2019 CS420 Machine Learning, Lecture 1A

(Home Reading Materials)

Mathematics for Machine Learning

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Areas of Mathematics Essential to Machine Learning

- Machine learning is part of both **statistics** and computer science
  - Probability
  - Statistical inference
  - Validation
  - Estimates of error, confidence intervals
- **Linear Algebra**
  - Hugely useful for compact representation of linear transformations on data
  - Dimensionally reduction techniques
- **Optimization** theory

Notations

- $a \in A$ set membership: *a* is member of set *A*
- $|B|$ cardinality: number of items in set *B*
- $\|\mathbf{v}\|$ norm: length of vector v
- $\sum$ summation
- $\int$ integral
- $\mathbf{x}, \mathbf{y}, \mathbf{z}$ vector (bold, lower case)
- $\mathbf{A}, \mathbf{B}$ matrix (bold, upper case)
- $y = f(x)$ function: assigns unique value in range of *y* to each value in domain of *x*
- $y = f(\mathbf{x})$ function on multiple variables

Probability Spaces

- A probability space models a *random process or experiment* with three components:
  - Ω, the set of possible outcomes O
    - number of possible outcomes = $|\Omega|$
    - Discrete space $|\Omega|$ is finite
    - Continuous space $|\Omega|$ is infinite
  - F, the set of possible events E
    - number of possible events = $|F|$
  - P, the probability distribution
    - function mapping each outcome and event to real number between 0 and 1 (the probability of O or E)
    - probability of an event is sum of probabilities of possible outcomes in event

Axioms of Probability

- Non-negativity:
  - for any event $E \in F, p(E) \geq 0$

- All possible outcomes:
  - $p(\Omega) = 1$

- Additivity of disjoint events:
  - For all events $E, E' \in F$ where $E \cap E' = \emptyset$,

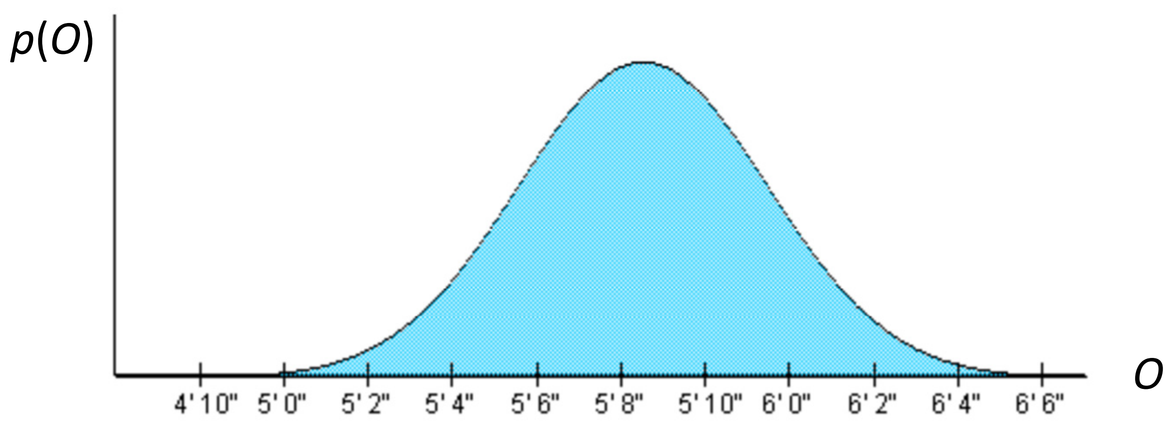
$$p(E \cup E') = p(E) + p(E')$$

Example of Discrete Probability Space

- Three consecutive flips of a coin
  - 8 possible outcomes: O = HHH, HHT, HTH, HTT, THH, THT, TTH, TTT
- 2^8=256 possible events
  - example: E = ($O \in$ { HHT, HTH, THH }), i.e. exactly two flips are heads
  - example: E = ($O \in$ { THT, TTT }), i.e. the first and third flips are tails
- If coin is fair, then probabilities of outcomes are equal
  - p(HHH) = p(HHT) = p(HTH) = p(HTT) = p(THH) = p(THT) = p(TTH) = p(TTT) = 1/8
  - example: probability of event E = (exactly two heads) is p(HHT) + p(HTH) + p(THH) = 3/8

Example of Continuous Probability Space

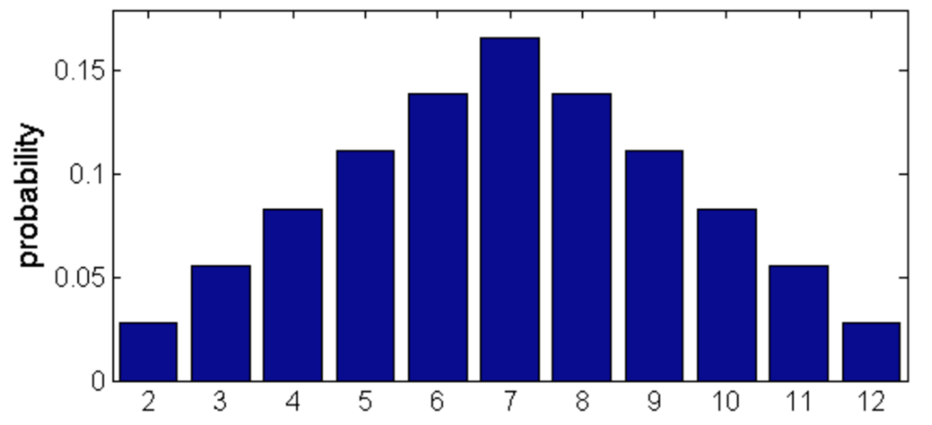
- Height of a randomly chosen American male
  - Infinite number of possible outcomes: *O* has some has some single value in range 2 feet to 8 feet
    - example: $E = (O \mid O < 5.5 \text{ feet})$, i.e. individual chosen is less than 5.5 feet tall
  - Infinite number of possible events
  - Probabilities of outcomes are not equal, and are described by a continuous function, $p(O)$



Probability Distributions

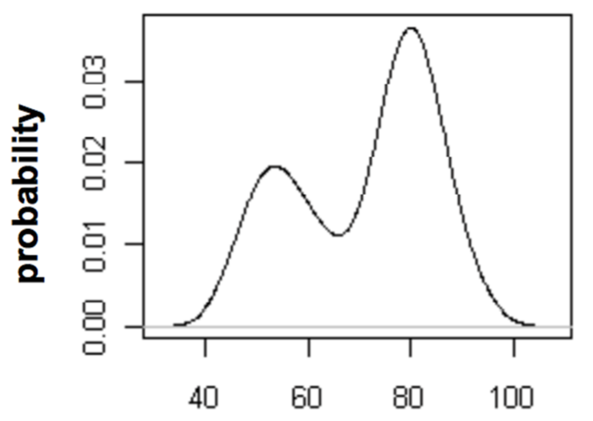
- Discrete: probability mass function (pmf)

example:
sum of two fair dice



- Continuous: probability density function (pdf)

example: waiting time
between eruptions of
Old Faithful (minutes)



Random Variables

- A random variable X is a function that associates a number x with each outcome O of a process
  - Common notation: $X(O) = x$, or just $X = x$
- Basically a way to redefine a probability space to a new probability space
  - X must obey axioms of probability
  - X can be discrete or continuous
- Example: X = number of heads in three flips of a coin
  - Possible values of X are 0, 1, 2, 3
  - $p(X = 0) = p(X = 3) = 1 / 8$, $p(X = 1) = p(X = 2) = 3 / 8$
  - Size of space (number of “outcomes”) reduced from 8 to 4
- Example: X = average height of five randomly chosen American men
  - Size of space unchanged, but pdf of X different than that for single man

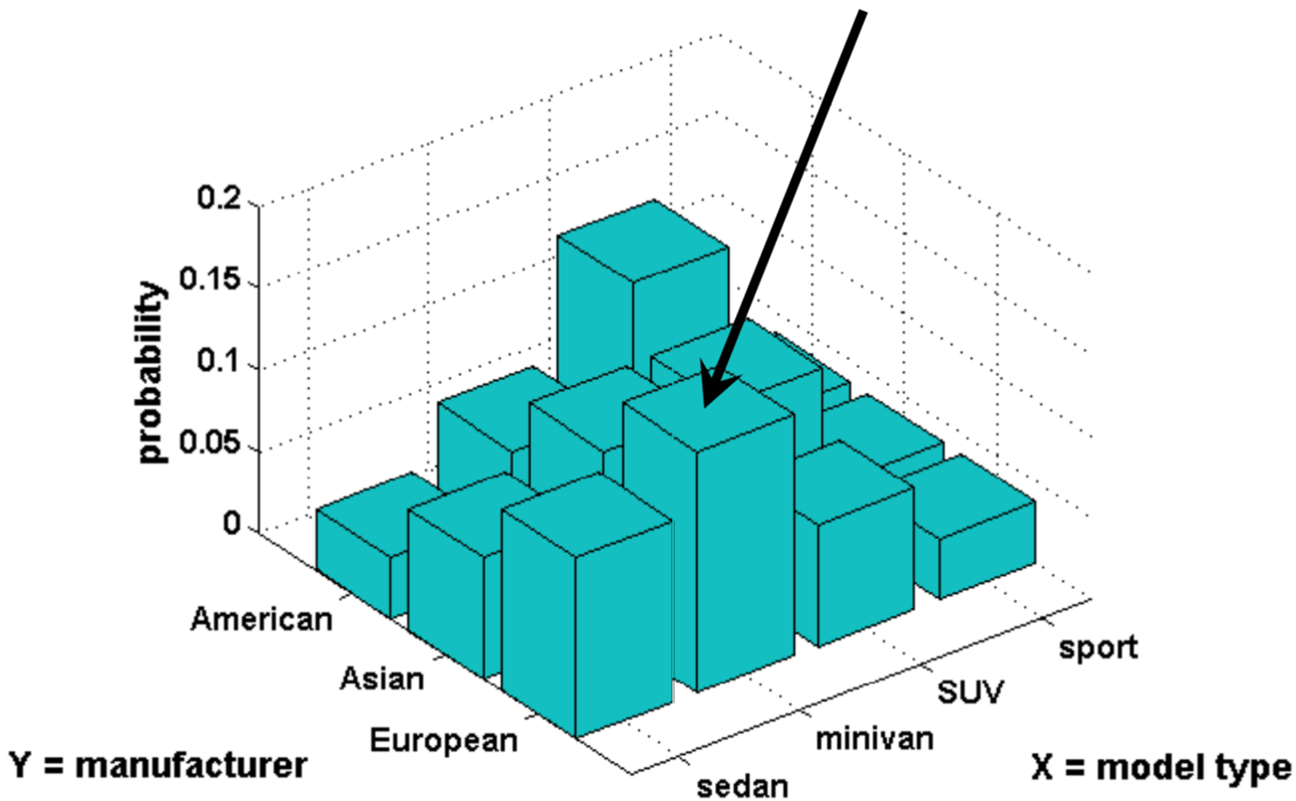
Multivariate Probability Distributions

- Scenario
  - Several random processes occur (doesn't matter whether in parallel or in sequence)
  - Want to know probabilities for each possible combination of outcomes
- Can describe as joint probability of several random variables
  - Example: two processes whose outcomes are represented by random variables *X* and *Y*. Probability that process *X* has outcome *x* and process *Y* has outcome *y* is denoted as

$$p(X = x, Y = y)$$

Example of Multivariate Distribution

joint probability: $p(\, X = \text{minivan},\ Y = \text{European}\,) = 0.1481$



Multivariate Probability Distributions

- Marginal probability
  - Probability distribution of a single variable in a joint distribution
  - Example: two random variables *X* and *Y*:

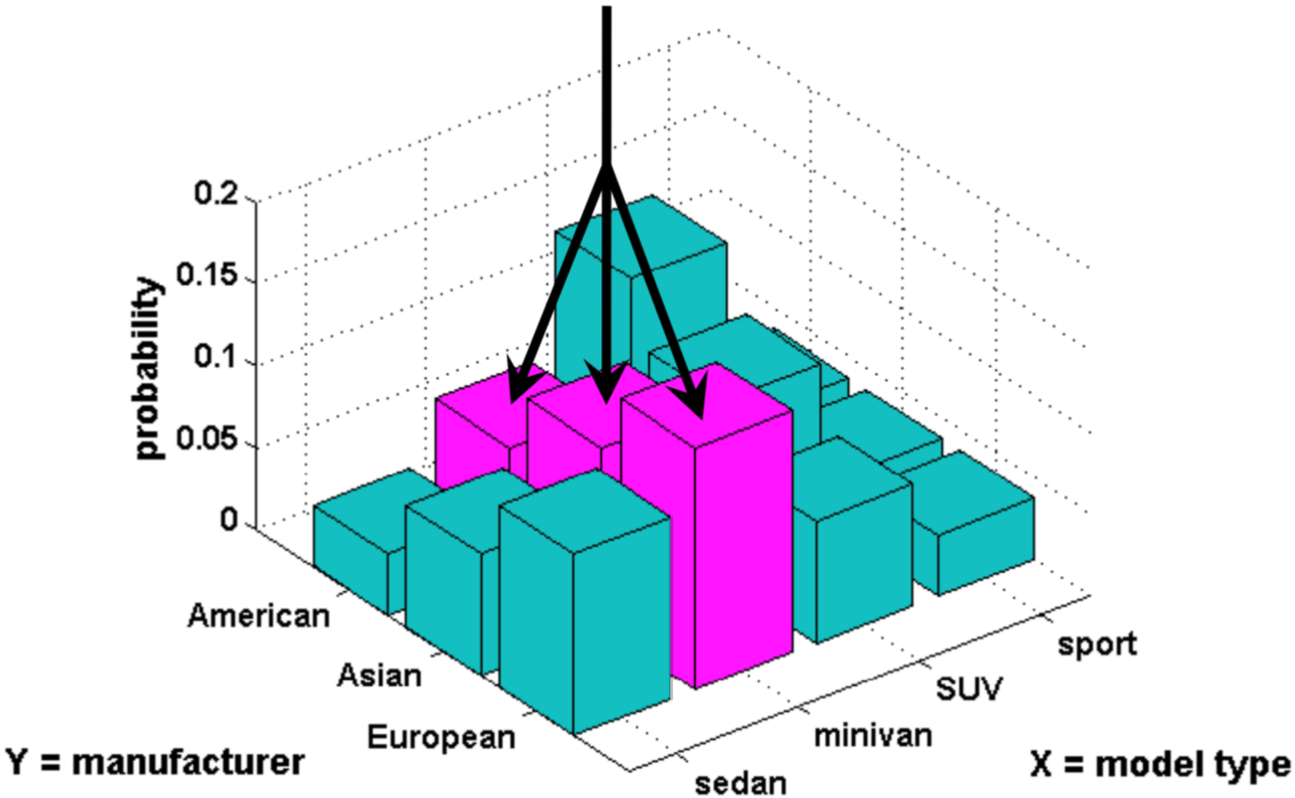
$$p(X = x) = \sum\nolimits_{b=\text{all values of } Y} p(X = x, Y = b)$$

- Conditional probability
  - Probability distribution of one variable given that another variable takes a certain value
  - Example: two random variables X and Y :

$$p(X = x | Y = y) = \frac{p(X=x, Y=y)}{p(Y=y)}$$

Example of Marginal Probability

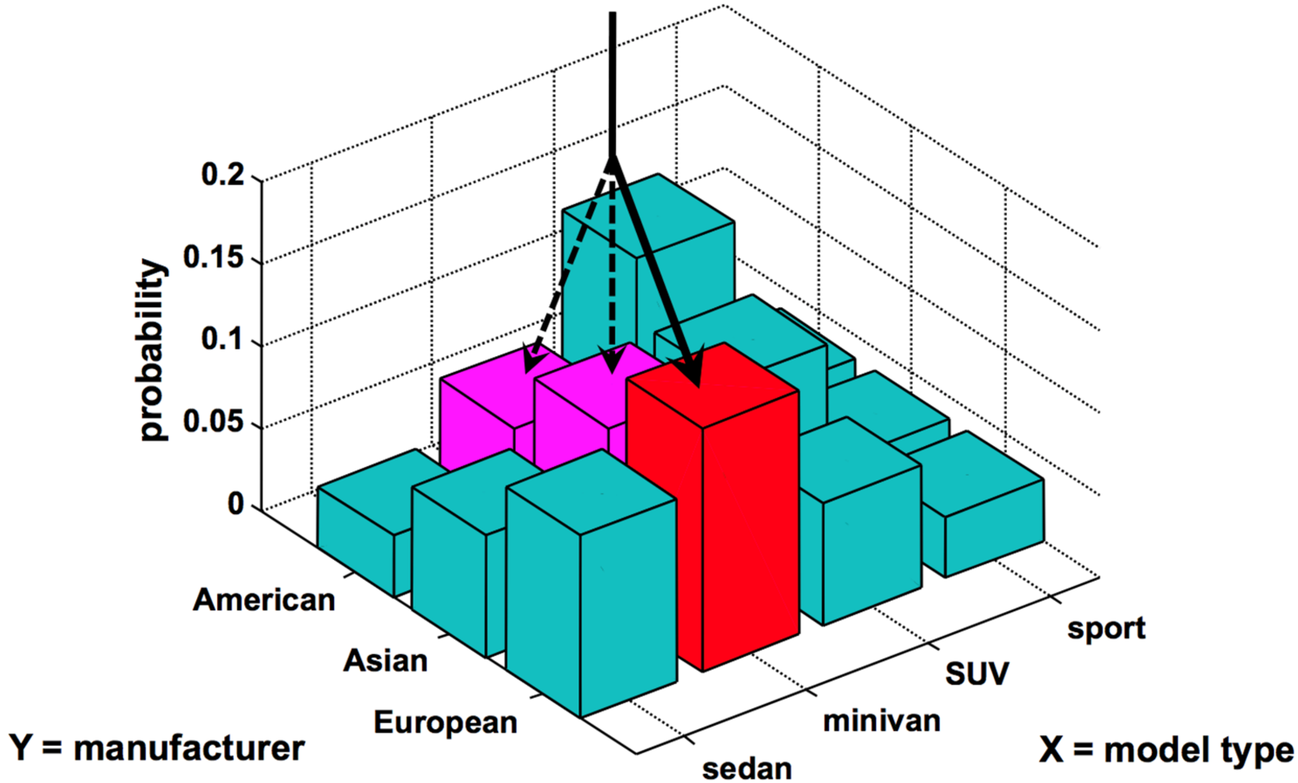
Marginal probability:
p(X = minivan) = 0.0741 + 0.1111 + 0.1481 = 0.3333



Example of Conditional Probability

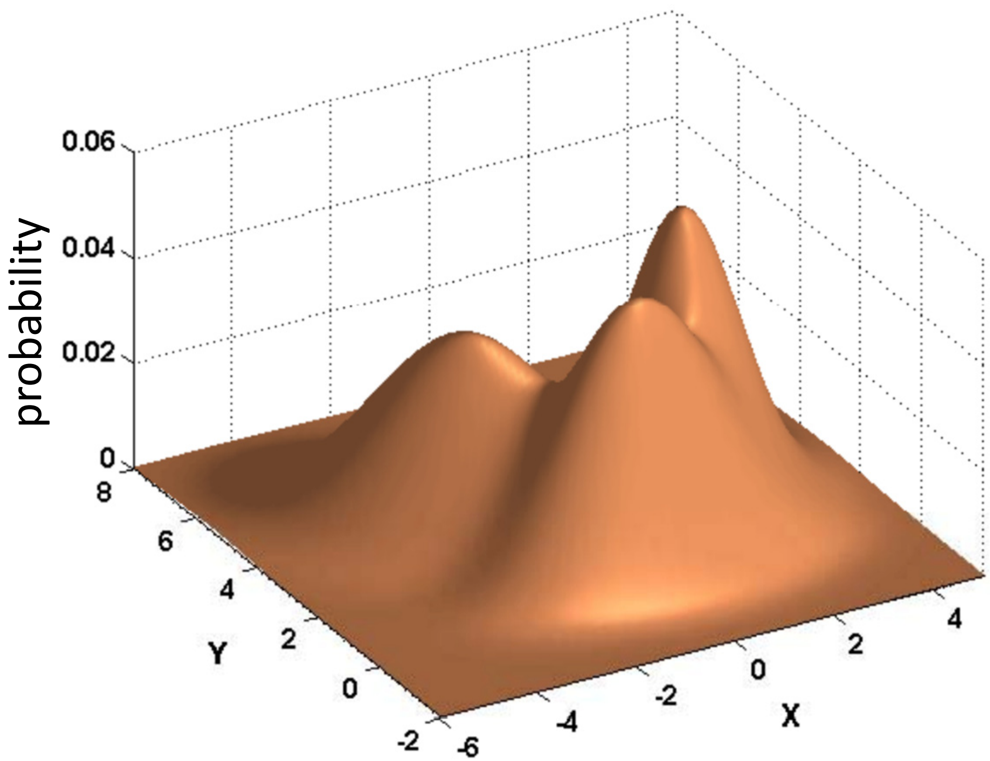
Conditional probability:

p(Y = European | X = minivan) = 0.1481 / (0.0741 + 0.1111 + 0.1481) = 0.4433



Continuous Multivariate Distribution

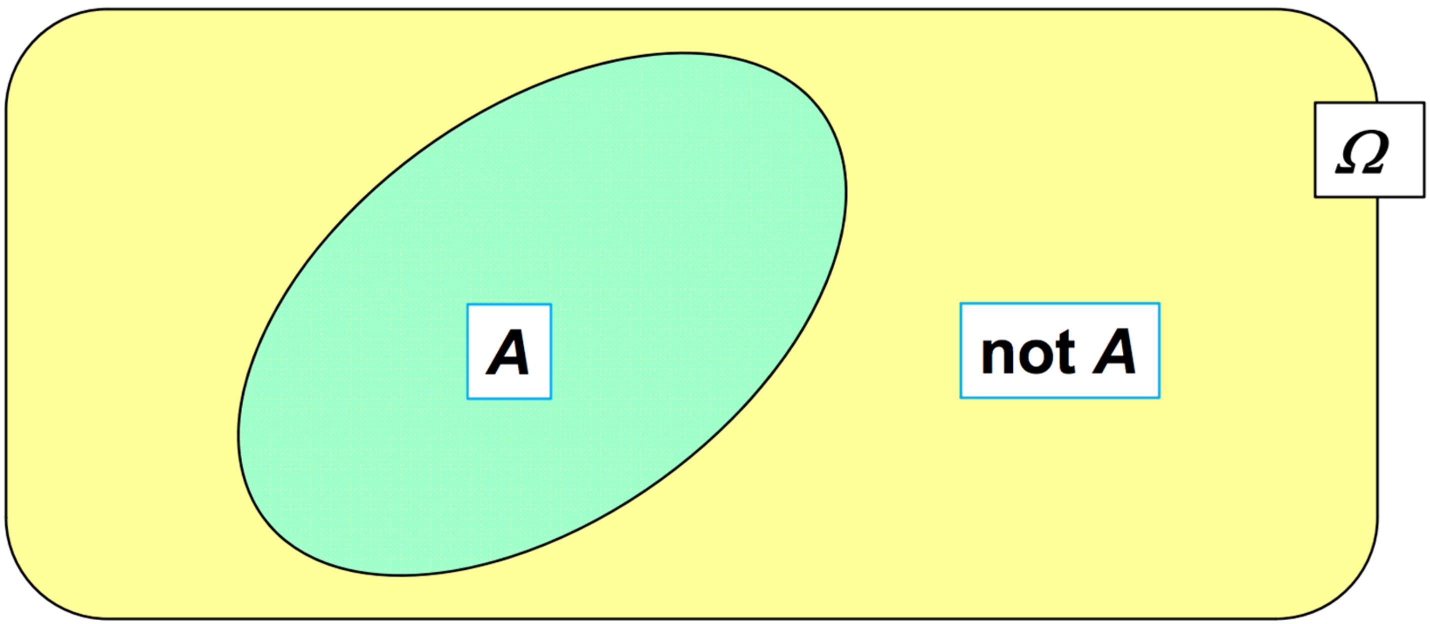
- Example: three-component Gaussian mixture in two dimensions



