

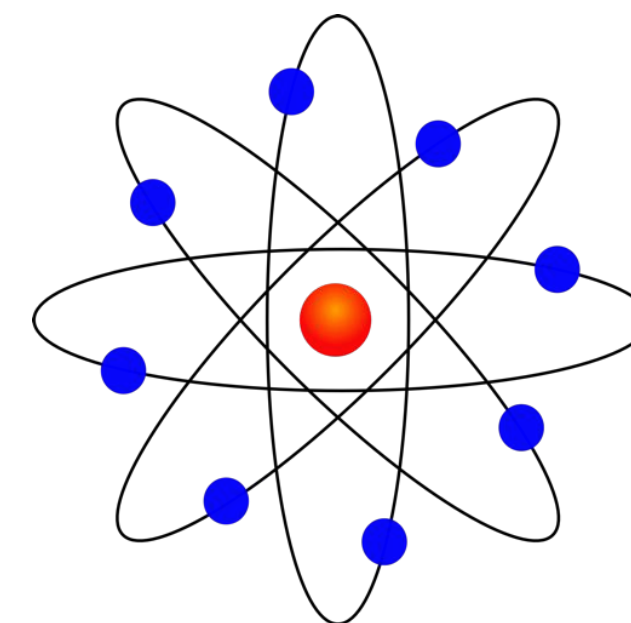
Overview



Rapid growth of massive datasets

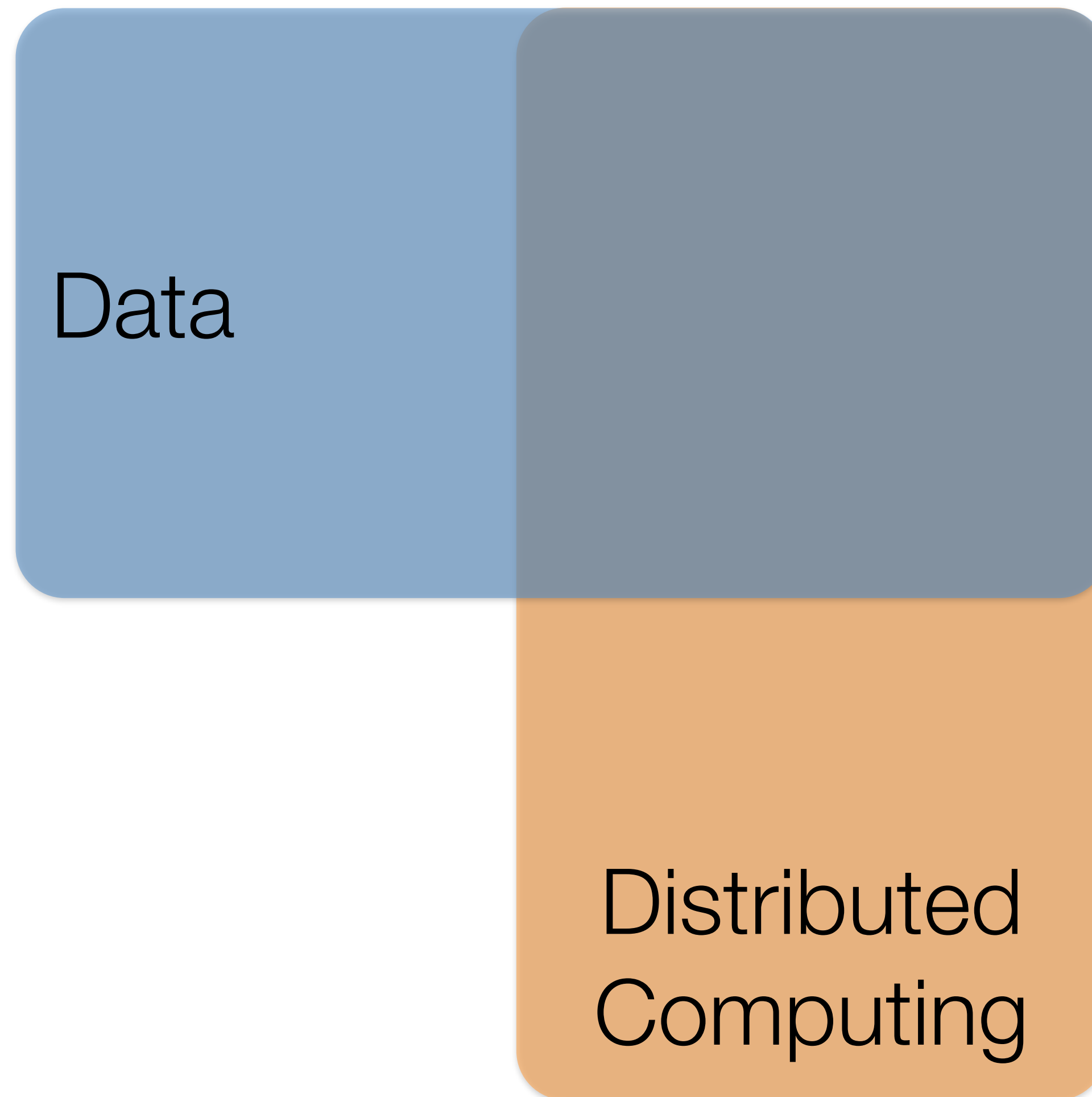
E.g., Online activity, Science, Sensor networks

Data



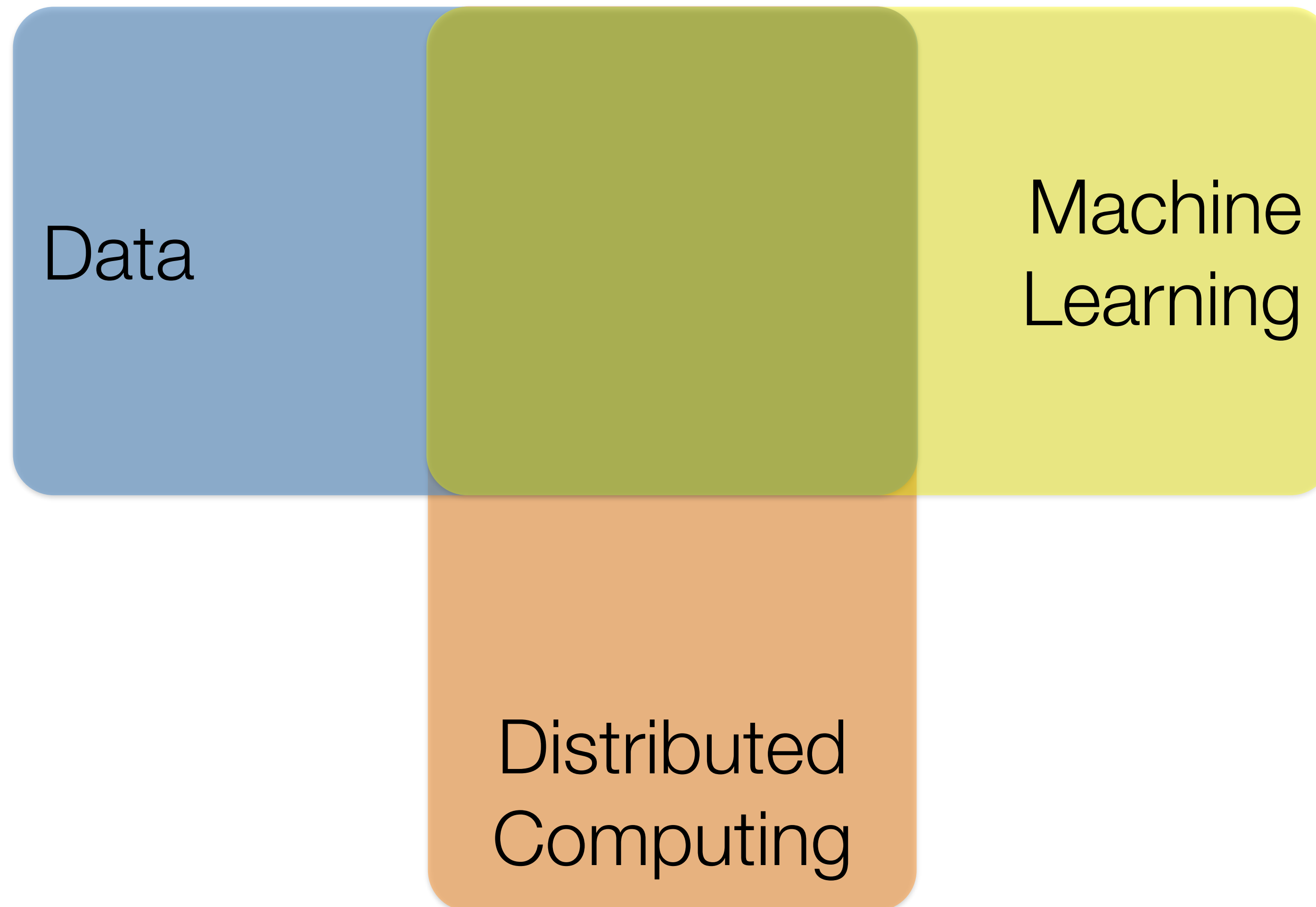
facebook®

Distributed Clusters are Pervasive



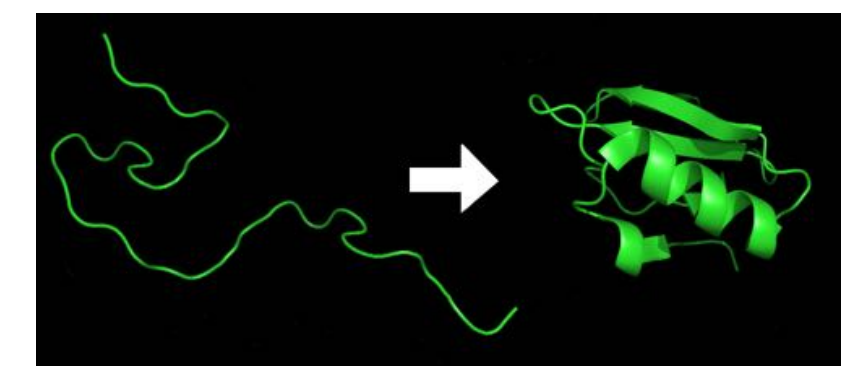
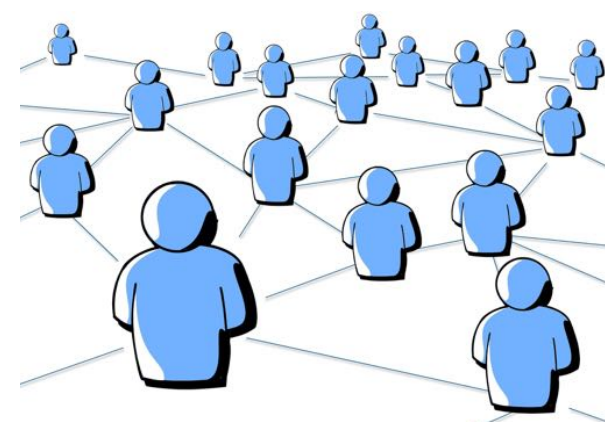
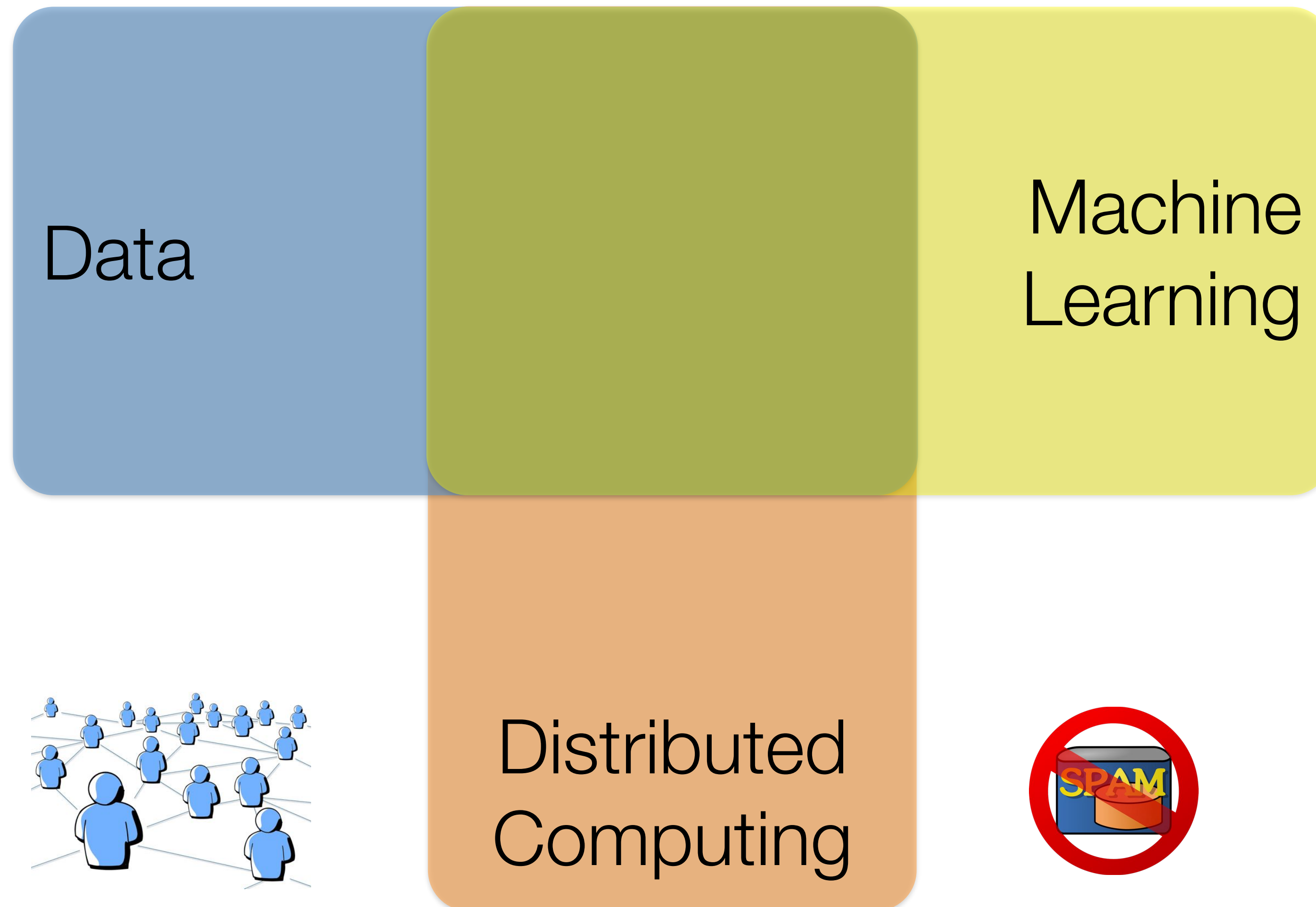
Mature Methods for Common Problems

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



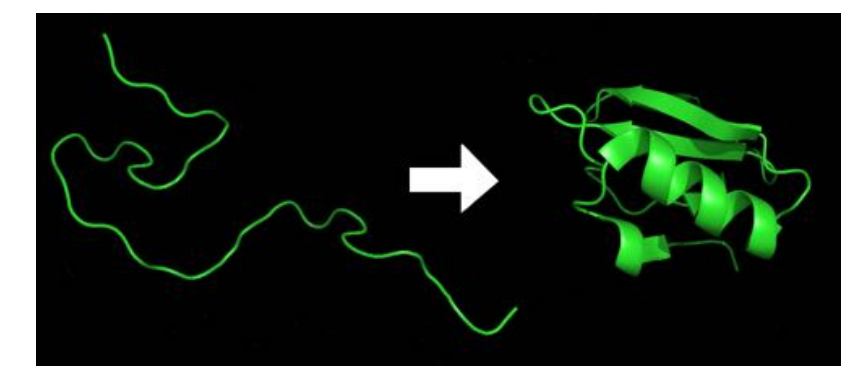
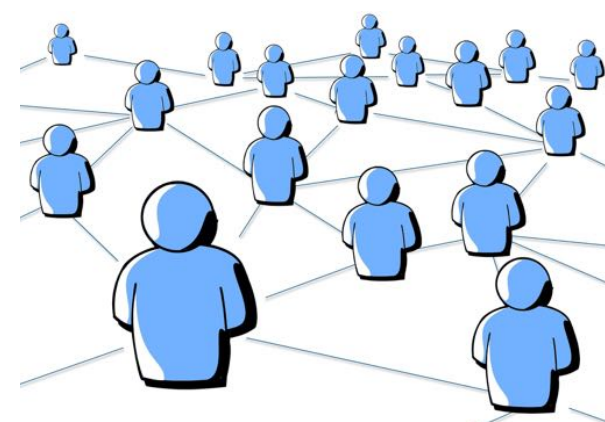
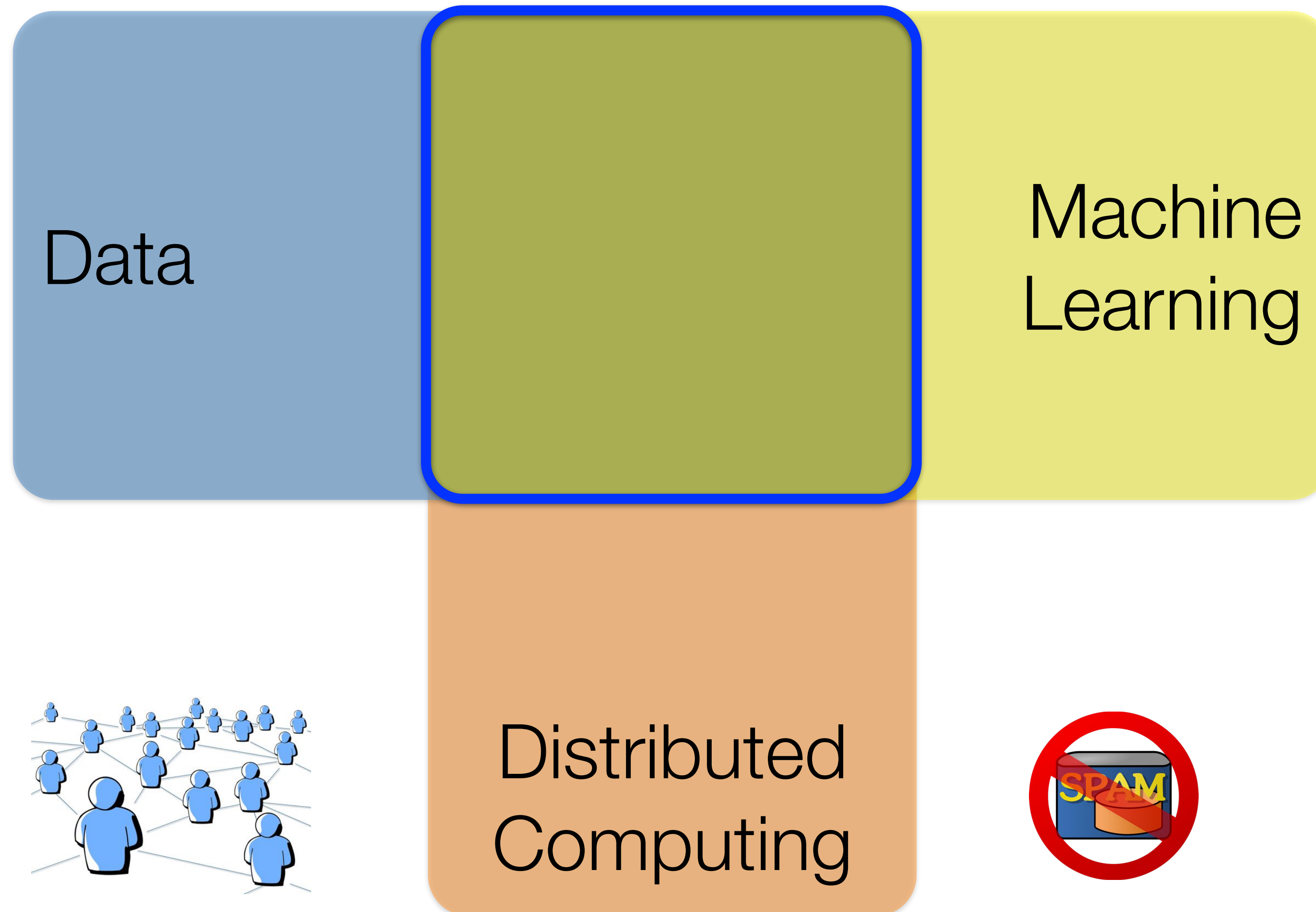
ML is Applied Everywhere

E.g., personalized recommendations, speech recognition, face detection, protein structure, fraud detection, spam filtering, playing chess or Jeopardy, unassisted vehicle control, medical diagnosis



