# APS1070

Foundations of Data Analytics and Machine Learning

Winter 2022

#### **Week 12:**

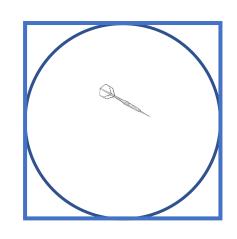
- Review Concepts
- Final Assessment Details
- Past Final Exam Questions



# **Review of Concepts**

### **Confidence Intervals**

> A numerical approach to estimate pi = 3.14159... by simulation



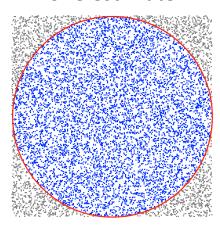
Probability = area of circle/area of square  $\frac{\pi r^2}{a^2} = \frac{\pi 1^2}{2^2} = \pi/4$  = in\_circle/num\_darts

----- Simulation Code -----

```
def throwDarts(num_darts):
    in_circle = 0
    for darts in range(num_darts):
        x = random.random()
        y = random.random()
        if (x*x + y*y) **0.5 <= 1.0:
            in_circle +=1
    return (4*in_circle/num_darts)

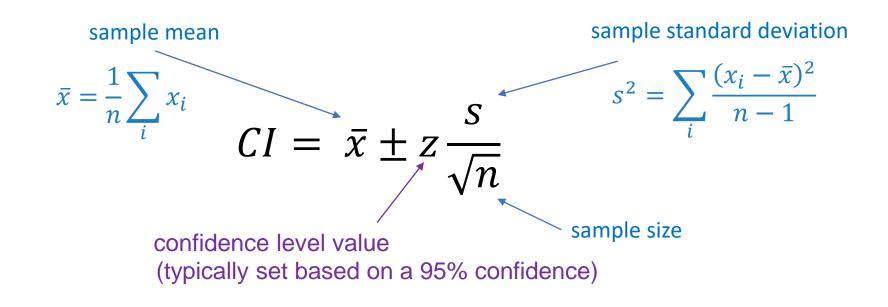
Estimate: 3.13868
Truth: 3.141592653589793</pre>
```

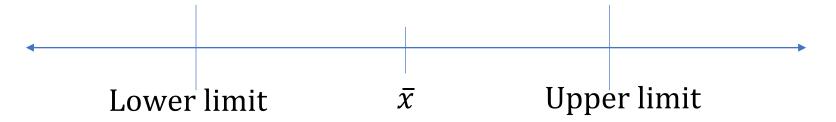
one estimate



### **Confidence Intervals**

> The equation for obtaining the confidence intervals is:

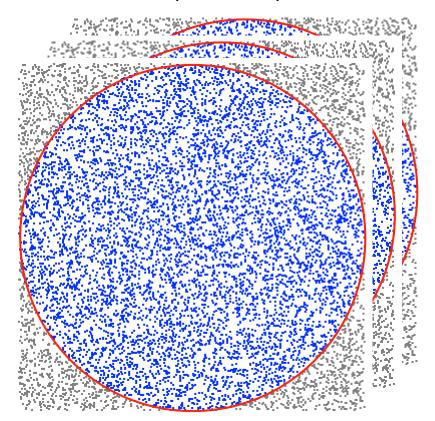




# Obtain More Samples

> Let us test this by repeating our simulation 100 times:

Repeat multiple times



#### ----- Simulation Code -----

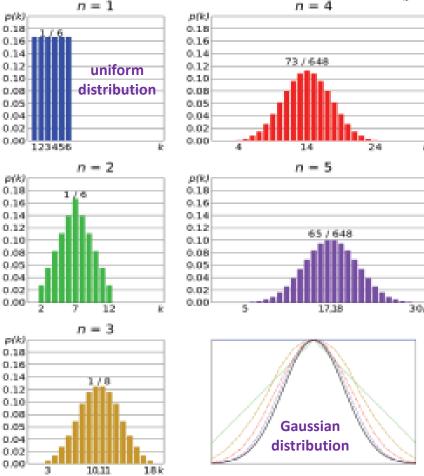
```
def getEst(num darts, num trials):
 estimates = []
  for t in range(num trials):
   guess = throwDarts(num darts)
    estimates.append(guess)
  s dev = np.std(np.array(estimates),ddof=1)
  s err = s dev/(len(estimates)**.5)
  cur est = sum(estimates)/len(estimates)
  return (s mean, s err)
```

# **Central Limit Theory**

- Q: What happens when you perform a measurement multiple times and compute the average.
- A: By the central limit theory the distribution will become Gaussian, and the mean will be close to the population (true) mean.

