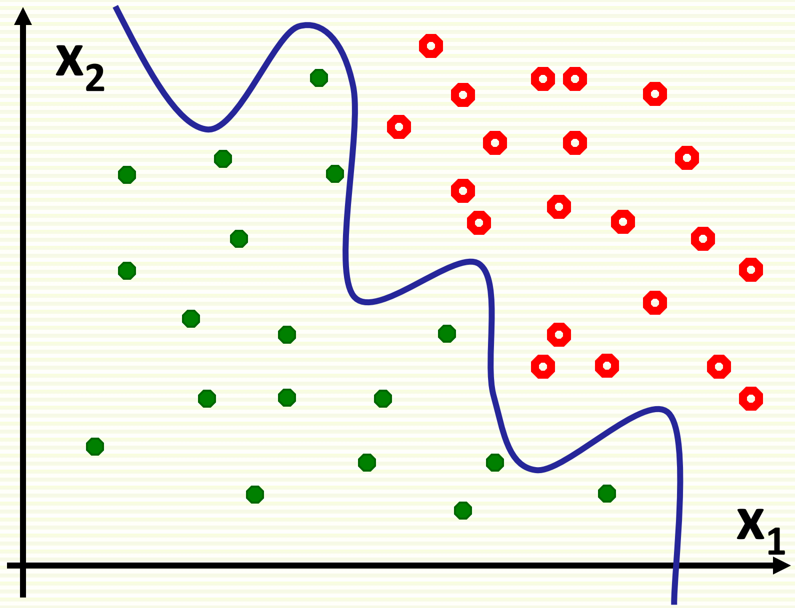
classification error 38%

best setting of **w**



classification error 4%

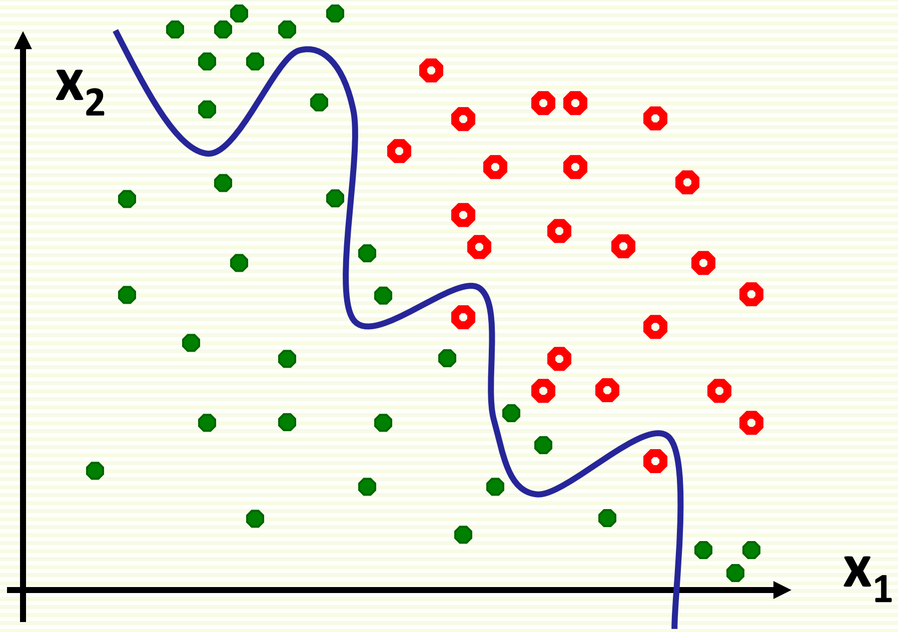
Training Stage: More Complex Classifier



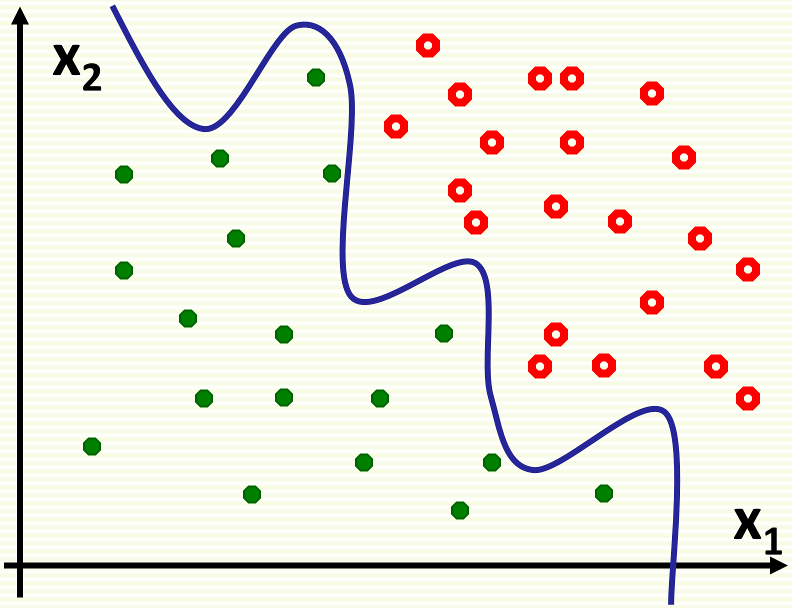
- for example if **f**(**x**,**w**) is a polynomial of high degree
- 0% classification error

Test Classifier on New Data