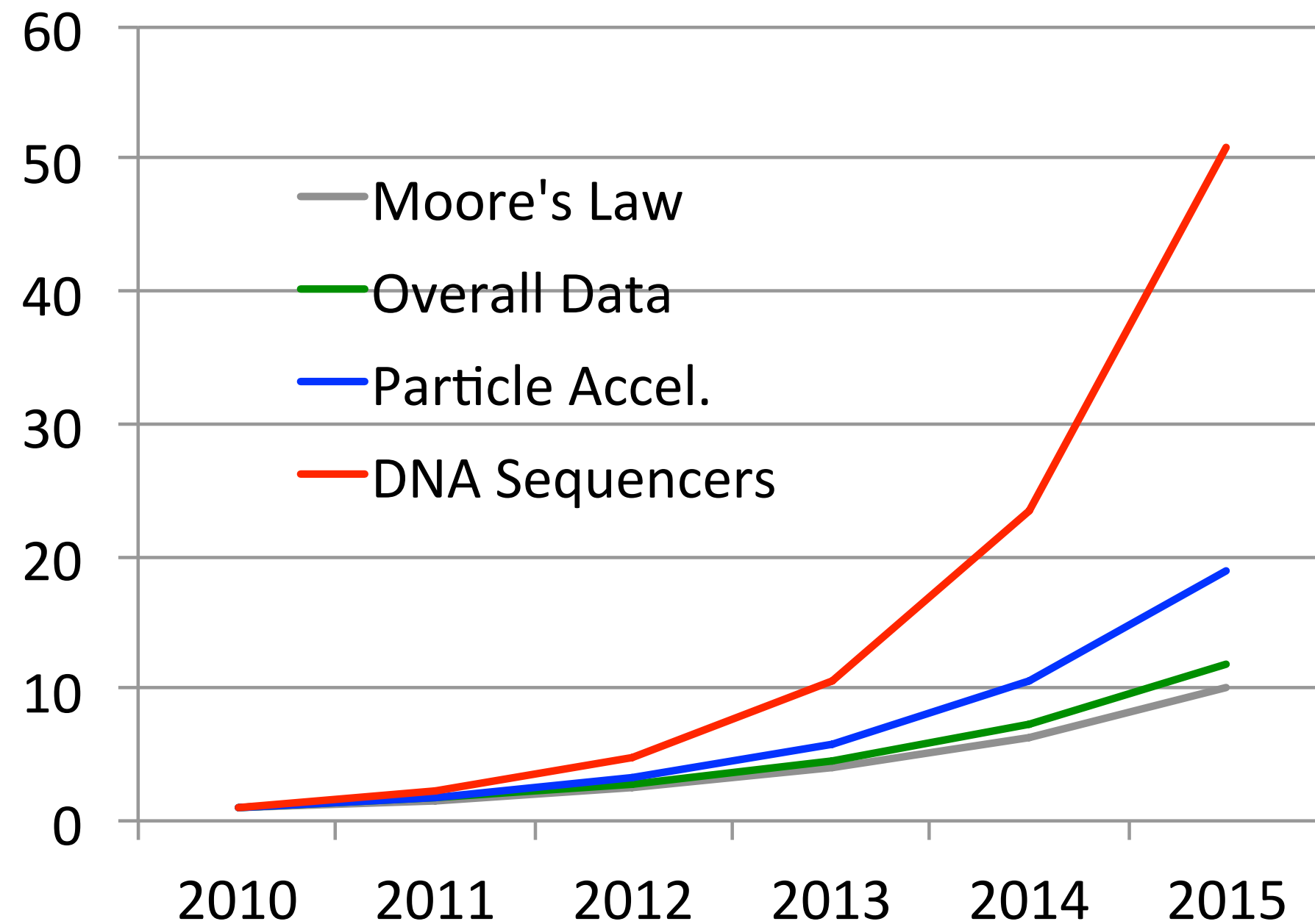
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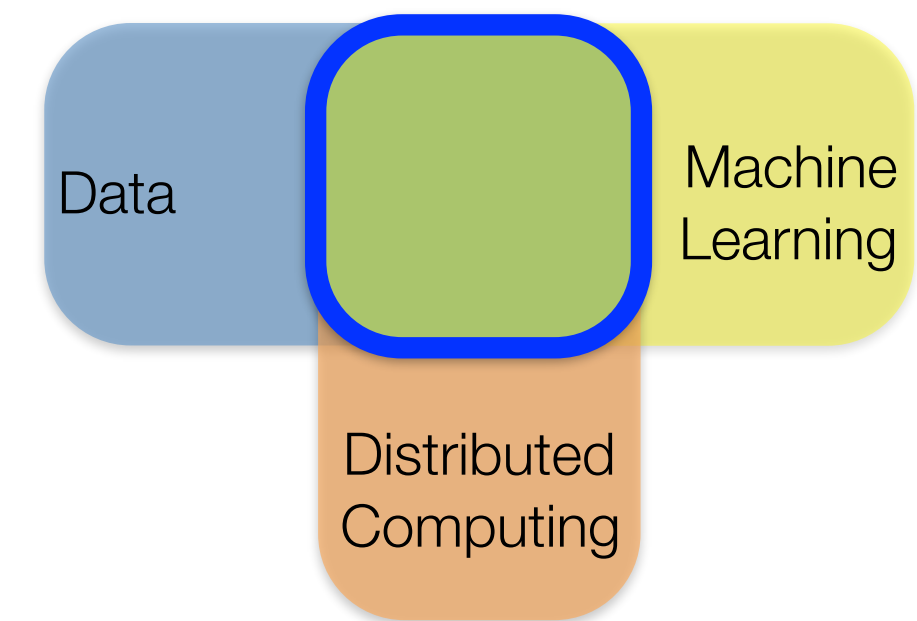
Challenge: Scalability

Classic ML techniques are not always suitable for modern datasets



Data Grows Faster
than Moore's Law

[IDC report, Kathy Yelick, LBNL]



Course Goals

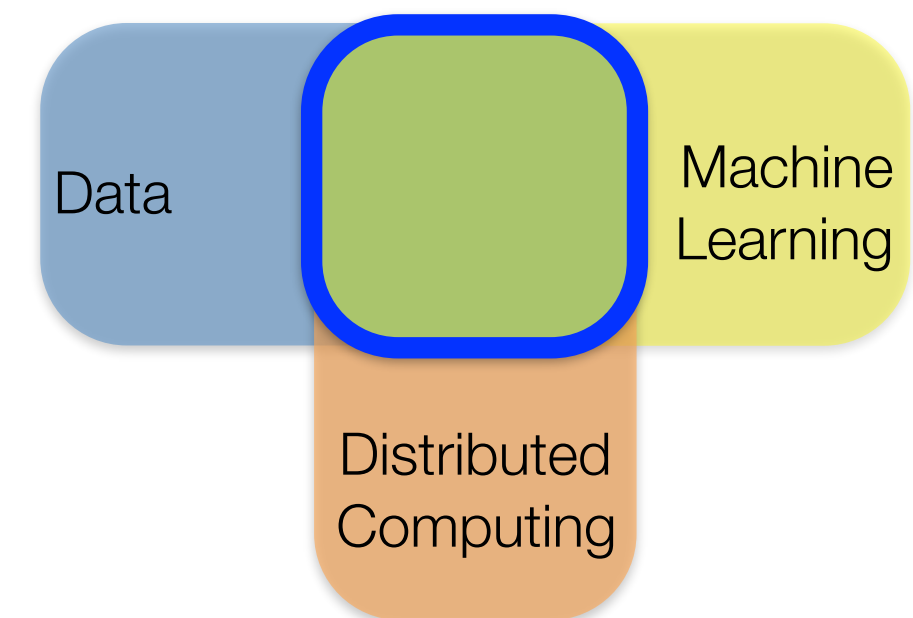
Focus on scalability challenges for common ML tasks

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

BerkeleyX CS105x - Introduction to Apache Spark

- Fundamentals of Spark

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

Schedule

4 weeks of lectures, 4 Spark coding labs

- Week 1: ML Overview, Math Review, Spark RDD Overview
- Week 2: Distributed ML Principles and Linear Regression
- Week 3: Classification with Click-through Rate Prediction
- Week 4: Exploratory Analysis with Brain Imaging Data

Distributed Computing and Apache Spark



How to Handle Massive Data?

Traditional tools (Matlab, R, Excel, etc.) run on a single machine

How to Handle Massive Data?

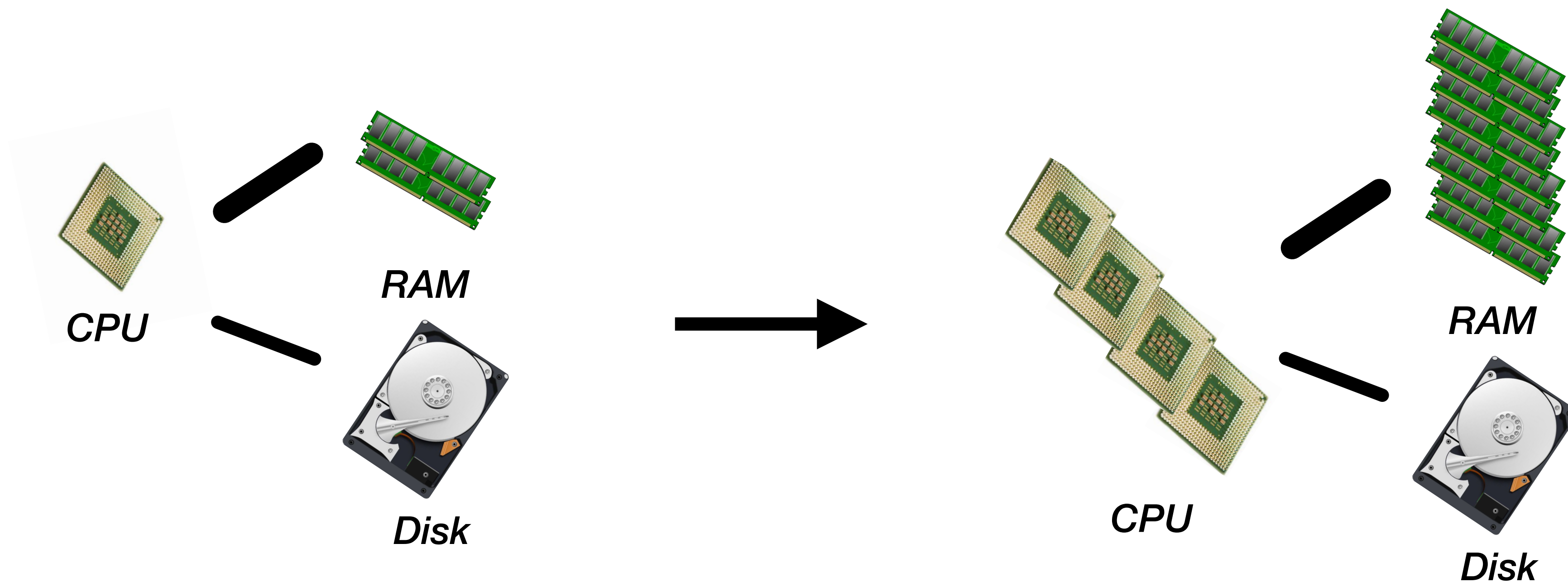
Need more hardware to store / process modern data

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

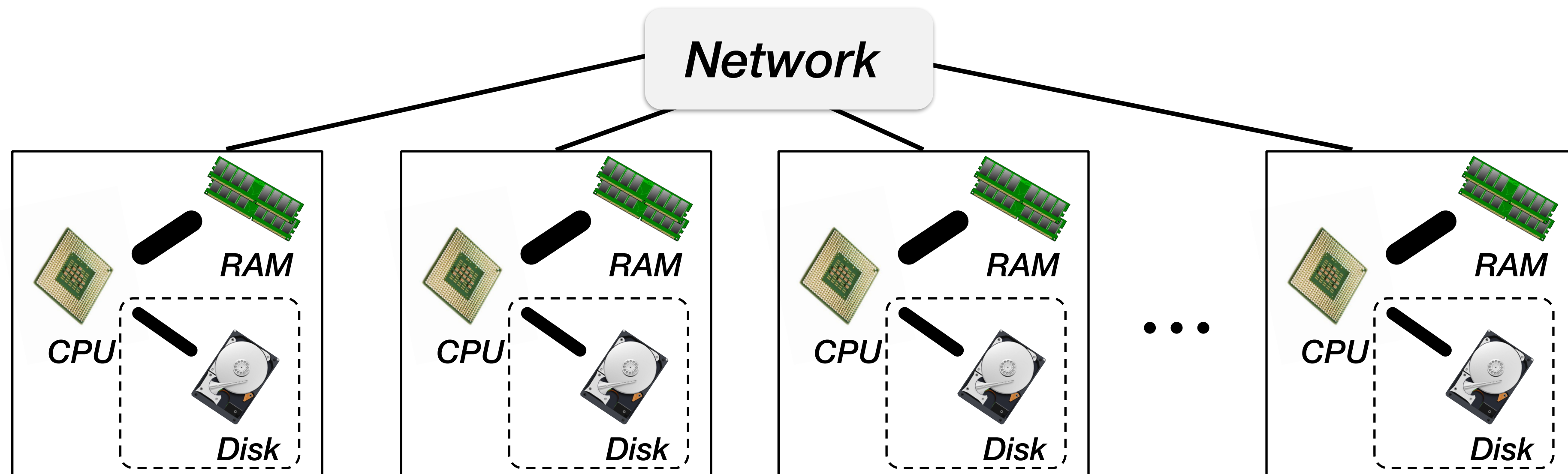


How to Handle Massive Data?

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

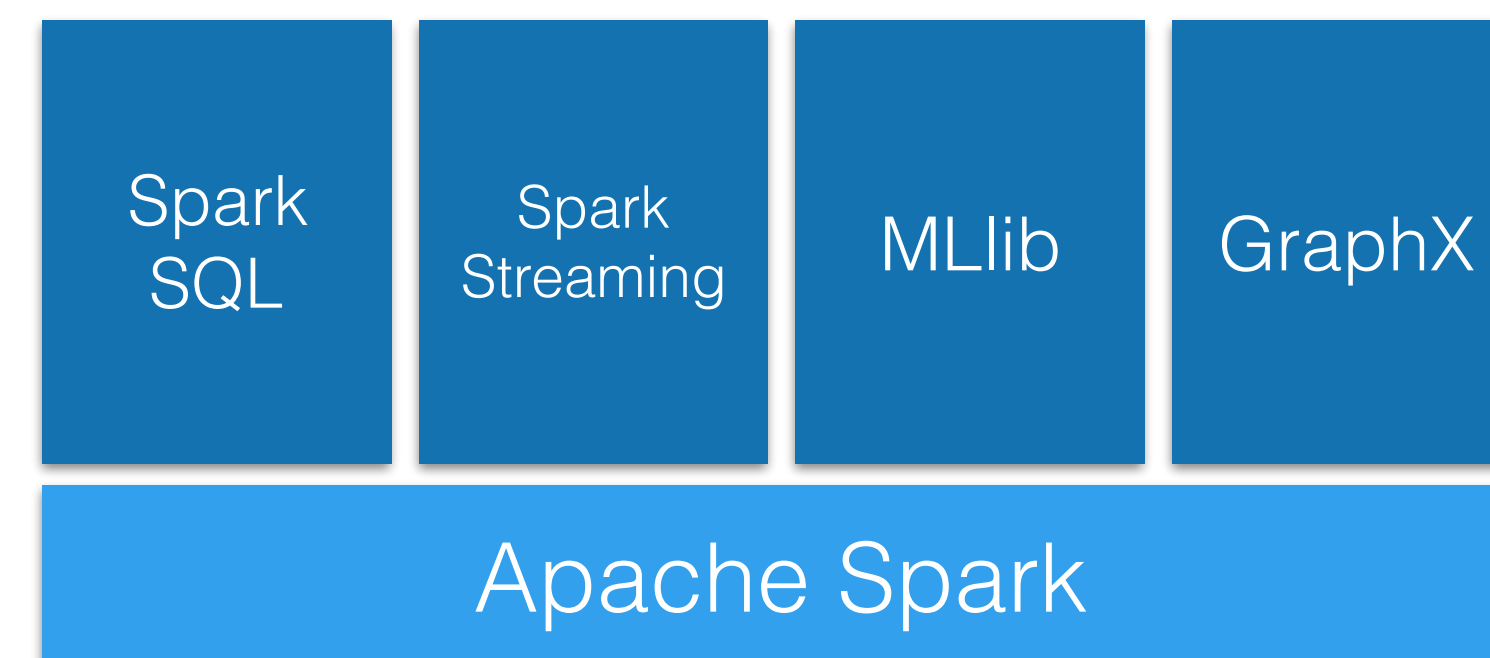
Well-suited for machine learning

- 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

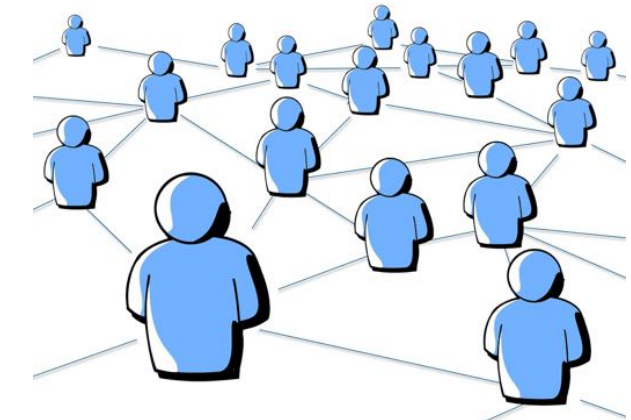
- Computer Science
- Probability and Statistics
- Optimization
- Linear Algebra

