Optimization and Machine Learning SI151

Lu Sun

School of Information Science and Technology

ShanghaiTech University

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Today:

- Introduction to machine learning and optimization
- Course logistics
- Overview of machine learning
- Overview of supervised learning I

Readings:

- The Elements of Statistical Learning (ESL), Chapters 1 and 2
- Pattern Recognition and Machine Learning (PRML), Chapter 1

Introduction to Machine Learning and Optimization

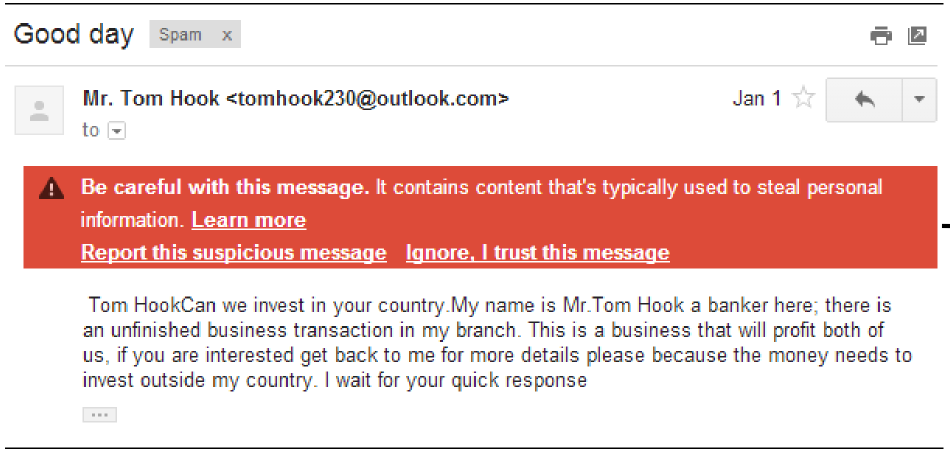
Machine Learning

"Machine learning (ML) is the scientific study of algorithms and statistical models that computer systems use to perform a specific task without using explicit instructions, relying on patterns and inference instead."

------Wikipedia

ML: Study of algorithms that

- improve their performance P
- at some task T
- with experience E



spam
vs
email

Well-defined ML task: <P, T, E>

Optimization in Machine Learning

Optimization problems arise in nearly everything we do in Machine Learning.
Typically, practical ML problems are solved mathematically by

translate  into $P: \min_{x \in D} f(X)$ $\rightarrow$ 

Conceptual idea *Optimization problem* *Solution*

This course: how to solve P.

Learning to Detect Spam Emails

- Data:
  - 4601 email messages
  - Each is labeled by email (+) or spam (-)
  - The relative frequencies of the 57 most commonly occurring words and punctuation marks in the message
- Classify:
  - label future messages email (+) or spam (-)
- Supervised learning problem on categorical data:

  Binary classification problem

Table: Words with largest difference between spam and email shown.

	spam	email
george	0.00	1.27
you	2.26	1.27
your	1.38	0.44
hp	0.02	0.90
free	0.52	0.07
hpl	0.01	0.43
!	0.51	0.11
our	0.51	0.18
re	0.13	0.42
edu	0.01	0.29
remove	0.28	0.01

Learning to Detect Spam Emails

- Examples of rules for prediction:
  - If (%george<0.6) and (%you>1.5)
    then `spam`
    else `email`
  - If (0.2·%you-0.3·%george)>0
    then `spam`
    else `email`
- Tolerance to errors:
  - Tolerant to letting through some spam (false positive)
  - No tolerance towards throwing out email (false negative)

Table: Words with largest difference between spam and email shown.

	spam	email
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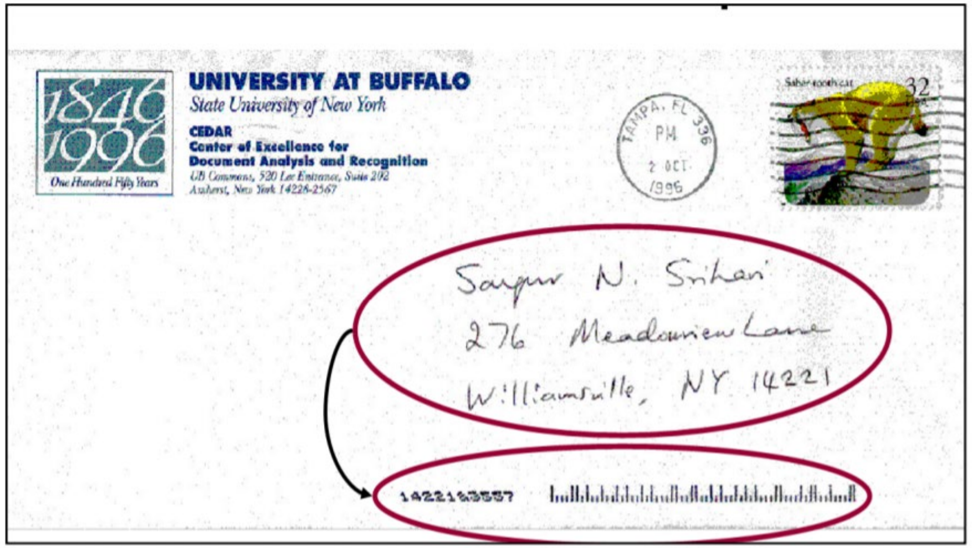
!	0.51	0.11
our	0.51	0.18
re	0.13	0.42
edu	0.01	0.29
remove	0.28	0.01

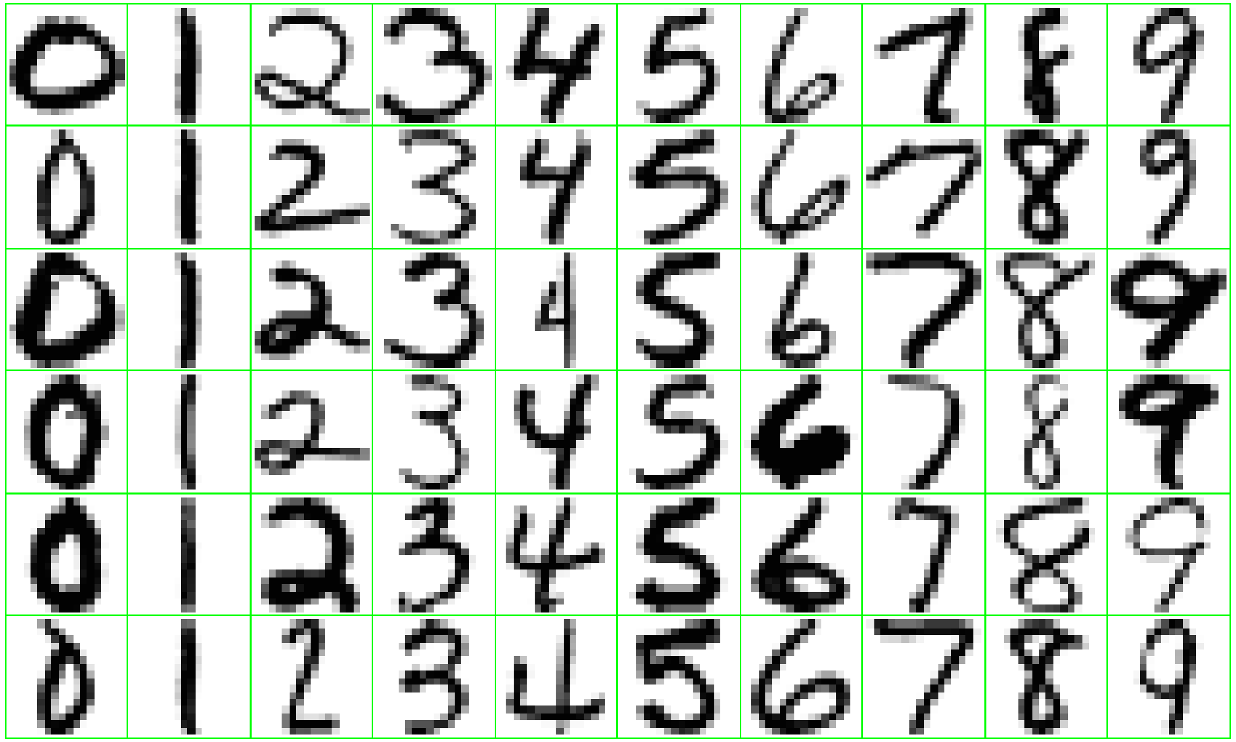
Learning to Recognize Handwritten Digits

Data: images are single digits 16x16 8-bit gray-scale, normalized for size and orientation

