# Machine, Data and Learning

Based on Chapter 1 of Python Machine Learning by Example

Selected slides for lectures from Jan 10 to 27

# Machine Learning

- Scientific study of algorithms and statistical models that computer systems use
  - To perform a specific task effectively without using explicit instructions
  - Rely on patterns and inference instead.
- Involves
  - Building a **mathematical model** based on sample data, known as "training data“ to make predictions or decisions
  - No explicit programming done to perform the task

# Machine Learning

- Term coined around 1960
- Why learn ? Why not just hire enough programmers and code in rules ?
  - Lots of patterns for an activity/event
  - Events can be dynamic
  - **Data** is increasing exponentially
  - **Data** is also in various formats [Text, Audio, Video]
  - Higher quality **data** due to cheaper storage
- Can be broadly classified into three categories
  - Unsupervised, Supervised and Reinforcement learning

# Unsupervised Learning

- Takes a set of data points that contains only inputs and finds structure in data E.g., Grouping or Clustering of data points

- **Marketing:** Finding groups of customers with similar behavior given a large database of customer data containing their properties and past buying records.
- **Biology:** Classification of plants and animals given their features.
- **Earthquake studies:** Clustering observed earthquake epicenters to identify dangerous zones.
- **World Wide Web:** Clustering weblog data to discover groups of similar access patterns.

# Supervised Learning

- Builds mathematical model using data set that has both inputs and desired outputs E.g., Classification and Regression tasks

| User ID | Gender | Age | Salary | Purchased |
|---|---|---|---|---|
| 15624510 | Male | 19 | 19000 | 0 |
| 15810944 | Male | 35 | 20000 | 1 |
| 15668575 | Female | 26 | 43000 | 0 |
| 15603246 | Female | 27 | 57000 | 0 |
| 15804002 | Male | 19 | 76000 | 1 |
| 15728773 | Male | 27 | 58000 | 1 |
| 15598044 | Female | 27 | 84000 | 0 |
| 15694829 | Female | 32 | 150000 | 1 |
| 15600575 | Male | 25 | 33000 | 1 |
| 15727311 | Female | 35 | 65000 | 0 |
| 15570769 | Female | 26 | 80000 | 1 |
| 15606274 | Female | 26 | 52000 | 0 |
| 15746139 | Male | 20 | 86000 | 1 |
| 15704987 | Male | 32 | 18000 | 0 |
| 15628972 | Male | 18 | 82000 | 0 |
| 15697686 | Male | 29 | 80000 | 0 |
| 15733883 | Male | 47 | 25000 | 1 |

