University of Idaho
Department of Computer Science

CS 487/587 Adversarial Machine Learning

Dr. Alex Vakanski

Lecture 3

Mathematics for Machine Learning

Lecture Outline

- Linear algebra
  - Vectors
  - Matrices
  - Eigen decomposition
- Differential calculus
- Optimization algorithms
- Probability
  - Random variables
  - Probability distributions
- Information theory

Notation

• a, b, c	Scalar (integer or real)
• $\mathbf{x}, \mathbf{y}, \mathbf{z}$	Vector (bold-font, lower case)
• $\mathbf{A}, \mathbf{B}, \mathbf{C}$	Matrix (bold-font, upper-case)
• $\mathsf{\mathbf{A}}, \mathsf{\mathbf{B}}, \mathsf{\mathbf{C}}$	Tensor (bold-font, upper-case)
• X, Y, Z	Random variable (normal font, upper-case)
• $a \in \mathcal{A}$	Set membership: a is member of set $\mathcal{A}$
• $\lvert\mathcal{A}\rvert$	Cardinality: number of items in set $\mathcal{A}$
• $\lVert\mathbf{v}\rVert$	Norm of vector $\mathbf{v}$
• $\mathbf{u} \cdot \mathbf{v}$ or $\langle\mathbf{u}, \mathbf{v}\rangle$	Dot product of vectors $\mathbf{u}$ and $\mathbf{v}$
• $\mathbb{R}$	Set of real numbers
• $\mathbb{R}^n$	Real numbers space of dimension n
• $y = f(x)$ or $x \mapsto f(x)$	Function (map): assign a unique value $f(x)$ to each input value x
• $f: \mathbb{R}^n \rightarrow \mathbb{R}$	Function (map): map an n-dimensional vector into a scalar

Notation

$\mathbf{A} \odot \mathbf{B}$	Element-wise product of matrices $\mathbf{A}$ and $\mathbf{B}$
$\mathbf{A}^{\dagger}$	Pseudo-inverse of matrix $\mathbf{A}$
$\frac{d^n f}{dx^n}$	n-th derivative of function f with respect to x
$\nabla_{\mathbf{x}} f(\mathbf{x})$	Gradient of function f with respect to $\mathbf{x}$
$\mathbf{H}_f$	Hessian matrix of function f
$X \sim P$	Random variable X has distribution P
$P(X\|Y)$	Probability of X given Y
$\mathcal{N}(\mu, \sigma^2)$	Gaussian distribution with mean μ and variance σ^2
$\mathbb{E}_{X \sim P}[X]$	Expectation of X drawn from P
$\mathrm{Var}(X)$	Variance of X
$\mathrm{Cov}(X, Y)$	Covariance of X and Y
$\mathrm{corr}(X, Y)$	Correlation coefficient for X and Y
$D_{KL}(P\|\|Q)$	Kullback-Leibler divergence for distributions P and Q
$CE(P, Q)$	Cross-entropy for distributions P and Q

Vectors

- *Vector* definition
  - **Computer science**: *vector* is a one-dimensional array of ordered real-valued scalars
  - **Mathematics**: *vector* is a quantity possessing both magnitude and direction, represented by an arrow indicating the direction, and the length of which is proportional to the magnitude
- Vectors are written in column form or in row form
  - Denoted by bold-font lower-case letters

$$\mathbf{x} = \begin{bmatrix} 1 \\ 7 \\ 0 \\ 1 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} 1 & 7 & 0 & 1 \end{bmatrix}^T$$

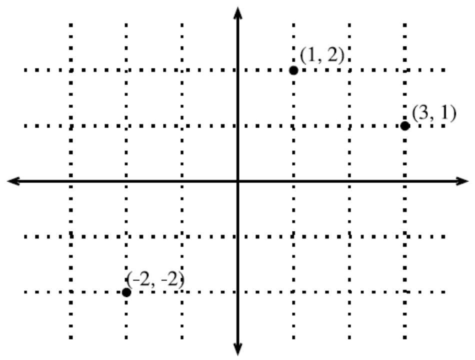
- For a general form vector with n elements, the vector lies in the n-dimensional space $\mathbf{x} \in \mathbb{R}^n$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

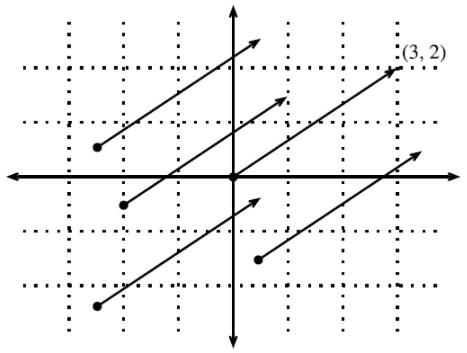
Geometry of Vectors

Vectors

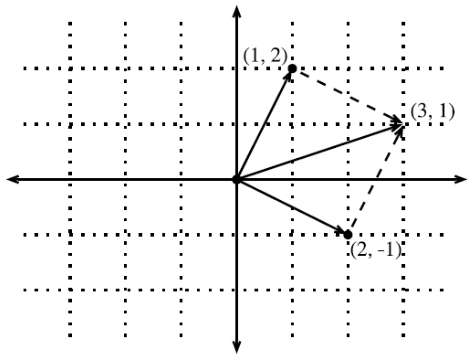
- First interpretation of a vector: point in space
  - E.g., in 2D we can visualize the data points with respect to a coordinate origin



- Second interpretation of a vector: direction in space
  - E.g., the vector $\vec{\mathbf{v}} = [3, 2]^T$ has a direction of 3 steps to the right and 2 steps up
  - The notation $\vec{\mathbf{v}}$ is sometimes used to indicate that the vectors have a direction
  - All vectors in the figure have the same direction



- Vector addition
  - We add the coordinates, and follow the directions given by the two vectors that are added

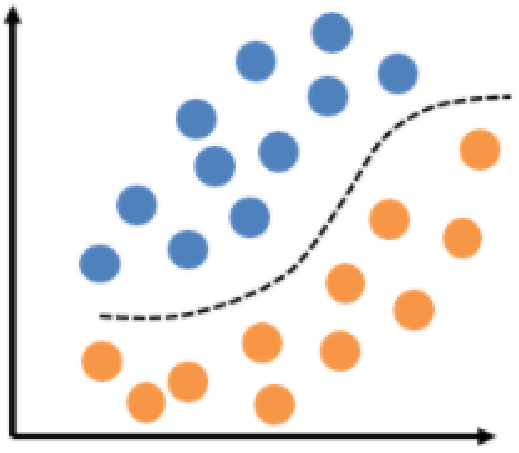


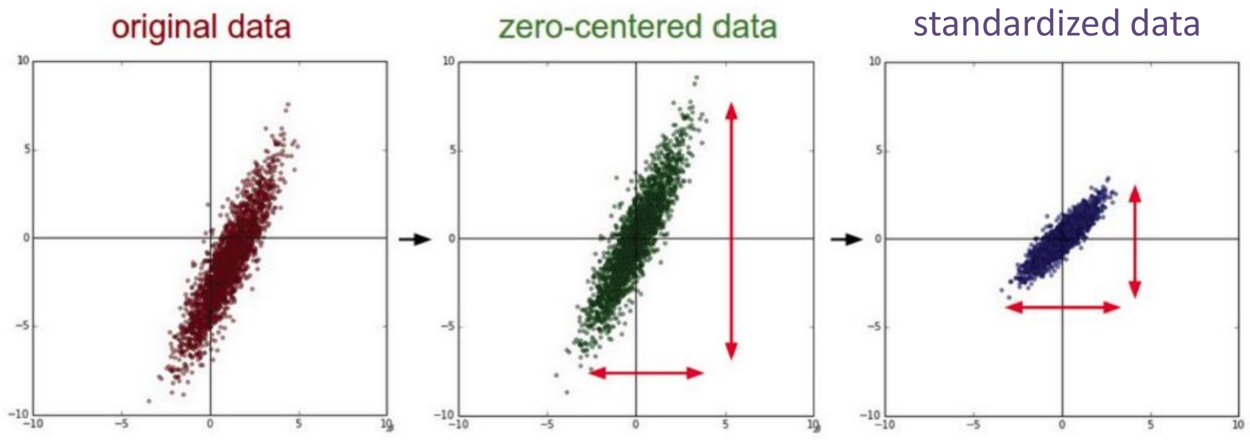
Picture from: http://d2l.ai/chapter_appendix-mathematics-for-deep-learning/geometry-linear-algebraic-ops.html#geometry-of-vectors

