Overview



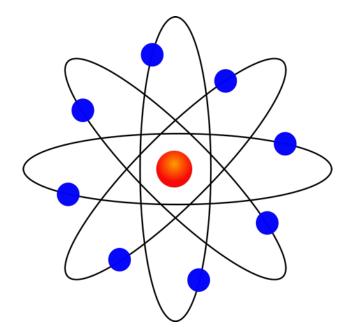


Rapid growth of massive datasets

E.g., Online activity, Science, Sensor networks

Data





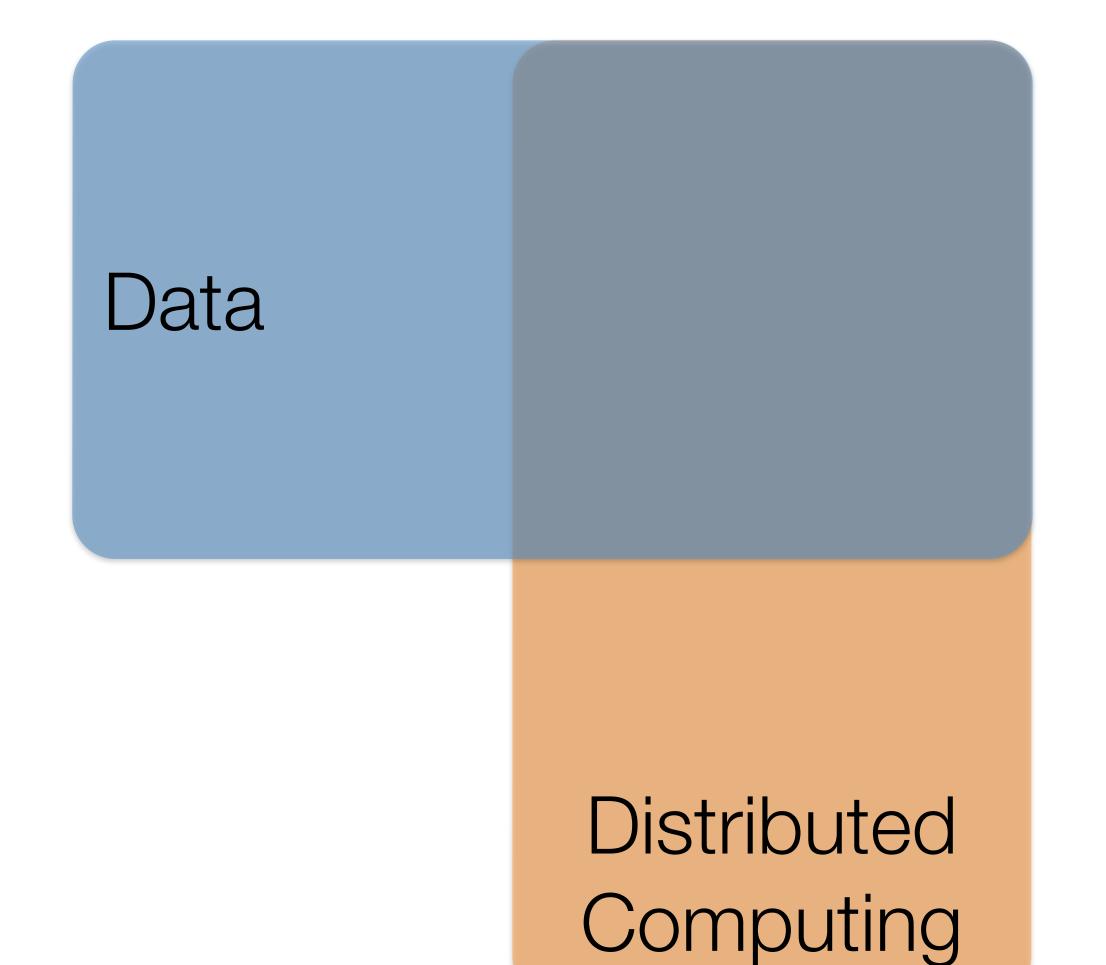








Distributed Clusters are Pervasive











Mature Methods for Common Problems

e.g., classification, regression, collaborative filtering, clustering

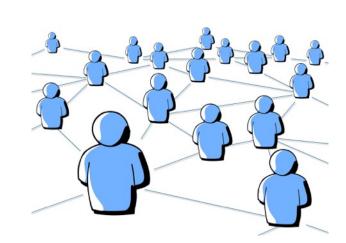
Machine Data Learning Distributed Computing

ML is Applied Everywhere

E.g., Personalized recommendations, Speech recognition, Face detection, Protein structure, Fraud detection, Spam filtering, Playing chess or Jeopardy, Unassisted vehicle control, Medical diagnosis, ...

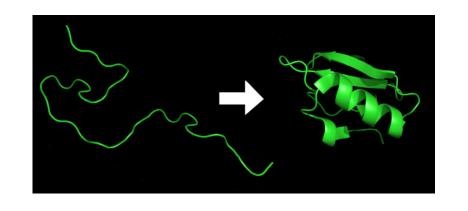
Data Machine Learning





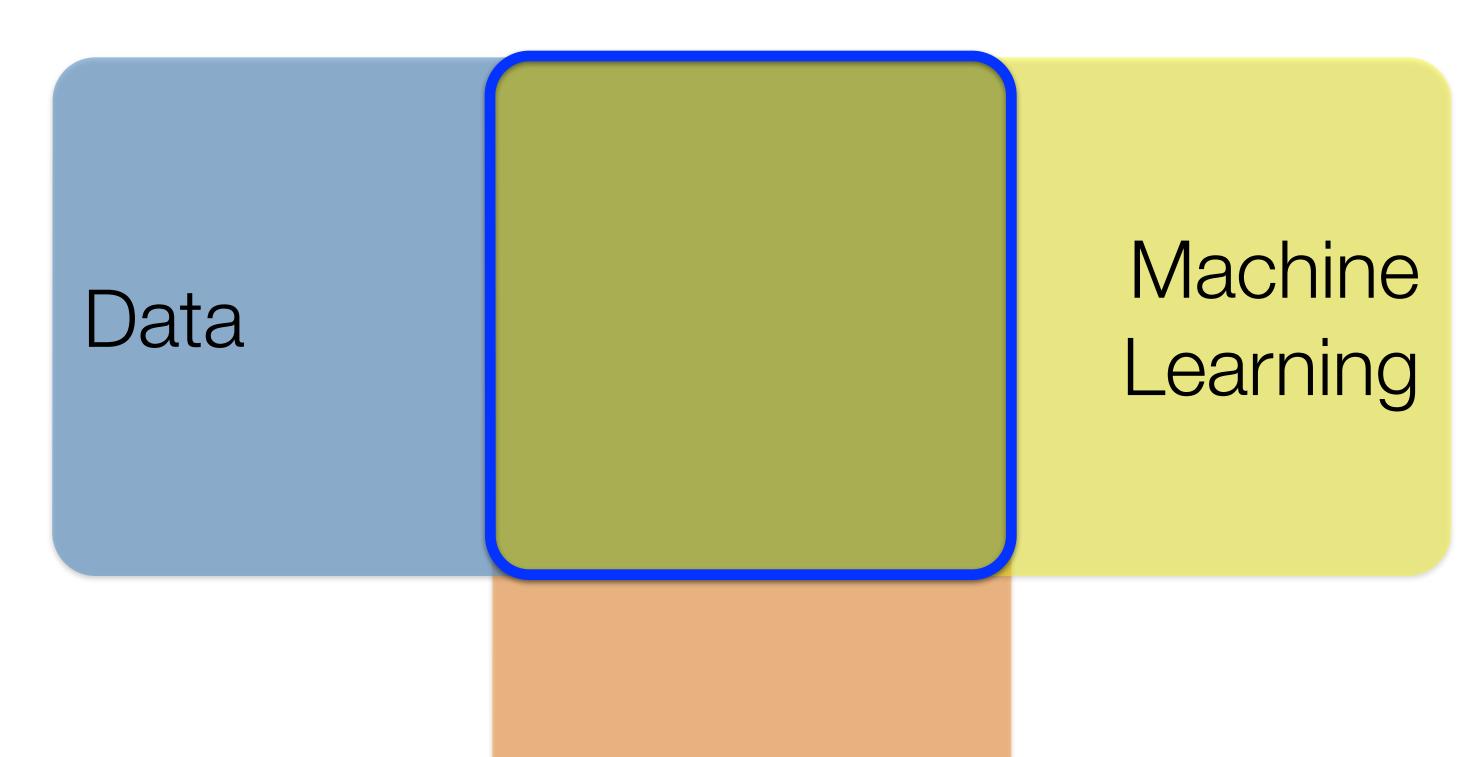
Distributed Computing



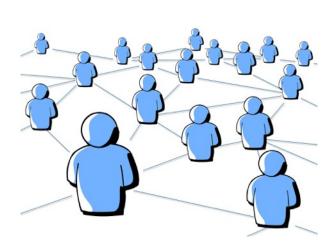


ML is Applied Everywhere

E.g., Personalized recommendations, Speech recognition, Face detection, Protein structure, Fraud detection, Spam filtering, Playing chess or Jeopardy, Unassisted vehicle control, Medical diagnosis, ...

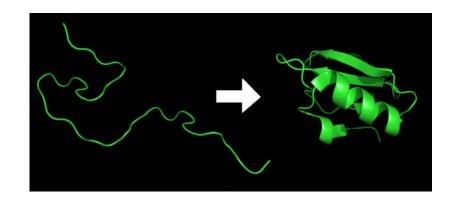






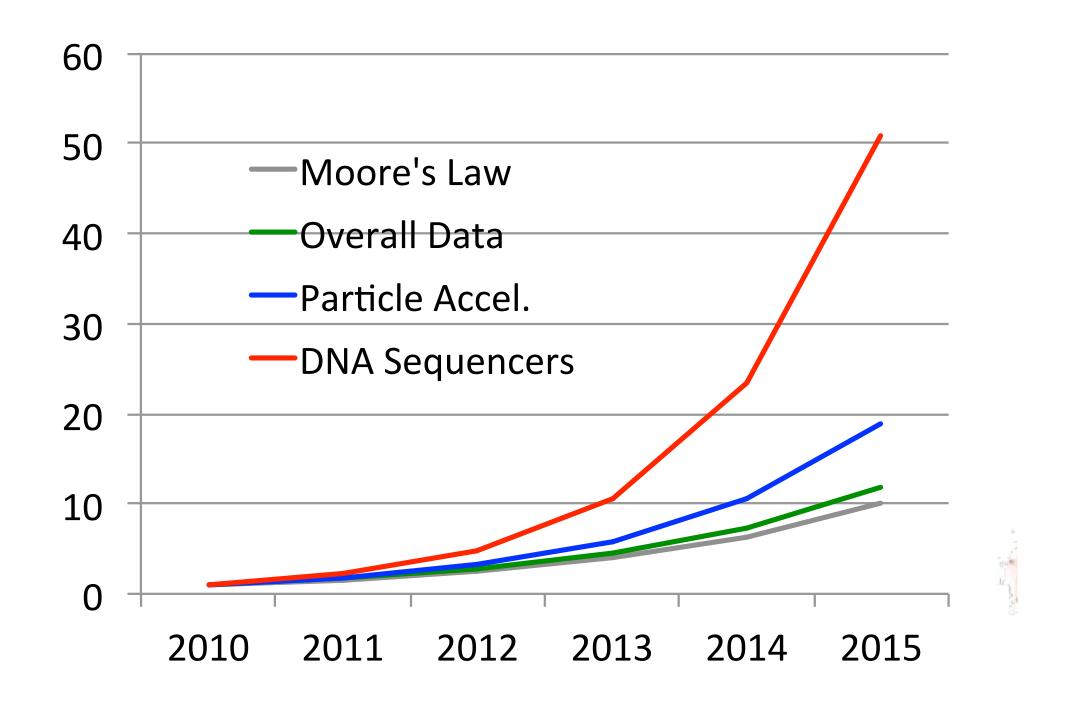
Distributed Computing



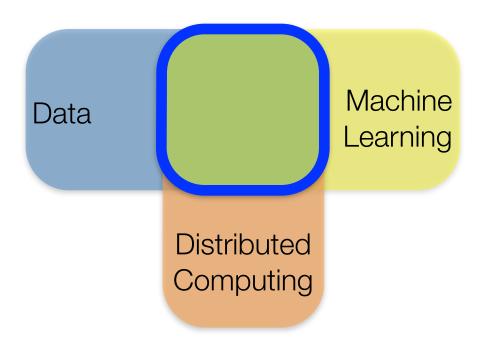


Challenge: Scalability

Classic ML techniques are not always suitable for modern datasets



Data Grows Faster than Moore's Law [IDC report, Kathy Yelick, LBNL]



Course Goals

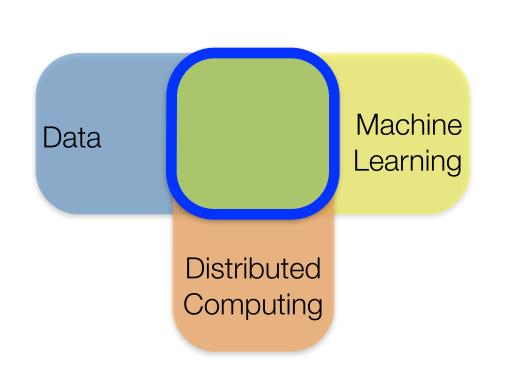
Focus on scalability challenges for common ML tasks

How can we use raw data to train statistical models?