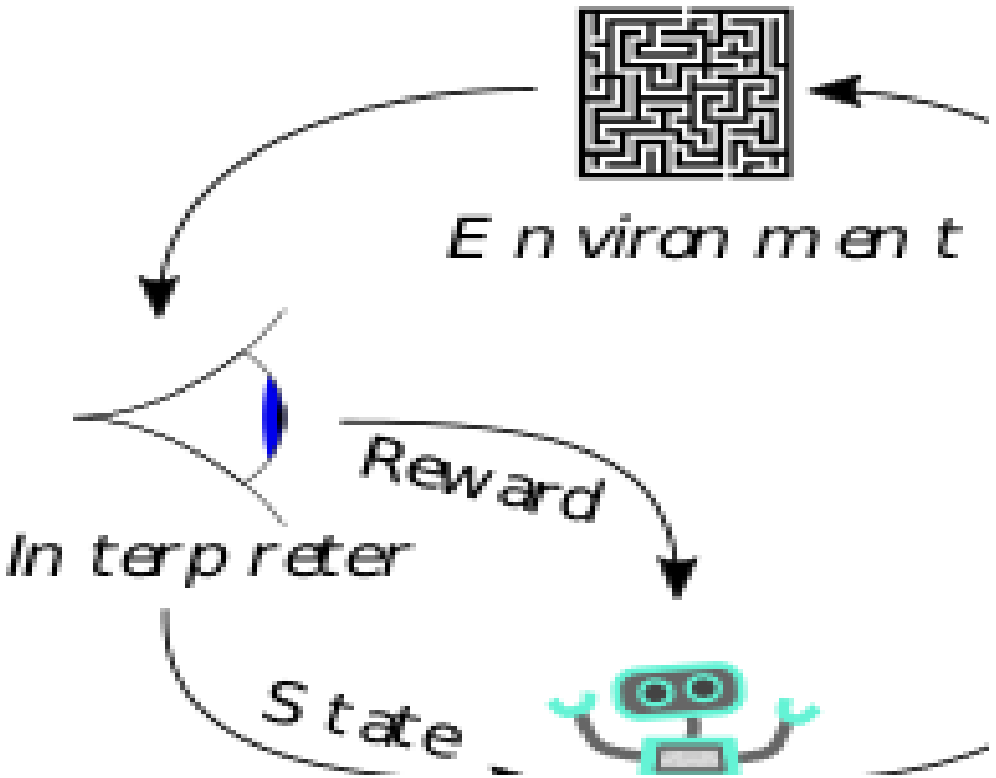
Figure A: CLASSIFICATION

| Temperature | Pressure | Relative Humidity | Wind Direction | Wind Speed |
|---|---|---|---|---|
| 10.69261758 | 986.882019 | 54.19337313 | 195.7150879 | 3.278597116 |
| 13.59184184 | 987.8729248 | 48.0648859 | 189.2951202 | 2.909167767 |
| 17.70494885 | 988.1119385 | 39.11965597 | 192.9273834 | 2.973036289 |
| 20.95430404 | 987.8500366 | 30.66273218 | 202.0752869 | 2.965289593 |
| 22.9278274 | 987.2833862 | 26.06723423 | 210.6589203 | 2.798230886 |
| 24.04233986 | 986.2907104 | 23.46918024 | 221.1188507 | 2.627005816 |
| 24.41475295 | 985.2338867 | 22.25082295 | 233.7911987 | 2.448749781 |
| 23.93361956 | 984.8914795 | 22.35178837 | 244.3504333 | 2.454271793 |
| 22.68800023 | 984.8461304 | 23.7538641 | 253.0864716 | 2.418341875 |
| 20.56425726 | 984.8380737 | 27.07867944 | 264.5071106 | 2.318677425 |
| 17.76400389 | 985.4262085 | 33.54900114 | 280.7827454 | 2.343950987 |
| 11.25680746 | 988.9386597 | 53.74139903 | 68.15406036 | 1.650191426 |
| 14.37810685 | 989.6819458 | 40.70884681 | 72.62069702 | 1.553469896 |
| 18.45114201 | 990.2960205 | 30.85038484 | 71.70604706 | 1.005017161 |
| 22.54895853 | 989.9562988 | 22.81738811 | 44.66042709 | 0.264133632 |
| 24.23155922 | 988.796875 | 19.74790765 | 318.3214111 | 0.329656571 |

Figure B: REGRESSION

# Reinforcement Learning

- Concerned with how software agents should take actions in an environment to maximize cumulative reward E.g. Autonomous vehicles, Computer games



# Some Applications

- Search engines
- Information retrieval
- Recommendation systems
- Credit card fraud detection
- Disease diagnosis
- Election prediction
- Image processing
- Speech translation
- …

# AlphaGo

- First computer Go program to defeat a 9-dan professional player
- Uses Monte Carlo Tree search algorithm based on knowledge learned by a deep learning method
- Beat World No. 1 ranked player in 2017
  - Retired after this match
- https://deepmind.com/research/alphago/
- https://www.youtube.com/watch?v=WXuK6gekU1Y

- AlphaGo Zero – Version without human data and stronger than AlphaGo [defeated 100-0]

# AlphaZero & MuZero

- AlphaZero, a generalized version of AlphaGo Zero Took 4 hours to learn Chess and defeat reigning world computer chess champion 28 to 0 in 100 matches
- https://www.youtube.com/watch?time_continue=7&v=tXlM99xPQC8

- MuZero: Master games without knowing rules
- Uses approach similar to AlphaZero, developed in 2019
- Trained via self-play and play against AlphaZero with no access to rules, opening books or endgame tables
- Viewed as significant advancement over AlphaZero

# AlphaFold: solution to a 50 year old grand challenge in biology

- https://deepmind.com/blog/article/alphafold-a-solution-to-a-50-year-old-grand-challenge-in-biology
- Figuring out what shapes proteins fold into is known as the “protein folding problem” - grand challenge in biology for the past 50 years
- Focus of intensive scientific research for many years, using a variety of experimental techniques such as nuclear magnetic resonance and X-ray crystallography.