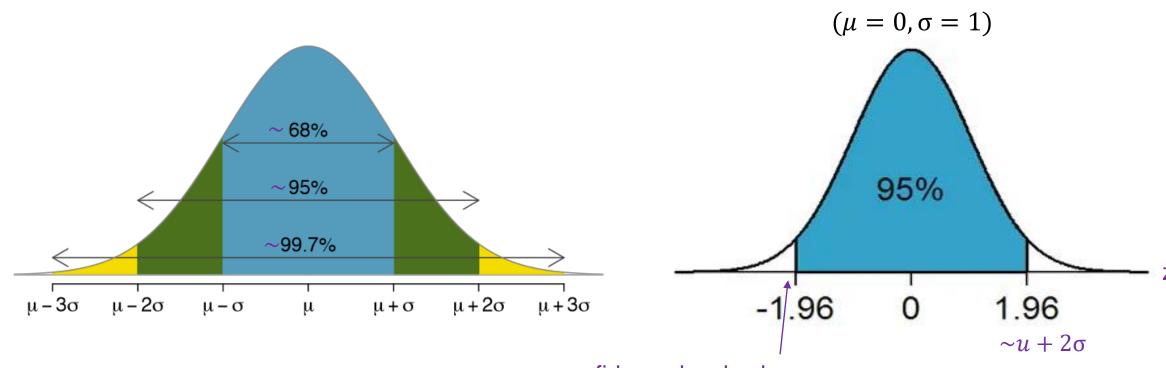
#### Example: rolling a die many times





## Gaussian Distribution

What does a 95% confidence really mean?

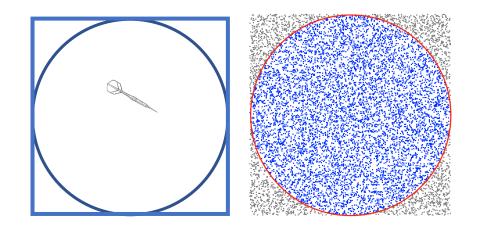


confidence level value (typically set based on a 95% confidence)

Normalized Gaussian

## **Confidence Intervals**

Calculating for our example...

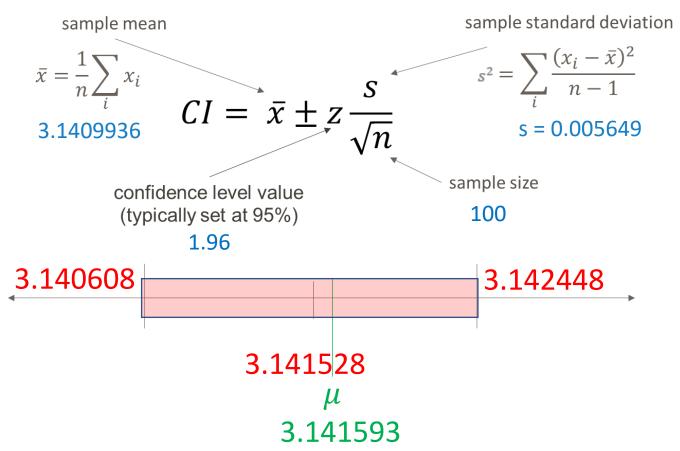


one sample mean

Sample Mean: 3.141528

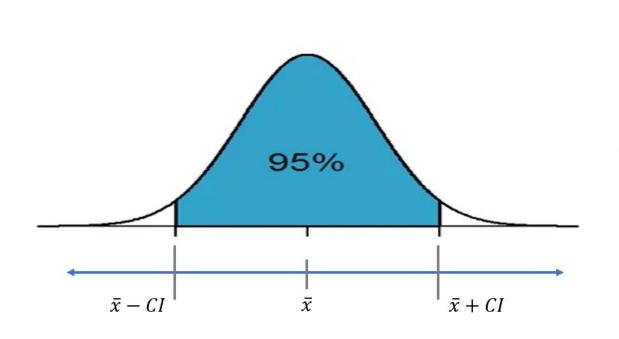
CI: 3.140608 to 3.142448

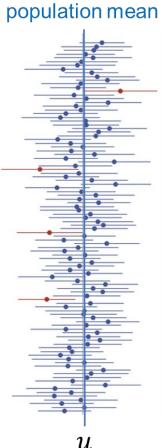
True Mean: 3.141592653589793



## **Confidence Intervals**

What does a 95% confidence really mean?



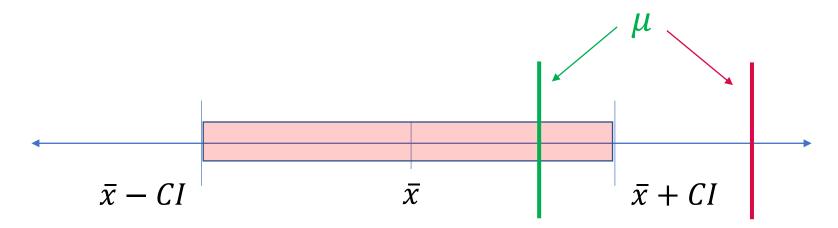


- If we were to repeat the simulation to obtain 100 sample means, then the confidence interval will contain the population mean ~95 times.
- And ~5 of the times, the interval will not contain the population mean.