- The goal is for classifier to perform well on new data
- Test "wiggly" classifier on new data: 25% error



Overfitting



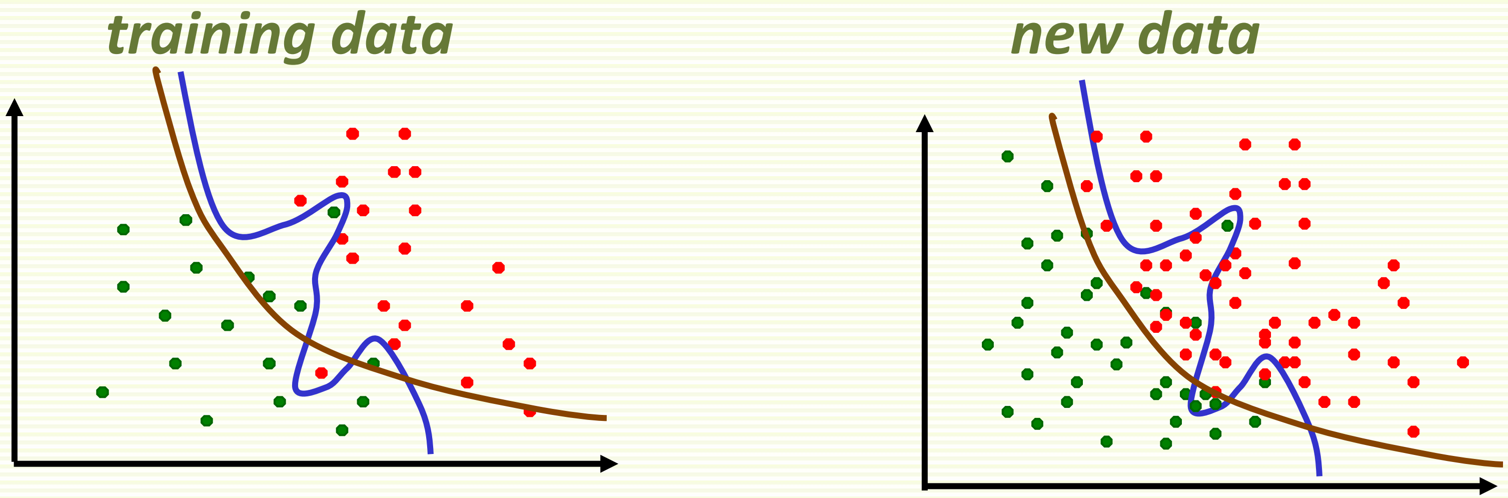
- Have only limited amount of data for training
- Overfitting
  - complex model often have too many parameters to fit reliably with a limited amount of training data
  - Complex model may adapt too closely to the random noise of the training data