Complement Rule

- Given: event A, which can occur or not

$$p(\text{not } A) = 1 - p(A)$$

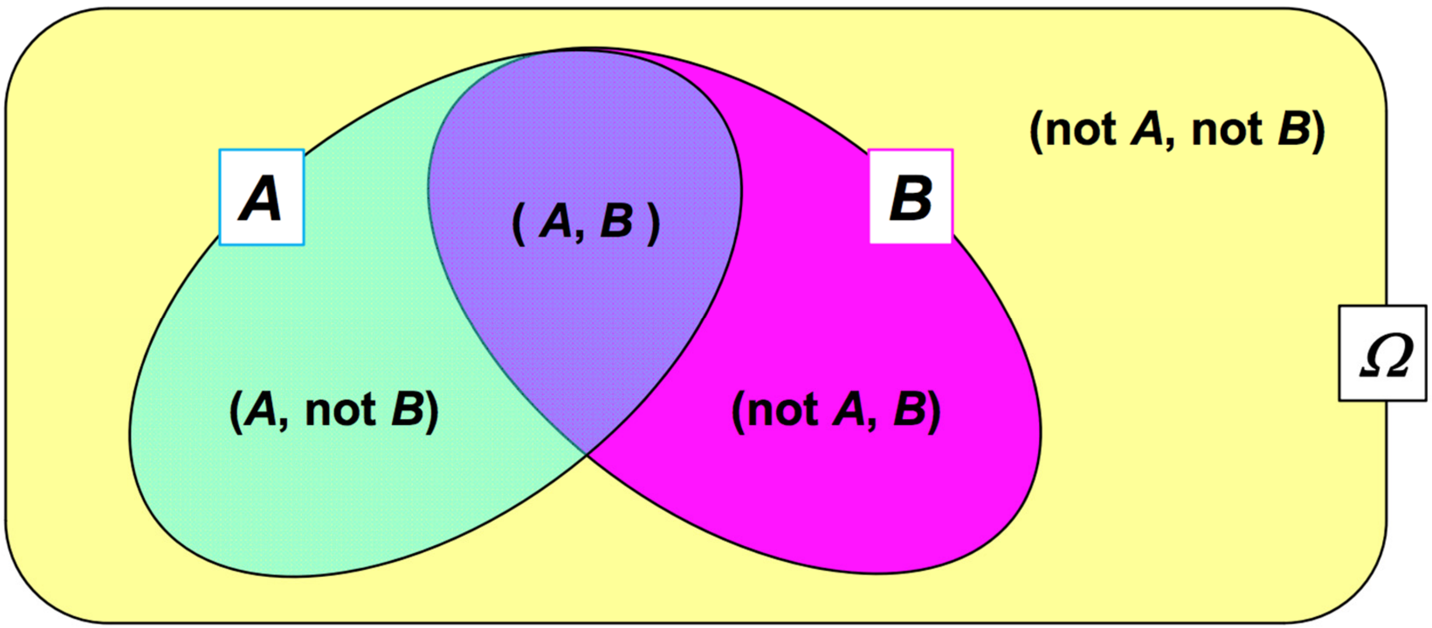


areas represent relative probabilities

Product Rule

- Given: events A and B, which can co-occur (or not)

$$p(A, B) = p(A|B) \cdot p(B)$$

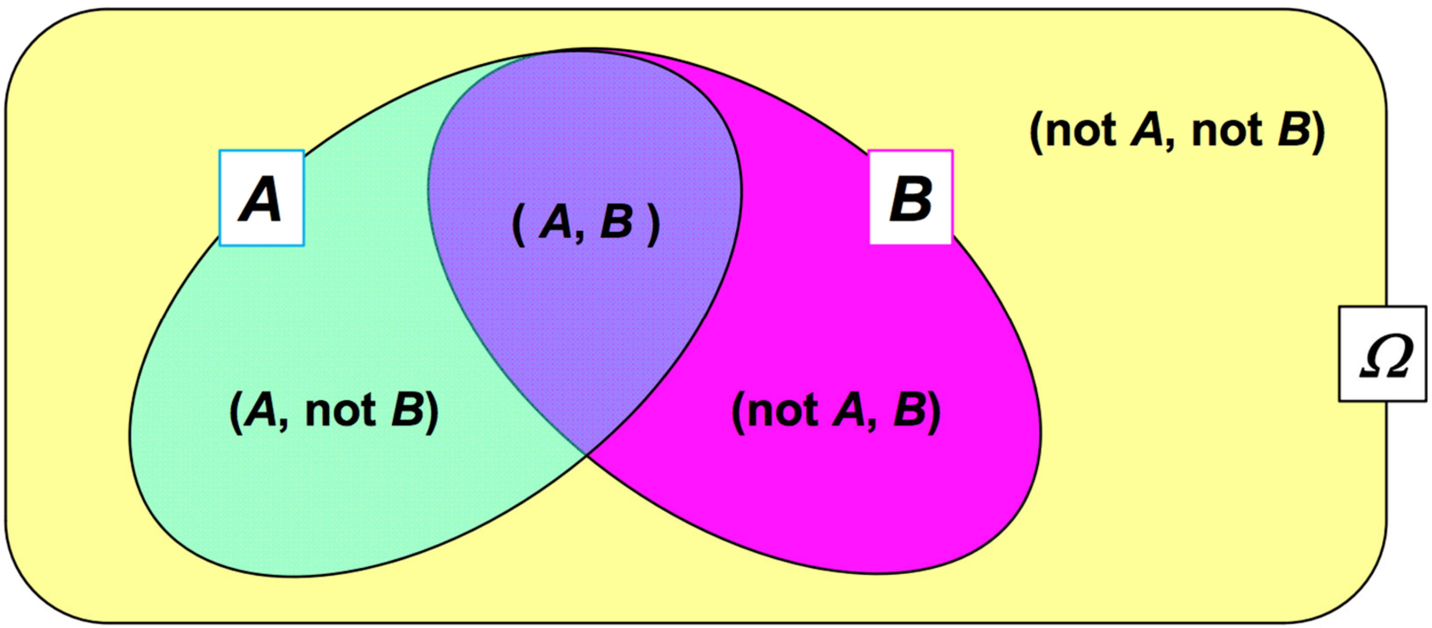


areas represent relative probabilities

Rule of Total Probability

- Given: events A and B, which can co-occur (or not)

$$
\begin{aligned}
p(A) =& p(A, B) + p(A, \text{not } B) \\
=& p(A|B) \cdot p(B) + p(A|\text{not } B) \cdot p(\text{not } B)
\end{aligned}
$$

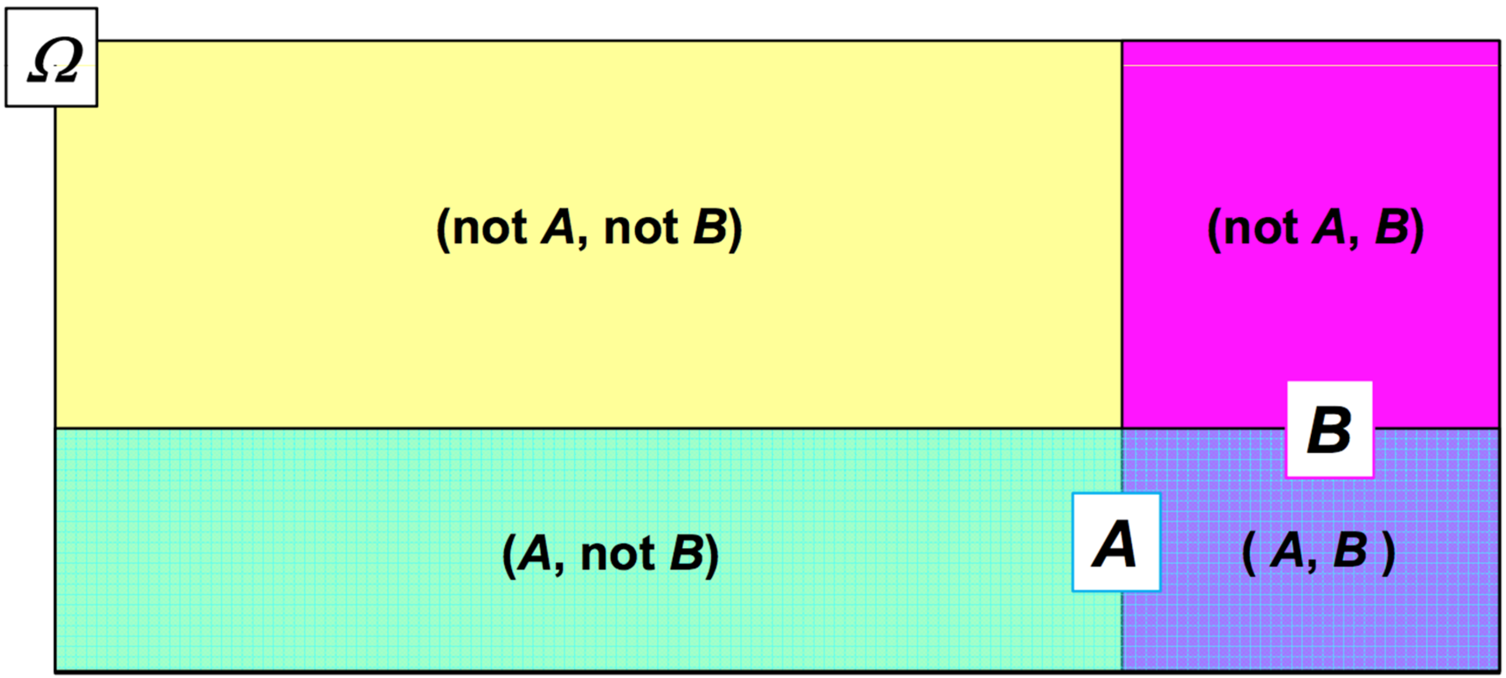


areas represent relative probabilities

Independence

- Given: events A and B, which can co-occur (or not)

$$p(A|B) = p(A) \quad \text{or} \quad p(A,B) = p(A) \cdot p(B)$$



areas represent relative probabilities

Example of Independence/Dependence

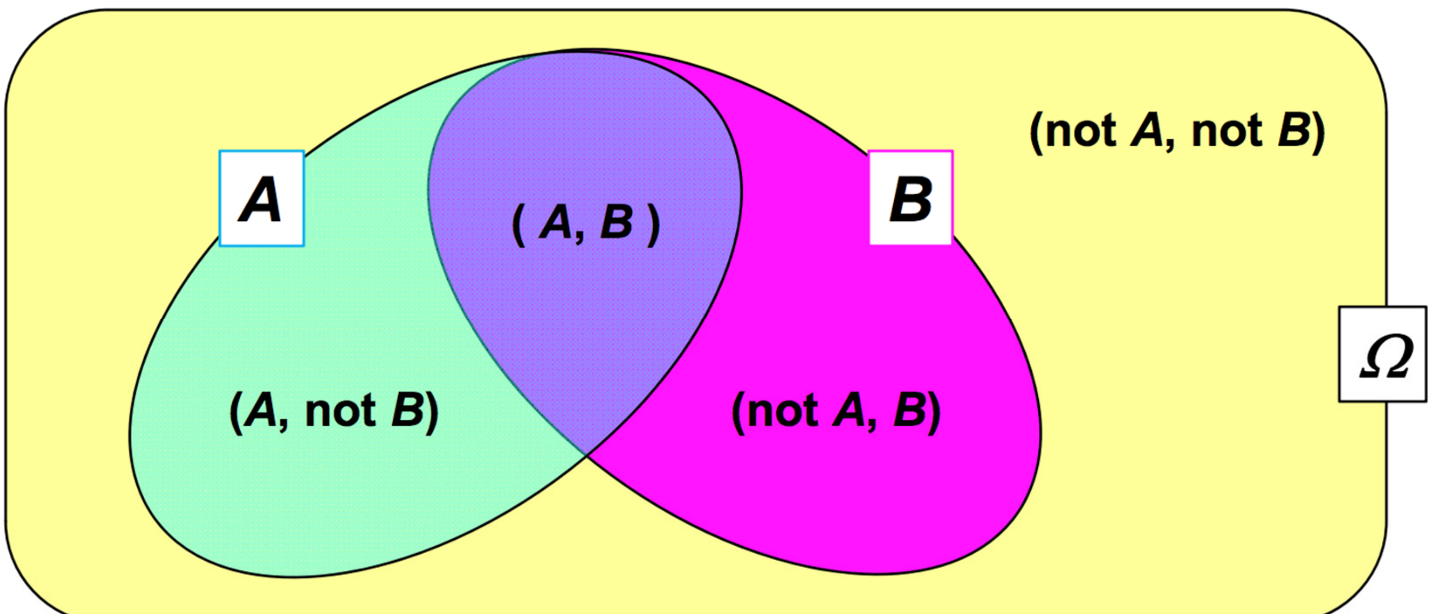
- Independence:
  - Outcomes on multiple flips of a coin
  - Height of two unrelated individuals
  - Probability of getting a king on successive draws from a deck, if card from each draw is ***replaced***

- Dependence:
  - Height of two related individuals
  - Probability of getting a king on successive draws from a deck, if card from each draw is ***not replaced***

Bayes Rule

- A way to find conditional probabilities for one variable when conditional probabilities for another variable are known.

