CARTE-Enbridge Bootcamp

Basics of Machine Learning

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Centre for Analytics and Artificial Intelligence Engineering

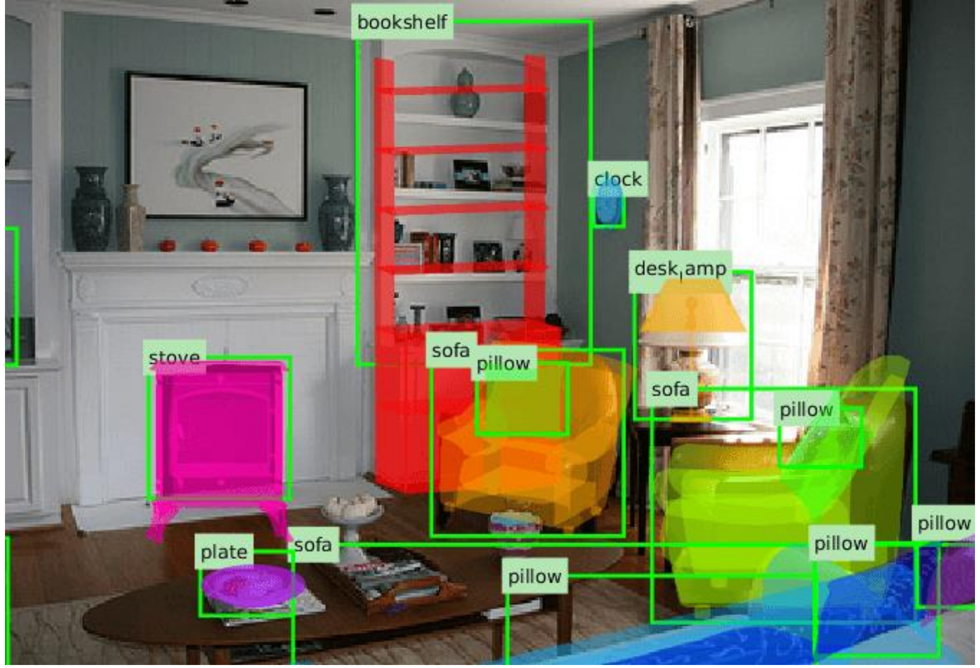
Artificial Intelligence

Getting computers to behave intelligently:

- Perform **non-trivial tasks** as well as humans do
- Perform **tasks that even humans struggle with**

Many sub-goals:

- Perception
- Reasoning
- Control
- Planning



My poker face: AI wins multiplayer game for first time

Pluribus wins 12-day session of Texas hold'em against some of the world's best human players

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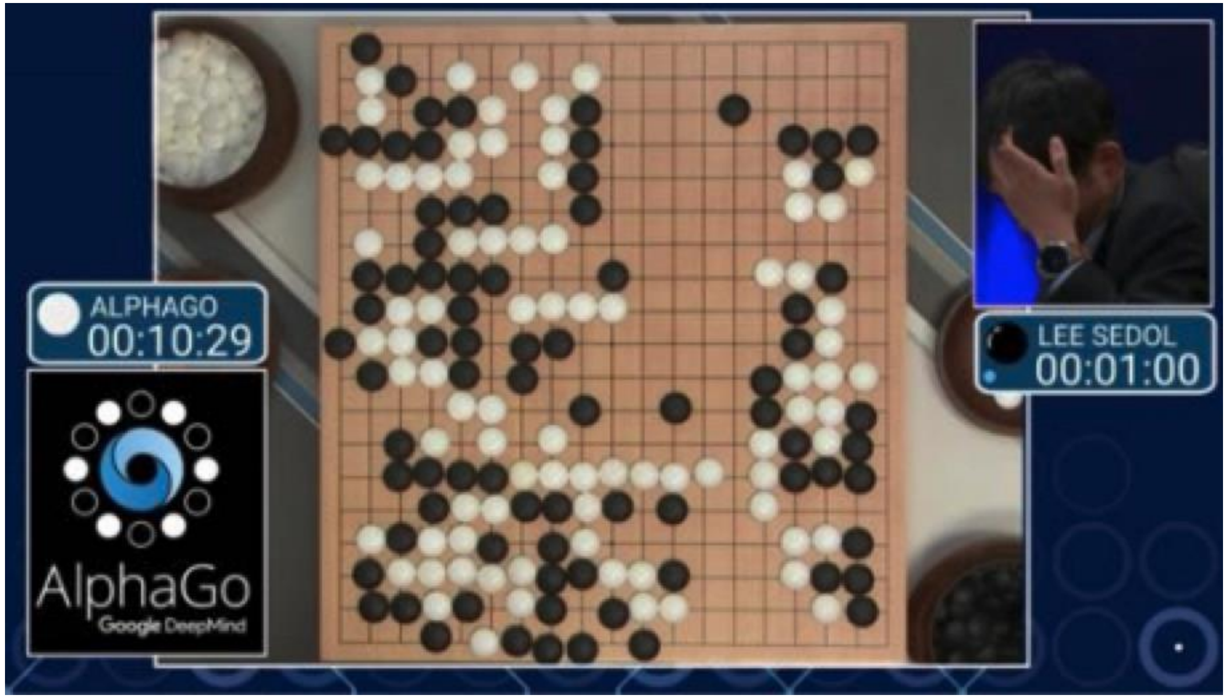
Speech Recognition Perception + Reasoning