- Study typical ML pipelines
- Classification, regression, exploratory analysis

How can we do so at scale?

- Study distributed machine learning algorithms
- Implement distributed pipelines in Apache Spark using real datasets
- Understand details of MLlib (Spark's ML library)



Prerequisites

Basic Python, ML, math background

First week provides review of ML and useful math concepts

Self-assessment exam has pointers to review material

http://cs.ucla.edu/~ameet/self_assessment.pdf

Assumes no knowledge of Spark

Second week introduces Spark

Schedule

5 weeks of lectures, 5 Spark coding labs, 1 setup lab

- Week 0: Setup software environment
- Week 1: ML overview, Math review
- Week 2: Spark Overview [from CS100.1x]
- Week 3: Distributed ML Principles and Linear Regression
- Week 4: Classification with Click-through Rate Prediction
- Week 5: Exploratory Analysis with Brain Imaging Data

Distributed Computing and Apache Spark



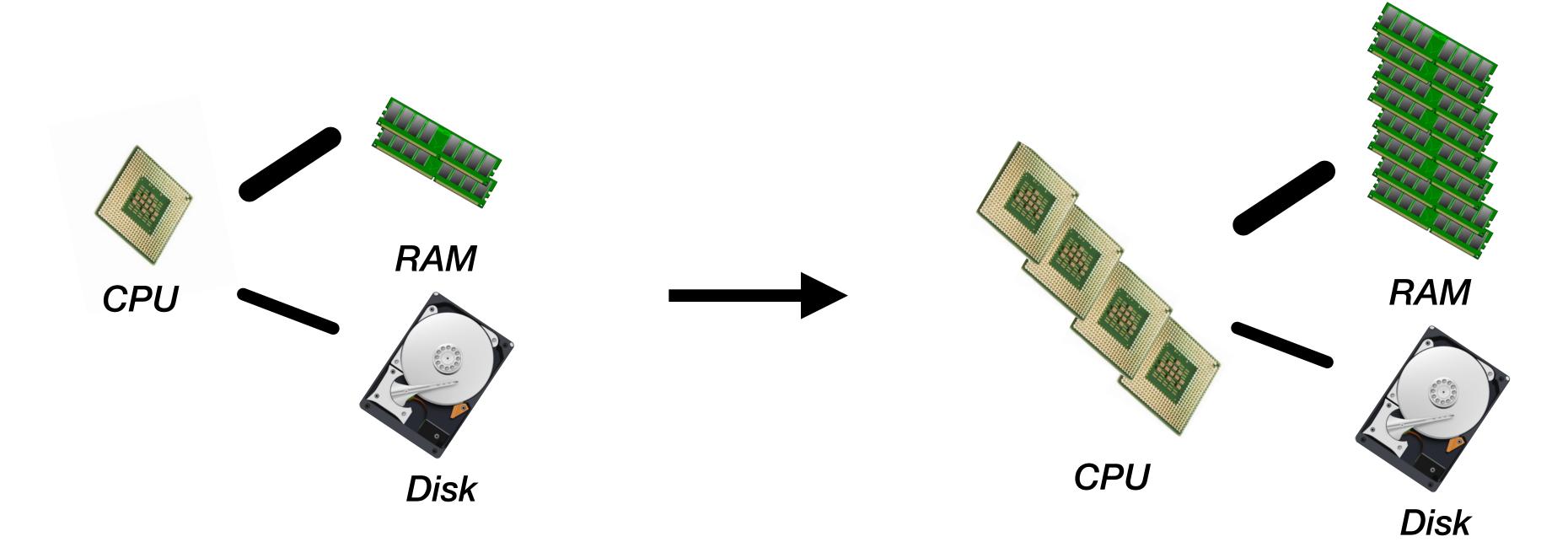


How to Handle Massive Data?

Need more hardware to store / process modern data

Scale-up (one big machine)

- Can be very fast for medium scale problems
- Expensive, specialized hardware
- Eventually hit a wall

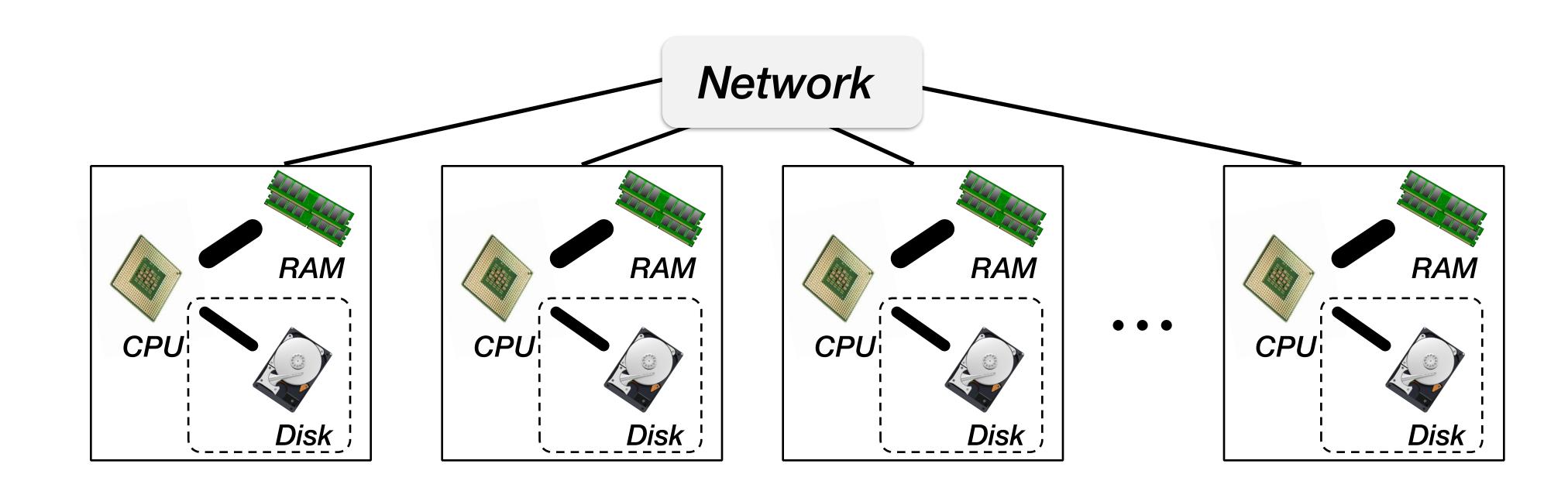


How to Handle Massive Data?

Need more hardware to store / process modern data

Scale-out (distributed, e.g., cloud-based)

- Commodity hardware, scales to massive problems
- Need to deal with network communication
- Added software complexity



What is Apache Spark?

General, open-source cluster computing engine

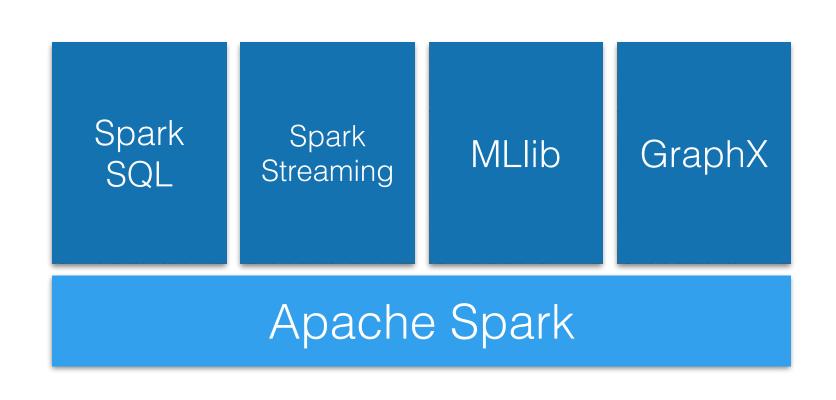
Well-suited for machine learning

- Fast iterative procedures
- Efficient communication primitives

Simple and Expressive

- APIs in Scala, Java, Python, R
- Interactive Shell

Integrated Higher-Level Libraries



What is Machine Learning?





A Definition

Constructing and studying methods that learn from and make predictions on data

Broad area involving tools and ideas from various domains

- Computer Science
- Probability and Statistics
- Optimization
- Linear Algebra

Some Examples

Face recognition

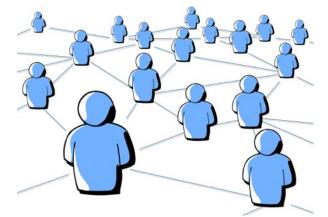
Link prediction



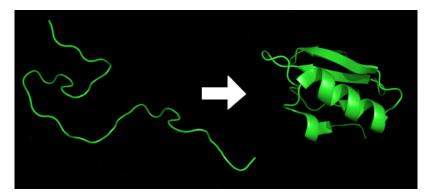
Protein structure prediction

Games, e.g., Backgammon or Jeopardy











Terminology

Observations. Items or entities used for learning or evaluation, e.g., emails

Features. Attributes (typically numeric) used to represent an observation, e.g., length, date, presence of keywords

Labels. Values / categories assigned to observations, e.g., spam, not-spam

Training and Test Data. Observations used to train and evaluate a learning algorithm, e.g., a set of emails along with their labels

- Training data is given to the algorithm for training
- Test data is withheld at train time

Two Common Learning Settings

Supervised learning. Learning from labeled observations

Labels 'teach' algorithm to learn mapping from observations to labels

Unsupervised learning. Learning from unlabeled observations

- Learning algorithm must find latent structure from features alone
- Can be goal in itself (discover hidden patterns, exploratory data analysis)
- Can be means to an end (preprocessing for supervised task)

Examples of Supervised Learning

Classification. Assign a category to each item, e.g., spam detection

- Categories are discrete
- Generally no notion of 'closeness' in multi-class setting

Regression. Predict a real value for each item, e.g., stock prices

- Labels are continuous
- Can define 'closeness' when comparing prediction with label

Examples of Unsupervised Learning

Clustering. Partition observations into homogeneous regions, e.g., to identify "communities" within large groups of people in social networks

Dimensionality Reduction. Transform an initial feature representation into a more concise representation, e.g., representing digital images