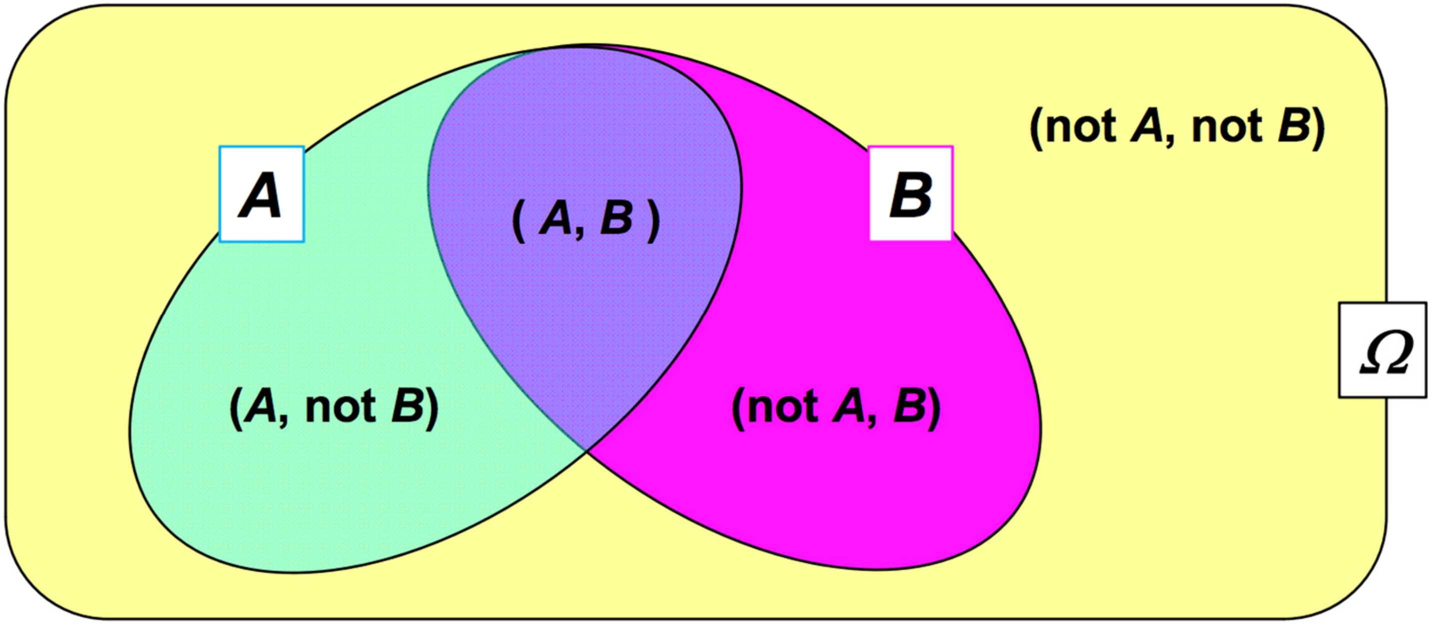
$$p(B|A) = \frac{p(A|B) \cdot p(B)}{p(A)}$$



Bayes Rule

$$p(B|A) \propto p(A|B) \cdot p(B)$$

$$\text{posterior probability} \propto \text{likelihood} \times \text{prior probability}$$



Example of Bayes Rule

- In recent years, it has rained only 5 days each year in a desert. The weatherman is forecasting rain for tomorrow. When it actually rains, the weatherman has forecast rain 90% of the time. When it doesn't rain, he has forecast rain 10% of the time. What is the probability it will rain tomorrow?
- Event A: The weatherman has forecast rain.
- Event B: It rains.
- We know:
  - $P(B) = 5/365 = 0.0137$ [It rains 5 days out of the year.]
  - $P(\text{not } B) = 1\text{-}0.0137 = 0.9863$
  - $P(A|B) = 0.9$ [When it rains, the weatherman has forecast rain 90% of the time.
  - $P(A|\text{not } B)=0.1$ [When it does not rain the weatherman has forecast rain 10% of the time.]

Example of Bayes Rule, cont'd

- We want to know *P*(B|A), the probability it will rain tomorrow, given a forecast for rain by the weatherman. The answer can be determined from Bayes rule:

$$
\begin{aligned}
p(B|A) =& p(A|B) \cdot p(B)/p(A) \\
p(A) =& p(A|B) \cdot p(B) + p(A|\text{not } B) \cdot p(\text{not } B) \\
=& 0.9 \times 0.0137 + 0.1 \times 0.9863 = 0.1110 \\
p(B|A) =& 0.9 \times 0.0137/0.1110 = 0.1111
\end{aligned}
$$

- The result seems unintuitive but is correct. Even when the weatherman predicts rain, it only rains only about 11% of the time, which is much higher than average.

Expected Value

- Given:
  - A discrete random variable *X*, with possible values $X = x_1, x_2, \ldots, x_n$
  - Probabilities $p(X = x_i)$ that *X* takes on the takes on the various values of x_i
  - A function $y_i = f(x_i)$ defined on *X*

- The expected value of *f* is the probability-weighted "average" value of $f(x_i)$:

$$\mathbb{E}(f) = \sum_i p(x_i) f(x_i)$$

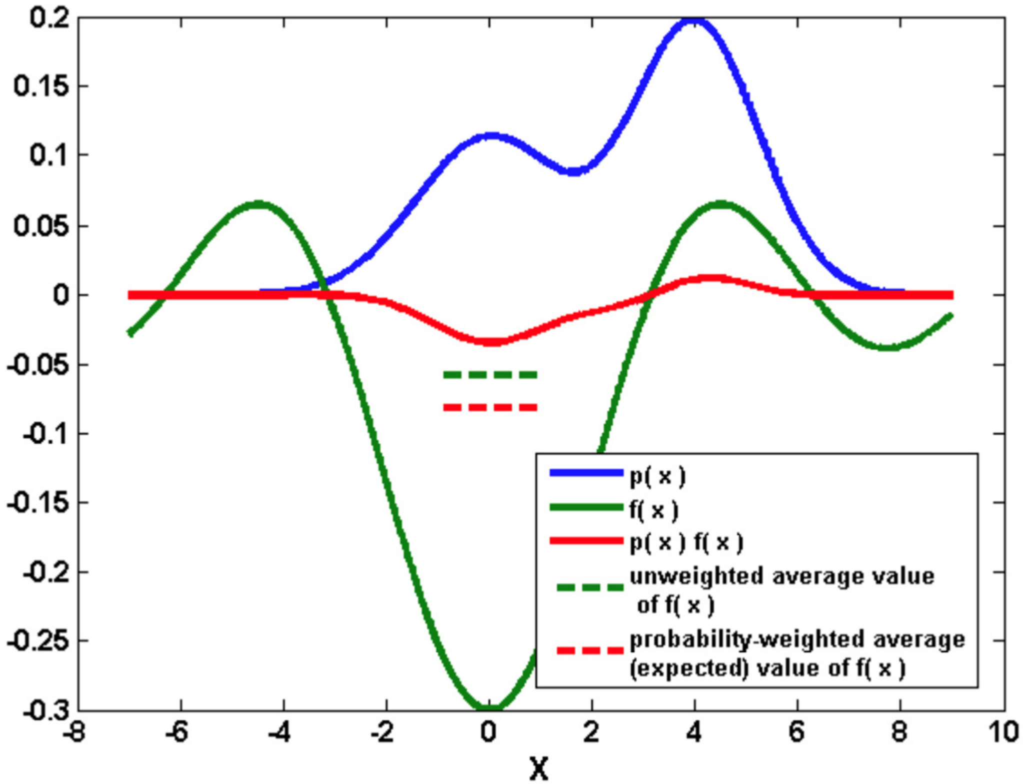
Example of Expected Value

- Process: game where one card is drawn from the deck
  - If face card, the dealer pays you \$10
  - If not a face card, you pay dealer \$4
- Random variable X = {face card, not face card}
  - *P*(face card) = 3/13
  - *P*(not face card) = 10/13
- Function *f*(*X*) is payout to you
  - *f*(face card) = 10
  - *f* (not face card) = -4
- Expected value of payout is

$$\mathbb{E}(f) = \sum_i p(x_i) f(x_i) = 3/13 \cdot 10 + 10/13 \cdot -4 = -0.77$$

Expected Value in Continuous Spaces

$$\mathbb{E}(f) = \int_{x=a \to b} p(x) f(x)$$



Common Forms of Expected Value (1)

- Mean μ

$$f(x_i) = x_i \quad \Longrightarrow \quad \mu = \mathbb{E}(f) = \sum_i p(x_i) x_i$$

  - Average value of $X = x_i$, taking into account probability of the various x_i
  - Most common measure of "center" of a distribution

- Estimate mean from actual samples

$$\mu = \frac{1}{N} \sum_{i=1}^{N} x_i$$

Common Forms of Expected Value (2)

- Variance σ^2

$$f(x_i) = (x_i - \mu) \quad \Longrightarrow \quad \sigma^2 = \sum_i p(x_i) \cdot (x_i - \mu)^2$$

  - Average value of squared deviation of $X = x_i$ from mean μ, taking into account probability of the various x_i
  - Most common measure of “spread” of a distribution
  - σ is the standard deviation

- Estimate variance from actual samples:

$$\sigma^2 = \frac{1}{N-1} \sum_{i=1}^{n} (x_i - \mu)^2$$

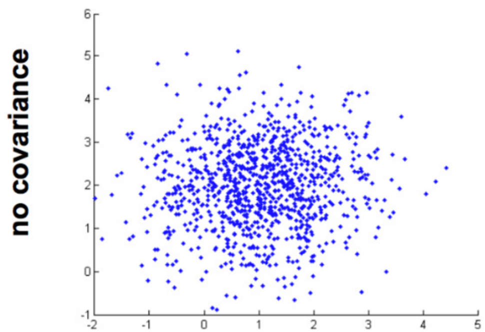
https://www.zhihu.com/question/20099757

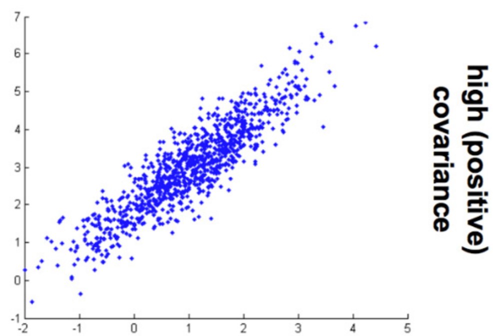
Common Forms of Expected Value (3)

- Covariance

$$f(x_i) = (x_i - \mu_x), \quad g(y_i) = (y_i - \mu_y)$$
$$cov(x, y) = \sum_i p(x_i, y_i) \cdot (x_i - \mu_x) \cdot (y_i - \mu_y)$$

  - Measures tendency for *x* and *y* to deviate from their means in same (or opposite) directions at same time