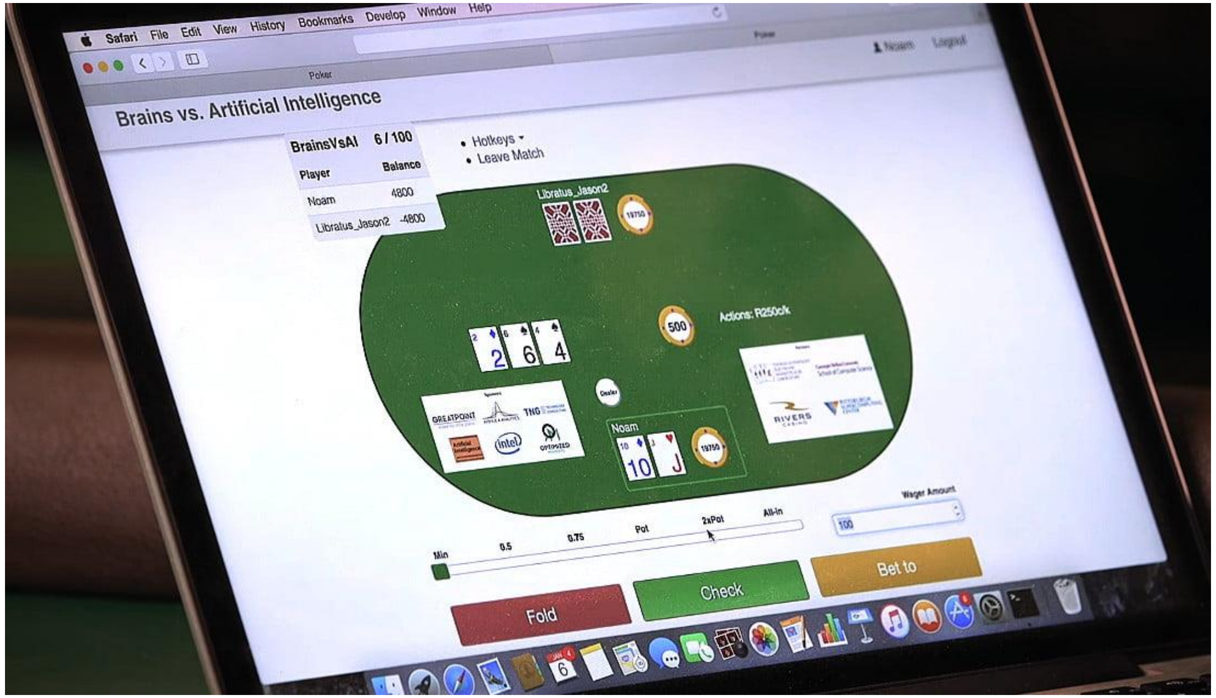
Autonomous Driving

Perception + Reasoning
Control + Planning

Game Playing

Reasoning + Planning



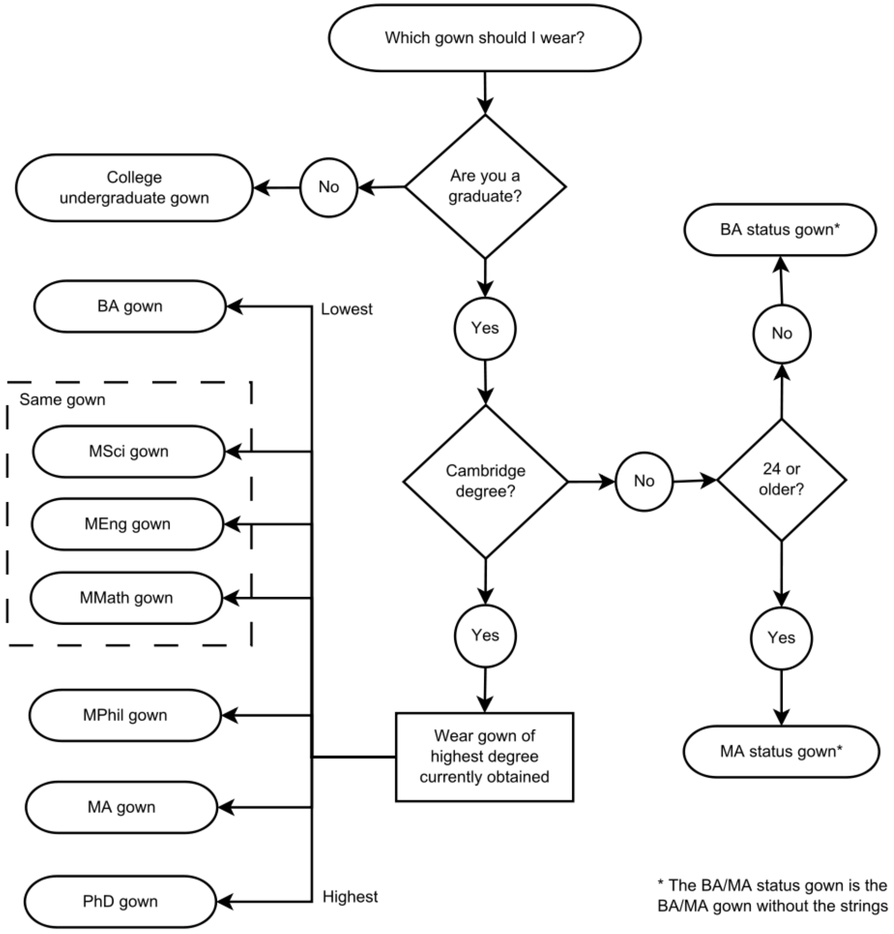


Knowledge-Based AI

Write programs that simulate how people solve the problem

Fundamental limitations:

- Will never get better than a person
- Requires deep domain knowledge
- We don't know how we do some things (e.g., riding a bicycle)



Data-Based AI = Machine Learning

Write **programs that learn** the task **from examples**

- ☑ No need to know how we do it as humans
- ☑ Performance should improve with more examples

- ✕ May need **many examples**!
- ✕ May not understand how the program works!