Classify: newly written digits



https://cedar.buffalo.edu/~srihari/CSE574/Chap1/1.1%20ML-Overview.pdf



- Non-binary classification problem
- Low tolerance to misclassifications

Learning to Diagnose Prostate Cancer

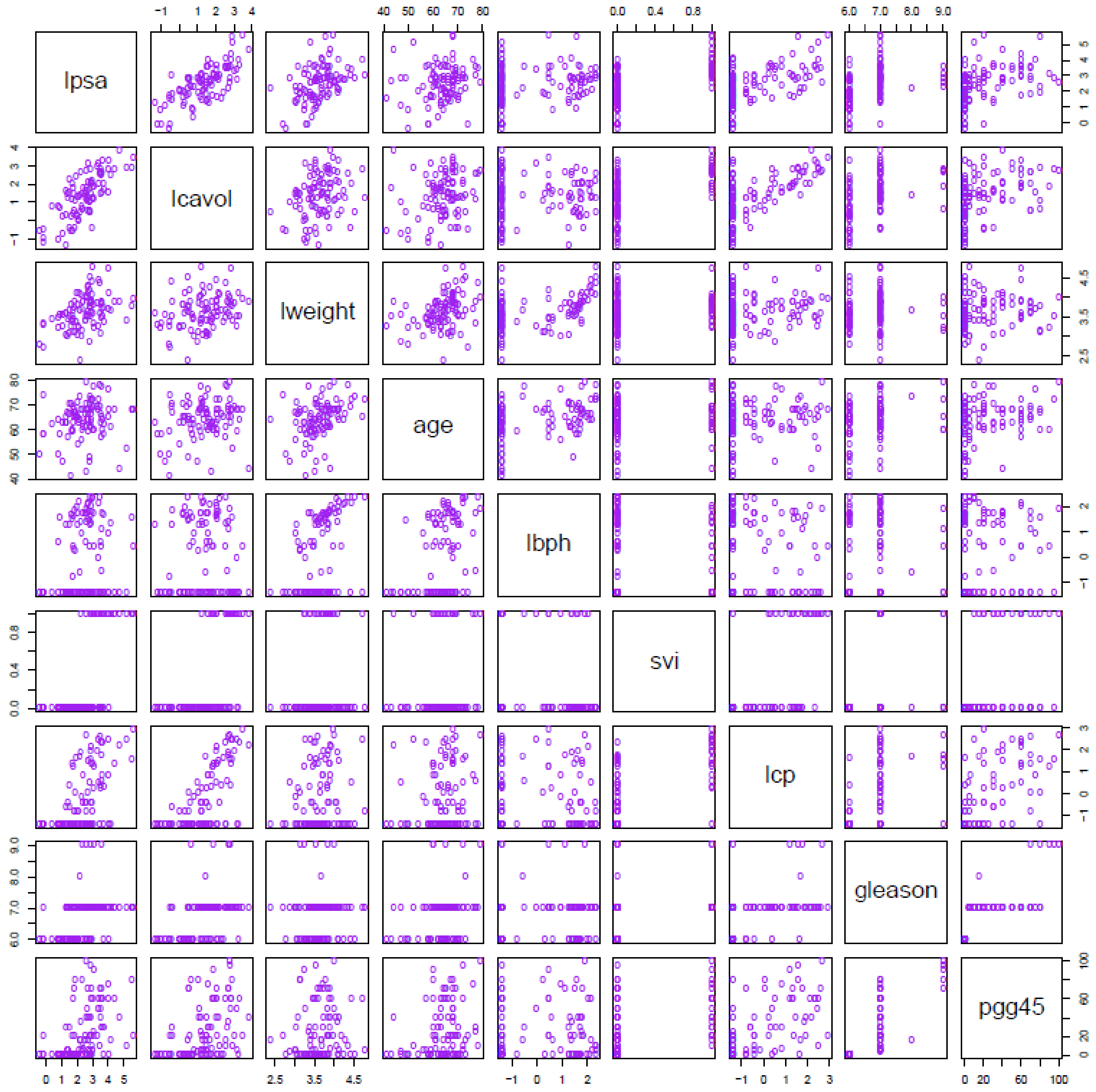
- Data (by Stamey et al. 1989):
  - Given:

`lcavol`	log cancer volume
`lweight`	log prostate weight
`age`	age
`lbph`	log benign hyperplasia amount
`svi`	seminal vesicle invasion
`lcp`	log capsular penetration
`gleason`	gleason score
`pgg45`	percent gleason scores 4 or 5

  - Predict:

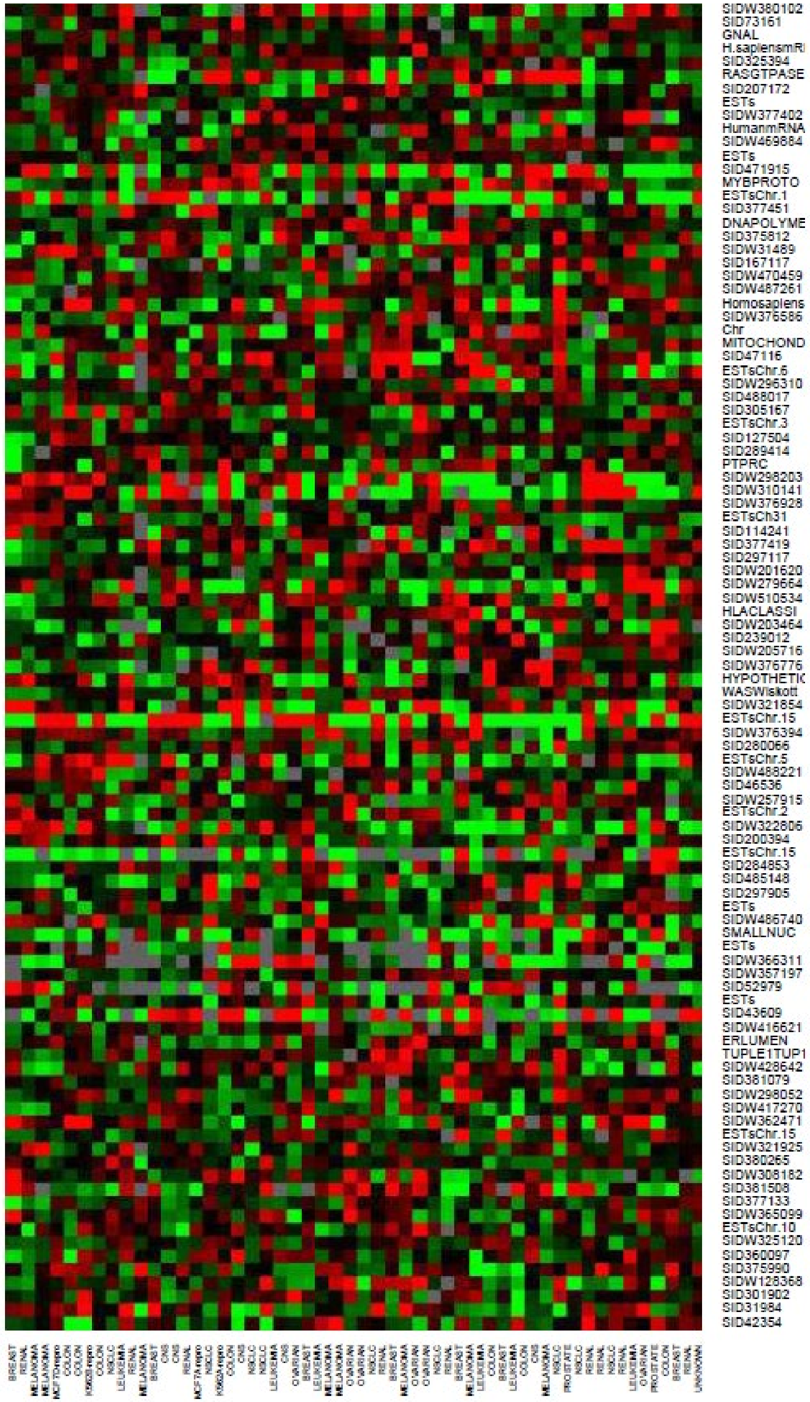
`lpsa`	log of prostate specific antigen

- Supervised learning problem on quantitative data: Regression problem.



Learning to Analyze DNA Data

- Data:
  - Color intensities signifying the abundance levels of mRNA for a number of genes (6830) in several (64) different cell states (samples).
  - Red: over-expressed gene
  - Green: under-expressed gene
  - Gray: gene with missing values
  - Black: normally expressed gene (according to some predefined background)
- Questions:
  1. Which genes show similar expression over the samples – Unsupervised learning
  2. Which samples show similar expression over the genes – Unsupervised learning
  3. Which genes are highly over or under expressed in certain cancers – Supervised learning

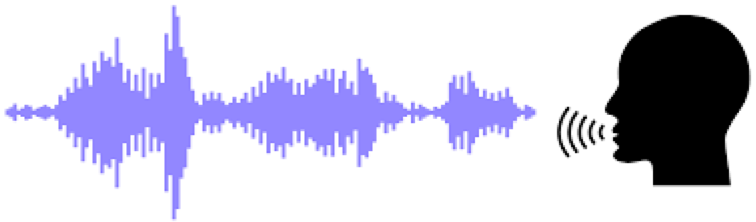


genes (100)

samples (64)

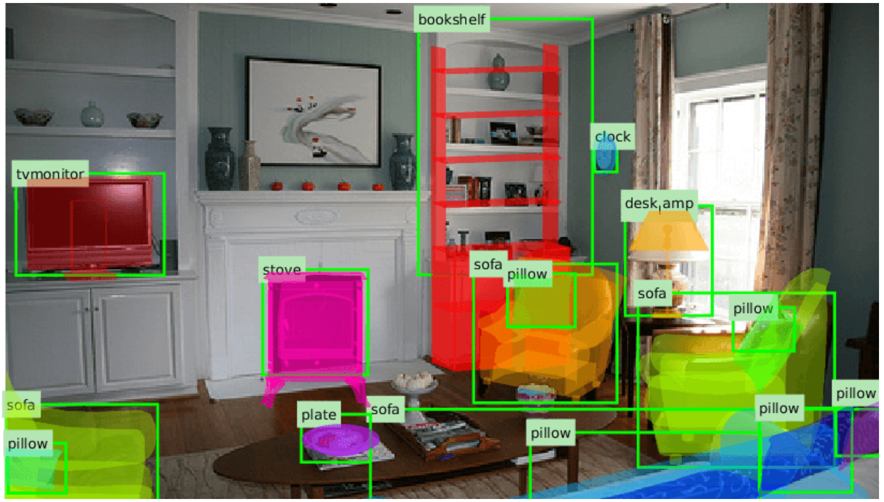
Machine Learning – Practice

Text analysis

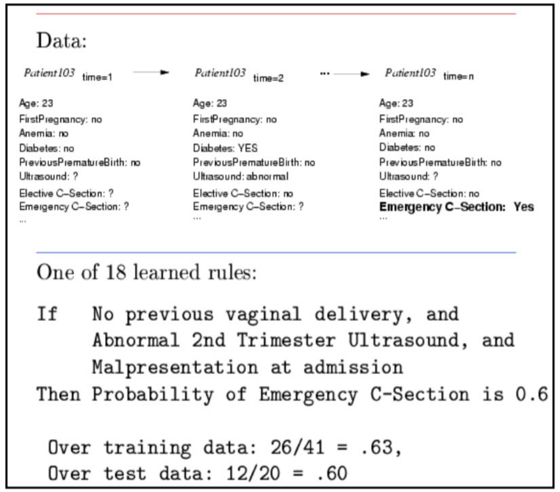


Speech recognition

Control learning



Object recognition



Data:

Patient103 time=1 → Patient103 time=2 ... → Patient103 time=n

Patient103 time=1	Patient103 time=2	Patient103 time=n
Age: 23	Age: 23	Age: 23
FirstPregnancy: no	FirstPregnancy: no	FirstPregnancy: no
Anemia: no	Anemia: no	Anemia: no
Diabetes: no	Diabetes: YES	Diabetes: no
PreviousPrematureBirth: no	PreviousPrematureBirth: no	PreviousPrematureBirth: no
Ultrasound: ?	Ultrasound: abnormal	Ultrasound: ?
Elective C–Section: ?	Elective C–Section: no	Elective C–Section: no
Emergency C–Section: ?	Emergency C–Section: ?	**Emergency C–Section: Yes**
...	...	...