- Estimate covariance from actual samples

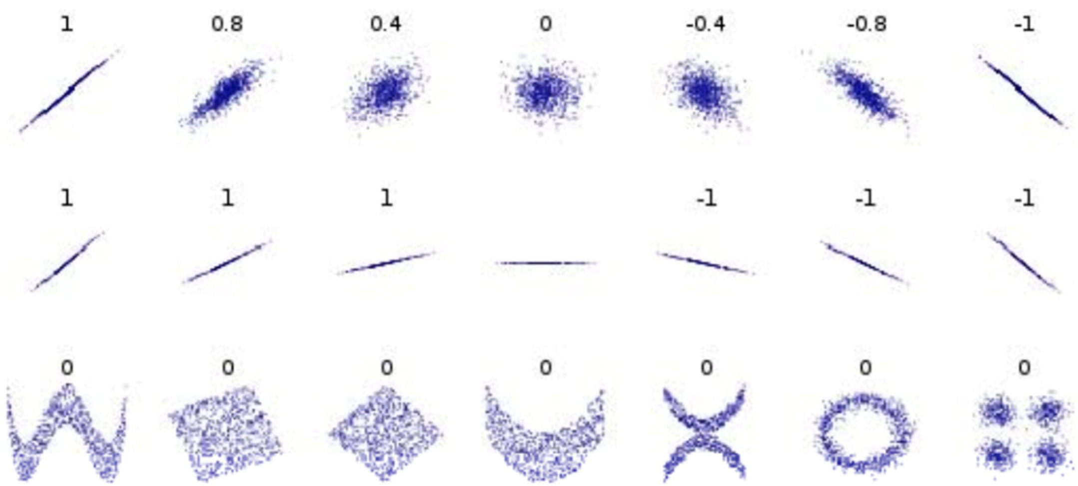
$$cov(x, y) = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \mu_x)(y_i - \mu_y)$$

Correlation

- Pearson's correlation coefficient is covariance normalized by the standard deviations of the two variables

$$corr(x, y) = \frac{cov(x, y)}{\sigma_x \sigma_y}$$

  - Always lies in range -1 to 1
  - Only reflects *linear dependence* between variables



Linear dependence with noise

Linear dependence without noise

Various nonlinear dependencies

Estimation of Parameters

- Suppose we have random variables $X_1, . . . , X_n$ and corresponding observations $x_1, . . . , x_n$.
- We prescribe a parametric model and fit the parameters of the model to the data.
- How do we choose the values of the parameters?

Maximum Likelihood Estimation(MLE)

- The basic idea of MLE is to maximize the probability of the data we have seen.

$$\hat{\theta}_{MLE} = \arg\max_{\theta} \mathcal{L}(\theta)$$

- where L is the likelihood function

$$\mathcal{L}(\theta) = p(x_1, \ldots, x_n; \theta)$$

- Assume that $X_1, \ldots, X_n$ are i.i.d, then we have

$$\mathcal{L}(\theta) = \prod_{i=1}^{n} p(x_i; \theta)$$

- Take log on both sides, we get log-likelihood

$$\log \mathcal{L}(\theta) = \sum_{i=1}^{n} \log p(x_i; \theta)$$

Example

- X_i are independent Bernoulli random variables with unknown parameter ϑ.

$$f(x_i;\theta) = \theta^{x_i}(1-\theta)^{1-x_i}$$

$$\mathcal{L}(\theta) = \prod_{i=1}^{n} f(x_i;\theta) = \theta^{\sum x_i}(1-\theta)^{n-\sum x_i}$$

$$\log\mathcal{L}(\theta) = (\sum x_i)\log\theta + (n - \sum x_i)\log(1-\theta)$$

$$\frac{\partial \log\mathcal{L}(\theta)}{\partial\theta} = 0 \Rightarrow \hat{\theta} = \frac{\sum_{i=1}^{n} x_i}{n}$$

Maximum A Posteriori Estimation (MAP)

- We assume that the parameters are a random variable, and we specify a prior distribution p(θ).

- Employ Bayes' rule to compute the posterior distribution

$$p(\theta|x_1,\ldots,x_n) \propto p(\theta)p(x_1,\ldots,x_n|\theta)$$

- Estimate parameter θ by maximizing the posterior

$$\hat{\theta}_{MAP} = \arg\max_{\theta} p(\theta)p(x_1,\ldots,x_n|\theta)$$

$$\hat{\theta}_{MAP} = \arg\max_{\theta} \log p(\theta) + \sum_{i=1}^{n} \log(x_i|\theta)$$

Example

- X_i are independent Bernoulli random variables with unknown parameter ϑ. Assume that ϑ satisfies normal distribution.
- Normal distribution:

$$\mathcal{N}(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- Maximize:

$$\arg\max_{\theta} -\frac{(\theta-\mu)^2}{2\sigma^2} + (\sum x_i)\log\theta + (n - \sum x_i)\log(1-\theta)$$

Comparison between MLE and MAP

- MLE: For which ϑ is $X_1, \ldots, X_n$ most likely?

- MAP: Which ϑ maximizes $p(\vartheta | X_1, \ldots, X_n)$ with prior $p(\vartheta)$?

- The prior can be regard as regularization - to reduce the overfitting.

Example

- Flip a unfair coin 10 times. The result is HHTTHHHHHT

$$f(x_i;\theta) = \theta^{x_i}(1-\theta)^{1-x_i}$$

- x_i = 1 if the result is head.

- MLE estimates ϑ = 0.7

- Assume the prior of ϑ is N(0.5,0.01), MAP estimates ϑ=0.558

What happens if we have more data?

- Flip the unfair coins 100 times, the result is 70 heads and 30 tails.
  - The result of MLE does not change, $\vartheta = 0.7$
  - The estimation of MAP becomes $\vartheta = 0.663$

- Flip the unfair coins 1000 times, the result is 700 heads and 300 tails.
  - The result of MLE does not change, $\vartheta = 0.7$
  - The estimation of MAP becomes $\vartheta = 0.696$

Unbiased Estimators

- An estimator of a parameter is unbiased if the expected value of the estimate is the same as the true value of the parameters.
- Assume X_i is a random variable with mean μ and variance σ^2

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$$

$$\mathbb{E}(\bar{X}) = \mathbb{E}(\frac{1}{n}\sum_{i=1}^{n} X_i) = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}(X_i) = \frac{1}{n}n\mu = \mu$$

- $\bar{X}$ is unbiased estimation

Estimator of Variance

- Assume X_i is a random variable with mean μ and variance σ^2
- Is $\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2$ unbiased?

$$
\begin{aligned}
\hat{\sigma}^2 =& \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2 \\
=& \frac{1}{n}\sum_{i=1}^{n}(X_i^2 - 2X_i\bar{X} + \bar{X}^2) \\
=& \frac{1}{n}\sum_{i=1}^{n}X_i^2 - 2\bar{X}\frac{1}{n}\sum_{i=1}^{n}X_i + \frac{1}{n}n\bar{X}^2 \\
=& \frac{1}{n}\sum_{i=1}^{n}X_i^2 - \bar{X}^2
\end{aligned}
$$

Estimator of Variance

$$\begin{aligned}
\mathbb{E}(\hat{\sigma}^2) =& \mathbb{E}[\frac{1}{n}\sum_{i=1}^{n} X_i^2 - \bar{X}^2] \\
=& \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}(X_i^2) - \mathbb{E}(\bar{X}^2) \\
=& \frac{1}{n}\sum_{i=1}^{n} (\sigma^2 + \mu^2) - (\sigma^2/n + \mu^2) \\
=& \sigma^2 - \sigma^2/n \\
=& \frac{(n-1)\sigma^2}{n} \neq \sigma^2
\end{aligned}$$

- where we use

$var(X) = \sigma^2 = E(X^2) - \mu^2$, $var(\bar{X}) = \sigma^2/n = E(\bar{X}^2) - \mu^2$

Estimator of Variance

$$\hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$$

$$\mathbb{E}(\hat{\sigma}^2) = \sigma^2$$

- $\hat{\sigma}^2$ is a unbiased estimation

Linear Algebra Applications

- Why vectors and matrices?
  - Most common form of data organization for machine vector organization for machine learning is a 2D array, where
    - rows represent samples
    - columns represent attributes
  - Natural to think of each sample as a vector of attributes, and whole array as a matrix

vector

Refund	Marital Status	Taxable Income	Cheat
Yes	Single	125K	No
No	Married	100K	No
No	Single	70K	No
Yes	Married	120K	No
No	Divorced	95K	Yes
No	Married	60K	No
Yes	Divorced	220K	No
No	Single	85K	Yes
No	Married	75K	No
No	Single	90K	Yes

matrix

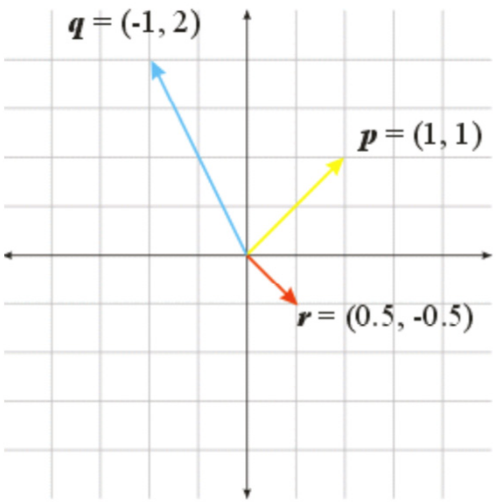
Vectors

- Definition: an *n*-tuple of values
  - *n* referred to as the *dimension* of the vector
- Can be written in column form or row form

$$x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \qquad x^\top = \begin{pmatrix} x_1 & \cdots & x_n \end{pmatrix}$$

$\top$ means "transpose"

- Can think of a vector as
  - a point in space *or*
  - a directed line segment with a magnitude and direction



Vector Arithmetic

- Addition of two vectors
  - add corresponding elements

$$\mathbf{z} = \mathbf{x} + \mathbf{y} = \begin{pmatrix} x_1 + y_1 & \cdots & x_n + y_n \end{pmatrix}^\top$$

- Scalar multiplication of a vector
  - multiply each element by scalar

$$\mathbf{y} = a\mathbf{x} = \begin{pmatrix} ax_1 & \cdots & ax_n \end{pmatrix}^\top$$

- Dot product of two vectors
  - Multiply corresponding elements, then add products

$$a = \mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{n} x_i y_i$$

  - Result is a <u>scalar</u>

Vector Norms

- A norm is a function $\|\cdot\|$ that satisfies:
  - $\|\mathbf{x}\| \geq 0$ with equality if and only if $\mathbf{x} = 0$
  - $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$
  - $\|a\mathbf{x}\| = |a|\|\mathbf{x}\|$
- 2-norm of vectors

$$\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2}$$

- Cauchy-Schwarz inequality

$$\mathbf{x} \cdot \mathbf{y} \leq \|\mathbf{x}\|_2 \|\mathbf{y}\|_2$$

Matrices

- Definition: an $m \times n$ two-dimensional array of values
  - *m* rows
  - *n* columns
- Matrix referenced by two-element subscript
  - first element in subscript is row
  - Second element in subscript is column
  - example: $\mathbf{A}_{24}$ or a_{24} is element in second row, fourth column of ***A***

$$\mathbf{A} = \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{pmatrix}$$

Matrices

- A vector can be regarded as special case of a matrix, where one of matrix dimensions is 1.
- Matrix transpose (denoted $^\top$)
  - swap columns and rows
  - $m \times n$ matrix becomes n x m matrix
  - example:

$$\mathbf{A} = \begin{pmatrix} 2 & 7 & -1 & 0 & 3 \\ 4 & 6 & -3 & 1 & 8 \end{pmatrix} \qquad \mathbf{A}^\top = \begin{pmatrix} 2 & 4 \\ 7 & 6 \\ -1 & -3 \\ 0 & 1 \\ 3 & 8 \end{pmatrix}$$

Matrix Arithmetic

- Addition of two matrices
  - matrices must be same size
  - add corresponding elements:
    $$c_{ij} = a_{ij} + b_{ij}$$
  - result is a matrix of same size

$$\mathbf{C} = \mathbf{A} + \mathbf{B} = \begin{pmatrix} a_{11} + b_{11} & \cdots & a_{1n} + b_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} + b_{m1} & \cdots & a_{mn} + b_{mn} \end{pmatrix}$$

- Scalar multiplication of a matrix
  - multiply each element by scalar:
    $$b_{ij} = d \cdot a_{ij}$$
  - result is a matrix of same size

$$\mathbf{B} = d \cdot \mathbf{A} = \begin{pmatrix} d \cdot a_{11} & \cdots & d \cdot a_{1n} \\ \vdots & \ddots & \vdots \\ d \cdot a_{m1} & \cdots & d \cdot a_{mn} \end{pmatrix}$$