Machine Learning:

Study of algorithms that

- Improve their performance P
- At some task T
- With experience E

Well defined task: <P,T,E>

The Machine Learning Process

Experience

- Examples of the form
  (input, correct output)

Task

- Mapping from input to output

Performance

- ”Loss function” that measures error w.r.t. desired outcome

Choices in ML Problem Formulation

Experience

- Examples of the form
  (input, correct output)

Task

- Mapping from input to output

Performance

- "Loss function" that measures error w.r.t. desired outcome

Loan Applications

- What historical examples do I have? What is a correct output?
- Predict probability of default? Loan decision? Credit score?
- Do I care more about minimizing False Positives? False negatives?

Machine Learning:

Study of algorithms that

- Improve their performance P Optimization, Evaluation
- At some task T Classification, regression, clustering
- With experience E Tabular, image, sequence

Well defined task: <P,T,E>

How will I rate “Chopin’s 5^{th} Symphony”?

Song	Rating
Some nights	☆☆☆☆☆
Skyfall	☆
Comfortably numb	☆☆☆
We are young	☆☆☆☆
…	…
…	…
Chopin’s 5^{th}	???

Classification: Three Elements

1. Data:
   - x: data example with d attributes
   - y: label of example (what you care about)

2. Classification model: a function $f_{(a,b,c,\ldots)}$
   - Maps from X to Y
   - (a,b,c,…) are the parameters

3. Loss function:
   - Penalizes the model's mistakes

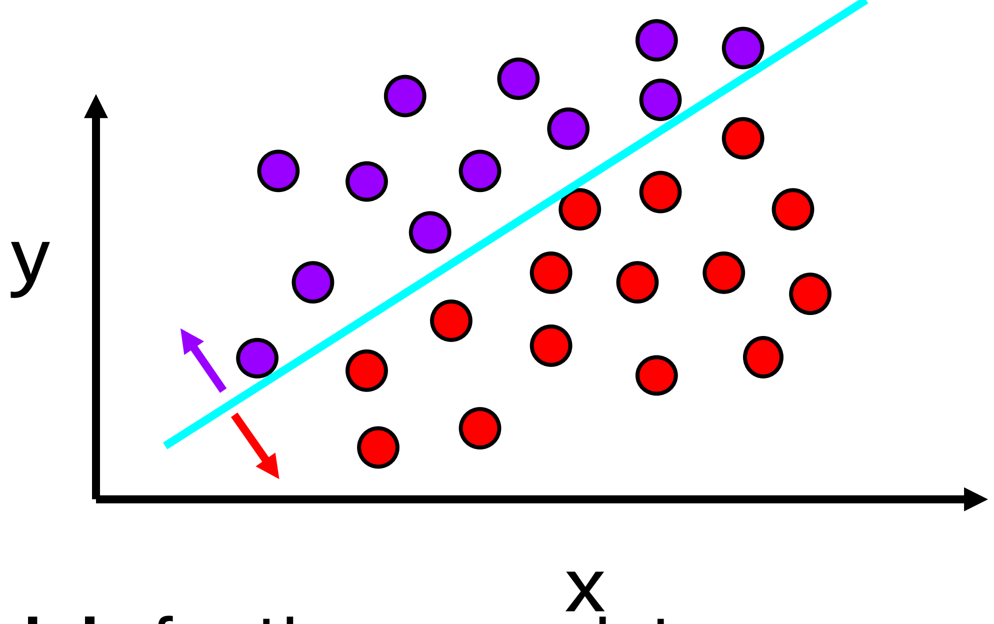
Song	Rating
Some nights	☆☆☆☆☆
Skyfall	☆
Comfortably numb	☆☆☆
We are young	☆☆☆☆
…	…
…	…
Chopin's 5th	???

Terminology Explanation

Song	Artist	Length	…	Rating
Some nights	Fun	4:23	…	☆☆☆☆☆
Skyfall	Adele	4:00	…	☆
Comf. Numb	Pink Floyd	6:13	…	☆☆☆
We are young	Fun	3:50	…	☆☆☆☆
…	…	…	…	…
…	…	…	…	…
Chopin's 5^{th}	Chopin	5:32	…	???

Data example = data instance
Attribute = feature = dimension
Label = target attribute

What is a "model"?



A **useful approximation** of the world

Typically, there are **many reasonable models** for the same data

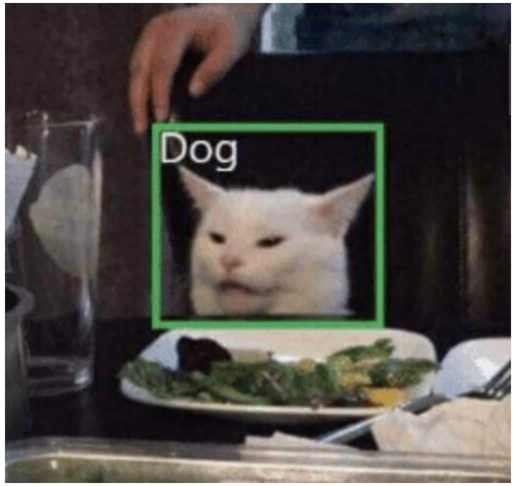
Training a model = finding appropriate values for (a,b,c,…)

- An **optimization** problem
- "appropriate" = **minimizes the Loss (cost)** function
- We will focus on a common training algorithm later on

Classification Loss Function

- How unhappy are you with the answer that the model gave?

- **L(y, f(x))** = 1 if: **y ≠ f(x)**
  0 otherwise



- **0-1 loss** function: intuitive but hard to optimize = train

- In practice, we use **approximations** of the 0-1 loss – getting warmer or getting colder

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Why should this work at all?