Geometry of Vectors

Vectors

- The geometric interpretation of vectors as points in space allow us to consider a training set of input examples in ML as a collection of points in space
  - Hence, classification can be viewed as discovering how to separate the clusters of points belonging to different classes (left picture)
    - Rather than distinguishing images containing cars, planes, buildings, for example
  - Or, it can help to visualize zero-centering and standardization of training data (right figure)



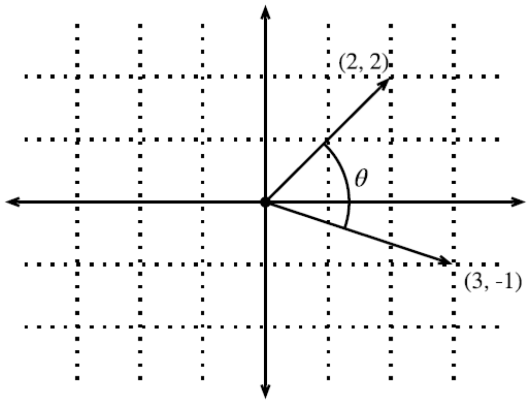


Dot Product and Angles

Vectors

- *Dot product* of vectors, $\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^T \mathbf{v} = \sum_i u_i \cdot v_i$
  - It is also referred to as inner product, or scalar product of vectors
  - The dot product $\mathbf{u} \cdot \mathbf{v}$ is also often denoted by $\langle \mathbf{u}, \mathbf{v} \rangle$
- The dot product is a symmetric operation, $\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^T \mathbf{v} = \mathbf{v}^T \mathbf{u} = \mathbf{v} \cdot \mathbf{u}$
- Geometric interpretation of a dot product: angle between two vectors
  - I.e., dot product $\mathbf{v} \cdot \mathbf{w}$ over the norms of the vectors is $\cos(\theta)$

$$\mathbf{u} \cdot \mathbf{v} = \|\mathbf{u}\|\|\mathbf{v}\| cos(\theta) \qquad \cos\theta = \frac{\mathbf{u} \cdot \mathbf{v}}{\|\mathbf{u}\|\|\mathbf{v}\|}$$



- If two vectors are orthogonal: $\theta = 90°$, i.e., $\cos(\theta) = 0$, then $\mathbf{u} \cdot \mathbf{v} = 0$
- Also, in ML the term $\cos\theta = \frac{\mathbf{u} \cdot \mathbf{v}}{\|\mathbf{u}\|\|\mathbf{v}\|}$ is sometimes employed as a measure of closeness of two vectors/data instances, and it is referred to as cosine similarity

Picture from: http://d2l.ai/chapter_appendix-mathematics-for-deep-learning/geometry-linear-algebraic-ops.html#geometry-of-vectors

Norm of a Vector

- A vector ***norm*** is a function that maps a vector to a scalar value
  - E.g., the norm can be a measure of the size of the vector
- The norm f should satisfy the following properties:
  - Scaling: $f(\alpha\mathbf{x}) = |\alpha| f(\mathbf{x})$
  - Triangle inequality: $f(\mathbf{x}+\mathbf{y}) \le f(\mathbf{x}) + f(\mathbf{y})$
  - Must be non-negative: $f(\mathbf{x}) \ge 0$
- The general ℓ_p norm of a vector $\mathbf{x}$ is obtained as: $\|\mathbf{x}\|_p = \left(\sum_{i=1}^{n} |x_i|^p\right)^{\frac{1}{p}}$
  - On next page we will review common norms, obtained for $p = 1, 2,$ and ∞

Norm of a Vector

- For $p = 2$, we have ℓ_2 norm
  - Also called **Euclidean norm**
  - It is the most often used norm
  - ℓ_2 norm is often denoted just as $\|\mathbf{x}\|$ with the subscript 2 omitted

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

- For $p = 1$, we have ℓ_1 norm
  - Uses the absolute values of the elements
  - Discriminate between zero and non-zero elements

$$\|\mathbf{x}\|_1 = \sum_{i=1}^{n} |x_i|$$

- For $p = \infty$, we have ℓ_∞ norm
  - Known as **infinity norm**, or **max norm**
  - Outputs the absolute value of the largest element

$$\|\mathbf{x}\|_\infty = \max_i |x_i|$$

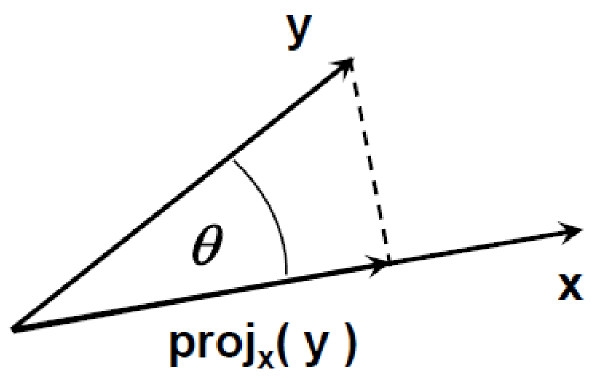
- ℓ_0 norm outputs the number of non-zero elements
  - It is not an ℓ_p norm, and it is not really a norm function either (it is incorrectly called a norm)

Vector Projection

Vectors

- *Orthogonal projection* of a vector **y** onto vector **x**
  - The projection can take place in any space of dimensionality ≥ 2
  - The unit vector in the direction of **x** is $\frac{\mathbf{x}}{\|\mathbf{x}\|}$
    - A unit vector has norm equal to 1
  - The length of the projection of **y** onto **x** is $\|\mathbf{y}\| \cdot cos(\theta)$
  - The orthogonal project is the vector $\mathbf{proj_x(y)}$

$$\mathbf{proj_x}(\mathbf{y}) = \frac{\mathbf{x} \cdot \|\mathbf{y}\| \cdot cos(\theta)}{\|\mathbf{x}\|}$$

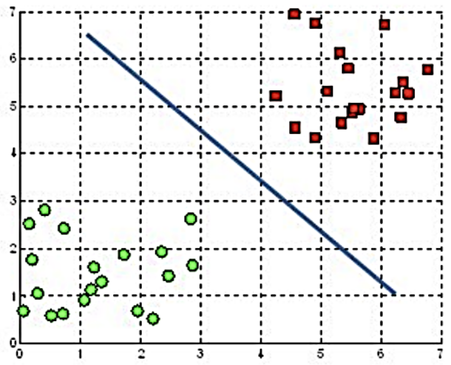


Picture from: Jeff Howbert — Machine Learning Math Essentials

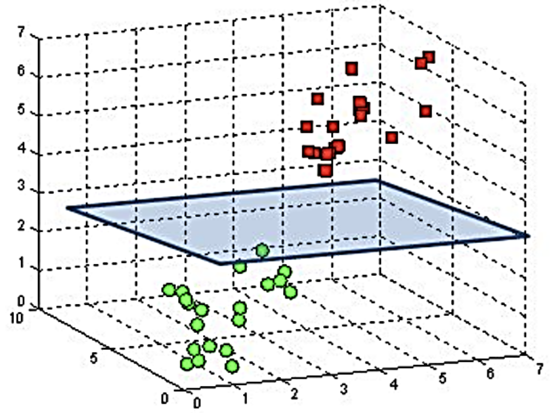
Hyperplanes

- ***Hyperplane*** is a subspace whose dimension is one less than that of its ambient space
  - In a 2D space, a hyperplane is a straight line (i.e., 1D)
  - In a 3D, a hyperplane is a plane (i.e., 2D)
  - In a d-dimensional vector space, a hyperplane has $d - 1$ dimensions, and divides the space into two half-spaces
- Hyperplane is a generalization of a concept of plane in high-dimensional space
- In ML, hyperplanes are decision boundaries used for linear classification
  - Data points falling on either sides of the hyperplane are attributed to different classes

