18-661: Introduction to ML for Engineers

MLE/MAP and Linear Algebra Review

Spring 2025

ECE – Carnegie Mellon University

Announcements

- No class on Monday Jan 20th, MLK day
- Self-assessment math quiz available on Gradescope until Friday. Recitations on Friday will go over the math quiz questions and solutions.
- Math review resources posted on Piazza
- HW1 will be released later this week

Registration

- If you're not registered, we encourage you to stay patient (waitlists are gradually clearing).
- You are welcome to keep attending the lectures until the waitlists are sorted out

Direct all waitlist-related questions to:
ece-waitlists@andrew.cmu.edu

Outline

1. Recap: Probability Review
2. A Simple Learning Problem: MLE/MAP Estimation
3. Linear Algebra Review

Recap: Probability Review

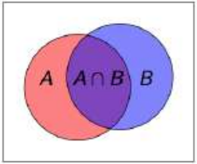
Probability Terminology

Name	Type	Symbol	Meaning
Sample Space	set	Ω, S	possible outcomes
Event Space	a set of subsets (of Ω)	$\mathcal{F}$, E	the events that have probabilities
Probability Measure	measure	P, π	assigns probabilities to events
Probability Space	a triple	$(\Omega, \mathcal{F}, P)$	

- Rolling a fair die
  - Ω: $\{1, 2, 3, 4, 5, 6\}$
  - $\mathcal{F} = \{\{1\}, \{2\}, \ldots, \{1, 2\}, \ldots, \{1, 2, 3\}, \ldots, \{1, 2, 3, 4, 5, 6\}, \{\}\}$
  - $P(\text{rolling an odd number}) = P(\{1, 3, 5\}) = \frac{1}{2}$
- Tossing a fair coin twice
  - Ω: $\{HH, HT, TH, TT\}$
  - $\mathcal{F} = \{\{HH\}, \{HT\}, \ldots, \{HH, HT\}, \ldots, \{HH, HT, TH, TT\}, \{\}\}$
  - $P(\text{first flip is heads}) = P(\{HH, HT\}) = \frac{1}{2}$

Axioms of Probability

The probability measure satisfies the following properties:



- $0 \leq P(A) \leq 1$
- $P(\Omega) = 1, \; P(\varnothing) = 0$
- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$

Consider two events $A, B \in \mathcal{F}$.

- The conditional probability of A given B is given by: $P(A \mid B) = \frac{P(A \cap B)}{P(B)}$.
- Bayes rule: $P(A \mid B) = \frac{P(B|A)P(A)}{P(B)}$, which can be derived from

$$P(B \mid A)P(A) = P(A \cap B) = P(A \mid B)P(B)$$

Random Variables

Formally, a random variable is a function $X : \Omega \to \mathbb{R}$ that assigns a numerical value to each outcome s within a probability space $(\Omega, \mathcal{F}, P)$.

Example: Rolling a fair die

- Ω: $\{1, 2, 3, 4, 5, 6\}$
- $\mathcal{F} = \{\{1\}, \{2\}, \ldots, \{1, 2\}, \ldots, \{1, 2, 3\}, \ldots, \{1, 2, 3, 4, 5, 6\}, \{\}\}$
- $X(S) = S$ for each $S \in \Omega$

The expectation of a random variable, $\mathbb{E}[X]$, is defined as $\sum_{s \in \Omega} X(s)P(s)$, i.e., the average value of X.

- $\mathbb{E}[X] = \sum_{s=1}^{6} sP(s) = \frac{1+2+3+4+5+6}{6} = \frac{7}{2}$

The variance of a random variable is $\mathrm{Var}(X) = \mathbb{E}\left[(X - \mathbb{E}[X])^2\right]$, which measures how much X can vary from its expected value $\mathbb{E}[X]$.