Let's test it out in code!

# Hypothesis Testing

> Q: How does confidence interval relate to hypothesis testing?



A: Null hypothesis is that the sample and population mean come from the same distribution. If CI overlaps with population mean, then we do not reject the null hypothesis. Otherwise, we reject the null hypothesis.

# Hypothesis Testing

- In the example we implanted what is referred to as a z-test.
  One of the requirements of a z-test is that we know the population variance.
  - ➢ or often if we have n > 30 samples we can assume that the sample variance is close enough.
- Alternatively, we can apply a t-test which uses a slightly different distribution that works well when population variance is unknown.

# **Short Break**

## Two or More samples

➤ We can also do a hypothesis test between two or more samples. That is, we can test if samples have the same population mean (Null Hypothesis):

H<sub>0</sub>: 
$$\mu_1 = \mu_2$$
 H<sub>0</sub>:  $\mu_1 = \mu_2 \dots = \mu_m$  H<sub>a</sub>:  $\mu_1 \neq \mu_2 \dots \neq \mu_m$  two sample t-test or ANOVA

If we reject the null hypothesis then the means are different.

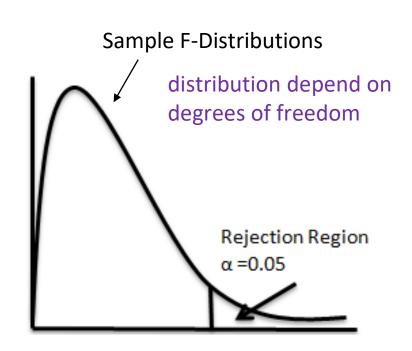
## **ANOVA**

$$H_0$$
:  $\mu_1 = \mu_2 ... = \mu_m$   
 $H_a$ :  $\mu_1 \neq \mu_2 ... \neq \mu_m$ 

### **ANOVA**

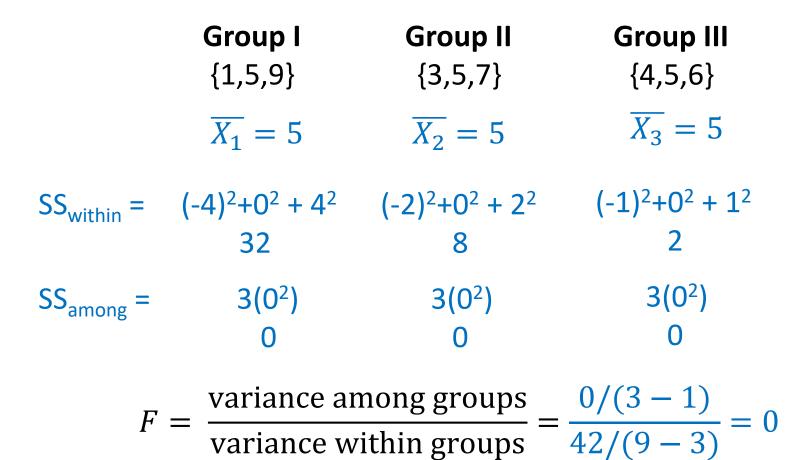
- ➤ To perform a statistical test on whether **more than two population means are equal** we can use Analysis of Variance (ANOVA).
- The approach:
  - 1. Find sum of squared differences within groups div. by dof
  - 2. Find sum of square **differences among group** div. by dof
  - 3. Ratio provides F value which is compared to the F distribution based on desired critical value or significance.

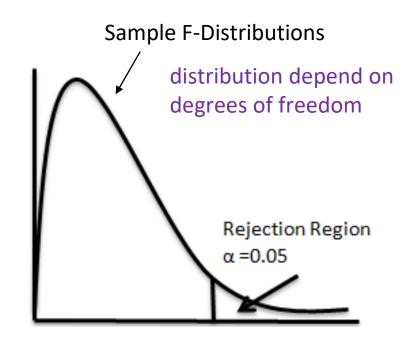
$$F = \frac{\text{variance among groups}}{\text{variance within groups}} = \frac{\text{SS}_{\text{among}}/(k-1)}{\text{SS}_{\text{within}}/(N-k)}$$