A hyperplane in $\mathbb{R}^2$ is a line



A hyperplane in $\mathbb{R}^3$ is a plane

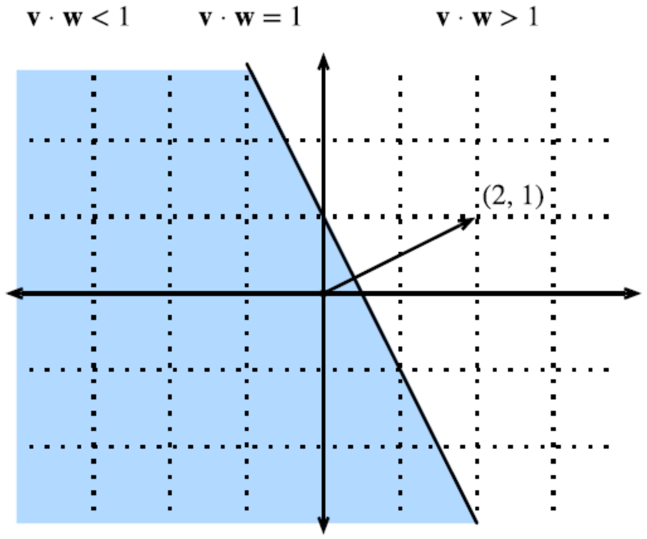


Picture from: https://kgpdag.wordpress.com/2015/08/12/svm-simplified/

Hyperplanes

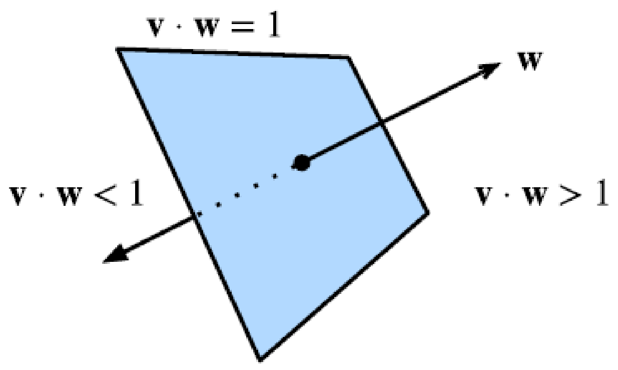
Hyperplanes

- For example, for a given data point $\mathbf{w} = [2, 1]^T$, we can use dot-product to find the hyperplane for which $\mathbf{w} \cdot \mathbf{v} = 1$
  - The solution to $\mathbf{w} \cdot \mathbf{v} = 1$ is the set of points that lay on the line that is orthogonal to the vector $\mathbf{w}$ (the line is $2x + y = 1$)



$\mathbf{v} \cdot \mathbf{w} < 1$
$\mathbf{v} \cdot \mathbf{w} = 1$
$\mathbf{v} \cdot \mathbf{w} > 1$
(2, 1)

- In a 3D space, the points that satisfy $\mathbf{w} \cdot \mathbf{v} = 1$ lay on a plane that is orthogonal to the vector $\mathbf{w}$
  - The inequalities $\mathbf{w} \cdot \mathbf{v} > 1$ and $\mathbf{w} \cdot \mathbf{v} < 1$ define the two subspaces that are created by the plane
  - The same concept applies to high-dimensional spaces as well



$\mathbf{v} \cdot \mathbf{w} = 1$
$\mathbf{w}$
$\mathbf{v} \cdot \mathbf{w} < 1$
$\mathbf{v} \cdot \mathbf{w} > 1$

Picture from: http://d2l.ai/chapter_appendix-mathematics-for-deep-learning/geometry-linear-algebraic-ops.html#hyperplanes

Matrices

- ***Matrix*** is a rectangular array of real-valued scalars arranged in m horizontal rows and n vertical columns
  - Each element a_{ij} belongs to the i^{th} row and j^{th} column
  - The elements are denoted a_{ij} or $\mathbf{A}_{ij}$ or $[\mathbf{A}]_{ij}$ or $\mathbf{A}(\boldsymbol{i}, \boldsymbol{j})$

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

- For the matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, the size (dimension) is $m \times n$ or (m, n)
  - Matrices are denoted by bold-font upper-case letters

Matrices

Matrices

- Addition or subtraction $\left(\mathbf{A} \pm \mathbf{B}\right)_{i,j} = \mathbf{A}_{i,j} \pm \mathbf{B}_{i,j}$

$$\begin{bmatrix} 1 & 3 & 1 \\ 1 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 5 \\ 7 & 5 & 0 \end{bmatrix} = \begin{bmatrix} 1+0 & 3+0 & 1+5 \\ 1+7 & 0+5 & 0+0 \end{bmatrix} = \begin{bmatrix} 1 & 3 & 6 \\ 8 & 5 & 0 \end{bmatrix}$$

- Scalar multiplication $\left(c\mathbf{A}\right)_{i,j} = c \cdot \mathbf{A}_{i,j}$

$$2 \cdot \begin{bmatrix} 1 & 8 & -3 \\ 4 & -2 & 5 \end{bmatrix} = \begin{bmatrix} 2 \cdot 1 & 2 \cdot 8 & 2 \cdot -3 \\ 2 \cdot 4 & 2 \cdot -2 & 2 \cdot 5 \end{bmatrix} = \begin{bmatrix} 2 & 16 & -6 \\ 8 & -4 & 10 \end{bmatrix}$$

- Matrix multiplication $\left(\mathbf{AB}\right)_{i,j} = \mathbf{A}_{i,1}\mathbf{B}_{1,j} + \mathbf{A}_{i,2}\mathbf{B}_{2,j} + \cdots + \mathbf{A}_{i,n}\mathbf{B}_{n,j}$
    - Defined only if the number of columns of the left matrix is the same as the number of rows of the right matrix
    - Note that $\mathbf{AB} \neq \mathbf{BA}$

$$\begin{bmatrix} \underline{2} & \underline{3} & \underline{4} \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & \underline{1000} \\ 1 & \underline{100} \\ 0 & \underline{10} \end{bmatrix} = \begin{bmatrix} 3 & \underline{2340} \\ 0 & 1000 \end{bmatrix}$$

Matrices

- *Transpose* of the matrix: $\mathbf{A}^T$ has the rows and columns exchanged

$$\left(\mathbf{A}^T\right)_{i,j} = \mathbf{A}_{j,i} \qquad \begin{bmatrix} 1 & 2 & 3 \\ 0 & -6 & 7 \end{bmatrix}^{\mathrm{T}} = \begin{bmatrix} 1 & 0 \\ 2 & -6 \\ 3 & 7 \end{bmatrix}$$

  - Some properties

$$\mathbf{A}+\mathbf{B}=\mathbf{B}+\mathbf{A} \qquad \mathbf{A}(\mathbf{B}+\mathbf{C})=\mathbf{AB}+\mathbf{AC}$$
$$(\mathbf{A}+\mathbf{B})^T=\mathbf{A}^T+\boldsymbol{B}^T \qquad \mathbf{A}(\mathbf{BC})=(\mathbf{AB})\mathbf{C}$$
$$(\mathbf{A}^T)^T=\mathbf{A} \qquad (\mathbf{AB})^T=\boldsymbol{B}^T\mathbf{A}^T$$

- *Square matrix*: has the same number of rows and columns
- *Identity matrix* ($\mathbf{I}_n$): has ones on the main diagonal, and zeros elsewhere
  - E.g.: identity matrix of size 3×3 : $\mathbf{I}_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

Matrices

- *Determinant* of a matrix, denoted by $\det(\mathbf{A})$ or $|\mathbf{A}|$, is a real-valued scalar encoding certain properties of the matrix
  - E.g., for a matrix of size 2×2:

$$\det\left(\begin{bmatrix} a & b \\ c & d \end{bmatrix}\right) = ad - bc$$

  - For larger-size matrices the determinant of a matrix id calculated as

$$\det(\mathbf{A}) = \sum_j a_{ij}(-1)^{i+j} det\left(\mathbf{A}_{(i,j)}\right)$$

  - In the above, $\mathbf{A}_{(i,j)}$ is a minor of the matrix obtained by removing the row and column associated with the indices i and j
- *Trace* of a matrix is the sum of all diagonal elements

$$\mathrm{Tr}(\mathbf{A}) = \sum_i a_{ii}$$

- A matrix for which $\mathbf{A} = \mathbf{A}^T$ is called a *symmetric matrix*

Matrices

- Elementwise multiplication of two matrices **A** and **B** is called the ***Hadamard product*** or ***elementwise product***
  - The math notation is $\odot$

$$\mathbf{A} \odot \mathbf{B} = \begin{bmatrix} a_{11}b_{11} & a_{12}b_{12} & \cdots & a_{1n}b_{1n} \\ a_{21}b_{21} & a_{22}b_{22} & \cdots & a_{2n}b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}b_{m1} & a_{m2}b_{m2} & \cdots & a_{mn}b_{mn} \end{bmatrix}$$

Matrix-Vector Products

Matrices

- Consider a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ and a vector $\mathbf{x} \in \mathbb{R}^n$
- The matrix can be written in terms of its row vectors (e.g., $\mathbf{a}_1^T$ is the first row)

$$\mathbf{A} = \begin{bmatrix} \mathbf{a}_1^\top \\ \mathbf{a}_2^\top \\ \vdots \\ \mathbf{a}_m^\top \end{bmatrix}$$