Typical Supervised Learning Pipeline

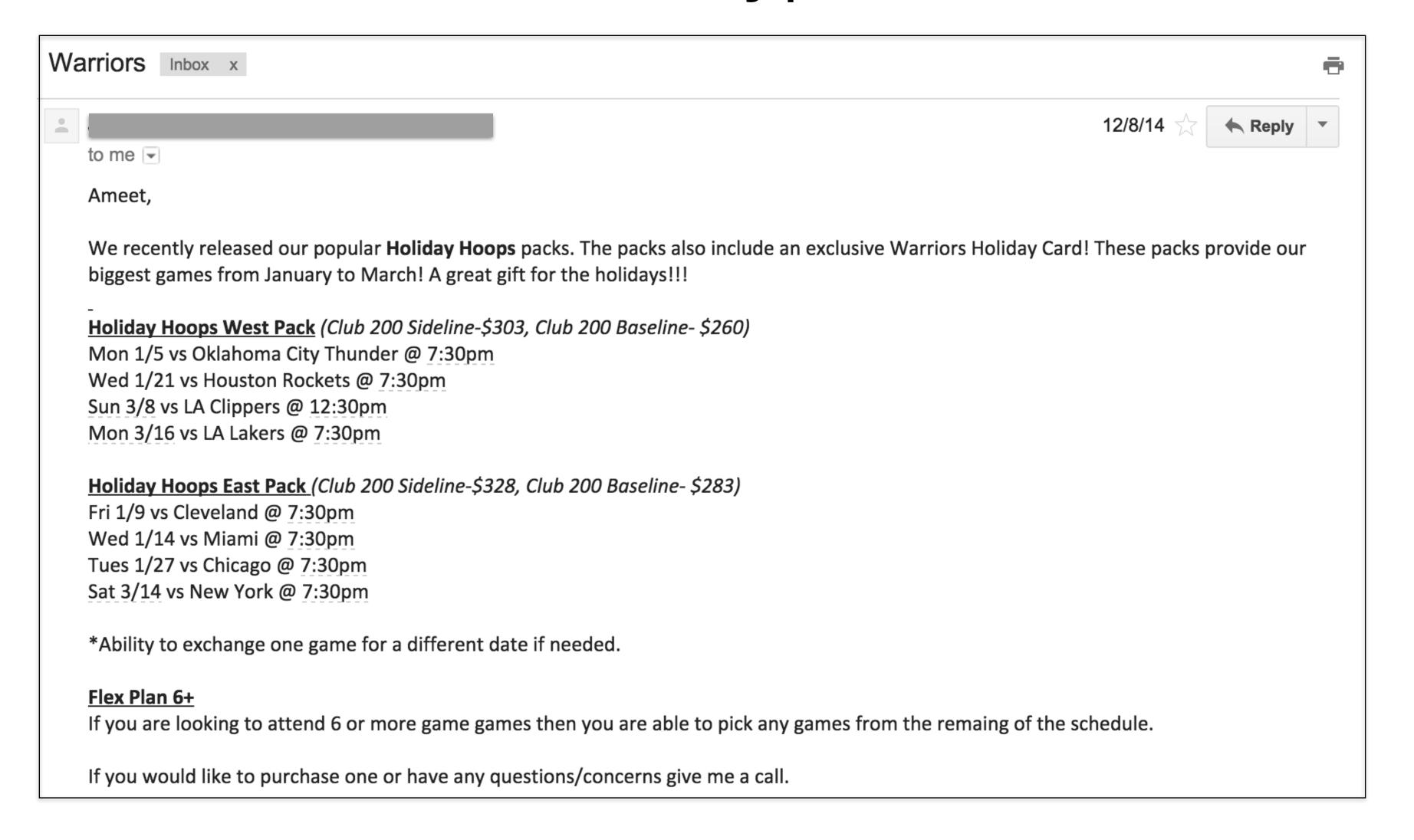




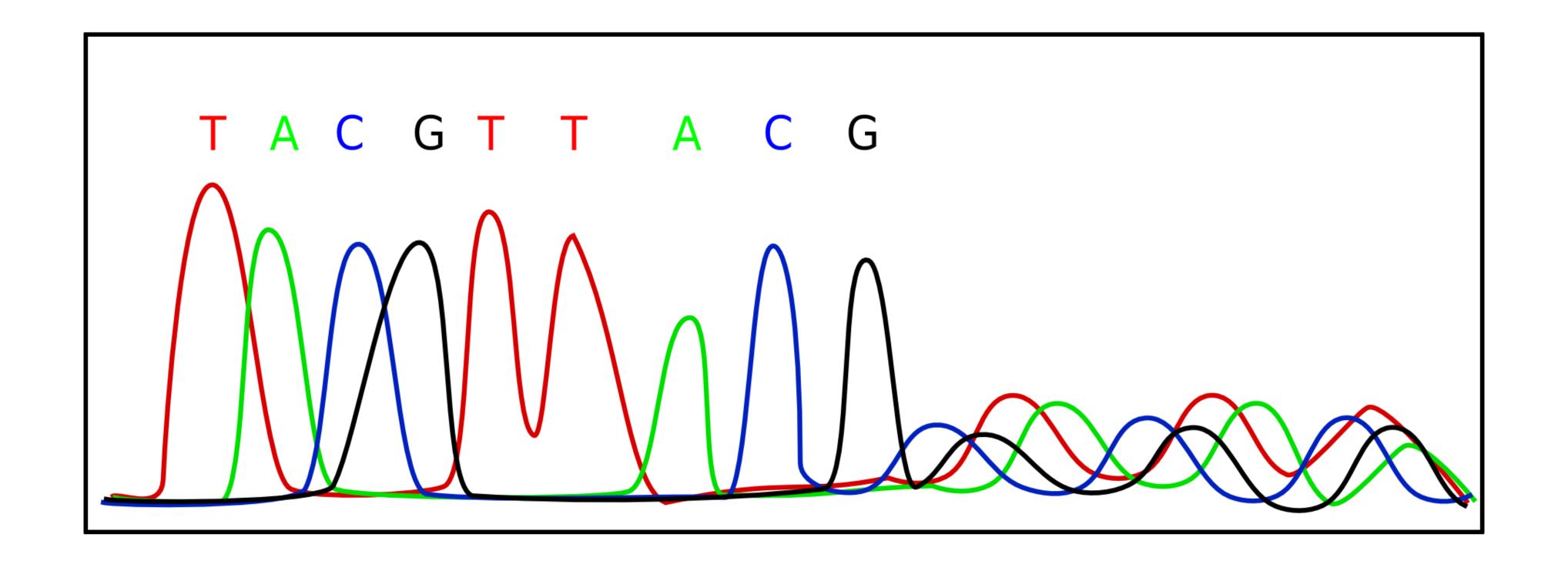
Raw data comes from many sources

Web hypertext

```
1 <!DOCTYPE html PUBLIC "-//W3C//DTD
   XHTML 1.0 Transitional//EN"
 2 "http://www.w3.org/TR/xhtml1/DTD/
   xhtml1-transitional.dtd">
 4 <html xmlns="http://www.w3.org/1999/
   xhtml">
 5
      <head>
           <meta http-equiv="Content-</pre>
  Type" content=
         "text/html; charset=us-
   ascii" />
          <script type="text/</pre>
   javascript">
               function reDo() {top.
   location.reload();}
               if (navigator.appName ==
10
   'Netscape') {top.onresize = reDo;}
               dom=document.
11
   getElementById;
12
      </script>
      </head>
13
       <body>
14
15
      </body>
16 </html>
```



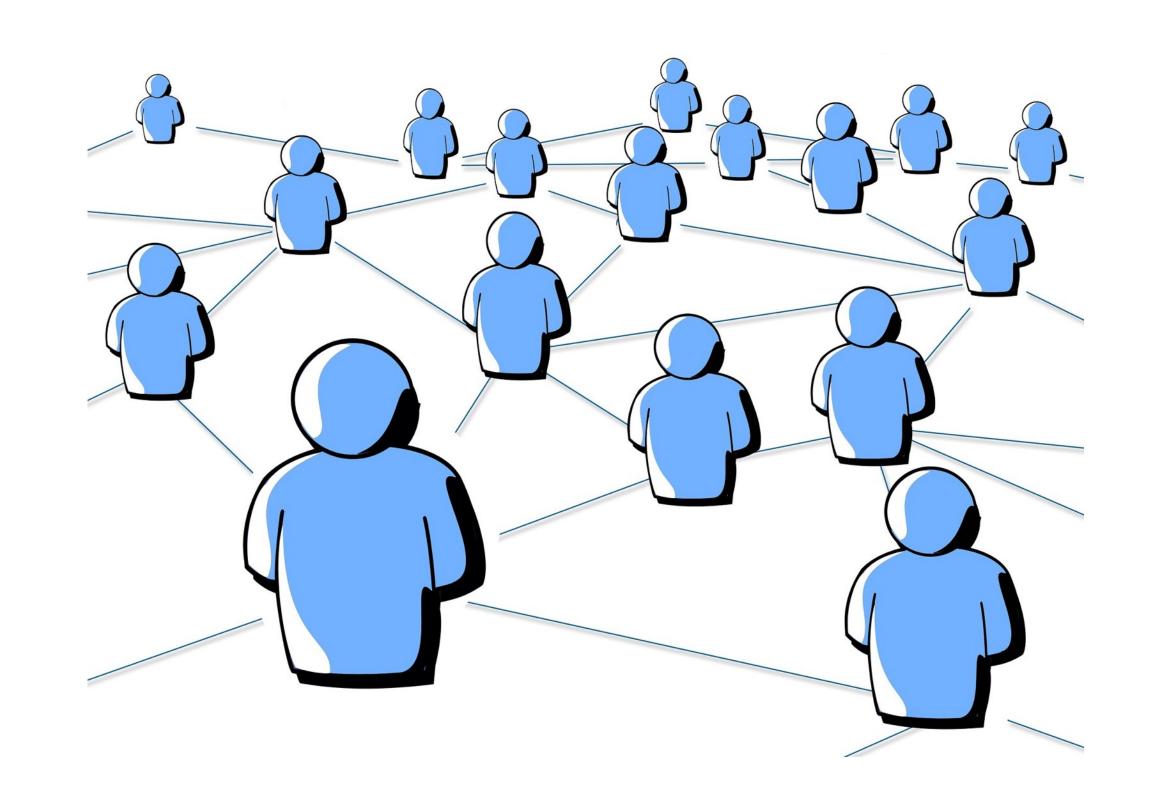
Email



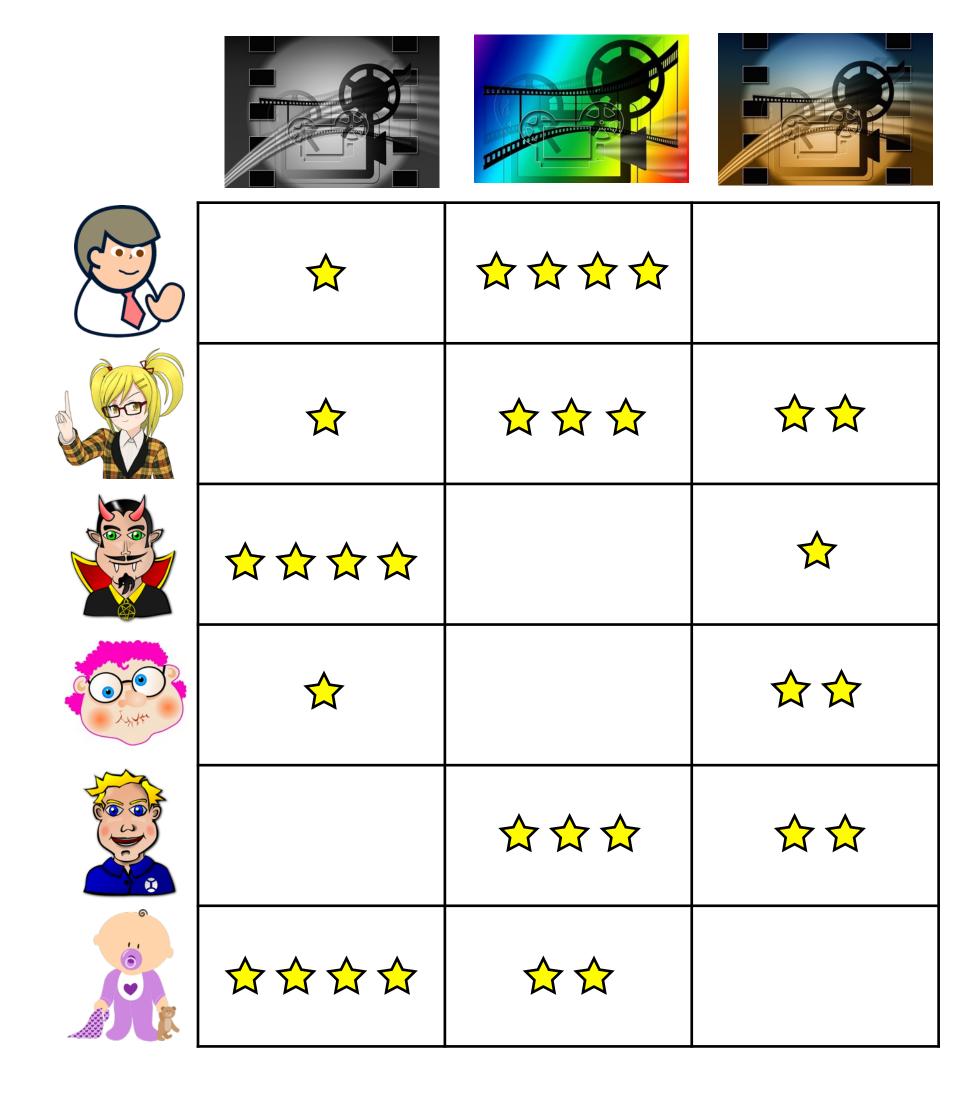
Genomic Data, e.g., SNPs



(Social) Networks / Graphs



User Ratings





Feature Extraction

Initial observations can be in arbitrary format

We extract features to represent observations

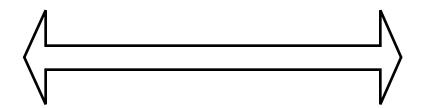
We can incorporate domain knowledge

We typically want numeric features

Success of entire pipeline often depends on choosing good descriptions of observations!!