# Example 1: ANOVA

Given scores from a test for 9 students: {1,3,4,5,5,5,6,7,9}

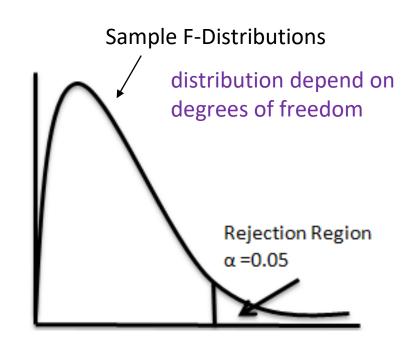




# Example 2: ANOVA

Given scores from a test for 9 students: {1,3,4,5,5,5,6,7,9}

	<b>Group A</b> {1,3,5}	<b>Group B</b> {5,7,9}	<b>Group C</b> {4,5,6}
	$\overline{X_1} = 3$	$\overline{X_2} = 7$	$\overline{X_3} = 5$
SS <sub>within</sub> =	$(-2)^2+0^2+2^2$	$(-2)^2+0^2+2^2$	$(-1)^2+0^2+1^2$
SS <sub>among</sub> =	3(3-5) <sup>2</sup> 12	3(7-5) <sup>2</sup> 12	3(5-5) <sup>2</sup> 0
$F = \frac{\text{variance among groups}}{\text{variance within groups}} = \frac{24/(3)}{18/(9)}$			$=\frac{24/(3-1)}{18/(9-3)}=4$



# Application: Feature Selection

- > ANOVA can also be used for feature selection
- ➤ F-value score -> checks that when grouping the numerical feature by target vector, the means of each group is significantly different.

# **Application: Feature Selection**

- > ANOVA can also be used for feature selection
- F-value score -> checks that when grouping the numerical feature by target vector, the means of each group is significantly different.

- Examples of ANOVA for Feature Selection in Machine Learning:
  - https://chrisalbon.com/machine learning/feature selection/anova fvalue for feature selection/
  - https://towardsdatascience.com/anova-for-feature-selection-in-machine-learning-d9305e228476

# **Programming Checklist**

- Python Basics
  - int, float, bool, operations, display,
  - ☐ lists, tuples, dictionaries, sets and mutability
  - conditionals, loops, functions, list comprehension, files
  - object-oriented programming, class, methods
- Analysis of Algorithms and Asymptotic Notation
  - array search, sorting, hashing
- Common Data Science Packages
  - ☐ Jupyter notebook
  - pandas, numpy, scipy, matplotlib, scikit-learn
- Automatic Differentiation
- Github Basics





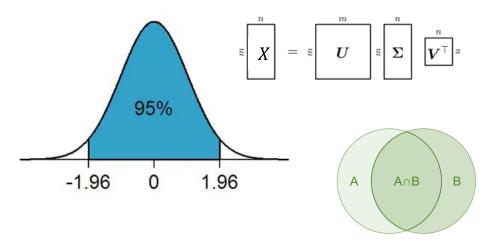




## **Mathematics Checklist**

- Discrete Math
  - □ sets, union and intersection, combinations, permutations
- Probability Theory
  - summary statistics, expectation, covariance,
  - multivariate gaussians and basic distributions
  - confidence intervals, hypothesis testing, ANOVA
- Linear Algebra
  - change of variables, projections, data augmentation
  - determinant, eigenvalue decomposition, trace, rank
  - ☐ matrix inverse, PCA, SVD and dimensionality reduction
- Vector Calculus
  - Jacobians/gradients, matrix derivatives

$$B = \begin{bmatrix} -7 & -7 & 6 \\ 2 & 1 & -1 \\ 4 & 5 & -4 \end{bmatrix}$$

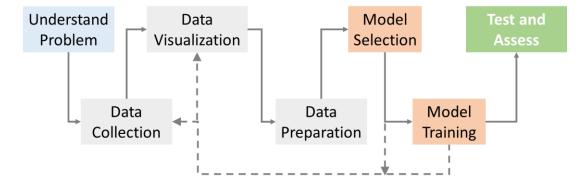


$$F_X(x) = \int_{-\infty}^x f_X(t) \, dt.$$

# Machine Learning and Analytics Checklist

- Instance Based Learning
  - ☐ KNN, decision trees, clustering strategies
- Model Based Learning
  - linear/logistic regression, MLE approach
  - feature mapping and polynomial regression
  - mixture of Gaussians for anomaly detection
  - deep learning overview and PyTorch
- Machine Learning Taxonomy
  - parametric/nonparametric,
  - classification/ regression,
  - supervised/unsupervised,
  - Model- and instance-based learning

- Discrete and Continuous Optimization
  - gradient descent, regularization and convexity
  - greedy algorithms and set cover
- Performance Metrics
  - generalization, overfitting, bias/variance
  - precision and recall, Confusion Matrix, ROC
  - cross-validation



## Final Assessment Details

### Final Assessment Details

#### When

- Crowdmark Opens: April 12 at 9am (Toronto Time)
- ➤ Crowdmark Closes: April 13 at 3pm (Toronto Time)— latest time to start is April 13 at 11:30am Late submission: A grade of zero for the final assessment (as per syllabus)
- Crowdmark invites will be sent by email.
- Submit answer to each question separately with legible handwriting.