- The matrix-vector product is a column vector of length m, whose i^{th} element is the dot product $\mathbf{a}_i^T\mathbf{x}$

$$\mathbf{A}\mathbf{x} = \begin{bmatrix} \mathbf{a}_1^\top \\ \mathbf{a}_2^\top \\ \vdots \\ \mathbf{a}_m^\top \end{bmatrix} \mathbf{x} = \begin{bmatrix} \mathbf{a}_1^\top \mathbf{x} \\ \mathbf{a}_2^\top \mathbf{x} \\ \vdots \\ \mathbf{a}_m^\top \mathbf{x} \end{bmatrix}$$

- Note the size: $\mathbf{A}(m \times n) \cdot \mathbf{x}(n \times 1) = \mathbf{A}\mathbf{x}(m \times 1)$

Matrix-Matrix Products

Matrices

- To multiply two matrices $\mathbf{A} \in \mathbb{R}^{n \times k}$ and $\mathbf{B} \in \mathbb{R}^{k \times m}$

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nk} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1m} \\ b_{21} & b_{22} & \cdots & b_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ b_{k1} & b_{k2} & \cdots & b_{km} \end{bmatrix}$$

- We can consider the matrix-matrix product as dot-products of rows in **A** and columns in **B**

$$\mathbf{C} = \mathbf{AB} = \begin{bmatrix} \mathbf{a}_1^\top \\ \mathbf{a}_2^\top \\ \vdots \\ \mathbf{a}_n^\top \end{bmatrix} \begin{bmatrix} \mathbf{b}_1 & \mathbf{b}_2 & \cdots & \mathbf{b}_m \end{bmatrix} = \begin{bmatrix} \mathbf{a}_1^\top \mathbf{b}_1 & \mathbf{a}_1^\top \mathbf{b}_2 & \cdots & \mathbf{a}_1^\top \mathbf{b}_m \\ \mathbf{a}_2^\top \mathbf{b}_1 & \mathbf{a}_2^\top \mathbf{b}_2 & \cdots & \mathbf{a}_2^\top \mathbf{b}_m \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{a}_n^\top \mathbf{b}_1 & \mathbf{a}_n^\top \mathbf{b}_2 & \cdots & \mathbf{a}_n^\top \mathbf{b}_m \end{bmatrix}$$

- Size: $\mathbf{A}(n \times k) \cdot \mathbf{B}(k \times m) = \mathbf{C}(n \times m)$

Linear Dependence

Matrices

- For the following matrix $\mathbf{B} = \begin{bmatrix} 2 & -1 \\ 4 & -2 \end{bmatrix}$
- Notice that for the two columns $\mathbf{b}_1 = [2, 4]^T$ and $\mathbf{b}_2 = [-1, -2]^T$, we can write $\mathbf{b}_1 = -2 \cdot \mathbf{b}_2$
  - This means that the two columns are linearly dependent
- The weighted sum $a_1\mathbf{b}_1 + a_2\mathbf{b}_2$ is referred to as a linear combination of the vectors $\mathbf{b}_1$ and $\mathbf{b}_2$
  - In this case, a linear combination of the two vectors exist for which $\mathbf{b}_1 + 2 \cdot \mathbf{b}_2 = \mathbf{0}$
- A collection of vectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k$ are ***linearly dependent*** if there exist coefficients $a_1, a_2, \dots, a_k$ not all equal to zero, so that

$$\sum_{i=1}^{k} a_i \mathbf{v_i} = 0$$

- If there is no linear dependence, the vectors are ***linearly independent***

Matrix Rank

- For an $n \times m$ matrix, the *rank* of the matrix is the largest number of linearly independent columns
- The matrix $\mathbf{B}$ from the previous example has $rank(\mathbf{B}) = 1$, since the two columns are linearly dependent

$$\mathbf{B} = \begin{bmatrix} 2 & -1 \\ 4 & -2 \end{bmatrix}$$

- The matrix $\mathbf{C}$ below has $rank(\mathbf{C}) = 2$, since it has two linearly independent columns
    - I.e., $\mathbf{c}_4 = -1 \cdot \mathbf{c}_1$, $\mathbf{c}_5 = -1 \cdot \mathbf{c}_3$, $\mathbf{c}_2 = 3 \cdot \mathbf{c}_1 + 3 \cdot \mathbf{c}_3$

$$\mathbf{C} = \begin{bmatrix} 1 & 3 & 0 & -1 & 0 \\ -1 & 0 & 1 & 1 & -1 \\ 0 & 3 & 1 & 0 & -1 \\ 2 & 3 & -1 & -2 & 1 \end{bmatrix}$$

Inverse of a Matrix

Matrices

- For a square $n \times n$ matrix $\mathbf{A}$ with rank n, $\mathbf{A}^{-1}$ is its ***inverse matrix*** if their product is an identity matrix $\mathbf{I}$

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$$

- Properties of inverse matrices

$$\left(\mathbf{A}^{-1}\right)^{-1} = \mathbf{A}$$

$$\left(\mathbf{A}\mathbf{B}\right)^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$$

- If $\det(A) = 0$ (i.e., $\text{rank}(A) < n$), then the inverse does not exist
  - A matrix that is not invertible is called a singular matrix
- Note that finding an inverse of a large matrix is computationally expensive
  - In addition, it can lead to numerical instability
- If the inverse of a matrix is equal to its transpose, the matrix is said to be orthogonal matrix

$$\mathbf{A}^{-1} = \mathbf{A}^{T}$$

Pseudo-Inverse of a Matrix

- ***Pseudo-inverse*** of a matrix
  - Also known as Moore-Penrose pseudo-inverse
- For matrices that are not square, the inverse does not exist
  - Therefore, a pseudo-inverse is used
- If $m < n$, then the pseudo-inverse is $\mathbf{A}^{\dagger} = \left(\mathbf{A}^{\mathrm{T}}\mathbf{A}\right)^{-1}\mathbf{A}^{T}$ and $\mathbf{A}^{\dagger}\mathbf{A} = \mathbf{I}$
  - E.g., for a matrix with dimension $\mathbf{X}_{2\times3}$, a pseudo-inverse can be found of size $\mathbf{X}^{\dagger}_{3\times2}$, so that $\mathbf{X}^{\dagger}_{3\times2}\mathbf{X}_{2\times3} = \mathbf{I}_{3\times3}$
- If $m > n$, then the pseudo-inverse is $\mathbf{A}^{\dagger} = \mathbf{A}^{T}\left(\mathbf{A}\mathbf{A}^{\mathrm{T}}\right)^{-1}$ and $\mathbf{A}\mathbf{A}^{\dagger} = \mathbf{I}$
  - E.g., for a matrix with dimension $\mathbf{X}_{3\times2}$, a pseudo-inverse can be found of size $\mathbf{X}^{\dagger}_{2\times3}$, so that $\mathbf{X}_{3\times2}\mathbf{X}^{\dagger}_{2\times3} = \mathbf{I}_{3\times3}$

Tensors

- *Tensors* are n-dimensional arrays of scalars
  - Vectors are first-order tensors, $\mathbf{v} \in \mathbb{R}^n$
  - Matrices are second-order tensors, $\mathbf{A} \in \mathbb{R}^{m \times n}$
  - E.g., a fourth-order tensor is $\mathsf{T} \in \mathbb{R}^{n_1 \times n_2 \times n_3 \times n_4}$
- Tensors are denoted with upper-case letters of a special font face (e.g., X, Y, Z)
- RGB images are third-order tensors, i.e., as they are 3-dimensional arrays
  - The 3 axes correspond to width, height, and channel
  - E.g., $224 \times 224 \times 3$
  - The channel axis corresponds to the color channels (red, green, and blue)