Some Examples

Face recognition



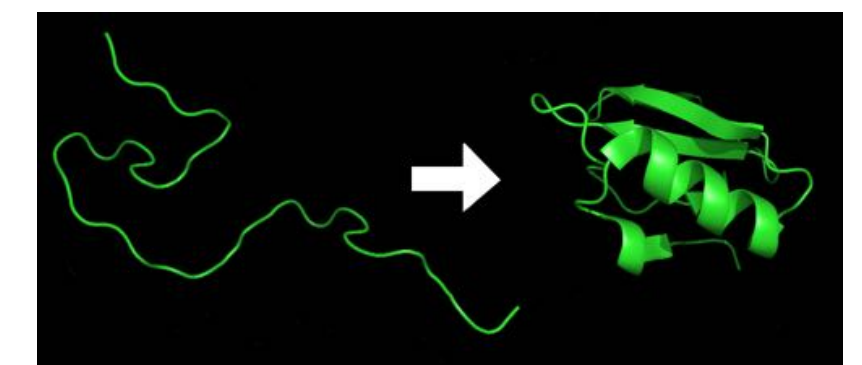
Link prediction



Text or document classification, e.g., spam detection



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



Obtain Raw Data

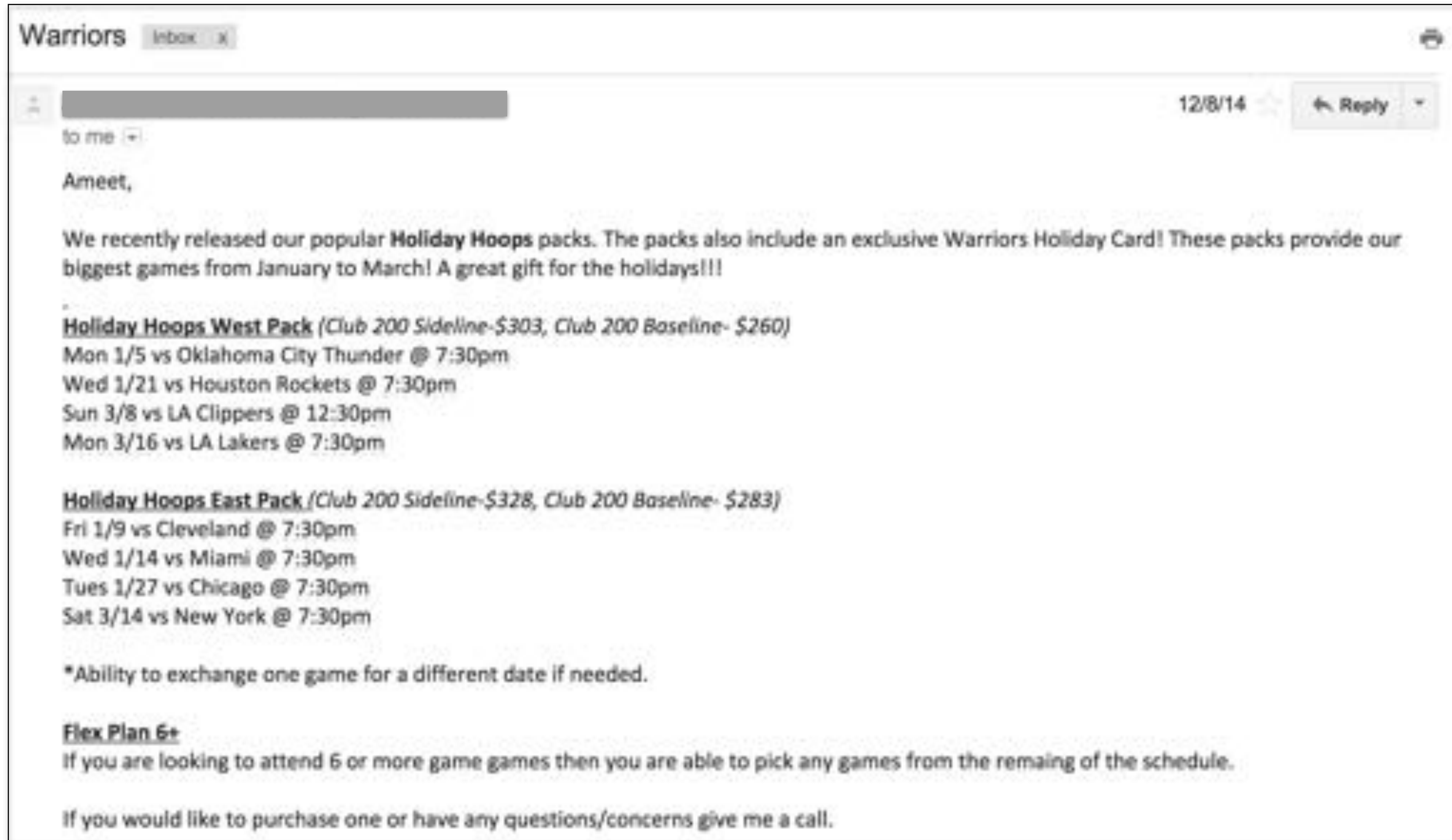
Raw data comes from many sources

Data Types

Web hypertext

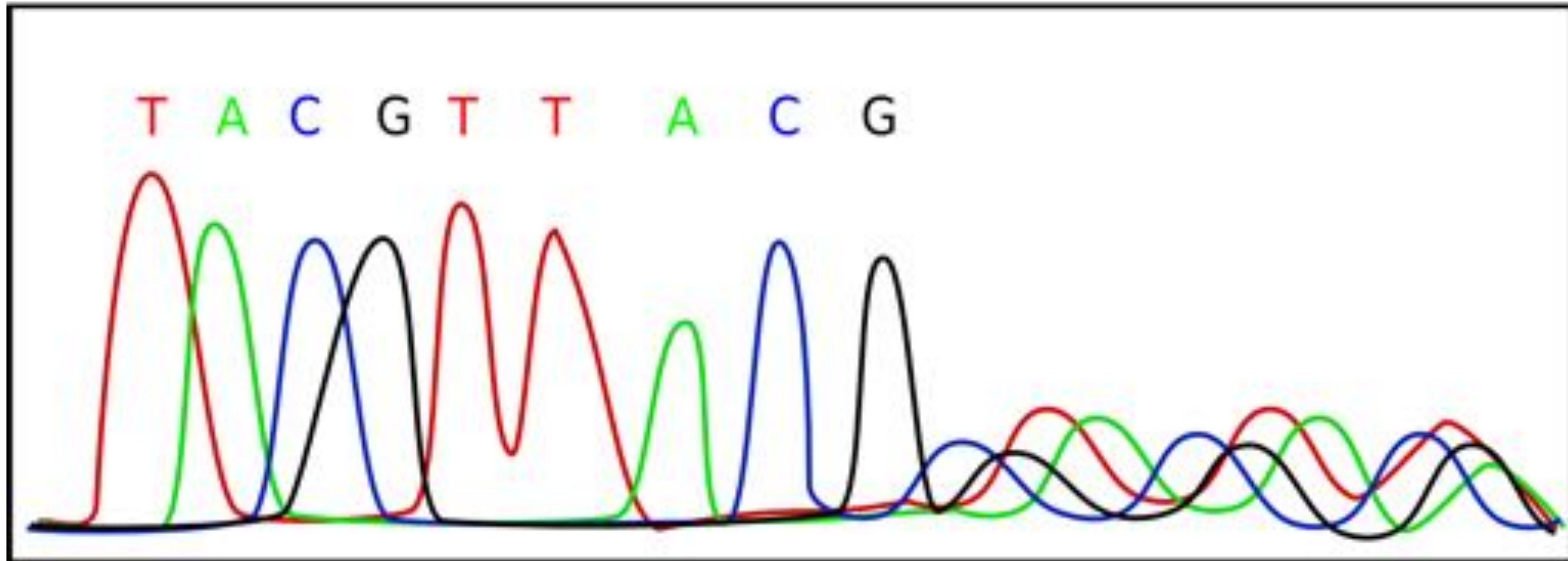
```
1 <!DOCTYPE html PUBLIC "-//W3C//DTD
  XHTML 1.0 Transitional//EN"
2 "http://www.w3.org/TR/xhtml1/DTD/
  xhtml1-transitional.dtd">
3
4 <html xmlns="http://www.w3.org/1999/
  xhtml">
5   <head>
6     <meta http-equiv="Content-
  Type" content=
7       "text/html; charset=us-
  ascii" />
8     <script type="text/
  javascript">
9       function reDo() {top.
  location.reload();}
10      if (navigator.appName ==
  'Netscape') {top.onresize = reDo;}
11      dom=document.
  getElementById;
12    </script>
13  </head>
14  <body>
15  </body>
16 </html>
```

Data Types



Email

Data Types



Genomic Data, e.g., SNPs

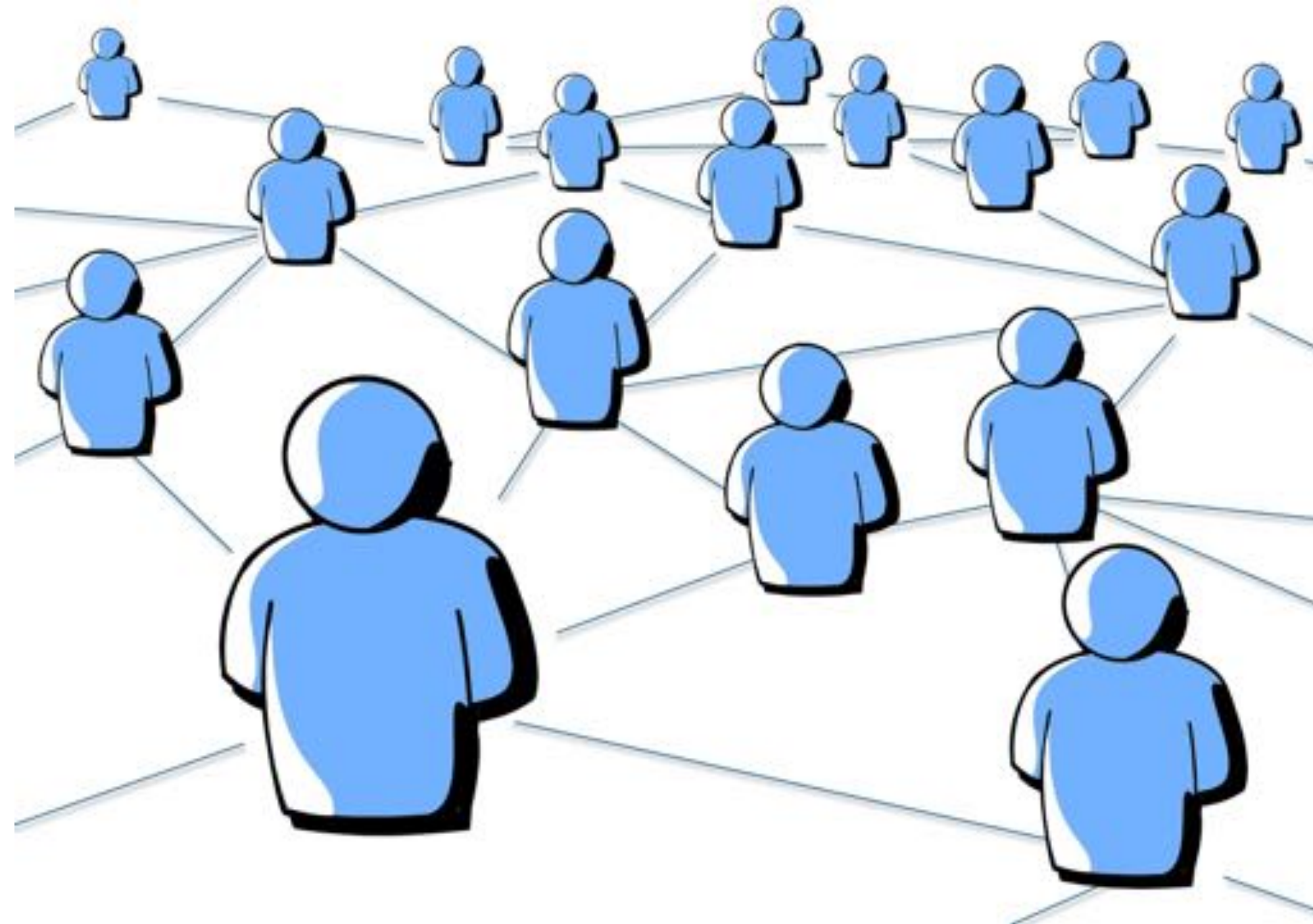
Data Types



Images










Data Types

(Social) Networks / Graphs

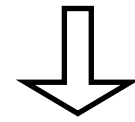


Data Types

User Ratings

			
	★	★★★★	
	★	★★★	★★
	★★★★		★
	★		★★
		★★★	★★
	★★★★	★★	

Obtain Raw Data



Feature Extraction

Initial observations can be in arbitrary format

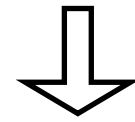
We extract *features* to represent observations

We can incorporate domain knowledge

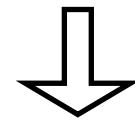
We typically want numeric features

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

Obtain Raw Data

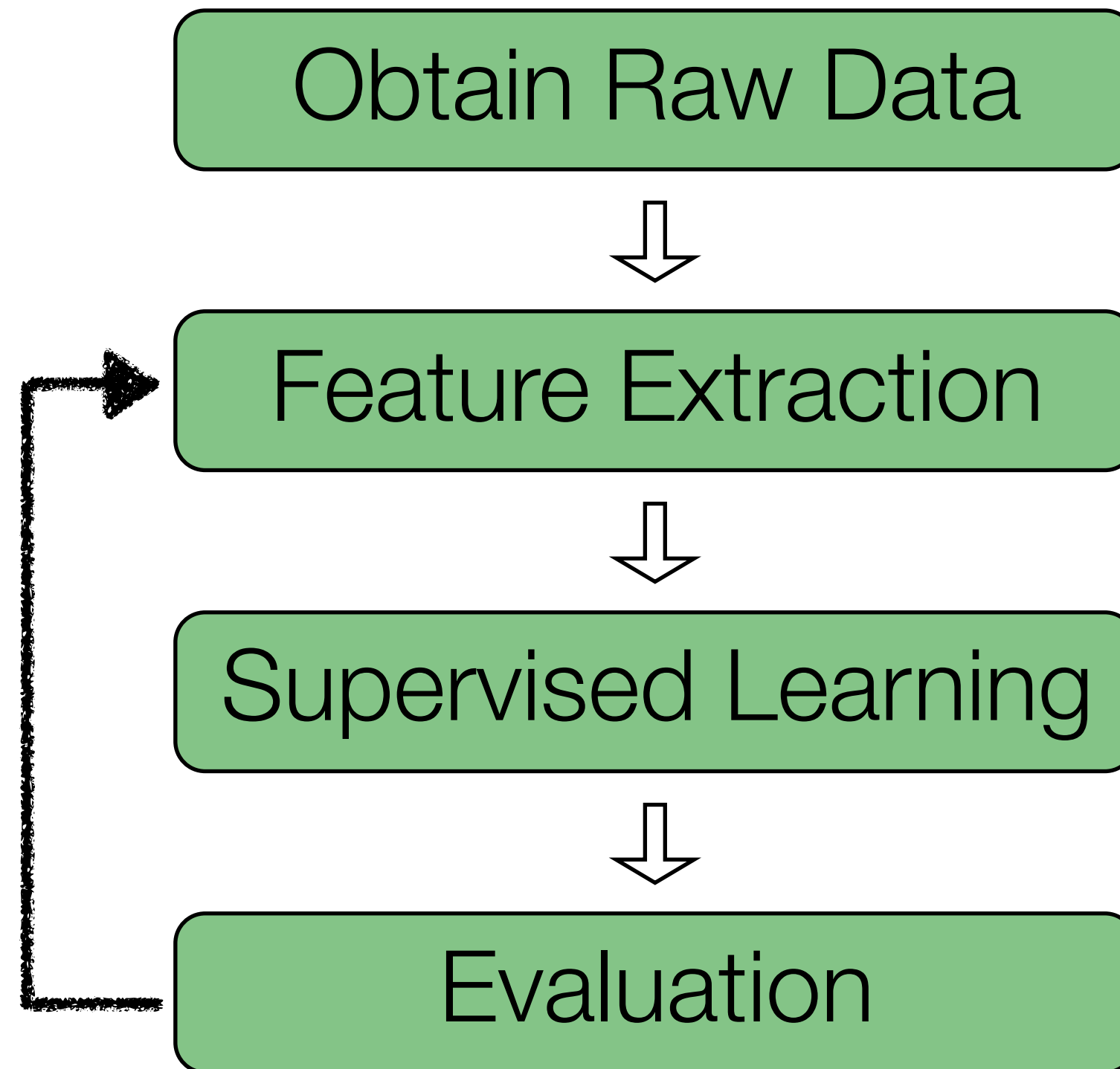


Feature Extraction



Supervised Learning

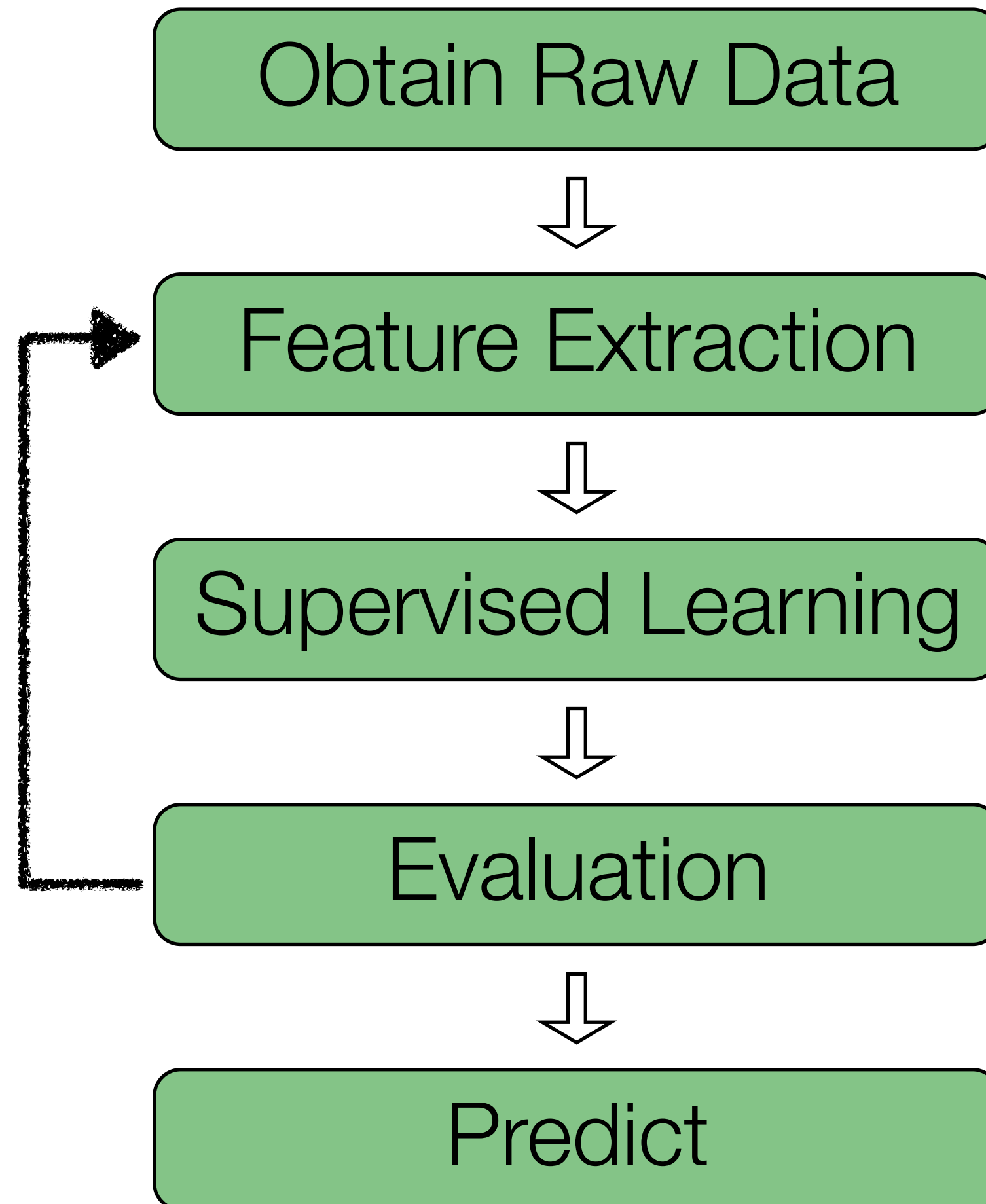
Train a supervised model using labeled data,
e.g., Classification or Regression model



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...