The main theoretical basis of ML:

With a **sufficient amount of "similar" data**

+

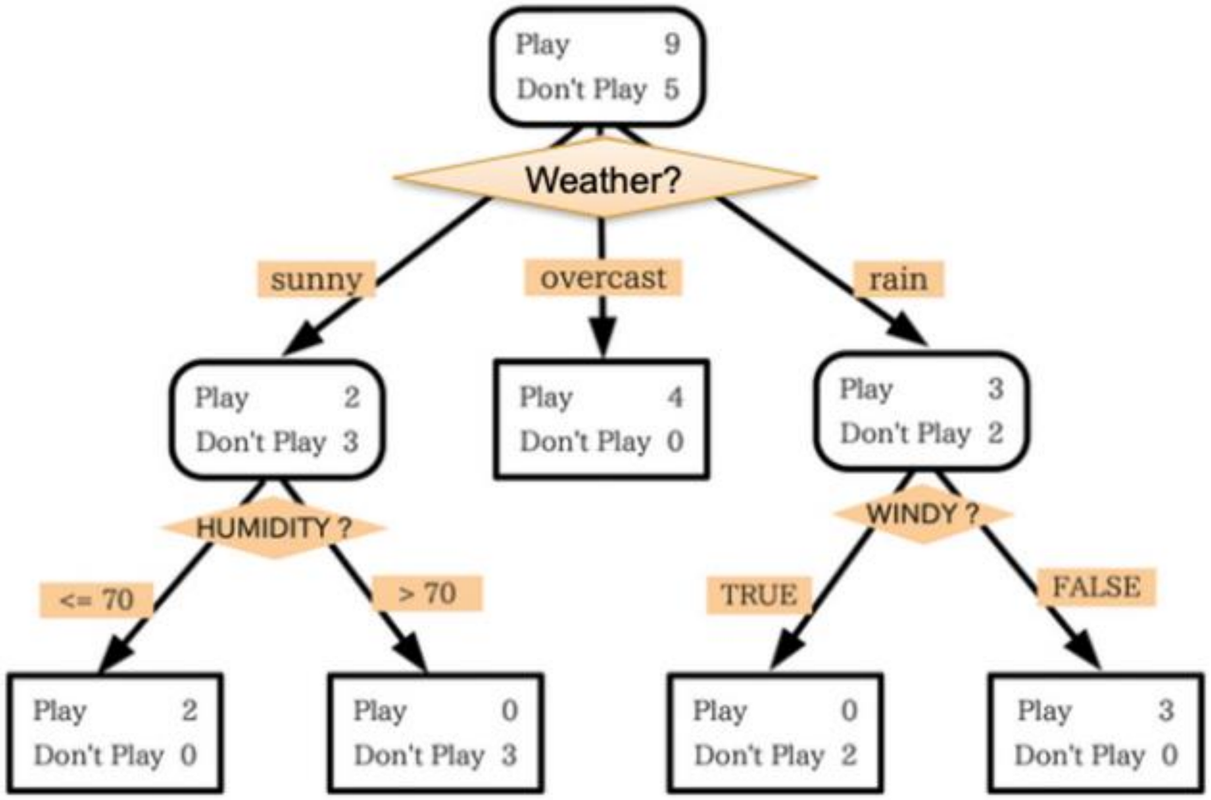
an **expressive model class**:

Minimizing the loss function on the training data yields a highly accurate model on **unseen test data**, with high probability

Decision Trees: To play tennis or not to?

- **Data**: attributes describing the weather; (sunny? humidity level, ...)
- **Target**: 1if it's good to **Play**, 0 otherwise

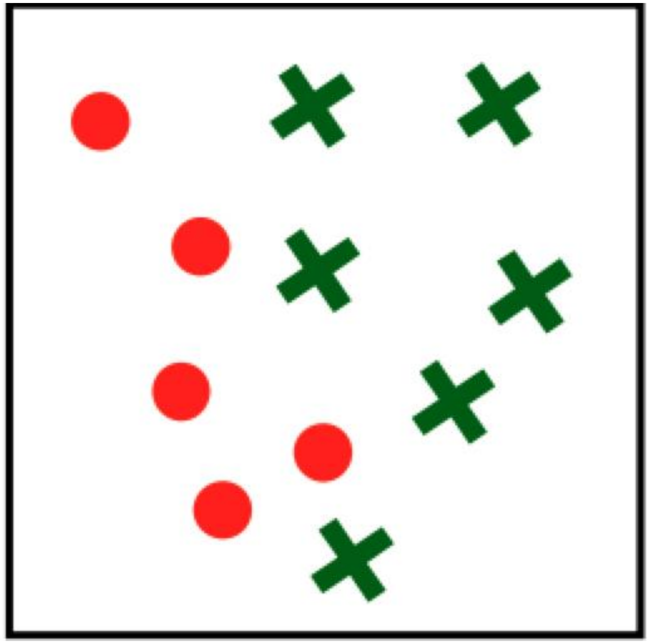
- **Model:** $f_T(x)$
- **Model parameters**: T, the tree structure (and size)