- $\mathrm{Var}[X] = \sum_{s=1}^{6} \frac{1}{6}(s - \frac{7}{2})^2 = \frac{35}{12}$

Some Other Concepts that You Should Know

- Discrete and continuous random variables
- PMF (probability mass function), PDF (probability density function), CDF (cumulative distribution function) of random variables
- Entropy of a random variable

Some of these will be covered in HW1

A Simple Learning Problem: MLE/MAP Estimation

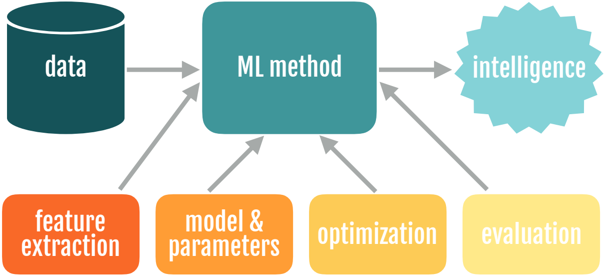
Dogecoin

- Scenario: You find a coin on the ground.

- *You ask yourself: Is this a fair or biased coin? What is the probability that I will flip a heads?*

- You flip the coin 10 times ...
- It comes up as 'H' 8 times and 'T' 2 times
- Can we learn the bias of the coin from this data?

Recall: Machine Learning Pipeline



Two methods that we will discuss today:

- Maximum likelihood Estimation (MLE)
- Maximum a posteriori Estimation (MAP)

Maximum Likelihood Estimation (MLE)

- **Data**: Observed sequence D of n_H heads and n_T tails
- **Model**: Each flip follows a Bernoulli distribution

$$P(H) = \theta,\ P(T) = 1 - \theta,\ \theta \in [0, 1]$$

Thus, the likelihood of observing sequence D is

$$P(D \mid \theta) = \theta^{n_H}(1-\theta)^{n_T}$$

- Question: Given this model and the data we've observed, can we calculate an estimate of θ?
- **MLE**: Choose θ that maximizes the *likelihood* of the observed data

$$\hat{\theta}_{MLE} = \arg\max_{\theta} P(D \mid \theta)$$

How to Solve?

- $\log(x)$ is a monotone increasing function; will not affect the arg max

$$\begin{aligned}
\hat{\theta}_{MLE} &= \arg\max_{\theta} P(D \mid \theta) \\
&= \arg\max_{\theta} \log P(D \mid \theta) \\
&= \arg\max_{\theta} \log\left(\theta^{n_H}(1-\theta)^{n_T}\right) \\
&= \arg\max_{\theta} \underbrace{n_H \log(\theta) + n_T log(1-\theta)}_{\text{concave}}
\end{aligned}$$

- Take derivative $\frac{\partial}{\partial\theta} \log P(D \mid \theta)$ and set equal to zero

$$\begin{aligned}
0 &= \frac{\partial}{\partial\theta}\left(n_H \log(\theta) + n_T log(1-\theta)\right) \\
&= \frac{n_H}{\theta} - \frac{n_T}{1-\theta} \\
\implies \hat{\theta}_{MLE} &= \frac{n_H}{n_H + n_T}
\end{aligned}$$

Going Back to Our Scenario

- You flip the coin 10 times . . .
- It comes up as 'H' 8 times and 'T' 2 times

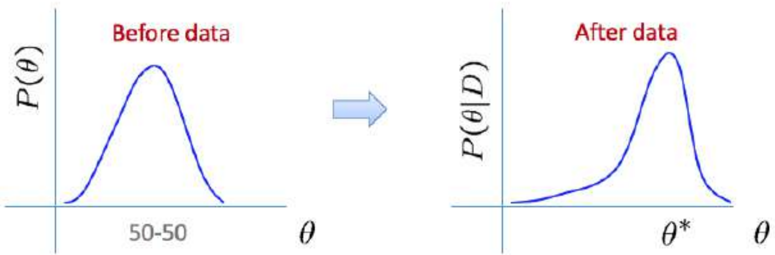
- Can we learn the bias θ of the coin from this data?

$$\hat{\theta}_{MLE} = \frac{n_H}{n_H + n_T} = 0.8$$

Here, we are trusting the data completely. But there could be too little data or noisy data

What about Prior Knowledge?