One of 18 learned rules:

```
If   No previous vaginal delivery, and
     Abnormal 2nd Trimester Ultrasound, and
     Malpresentation at admission
Then Probability of Emergency C-Section is 0.6

 Over training data: 26/41 = .63,
 Over test data: 12/20 = .60
```

Mining databases

- Logistic regression
- SVM
- Neural networks
- Hidden Markov models
- Reinforcement learning
- Bayesian methods
- ……

Machine Learning – Theory

PAC Learning Theory
(by Leslie Valiant, 1984)

examples (m)

hypothesis complexity (H)

failure probability (δ)

error rate (ε)

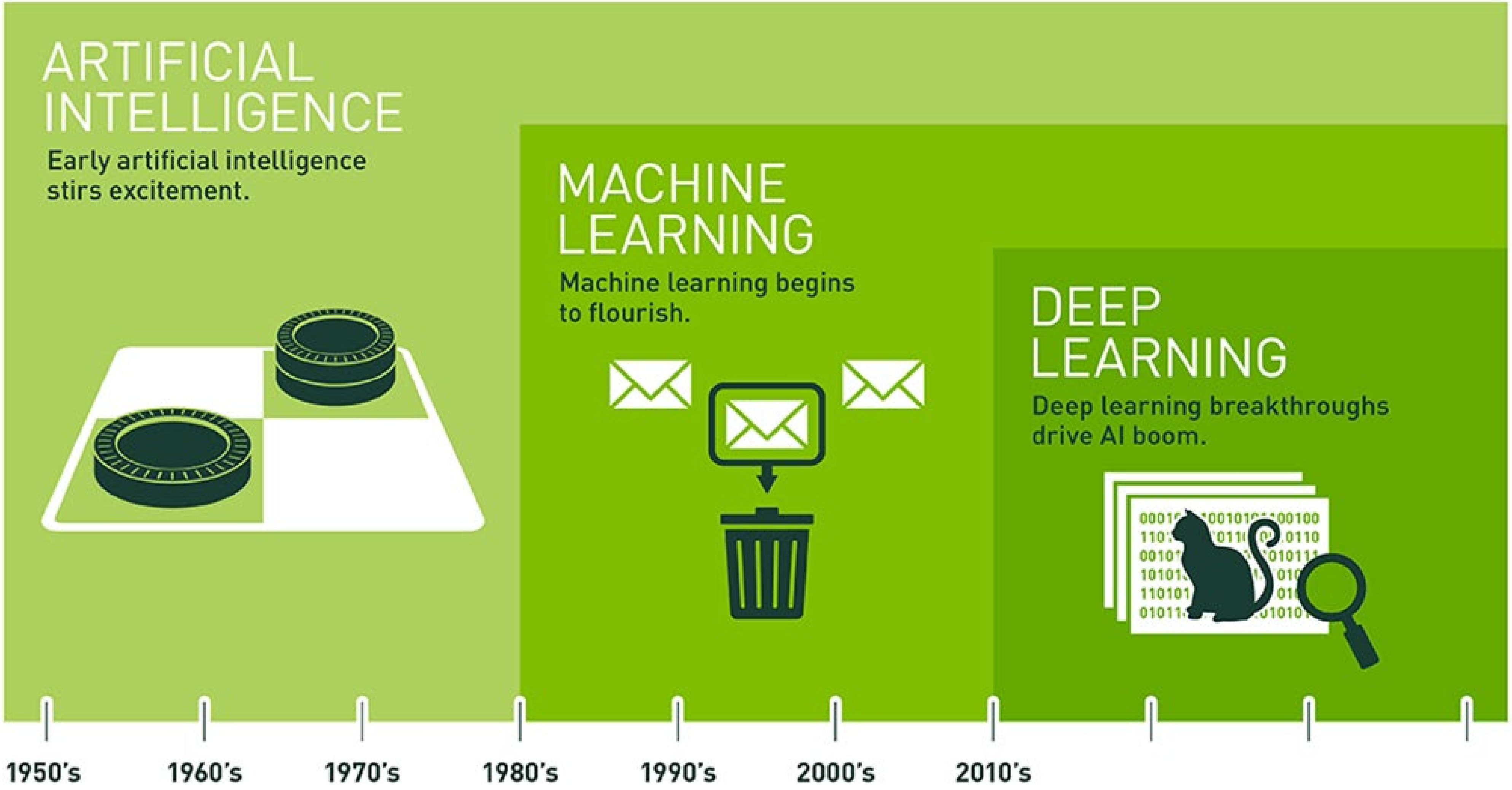
$$m \geq \frac{1}{\varepsilon}\left(ln|H| + \ln(\frac{1}{\delta})\right)$$

PAC: Probably Approximately Correct

Other theories for

- Reinforcement learning
- Semi-supervised learning
- ……

Defining Artificial Intelligence



What You Will Learn in This Course

- The primary machine learning and optimization algorithms
  - Ridge regression, lasso, logistic regression, SVM, neural networks, graphical models, unsupervised learning, reinforcement learning…
  - Convex optimization, gradient methods, proximal methods, ADMM, …

- Underlying statistical and computational theory

- Enable to apply the algorithms to solve practical problems

- Enough to read and understand related research papers.

Course Logistics

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- Research Interests
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Optimization and Machine Learning SI151

General information

- Time: Tue. & Thu., 08:15-09:55
- Online: Blackboard, Piazza & Gradescope
- 16 weeks (64 credit hours)
- Machine learning in weeks 1-12; convex optimization in weeks 13-16

All class communication via Piazza

- https://piazza.com/class/klfa86is5z91mz
- announcements and discussion
- read it regularly
- post all questions/comments there
- direct email is not a good idea

Optimization and Machine Learning SI151

Grading

- Homework: 30%
- Course project: 30%
- Final exam: 40%

Highlights

- Please write your HW, project and exam in English
- For late HW or project, the score will be exponentially decreased
- Once any plagiarism or cheating is confirmed, relevant assignments or exams will receive 0 points

Optimization and Machine Learning SI151

Recommended textbooks

- **The Elements of Statistical Learning: Data Mining, Inference and Prediction**, Trevor Hastie, Robert Tibshirani, and Jerome H. Friedman
- **Pattern Recognition and Machine Learning**, Christopher Bishop
- **Machine Learning**, Tom M. Mitchell
- **Convex Optimization**, Stephen Boyd and Lieven Vandenberghe