Overfitting: Extreme Example

- 2 class problem: face and non-face images
- Memorize (i.e. store) all the “face” images
- For a new image, see if it is one of the stored faces
  - if yes, output “face” as the classification result
  - If no, output “non-face”
  - also called “rote learning”
- **problem**: new “face” images are different from stored “face” examples
  - zero error on stored data, 50% error on test (new) data
  - decision boundary is very irregular
- Rote learning is memorization without generalization

slide is modified from Y. LeCun

Generalization



- The ability to produce correct outputs on previously unseen examples is called **generalization**
- Big question of learning theory: how to get good generalization with a limited number of examples
- Intuitive idea: favor simpler classifiers
  - William of Occam (1284-1347): "entities are not to be multiplied without necessity"
- Simpler decision boundary may not fit ideally to the training data but tends to generalize better to new data

Training and Testing

- How to diagnose overfitting?
- Divide all labeled samples $\mathbf{x}^1, \mathbf{x}^2, \ldots \mathbf{x}^n$ into *training* set and *test* set
- Use training set (training samples) to tune classifier weights **w**
- Use test set (test samples) to see how well classifier with tuned weights **w** work on unseen examples
- Thus there are 2 main phases in classifier design
  1. training
  2. testing

Training Phase

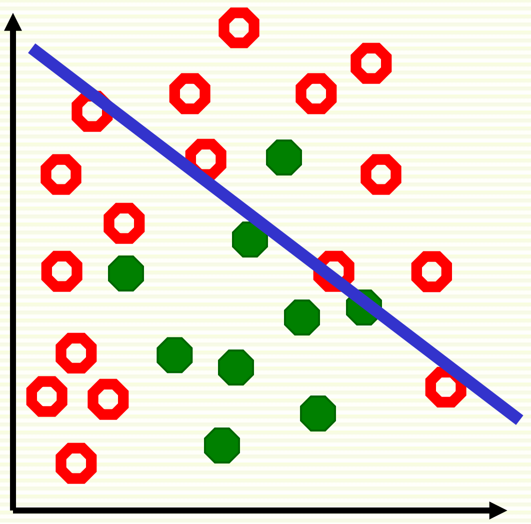
- Find weights $\mathbf{w}$ s.t. $f(\mathbf{x}^i,\mathbf{w}) = \mathbf{y}^i$ "as much as possible" for *training* samples $\mathbf{x}^i$
  - "as much as possible" needs to be defined
    - usually some penalty whenever $f(\mathbf{x}^i,\mathbf{w}) \neq \mathbf{y}^i$
    - penalty defined with loss function $\mathbf{L}(\mathbf{f}(\mathbf{x}^i,\mathbf{w}),\ \mathbf{y}^i)$
  - how to search for such $\mathbf{w}$?
    - usually through optimization, can be quite time consuming
  - classification error on training data is called *training error*

Testing Phase

- The goal is good performance on unseen examples
- Evaluate performance of the trained classifier **f**(**x**,**w**) on the test samples (unseen labeled samples)
- Testing on unseen labeled examples lets us approximate how well classifier will perform in practice
- If testing results are poor, may have to go back to the training phase and redesign **f**(**x**,**w**)
- Classification error on test data is called *test error*
- Side note
  - when we “deploy” the final classifier **f**(**x**,**w**) in practice, this is also called testing

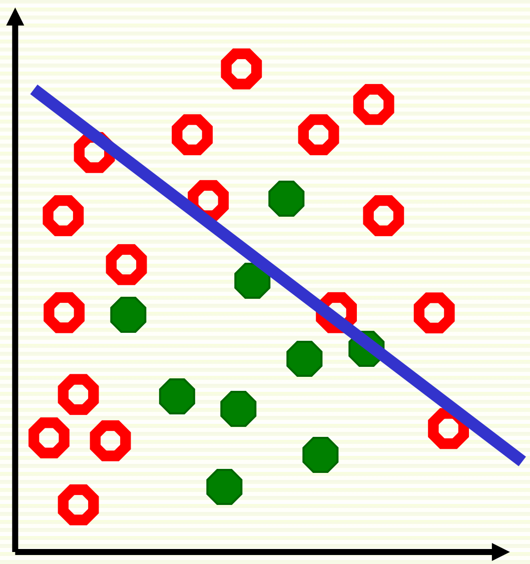
Underfitting

- Can also underfit data, i.e. too simple decision boundary
  - chosen hypothesis space is not expressive enough
- No linear decision boundary can well separate the samples
- Training error is too high
  - test error is, of course, also high