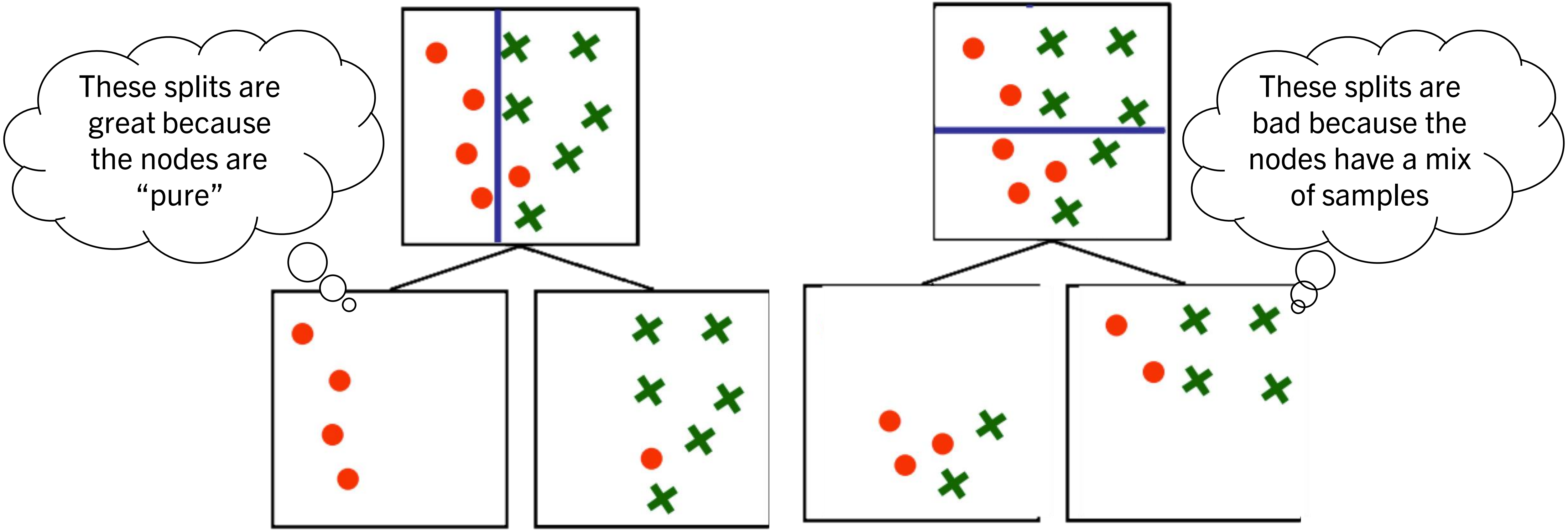
Training (fitting) a Decision Tree

How to choose the attribute/value to split on at each level of the tree?

- Two classes (red circles / green crosses)
- Two attributes: X and Y
- 11 points in training data
- Idea: construct a decision tree such that the leaf nodes correctly predict the class for all the training examples

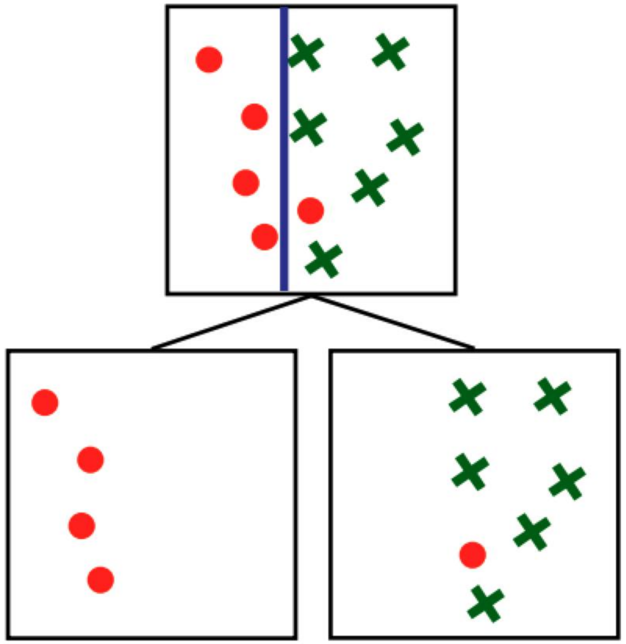


Training (fitting) a Decision Tree



Training (fitting) a Decision Tree

1. Find the **best attribute** to split on
2. Find the **best split** on the chosen attribute
3. Repeat 1 & 2 until **stopping criterion** is met



Common **stopping criteria**:

- Node contains very few data points
- Node is pure: most training data in node have same label

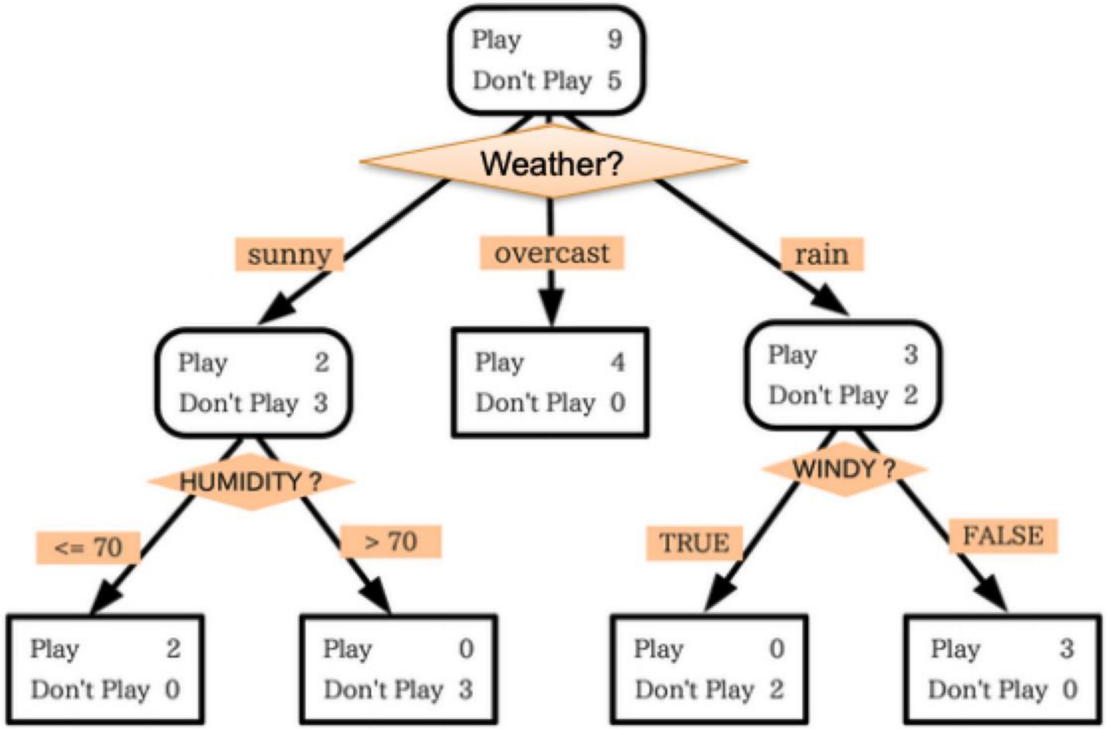
Final words on Decision Trees

Advantages

- Simple interpretation
- Fast predictions
- Handles mixed-type attributes

Caveats

- May be too simple for complex data
- Hard to figure out the right depth, stopping criterion, especially at the node level



Forecasting

Decision Trees predict discrete outcomes

- Given X features, what is y outcome?