Some useful online resources

- CMU, machine learning course

http://www.cs.cmu.edu/~ninamf/courses/601sp15/lectures.shtml

- Stanford, convex optimization course

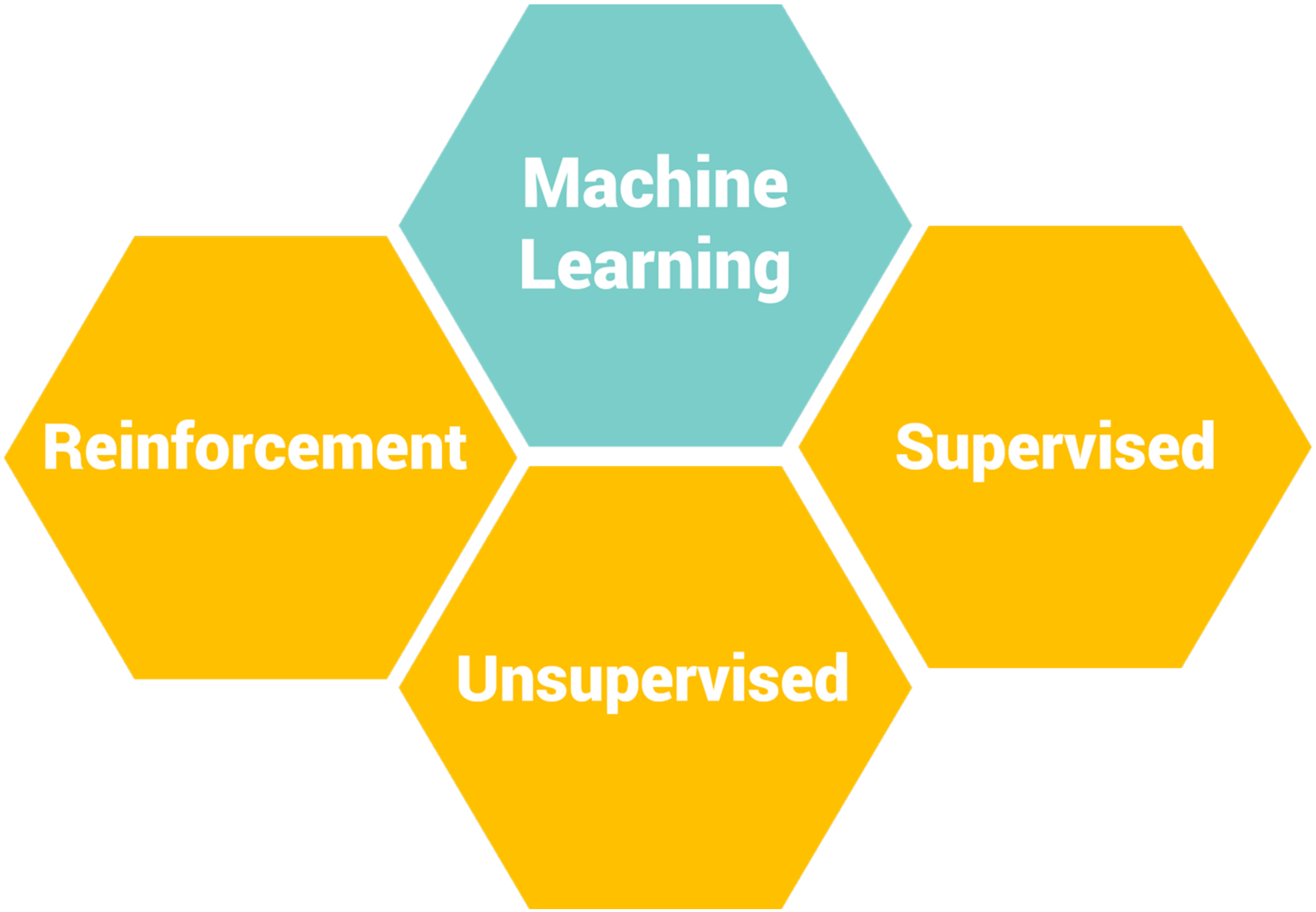
https://web.stanford.edu/~boyd/cvxbook/

- CMU, convex optimization

https://www.stat.cmu.edu/~ryantibs/convexopt/

Overview of Machine Learning

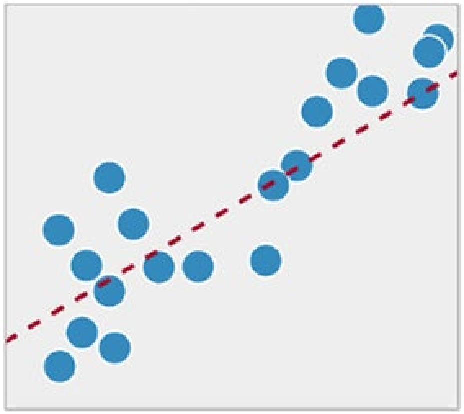
Different Classes of Machine Learning Problems



Supervised Learning

Train your model to map the input to the prediction output based on the **ground truth** labels in the training data

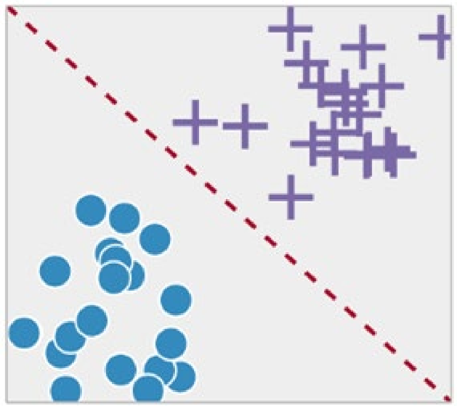
Regression



Learning a function for a **continuous** output

Eg. Predicting sales price of house.

Classification



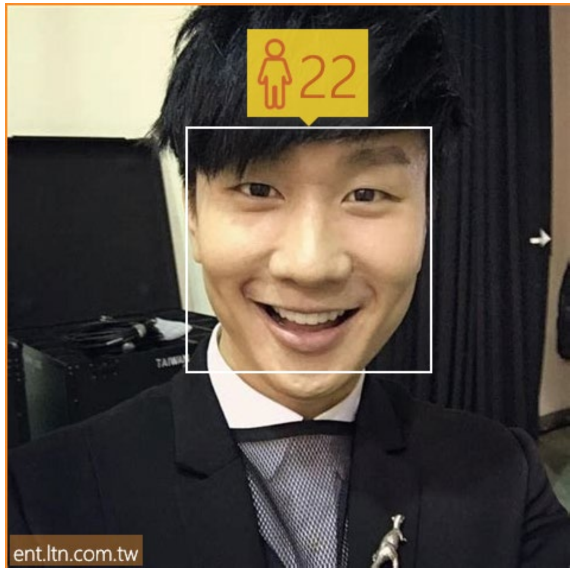
Learning a function for a **categorical** output

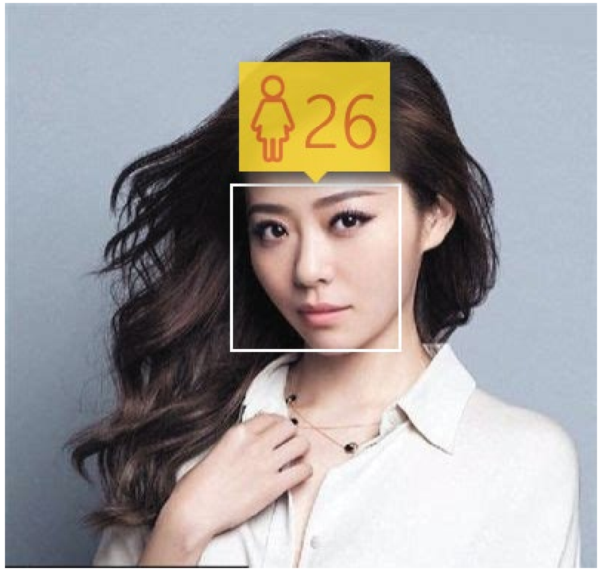
Eg. Classifying cats vs dogs in images.

Regression

Gives a **continuous output**.

Example: Age Prediction





《红秀》杂志封面

Classification

Gives a **discrete output.**

Example: Fruit Classification

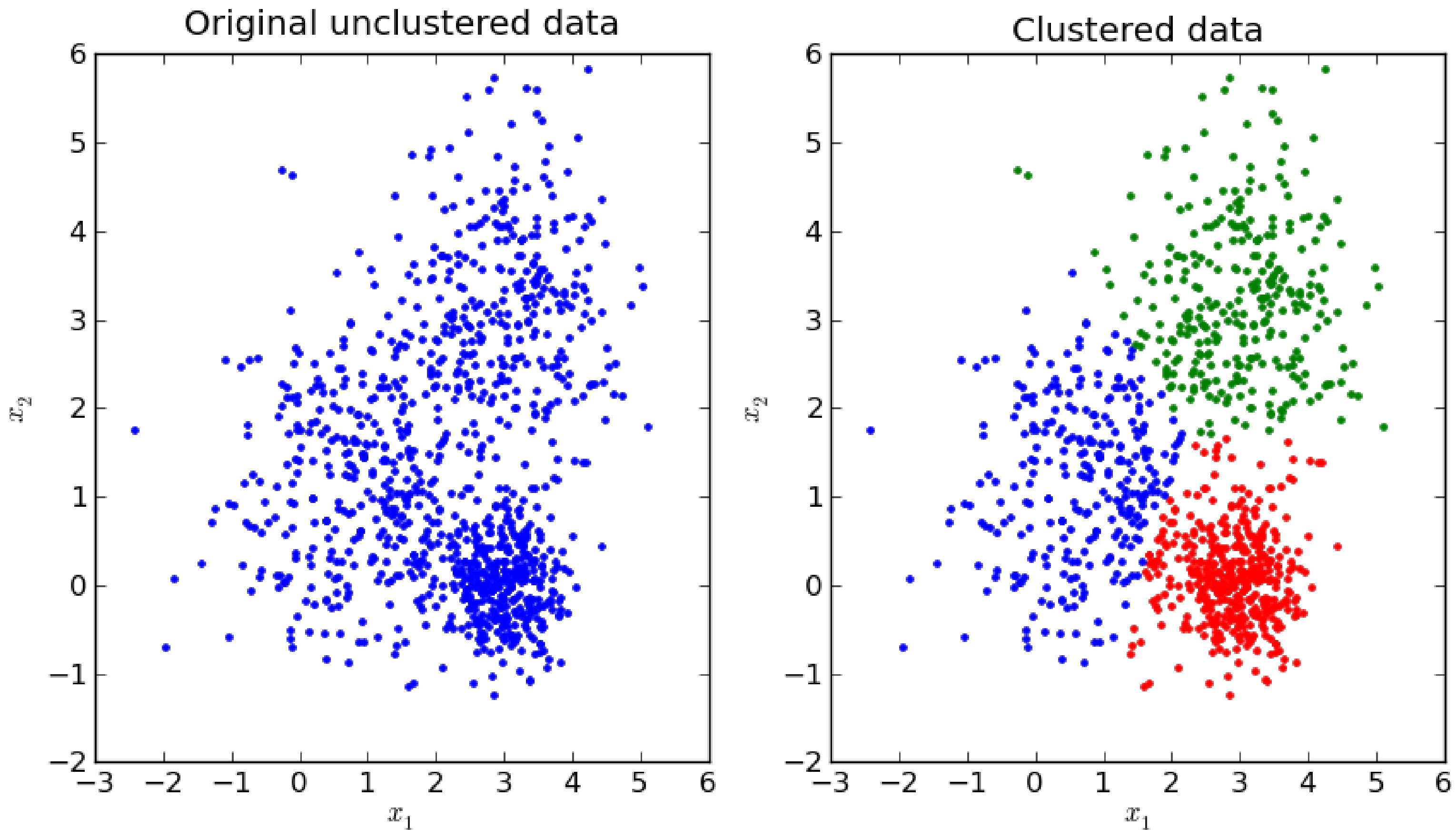
Some Basic Terminology

Features/ Attributes					Target Variable
Colour	Mass	Shape	Seeds	Country	Fruit
Red	100g	Round	Yes	Canada	Apple
Yellow	647 g	Curved	No	Australia	Banana