#### Duration

- > Limited window to start the exam and submit it (a countdown starts as soon as you access the assessment)
- ➤ 2.5 hour for the exam + 30 minutes for taking pictures and uploading on crowdmark + 30 minutes for all contingencies = 3.5-hour in total

### Final Assessment Details

- Material in the final exam:
  - > Weeks 1 to 12 of lectures
  - > Use course material + online resources with citation NO HELP FROM OTHERS!!
- Sign Honour Code
  - > All work must be your own; all work must be completed without consulting with anyone else.
  - > Students suspected of plagiarism on a project, midterm or final assessment will be referred to the department for formal discipline for breaches of the Student Code of Conduct.
- Piazza will not be accessible during the exam.
- If needed, make assumptions and answer the questions. No need to contact us.
- In case of a logistic problem, you should email Samin + Sinisa + Ali immediately. There is no guarantee that we can respond to you before your time runs out.

# Final Assessment Topics

- Analytical concepts in learning
- Comparison of ML models
- Dimensionality reduction methods
- Matrix operations and transformations
- Eigenvectors and eigenvalues
- Gaussian Elimination
- Solving systems of linear equations
- Linear and non-linear regression
- Decision trees
- Artificial neural networks
- Backpropagation
- Vector calculus
- Analytical geometry

- ➤ Model-based learning
- ➤ Gradient descent
- ➤ Polynomial regression
- ➤ Regularization
- Numerical optimization
- Logistic regression
- ➤ Binary classification
- ➤ Abstract data types
- Performance measures
- **≻**Confusion matrix
- Receiver Operating Characteristic
- Design and implementation of ML models

### Final Assessment Format

- Multiple Choice and True /False
- Short Answer
- Calculations
- Descriptive and Analytical Answer
- Coding
  - > You may be asked to interpret and explain concepts and models similar to what you would have seen in lectures.
  - ➤ Google Colab is available to you should you find it useful, but it does not count as showing your working.

# Questions?

**≻**Piazza

# Sample Questions

#### Part I: Multiple Choice (Select only 1 answer per question)

- 1. Which of the following statements is true? [2]
  - a) In k-fold cross-validation, training data is divided into k folds, then the model is trained on k folds and validated on 1 fold, for a total of k-1 times (splits).
  - b) In *k*-fold cross-validation, training data is divided into *k folds*, then the model is trained on *k* folds and validated on 1 fold, for a total of *k* times (splits).
    - In k-fold cross-validation, training data is divided into k folds, then the model is trained on k-1 folds and validated on 1 fold, for a total of k times (splits).
  - d) In k-fold cross-validation, training data is divided into k folds, then the model is trained on k-1 folds and validated on 1 fold, for a total of k-1 times (splits).

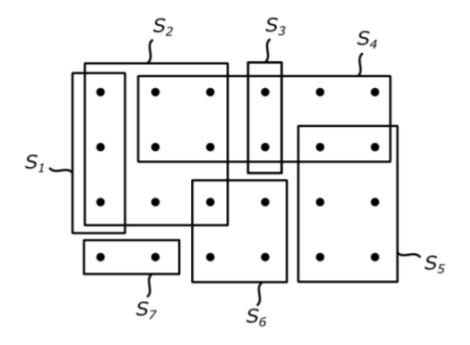
- 2. When performing PCA, the goal is to accomplish which of the following? [2]
  - Maximize the variance of the primary components and maximize the residuals.
  - Minimize the variance of the primary components and minimize the residuals.
  - c) Maximize the variance of the primary components and minimize the residuals.
    - d) Minimize the variance of the primary components and maximize the residuals.

3. The schematic to the right has sets  $S_1$ ,  $S_2$ ,  $S_3$ ,  $S_4$ ,  $S_5$ ,  $S_6$  and  $S_7$ . What sets, and in what order, would a greedy algorithm select to cover the universe (i.e., cover each point) if all sets are weighted equally? [2]

#### <u>Answer</u>

In order of selection: S4, S2, S5, S6, S7

We exclude S1, S3



4. Is the matrix 
$$A = \begin{pmatrix} 1 & 2 & -1 \\ 1 & 0 & 3 \\ -2 & -4 & 2 \end{pmatrix}$$
 invertible? [2]

#### **Answer**

For n = 3 (known as Sarrus' rule),

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11}a_{22}a_{33} + a_{21}a_{32}a_{13} + a_{31}a_{12}a_{23}$$
$$- a_{31}a_{22}a_{13} - a_{11}a_{32}a_{23} - a_{21}a_{12}a_{33} .$$

5. Given that 
$$\binom{n}{r} = \frac{n!}{r!(n-r)!}$$
, prove that  $\binom{n}{r} = \binom{n}{n-r}$ . [2]

#### <u>Answer</u>

$$= \frac{n!}{(\boldsymbol{n} - \boldsymbol{r})! (\boldsymbol{n} - (\boldsymbol{n} - \boldsymbol{r})!}$$
$$= \frac{n!}{(\boldsymbol{n} - \boldsymbol{r})! r!}$$