- We believe the coin is *supposed* to be close to 50-50
- Rather than completely “trusting” the data as-is, we want to use the data to update our prior beliefs



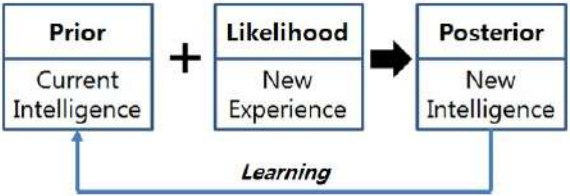
Bayesian Learning

- How to incorporate prior knowledge?
- Use Bayes' Rule:

$$P(\theta \mid D) = \frac{P(D \mid \theta)P(\theta)}{P(D)}$$

- Or, equivalently:

$$\underbrace{P(\theta \mid D)}_{\text{posterior}} \propto \underbrace{P(D \mid \theta)}_{\text{likelihood}} \underbrace{P(\theta)}_{\text{prior}}$$



MAP for Dogecoin

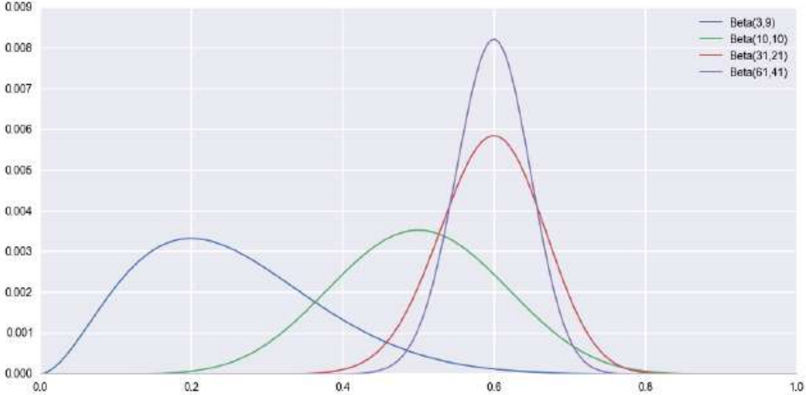
$$\hat{\theta}_{MAP} = \arg\max_{\theta} P(D \mid \theta) P(\theta)$$

- Recall that $P(D \mid \theta) = \theta^{n_H}(1-\theta)^{n_T}$
- How should we set the prior, $P(\theta)$?
- Common choice is to use the Beta distribution, $\theta \sim Beta(\alpha, \beta)$:

$$P(\theta) = \frac{1}{B(\alpha, \beta)} \theta^{\alpha-1}(1-\theta)^{\beta-1}, \text{where } B(\alpha, \beta) = \int_0^1 \theta^{\alpha-1}(1-\theta)^{\beta-1} d\theta$$

- Interpretation: $\alpha =$ number of expected heads, $\beta =$ number of expected tails. Larger value of $\alpha + \beta$ denotes more confidence (and smaller variance).

Beta Distribution



$\frac{\alpha}{\beta}$ controls left/right bias, $\alpha + \beta$ controls height of peak

MAP for Dogecoin

- A benefit of using the *Beta* distribution as a prior is that the posterior will also be a *Beta* distribution:

$$\begin{aligned}\hat{\theta}_{MAP} &= \arg\max_{\theta} P(D \mid \theta)P(\theta) \\ &= \arg\max_{\theta} \theta^{\alpha+n_H-1}(1-\theta)^{\beta+n_T-1} \\ &= \frac{\alpha+n_H-1}{\alpha+\beta+n_H+n_T-2}\end{aligned}$$

- Note that as $n_H + n_T \to \infty$, the effect of the prior disappears and we recover the MLE estimate

Putting It All Together

$$\hat{\theta}_{MLE} = \frac{n_H}{n_H + n_T}$$

$$\hat{\theta}_{MAP} = \frac{\alpha + n_H - 1}{\alpha + \beta + n_H + n_T - 2}$$

- Suppose $\theta^* := 0.5$ and we observe: $D = \{H, H, T, T, T, T\}$
- Scenario 1: We assume $\theta \sim Beta(4, 4)$. Which is more accurate – θ_{MLE} or θ_{MAP}?
  - $\theta_{MAP} = 5/12$, $\theta_{MLE} = 1/3$
- Scenario 2: We assume $\theta \sim Beta(1, 7)$. Which is more accurate – θ_{MLE} or θ_{MAP}?
  - $\theta_{MAP} = 1/6$, $\theta_{MLE} = 1/3$

Why Was This a ML Problem?