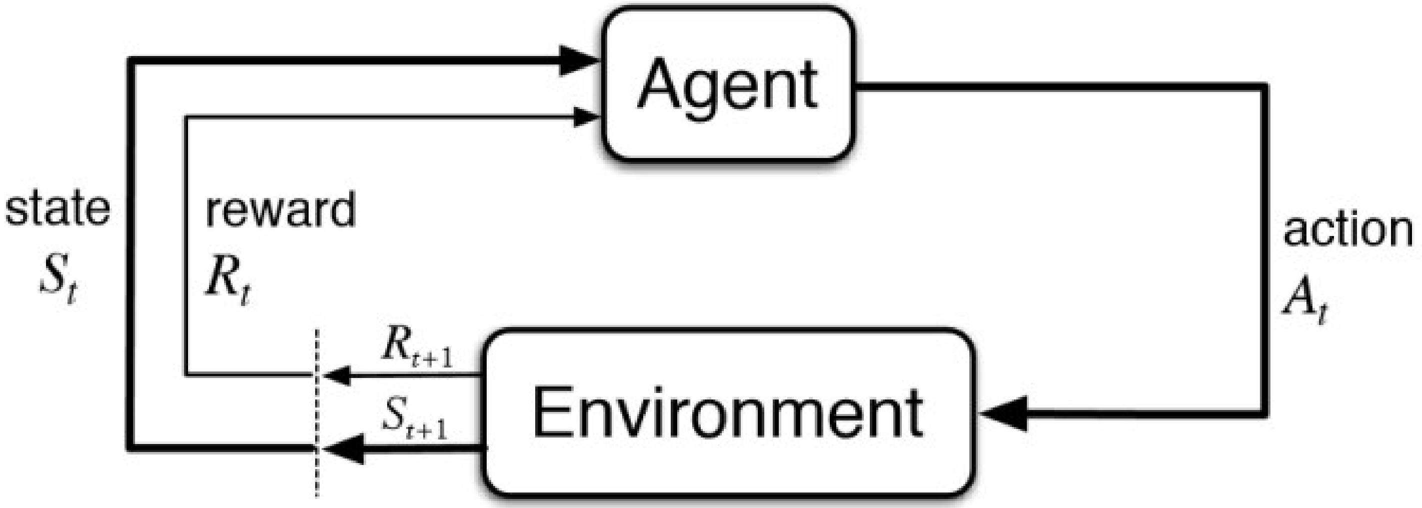
Features / attributes: how you would describe the fruit
Target variable: how you want to teach your model to recognize the fruit. (ground truth)

Unsupervised Learning

Train your model to learn how to difference input data, and make prediction on its own without training labels.



Reinforcement Learning



Your system learns to behave in an evolving environment and make prediction by learning from the outcome of specific actions.

Goal: learn the actions (Good) that **maximize** the reward.

Machine Learning Pipeline

1 Identify Problem

Carefully define the problem you want to solve. What specific question are you trying to answer?

2 Gather Data

Figure out what data is needed and where to retrieve it. Does similar data exist or do we need to generate it?

3 Process Data

Format data that can be interpreted by a computer. That includes cleaning, manipulating and extracting important features to feed into the training model.

4 Train Model

Training the dataset on your selected model. In practice, datasets are split into train, validation and test sets in order to measure model performance.

5 Evaluate Results

Does the trained model solve your initial problem? Does it satisfy your performance requirements?

6 Repeat!

Improve your model by reiterating the process!

Overview of Supervised Learning I

--- Variable Types and Terminology

Variable Types and Terminology

Input: a variable X. If X is a vector, its j-th element is X_j

an observation x_i
(scalar or vector)

Typically, we use i to denote the index of observations, while use j to denote the index of variables.

Model

Scalar

$$N \text{ observations} \left\{ \begin{array}{c} X \\ \hline x_1 \\ \vdots \\ x_i \\ \vdots \\ x_N \end{array} \right. \qquad \mathbf{x} \in \mathbb{R}^N$$

Vector

$$N \text{ observations} \left\{ \begin{array}{ccccc} X_1 & \cdots & X_j & \cdots & X_p \\ \hline \text{—} & & x_1^T & & \text{—} \\ & & \vdots & & \\ \text{—} & & x_i^T & & \text{—} \\ & & \vdots & & \\ \text{—} & & x_N^T & & \text{—} \end{array} \right. \qquad \mathbf{X} \in \mathbb{R}^{N \times p}$$

p variables

Variable Types and Terminology

Input: a variable X. If X is a vector, its j-th element is X_j

an observation x_i

Model

Binary classification

coding

$= 2$ a binary digit. $\{0,1\}$ or $\{-1,1\}$

> 2 K binary digits. One is "on" at a time.

Multi-class classification

Output

qualitative: G → **classification**
(categorical or discrete)

quantitative: Y → **regression**

Variable Types and Terminology

Input: a variable X. If X is a vector, its j-th element is X_j

an observation x_i

Model

Output

- qualitative: G (categorical or discrete) → **classification**
- quantitative: Y → **regression**

Main question of this course:
Given the value of an input vector X,
make a good prediction $\hat{Y}$ of the output Y.

Overview of Supervised Learning I

--- Least Squares and Nearest Neighbors

Simple Approach 1: Least Squares

- Given inputs:

$$X^T = (X_1, X_2, \dots, X_p)$$

- Predict output Y via the model

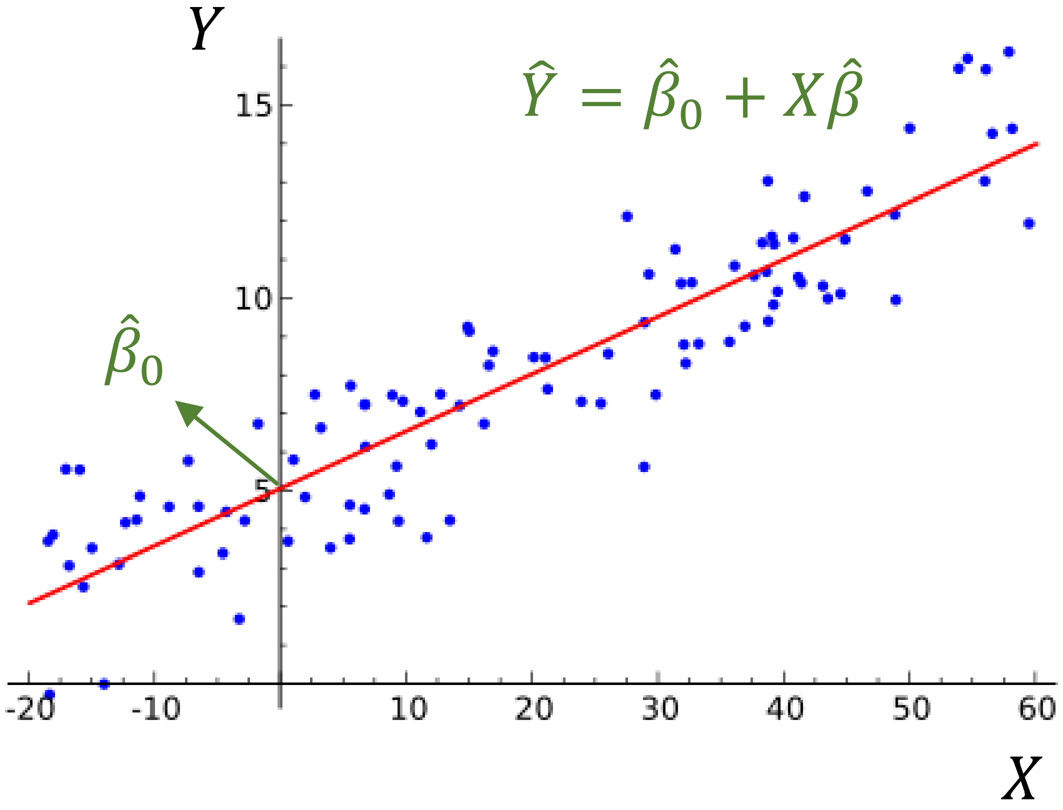
$$\hat{Y} = \hat{\beta}_0 + \sum_{j=1}^{p} X_j \hat{\beta}_j$$

$\hat{\beta}_0$: bias or intercept

- Include the constant variable 1 in X

$$\hat{Y} = X^T \hat{\beta}$$

- Here $\hat{Y}$ is a scalar. If the output $\hat{Y}$ is K-vector, then $\hat{\beta}$ is a $p \times K$ matrix of coefficients.



Multi-output regression

Simple Approach 1: Least Squares

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- Here $\hat{Y}$ is a scalar. If the output $\hat{Y}$ is K-vector, then $\hat{\beta}$ is a $p \times K$ matrix of coefficients.

- In the $(p + 1)$-dimensional input-output space, $(X, \hat{Y})$ represents a hyperplane
- If the constant is included in X, then the hyperplane goes through the origin