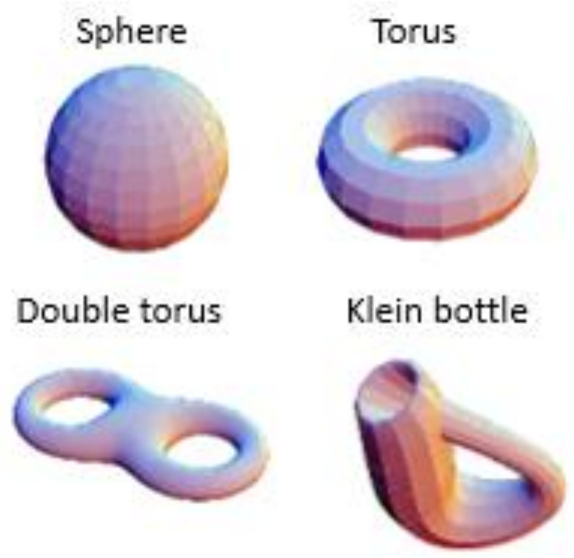
Manifolds

- Earlier we learned that hyperplanes generalize the concept of planes in high-dimensional spaces
  - Similarly, manifolds can be informally imagined as generalization of the concept of surfaces in high-dimensional spaces
- To begin with an intuitive explanation, the surface of the Earth is an example of a two-dimensional manifold embedded in a three-dimensional space
  - This is true because the Earth looks locally flat, so on a small scale it is like a 2-D plane
  - However, if we keep walking on the Earth in one direction, we will eventually end up back where we started
    - This means that Earth is not really flat, it only looks locally like a Euclidean plane, but at large scales it folds up on itself, and has a different global structure than a flat plane

Manifolds

Manifolds

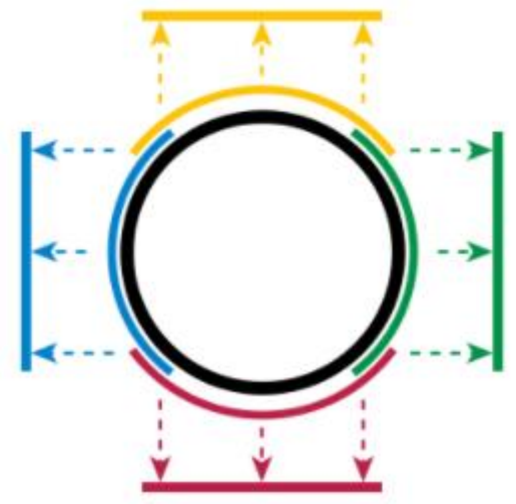
- Manifolds are studied in mathematics under topological spaces
- An *n*-dimensional ***manifold*** is defined as a topological space with the property that each point has a neighborhood that is homeomorphic to the Euclidean space of dimension *n*
  - This means that a manifold locally resembles Euclidean space near each point
  - Informally, a Euclidean space is locally smooth, it does not have holes, edges, or other sudden changes, and it does not have intersecting neighborhoods
  - Although the manifolds can have very complex structure on a large scale, resemblance of the Euclidean space on a small scale allows to apply standard math concepts
- Examples of 2-dimensional manifolds are shown in the figure
  - The surfaces in the figure have been conveniently cut up into little rectangles that were glued together
  - Those small rectangles locally look like flat Euclidean planes

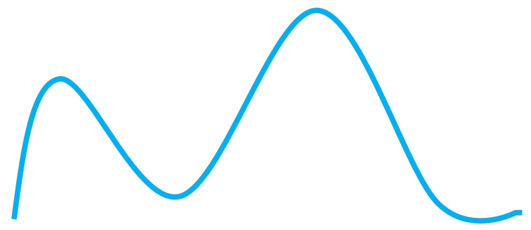


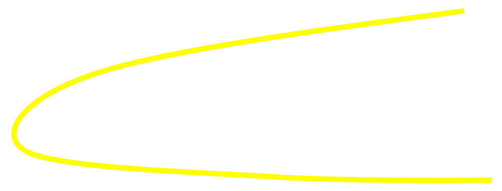
Picture from: http://bjlkeng.github.io/posts/manifolds/

Manifolds

- Examples of one-dimensional manifolds
  - Upper figure: a circle is a l-D manifold embedded in 2-D, where each arc of the circle locally resembles a line segment
  - Lower figures: other examples of 1-D manifolds
  - Note that a number 8 figure is not a manifold because it has an intersecting point (it is not Euclidean locally)
- It is hypothesized that in the real-world, high-dimensional data (such as images) lie on low-dimensional manifolds embedded in the high-dimensional space
  - E.g., in ML, let's assume we have a training set of images with size 224 × 224 × 3 pixels
  - Learning an arbitrary function in such high-dimensional space would be intractable
  - Despite that, all images of the same class ("cats" for example) might lie on a low-dimensional manifold
  - This allows function learning and image classification



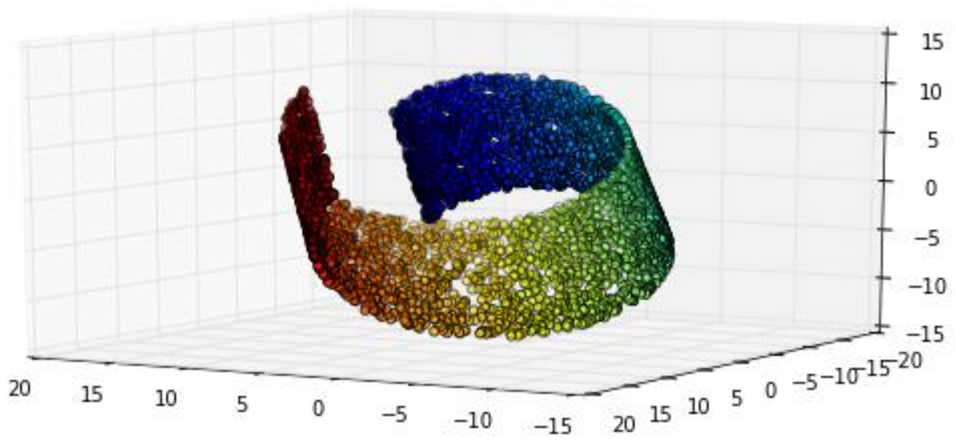


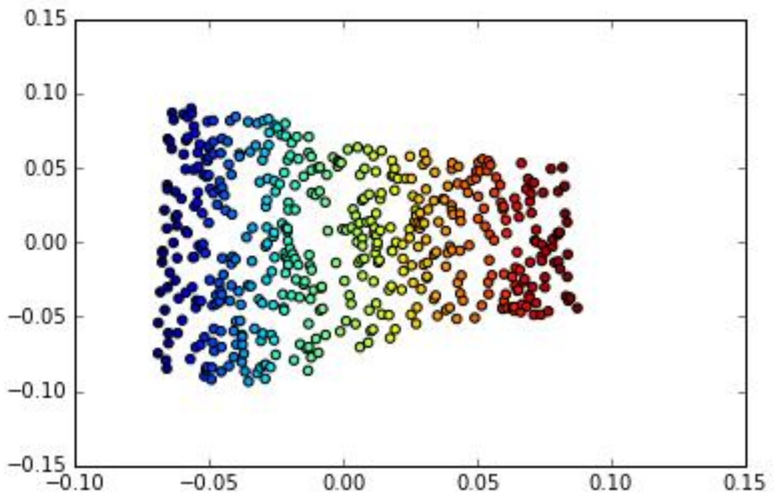


Picture from: http://bjlkeng.github.io/posts/manifolds/

Manifolds

- Example:
    - The data points have 3 dimensions (left figure), i.e., the input space of the data is 3-dimensional
    - The data points lie on a 2-dimensional manifold, shown in the right figure
    - Most ML algorithms extract lower-dimensional data features that enable to distinguish between various classes of high-dimensional input data
        - The low-dimensional representations of the input data are called embeddings





Eigen Decomposition

- *Eigen decomposition* is decomposing a matrix into a set of eigenvalues and eigenvectors
- *Eigenvalues* of a square matrix **A** are scalars λ and *eigenvectors* are non-zero vectors **v** that satisfy

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

- Eigenvalues are found by solving the following equation

$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0$$

- If a matrix **A** has n linearly independent eigenvectors $\{\mathbf{v}^1, \dots, \mathbf{v}^n\}$ with corresponding eigenvalues $\{\lambda_1, \dots, \lambda_n\}$, the eigen decomposition of **A** is given by

$$\mathbf{A} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{-1}$$

  - Columns of the matrix **V** are the eigenvectors, i.e., $\mathbf{V} = [\mathbf{v}^1, \dots, \mathbf{v}^n]$
  - $\boldsymbol{\Lambda}$ is a diagonal matrix of the eigenvalues, i.e., $\boldsymbol{\Lambda} = [\lambda_1, \dots, \lambda_n]$
- To find the inverse of the matrix A, we can use $\mathbf{A}^{-1} = \mathbf{V}\boldsymbol{\Lambda}^{-1}\mathbf{V}^{-1}$
  - This involves simply finding the inverse $\boldsymbol{\Lambda}^{-1}$ of a diagonal matrix