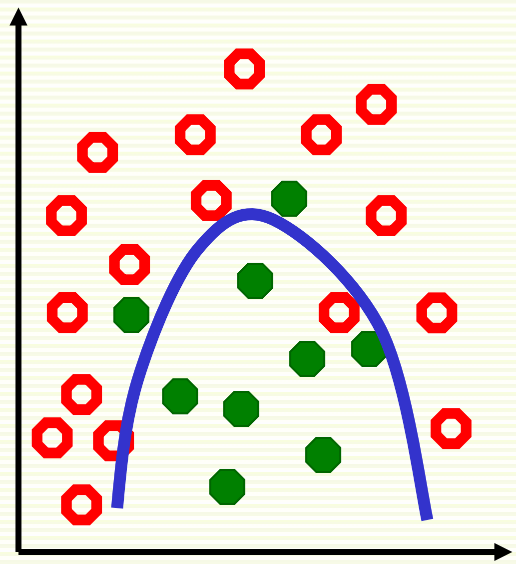
Underfitting → Overfitting

underfitting



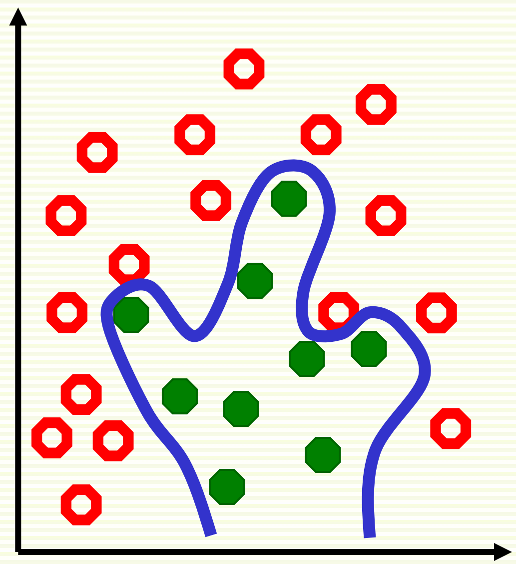
- high training error
- high test error

"just right"