$$f(X) = X^T \beta$$

is a linear function

- Its gradient

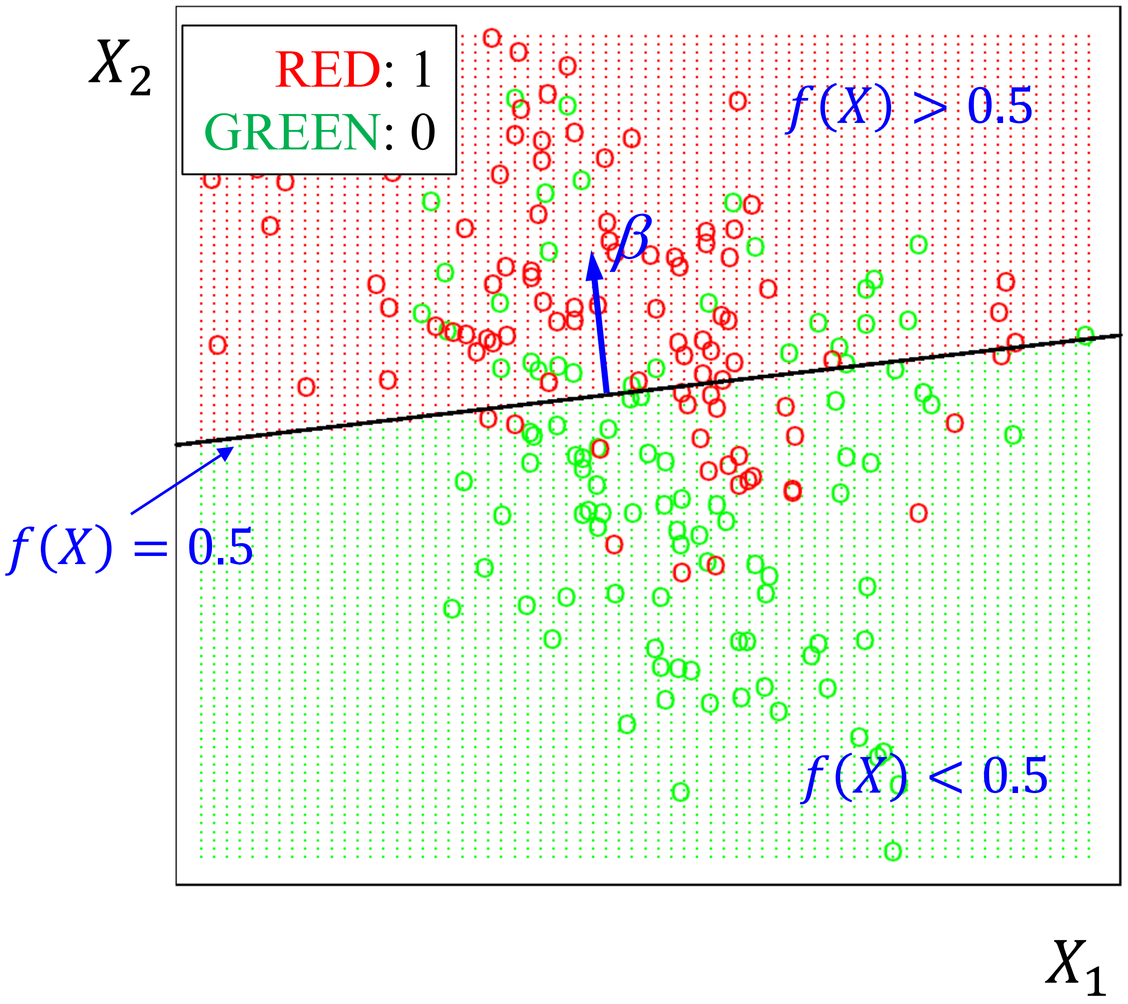
$$\boxed{f'(X) = \beta}$$

is a vector that points in the steepest uphill direction.

For the derivatives of vectors and matrices, please refer to:

- **The Matrix Cookbook**. Kaare Brandt Petersen and Michael Syskind Pedersen

Simple Approach 1: Least Squares



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Simple Approach 1: Least Squares

- Training procedure:
  Method of *least-squares*
- N = #observations
- Minimize the *residual sum of squares*

$$\mathrm{RSS}(\beta) = \sum_{i=1}^{N} (y_i - x_i^T \beta)^2$$

  Or equivalently,

$$\begin{aligned}\mathrm{RSS}(\beta) &= (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) \\ &= \|\mathbf{y} - \mathbf{X}\beta\|_2^2\end{aligned}$$

- This quadratic function always has a global minimum, but it may not be unique.

Note: for an arbitrary vector $\boldsymbol{a}$, we have the squared ℓ_2-norm $\|\boldsymbol{a}\|_2^2 = \boldsymbol{a}^T \boldsymbol{a}$.

Simple Approach 1: Least Squares

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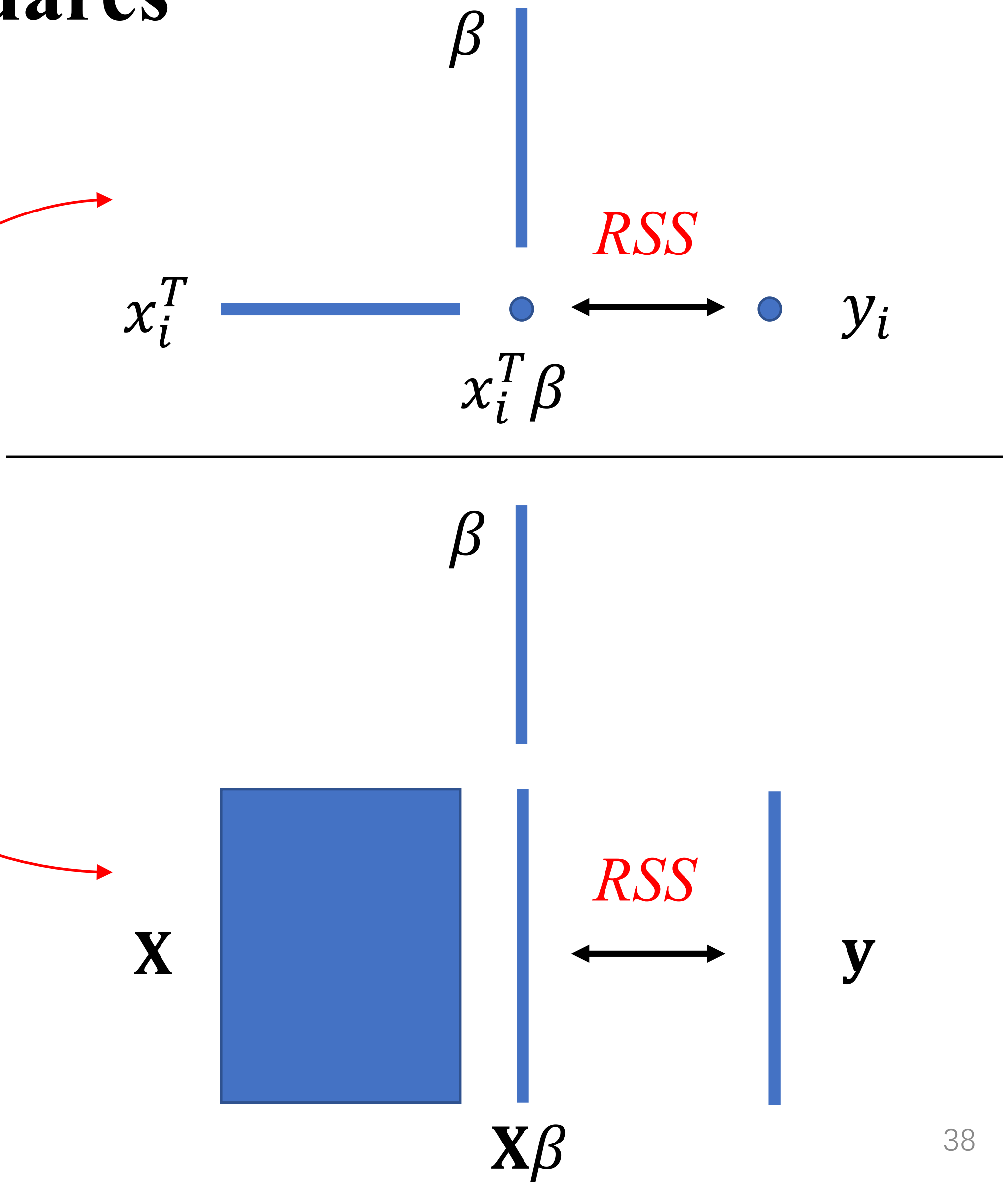
$$= \|\mathbf{y} - \mathbf{X}\beta\|_2^2$$

- This quadratic function always has a global minimum, but it may not be unique.

Q: What is the difference among x_i, x_i^T, $\mathbf{x}$, X and $\mathbf{X}$?



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$$= \|\mathbf{y} - \mathbf{X}\beta\|_2^2$$

- This quadratic function always has a global minimum, but it may not be unique.

- Differentiating w.r.t. β yields the *normal equations*

$$\mathbf{X}^T (\mathbf{y} - \mathbf{X}\beta) = 0$$

- If $\mathbf{X}^T\mathbf{X}$ is nonsingular, then the unique solution is

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

- The fitted value at an arbitrary input x_0 is

$$\hat{y}(x_0) = x_0^T \hat{\beta}$$

- The entire fitted surface is characterized by $\hat{\beta}$.

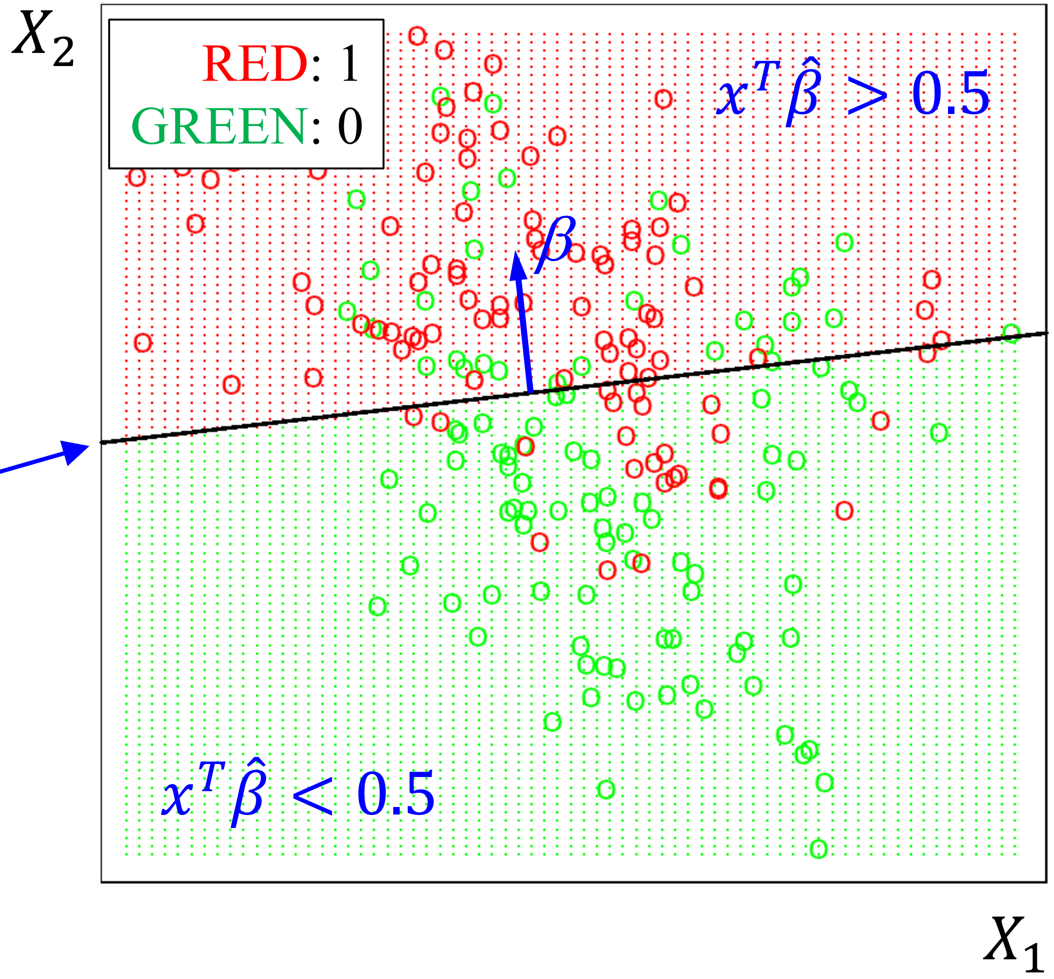
Simple Approach 1: Least Squares

Example:

- Data on two inputs X_1 and X_2.
- Output variable has values GREEN (coded 0) and RED (coded 1).
- 100 points per class.
- Regression line is defined by

$$x^T\hat{\beta} = 0.5.$$

- Easy but many misclassifications if the problem is not linear.