What about something **continuous?**

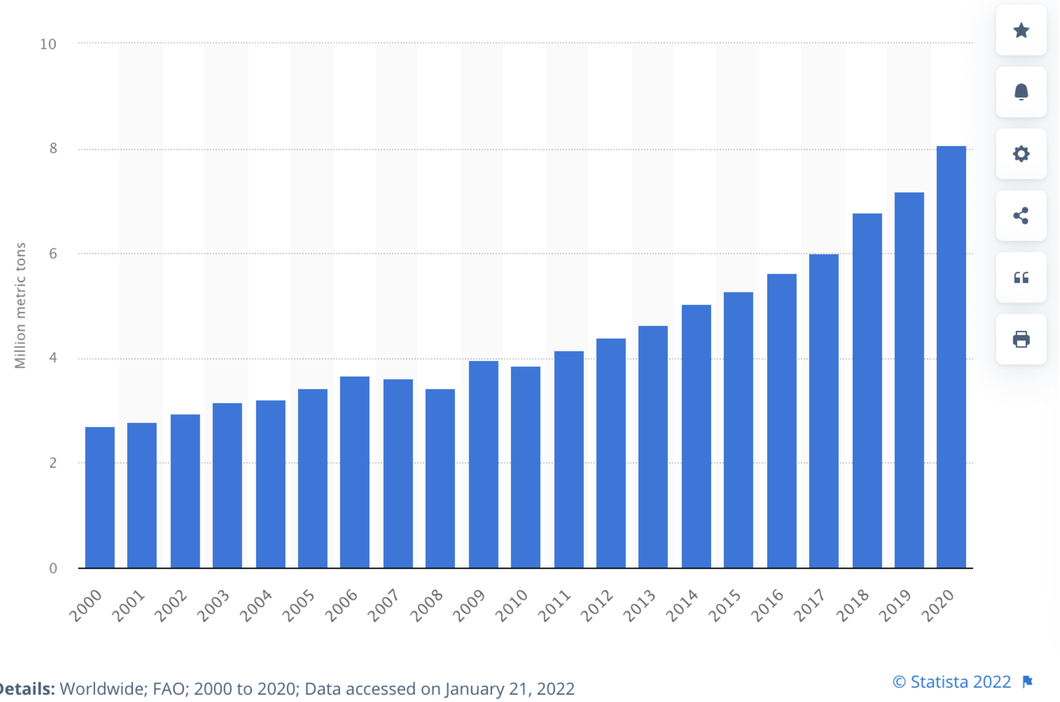
- How is something likely to change over time?

- Time series data tracks a value over time
  - e.g. temperature in one location, company sales data
- Often we want to predict what will happen *next*, i.e. in sequence