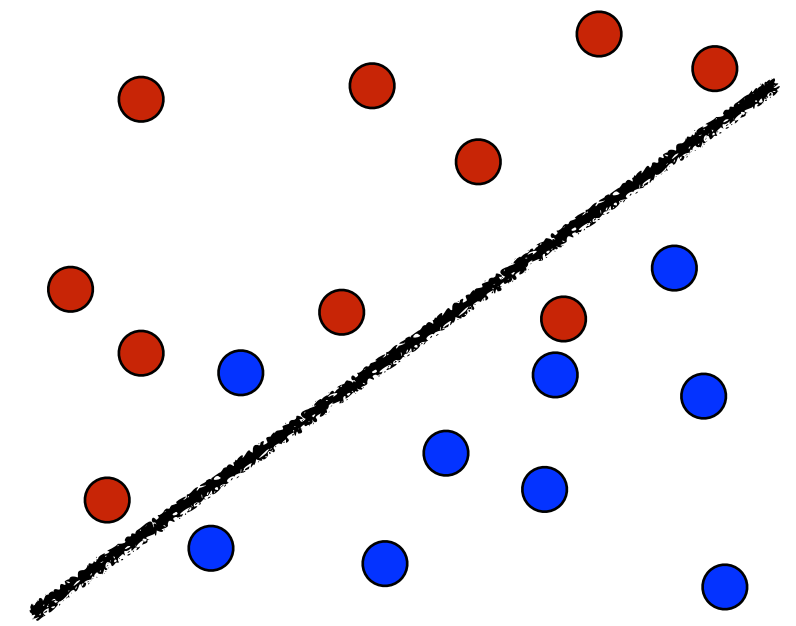


Once we're happy with our model, we can use it to make predictions on future observations, i.e., data without a known label

Sample Classification Pipeline



Classification

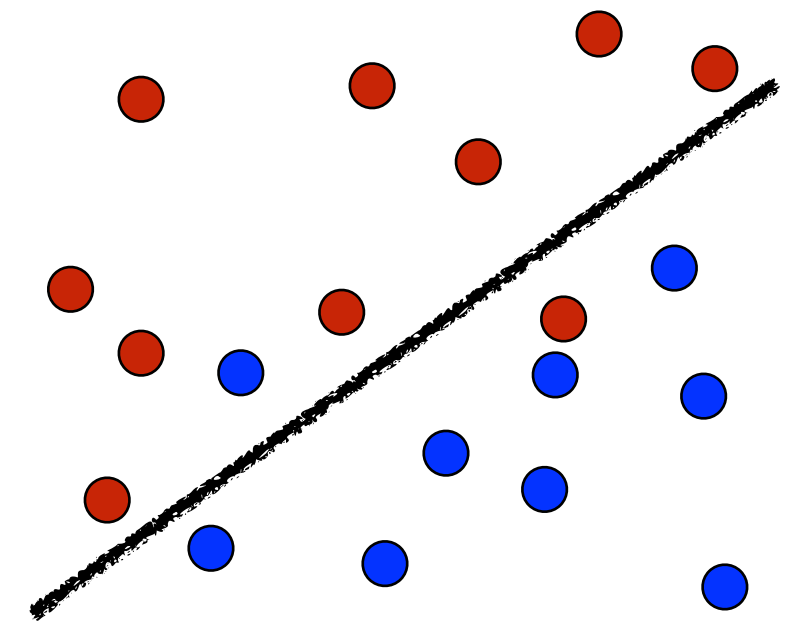


Goal: Learn a mapping from observations to discrete labels given a set of training examples (supervised learning)

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 \rightarrow {fraud, not fraud}

Face detection: Images \rightarrow set of people

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

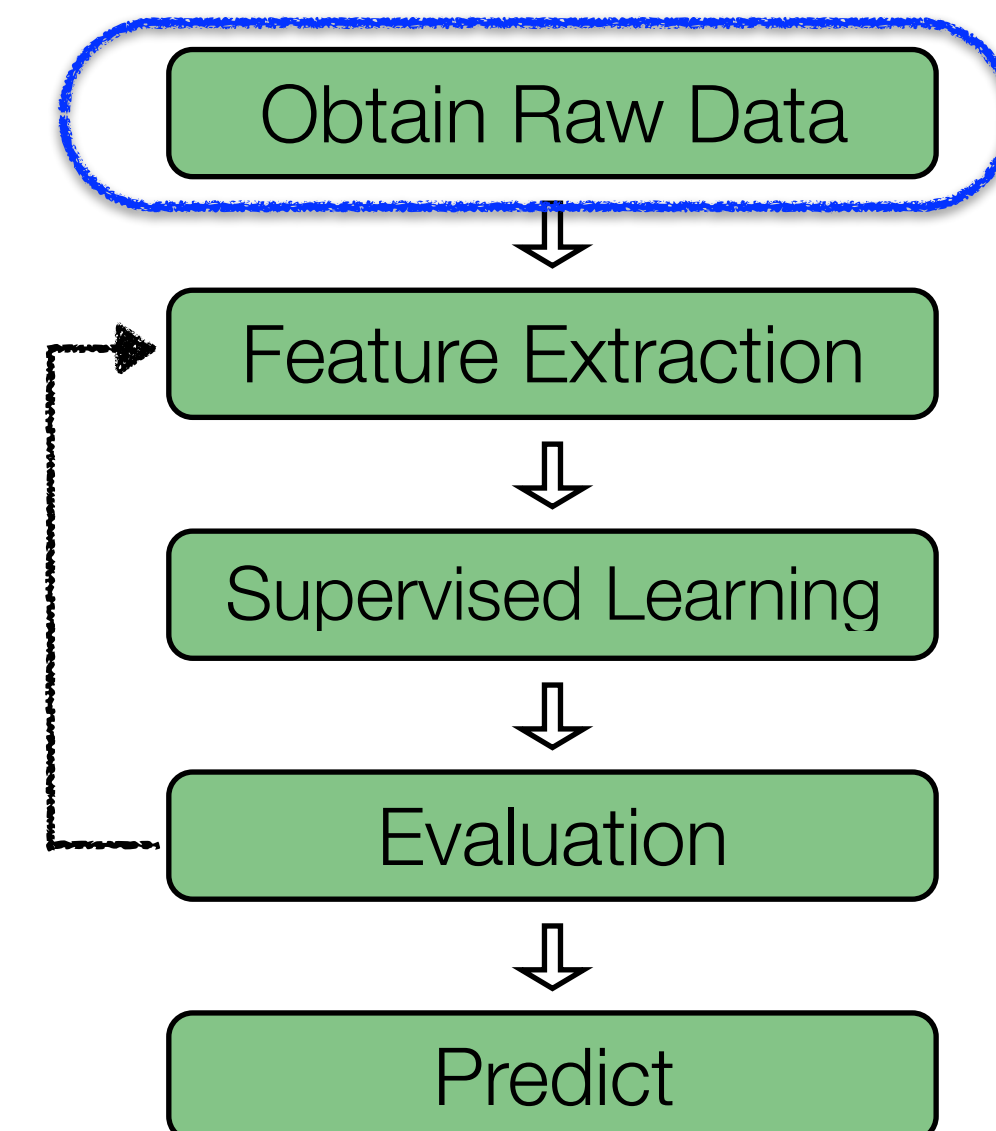
Clickthrough rate prediction: User and ads \rightarrow {click, no click}

Many others...

Classification Pipeline



Raw data consists of a set of labeled training observations



E.g., Spam Classification

Observation

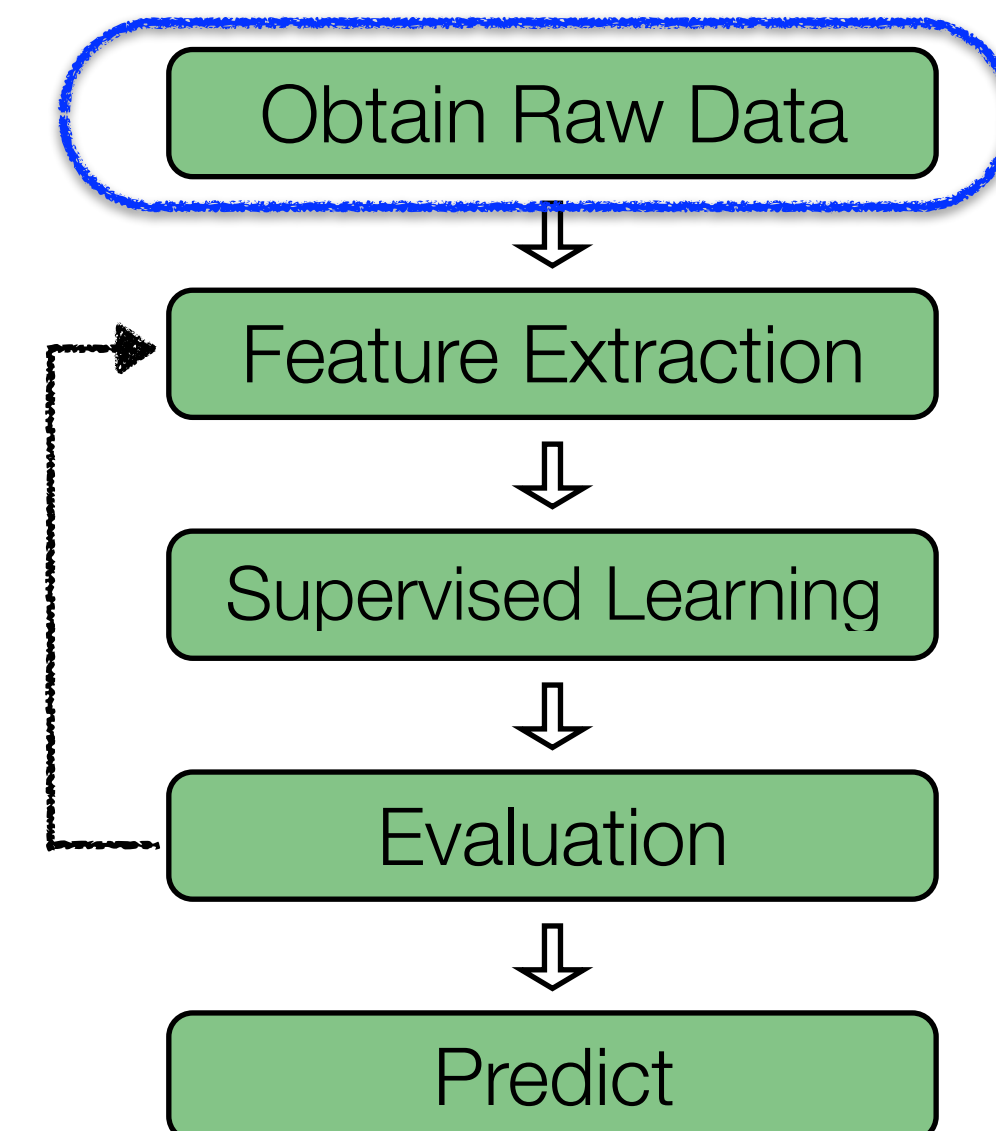
Label

From: illegitimate@bad.com
"Eliminate your debt by
giving us your money..."

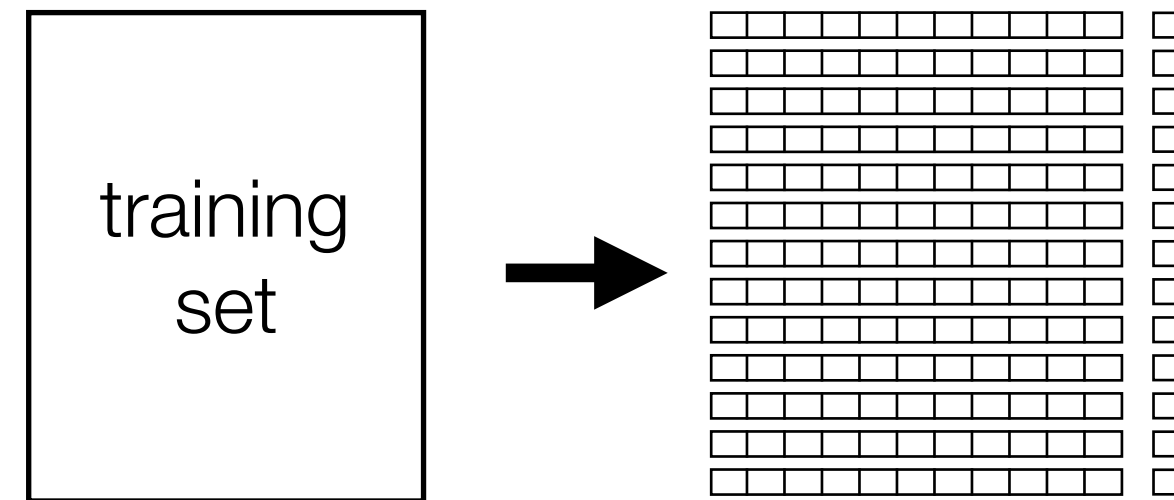
spam

From: bob@good.com
"Hi, it's been a while!
How are you? ..."

not-spam

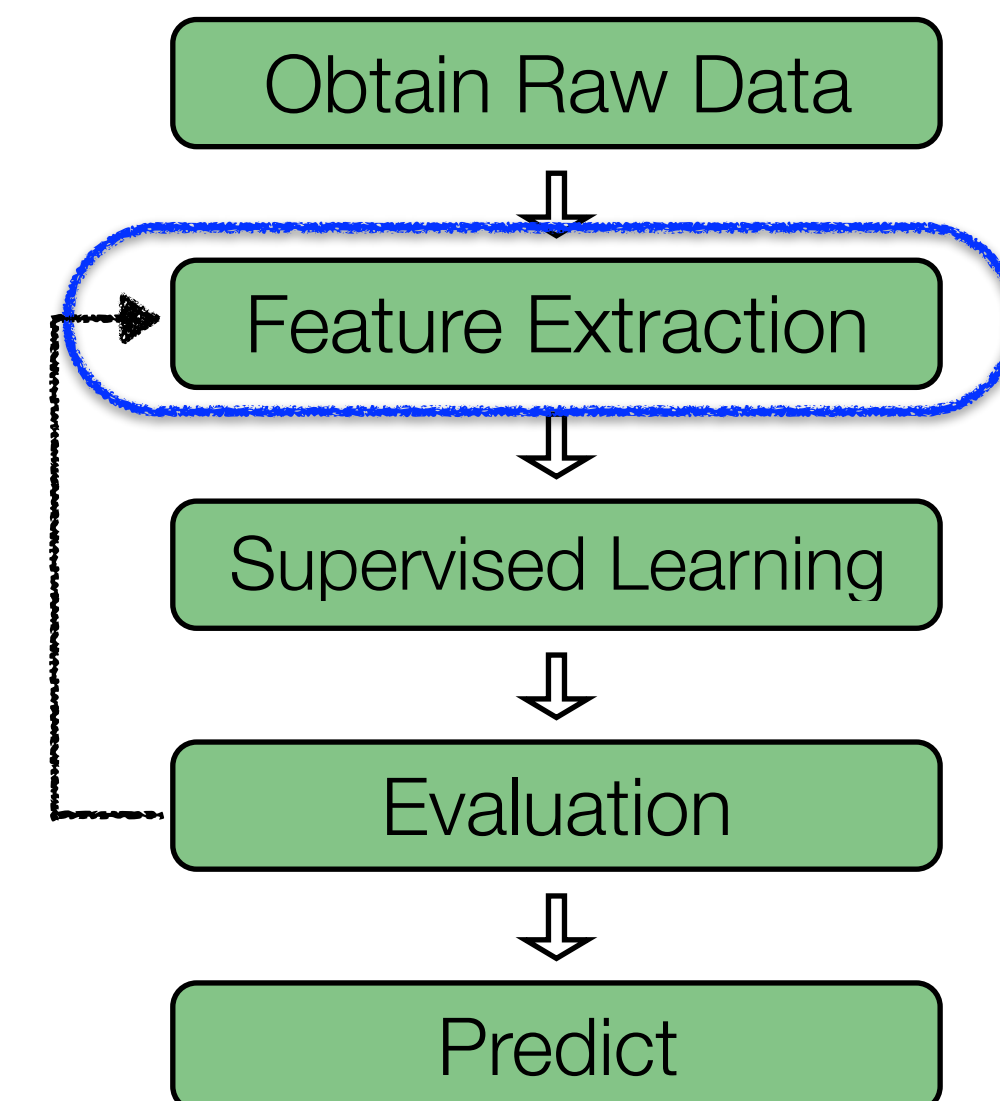


Classification Pipeline



Feature extraction typically transforms each observation 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”