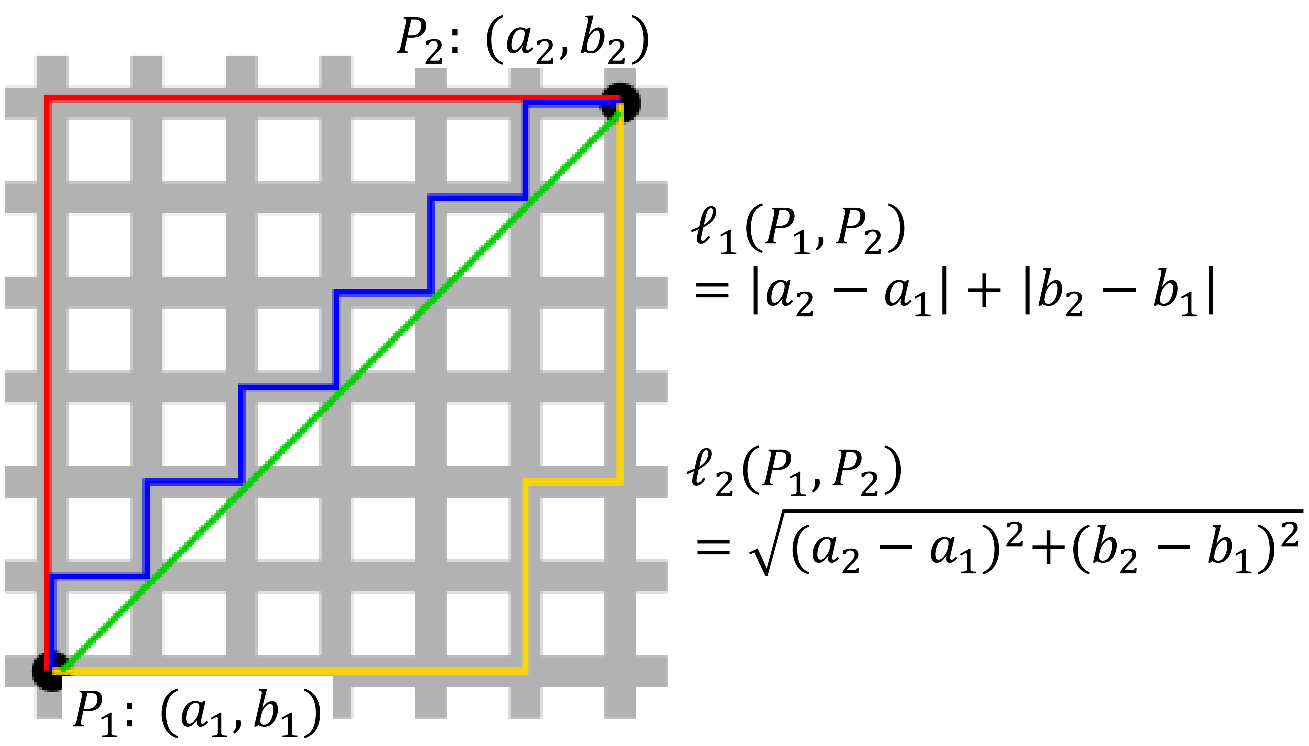


Simple Approach 2: Nearest Neighbors

- Use observations in the training set closest to the given input.

$$\hat{Y}(x) = \frac{1}{k}\sum_{x_i \in N_k(x)} y_i.$$

- $N_k(x)$ is the set of the k closest points to x is the training sample
- Average the outcome of the k closest training sample points



Taxicab geometry ($\boldsymbol{\ell_1}$) versus **Euclidean distance ($\boldsymbol{\ell_2}$)** : In taxicab geometry, the red, yellow, and blue paths all have the same shortest path length of 12. In Euclidean geometry, the green line has length $6\sqrt{2} \approx 8.49$ and is the unique shortest path.

Simple Approach 2: Nearest Neighbors

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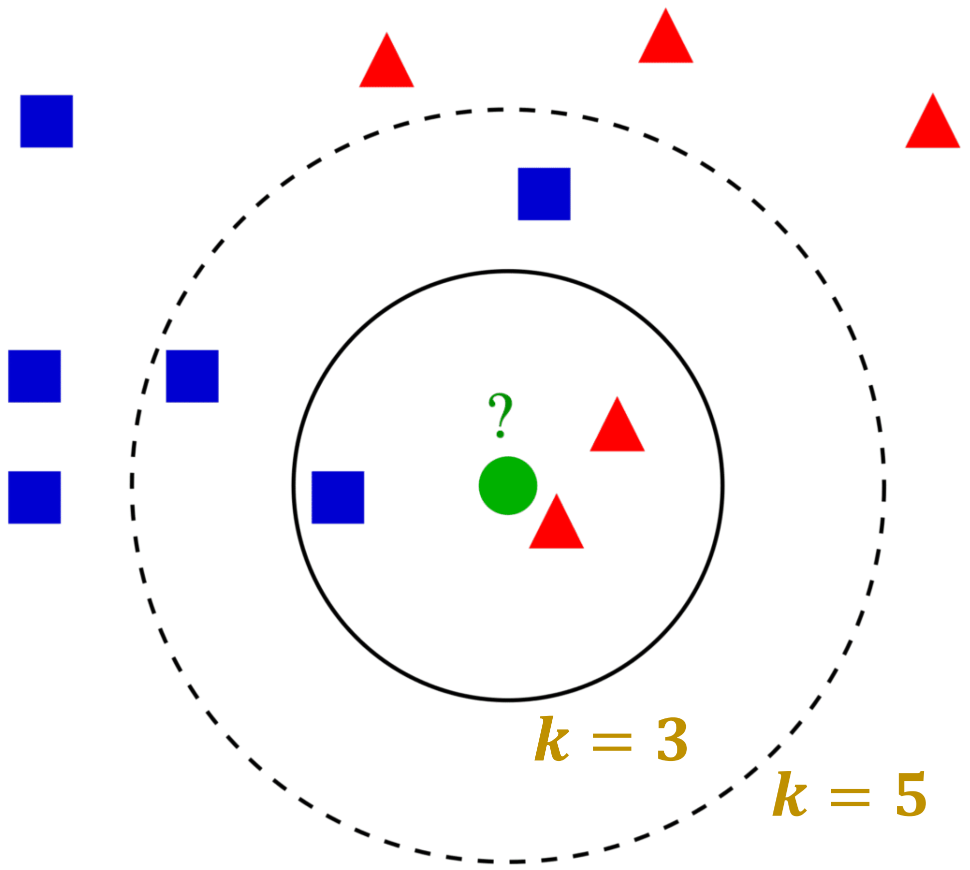

Simple Approach 2: Nearest Neighbors

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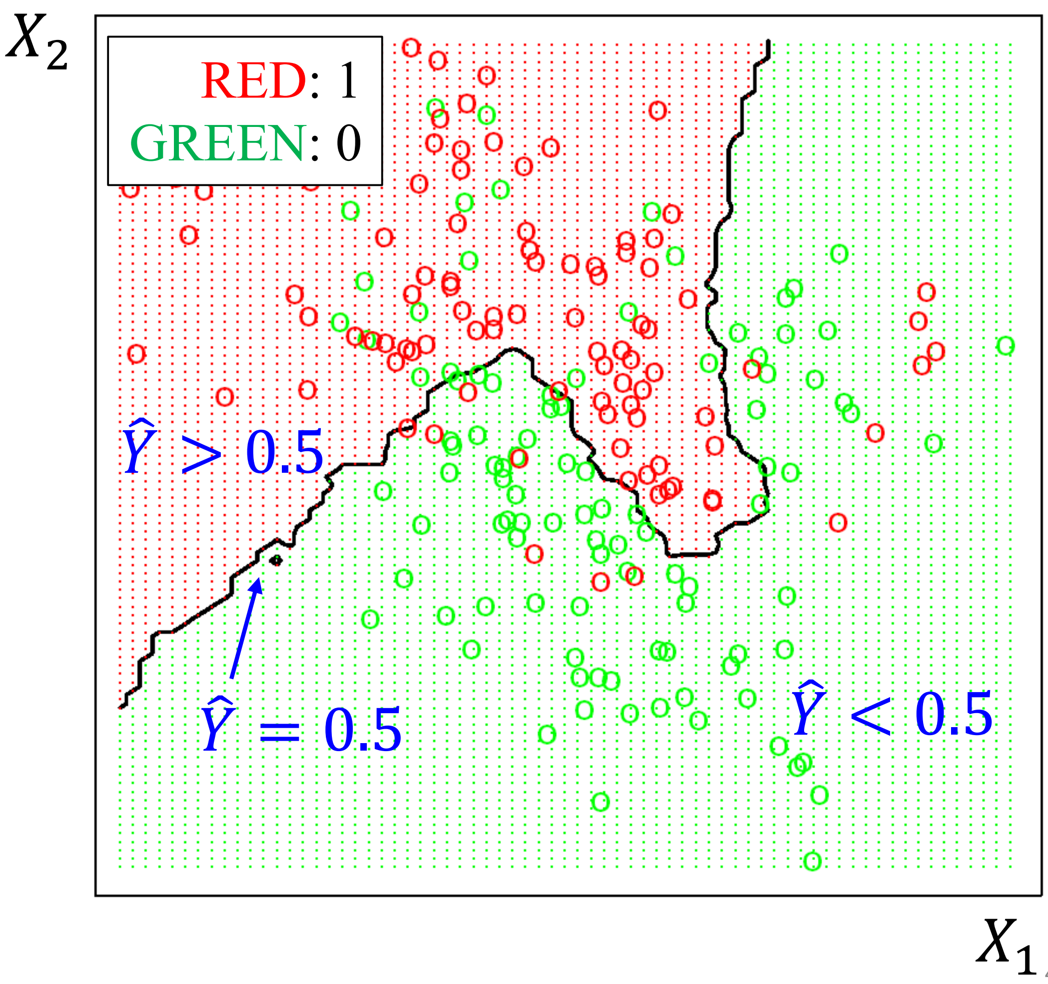
$$\hat{Y}(x) = \frac{1}{k}\sum_{x_i \in N_k(x)} y_i.$$