# AlphaFold

- Number of ways a protein could theoretically fold before settling into its final 3D structure is astronomical.
- Cyrus Levinthal estimated 10^300 possible conformations for a typical protein.
- Estimated would take longer than the age of universe to enumerate all possible configurations. Yet in nature, proteins fold spontaneously, some within milliseconds - referred to as Levinthal's paradox.

# Generalization & Goodness of Fit

- **Generalization** refers to how well the concepts learned by a ML model generalizes to specific examples or data not yet seen by the model.
  - …
- **Goodness of fit** describes how well a model fits for a set of observations.
  - Overfitting and Underfitting

# Overfitting

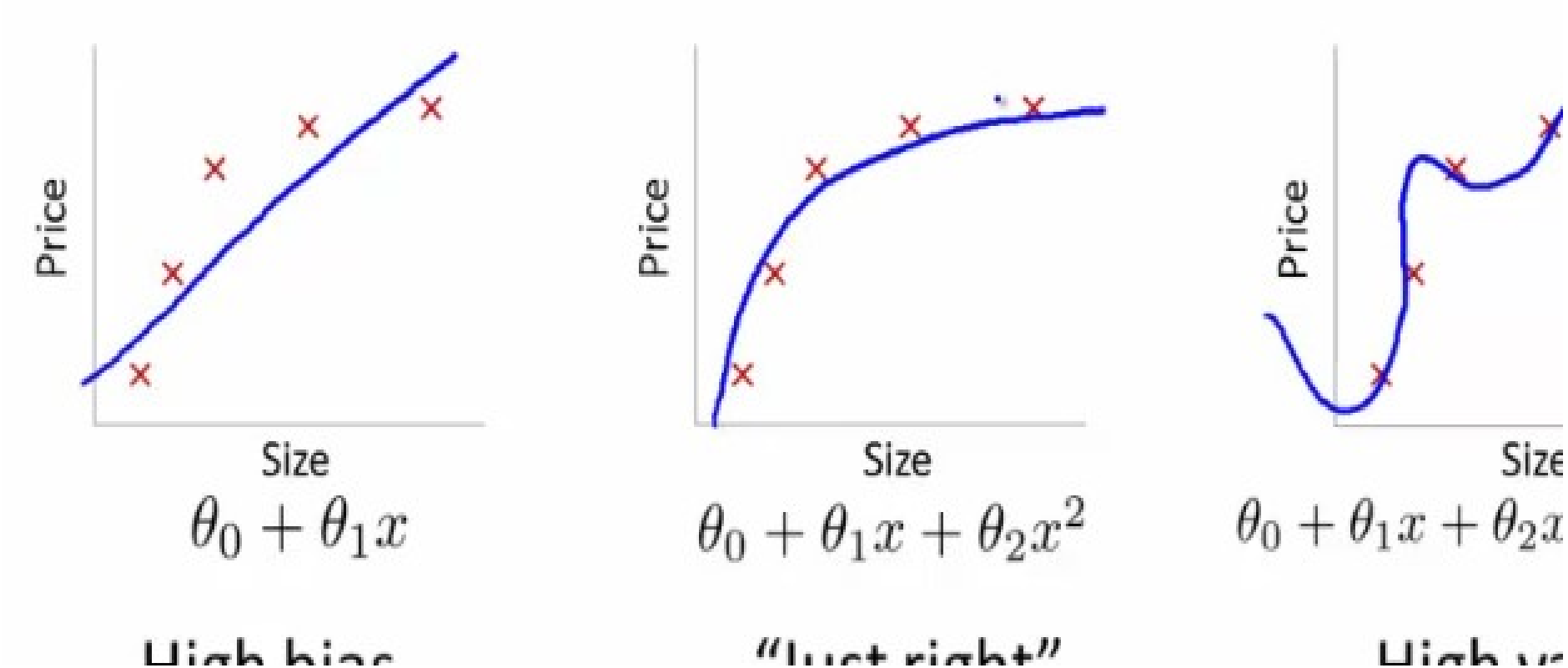
- Phenomenon of extracting too much information from training sets or memorization can cause overfitting
  - Makes ML model work well with training data called **low bias**
  - Bias refers to error due to incorrect assumptions in learning algorithm
  - However, does not generalize well or derive patterns, performs poorly on test datasets called **high variance**
  - Variance measures error due to small fluctuations in training set