Eigen Decomposition

Eigen Decomposition

- Decomposing a matrix into eigenvalues and eigenvectors allows to analyze certain properties of the matrix
  - If all eigenvalues are positive, the matrix is positive definite
  - If all eigenvalues are positive or zero-valued, the matrix is positive semidefinite
  - If all eigenvalues are negative or zero-values, the matrix is negative semidefinite
    - Positive semidefinite matrices are interesting because they guarantee that $\forall \mathbf{x}, \mathbf{x}^T \mathbf{A} \mathbf{x} \geq 0$
- Eigen decomposition can also simplify many linear-algebraic computations
  - The determinant of A can be calculated as

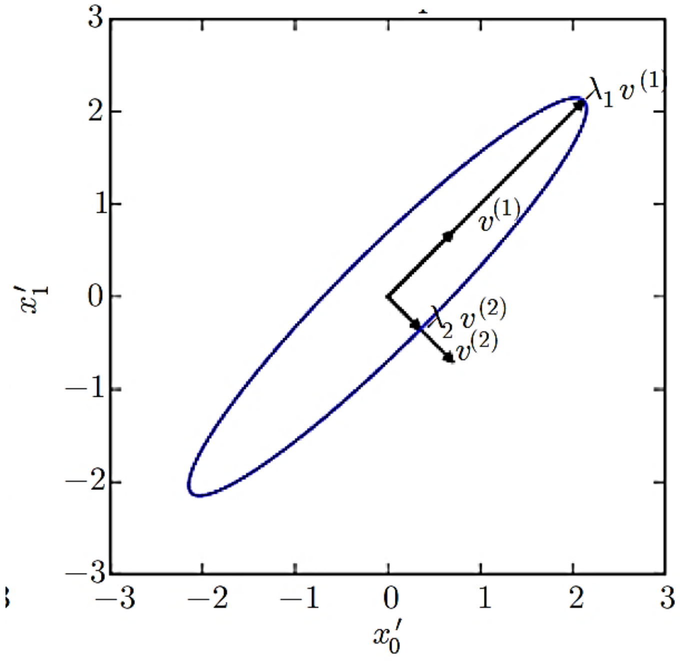
$$\det(\mathbf{A}) = \lambda_1 \cdot \lambda_2 \cdots \lambda_n$$

  - If any of the eigenvalues are zero, the matrix is singular (it does not have an inverse)
- However, eigen decomposition is defined only for square matrices
  - Also, in some cases the decomposition may involve complex numbers
  - Still, every real symmetric matrix is guaranteed to have an eigen decomposition according to $\mathbf{A} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{-1}$, where $\mathbf{V}$ is an orthogonal matrix

Eigen Decomposition

Eigen Decomposition

- Geometric interpretation of the eigenvalues and eigenvectors is that they allow to stretch the space in specific directions
  - Figure: the two eigenvectors $\mathbf{v}^1$ and $\mathbf{v}^2$ are multiplied with the eigenvalues λ_1 and λ_2
    - We can see how the space is scaled in the direction of the larger eigenvalue λ_1
- E.g., this is used for dimensionality reduction with PCA (principal component analysis) where the eigenvectors corresponding to the largest eigenvalues are used for extracting the most important data dimensions



Picture from: Goodfellow (2017) – Deep Learning

Singular Value Decomposition

- ***Singular value decomposition*** (SVD) provides another way to factorize a matrix, into singular vectors and singular values
  - SVD is more generally applicable than eigen decomposition
  - Every real matrix has an SVD, but the same is not true of the eigen decomposition
    - E.g., if a matrix is not square, the eigen decomposition is not defined, and we must use SVD
- SVD of an $m \times n$ matrix $\mathbf{A}$ is given by

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^{\boldsymbol{T}}$$

  - $\mathbf{U}$ is an $m \times m$ matrix, $\mathbf{D}$ is an $m \times n$ matrix, and $\mathbf{V}$ is an $n \times n$ matrix
  - The elements along the diagonal of $\mathbf{D}$ are known as the singular values of A
  - The columns of $\mathbf{U}$ are known as the left-singular vectors
  - The columns of $\mathbf{V}$ are known as the right-singular vectors
- For a non-square matrix $\mathbf{A}$, the squares of the singular values σ_i are the eigenvalues λ_i of $\mathbf{A}^{\boldsymbol{T}}\mathbf{A}$, i.e., $\sigma_i^2 = \lambda_i$ for $i = 1,2, \dots, n$
- Applications of SVD include computing the pseudo-inverse of non-square matrices, matrix approximation, determining the matrix rank

Matrix Norms

- ***Frobenius norm*** – calculates the square-root of the summed squares of the elements of matrix **X**
  - This norm is similar to Euclidean norm of a vector

$$\|\mathbf{X}\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} x_{ij}^2}$$

- ***Spectral norm*** – is the largest singular value of matrix **X**
  - Denoted $\|\mathbf{X}\|_2$
  - The singular values of **X** are $\sigma_1, \sigma_2, \ldots, \sigma_m$

$$\|\mathbf{X}\|_2 = \sigma_{max}(\mathbf{X})$$

- ***$L_{2,1}$ norm*** – is the sum of the Euclidean norms of the columns of matrix **X**

$$\|\mathbf{X}\|_{2,1} = \sum_{j=1}^{n}\sqrt{\sum_{i=1}^{m} x_{ij}^2}$$

- ***Max norm*** – is the largest element of matrix **X**

$$\|\mathbf{X}\|_{\max} = \max_{i,j}\left(x_{ij}\right)$$

Differential Calculus

- For a function $f: \mathbb{R} \rightarrow \mathbb{R}$, the ***derivative*** of f is defined as

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- If $f'(a)$ exists, f is said to be differentiable at a
- If $f'(c)$ is differentiable for $\forall c \in [a, b]$, then f is differentiable on this interval
  - We can also interpret the derivative $f'(x)$ as the instantaneous rate of change of $f(x)$ with respect to x
  - I.e., for a small change in x, what is the rate of change of $f(x)$
- Given $y = f(x)$, where x is an independent variable and y is a dependent variable, the following expressions are equivalent:

$$f'(x) = f' = \frac{dy}{dx} = \frac{df}{dx} = \frac{d}{dx} f(x) = Df(x) = D_x f(x)$$

- The symbols $\frac{d}{dx}$, D, and D_x are differentiation operators that indicate operation of differentiation

Differential Calculus

- The following rules are used for computing the derivatives of explicit functions
  - **Derivative of constants.** $\frac{d}{dx}c = 0$.
  - **Derivative of linear functions.** $\frac{d}{dx}(ax) = a$.
  - **Power rule.** $\frac{d}{dx}x^n = nx^{n-1}$.
  - **Derivative of exponentials.** $\frac{d}{dx}e^x = e^x$.
  - **Derivative of the logarithm.** $\frac{d}{dx}\log(x) = \frac{1}{x}$.
  - **Sum rule.** $\frac{d}{dx}(g(x) + h(x)) = \frac{dg}{dx}(x) + \frac{dh}{dx}(x)$.
  - **Product rule.** $\frac{d}{dx}(g(x) \cdot h(x)) = g(x)\frac{dh}{dx}(x) + \frac{dg}{dx}(x)h(x)$.
  - **Chain rule.** $\frac{d}{dx}g(h(x)) = \frac{dg}{dh}(h(x)) \cdot \frac{dh}{dx}(x)$.

Higher Order Derivatives

Differential Calculus

- The derivative of the first derivative of a function $f(x)$ is the ***second derivative*** of $f(x)$

$$\frac{d^2 f}{dx^2} = \frac{d}{dx}\left(\frac{df}{dx}\right)$$

- The second derivative quantifies how the rate of change of $f(x)$ is changing
  - E.g., in physics, if the function describes the displacement of an object, the first derivative gives the velocity of the object (i.e., the rate of change of the position)
  - The second derivative gives the acceleration of the object (i.e., the rate of change of the velocity)
- If we apply the differentiation operation any number of times, we obtain the n-th derivative of $f(x)$

$$f^{(n)}(x) = \frac{d^n f}{dx^n} = \left(\frac{d}{dx}\right)^n f(x)$$

Taylor Series

Differential Calculus

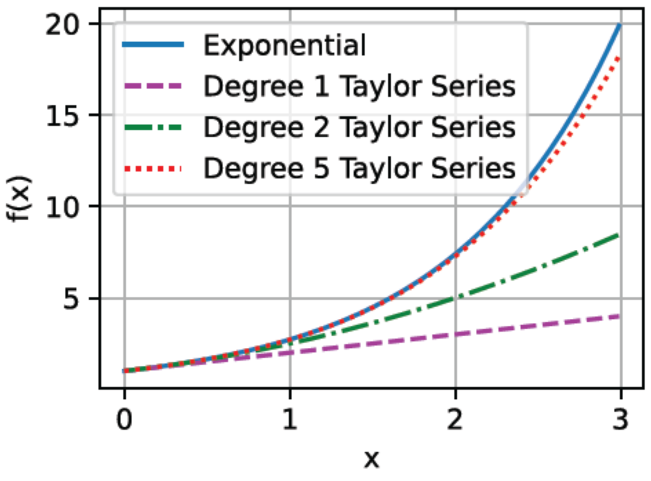
- ***Taylor series*** provides a method to approximate any function $f(x)$ at a point x_0 if we have the first n derivatives $\{f(x_0), f^{(1)}(x_0), f^{(2)}(x_0), \ldots, f^{(n)}(x_0)\}$
- For instance, for $n = 2$, the second-order approximation of a function $f(x)$ is

$$f(x) \approx \frac{1}{2}\frac{d^2 f}{dx^2}\bigg|_{x_0}(x - x_0)^2 + \frac{df}{dx}\bigg|_{x_0}(x - x_0) + f(x_0)$$