Time Series Data: Three Main Components

1. Trend: the long-term trajectory of the data

Avocado production is steadily increasing year-on-year

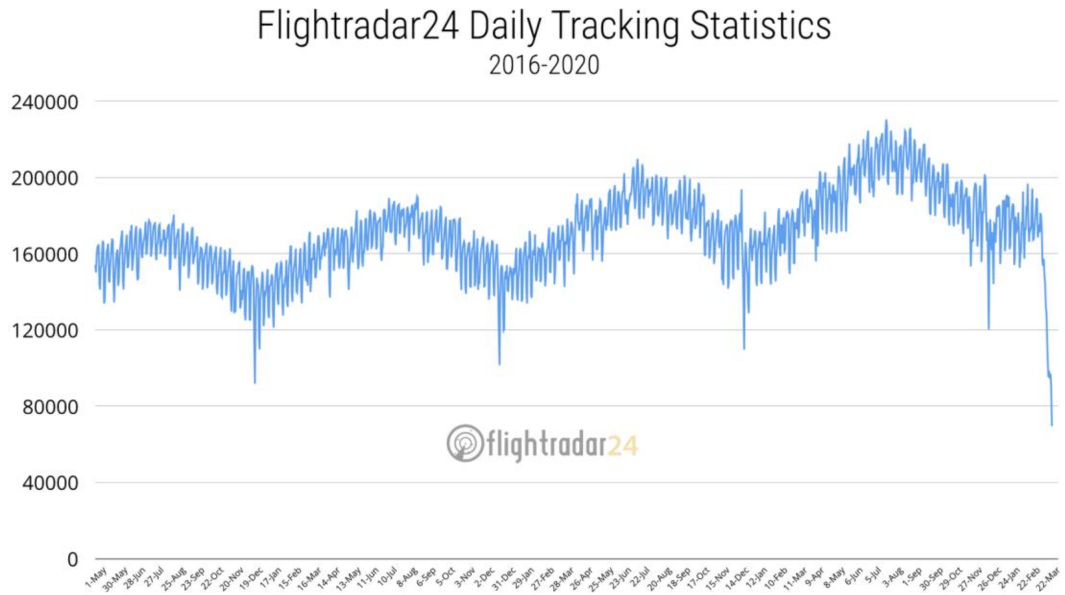


Details: Worldwide; FAO; 2000 to 2020; Data accessed on January 21, 2022

Time Series Data: Three Main Components

2. Seasonality: how the data changes according to the calendar

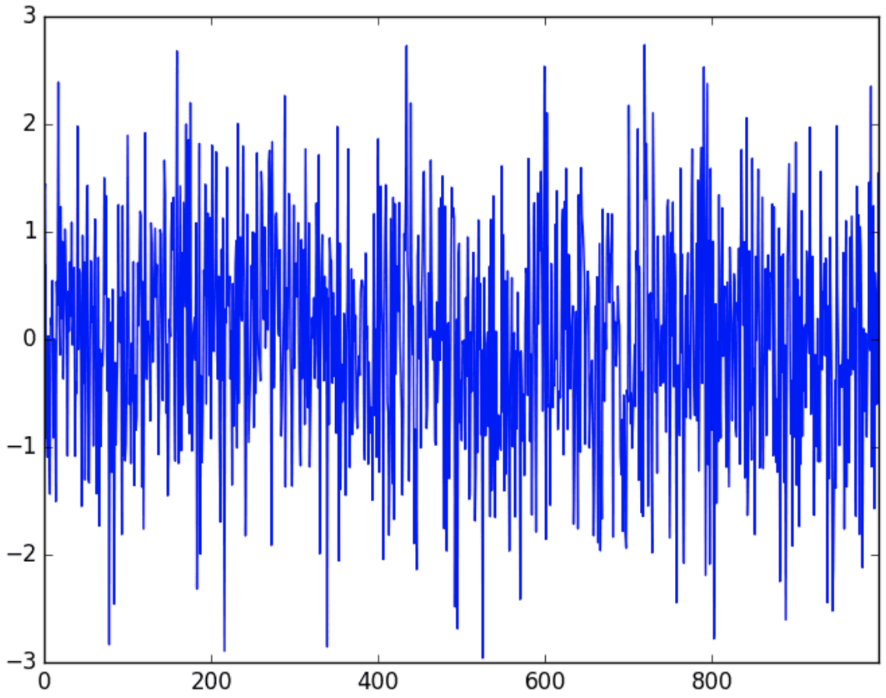
This is highly domain specific – e-commerce platforms experience the most sales around Christmas, but homes are sold most frequently in the summer



Time Series Data: Three Main Components

3. Noise: The random element left over

Noise comes from short-term changes that are unpredictable. More noise makes it harder to anticipate change



White noise (Image by Morn from Wiki Media Commons)

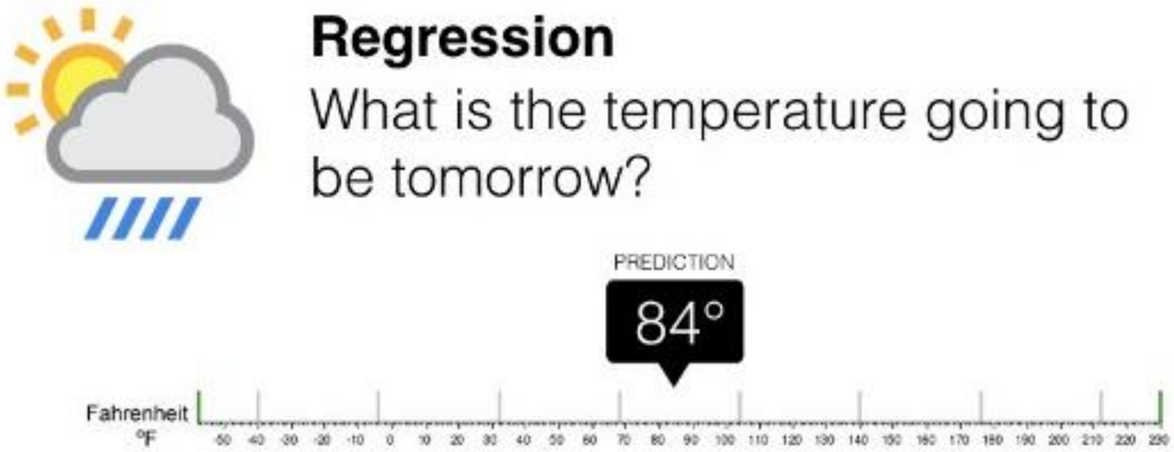
Regression

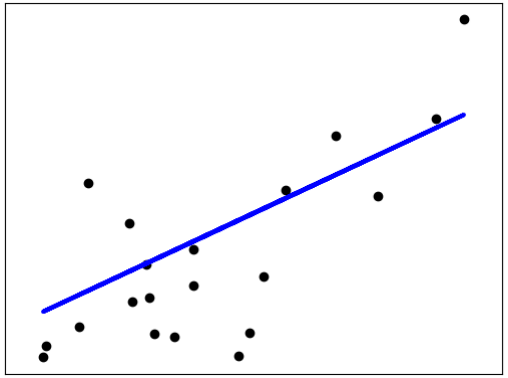
Examples:

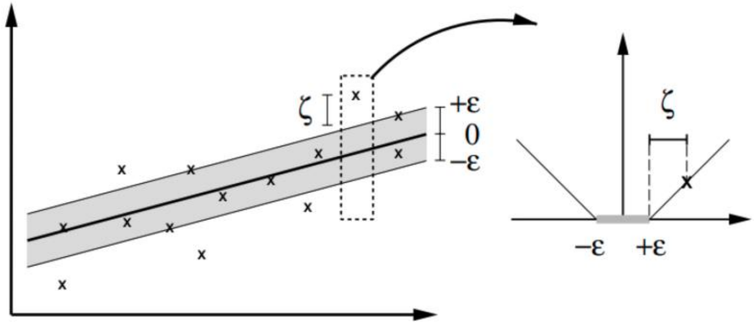
- Stock price prediction
- Forecasting epidemics
- Weather prediction

