# Day 2: Linear Regression Summer STEM: Machine Learning

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#### Outline

- 1 Review of Day 1
- 2 Lab: Simple Linear Mode
- 3 Lab: Goodness of Fit
- 4 Statistics for the LS Solutio
- 5 Least Squares Solution
- 6 Extension to Multivariable Dat
- 7 Lab: Robot Arm Calibratio



## What is Machine Learning

- Learn the algorithm from known data to generate the rules
- Make predictions on unknown data using these rules
- Very effective tool where human expertise is not available

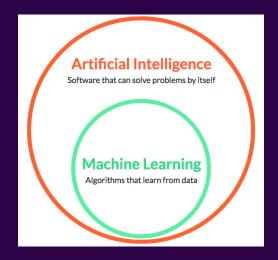


# Artificial Intelligence

- Search
- Reasoning and Problem Solving
- Knowledge Representation
- Planning
- Learning
- Perception
- Natural Language Processing
- Motion and Manipulation
- Social and General Intelligence



## Machine Learning



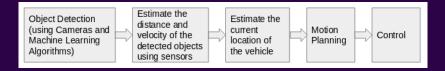


#### Autonomous vs. Automated





#### Autonomous Example: Driver-less Cars





# Why is Machine Learning so Prevalent?

- Database mining
- Medical records
- Computational biology
- Engineering
- Recommendation systems
- Understanding the human brain



# Why Now?

- Big Data
  - Massive storage. Large data centers
  - Massive connectivity
  - Sources of data from internet and elsewhere
- Computational advances
  - Distributed machines, clusters
  - GPUs and hardware



Review Lab Lab Stats LS Multivariable

# Supervised Learning

- In supervised learning, we are given a data set and already know what our correct output should look like, having the idea that there is a relationship between the input and the output.
- Supervised learning problems are categorized into "regression" and "classification" problems.
  - In a regression problem, we are trying to predict results within a continuous output, meaning that we are trying to map input variables to some continuous function.
  - In a classification problem, we are instead trying to predict results in a discrete output. In other words, we are trying to map input variables into discrete categories.



# Supervised Learning - Examples

- Regression Given a picture of a person, we have to predict their age on the basis of the given picture
- Classification Given a patient with a tumor, we have to predict whether the tumor is malignant or benign



# Unsupervised Learning

- Unsupervised learning allows us to approach problems with little or no idea what our results should look like. We can derive structure from data where we don't necessarily know the effect of the target variables.
- We can derive this structure by clustering the data based on relationships among the variables in the data.
- Example: Grouping individual voices from a mesh of sounds.



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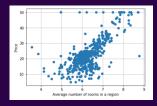


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#### Linear Model

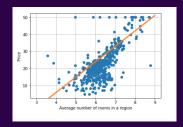
#### ■ Data Representation:

- y = variable you are trying to predict. Also referred to as: Dependent variable, response variable, target variable etc.
- $\blacksquare$  x = what you are using to predict. Also referred to as: Independent variable, attribute, predictor etc.
- Set of points,  $(x_i, y_i)$ , i = 1, ..., n. Each data point is called a sample.
- An efficient way to visualize the data is by plotting *y* vs *x* in a scatter plot.





- Assume a linear relationship y = b + wx
  - $\bullet$  b = intercept
  - $\mathbf{w} = \mathsf{slope}$
- $\mathbf{w} = (b, w) = (w_0, w_1)$  are the parameters of the model



■ Let's go to the lab to understand this further.



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#### Is Your Model a Good Fit?

- How would you determine if your model is a good fit or not?
- Talk with your classmates next to you to see whose model fits the data the best
  - How will you determine this?
  - Is there a quantitative way?
  - Write python code if so.



Lab

#### **Error Functions**

- An **error function** quantifies the discrepancy between your model and the data.
  - They are non-negative, and go to zero as the model gets better.
- Common Error Functions:
  - Mean Squared Error:  $MSE = \frac{1}{N} \sum_{i=1}^{N} (y_i \hat{y}_i)^2$
  - Mean Absolute Error:  $MAE = \frac{1}{N} \sum_{i=1}^{N} |y_i \hat{y}_i|$
- In later units, we will refer to these as cost functions or loss functions.
- Compute MSE on your model
- How do we interpret MSE? MAE?
  - RMSE?