6. We have  $x = [1,1,2]^T \in \mathbb{R}^3$  and  $y = [1,0,3]^T \in \mathbb{R}^3$ . What is the angle between vectors? [2]

#### <u>Answer</u>

$$\cos(w) = \frac{x^T y}{\sqrt{x^T x y^T y}} = \frac{7}{\sqrt{6*10}} \rightarrow w = 25.4 \ degrees$$

7. Calculate the Jacobian  $J_F(x_1, x_2, x_3)$  of the function  $F: \mathbb{R}^3 \to \mathbb{R}^4$ , which has components: [2]

$$y_1 = x_1 + 2x_3^2$$
;  $y_2 = x_1 \sin x_2$ ;  $y_3 = x_2 \exp(x_3)$ ;  $y_4 = x_1 + x_2$ 

#### **Answer**

$$\begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \frac{\partial y_1}{\partial x_3} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \frac{\partial y_2}{\partial x_3} \\ \frac{\partial y_3}{\partial x_1} & \frac{\partial y_3}{\partial x_2} & \frac{\partial y_3}{\partial x_3} \\ \frac{\partial y_4}{\partial x_1} & \frac{\partial y_4}{\partial x_2} & \frac{\partial y_4}{\partial x_3} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 4x_3 \\ \sin(x_2) & x_1 \cos(x_2) & 0 \\ 0 & \exp(x_3) & x_2 \exp(x_3) \\ 1 & 1 & 0 \end{bmatrix}$$

8. Consider functions  $f: \mathbb{R}^3 \to \mathbb{R}^1$  and  $x: \mathbb{R}^1 \to \mathbb{R}^3$ , where:

$$f(\mathbf{x}) = x_1 + 2x_2^2 + x_3 ; \mathbf{x}(t) = \begin{bmatrix} t \\ 3t \\ \exp(t) \end{bmatrix}$$

Calculate the gradient  $\frac{df}{dt}$  using the chain rule. [2]

<u>Answer</u>

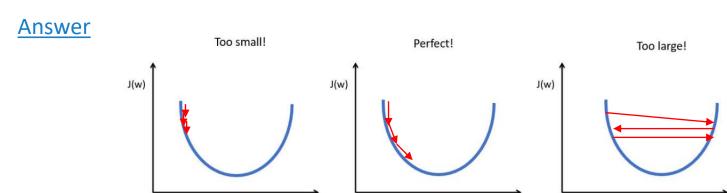
$$\begin{bmatrix} \frac{df}{dx_1} & \frac{df}{dx_2} & \frac{df}{dx_3} \end{bmatrix} \begin{bmatrix} \frac{dx_1}{dt} \\ \frac{dx_2}{dt} \\ \frac{dt}{dt} \end{bmatrix} = \begin{bmatrix} 1 & 12t & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 3 & \exp(t) \end{bmatrix} = 1 + 36t + \exp(t)$$

In general, is using a gradient descent algorithm a good choice for finding optimal hyperparameters? Why or why not? [2]

#### **Answer**

No. Gradient descent requires a smooth function to optimize, and ideally a convex function in order to find the global minimum. This is usually not the case for hyperparameters.

10. What is a learning rate? Explain what happens if it is set too high or too low (you may use a schematic/drawing if helpful). [2]



Learning rate is the step size taken in the opposite direction of the gradient.

11. You have the following code:

How efficient is this code in terms of big O notation (what is the order of the algorithm's runtime)? [hint:  $\sum_{k=1}^{n} k^3 = \frac{n^2(n+1)^2}{4}$ ] [2]

#### **Answer**

The loop is performed 1, 8, 27, ..., 
$$n^3$$
 times,  $\sum_{k=1}^n k^3 = \frac{n^2(n+1)^2}{4} = \frac{n^2(n^2+2n+1)}{4} = \frac{n^4+2n^3+n^2}{4} \to O(n^4)$ 

12. The input parameter *x* of "my\_function" is training data with features as columns and examples as rows.

a) What is the purpose of this function, specifically? [2]

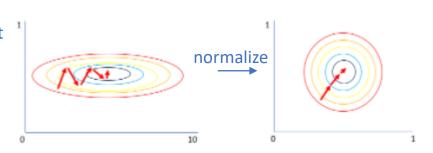
def my\_function(x):
 return (x - x.mean()) / x.std

 b) Describe why this type of process is important to gradient descent and K-Nearest Neighbor algorithms. [2]

#### **Answer**

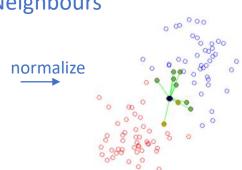
- a. Normalize each dimension by zero mean and unit variance.
- b. Gradient descent

gradient does not point towards minimum, hence takes longer to converge



K-Nearest Neighbours

All nearest neighbours align in direction of the axis with the smaller range.