- Similarly, the approximation of $f(x)$ with a Taylor polynomial of n-degree is

$$f(x) \approx \sum_{i=0}^{n} \frac{1}{i!}\frac{d^{(i)} f}{dx^i}\bigg|_{x_0}(x - x_0)^i$$

- For example, the figure shows the first-order, second-order, and fifth-order polynomial of the exponential function $f(x) = e^x$ at the point $x_0 = 0$



Picture from: http://d2l.ai/chapter_appendix-mathematics-for-deep-learning/single-variable-calculus.html

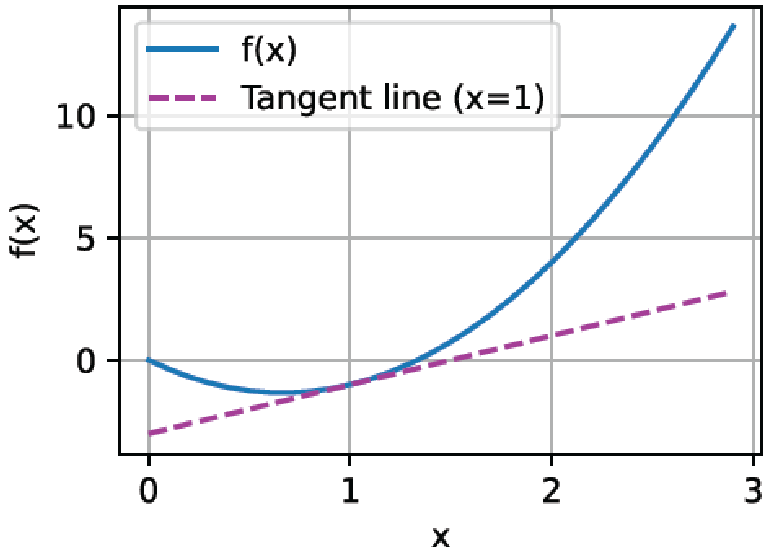
Geometric Interpretation

- To provide a geometric interpretation of the derivatives, let's consider a first-order Taylor series approximation of $f(x)$ at $x = x_0$

$$f(x) \approx f(x_0) + \left.\frac{df}{dx}\right|_{x_0} (x - x_0)$$

- The expression approximates the function $f(x)$ by a line which passes through the point $\left(x_0, f(x_0)\right)$ and has slope $\left.\frac{df}{dx}\right|_{x_0}$ (i.e., the value of $\frac{df}{dx}$ at the point x_0)

- Therefore, the first derivative of a function is also the slope of the tangent line to the curve of the function



Picture from: http://d2l.ai/chapter_appendix-mathematics-for-deep-learning/single-variable-calculus.html

Partial Derivatives

- So far, we looked at functions of a single variable, where $f: \mathbb{R} \to \mathbb{R}$
- Functions that depend on many variables are called multivariate functions
- Let $y = f(\mathbf{x}) = f(x_1, x_2, \dots, x_n)$ be a multivariate function with n variables
  - The input is an n-dimensional vector $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$ and the output is a scalar y
  - The mapping is $f: \mathbb{R}^n \to \mathbb{R}$
- The ***partial derivative*** of y with respect to its ith parameter x_i is

$$\frac{\partial y}{\partial x_i} = \lim_{h \to 0} \frac{f(x_1, x_2, \dots, x_i + h, \dots, x_n) - f(x_1, x_2, \dots, x_i, \dots, x_n)}{h}$$

- To calculate $\frac{\partial y}{\partial x_i}$ (∂ pronounced "del" or we can just say "partial derivative"), we can treat $x_1, x_2, \dots, x_{i-1}, \quad x_{i+1} \dots, x_n$ as constants and calculate the derivative of y only with respect to x_i
- For notation of partial derivatives, the following are equivalent:

$$\frac{\partial y}{\partial x_i} = \frac{\partial f}{\partial x_i} = \frac{\partial}{\partial x_i} f(\mathbf{x}) = f_{x_i} = f_i = D_i f = D_{x_i} f$$

Gradient

Differential Calculus

- We can concatenate partial derivatives of a multivariate function with respect to all its input variables to obtain the ***gradient*** vector of the function
- The gradient of the multivariate function $f(\mathbf{x})$ with respect to the n-dimensional input vector $\mathbf{x} = [x_1, x_2, \ldots, x_n]^T$, is a vector of n partial derivatives

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \left[\frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2}, \ldots, \frac{\partial f(\mathbf{x})}{\partial x_n}\right]^T$$

- When there is no ambiguity, the notations $\nabla f(\mathbf{x})$ or $\nabla_{\mathbf{x}} f$ are often used for the gradient instead of $\nabla_{\mathbf{x}} f(\mathbf{x})$
  - The symbol for the gradient is the Greek letter ∇ (pronounced "nabla"), although $\nabla_{\mathbf{x}} f(\mathbf{x})$ is more often it is pronounced "gradient of f with respect to $\mathbf{x}$"
- In ML, the gradient descent algorithm relies on the opposite direction of the gradient of the loss function $\mathcal{L}$ with respect to the model parameters θ ($\nabla_{\theta}\mathcal{L}$) for minimizing the loss function
  - Adversarial examples can be created by adding perturbation in the direction of the gradient of the loss $\mathcal{L}$ with respect to input examples x ($\nabla_x \mathcal{L}$) for maximizing the loss function

Hessian Matrix

Differential Calculus

- To calculate the second-order partial derivatives of multivariate functions, we need to calculate the derivatives for all combination of input variables
- That is, for a function $f(\mathbf{x})$ with an n-dimensional input vector $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$, there are n^2 second partial derivatives for any choice of i and j

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial}{\partial x_i}\left(\frac{\partial f}{\partial x_j}\right)$$

- The second partial derivatives are assembled in a matrix called the ***Hessian***

$$\mathbf{H}_f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{bmatrix}$$

- Computing and storing the Hessian matrix for functions with high-dimensional inputs can be computationally prohibitive
  - E.g., the loss function for a ResNet50 model with approximately 23 million parameters, has a Hessian of 23 M × 23 M = 529 T (trillion) parameters

Jacobian Matrix

Differential Calculus

- The concept of derivatives can be further generalized to vector-valued functions (or, vector fields) $f: \mathbb{R}^n \to \mathbb{R}^m$
- For an n-dimensional input vector $\mathbf{x} = [x_1, x_2, \ldots, x_n]^T \in \mathbb{R}^n$, the vector of functions is given as

$$\mathbf{f}(\mathbf{x}) = [f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_m(\mathbf{x})]^T \in \mathbb{R}^m$$

- The matrix of first-order partial derivates of the vector-valued function $\mathbf{f}(\mathbf{x})$ is an $m \times n$ matrix called a ***Jacobian***

$$\mathbf{J} = \begin{bmatrix} \frac{\partial f_1(\mathbf{x})}{\partial x_1} & \cdots & \frac{\partial f_1(\mathbf{x})}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m(\mathbf{x})}{\partial x_1} & \cdots & \frac{\partial f_m(\mathbf{x})}{\partial x_n} \end{bmatrix}$$

  - For example, in robotics a robot Jacobian matrix gives the partial derivatives of the translational and angular velocities of the robot end-effector with respect to the joints (i.e., axes) velocities