- $N_k(x)$ is the set of the k closest points to x is the training sample
- Average the outcome of the k closest training sample points
- Fewer misclassifications

15-nearest neighbors averaging



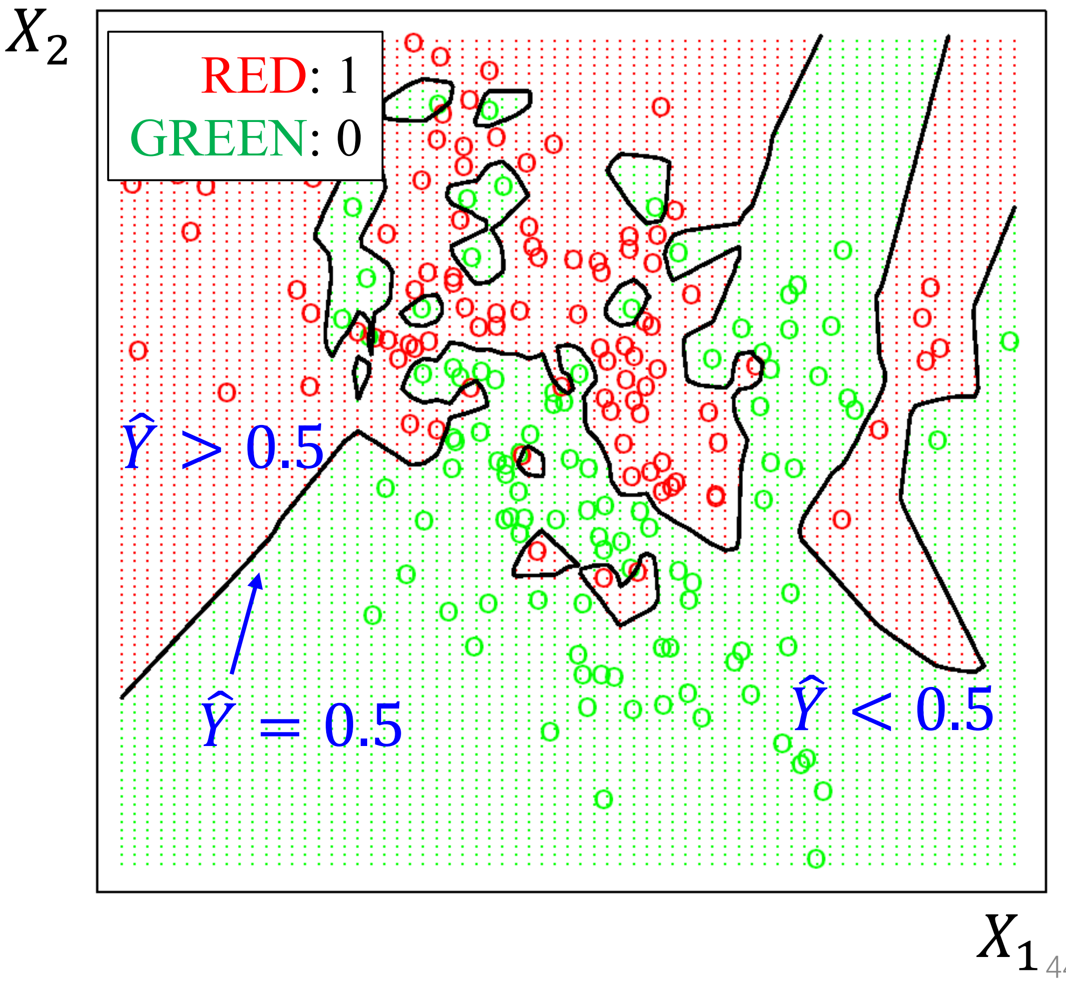
Simple Approach 2: Nearest Neighbors

- Use observations in the training set closest to the given input.

$$\hat{Y}(x) = \frac{1}{k}\sum_{x_i \in N_k(x)} y_i.$$

- $N_k(x)$ is the set of the k closest points to x is the training sample
- Average the outcome of the k closest training sample points
- No misclassifications: overtraining

1-nearest neighbors averaging



Simple Approach 2: Nearest Neighbors

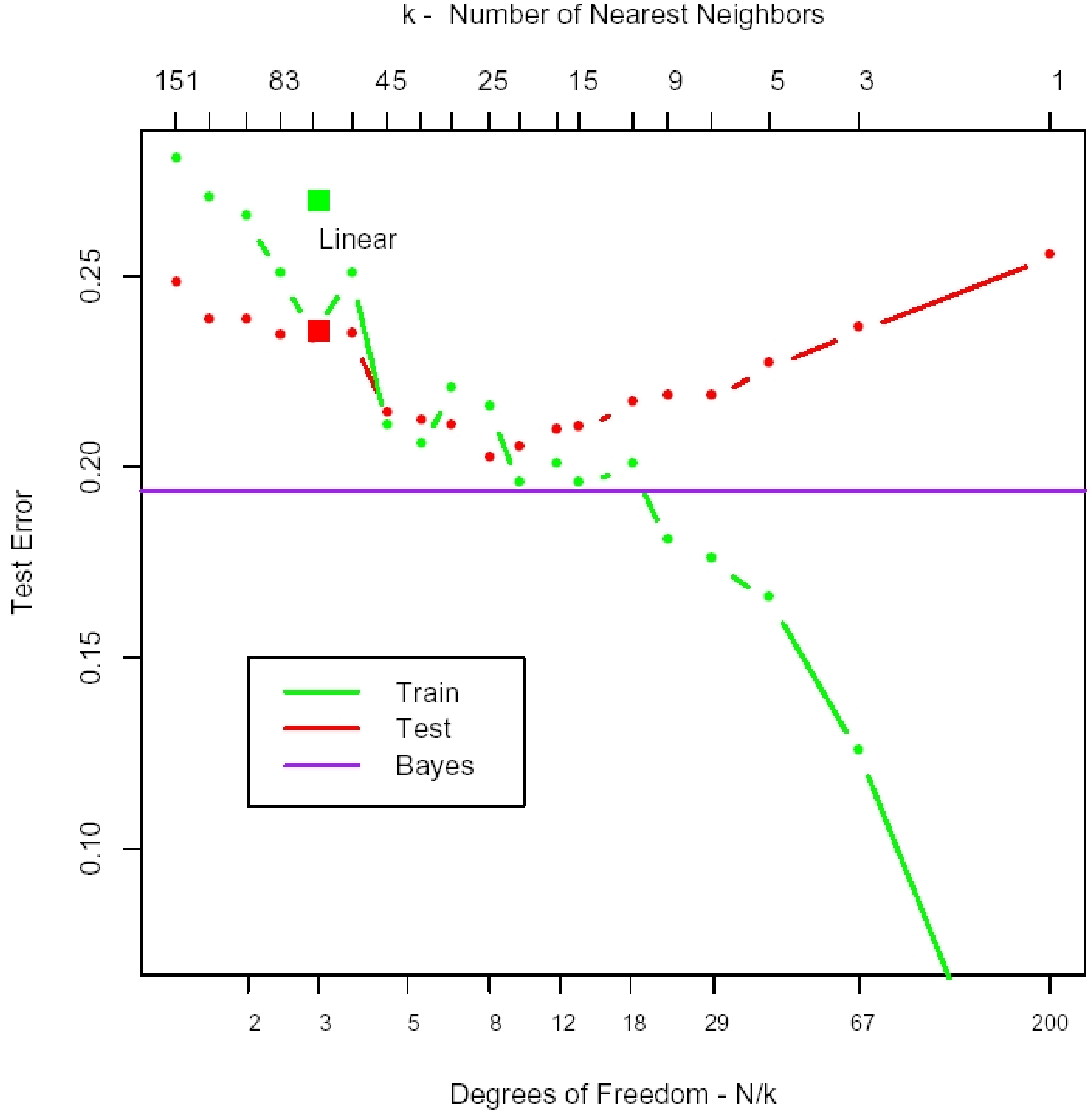
Pros:

- Simple algorithm, easy to implement (good baseline)
- No training time
- Easily scalable to multiple classes
- Works for “unusual” data distributions

Cons:

- Expensive query for test instances (time intensive)
- Memory intensive: stores data instead of parameters
- Not suitable for high-dimension data (curse of dimensionality)

Comparison of the Two Simple Approaches



Comparison of the Two Approaches

Linear regression	***k*-nearest neighbors**
p parameters (p = #variables)	$\frac{N}{k}$ parameters (k: hyperparameter) (N = #observations)
Low variance (robust)	High variance (not robust)
High bias (strong assumption)	Low bias (mild assumption)

Appendix

Symbol	Statistics	Machine Learning
X	variable, covariable predictor independent variable	feature attribute
Y	response dependent variable	label
x_i	observation data point	example instance
β	weights coefficients	parameters
$f(\cdot)$	model	learner

Difference between Statistics and Machine Learning in Terminology