Machine learning is: the study of methods that

improve their performance (the accuracy of the predicted probability)

on some task (predicting the probability of 'heads')

with experience (the more coin flips we see, the better our guess)

Learning Involves ...

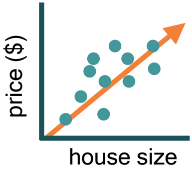
- Collect some data
  - e.g., coin flips
- Set up the problem: Choose a model / loss function
  - e.g., Bernoulli model, data likelihood, prior distribution
- Solve the problem: Choose an optimization procedure
  - e.g., set derivative of log to zero and solve to find MLE/MAP

Key idea: these are *choices*. It's important to understand the implications of these choices and evaluate their trade-offs for the problem at hand.

Linear Algebra Review

Recall: Task 1: Regression

How much should you sell your house for?



input: houses & features **learn**: $x \to y$ relationship **predict**: y (*continuous*)

Data Can be Compactly Represented by Matrices

- Learn parameters (w_1, w_0) of the orange line $y = w_1 x + w_0$

Sq.ft

$$\text{House 1: } 1000 \times w_1 + w_0 = 200,000$$

$$\text{House 2: } 2000 \times w_1 + w_0 = 350,000$$

- Rewriting in vector form:

$$\begin{bmatrix} 1000 \\ 2000 \end{bmatrix} w_1 + \begin{bmatrix} 1 \\ 1 \end{bmatrix} w_0 = \begin{bmatrix} 200,000 \\ 350,000 \end{bmatrix}$$

- Can represent compactly in matrix notation

$$\begin{bmatrix} 1000 & 1 \\ 2000 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_0 \end{bmatrix} = \begin{bmatrix} 200,000 \\ 350,000 \end{bmatrix}$$

Some Concepts That You Should Know

- Determinants and Matrix Invertibility
- Vector Norms – L1, L2; Inner Products
- Eigenvalues and Eigenvectors
- Singular Value Decomposition
- Covariance Matrices and Positive Semi-definite-ness

Excellent Resources:

- Essence of Linear Algebra YouTube Series by 3Blue1Brown
- Prof. Gilbert Strang's course at MIT
- Matrix Cookbook (link posted on the course website)

Matrix Multiplication

- For two matrices $A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{n \times p}$, their product is:

$$AB = C \in R^{m \times p} \iff C_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj}$$

- Multiplication is undefined with the number of columns in $A \neq$ the number of rows in B (except in case: cA where $c \in \mathbb{R}$ is a scalar)
- Special cases:
  - Inner product: $x, y \in \mathbb{R}^n, \quad x^\top y \in \mathbb{R} = \sum_{i=1}^{n} x_i y_i$
  - Matrix-vector product: $A \in \mathbb{R}^{m \times n}, x \in \mathbb{R}^n \iff Ax \in \mathbb{R}^m$

$$A = \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \dots & a_n \\ | & | & & | \end{bmatrix}, \; Ax \in \mathbb{R}^m = \sum_{i=1}^{n} a_i x_i$$

Important Properties

- Associative: $A(BC) = (AB)C$
- Distributive: $A(B + C) = AB + AC$
- *Not* Commutative: $AB \neq BA$ (except in special cases)
- Transpose: $(AB)^\top = B^\top A^\top$

Matrix Inverse

- The inverse of a matrix $A \in \mathbb{R}^{n\times n}$ is a matrix $A^{-1} \in \mathbb{R}^{n\times n}$ such that:

$$AA^{-1} = A^{-1}A = I_n$$

- If A^{-1} exists, then A is called invertible or non-singular
- Matrix A is invertible iff $\det(A) \neq 0$.
- If A^{-1} exists, then it is unique.
- Let us solve the house-price prediction problem

$$\begin{bmatrix} 1000 & 1 \\ 2000 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_0 \end{bmatrix} = \begin{bmatrix} 200,000 \\ 350,000 \end{bmatrix}$$