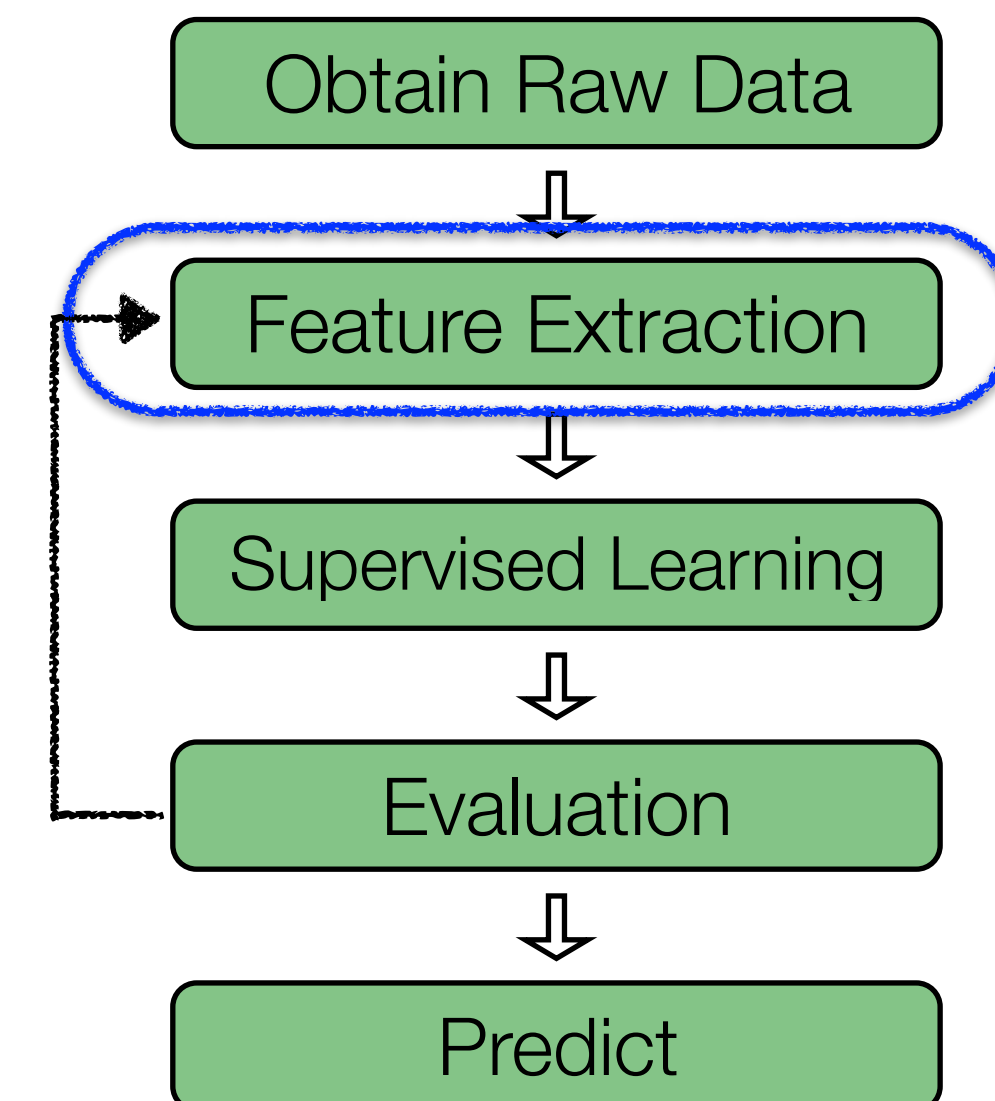
From: illegitimate@bad.com

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

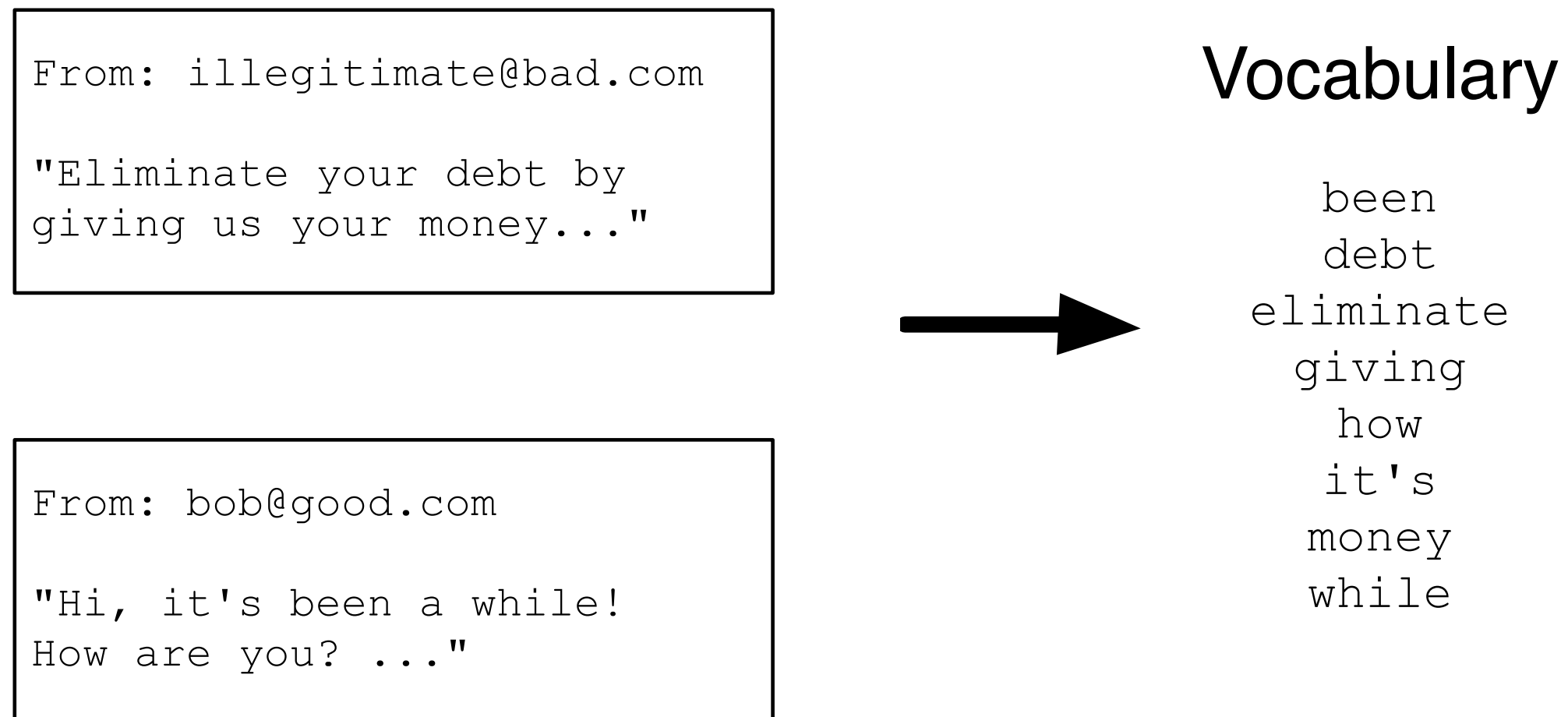
From: bob@good.com

"Hi, it's been a while!
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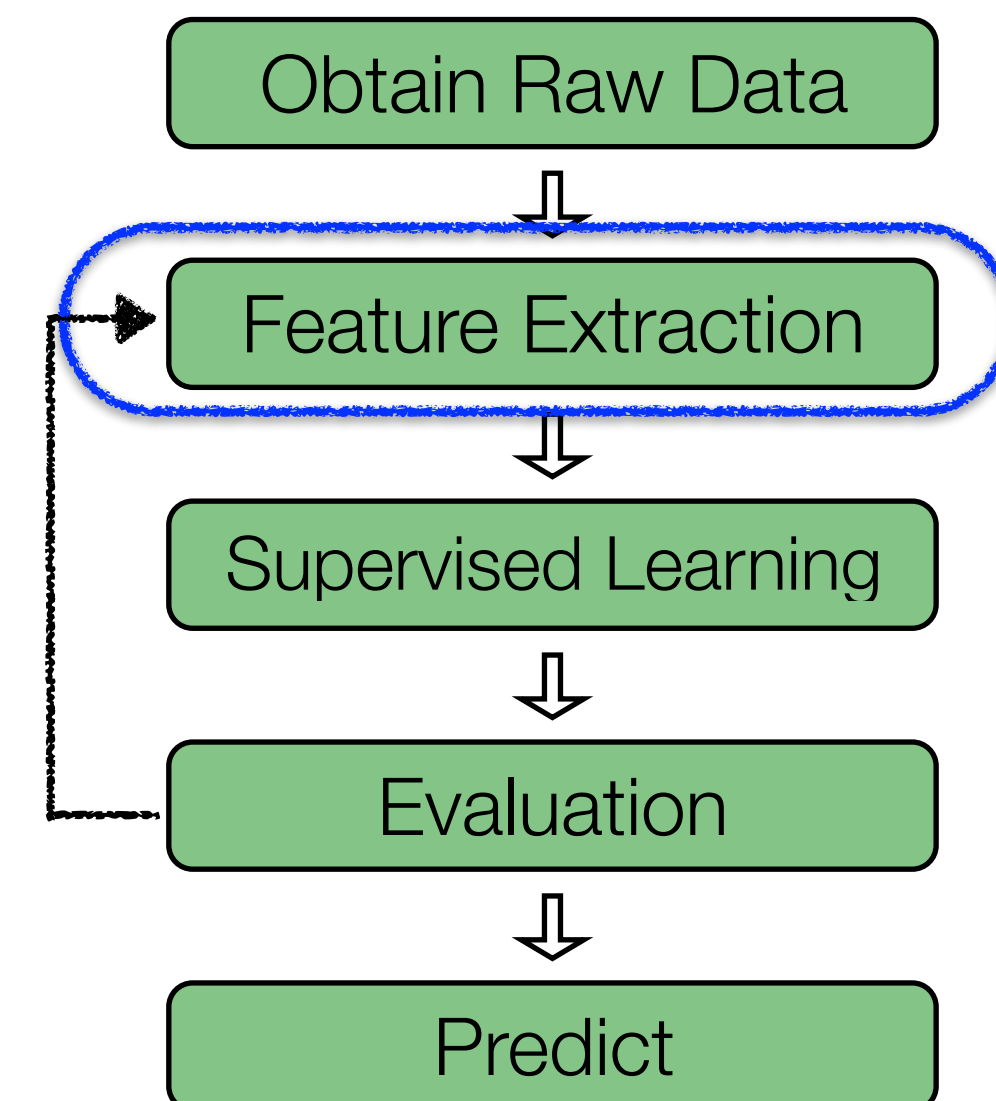
Observations are documents



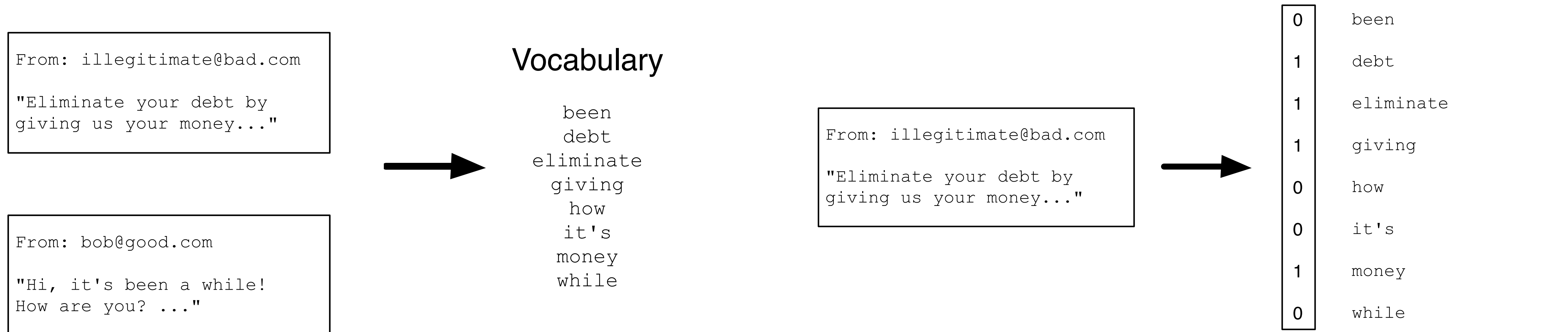
E.g., “Bag of Words”



Observations are documents
Build Vocabulary



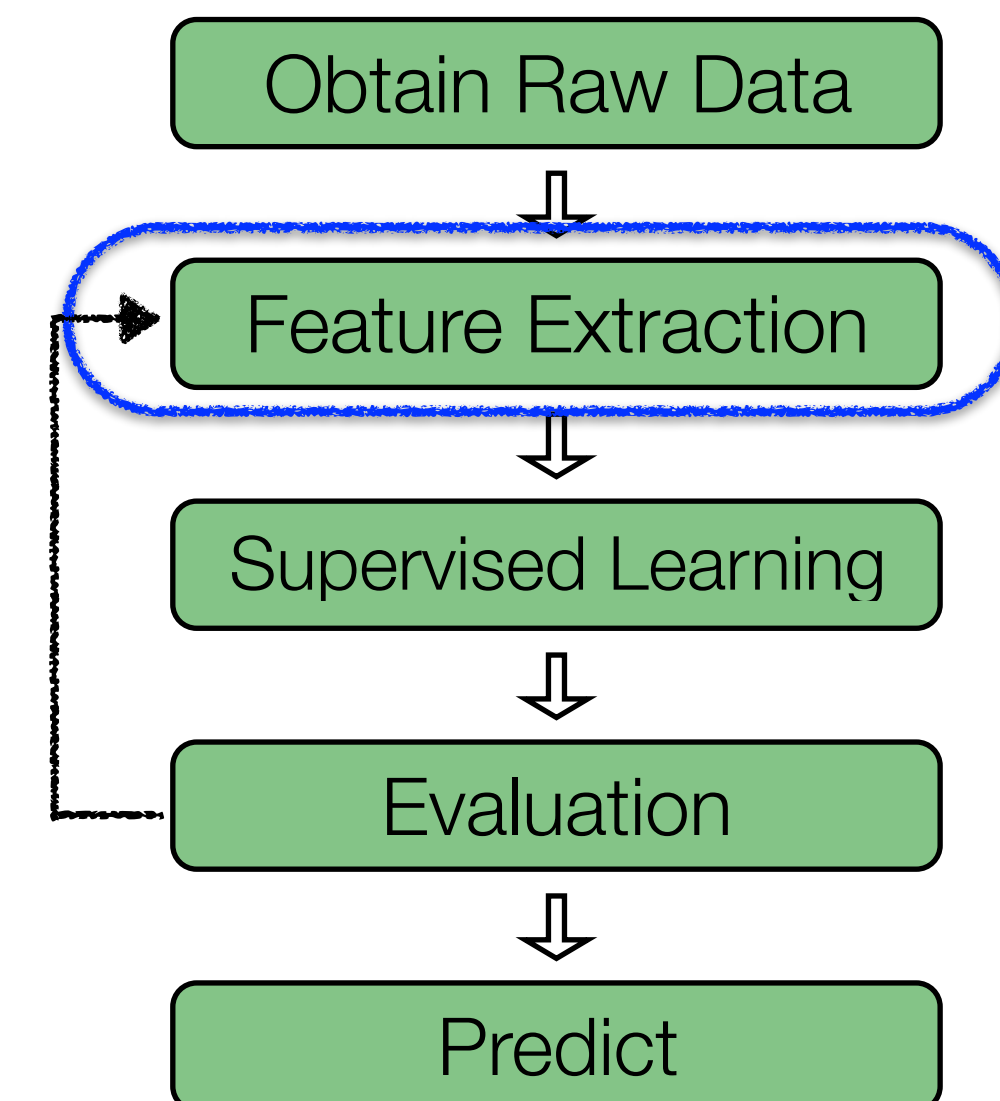
E.g., “Bag of Words”



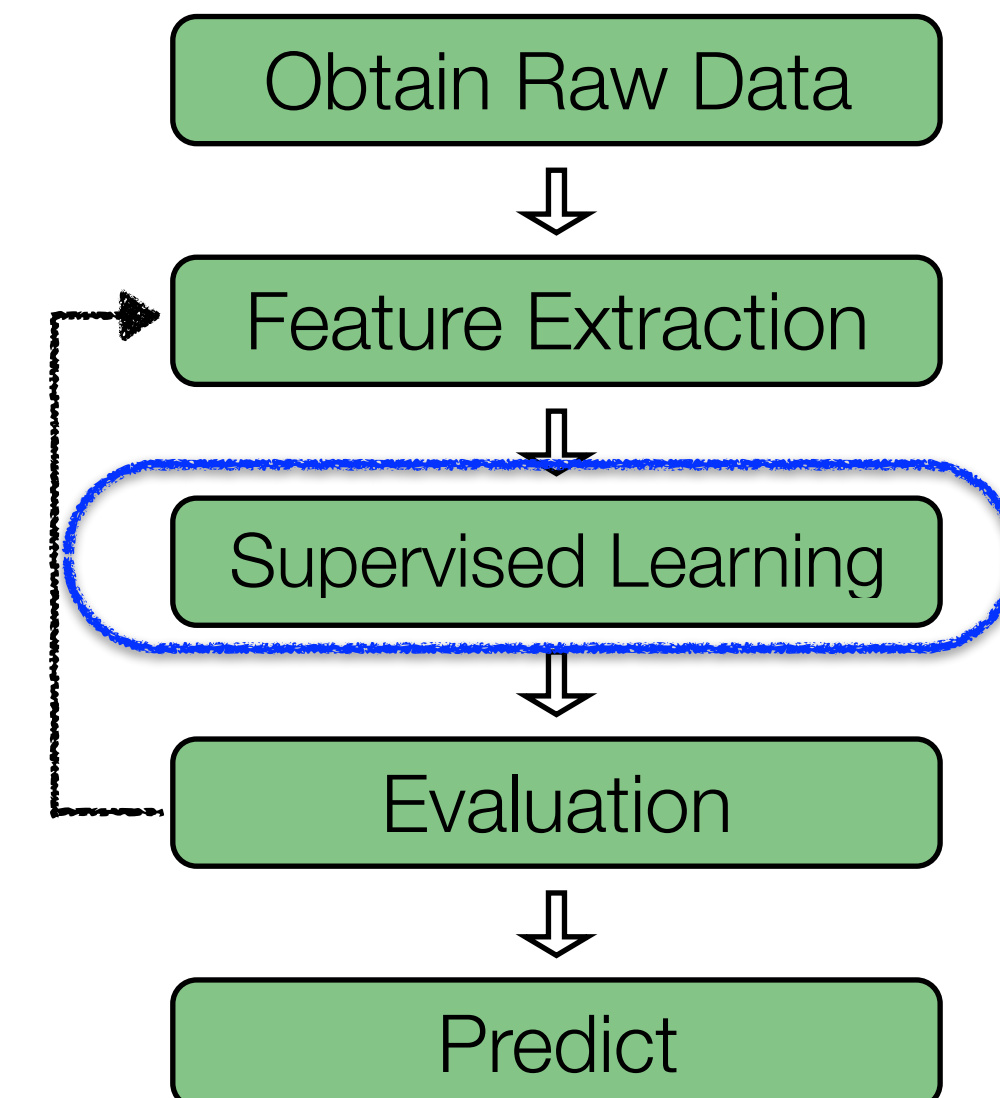
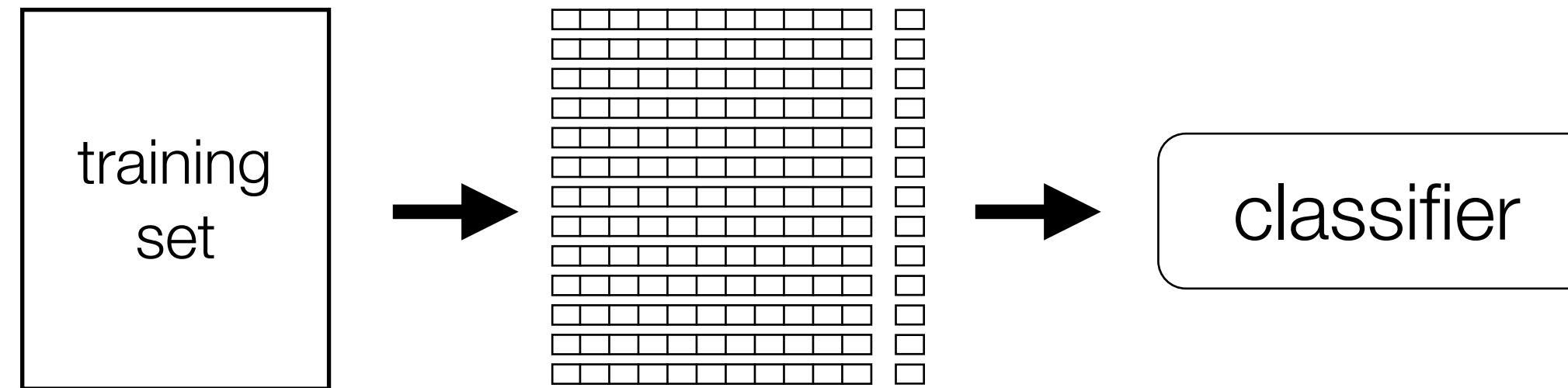
Observations are documents