Feature Extraction



Unsupervised Learning

Preprocessing step for supervised learning

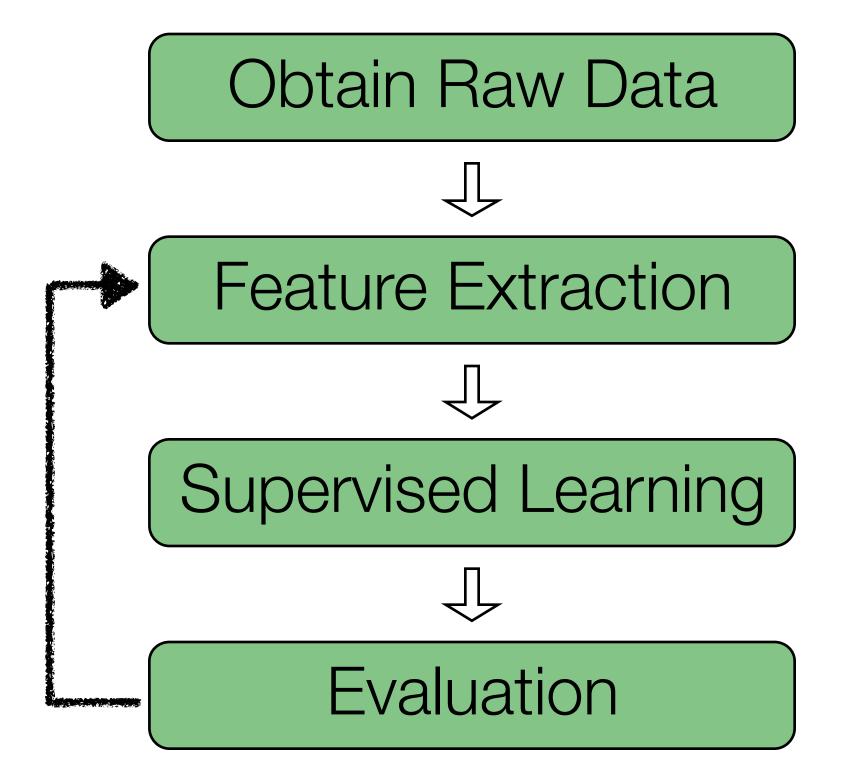


Feature Extraction



Supervised Learning

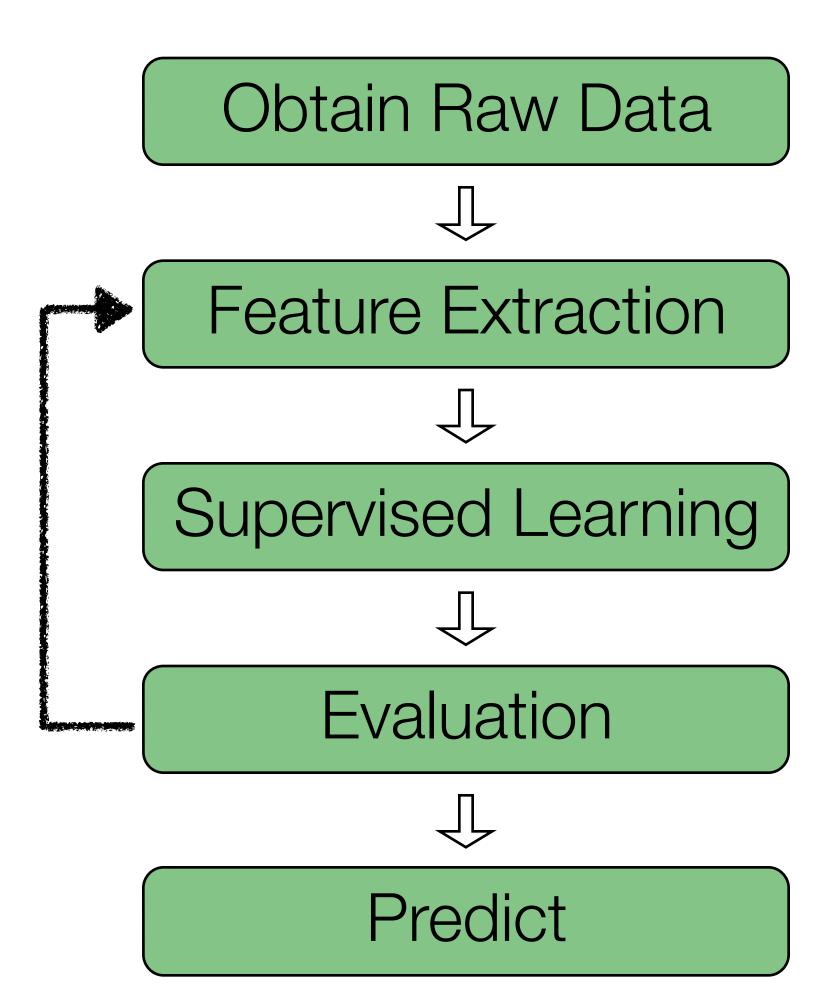
Train a supervised model using labeled data, e.g., Classification or Regression model



Q: How do we determine the quality of the model we've just trained?

A: We can evaluate it on test / hold-out data, i.e., labeled data not used for training

If we don't like the results, we iterate...



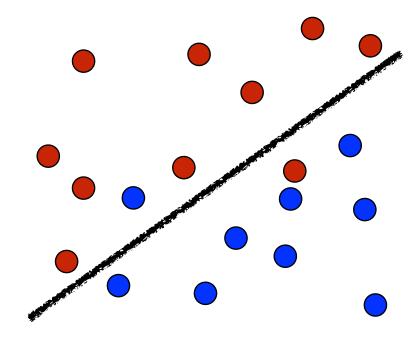
Once we're happy with our model, we can use it to make predictions on future observations, i.e., data without a known label

Sample Classification Pipeline





Classification

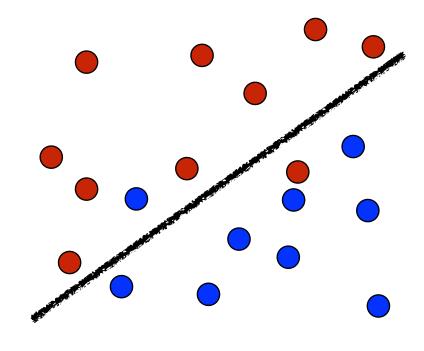


Goal: Learn a mapping from observations to discrete labels given a set of training examples (supervised learning)

Example: Spam Classification

- Observations are emails
- Labels are {spam, not-spam} (Binary Classification)
- Given a set of labeled emails, we want to predict whether a new email is spam or not-spam

Other Examples



Fraud detection: User activity → {fraud, not fraud}

Face detection: Images → set of people

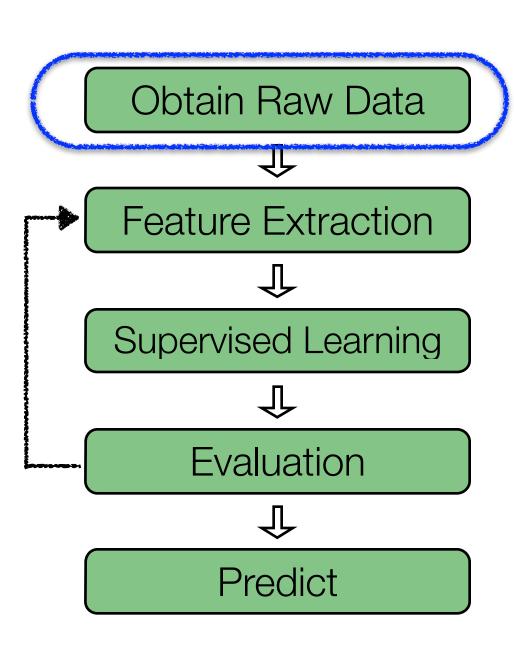
Link prediction: Users → {suggest link, don't suggest link}

Clickthrough rate prediction: User and ads → {click, no click}

Many others...

training set

Raw data consists of a set of labeled training observations



E.g., Spam Classification

Observation

Label

From: illegitimate@bad.com

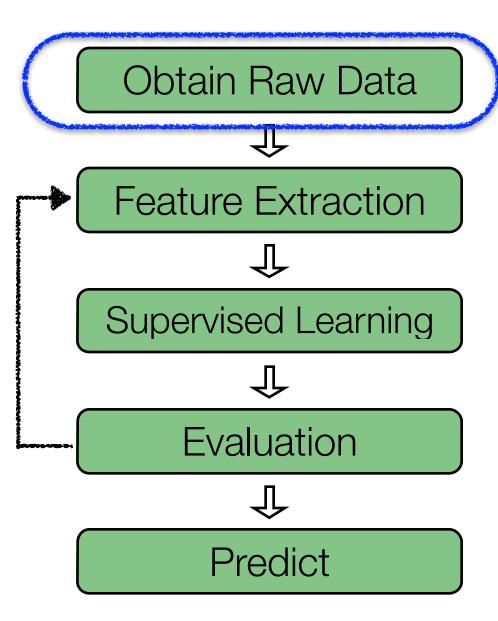
"Eliminate your debt by giving us your money..."

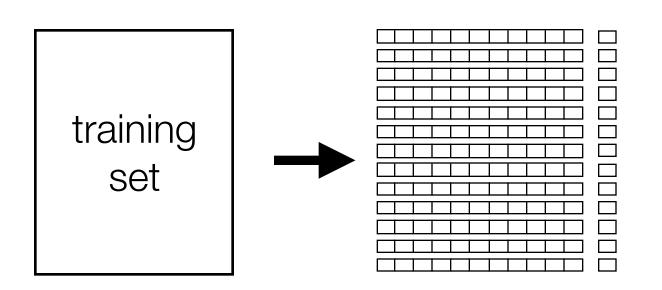
spam

From: bob@good.com

"Hi, it's been a while!
How are you? ..."

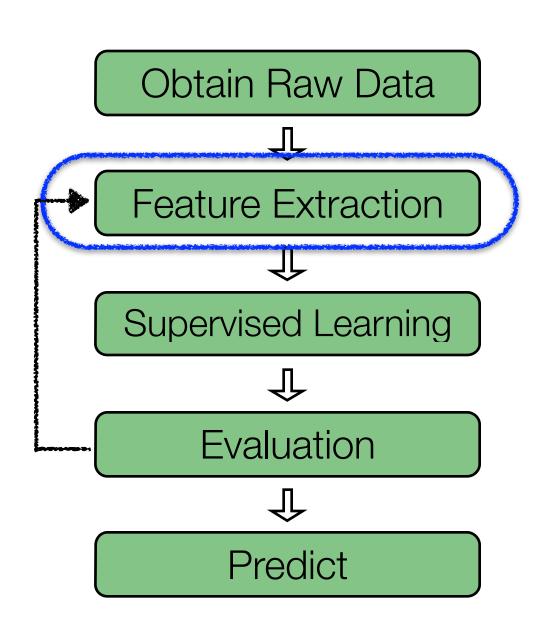
not-spam





Feature extraction typically transforms each observations into a vector of real numbers (features)

Success or failure of a classifier often depends on choosing good descriptions of observations!!



E.g., "Bag of Words"

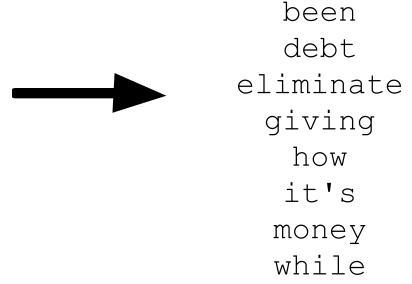
From: illegitimate@bad.com

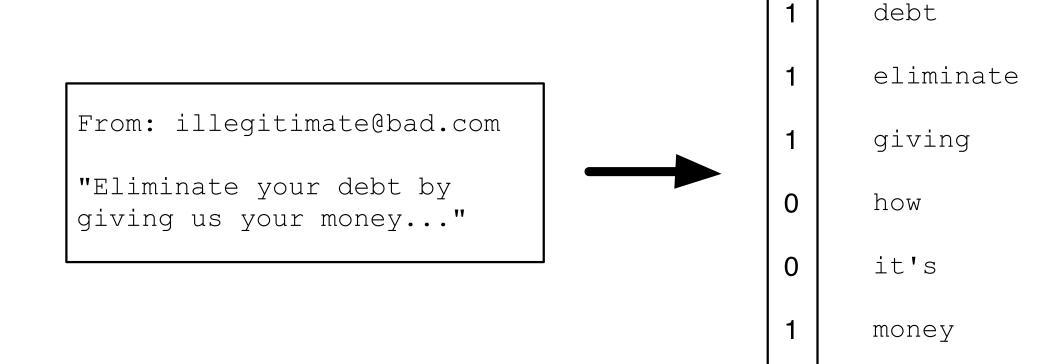
"Eliminate your debt by
giving us your money..."

From: bob@good.com

"Hi, it's been a while!
How are you? ..."