- 13. Consider a differentiable loss function l(w, x, y) and a dataset D. You're asked to optimize the average loss  $\frac{1}{N}\sum_{i=1}^{N}l(w, x^{(i)}, y^{(i)})$  with respect to w. Write pseudocode implementing mini-batch gradient descent optimization using a decaying learning rate (i.e., a learning rate that is reduced by  $\alpha_D$  every epoch), with the following inputs: **[4]** 
  - Differentiable loss l(w, x, y) with gradient  $\nabla_w l(w, x, y)$ .
  - Dataset  $D = (x^{(1)}, y^{(1)}), ... (x^{(N)}, y^{(N)}).$
  - Mini-batch size m, initial weights  $w_0$  and number of steps T.
  - Initial learning rate  $\alpha_0$  and learning rate decay  $\alpha_D$ .

Note that your pseudo-code is just a representation of your algorithm written in plain English. Keep your pseudo-code simple and concise. Please use indentation and control structures. State any assumptions you make.

#### **Answer**

```
Initial weight w = w_0
Initial alpha = a_0
For each EPOCH
        shuffle the training data
        For each Iteration (T)
                pick a mini batch
                compute the gradients: delta (w,x,y)
                update the weights: w = w - alpha * delta
       Update the LR: alpha = alpha * a_d
```

## **Short Break**

#### 2. [2] We have that

$$f(\mathbf{x}) = f(x_1, x_2, x_3) = ln(x_1 x_2) - \frac{x_3}{2}$$

$$\mathbf{x}(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \end{bmatrix} = \begin{bmatrix} e^t \\ -\cos(t) \\ 2t \end{bmatrix}$$

Calculate the gradient  $\frac{df}{dt}$ . Show all your calculations.

#### **Answer**

Given that 
$$ln(x_1x_2) = ln(x_1) + ln(x_2)$$

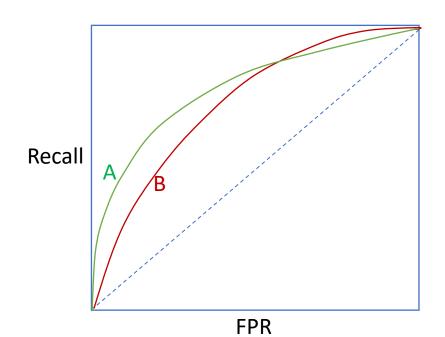
$$\frac{df}{dt} = \frac{df}{dx}\frac{dx}{dt} = \begin{bmatrix} \frac{df}{dx_1} & \frac{df}{dx_2} & \frac{df}{dx_3} \end{bmatrix} \begin{bmatrix} \frac{dx_1}{dt} \\ \frac{dx_2}{dt} \\ \frac{dt}{dt} \end{bmatrix}$$

$$= \left[\frac{1}{x_1} \quad \frac{1}{x_2} \quad -\frac{1}{2}\right] \begin{bmatrix} e^t \\ \sin(t) \\ 2 \end{bmatrix}$$

$$= \left[\frac{1}{e^t} \quad -\frac{1}{\cos(t)} \quad -\frac{1}{2}\right] \begin{bmatrix} e^t \\ \sin(t) \\ 2 \end{bmatrix} = 1 - \tan(t) - 1$$

$$= -\tan(t)$$

3. [3] Binary classification Model A achieves a top F1 score of F1<sub>A</sub> and an area under the ROC curve (AUC) of AUC<sub>A</sub>, whereas binary classification Model B achieves a top F1 score of F1<sub>B</sub> and an AUC of AUC<sub>B</sub>, on the same dataset. If AUC<sub>A</sub> > AUC<sub>B</sub>., is it implied that F1<sub>A</sub> > F1<sub>B</sub>? Why?

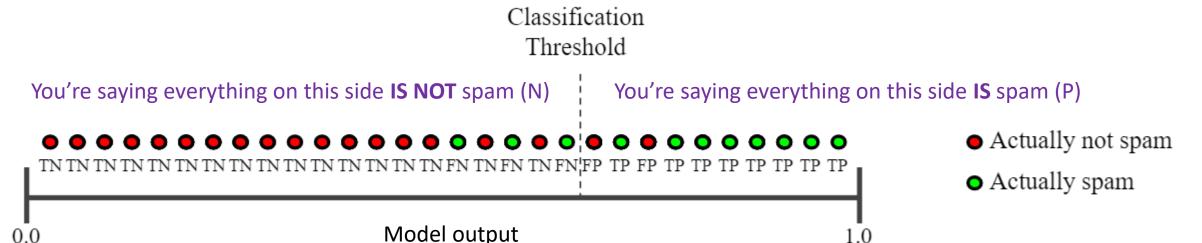


#### <u>Answer</u>

No, F1<sub>A</sub> > F1<sub>B</sub> is not implied. AUC is the area under the ROC curve, which plots TPR ( $TPR = \frac{TP}{TP+FN}$ ) vs FPR ( $FPR = \frac{FP}{FP+TN}$ ). F1 score is  $(\frac{2TP}{2TP+FP+FN})$  calculated at a single threshold. **Top F1 score is sensitive** to the "best" threshold, whereas AUC is an aggregate measure across all possible thresholds .