# Underfitting

- Model is underfit if it does not perform well on training sets and will not do so on test sets
- Occurs when we are not using enough data to train or if we try to fit wrong model to the data
  - E.g., if you do not read enough material for exam or if you prepare wrong syllabus
- Called **high bias** in ML although **variance is low** [i.e. consistent but in a bad way]
- May need to increase number of features since it expands the hypothesis space.

# Goodness of fit

- For same data:



# Bias-Variance Tradeoff

- If the model is too simple and has very few parameters then it may have high bias and low variance
- If the model has large number of parameters it may have high variance and low bias
- We need to find a right/good **balance** without overfitting or underfitting the data
- As more parameters are added to a model
  - Complexity of the model rises
  - Variance becomes primary concern while bias falls steadily.

# Bias-Variance Tradeoff

- Suppose a training set consists of points x1, …, xn and real values yi associated with each point xi
- We assume there is a function y = f(x) + Ɛ, where the noise Ɛ has zero mean and variance $\sigma^2$
- Find $\hat{f}(x)$, tht approximates f(x) as well as possible
- To measure how well the approximation was performed, we minimize the mean square error $(y - \hat{f}(x))^2$
- A number of algorithms exist to find $\hat{f}(x)$, that generalizes to points outside of our training set

# Bias-Variance Tradeoff

- Variance measures how far a set of (random) numbers are spread out from their average value.
- Measured as expectation of the squared deviation of a random variable from its mean.

$$Var(X) = E[(x - \mu)^2]$$

$$Var(X) = E[(x - E[x])^2]$$

$$= E[x^2 - 2xE[x] + E[x]^2)$$

$$= E[x^2] - 2E[x]E[x] + E[x]^2$$

$$= E[x^2] - E[x]^2$$

# Bias-Variance Tradeoff

- Turns out expected (mean squared) error of $\hat{f}$ on an unseen sample in general can be decomposed as:

$$E\left[\left(y - \hat{f}(x)\right)^2\right] = (Bias[\hat{f}(x)])^2 + Var[\hat{f}(x)] + \sigma^2$$

where,

$$Bias\left(\hat{f}(x)\right) = E[\hat{f}(x) - f(x)]$$

$$= E[\hat{f}(x)] - E[f(x)] = E[\hat{f}(x)] - f(x)$$

$$Since\ f\ is\ deterministic, E[f] = f$$

and

$$Var[\hat{f}(x)] = E[\hat{f}(x)^2] - E[\hat{f}(x)]^2$$

Note that all three terms are positive

# Bias-Variance Tradeoff

- Notations:

$$Var[x] = E[x^2] - (E[x])^2$$

$$E[X^2] = Var(X) + (E[x])^2$$

$$Given\ y = f + \varepsilon\ and\ E[\varepsilon] = 0, E[y] = E[f + \varepsilon] = E[f] = f$$

$$Since\ Var[\varepsilon] = \sigma^2, Var[y] = E[(y - E[y])^2] = E[(y - f)^2]$$

$$= E[(f + \varepsilon - f)^2] = E[\varepsilon^2] = Var[\varepsilon] + (E[\varepsilon])^2 = \sigma^2$$