Build Vocabulary

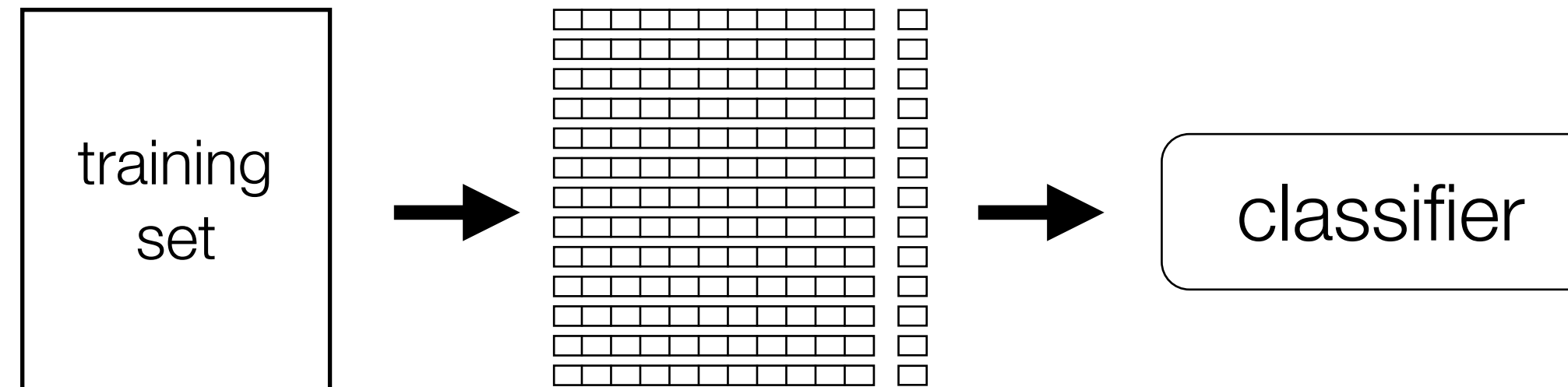
Derive feature vectors from Vocabulary



Classification Pipeline



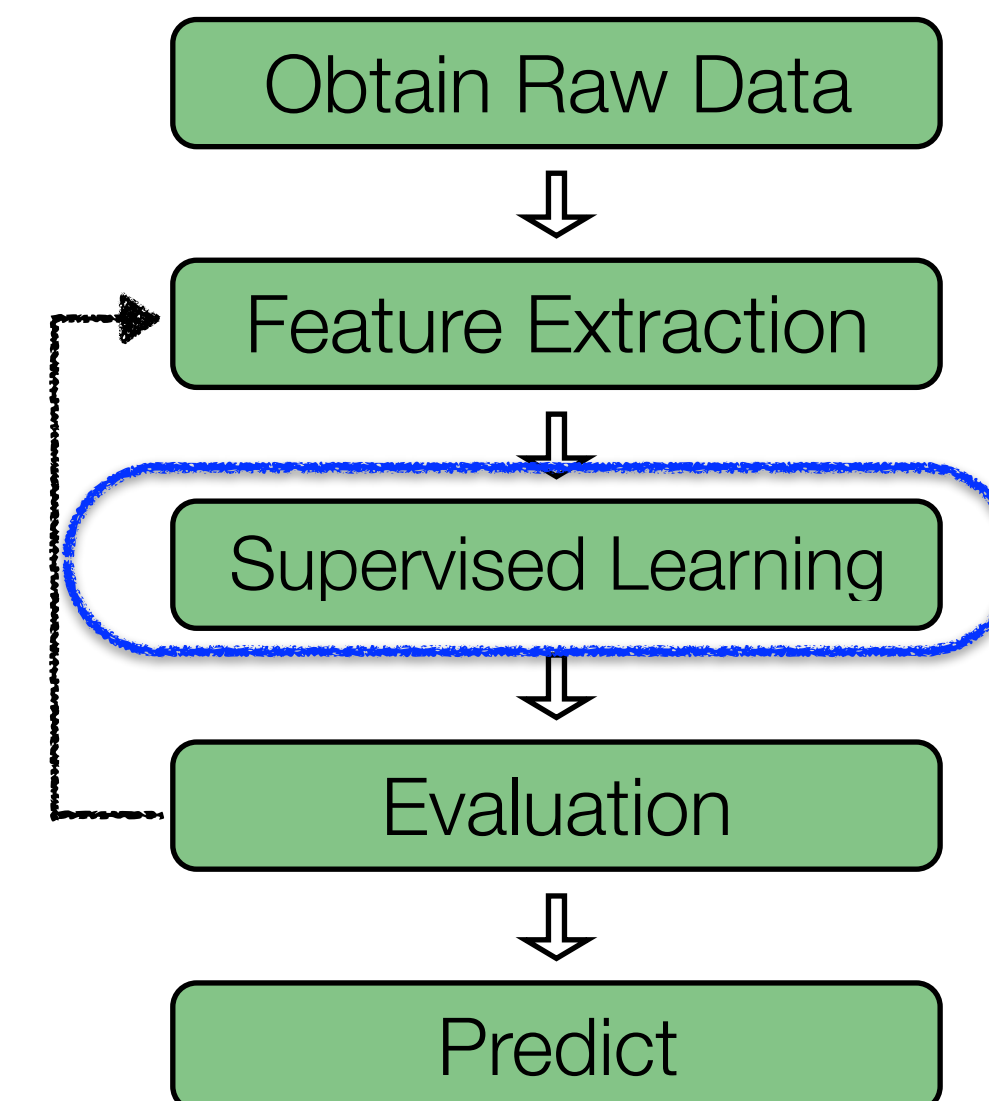
Classification Pipeline



Supervised Learning: Train classifier using training data

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

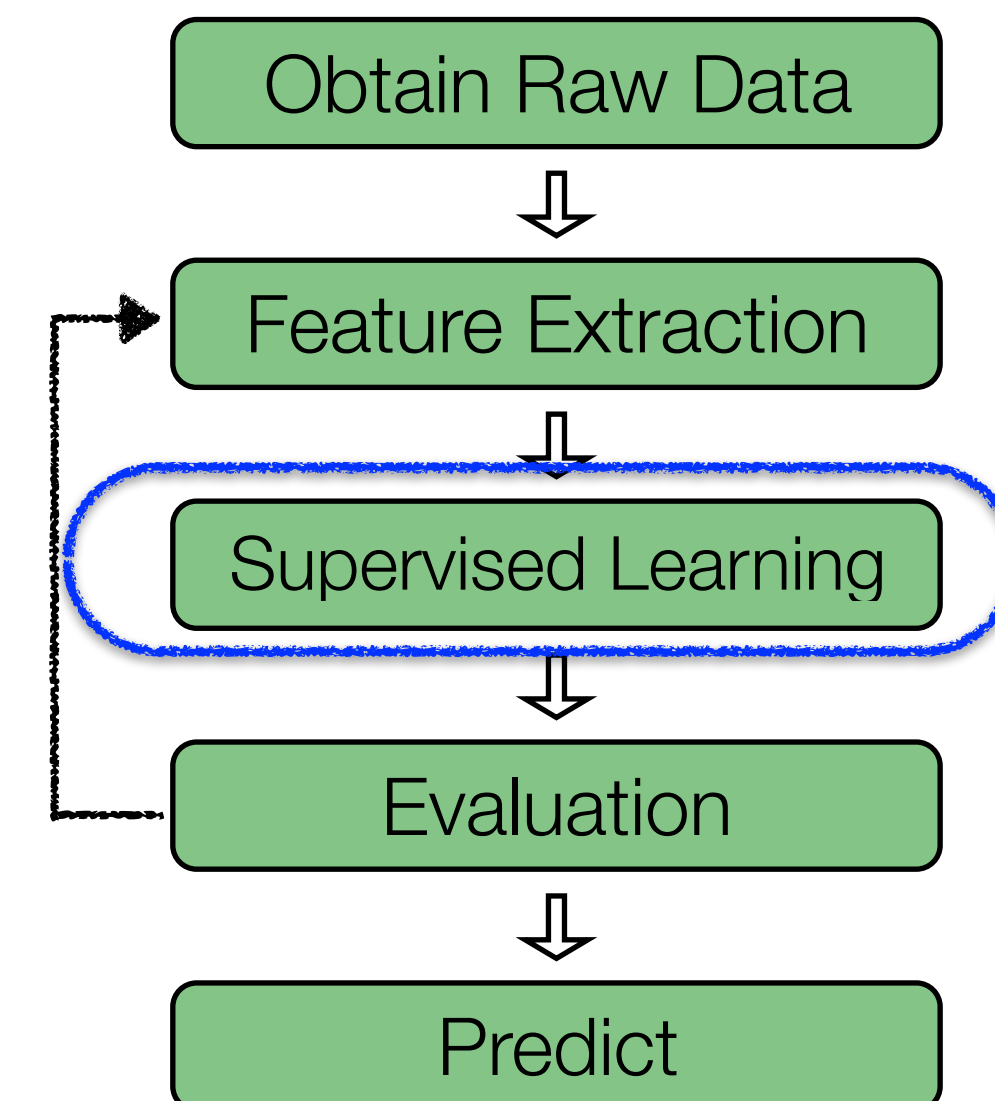
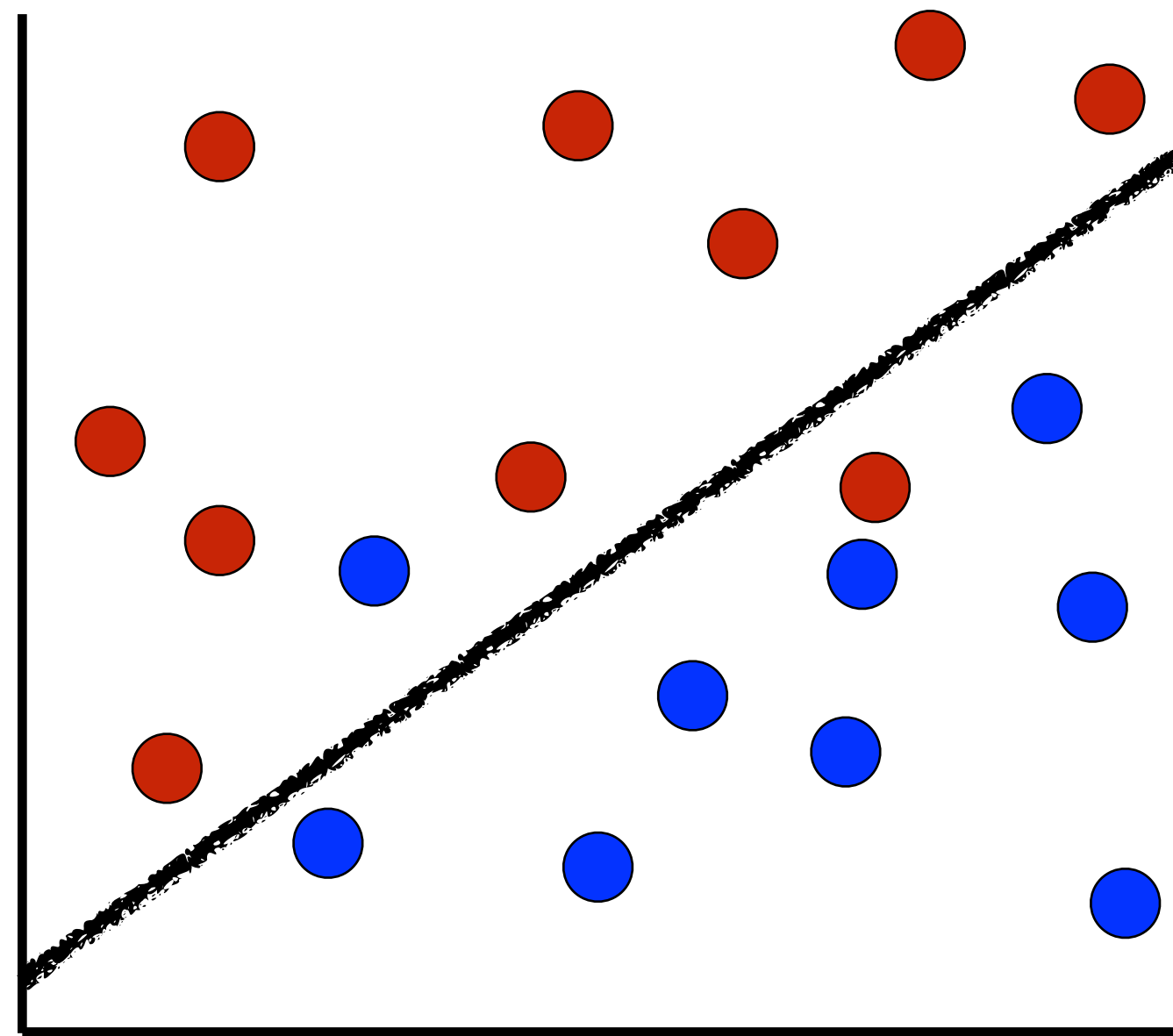
Training (especially at scale) often involves iterative computations, e.g., gradient descent



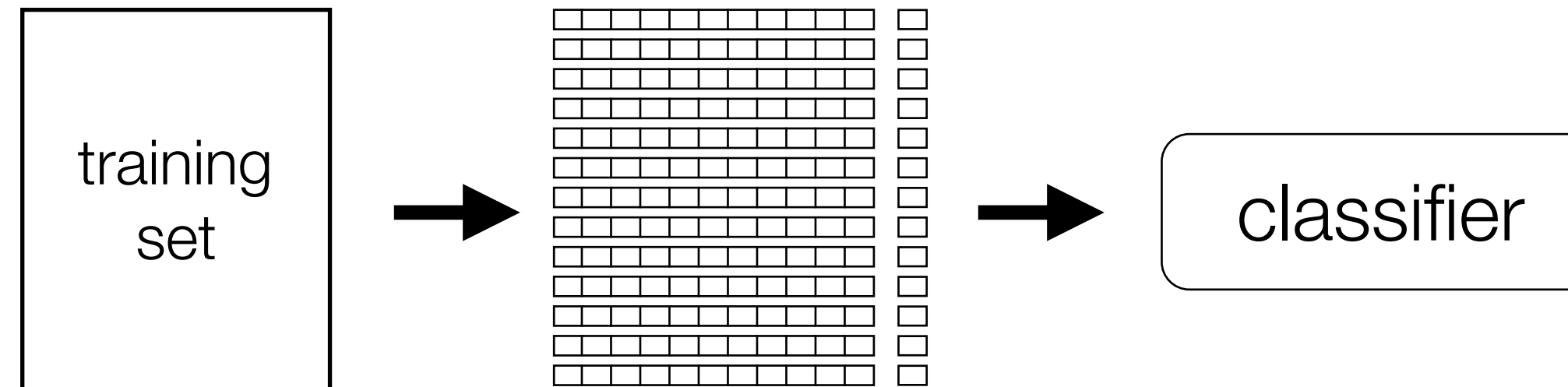
E.g., Logistic Regression

Goal: Find linear decision boundary

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



Classification Pipeline



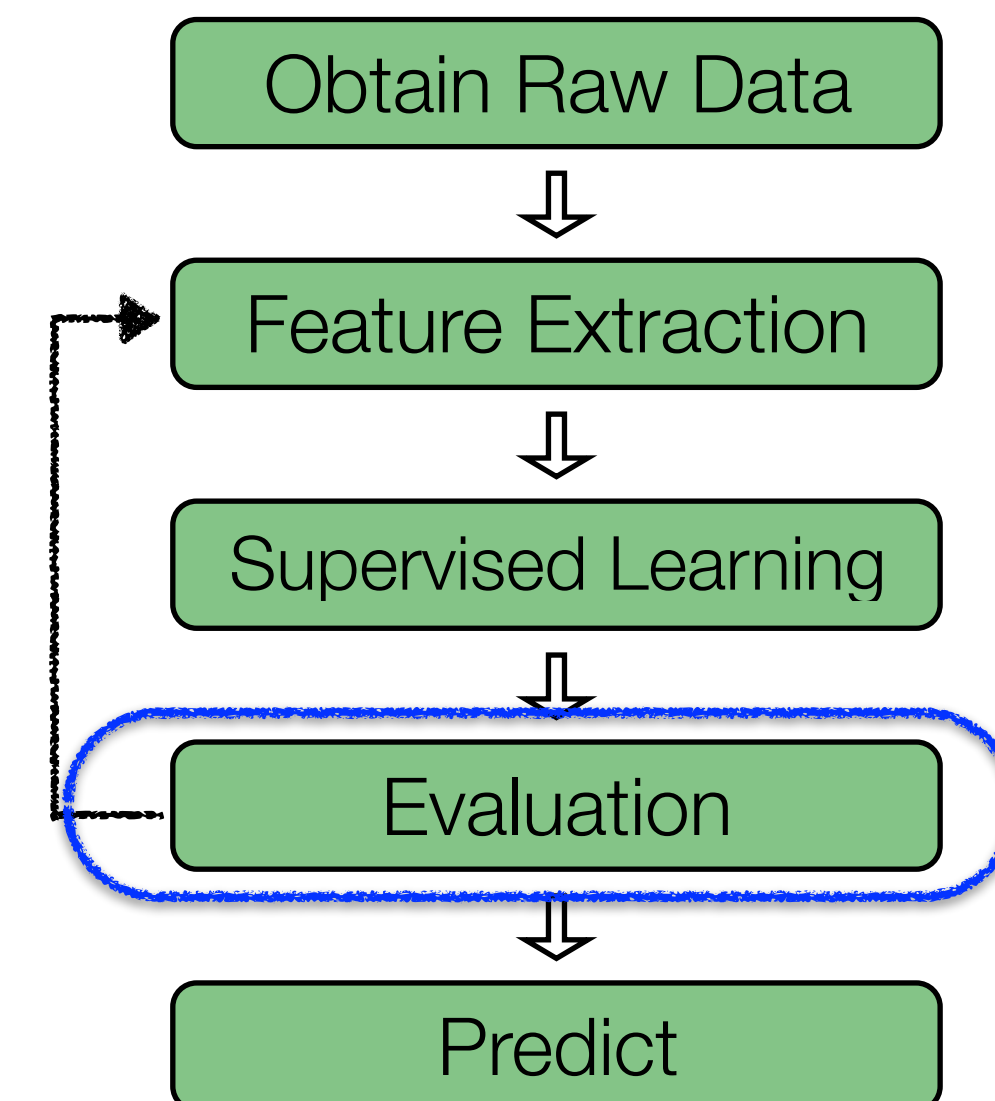
How can we evaluate the quality of our classifier?

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'



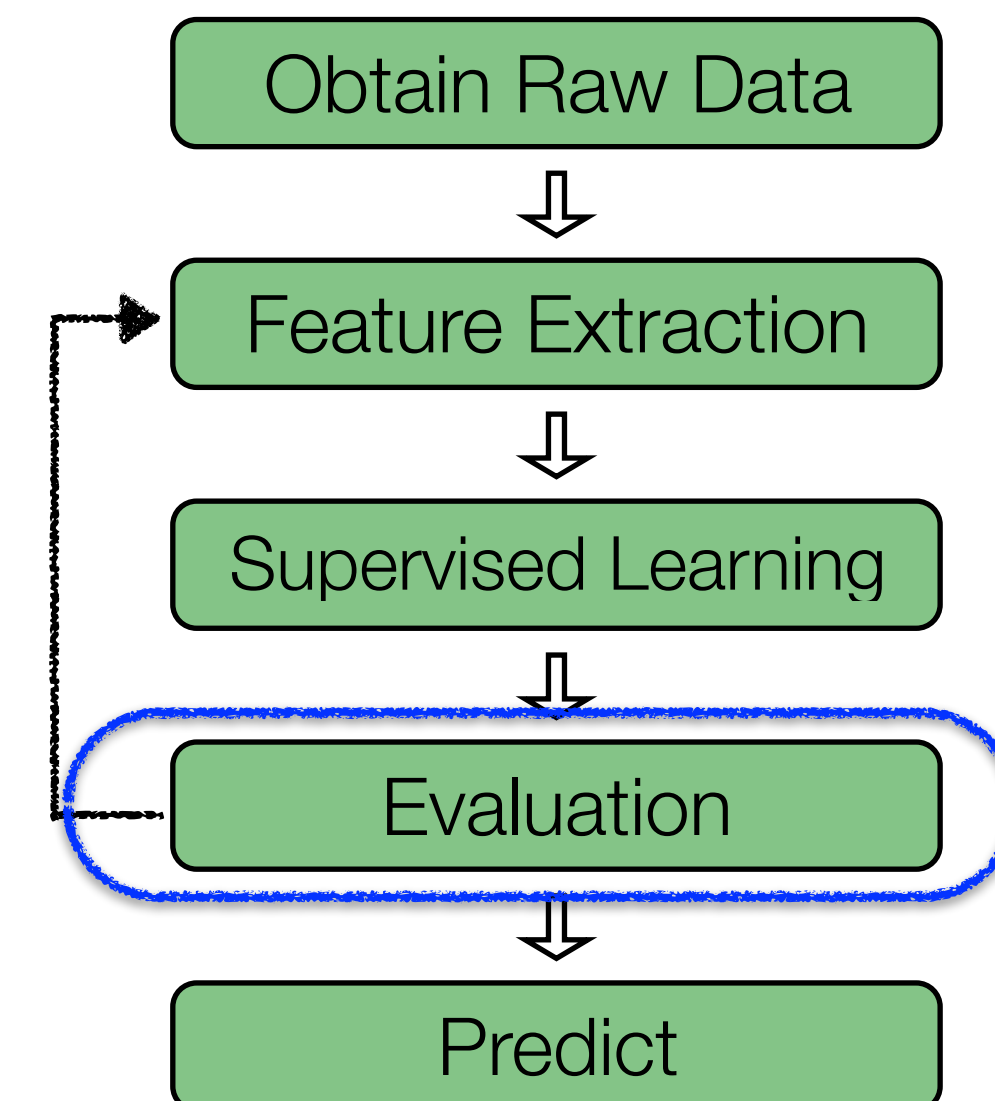
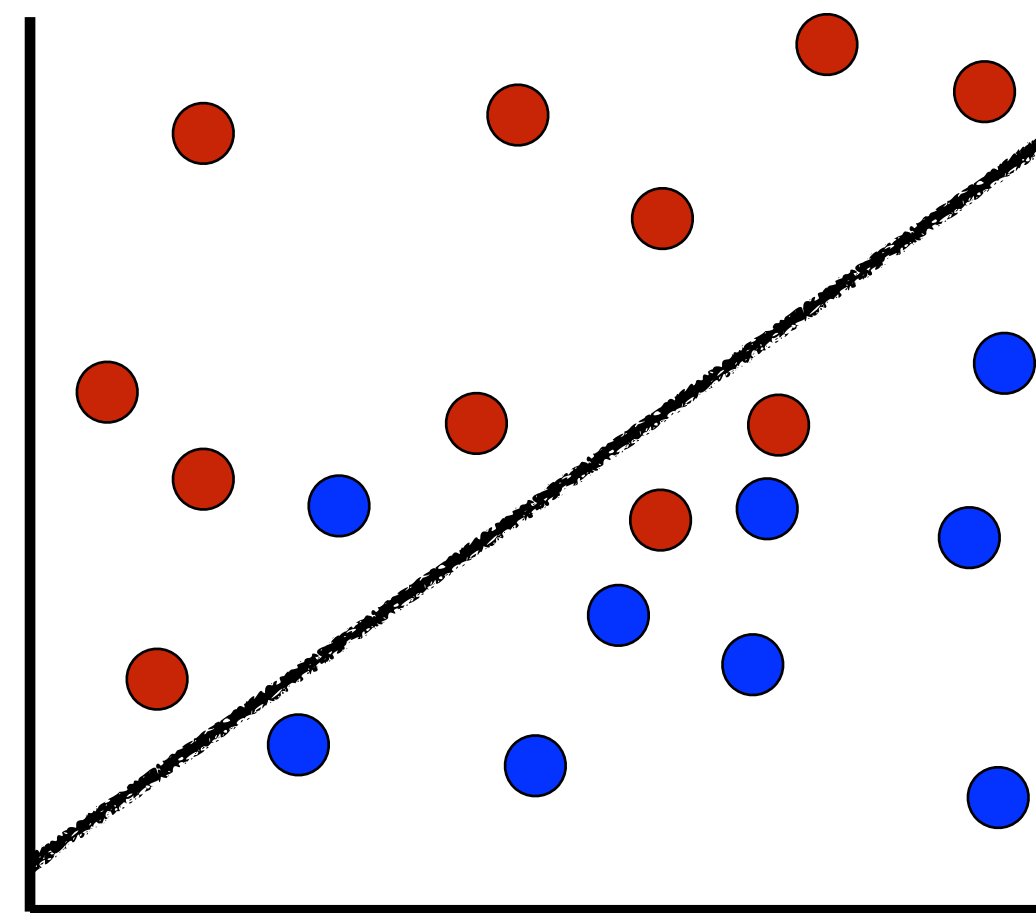
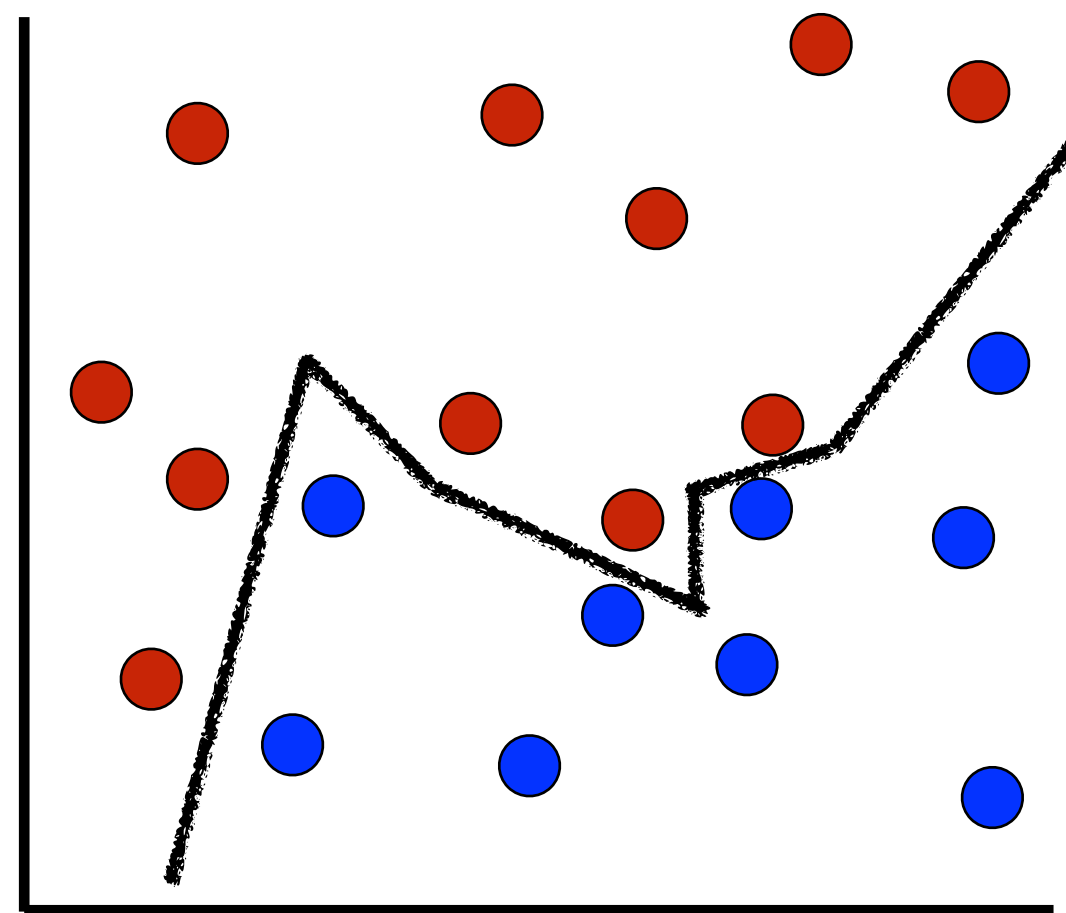
Overfitting and Generalization