Matrix Arithmetic

- Matrix-matrix multiplication
  - the column dimension of the previous matrix must match the row dimension of the following matrix

$$\mathbf{C}_{p\times n} = \mathbf{A}_{p\times m}\mathbf{B}_{m\times n} \qquad c_{ij} = \sum_{k=1}^{m} a_{ik} b_{kj}$$

- Multiplication is associative

$$\mathbf{A}\cdot(\mathbf{B}\cdot\mathbf{C}) = (\mathbf{A}\cdot\mathbf{B})\cdot\mathbf{C}$$

- Multiplication is not commutative

$$\mathbf{A}\cdot\mathbf{B} \neq \mathbf{B}\cdot\mathbf{A}$$

- Transposition rule

$$(\mathbf{A}\cdot\mathbf{B})^\top = \mathbf{B}^\top\cdot\mathbf{A}^\top$$

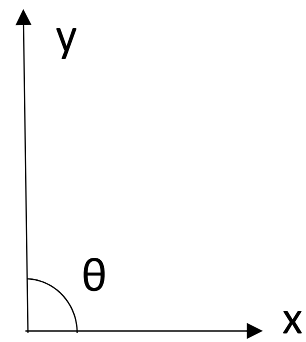
Orthogonal Vectors

- Alternative form of dot product:

$$\mathbf{x}^\top \mathbf{y} = \|\mathbf{x}\| \|\mathbf{y}\| \cos \theta$$

- A pair of vector x and y are *orthogonal* if

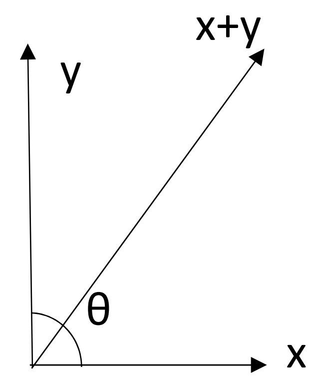
$$\mathbf{x}^\top \mathbf{y} = 0$$



- A set of vectors S is orthogonal if its elements are pairwise orthogonal
  - for $\mathbf{x}, \mathbf{y} \in S, \mathbf{x} \neq \mathbf{y} \Rightarrow \mathbf{x}^\top \mathbf{y} = 0$
- A set of vectors S is orthonormal if it is orthogonal and, every $\mathbf{x} \in S$ has $\|\mathbf{x}\| = 1$

Orthogonal Vectors

- Pythagorean theorem:
  - If x and y are orthogonal, then
    $$\|\mathbf{x}+\mathbf{y}\|^2 = \|\mathbf{x}\|^2 + \|\mathbf{y}\|^2$$
  - Proof: we know $\mathbf{x}^\top \mathbf{y} = 0$, then
    $$\begin{aligned}\|\mathbf{x}+\mathbf{y}\|^2 &= (\mathbf{x}+\mathbf{y})^\top(\mathbf{x}+\mathbf{y}) \\ &= \|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 + \mathbf{x}^\top\mathbf{y} + \mathbf{y}^\top\mathbf{x} \\ &= \|\mathbf{x}\|^2 + \|\mathbf{y}\|^2\end{aligned}$$



- General case: a set of vectors is orthogonal

$$\|\sum_{i=1}^{n}\mathbf{x}_i\|^2 = \sum_{i=1}^{n}\|\mathbf{x}_i\|^2$$

Orthogonal Matrices

- A square matrix $\mathbf{Q} \in \mathbb{R}^{n \times n}$ is orthogonal if

$$\mathbf{Q}^\top \mathbf{Q} = \mathbf{I} \quad \text{i.e., } \mathbf{Q}^\top = \mathbf{Q}^{-1}$$

- In terms of the columns of Q, the product can be written as

$$\begin{pmatrix} \mathbf{q}_1^\top \\ \mathbf{q}_2^\top \\ \vdots \\ \mathbf{q}_n^\top \end{pmatrix} \begin{pmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots \mathbf{q}_n \end{pmatrix} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}$$

Orthogonal Matrices

$$\begin{pmatrix} \mathbf{q}_1^\top \\ \mathbf{q}_2^\top \\ \vdots \\ \mathbf{q}_n^\top \end{pmatrix} \begin{pmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots \mathbf{q}_n \end{pmatrix} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}$$

$$\mathbf{q}_i^\top \mathbf{q}_j = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

- The columns of orthogonal matrix Q form an orthonormal basis

Orthogonal matrices

- The processes of multiplication by an orthogonal matrices preserves geometric structure
  - Dot products are preserved

$$(\mathbf{Qx}) \cdot (\mathbf{Qy}) = \mathbf{x} \cdot \mathbf{y}$$

$$(\mathbf{Qx})^\top (\mathbf{Qy}) = \mathbf{x}^\top \mathbf{Q}^\top \mathbf{Qy} = \mathbf{x}^\top \mathbf{y}$$

  - Lengths of vectors are preserved

$$\|\mathbf{Qx}\| = \|\mathbf{x}\|$$

  - Angles between vectors are preserved

$$\cos\theta = \frac{(\mathbf{Qx})^\top (\mathbf{Qy})}{\|\mathbf{Qx}\|\|\mathbf{Qy}\|} = \frac{\mathbf{x}^\top \mathbf{y}}{\|\mathbf{x}\|\|\mathbf{y}\|}$$

Tall Matrices with Orthonormal Columns

- Suppose matrix $\mathbf{Q} \in \mathbb{R}^{m \times n}$ is tall (m>n) and has orthogonal columns

- Properties:

$$\mathbf{Q}^\top \mathbf{Q} = \mathbf{I}$$

$$\mathbf{Q}\mathbf{Q}^\top \neq \mathbf{I}$$

Matrix Norms

- Vector p-norms:

$$\|\mathbf{x}\|_p = (|x_1|^p + |x_2|^p + \cdots + |x_n|^p)^{1/p}$$

- Matrix p-norms:

$$\|\mathbf{A}\|_p = \max_{\mathbf{x} \neq 0} \frac{\|\mathbf{A}\mathbf{x}\|_p}{\|\mathbf{x}\|_p}$$

- Example: 1-norm $\|\mathbf{A}\|_1 = \max_j \sum_{i=1}^{n} |a_{ij}|$

- Matrix norms which induced by vector norm are called operator norm.

General Matrix Norms

- A norm is a function $\|\cdot\|$ that satisfies:
  - $\|\mathbf{A}\| \geq 0$ with equality if and only if $\mathbf{A} = 0$
  - $\|\mathbf{A} + \mathbf{B}\| \leq \|\mathbf{A}\| + \|\mathbf{B}\|$
  - $\|\alpha \mathbf{A}\| = |\alpha| \|\mathbf{A}\|$

- Frobenius norm
  - The Frobenius norm of $\mathbf{A} \in \mathbb{R}^{m \times n}$ is:

$$\|\mathbf{A}\|_F = (\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2)^{1/2}$$

Some Properties

- $\|\mathbf{A}\|_F^2 = trace(\mathbf{A}^\top \mathbf{A})$

- $\|\mathbf{AB}\|_F = \|\mathbf{A}\|_F \|\mathbf{B}\|_F$

- Invariance under orthogonal Multiplication

  $$\|\mathbf{QA}\|_2 = \|\mathbf{A}\|_2 \qquad \|\mathbf{QA}\|_F = \|\mathbf{A}\|_F$$

  - Q is an orthogonal matrix

Eigenvalue Decomposition

- For a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, we say that a nonzero vector $\mathbf{x} \in \mathbb{R}^n$ is an eigenvector of A corresponding to eigenvalue λ if

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

- An eigenvalue decomposition of a square matrix A is

$$\mathbf{A} = \mathbf{X}\mathbf{\Lambda}\mathbf{X}^{-1}$$

- X is nonsingular and consists of eigenvectors of A
- $\mathbf{\Lambda}$ is a diagonal matrix with the eigenvalues of A on its diagonal.

Eigenvalue Decomposition

- Not all matrix has eigenvalue decomposition.
  - A matrix has eigenvalue decomposition if and only if it is diagonalizable.

- Real symmetric matrix has real eigenvalues.
- It’s eigenvalue decomposition is the following form:

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^\top$$

- Q is orthogonal matrix.

Singular Value Decomposition(SVD)

- every matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ has an SVD as follows:

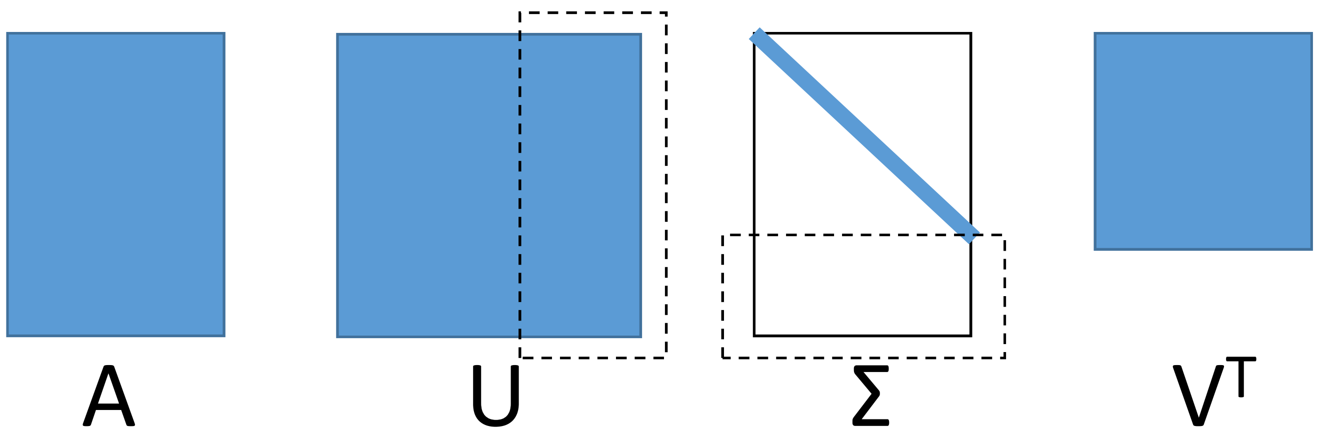
$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$$

- $\mathbf{U} \in \mathbb{R}^{m \times m}$ and $\mathbf{V} \in \mathbb{R}^{n \times n}$ are orthogonal matrices
- $\mathbf{\Sigma} \in \mathbb{R}^{m \times n}$ is a diagonal matrix with the singular values of A on its diagonal.
- Suppose the rank of A is r, the singular values of A is

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r \geq \sigma_{r+1} = \ldots \sigma_{min(m,n)} = 0$$

Full SVD and Reduced SVD

- Assume that $m \geq n$
  - Full SVD: *U* is $m \times m$ matrix, *Σ* is $m \times n$ matrix.
  - Reduced SVD: *U* is $m \times n$ matrix, *Σ* is $n \times n$ matrix.



Properties via the SVD

- The nonzero singular values of A are the square roots of the nonzero eigenvalues of $A^\top A$.

$$\mathbf{A}^\top\mathbf{A} = (\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top)^\top(\mathbf{U}\mathbf{\Sigma}\mathbf{V}) = \mathbf{V}\mathbf{\Sigma}^\top\mathbf{U}^\top\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top = \mathbf{V}(\mathbf{\Sigma}^\top\mathbf{\Sigma})\mathbf{V}^\top$$

- If $A=A^\top$, then the singular values of A are the absolute values of the eigenvalues of A.

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^\top = \mathbf{Q}|\mathbf{\Lambda}|sign(\mathbf{\Lambda})\mathbf{Q}^\top$$

Properties via the SVD

- $\|\mathbf{A}\|_2 = \sigma_1$

  $\|\mathbf{A}\|_F = \sqrt{\sigma_1^2 + \sigma_2^2 + \cdots + \sigma_r^2}$

- Denote $\mathbf{U} = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \dots & \mathbf{u}_m \end{pmatrix}$

$$\mathbf{V} = \begin{pmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \dots & \mathbf{v}_n \end{pmatrix}$$

$$\mathbf{A} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$$

Low-rank Approximation

- $$\mathbf{A} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$$
- For any 0 < *k* < *r*, define $\mathbf{A}_k = \sum_{i=1}^{k} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$
- Eckart-Young Theorem:

$$\min_{rank(\mathbf{B}) \le k} \|\mathbf{A} - \mathbf{B}\|_2 = \|\mathbf{A} - \mathbf{A}_k\|_2 = \sigma_{k+1}$$

$$\min_{rank(\mathbf{B}) \le k} \|\mathbf{A} - \mathbf{B}\|_F = \|\mathbf{A} - \mathbf{A}_k\|_F = \sqrt{\sigma_{k+1}^2 + \cdots + \sigma_r^2}$$

- A_k is the best rank-k approximation of A.