Vocabulary

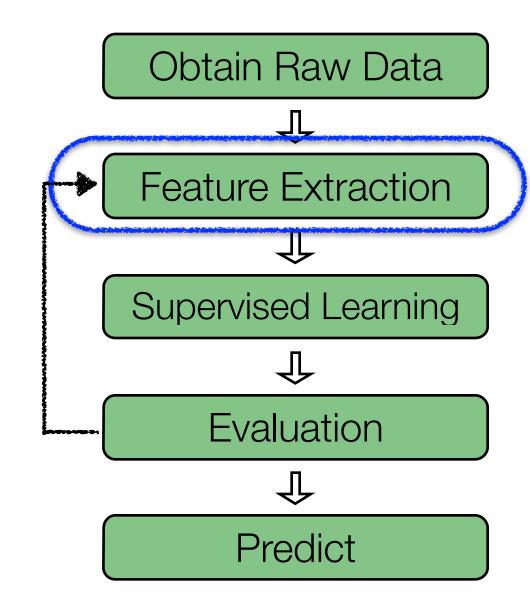




Observations are documents

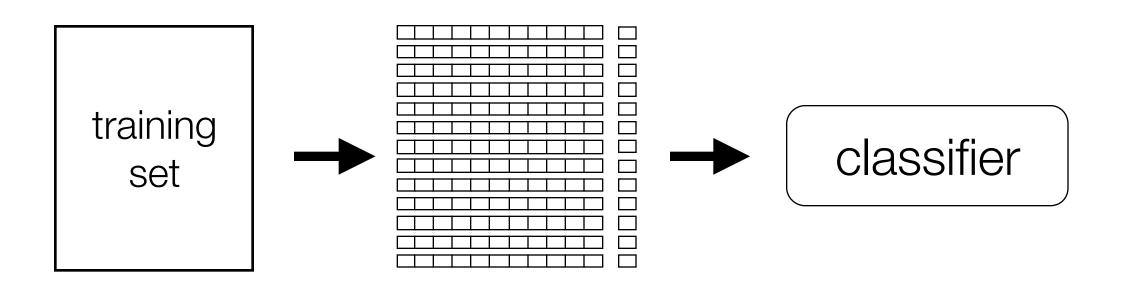
Build Vocabulary

Derive feature vectors from Vocabulary



been

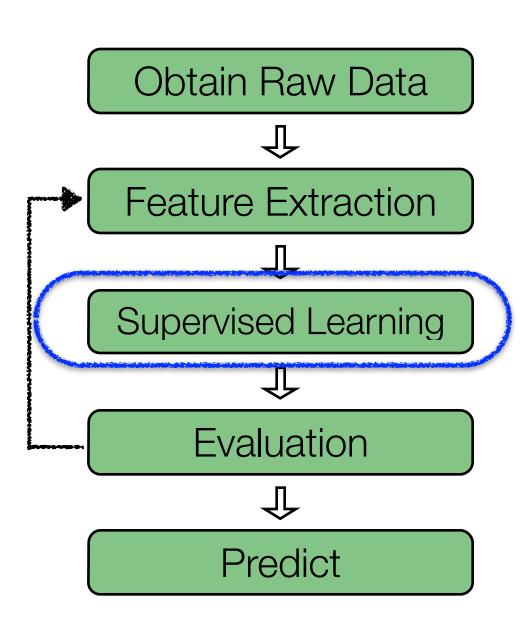
while



Supervised Learning: Train classifier using training data

 Common classifiers include Logistic Regression, SVMs, Decision Trees, Random Forests, etc.

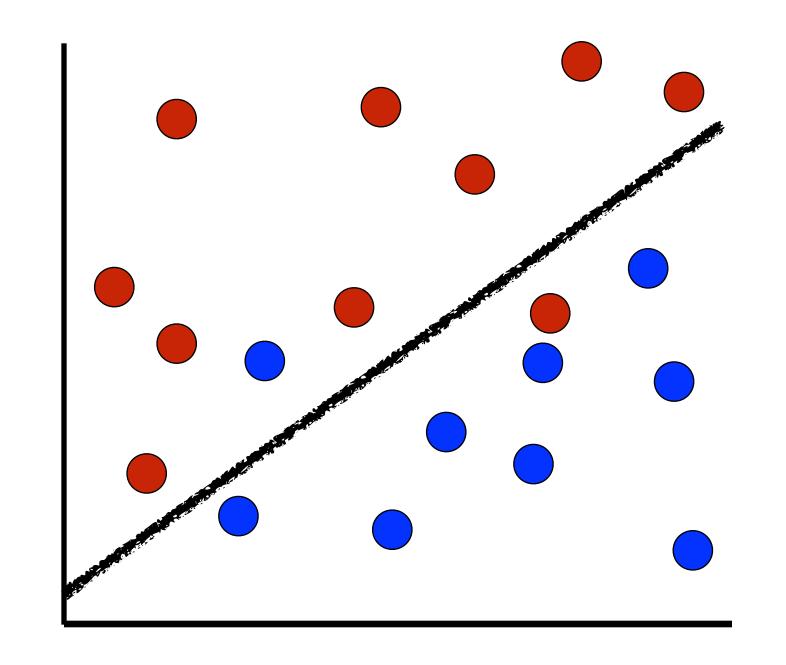
Training (especially at scale) often involves iterative computations, e.g., gradient descent

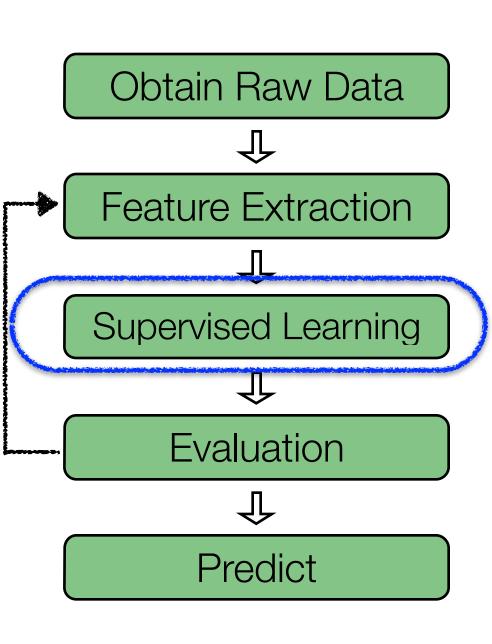


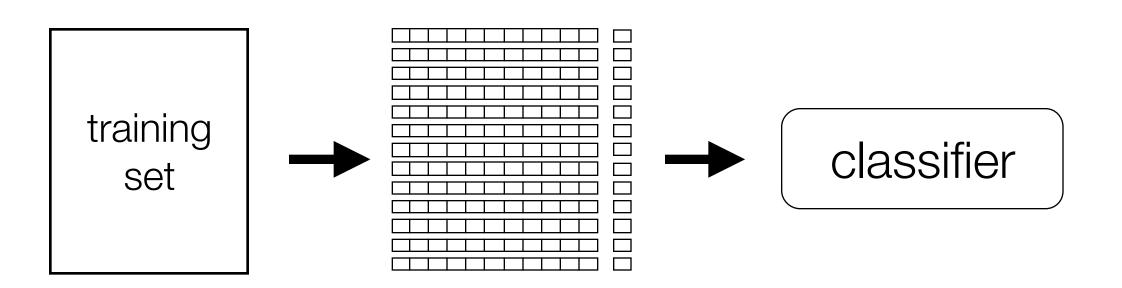
E.g., Logistic Regression

Goal: Find linear decision boundary

- Parameters to learn are feature weights and offset
- Nice probabilistic interpretation
- Covered in more detail later in course







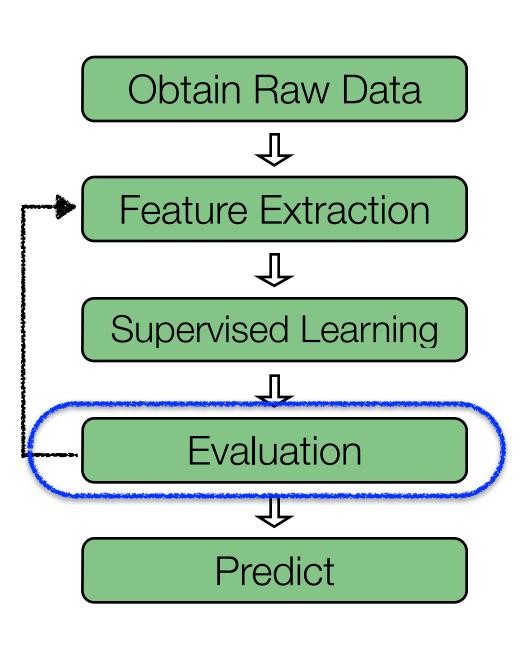
How can we evaluate the quality of our classifier?

We want good predictions on unobserved data

• 'Generalization' ability

Accuracy on training data is overly optimistic since classifier has already learned from it

We might be 'overfitting'



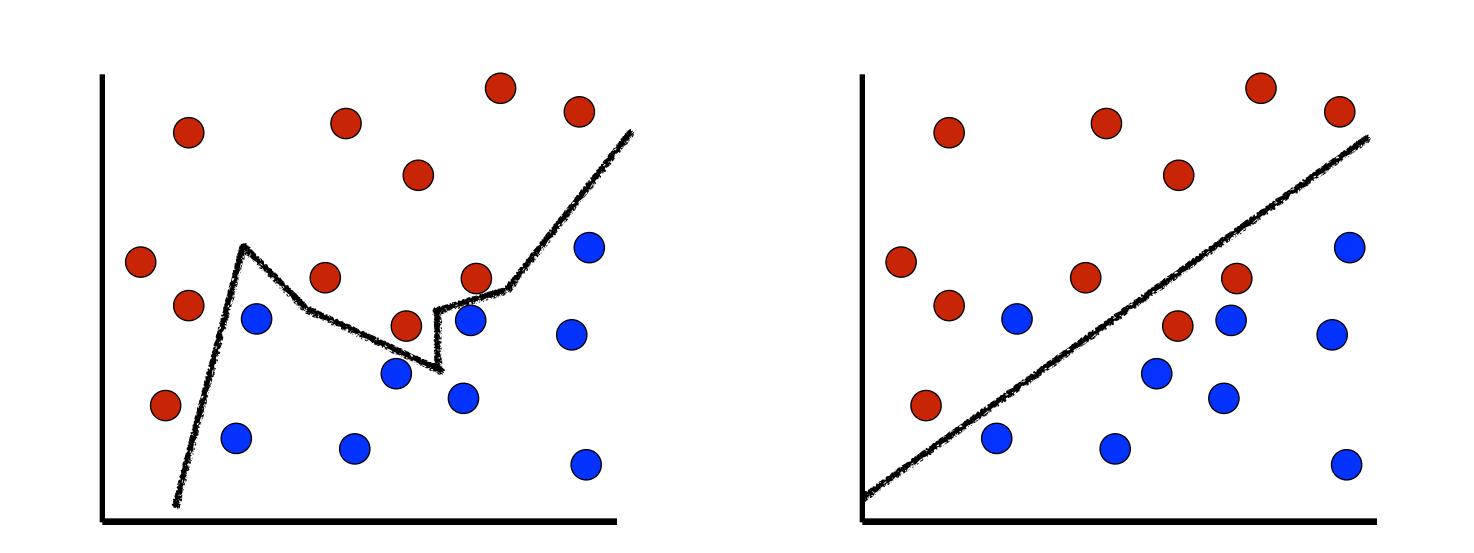
Overfitting and Generalization

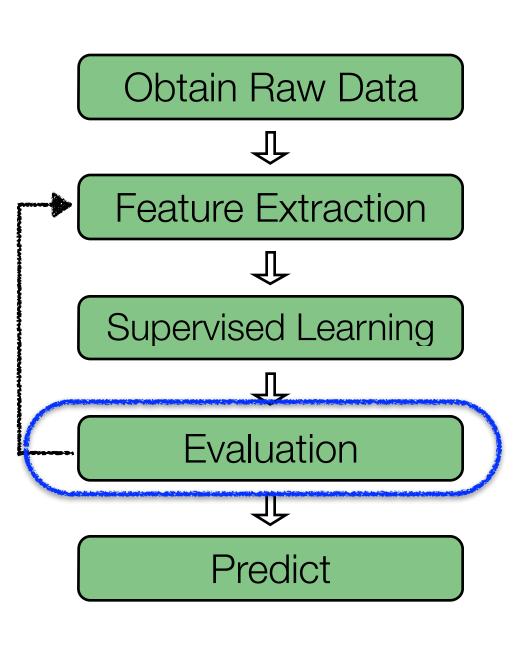
Fitting training data does not guarantee generalization, e.g., lookup table