Matrix Inverse

- Let us solve the house-price prediction problem

$$\begin{bmatrix} 1000 & 1 \\ 2000 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_0 \end{bmatrix} = \begin{bmatrix} 200,000 \\ 350,000 \end{bmatrix} \tag{1}$$

$$\begin{bmatrix} w_1 \\ w_0 \end{bmatrix} = \left(\begin{bmatrix} 1000 & 1 \\ 2000 & 1 \end{bmatrix} \right)^{-1} \begin{bmatrix} 200,000 \\ 350,000 \end{bmatrix} \tag{2}$$

$$= \frac{1}{-1000} \begin{bmatrix} 1 & -1 \\ -2000 & 1000 \end{bmatrix} \begin{bmatrix} 200,000 \\ 350,000 \end{bmatrix} \tag{3}$$

$$= \frac{1}{-1000} \begin{bmatrix} -150,000 \\ -5 \times 10^7 \end{bmatrix} \tag{4}$$

$$\begin{bmatrix} w_1 \\ w_0 \end{bmatrix} = \begin{bmatrix} 150 \\ 50,000 \end{bmatrix} \tag{5}$$

Norms and Loss Functions

- You could have data from many houses

$$\underbrace{\begin{bmatrix}1000 & 1\\ 2000 & 1\\ 1500 & 1\\ \vdots & \vdots\\ 2500 & 1\end{bmatrix}}_{A} \times \underbrace{\begin{bmatrix}w_1\\ w_0\end{bmatrix}}_{w} = \underbrace{\begin{bmatrix}200,000\\ 350,000\\ 300,000\\ \vdots\\ 450,000\end{bmatrix}}_{y}$$

- There isn't a $w = [w_1, w_0]^T$ that will satisfy all equations
- Want to find w that minimizes the difference between Aw, y
- But since this a vector, we need an operator that can map the vector $y - Aw$ to a scalar

Norms and Loss Functions

- A vector norm is any function $f : \mathbb{R}^n \to \mathbb{R}$ with
  - $f(x) \geq 0$ and $f(x) = 0 \iff x = 0$
  - $f(ax) = |a| f(x)$ for $a \in \mathbb{R}$
  - $f(x + y) \leq f(x) + f(y)$
- e.g., ℓ_2 norm: $\|x\|_2 = \sqrt{x^\top x} = \sqrt{\sum_{i=1}^n x_i^2}$
- e.g., ℓ_1 norm: $\|x\|_1 = \sum_{i=1}^n |x_i|$
- Question: What is the ℓ_1 norm of $y - Aw$ for the following problem?

$$\underbrace{\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 1.5 & 1 \\ 2.5 & 1 \end{bmatrix}}_{A} \times \underbrace{\begin{bmatrix} 1.5 \\ 0.5 \end{bmatrix}}_{w} = \underbrace{\begin{bmatrix} 2 \\ 3.5 \\ 3 \\ 4.5 \end{bmatrix}}_{y}$$

- Answer: $\|y - Aw\|_1 = 0.5$

Eigenvalues and Eigenvectors: Matrix as Linear Transformation (see 3Blue1Brown)

- How exactly does square matrix multiplication transform vectors?
- Its columns correspond to re-scaled and rotated unit vectors

$$\begin{bmatrix}1 & 2\\4 & 3\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}1\\4\end{bmatrix}, \quad \begin{bmatrix}1 & 2\\4 & 3\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}2\\3\end{bmatrix}$$

- Now we can express any vector as a linear combination of the above matrix-unit-vector products

$$\begin{aligned}\begin{bmatrix}1 & 2\\4 & 3\end{bmatrix}\begin{bmatrix}2\\1\end{bmatrix} &= \begin{bmatrix}1 & 2\\4 & 3\end{bmatrix}\left(2\begin{bmatrix}1\\0\end{bmatrix} + 1\begin{bmatrix}0\\1\end{bmatrix}\right)\\ \begin{bmatrix}1 & 2\\4 & 3\end{bmatrix}\begin{bmatrix}2\\1\end{bmatrix} &= 2\begin{bmatrix}1\\4\end{bmatrix} + 1\begin{bmatrix}2\\3\end{bmatrix}\\ &= \begin{bmatrix}4\\11\end{bmatrix}\end{aligned}$$