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

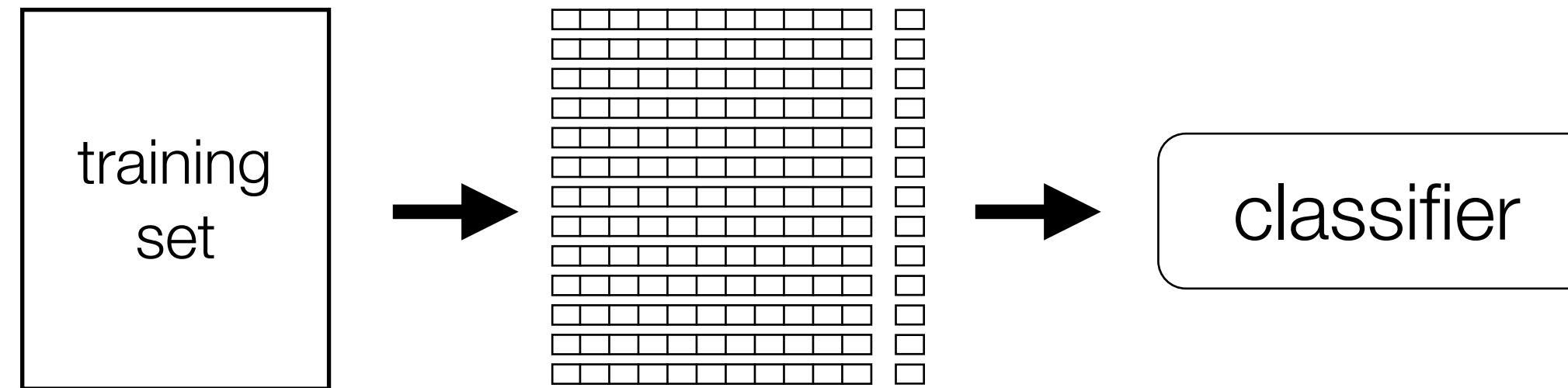
Left: perfectly fits training samples, but it is complex / overfitting

Right: misclassifies a few points, but simple / generalizes

Occam's razor

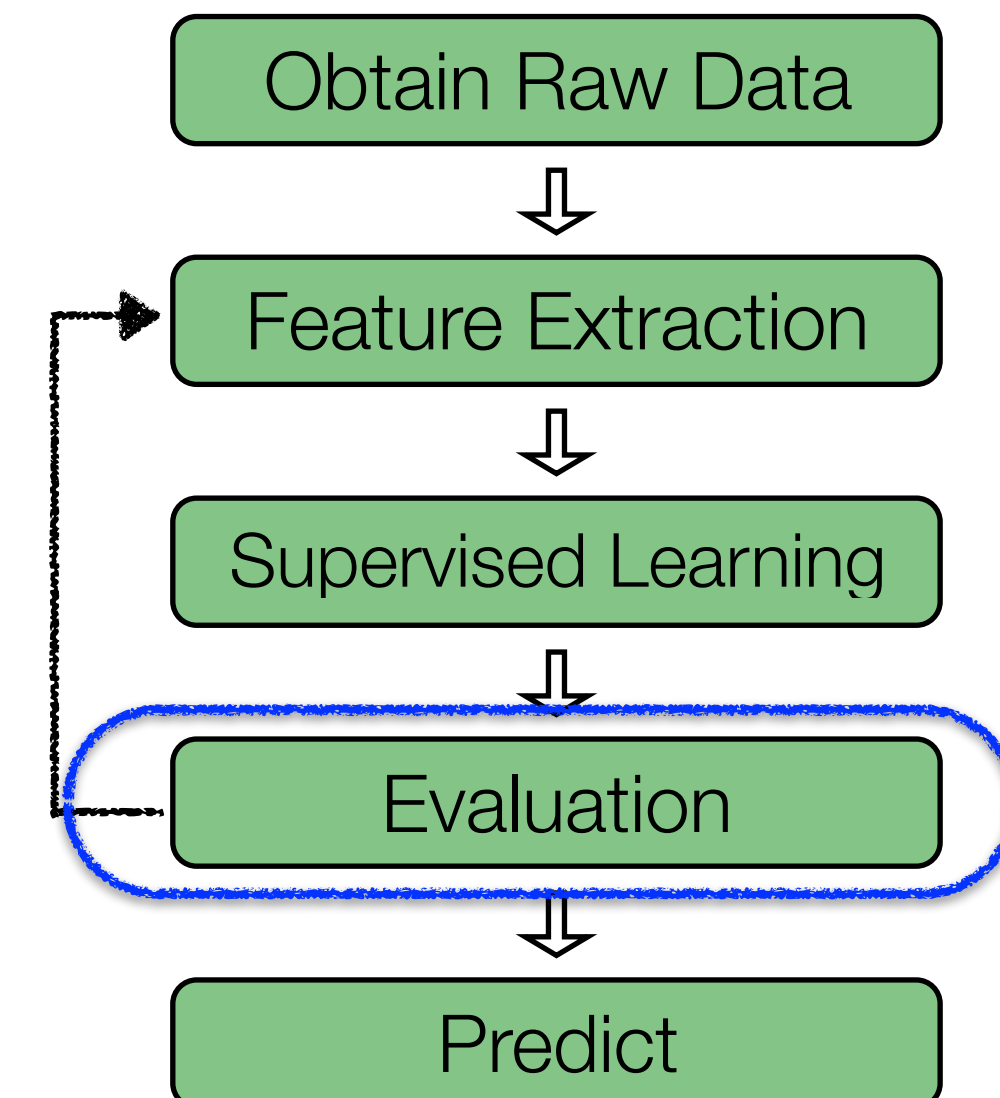


Classification Pipeline

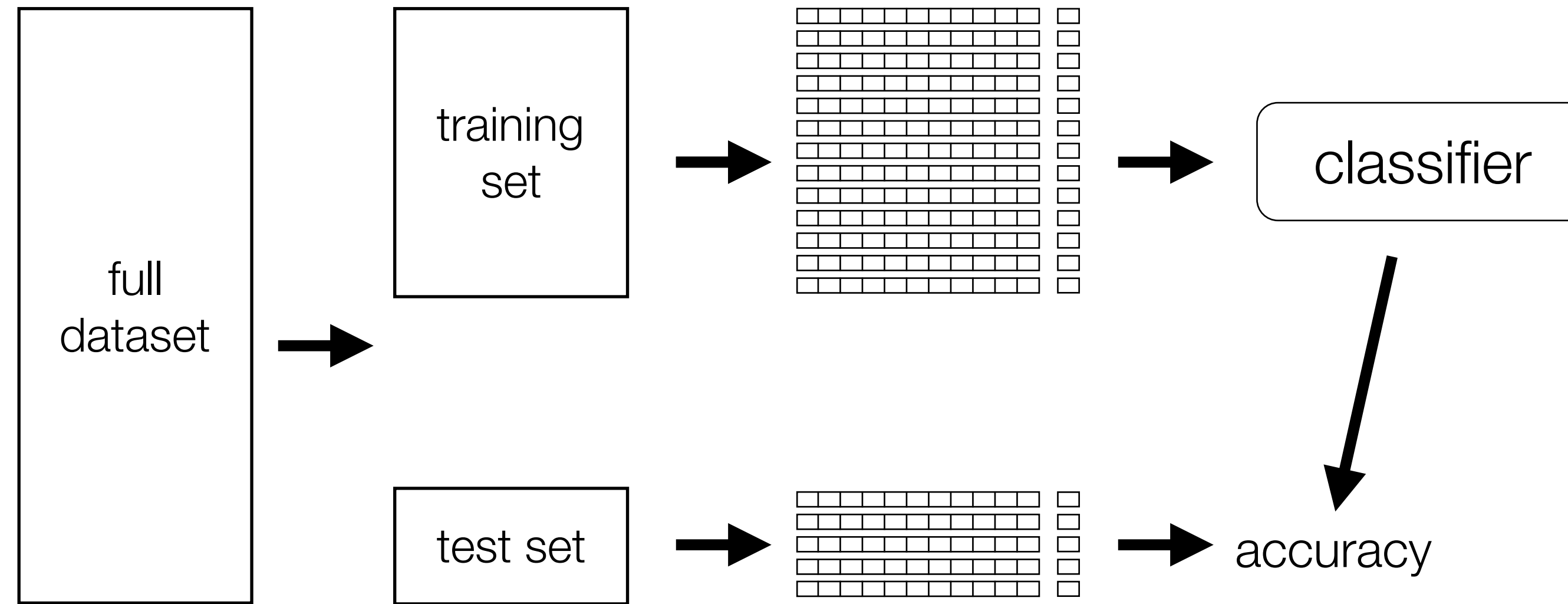


How can we evaluate the quality of our classifier?