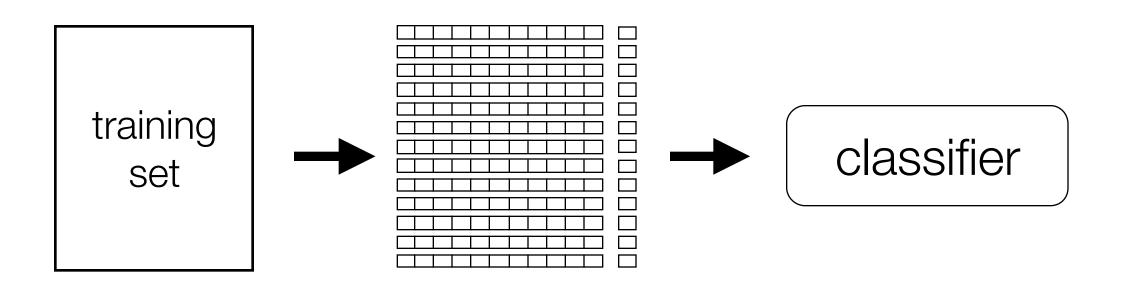
Left: perfectly fits training samples, but it is complex / overfitting

Right: misclassifies a few points, but simple / generalizes

Occam's razor

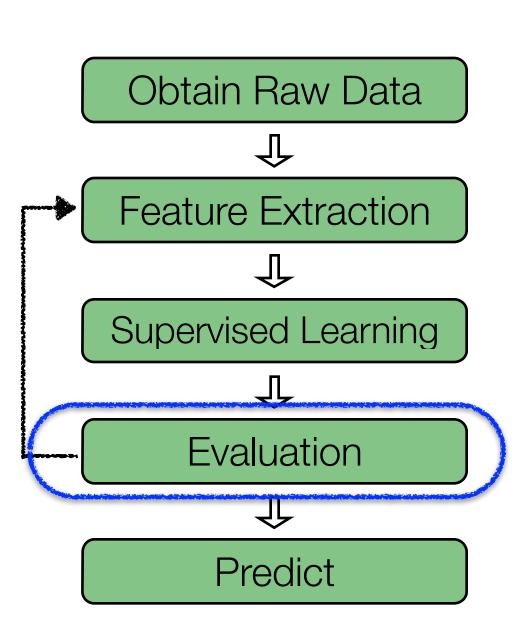


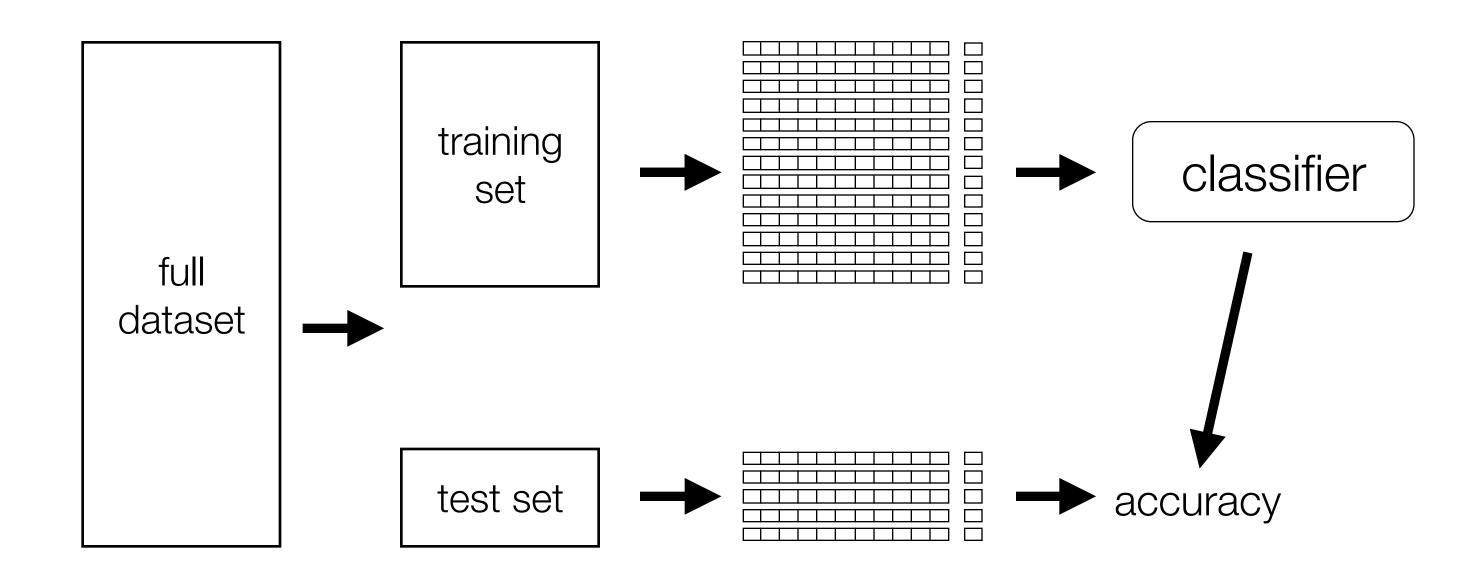




How can we evaluate the quality of our classifier?

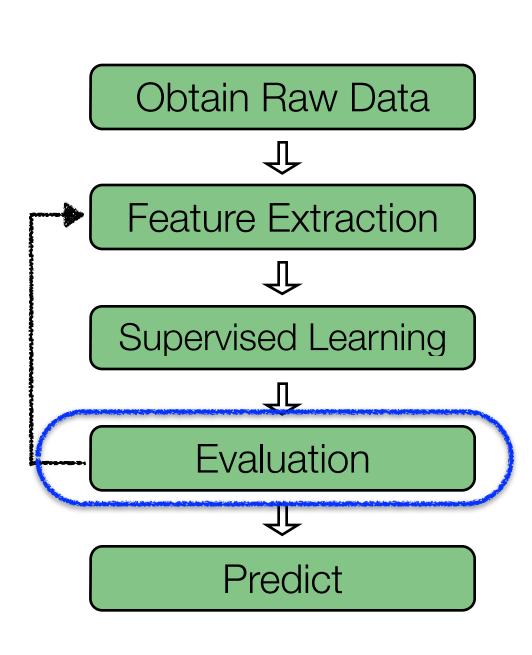
Idea: Create test set to simulate unobserved data

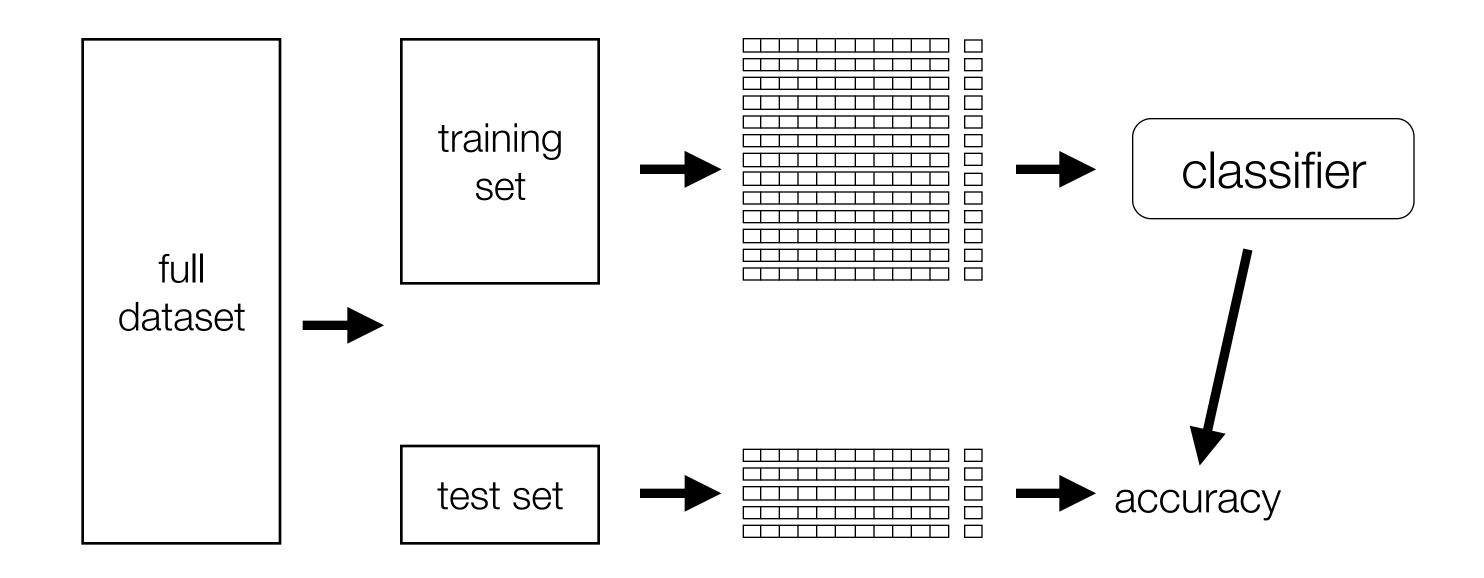




Evaluation: Split dataset into training / testing datasets

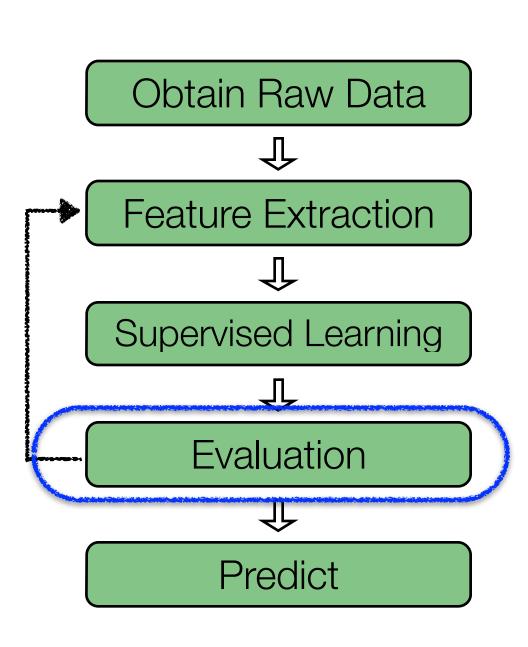
- Train on training set (don't expose test set to classifier)
- Make predictions on test set (ignoring test labels)
- Compare test predictions with underlying test labels

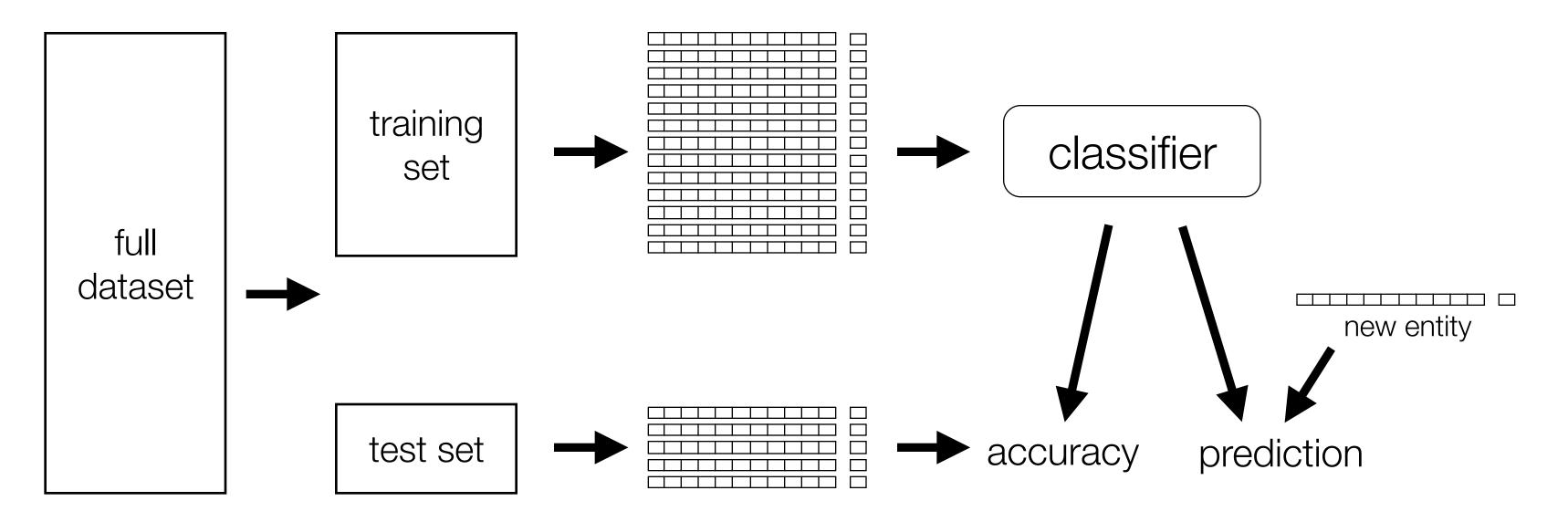




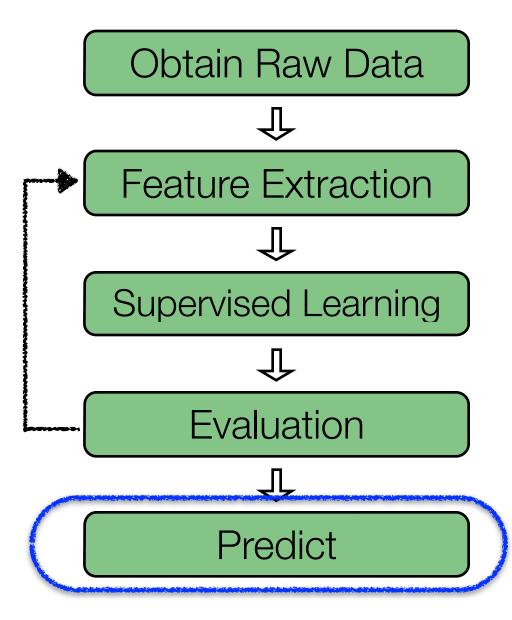
Evaluation: Split dataset into training / testing datasets