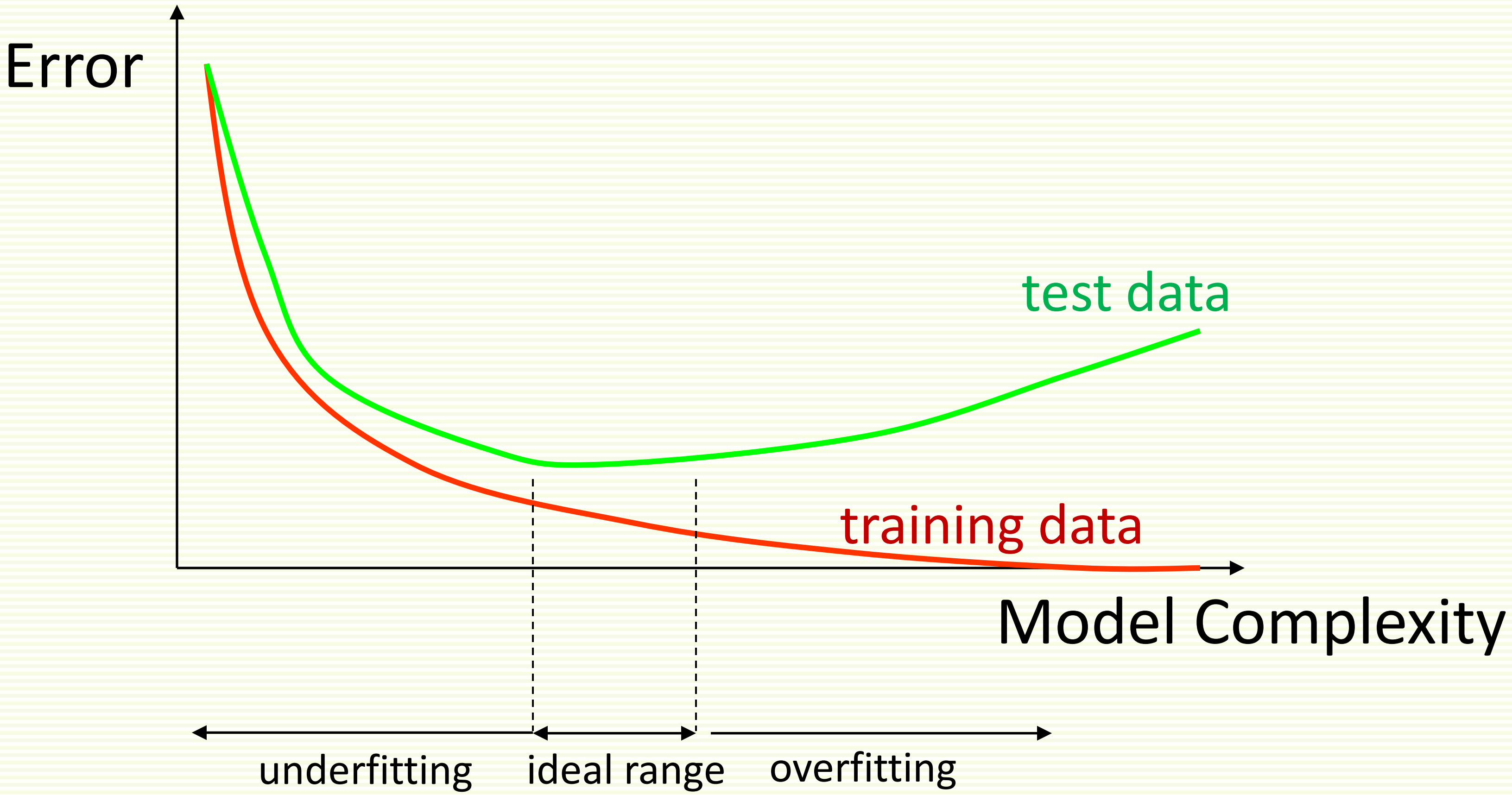
- low training error
- low test error

overfitting



- low training error
- high test error

How Overfitting affects Prediction



Fixing Underfitting/Overfitting

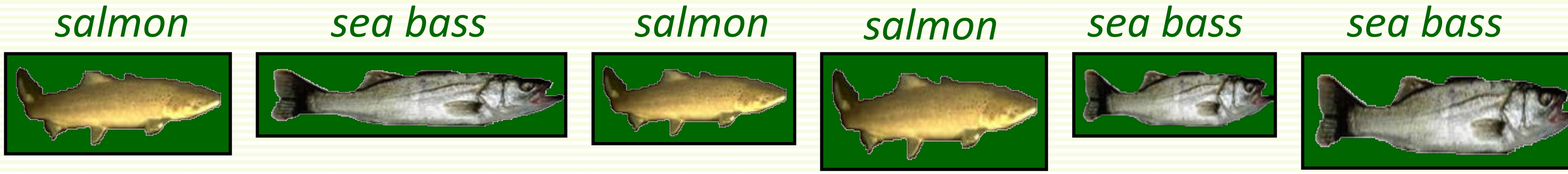
- Underfitting
  - add more features
  - use more complex **f**(**x**,**w**)
- Overfitting
  - remove features
  - collect more training data
  - use less complex **f**(**x**,**w**)

Sketch of Supervised Machine Learning

- Chose a hypothesis space **f**(**x**,**w**)
  - **w** are tunable weights
  - **x** is the input sample
  - tune **w** so that **f**(**x**,**w**) gives the correct label for training samples **x**
- Which hypothesis space **f**(**x**,**w**) to choose?
  - has to be expressive enough to model our problem well, i.e. to avoid ***underfitting***
  - yet not to complicated to avoid ***overfitting***

Classification System Design Overview

- Collect and label data by hand



- Split data into training and test sets
- Preprocess data (i.e. segmenting fish from background)

- Extract possibly discriminating features
  - length, lightness, width, number of fins,etc.
- Classifier design
  - Choose model for classifier
  - Train classifier on training data
- Test classifier on test data

we mostly look at these steps in the course

Basic Linear Algebra

- Basic Concepts in Linear Algebra
  - vectors and matrices
  - products and norms

Why Linear Algebra?

- For each example (e.g. a fish image), we extract a set of features (e.g. length, width, color)
- This set of features is represented as a *feature vector*
  - [length, width, color]

- All collected examples will be represented as collection of (feature) vectors

$[l_1, w_1, c_1]$ example 1

$[l_2, w_2, c_2]$ example 2

$[l_3, w_3, c_3]$ example 3

$$\longrightarrow \begin{bmatrix} l_1 & w_1 & c_1 \\ l_2 & w_2 & c_2 \\ l_3 & w_3 & c_3 \end{bmatrix}$$

matrix

- Often use linear classifiers since they are simple and computationally tractable

What is a Matrix?