We will look at:

- Linear Regression
- Ridge Regression
- LASSO







Linear Regression

Data: $S = \{(x_1, y_1), (x_2, y_2), \ldots, (x_i, y_i)\}$

x_i: data example with d attributes

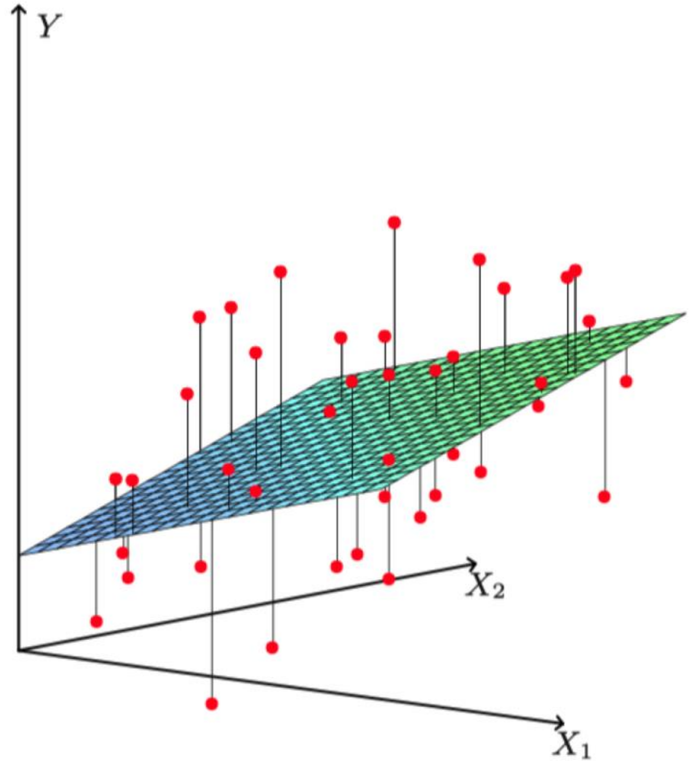
y_i: target of example (what you care about)

Model:

$$f(x; \boldsymbol{\beta}) = \beta_0 + \beta_1 x_1 + \cdots + \beta_d x_d$$

Loss function: Residual Sum of Squares

$$RSS(\boldsymbol{\beta}) = \sum_{i=1}^{n} \left(y_i - f(x_i; \boldsymbol{\beta})\right)^2$$



Ridge Regression

- Linear Regression uses all features; model may be complicated
- **Ridge Regression** penalizes large parameter values

Model:

$$f(x;\boldsymbol{\beta}) = \beta_0 + \beta_1 x_1 + \cdots + \beta_d x_d$$

Loss function: Residual Sum of Squares + penalty term

$$RSS(\boldsymbol{\beta}) = \sum_{i=1}^{n} \left(y_i - f(x_i;\boldsymbol{\beta})\right)^2 + \boldsymbol{\lambda} \sum_{j=0}^{d} \beta_j^2$$

Lasso Regression

- **As in Ridge Regression, Lasso** penalizes large parameters
- Penalizes **absolute** instead of squared coefficient values
- **Zeroes out** more coefficients **BUT** optimization is more involved

Model:

$$f(x;\boldsymbol{\beta}) = \beta_0 + \beta_1 x_1 + \cdots + \beta_d x_d$$

Loss function: Residual Sum of Squares + penalty term

$$RSS(\boldsymbol{\beta}) = \sum_{i=1}^{n} \big(y_i - f(x_i;\boldsymbol{\beta})\big)^2 + \lambda \sum_{j=0}^{d} |\beta_j|$$

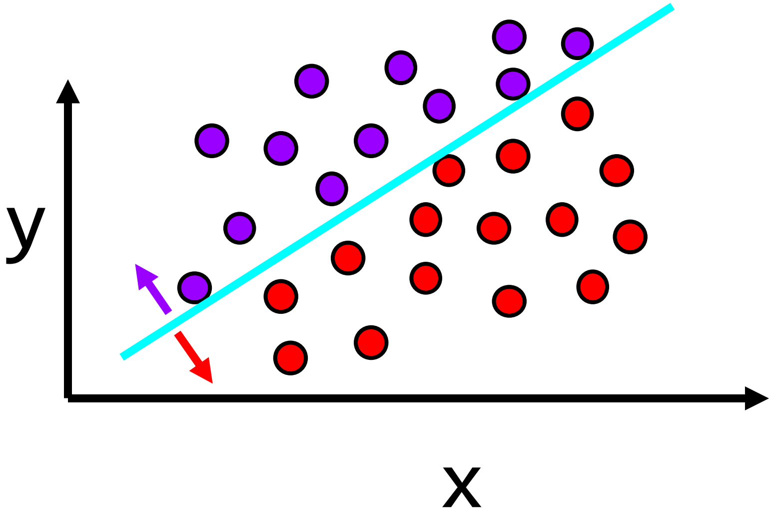
Example: Prostate Cancer

Stamey et al. (1989)

- x: cancer volume, prostate weight, age, …
- y: amount of prostate-specific antigen

Term	LS	Best Subset	Ridge	Lasso
Intercept	2.465	2.477	2.452	2.468
lcavol	0.680	0.740	0.420	0.533
lweight	0.263	0.316	0.238	0.169
age	−0.141		−0.046	
lbph	0.210		0.162	0.002
svi	0.305		0.227	0.094
lcp	−0.288		0.000	
gleason	−0.021		0.040	
pgg45	0.267		0.133	
Test Error	0.521	0.492	0.492	0.479
Std Error	0.179	0.143	0.165	0.164

Recap



- ML vs Knowledge-Based AI
- The ML mindset
- Classification: definition and assumptions
- Decision Trees
- Time-Series Data
- Regression