- Various ways to compare predicted and true labels
- Evaluation criterion is called a 'loss' function
- Accuracy (or 0-1 loss) is common for classification





Predict: Final classifier can then be used to make predictions on future observations, e.g., new emails we receive



Linear Algebra Review





Matrices

A matrix is a 2-dimensional array

$$\mathbf{A} = \begin{bmatrix} 3.3 & 5.3 & 4.5 \\ 1.0 & 4.5 & 3.4 \\ 6.3 & 1.0 & 2.2 \\ 4 \times 3 & 3.6 & 4.7 & 8.9 \end{bmatrix} A_{32}$$

Notation:

- Matrices are denoted by bold uppercase letters
- A_{ij} denotes the entry in *i*th row and *j*th column
- If \mathbf{A} is $n \times m$, it has n rows an m columns
- If \mathbf{A} is $n \times m$, then $\mathbf{A} \in \mathbb{R}^{n \times m}$

Vectors

A vector is a matrix with many rows and one column

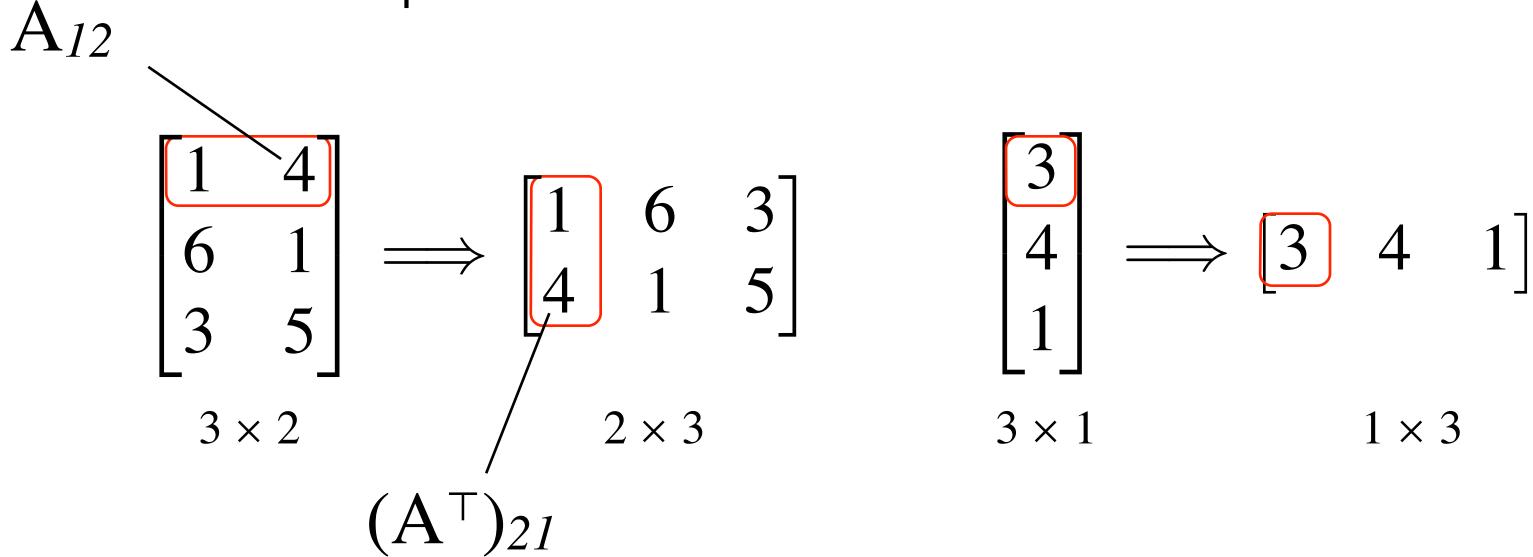
$$\mathbf{a} = \begin{bmatrix} 3.3 \\ 1.0 \\ 6.3 \\ 3.6 \end{bmatrix}$$

Notation:

- Vectors are denoted by bold lowercase letters
- a_i denotes the *i*th entry
- If \mathbf{a} is m dimensional, then $\mathbf{a} \in \mathbb{R}^m$

Transpose

Swap the rows and columns of a matrix



Properties of matrix transposes:

- $\bullet \ A_{ij} = (A^{\top})_{ji}$
- If \mathbf{A} is $n \times m$, then \mathbf{A}^{\top} is $m \times n$

Addition and Subtraction

These are element-wise operations

Addition:
$$\begin{bmatrix} 3 & 5 \\ 6 & 1 \end{bmatrix} + \begin{bmatrix} 4 & 5 \\ 8 & 12 \end{bmatrix} = \begin{bmatrix} 3+4 & 5+5 \\ 6+8 & 1+12 \end{bmatrix}$$
$$= \begin{bmatrix} 7 & 10 \\ 14 & 13 \end{bmatrix}$$

Subtraction:
$$\begin{bmatrix} 5 \\ 1 \end{bmatrix} - \begin{bmatrix} 4 \\ 3 \end{bmatrix} = \begin{bmatrix} 5 - 4 \\ 1 - 3 \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ -2 \end{bmatrix}$$

Addition and Subtraction

The matrices must have the same dimensions

$$\begin{bmatrix} 5 \\ 1 \end{bmatrix} - \begin{bmatrix} 4 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}$$

$$\begin{bmatrix} 3 & 5 & 4 \\ 6 & 1 & 2 \end{bmatrix} + \begin{bmatrix} 4 & 5 & 1 \\ 8 & 12 & 9 \end{bmatrix} = \begin{bmatrix} 7 & 10 & 5 \\ 14 & 13 & 11 \end{bmatrix}$$

$$\begin{bmatrix} 3 & 5 & 4 \\ 6 & 1 & 2 \end{bmatrix} + \begin{bmatrix} 4 & 5 \\ 8 & 12 \end{bmatrix}$$

Matrix Scalar Multiplication

We multiply each matrix element by the scalar value

$$3 \times \begin{bmatrix} 3 & 5 & 4 \\ 6 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 9 & 15 & 12 \\ 18 & 3 & 6 \end{bmatrix}$$

$$-0.5 \times \begin{bmatrix} 3 \\ 8 \end{bmatrix} = \begin{bmatrix} -1.5 \\ -4 \end{bmatrix}$$

Scalar Product

A function that maps two vectors to a scalar

$$\begin{bmatrix} 1 & 4 \\ 4 & -9 \\ 3 & -7 \end{bmatrix}$$

$$1 \times 4$$

Performs pairwise multiplication of vector elements

Scalar Product

A function that maps two vectors to a scalar

$$\begin{bmatrix} 1 \\ 4 \\ \cdot \\ 2 \\ -7 \end{bmatrix} = -9$$

$$1 \times 4 + 4 \times 2$$

Performs pairwise multiplication of vector elements

Scalar Product

A function that maps two vectors to a scalar

$$\begin{bmatrix} 1 \\ 4 \\ \cdot \\ 2 \\ -7 \end{bmatrix}$$

$$1 \times 4 + 4 \times 2 + 3 \times (-7) = -9$$

Performs pairwise multiplication of vector elements

The two vectors must be the same dimension

Also known as dot product or inner product

Matrix-Vector Multiplication

Involves repeated scalar products

$$\begin{bmatrix} 1 & 4 & 3 \\ 6 & 1 & 2 \end{bmatrix} \begin{bmatrix} 4 \\ 2 \\ -7 \end{bmatrix} = \begin{bmatrix} -9 \end{bmatrix}$$

$$1 \times 4 + 4 \times 2 + 3 \times (-7) = -9$$

Matrix-Vector Multiplication

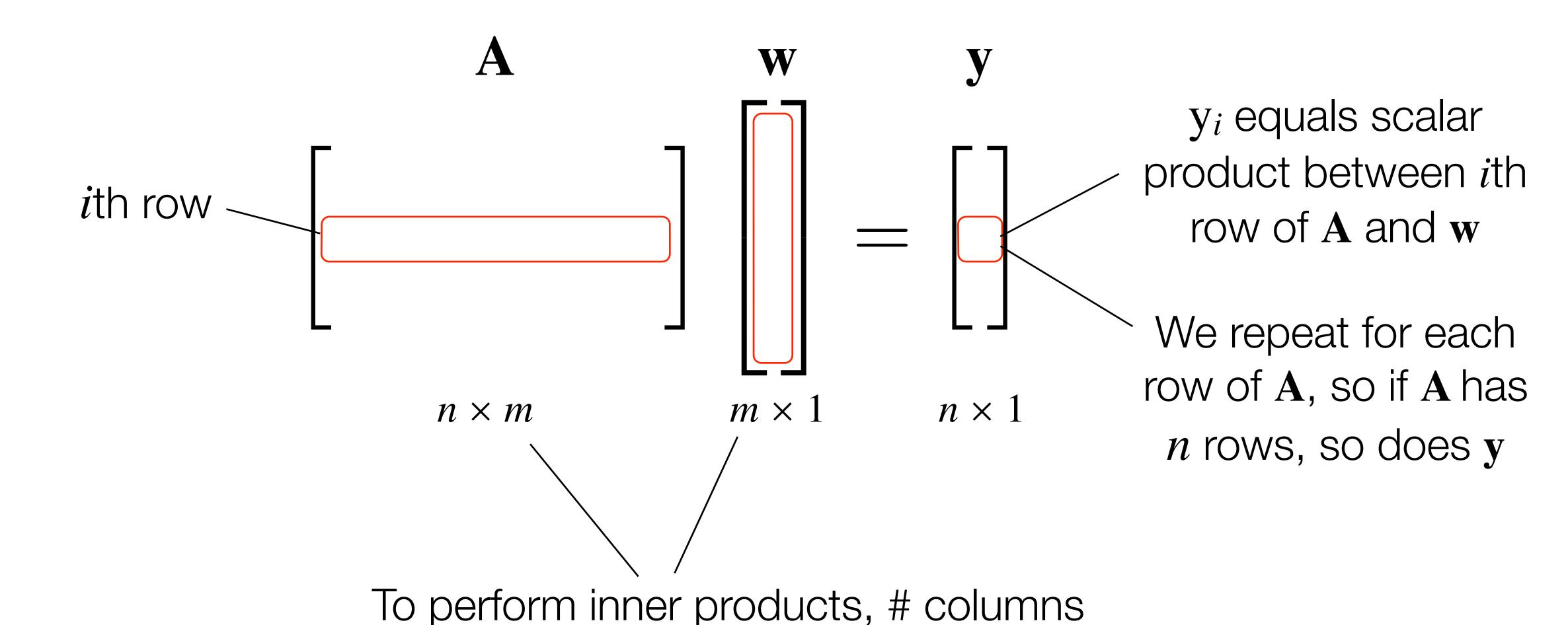
Involves repeated scalar products

$$\begin{bmatrix} 1 & 4 & 3 \\ 6 & 1 & 2 \end{bmatrix} \begin{bmatrix} 4 \\ 2 \\ -7 \end{bmatrix} = \begin{bmatrix} -9 \\ 12 \end{bmatrix}$$

$$1 \times 4 + 4 \times 2 + 3 \times (-7) = -9$$

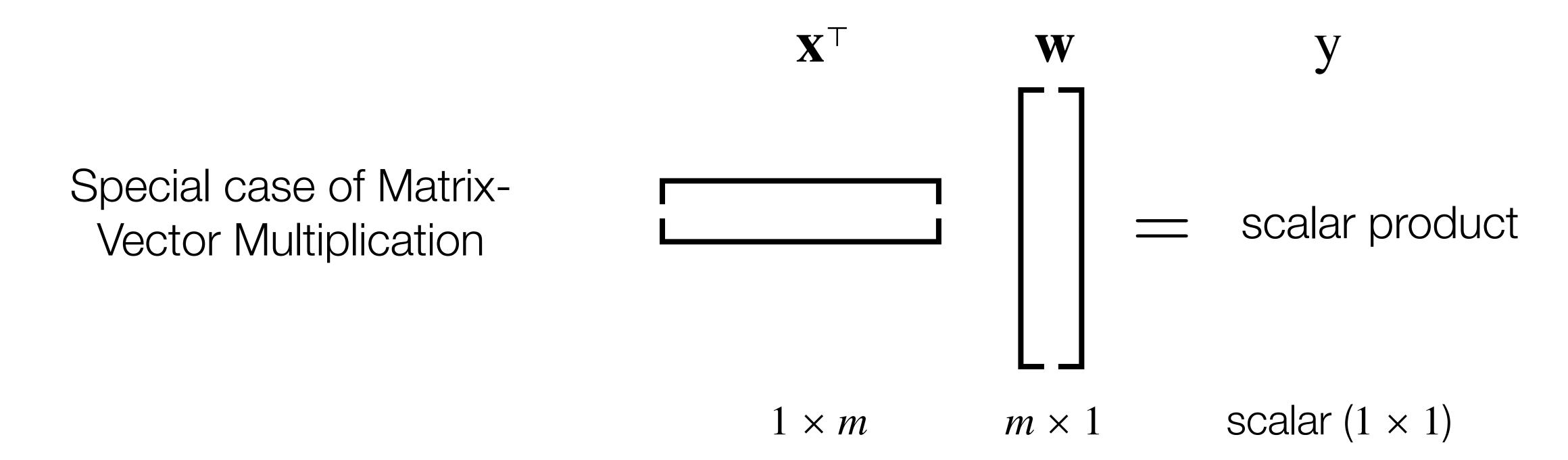
$$6 \times 4 + 1 \times 2 + 2 \times (-7) = 12$$