Example

- Image Compression

original
(390*390)

k=10

k=20

k=50

Positive (semi-)definite matrices

- A symmetric matrix A is positive semi-definite(PSD) if for all $\mathbf{x} \in \mathbb{R}^n, \mathbf{x}^\top \mathbf{A}\mathbf{x} \geq 0$

- A symmetric matrix A is positive definite(PD) if for all nonzero $\mathbf{x} \in \mathbb{R}^n, \mathbf{x}^\top \mathbf{A}\mathbf{x} > 0$

- Positive definiteness is a strictly stronger property than positive semi-definiteness.

- Notation: $\mathbf{A} \succeq 0$ if A is PSD, $\mathbf{A} \succ 0$ if A is PD

Properties of PSD matrices

- A symmetric matrix is PSD if and only if all of its eigenvalues are nonnegative.
  - Proof: let *x* be an eigenvector of *A* with eigenvalue *λ*.

$$0 \leq \mathbf{x}^\top \mathbf{A}\mathbf{x} = \mathbf{x}^\top(\lambda \mathbf{x}) = \lambda \mathbf{x}^\top \mathbf{x} = \lambda \|\mathbf{x}\|_2^2$$

- The eigenvalue decomposition of a symmetric PSD matrix is equivalent to its singular value decomposition.

Properties of PSD matrices

- For a symmetric PSD matrix *A*, there exists a unique symmetric PSD matrix *B* such that

$$\mathbf{B}^2 = \mathbf{A}$$

- Proof: We only show the existence of *B*
  - Suppose the eigenvalue decomposition is

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\top$$

  - Then, we can get *B*:

$$\mathbf{B} = \mathbf{U}\boldsymbol{\Lambda}^{\frac{1}{2}}\mathbf{U}^\top$$

$$\mathbf{B}^2 = \mathbf{U}\boldsymbol{\Lambda}^{\frac{1}{2}}\mathbf{U}^\top\mathbf{U}\boldsymbol{\Lambda}^{\frac{1}{2}}\mathbf{U}^\top = \mathbf{U}\boldsymbol{\Lambda}^{\frac{1}{2}}\boldsymbol{\Lambda}^{\frac{1}{2}}\mathbf{U}^\top = \mathbf{A}$$

Convex Optimization

Gradient and Hessian

- The gradient of $f : \mathbb{R}^d \to \mathbb{R}$ is

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_d} \end{pmatrix}$$

- The Hessian of $f : \mathbb{R}^d \to \mathbb{R}$ is

$$\nabla^2 f = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{pmatrix}$$

What is Optimization?

- Finding the minimizer of a function subject to constraints:

$$\min_x \; f(x)$$

$$s.t. \; g_i(x) \leq 0, i = 1, 2, \ldots, m$$

$$h_j(x) = 0, j = 1, 2, \ldots, n$$

Why optimization?

- Optimization is the key of many machine learning algorithms
  - Linear regression:

$$\min_{w} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

  - Logistic regression:

$$\min_{w} \sum_{i=1}^{n} \log(1 + \exp(-\mathbf{y}_i \mathbf{x}_i^\top \mathbf{w}))$$

  - Support vector machine:

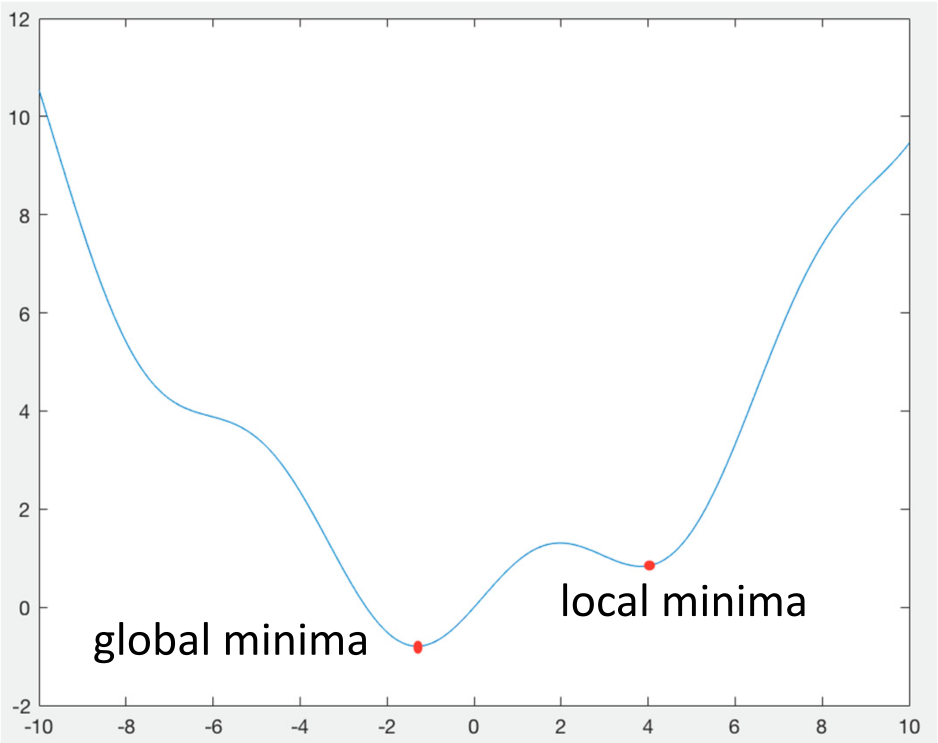
$$\min \|\mathbf{w}\|^2 + C \sum_{i=1}^{n} \xi_i$$

$$s.t.\ \xi_i \geq 1 - \mathbf{y}_i \mathbf{x}_i^\top \mathbf{w}$$

$$\xi_i \geq 0$$

Local Minima and Global Minima

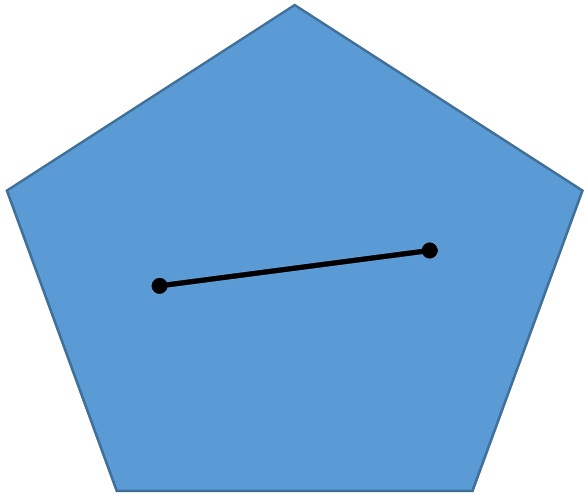
- Local minima
  - a solution that is optimal within a neighboring set
- Global minima
  - the optimal solution among all possible solutions

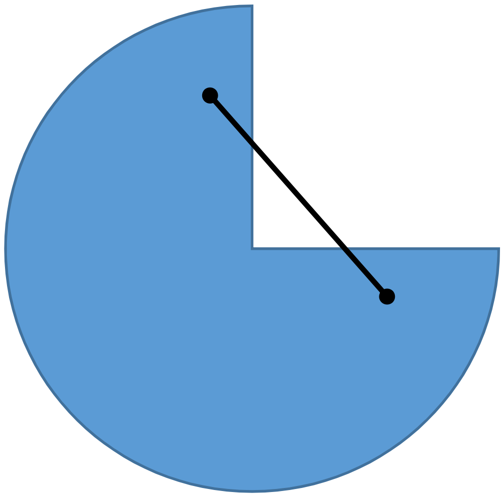


Convex Set

- A set $C \subseteq \mathbb{R}^n$ is convex if for any $x, y \in C$,

$$tx + (1-t)y \in C \text{ for all } \; t \in [0,1]$$





Example of Convex Sets

- Trivial: empty set, line, point, etc.

- Norm ball: $\{x : \|x\| \leq r\}$, for given radius *r*

- Affine space: $\{x : Ax = b\}$, given *A*, *b*

- Polyhedron: $\{x : Ax \leq b\}$, where inequality ≤ is interpreted component-wise.

Operations preserving convexity

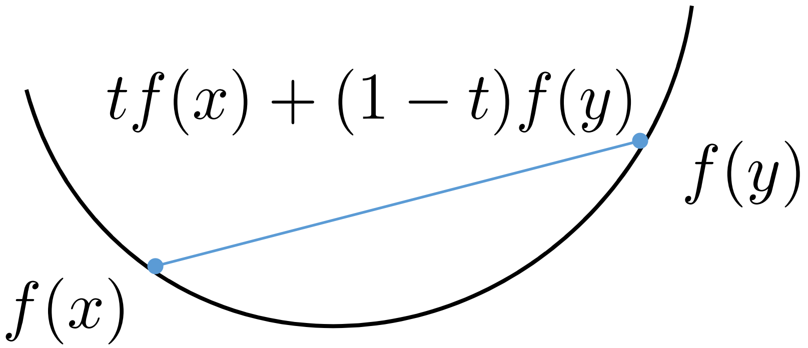
- Intersection: the intersection of convex sets is convex

- Affine images: if $f(x) = Ax + b$ and C is convex, then
$$f(C) = \{Ax + b : x \in C\}$$
is convex

Convex functions

- A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if for $x, y \in dom f$,

$$f(tx + (1-t)y) \leq tf(x) + (1-t)f(y), \text{ for all } t \in [0,1]$$



Strictly Convex and Strongly Convex

- Strictly convex:
  - $$f(tx + (1-t)y) < tf(x) + (1-t)f(y)$$
    $$\text{for } x \neq y \text{ and } 0 < t < 1$$
  - Linear function is not strictly convex.

- Strongly convex:
  - For $m > 0 : f(x) - \frac{m}{2}\|x\|^2$ is convex

- Strong convexity ⇒ strict convexity ⇒ convexity

Example of Convex Functions

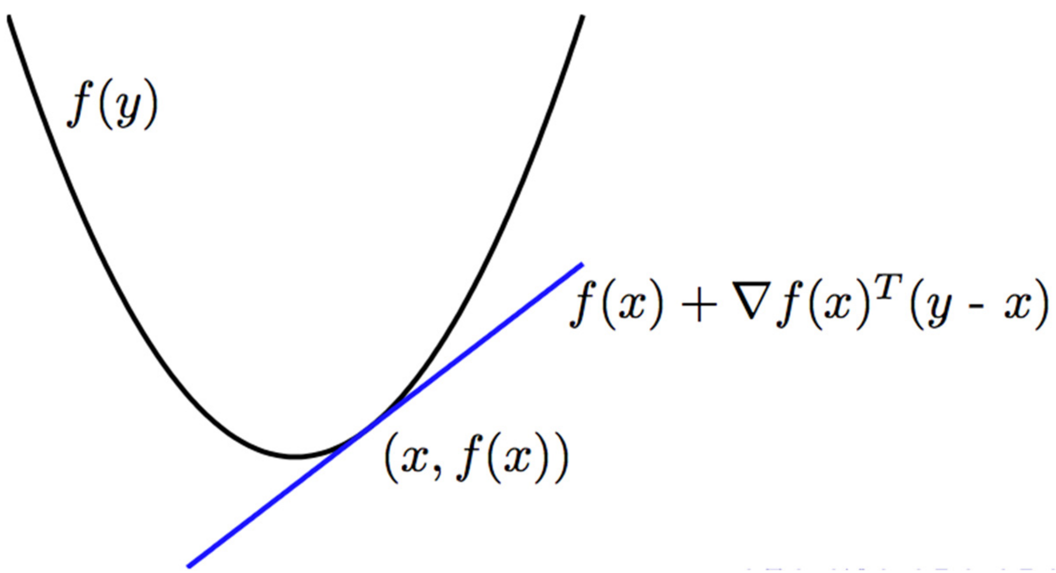
- Exponential function: e^{ax}
- logarithmic function log(*x*) is concave
- Affine function: $a^\top x + b$
- Quadratic function: $x^\top Q x + b^\top x + c$ is convex if Q is positive semidefinite (PSD)
- Least squares loss: $\|y - Ax\|_2^2$
- Norm: $\|x\|$ is convex for any norm

$$\|x\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2} \qquad \|x\|_1 = \sum_{i=1}^{n} |x_i|$$

First order convexity conditions

- Theorem:
- Suppose f is differentiable. Then f is convex if and only if for all $x, y \in dom f$

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x)$$



Second order convexity conditions

- Suppose f is twice differentiable. Then f is convex if and only if for all $x \in dom f$

$$\nabla^2 f(x) \succeq 0$$

Properties of convex functions

- If *x* is a local minimizer of a convex function, it is a global minimizer.