- A matrix is a set of elements, organized into rows and columns

$$\xrightarrow{\qquad\qquad\text{rows}\qquad\qquad}$$

$$\begin{array}{c|cc} & \left[\begin{array}{cccc} 2 & 7 & 6 & 10 \\ 1 & 4 & 4 & 9 \\ 6 & 4 & 9 & 6 \end{array}\right] & \begin{array}{l} \text{example 1} \\ \text{example 2} \\ \text{example 3} \end{array} \\ \text{columns} \downarrow & \begin{array}{cccc} \text{feature 1} & \text{feature 2} & \text{feature 3} & \text{feature 4} \end{array} & \end{array}$$

Basic Matrix Operations

- addition, subtraction, multiplication by a scalar

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} + \begin{bmatrix} e & f \\ g & h \end{bmatrix} = \begin{bmatrix} a+e & b+f \\ c+g & d+h \end{bmatrix}$$ add elements

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} - \begin{bmatrix} e & f \\ g & h \end{bmatrix} = \begin{bmatrix} a-e & b-f \\ c-g & d-h \end{bmatrix}$$ subtract elements

$$\alpha \cdot \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} \alpha \cdot a & \alpha \cdot b \\ \alpha \cdot c & \alpha \cdot d \end{bmatrix}$$ multiply every entry

Matrix Transpose

- **n** by **m** matrix A and its **m** by **n** transpose A^T

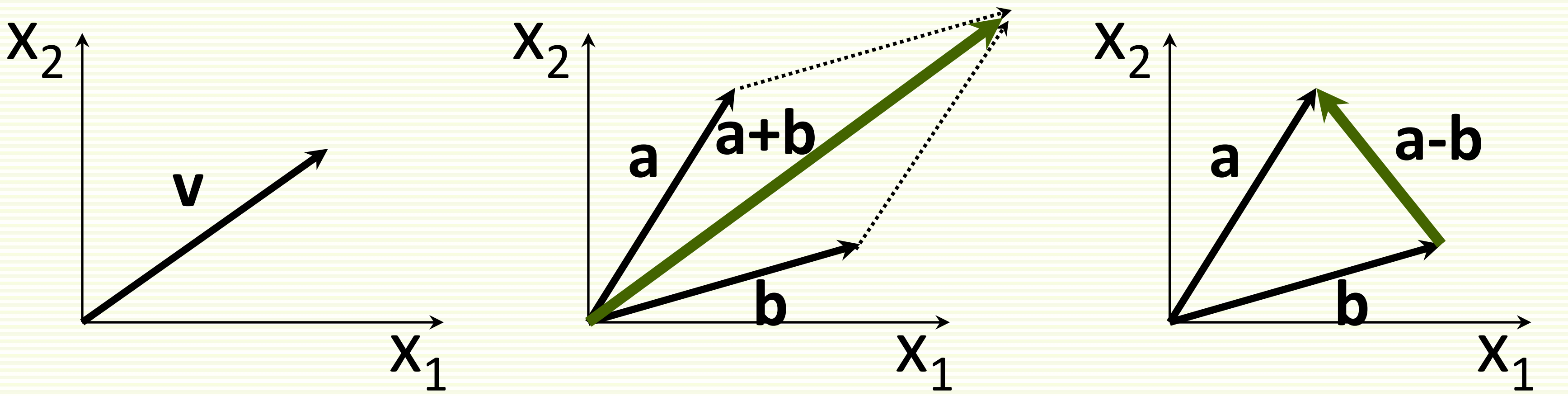
$$A = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2m} \\ \vdots & \vdots & \cdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nm} \end{bmatrix} \qquad A^T = \begin{bmatrix} x_{11} & x_{21} & \cdots & x_{n1} \\ x_{12} & x_{22} & \cdots & x_{n2} \\ \vdots & \vdots & \cdots & \vdots \\ x_{1m} & x_{2m} & \cdots & x_{nm} \end{bmatrix}$$