# Bias-Variance Tradeoff

- The expected error on an unseen sample x can be decomposed as:

$$
\begin{aligned}
E[(y-\hat{f})^2] &= E[(f+\varepsilon-\hat{f})^2] \\
&= E[(f+\varepsilon-\hat{f}+E[\hat{f}]-E[\hat{f}])^2] \\
&= E\left[(f-E[\hat{f}])^2\right] + E[\varepsilon^2] + E\left[(E(\hat{f})-\hat{f})^2\right] \\
&+ 2E[(f-E[\hat{f}])\varepsilon] + 2E[\varepsilon(E(\hat{f})-\hat{f})] + 2E[(E(\hat{f})-\hat{f})(f-E[\hat{f}])] \\
&= (f-E(\hat{f}))^2 + E(\varepsilon^2) + E[(E[\hat{f}]-\hat{f})^2] \\
&+ 2(f-E[\hat{f}])E(\varepsilon) + 2E(\varepsilon)E(E[\hat{f}]-\hat{f}] + 2E[E[\hat{f}]-\hat{f}](f-E[\hat{f}])
\end{aligned}
$$

# Bias-Variance Tradeoff

$$= (f - E[\hat{f}])^2 + E[\varepsilon^2] + E[(E[\hat{f}] - \hat{f})^2]$$
$$= (f - E[\hat{f}])^2 + Var[y] + Var[\hat{f}]$$
$$= Bias[\hat{f}]^2 + Var[y] + Var[\hat{f}]$$
$$= Bias[\hat{f}]^2 + \sigma^2 + Var[\hat{f}]$$

- Hence the derivation.

# Avoiding Overfitting

- A variety of techniques to avoid overfitting:
  - Cross-validation
  - Regularization
  - Feature selection
  - Dimensionality reduction

# Non-exhaustive Cross-validation

# Exhaustive Cross-validation

# Nested Cross-validation

- Popular way to tune parameters of an algorithm
- One version: k-fold cross validation with validation and test set
- Lets say parameter X needs tuning
  - Possible values 10, 20, 30, 40, 50

# Nested Cross-validation

- k = 7 in our example
  - One set each picked as Test and Validation, (k-2) picked for training
- For the picked Test set
  - Perform k-fold cross validation on Train & Validation set [Here k = 6]
  - Compute the average training error for each value of X
  - Pick the best X
- Repeat for each possible Test set [i.e. 7 times]
- Pick X that was returned maximum times to outer loop

# Regularization

# Regularization

- Let $\hat{f}(x) = \theta_0 + \theta_1 x^2 + \theta_3 x^2 + \theta_4 x^3$
- We want to minimize the MSE:

$$\frac{1}{m} * \min_{\theta_0,\theta_1,\theta_3,\theta_4} \sum_{i=1}^{m} (\hat{f}_\theta(x^{(i)}) - y^{(i)})^2$$

- where m is the number of training samples, theta's are the weight parameters
- Let MSE be represented by $J(\theta)$
- Lets say we want to penalize the higher order terms (2 and 3)

# Regularization

- Can add penalty terms say +1000 $\theta_3$ + 1000 $\theta_4$
- The effect of this would be that $\theta_3$ and $\theta_4$ need to be quite small to minimize error
- A significantly high penalty can actually convert a overfit problem to an underfit problem
  - Since all the terms with high regularization parameter would become 0 or close to 0
  - E.g. if all terms except $\theta_0$ have a high enough regularization parameter then $\hat{f}(x)$ can become a constant !!!

# Feature Selection

- Filter methods: …
- Wrapper methods: …
  - Recursive Feature Elimination
- Embedded methods: …

# Dimensionality Reduction

# Data Preprocessing

- A popular methodology in data mining is CRoss Industry Standard Process for data mining (CRISP DM)
- …

# Feature Engineering

- …
- **One-hot-encoding or one-of-K:** Refers to splitting the column which contains numerical *categorical data* to many columns depending on the number of categories present in that column.
  - Each column contains “0” or “1” corresponding to which column it has been placed.

# Feature Engineering

| Fruit | Categorical value of fruit | Price |
|---|---|---|
| apple | 1 | 5 |
| mango | 2 | 10 |
| apple | 1 | 15 |
| orange | 3 | 20 |

- After one hot encoding

| apple | mango | orange | price |
|---|---|---|---|
| 1 | 0 | 0 | 5 |
| 0 | 1 | 0 | 10 |
| 1 | 0 | 0 | 15 |
| 0 | 0 | 1 | 20 |

# Feature Engineering

- …