# A model has multiple F1's depending on the threshold

- Application spam detection
- Improving precision usually reduces recall, vice-versa



**Precision** 
$$tp/(tp+fp) = 8/(8+2) = 0.8$$

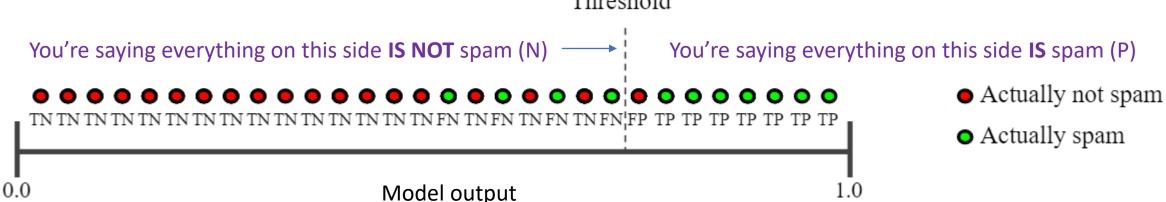
**Recall** 
$$tp/(tp+fn) = 8/(8+3) = 0.73$$

Source: ML Crash Course

# A model has multiple F1's depending on the threshold

- Application spam detection
- Improving precision usually reduces recall, vice-versa

Classification Threshold



**Precision** = 
$$7/(7+1) = 0.88$$

$$Recall = 7/(7+4) = 0.64$$

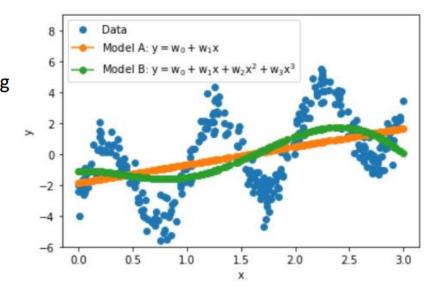
Source: ML Crash Course

- 4. [3] StandardScaler (in sklearn) is often used in linear regression models.
  - a. What does StandardScaler do?
  - b. Is it best practice to apply StandardScaler before or after splitting data into training and testing groups? Why?
  - c. Typically, is it useful to apply StandardScaler on targets, feature data, or both?

#### <u>Answer</u>

- a. StandardScaler scales features to 0 mean and unit variance.
- b. It's best to apply StandardScaler after splitting data, since you want to keep test data completely separate. If you scale before splitting, you're incorporating knowledge of test data properties into your model.
- c. StandardScaler is typically applied only on features (so any one feature does not dominate the others). There's usually no benefit to applying it on targets.

- 5. [3] Sam applies linear regression to data that has a single feature, x. A first model, Model A, makes predictions y using only a bias  $(w_0)$  and a weighted feature  $(w_1x)$ , i.e.  $y=w_0+w_1x$ . Unsatisfied, Sam then creates new features that are the x feature squared and cubed, yielding the model  $y=w_0+w_1x+w_2x_2^2+w_3x_3^2$  (Model B), which still isn't a great fit.
  - a. What minimum degree polynomial is needed to fit the data reasonably well? Why? [hint: count turning points (extremums) of polynomial]
  - b. Can you conceive of an alternate feature mapping scheme, where a single additional feature is added to Model A, that would fit the data well? Explain your reasoning.



#### **Answer**

- a. You'll need a polynomial of at least degree 7 to fit the data well there's an explanation  $\underline{\text{here}}$  1 more degree than the number of bumps.
- b. The idea here is to add a sinusoidal feature to Model A. The general equation for a sine function is:

$$y = a * sin(b * x)$$

Here the period is clearly 1, so  $1 = \frac{2\pi}{b}$  and  $b = 2\pi$ 

We could thus add a feature  $sin(2\pi x)$ , and expect a good fit.

- 6. [3] This term, several approaches to combat overfitting were discussed.
  - a. What is overfitting, and how do we know if a model is overfitted?
  - b. Describe two methods that are used to prevent overfitting. To what models do these methods apply? (ie are they general, or specific to certain types of models?)
  - c. What are the major advantages and disadvantages of these methods?

#### <u>Answer</u>

- a. Model has fit the subtleties in the training data that does not generalize to the test data. The model has low training error, but on a validation set, its error is high.
- b. Cross-validation and regularization are the most obvious methods here, but you could also discuss the removal of features, adding more data, etc. These generalize to all models.
- c. Cross-validation: allows you to use your data more effectively, but at the price of increased computation Regularization: limits the flexibility of the parameters which can be good and bad. Good in that it will limit the model's propensity to overfit, but bad in that sometimes it may be too restrictive.

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