Vectors

- Vector: N x 1 matrix

$$v = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

- **dot product** and **magnitude** defined on vectors only



vector addition

vector subtraction

More on Vectors

- n-dimensional row vector $x = \begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix}$

- Transpose of row vector is column vector $x^T = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$

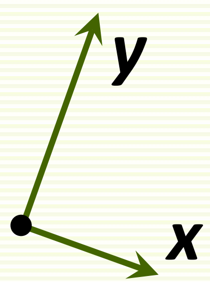
- *Vector* product (or *inner* or *dot* product)

$$\langle x, y \rangle = x \cdot y = x^T y = x_1 y_1 + x_2 y_2 + \dots + x_n y_n = \sum_{i=1 \dots n} x_i y_i$$

More on Vectors

- *Euclidian norm* or *length* $\|x\| = \sqrt{\langle x, x \rangle} = \sqrt{\sum_{i=1\ldots n} x_i^2}$
- If ||***x***|| =1 we say ***x*** is *normalized* or *unit* length
- angle *q* between vectors ***x*** and ***y*** : $\cos \boldsymbol{\theta} = \dfrac{x^T y}{\|x\|\|y\|}$
- inner product captures direction relationship

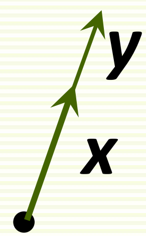
$\cos \boldsymbol{\theta} = 0$



$x^T y = 0$

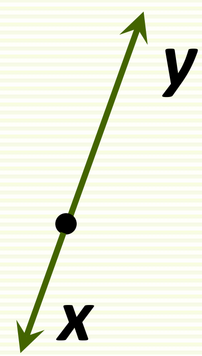
$x \perp y$

$\cos \theta = 1$



$x^T y = \|x\|\|y\| > 0$

$\cos \theta = -1$



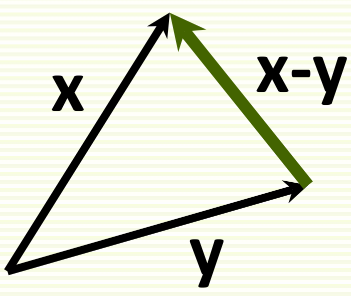
$x^T y = -\|x\|\|y\| < 0$

More on Vectors

- Vectors x and y are orthonormal if they are orthogonal and ||x|| = ||y|| =1

- Euclidian distance between vectors x and y

$$\|x - y\| = \sqrt{\sum_{i=1\ldots n} (x_i - y_i)^2}$$



Matrix Product

$$AB = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1d} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nd} \end{bmatrix} \begin{bmatrix} b_{11} & \cdots & b_{1m} \\ b_{21} & \cdots & b_{2m} \\ b_{31} & \cdots & b_{3m} \\ \vdots & \cdots & \vdots \\ b_{d1} & \cdots & b_{dm} \end{bmatrix} = \begin{bmatrix} & & \\ & c_{ij} & \\ & & \end{bmatrix}$$

$c_{ij} = \langle a^i, b_j \rangle$

a^i is row ***i*** of ***A***

b_j is column ***j*** of ***B***

- # of columns of A = # of rows of B
- even if defined, in general AB ≠ BA

MATLAB

- Starting matlab
  - xterm -fn 12X24
  - matlab
  - matlab -nodisplay
- Basic Navigation
  - quit
  - more
  - help general
- Scalars, variables, basic arithmetic
  - Clear
  - + - * / ^
  - help arith
- Relational operators
  - ==,&,|,~,xor
  - help relop
- Lists, vectors, matrices
  - A=[2 3;4 5]
  - A’
- Matrix and vector operations
  - find(A>3), colon operator
  - * / ^ .* ./ .^
  - eye(n),norm(A),det(A),eig(A)
  - max,min,std
  - help matfun
- Elementary functions
  - help elfun
- Data types
  - double
  - Char
- Programming in Matlab
  - .m files
  - scripts
  - function y=square(x)
  - help lang
- Flow control
  - if i== 1else end, if else if end
  - for i=1:0.5:2 … end
  - while i == 1 … end
  - Return
  - help lang
- Graphics
  - help graphics
  - help graph3d
- File I/O
  - load,save
  - fopen, fclose, fprintf, fscanf