Matrix-Vector Multiplication



in A must equal # rows of w

Scalar Product Revisited



Vectors assumed to be in column form (many rows, one column)

Transposed vectors are row vectors

Common notation for scalar product: $\mathbf{x}^{\mathsf{T}}\mathbf{w}$

Also involves several scalar products

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -5 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} 28 \\ \end{bmatrix}$$

$$9 \times 1 + 3 \times 3 + 5 \times 2 = 28$$

Also involves several scalar products

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -5 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} 28 & 18 \\ \end{bmatrix}$$

$$9 \times 1 + 3 \times 3 + 5 \times 2 = 28$$

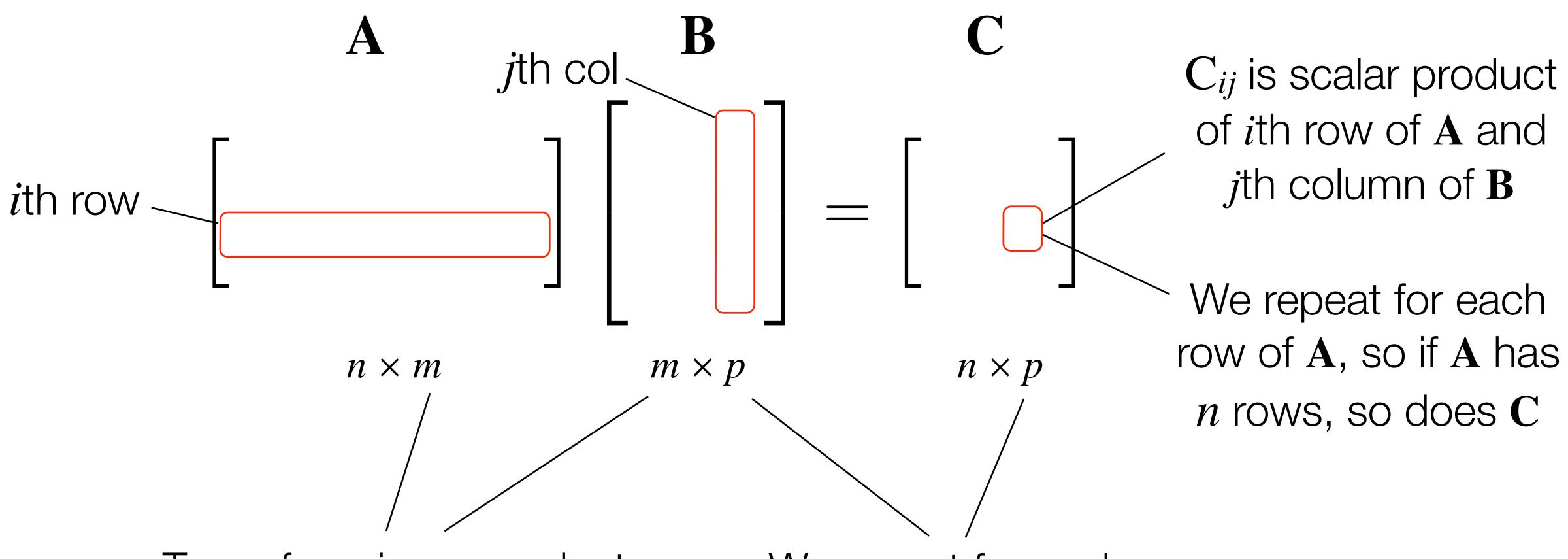
 $9 \times 2 + 3 \times (-5) + 5 \times 3 = 18$

Also involves several scalar products

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -5 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} 28 & 18 \\ 11 & 9 \end{bmatrix}$$

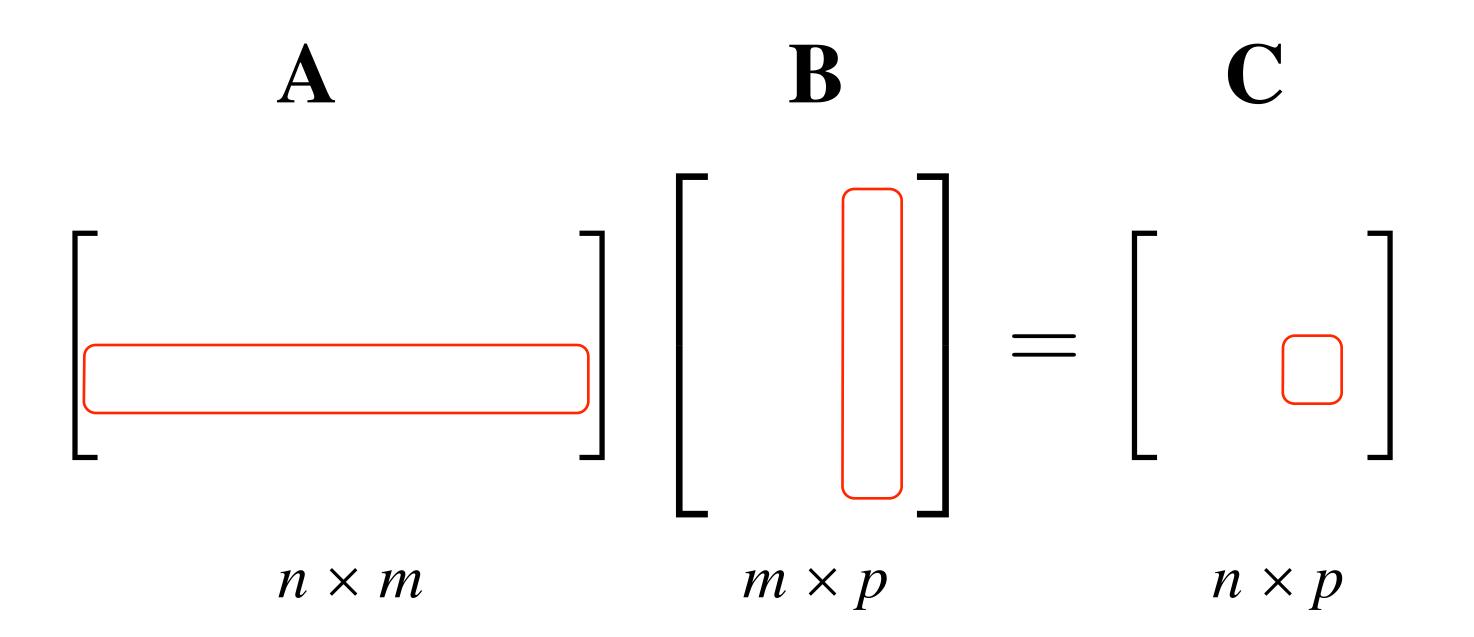
$$9 \times 1 + 3 \times 3 + 5 \times 2 = 28$$

 $9 \times 2 + 3 \times (-5) + 5 \times 3 = 18$



To perform inner products,
columns in **A** must equal
rows of **B**

We repeat for each column of ${\bf B}$, so if ${\bf B}$ has p columns, so does ${\bf C}$



Associative, i.e., (AB)C = A(BC)

Not commutative, i.e., $AB \neq BA$

Outer Product

Special case of Matrix-Matrix Multiplication involving two vectors

 C_{ij} is "inner product" of ith entry of x and jth entry of w

Identity Matrix

One is the scalar multiplication identity, i.e., $c \times 1 = c$

 I_n is the $n \times n$ identity matrix, i.e., $I_n A = A$ and $A I_m = A$ for any $n \times m$ matrix A

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix}$$

Identity matrices are square, with ones on the diagonal entries

Inverse Matrix

1/c is the scalar inverse, i.e., $c \times 1/c = 1$

Multiplying a matrix by its inverse results in the identity matrix

- For an $n \times n$ matrix **A**, **A**⁻¹ denotes its inverse (when it exists)
- $AA^{-1} = A^{-1}A = I_n$

Only a square matrix (when n = m) can have an inverse

Euclidean Norm for Vectors

The magnitude / length of a scalar is its absolute value

Vector norms generalize this idea for vectors

The Euclidean norm for $\mathbf{x} \in \mathbb{R}^m$ is denoted by $\|\mathbf{x}\|_2$

- Equals absolute value when m=1
- Related to scalar product: $\|\mathbf{x}\|_2^2 = \mathbf{x}^\top \mathbf{x}$

Big O Notation for Time and Space Complexity





Big O Notation

Describes how algorithms respond to changes in input size

- Both in terms of processing time and space requirements
- We refer to complexity and Big O notation synonymously

Required space proportional to units of storage

Typically 8 bytes to store a floating point number

Required time proportional to number of 'basic operations'

• Arithmetic operations $(+, -, \times, /)$, logical tests (<, >, ==)

Big O Notation

Notation: f(x) = O(g(x))

Can describe an algorithm's time or space complexity

Informal definition: f does not grow faster than g

Formal definition: $|f(x)| \le C|g(x)| \quad \forall x > N$

Ignores constants and lower-order terms

- \bullet For large enough x, these terms won't matter
- E.g., $x^2 + 3x \le Cx^2 \ \forall \ x > N$

E.g., O(1) Complexity

Constant time algorithms perform the same number of operations every time they're called

E.g., performing a fixed number of arithmetic operations

Similarly, constant space algorithms require a fixed amount of storage every time they're called

E.g., storing the results of a fixed number of arithmetic operations

E.g., O(n) Complexity

Linear time algorithms perform a number of operations proportional to the number of inputs

• E.g., adding two n-dimensional vectors requires O(n) arithmetic operations

Similarly, linear space algorithms require storage proportional to the size of the inputs

• E.g., adding two n-dimensional vectors results in a new n-dimensional vector which requires O(n) storage

E.g., $O(n^2)$ Complexity

Quadratic time algorithms perform a number of operations proportional to the square of the number of inputs

• E.g., outer product of two n-dimensional vectors requires $O(n^2)$ multiplication operations (one per each entry of the resulting matrix)

Similarly, quadratic space algorithms require storage proportional to the square of the size of the inputs

• E.g., outer product of two n-dimensional vectors requires $O(n^2)$ storage (one per each entry of the resulting matrix)

Time and Space Complexity Can Differ

Inner product of two *n*-dimensional vectors

- O(n) time complexity to multiply n pairs of numbers
- O(1) space complexity to store result (which is a scalar)

Matrix inversion of an $n \times n$ matrix

- $O(n^3)$ time complexity to perform inversion
- $O(n^2)$ space complexity to store result

E.g., Matrix-Vector Multiply

Goal: multiply an $n \times m$ matrix with an $m \times 1$ vector

Computing result takes O(nm) time

- There are *n* entries in the resulting vector
- Each entry computed via dot product between two *m*-dimensional vectors (a row of input matrix and input vector)

Storing result takes O(n) space

• The result is an *n*-dimensional vector

E.g., Matrix-Matrix Multiply

Goal: multiply an $n \times m$ matrix with an $m \times p$ matrix

Computing result takes O(npm) time

- There are *np* entries in the resulting matrix
- Each entry computed via dot product between two *m*-dimensional vectors

Storing result takes O(np) space

• The result is an $n \times p$ matrix