Eigenvalues and Eigenvectors

- For $A \in \mathbb{R}^{n \times n}, \lambda$ is an eigenvalue and $x \neq 0$ is an eigenvector if $Ax = \lambda x$.
- Eigenvalues are the roots of $\det(A - \lambda I_n) = 0$
- Eigenvectors are non-zero solutions of $Ax = \lambda x$
- Viewing A as a linear transformation
  - The vectors that remain unchanged and only get re-scaled are the eigenvectors.
  - Their scaling factors are the eigenvalues!
- Question: Find the eigenvalues and eigenvectors of

$$\begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix}$$

Eigenvalues and Eigenvectors

- Question: Find the eigenvalues and eigenvectors of

$$\begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix}$$

- Eigenvalues:

$$\begin{aligned} \det\left(\begin{bmatrix} 1-\lambda & 2 \\ 4 & 3-\lambda \end{bmatrix}\right) &= 0 \\ (1-\lambda)(3-\lambda) - 8 &= 0 \\ \lambda^2 - 4\lambda - 5 &= 0 \\ (\lambda-5)(\lambda+1) &= 0 \\ \lambda = 5, \lambda &= -1 \end{aligned}$$

Eigenvalues and Eigenvectors

- Question: Find the eigenvalues and eigenvectors of

$$\begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix}$$

- Eigenvalues: $\lambda = 5, \lambda = -1$
- Eigenvectors:

$$\begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 5 \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \implies \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = -1 \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \implies \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

Eigenvalue Decomposition

- Group the eigenvectors and eigenvalues into the following matrices.

$$P = \begin{bmatrix} 1 & -1 \\ 2 & 1 \end{bmatrix}$$

$$\Lambda = \begin{bmatrix} 5 & 0 \\ 0 & -1 \end{bmatrix}$$

- If the eigenvectors are linearly independent, we can express A as

$$\begin{aligned} A &= P\Lambda P^{-1} \\ &= \begin{bmatrix} 1 & -1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 5 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 2 & 1 \end{bmatrix}^{-1} \end{aligned}$$

EigenValue Decomposition

- Why is this useful?
- Suppose we want to find powers of A, eg. A^4
- One option, that is quite tedious is:

$$A^4 = \begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix}$$

- Instead we could use the eigenvalue decomposition

$$\begin{aligned} A^4 &= P\Lambda P^{-1} P\Lambda P^{-1} P\Lambda P^{-1} P\Lambda P^{-1} \\ &= P\Lambda^4 P^{-1} \\ &= \begin{bmatrix} 1 & -1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 5^4 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 2 & 1 \end{bmatrix}^{-1} \end{aligned}$$

Singular value decomposition (SVD)

- EVD only works for square, diagonalizable matrices
- SVD works for matrices of any size! It decomposes $A \in \mathbb{R}^{m \times n}$ as follows.
$$A = U \Sigma V^\top,$$
- $U \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{n \times n}$ are orthogonal matrices (*i.e.* $U^\top = U^{-1}$)
- $\Sigma \in \mathbb{R}^{m \times n}$ is a diagonal matrix with *singular values* of A denoted by σ_i appearing by non-increasing order: $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{\min(m,n)} \geq 0$.
- The squared singular values of A are the eigenvalues of the matrix $AA^\top$ or $A^\top A$, i.e., $\sigma_i(A) = \sqrt{\lambda_i(AA^\top)} = \sqrt{\lambda_i(A^\top A)}$
- V is the matrix of eigenvectors of $A^T A$
- U is the matrix of eigenvectors of AA^T

What You Should Know

Probability Concepts

- Axioms of probability
- Bayes' Rule
- MLE and MAP procedures
- Expectation and variance of random variables

Linear Algebra Concepts

- Determinants and matrix invertibility
- Vector Norms – $\ell 1$, $\ell 2$; Inner products
- Eigenvalues and eigenvectors
- Singular Value Decomposition
- Covariance matrices and positive semi-definite-ness