Idea: Create test set to simulate unobserved data

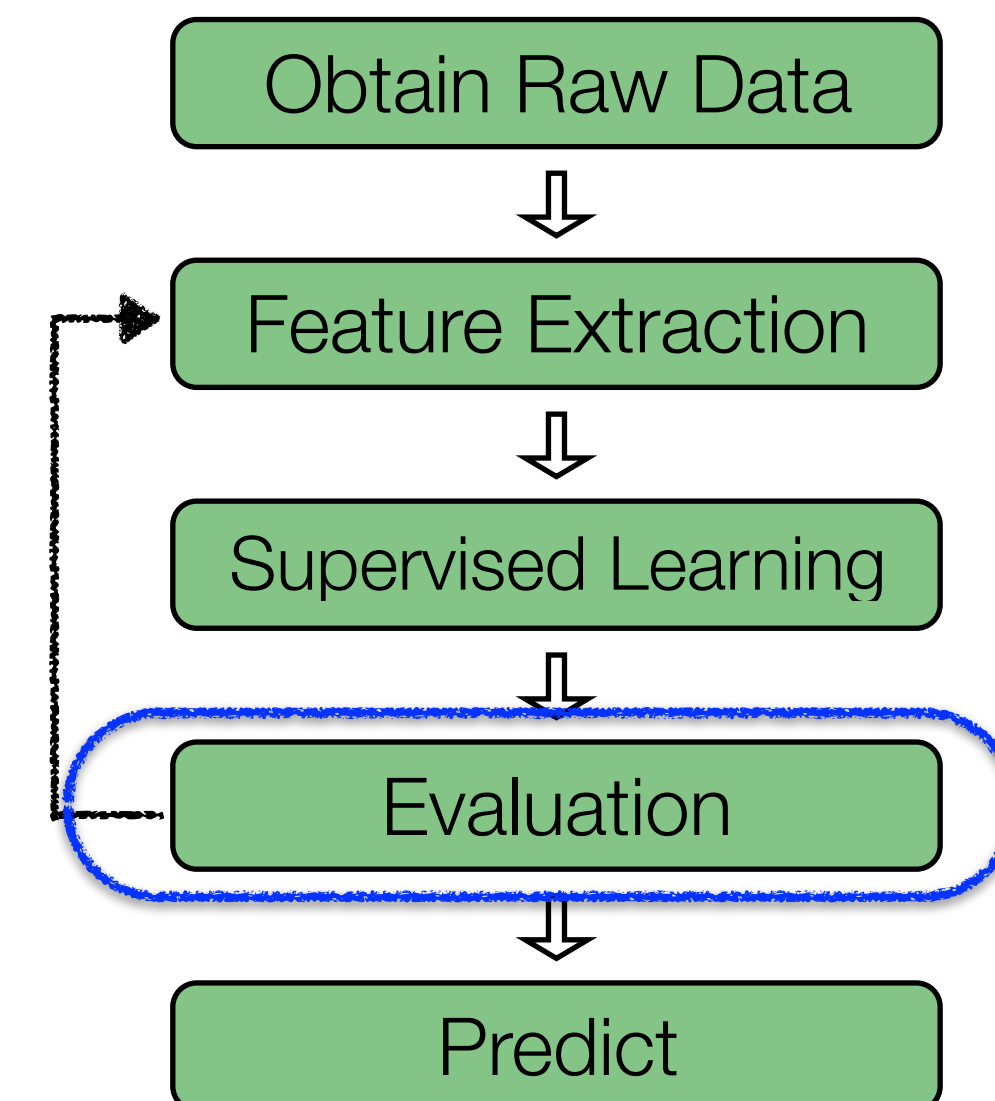


Classification Pipeline

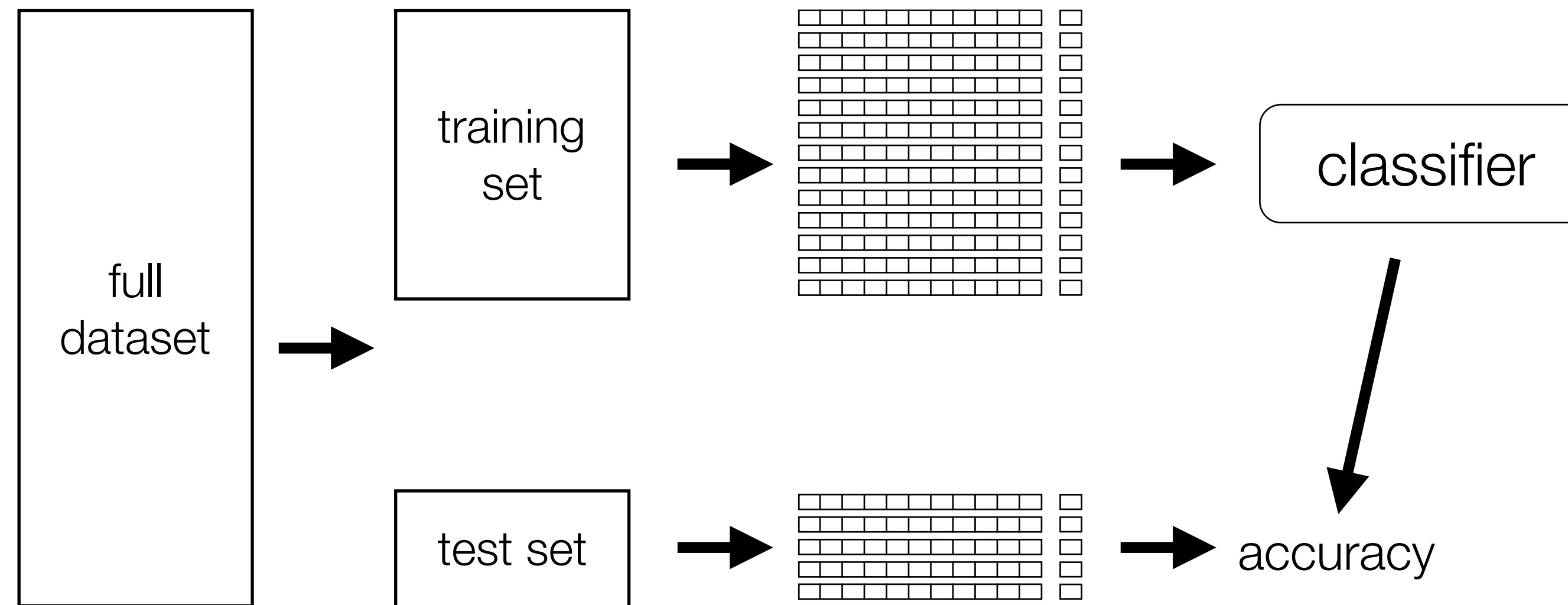


Evaluation: Split dataset into training / testing datasets

- 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

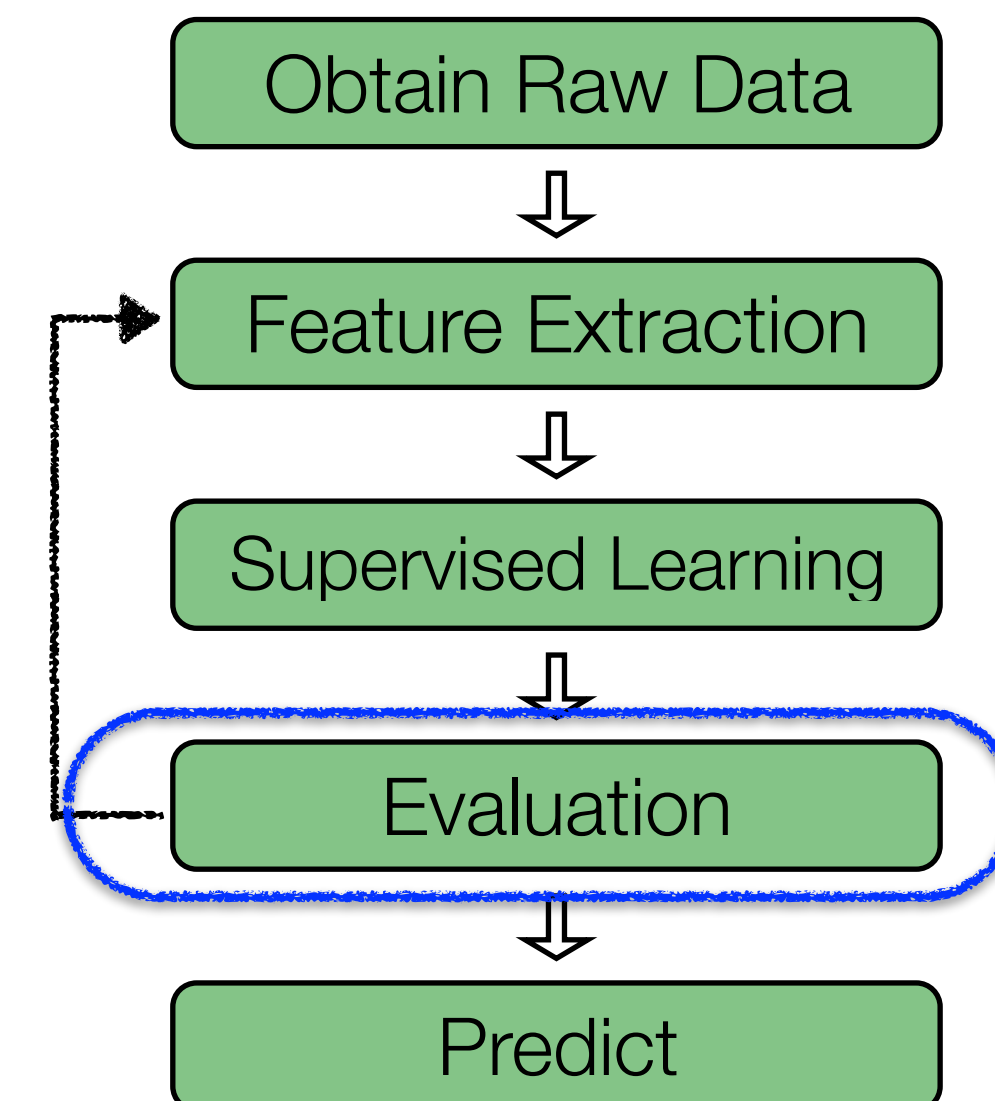


Classification Pipeline

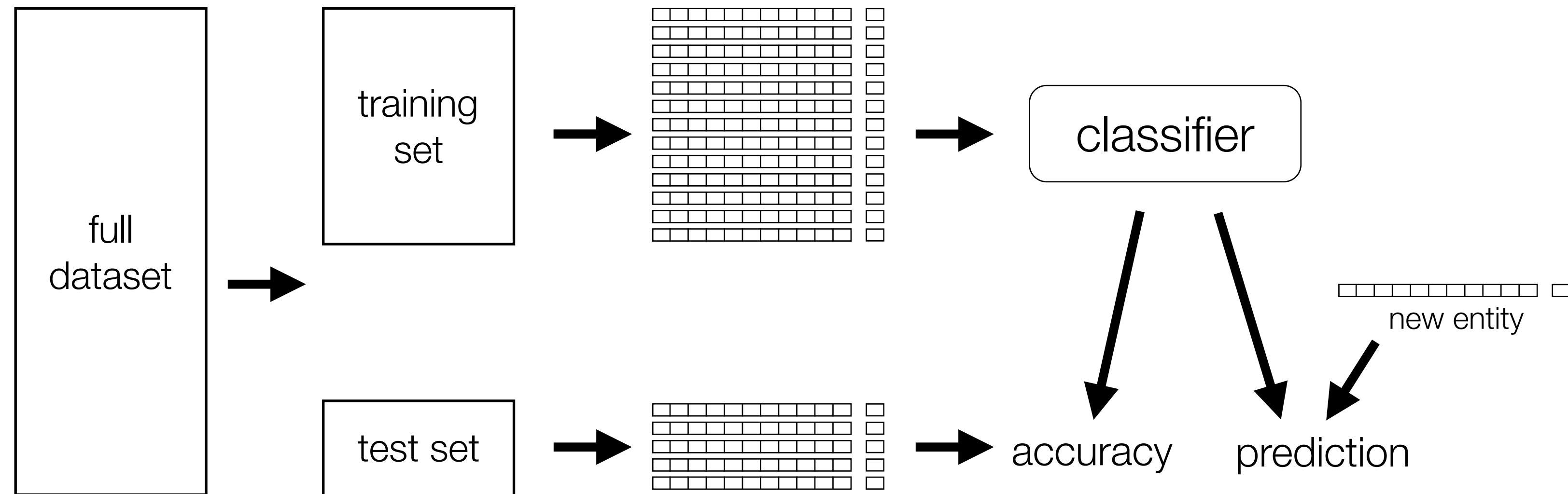


Evaluation: Split dataset into training / testing datasets

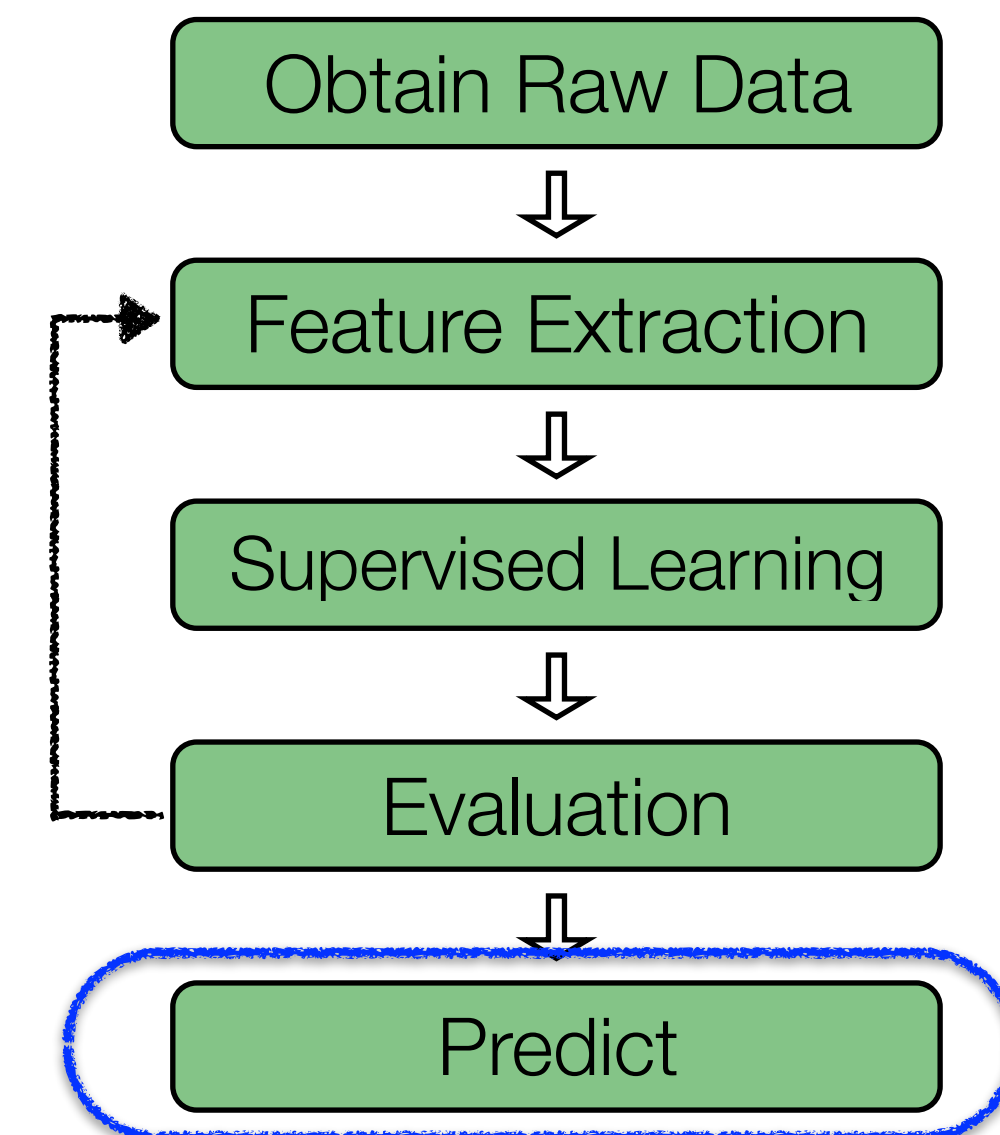
- Various ways to compare predicted and true labels
- Evaluation criterion is called a 'loss' function
- Accuracy (or 0-1 loss) is common for classification



Classification Pipeline



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

$$\begin{bmatrix} 3.3 & 5.3 & 4.5 \\ 1.0 & 4.5 & 3.4 \\ 6.3 & 1.0 & 2.2 \\ 3.6 & 4.7 & 8.9 \end{bmatrix}$$

Matrices

A matrix is a 2-dimensional array

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

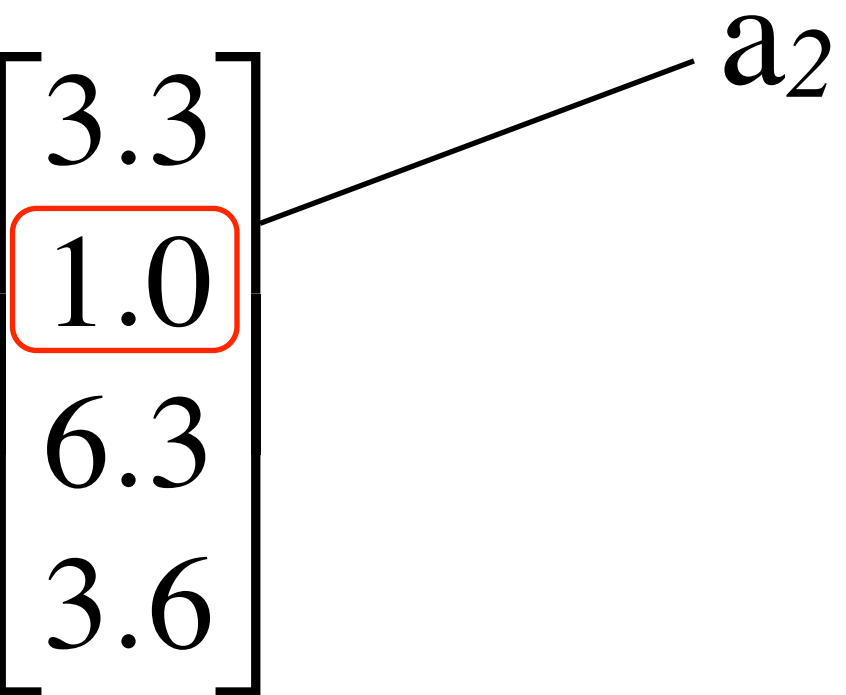
The element 3.3 is labeled A_{11} and the element 1.0 is labeled A_{32} .

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 and 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

$$\mathbf{a} = \begin{bmatrix} 3.3 \\ 1.0 \\ 6.3 \\ 3.6 \end{bmatrix}$$
A diagram showing a vector \mathbf{a} represented as a column matrix with four entries: 3.3, 1.0, 6.3, and 3.6. The entry 1.0 is highlighted with a red rectangular box. An arrow points from the label a_2 to this boxed entry, indicating it is the second component of the vector.

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

A_{12}

$$\begin{bmatrix} 1 & 4 \\ 6 & 1 \\ 3 & 5 \end{bmatrix}_{3 \times 2} \Rightarrow \begin{bmatrix} 1 & 6 & 3 \\ 4 & 1 & 5 \end{bmatrix}_{2 \times 3}$$

$(A^T)_{21}$

$$\begin{bmatrix} 3 \\ 4 \\ 1 \end{bmatrix}_{3 \times 1} \Rightarrow \begin{bmatrix} 3 & 4 & 1 \end{bmatrix}_{1 \times 3}$$

Properties of matrix transposes:

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

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

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

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

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

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

$$1 \times 4$$

Performs pairwise multiplication of vector elements

Scalar Product

A function that maps two vectors to a scalar

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

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

Performs pairwise multiplication of vector elements

Scalar Product

A function that maps two vectors to a scalar

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

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

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

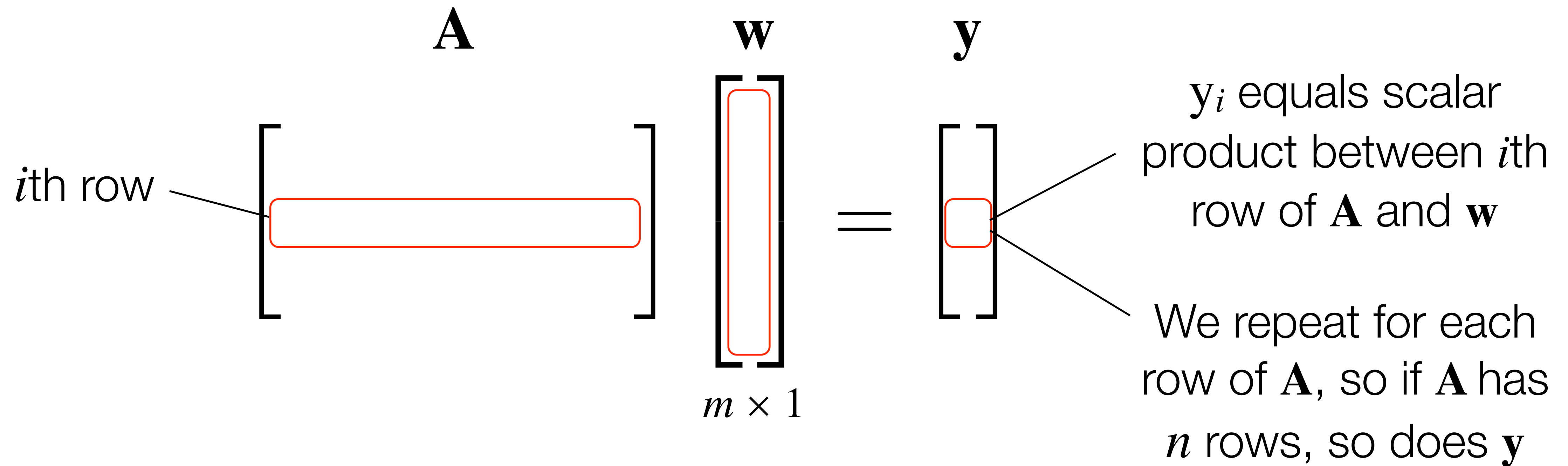
Involves repeated scalar products

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

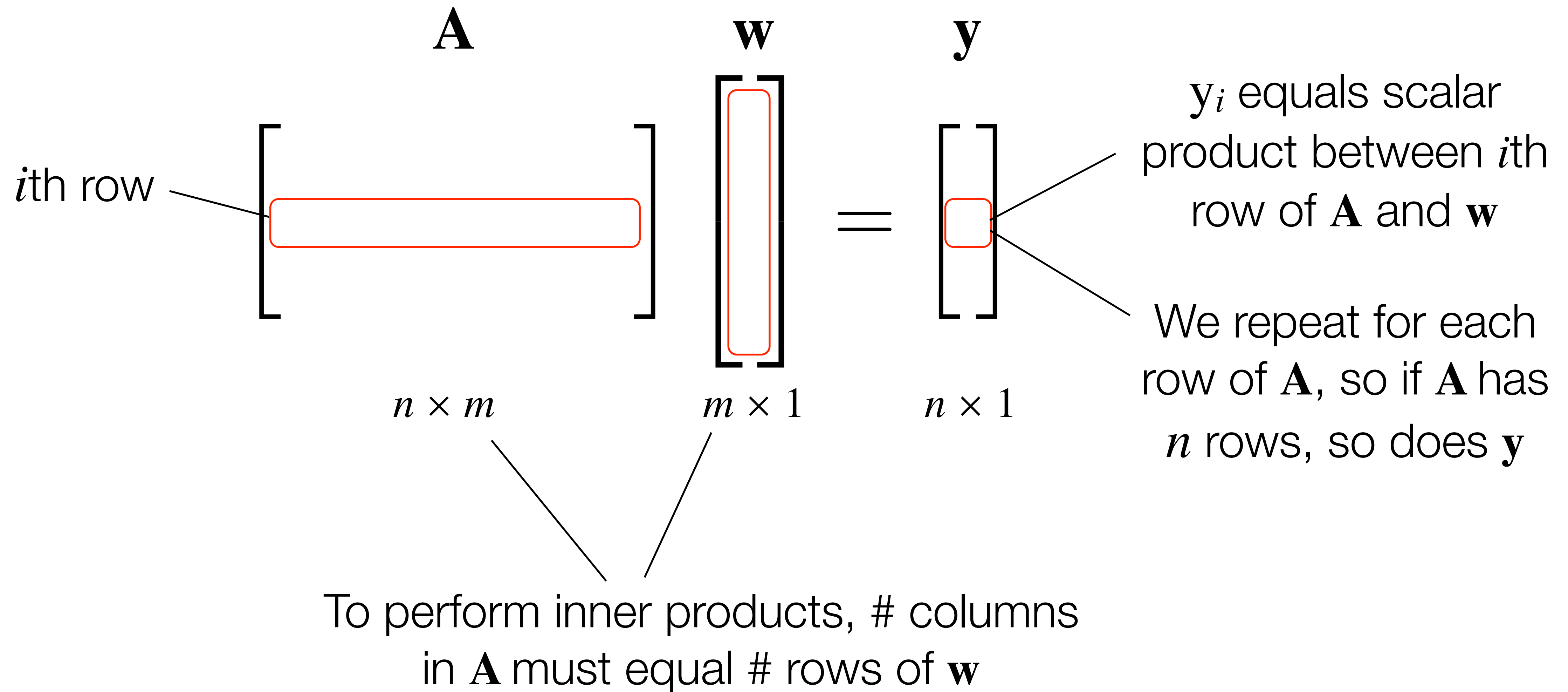
$$1 \times 4 + 4 \times 2 + 3 \times (-7) = -9$$

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

Matrix-Vector Multiplication



Matrix-Vector Multiplication



Scalar Product Revisited

Special case of Matrix-Vector Multiplication

$$\begin{array}{ccc} \mathbf{x}^\top & \mathbf{w} & y \\ \boxed{} & \boxed{} & = \text{scalar product} \\ 1 \times m & m \times 1 & \text{scalar } (1 \times 1) \end{array}$$

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

Transposed vectors are row vectors

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

Matrix-Matrix Multiplication

Also involves several scalar products

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

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

Matrix-Matrix Multiplication

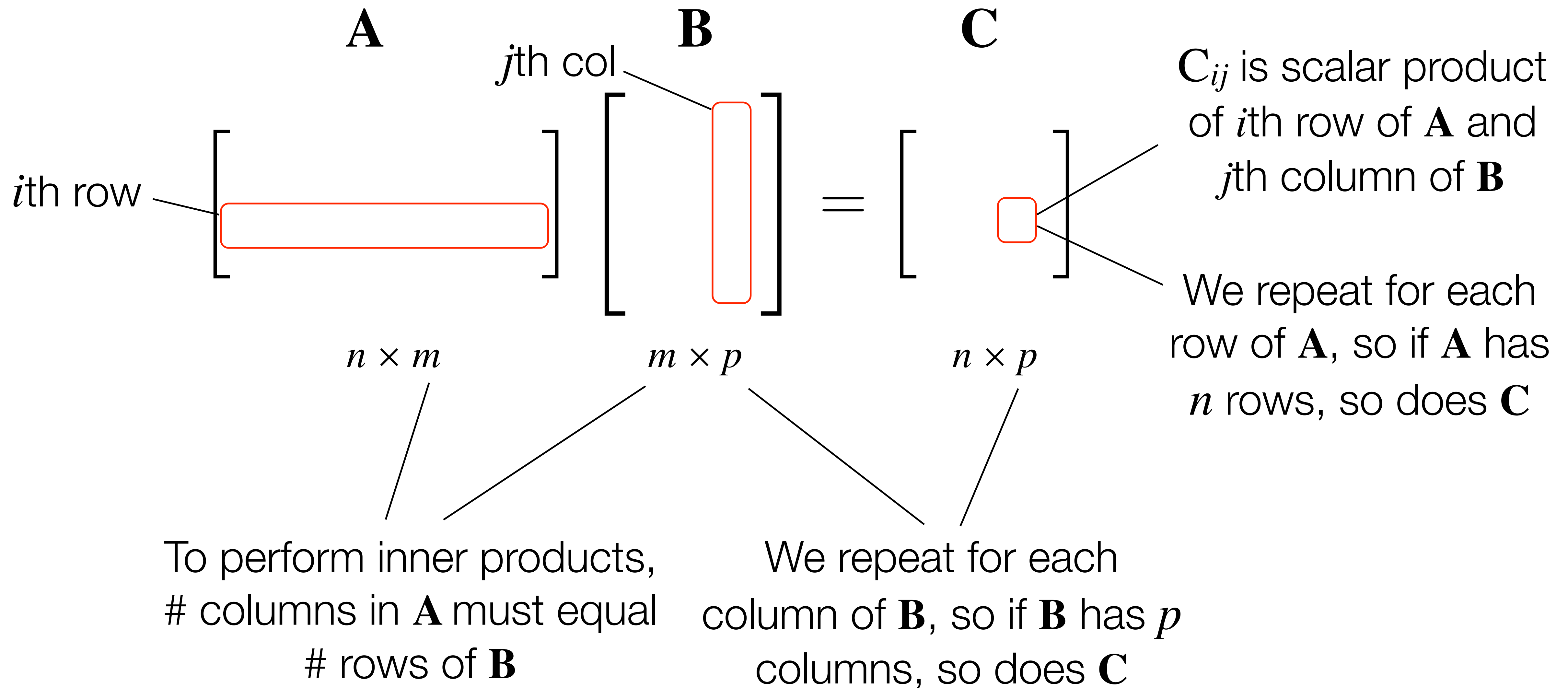
Also involves several scalar products

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

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

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

Matrix-Matrix Multiplication



Matrix-Matrix Multiplication

$$\begin{array}{ccc} \mathbf{A} & \mathbf{B} & \mathbf{C} \\ \left[\begin{array}{c} \text{---} \end{array} \right] & \left[\begin{array}{c} \text{---} \end{array} \right] & = \left[\begin{array}{c} \text{---} \end{array} \right] \\ n \times m & m \times p & n \times p \end{array}$$

Associative, i.e., $(\mathbf{AB})\mathbf{C} = \mathbf{A}(\mathbf{BC})$

Not commutative, i.e., $\mathbf{AB} \neq \mathbf{BA}$

Outer Product

Special case of Matrix-Matrix
Multiplication involving two vectors

$$\begin{array}{ccc} \mathbf{x} & \mathbf{w}^\top & \mathbf{C} \\ \left[\begin{array}{c} \square \end{array} \right] & \left[\begin{array}{c} \square \end{array} \right] & = \left[\begin{array}{c} \square \end{array} \right] \\ n \times 1 & 1 \times m & n \times m \end{array}$$

C_{ij} is “inner product” of i th entry of \mathbf{x} and j th entry of \mathbf{w}

Identity Matrix

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

\mathbf{I}_n is the $n \times n$ identity matrix, i.e., $\mathbf{I}_n \mathbf{A} = \mathbf{A}$ and $\mathbf{A} \mathbf{I}_m = \mathbf{A}$ for any $n \times m$ matrix \mathbf{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 \mathbf{A} , \mathbf{A}^{-1} denotes its inverse (when it exists)
- $\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}_n$

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 $\|\mathbf{x}\|_2$

- $\|\mathbf{x}\|_2 = \sqrt{x_1^2 + x_2^2 + \dots + x_m^2}$
- 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 (+, −, ×, /), 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: $|f(x)| \leq C|g(x)| \quad \forall x > N$

Ignores constants and lower-order terms

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

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

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