■ Load and visualize data



- Load and visualize data
  - $\blacksquare (x_i, y_i), i = 1, ..., n$

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- Find parameters that minimize the error function
  - $\blacksquare$  Select b, w to minimize the error function



#### Least Squares Fit

■ The **Least Squares Fit** is characterized by the minimization of the MSE error function:

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- Find the parameters,  $\mathbf{w} = (b, w) = (w_0, w_1)$ , that give the smallest MSE
- MSE is a useful metric because there exists an analytic solution to find the optimal parameters b and w



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- Mean:

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i, \quad \bar{y} = \frac{1}{N} \sum_{i=1}^{N} y_i$$

Stats

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Variance:

$$\sigma_x^2 = \frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})^2, \quad \sigma_y^2 = \frac{1}{N} \sum_{i=1}^N (y_i - \bar{y})^2$$



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■ Covariance:

$$\sigma_{xy} = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})(y_i - \bar{y})$$

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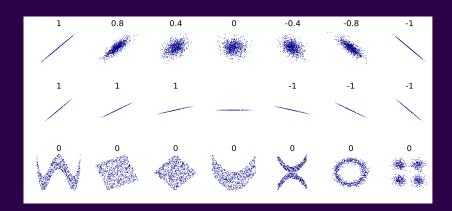
■ Correlation Coefficient:

$$\rho = \frac{\sigma_{xy}}{\sigma_x \sigma_y}$$

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#### Lab: Gaining Intuition





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$$\hat{y} = \bar{y} + \rho \frac{\sigma_y}{\sigma_x} (x - \bar{x})$$
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Prediction:

$$y_{new} = b + wx_{new}$$



■ Model:

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■ Prediction:

$$y_{new} = b + wx_{new}$$

Compute the LS fit model



# Lab: Find/Build and fit your own data

- 1 Find your a data set
  - Google: "[subject you're interested in] dataset"
  - https://archive.ics.uci.edu/ml/datasets.php
  - https://toolbox.google.com/datasetsearch
  - or -
- 2 Build your own data set
  - Only need 10+ samples



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Multivariable

■ Model: 
$$\hat{y} = b + w_1x_1 + w_2x_2 + ... + w_Dx_D$$

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Let 
$$\mathbf{x} = [1, x_1, x_2, ..., x_D]^T$$



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and  $\mathbf{w} = [w_0, w_1, ..., w_D]^T$   
So,  $\hat{y} = \mathbf{x}^T \mathbf{w}$ 



■ We want to minimize the squared error over all the samples:  $\sum_{i=1}^{N} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{N} (y_i - \mathbf{x}_i^T \mathbf{w})^2$ 



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we want to minimize the squared error over all 
$$\sum_{i=1}^{N} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{N} (y_i - \mathbf{x}_i^T \mathbf{w})^2$$
Design Matrix: Let,  $X = \begin{bmatrix} 1 & x_{1_1} & \cdots & x_{1_D} \\ 1 & x_{2_1} & \cdots & x_{2_D} \\ \vdots & & \ddots & \\ 1 & x_{N_1} & \cdots & x_{N_D} \end{bmatrix}$ 



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- Can express these conditions in matrix form:  $\mathbf{y} = X\mathbf{w}$
- Solution: Pseudo-Inverse



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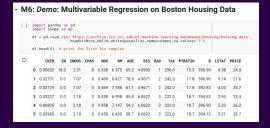
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  - There isn't a true solution to this equation.
- We say  $\mathbf{w}^*$  solves  $\mathbf{y} = X\mathbf{w}$  in the least squares sense, where

$$\mathbf{w}^{\star} = X^{\dagger}\mathbf{y}$$



### **Boston Housing Demo**

- Using multiple features to predicting house prices
  - Crime rate per capita, number of rooms, student-teacher ratio at local schools, ...
- Lets use a linear model that takes into account all the collected data





Lab

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#### Robot Arm Calibration

- Let's train a model based on the given data.
- In this lab we're going to:
  - Predict the *current* drawn
    - Predictors, X: Robot arm's joint angles, velocity, acceleration, strain gauge readings (load measurement).



#### Thank You!

- Next Class: Generalization Error
- How do our models hold up against prediction new data?



Lab