- Suppose *f* is differentiable and convex. Then, *x* is a global minimizer of *f*(*x*) if and only if

$$\nabla f(x) = 0$$

- Proof:
  - $\nabla f(x) = 0$. We have

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x) = f(x)$$

  - $\nabla f(x) \neq 0$. There is a direction of descent.

Gradient Descent

- The simplest optimization method.

- Goal:

$$\min_x f(x)$$

- Iteration:

$$x_{t+1} = x_t - \eta_t \nabla f(x_t)$$

- η_t is step size.

How to choose step size

- If step size is too big, the value of function can diverge.
- If step size is too small, the convergence is very slow.
- Exact line search:

$$\eta_t = \arg\min_{\eta} \; f(x - \eta \nabla f(x))$$

- Usually impractical.

Backtracking Line Search

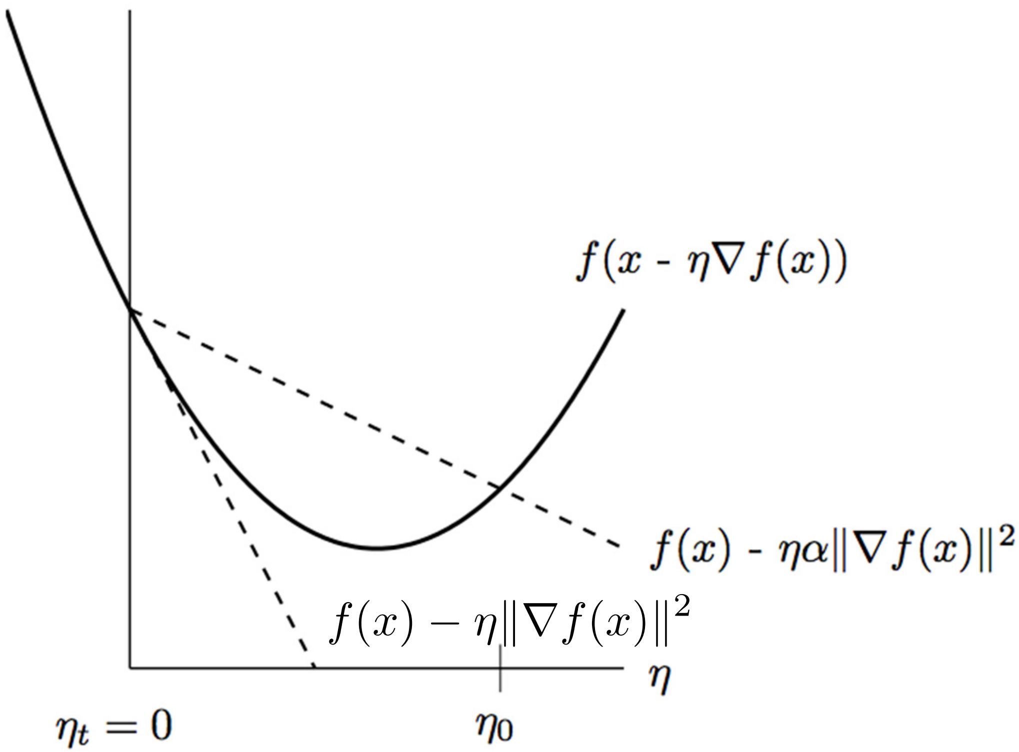
- Let $\alpha \in (0, 1/2], \beta \in (0, 1)$. Start with $\eta = 1$ and multiply $\eta = \beta\eta$ until

$$f(x - \eta \nabla f(x)) \leq f(x) - \alpha\eta \|\nabla f(x)\|^2$$

- Work well in practice.

Backtracking Line Search

- Understanding backtracking Line Search



$$f(x - \eta\nabla f(x)) \leq f(x) - \alpha\eta\|\nabla f(x)\|^2$$

Convergence Analysis

- Assume that f convex and differentiable.
- Lipschitz continuous:

$$\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2$$

- Theorem:
  - Gradient descent with fixed step size $\eta \leq 1/L$ satisfies

$$f(x_t) - f^* \leq \frac{\|x_0 - x^*\|_2^2}{2t\eta}$$

  - To get $f(x_t) - f^* \leq \epsilon$, we need $O(1/\epsilon)$ iterations.
  - Gradient descent with backtracking line search have the same order convergence rate.

Convergence Analysis under Strong Convexity

- Assume f is strongly convex with constant m.
- Theorem:
  - Gradient descent with fixed step size $t \leq 2/(m + L)$ or with backtracking line search satisfies

$$f(x_t) - f^* \leq c^t \frac{L}{2} \|x_0 - x^*\|_2^2$$

  - where $0 < c < 1$.
  - To get $f(x_t) - f^* \leq \epsilon$, we need $O(\log(1/\epsilon))$ iterations.
  - Called linear convergence.

Newton's Method

- Idea: minimize a second-order approximation

$$f(x+v) \approx f(x) + \nabla f(x)^\top v + \frac{1}{2} v^\top \nabla^2 f(x) v$$

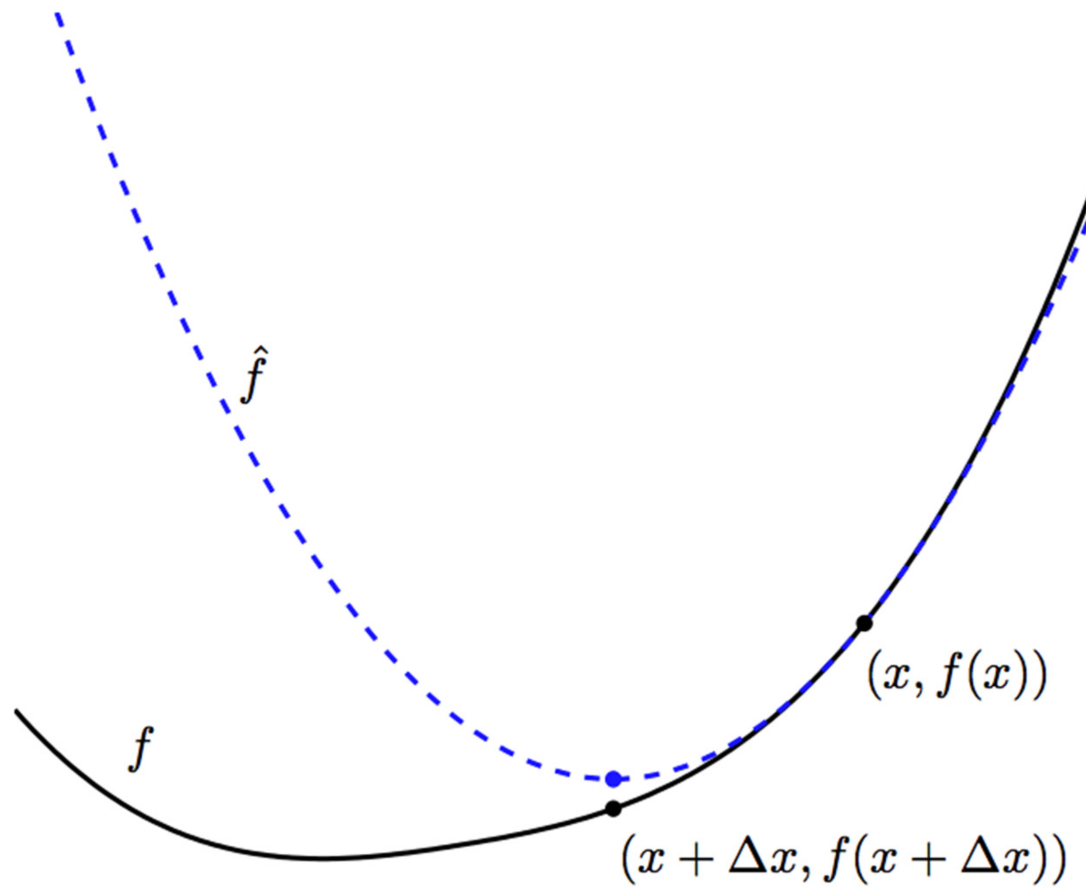
- Choose v to minimize above

$$v = -[\nabla^2 f(x)]^{-1} \nabla f(x)$$

- Newton step:

$$x_{t+1} = x_t - [\nabla^2 f(x_t)]^{-1} \nabla f(x_t)$$

Newton step



Newton's Method

- f is strongly convex
- $\nabla f(x), \nabla^2 f(x)$ are Lipschitz continuous
- Quadratic convergence:
  - convergence rate is O(log log(1/ϵ))
- Locally quadratic convergence: we are only guaranteed quadratic convergence after some number of steps k.

- Drawback: computing the inverse of Hessian is usually very expensive.
- Quasi-Newton, Approximate Newton...

Lagrangian

- Start with optimization problem:

$$\min_x \ f(x)$$

$$s.t. \ g_i(x) \le 0, i = 1, 2, \ldots, m$$

$$h_j(x) = 0, j = 1, 2, \ldots, n$$

- We define Lagrangian as

$$L(x, u, v) = f(x) + \sum_{i=1}^{m} u_i g_i(x) + \sum_{j=1}^{n} v_j h_j(x)$$

- where $u_i \ge 0$

Property

- Lagrangian

$$L(x,u,v) = f(x) + \sum_{i=1}^{m} u_i g_i(x) + \sum_{j=1}^{n} v_j h_j(x)$$

- For any *u* ≥ 0 and *v*, any feasible *x*,

$$L(x,u,v) \leq f(x)$$

Lagrange Dual Function

- Let C denote primal feasible set, f^* denote primal optimal value. Minimizing $L(x, u, v)$ over all x gives a lower bound on f^* for any $u \geq 0$ and v.

$$f^* \geq \min_{x \in C} L(x, u, v) \geq \min_{x} L(x, u, v) = g(u, v)$$

- Form dual function:

$$g(u, v) = \min_{x} L(x, u, v)$$

Lagrange Dual Problem

- Given primal problem

$$\min_{x} \ f(x)$$

$$s.t. \ g_i(x) \leq 0, i = 1, 2, \ldots, m$$

$$h_j(x) = 0, j = 1, 2, \ldots, n$$

- The Lagrange dual problem is:

$$\max_{u,v} \ g(u, v)$$

$$s.t. \ u \geq 0$$

Property

- Weak duality:

$$f^* \geq g^*$$

- The dual problem is a convex optimization problem (even when primal problem is not convex)

$$g(u, v) = \min_x \{f(x) + \sum_{i=1}^{m} u_i g_i(x) + \sum_{j=1}^{n} v_j h_j(x)\}$$

- *g*(*u*,*v*) is concave.

Strong duality

- In some problems we have observed that actually

$$f^* = g^*$$

  which is called strong duality.

- Slater's condition: if the primal is a convex problem, and there exists at least one strictly feasible *x*, i.e,

$$g_1(x) < 0, \ldots, g_m(x) < 0 \text{ and } h_1(x) = \ldots h_n(x) = 0$$

  then strong duality holds

Example

- Primal problem

$$\min_x \; x^\top x$$
$$s.t. \; Ax \le b$$

- Dual function

$$\begin{aligned} g(u) &= \min_x \{x^\top x + u^\top (Ax - b)\} \\ &= -\frac{1}{4} u^\top A A^\top u - b^\top u \end{aligned}$$

- Dual problem

$$\max_u \; -\frac{1}{4} u^\top A A^\top u - b^\top u, s.t. \; u \ge 0$$

- Slater's condition always holds.

References

- A majority part of this lecture is based on CSS 490 / 590 - Introduction to Machine Learning
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