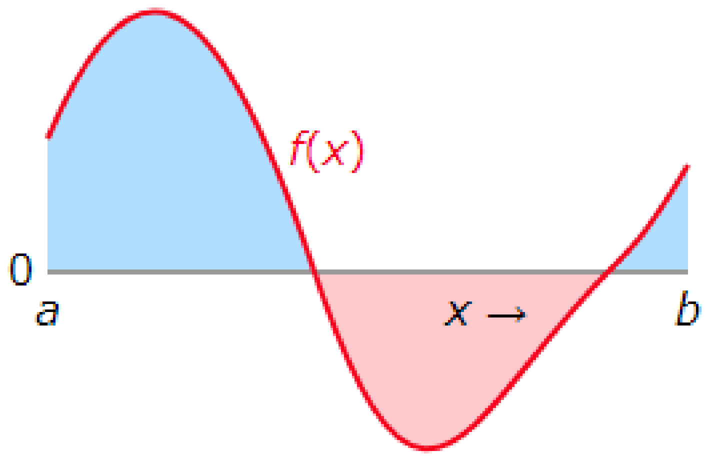
Integral Calculus

Integral Calculus

- For a function $f(x)$ defined on the domain $[a, b]$, the definite ***integral*** of the function is denoted

$$\int_a^b f(x)dx$$

- Geometric interpretation of the integral is the area between the horizontal axis and the graph of $f(x)$ between the points a and b
  - In this figure, the integral is the sum of blue areas (where $f(x) > 0$) minus the pink area (where $f(x) < 0$)



Picture from: https://mjo.osborne.economics.utoronto.ca/index.php/tutorial/index/1/clc/t

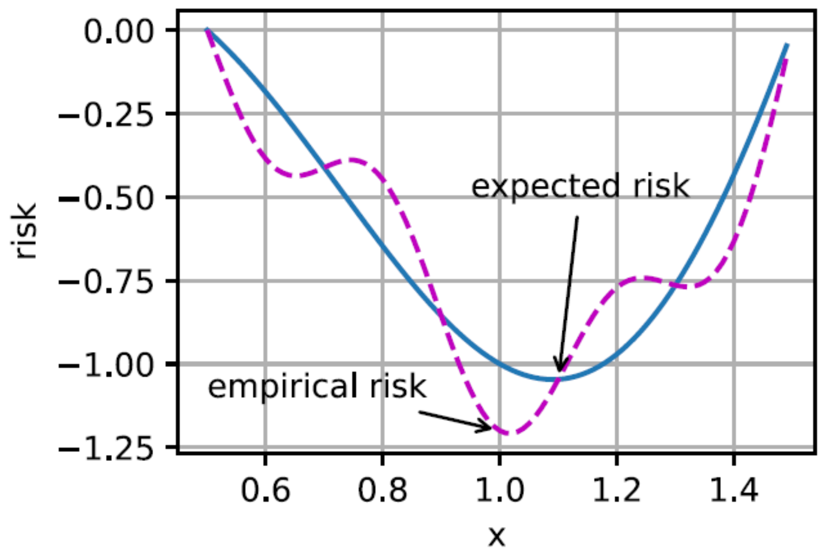
Optimization

- ***Optimization*** is concerned with optimizing an objective function — finding the value of an argument that minimizes of maximizes the function
  - Most optimization algorithms are formulated in terms of minimizing a function $f(x)$
  - Maximization is accomplished vie minimizing the negative of an objective function (e.g., minimize $-f(x)$)
  - In minimization problems, the objective function is often referred to as a cost function or loss function or error function
- Optimization is very important for machine learning
  - The performance of optimization algorithms affect the model's training efficiency
- Most optimization problems in machine learning are nonconvex
  - Meaning that the loss function is not a convex function
  - Nonetheless, the design and analysis of algorithms for solving convex problems has been very instructive for advancing the field of machine learning

Optimization

Optimization

- Optimization and machine learning have related, but somewhat different goals
  - Goal in optimization: minimize an objective function
    - For a set of training examples, reduce the training error
  - Goal in ML: find a suitable model, to predict on data examples
    - For a set of testing examples, reduce the generalization error
- For a given empirical function *g* (dashed purple curve), optimization algorithms attempt to find the point of minimum empirical risk (error on the training dataset)
- ML algorithms attempt to find the point of minimum expected risk, based on minimizing the error on a set of testing examples (blue curve)
    - Which may be at a different location than the minimum of the training examples

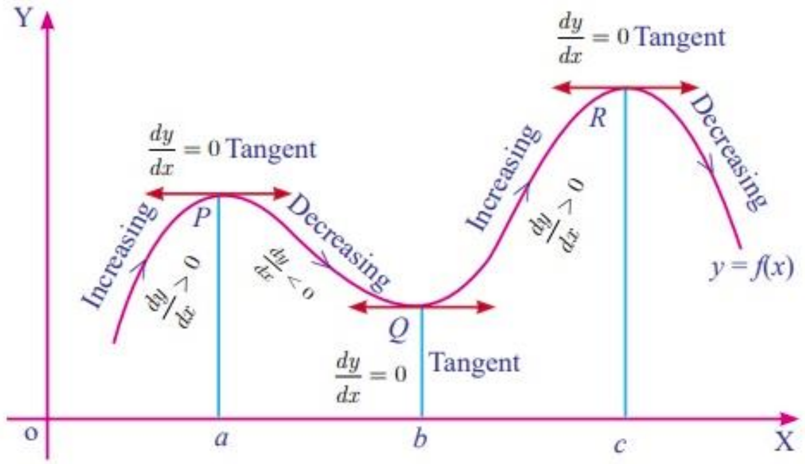


Picture from: http://d2l.ai/chapter_optimization/optimization-intro.html

Stationary Points

Optimization

- *Stationary points* (or critical points) of a differentiable function $f(x)$ of one variable are the points where the derivative of the function is zero, i.e., $f'(x) = 0$
- The stationary points can be:
  - *Minimum*, a point where the derivative changes from negative to positive
  - *Maximum*, a point where the derivative changes from positive to negative
  - *Saddle point*, derivative is either positive or negative on both sides of the point
- The minimum and maximum points are collectively known as extremum points
- The nature of stationary points can be determined based on the second derivative of $f(x)$ at the point
  - If $f''(x) > 0$, the point is a minimum
  - If $f''(x) < 0$, the point is a maximum
  - If $f''(x) = 0$, inconclusive, the point can be a saddle point, but it may not
- The same concept also applies to gradients of multivariate functions

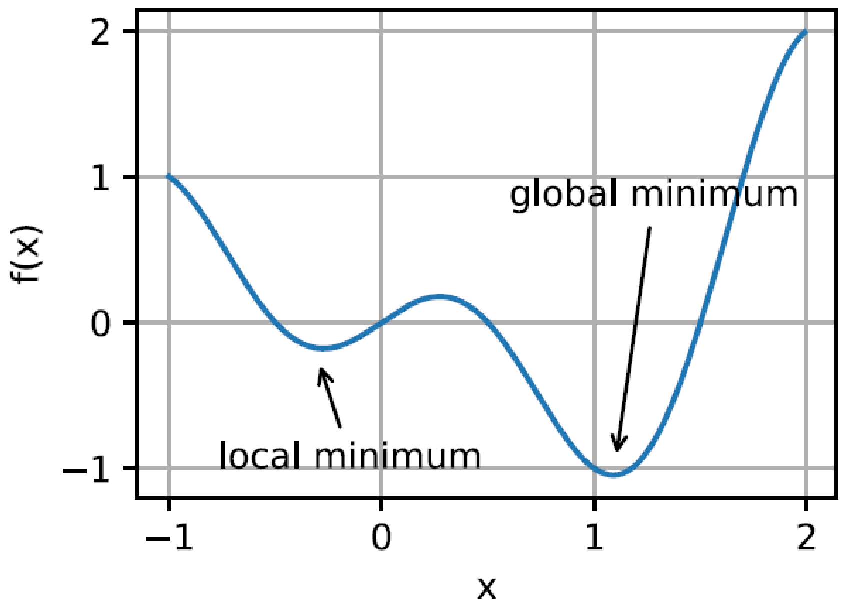


P, Q, R are called Stationary Points

Local Minima

Optimization

- Among the challenges in optimization of model's parameters in ML involve local minima, saddle points, vanishing gradients
- For an objective function $f(x)$, if the value at a point x is the minimum of the objective function over the entire domain of x, then it is the ***global minimum***
- If the value of $f(x)$ at x is smaller than the values of the objective function at any other points in the vicinity of x, then it is the ***local minimum***
  - The objective functions in ML usually have many local minima
    - When the solution of the optimization algorithm is near the local minimum, the gradient of the loss function approaches or becomes zero (vanishing gradients)
    - Therefore, the obtained solution in the final iteration can be a local minimum, rather than the global minimum

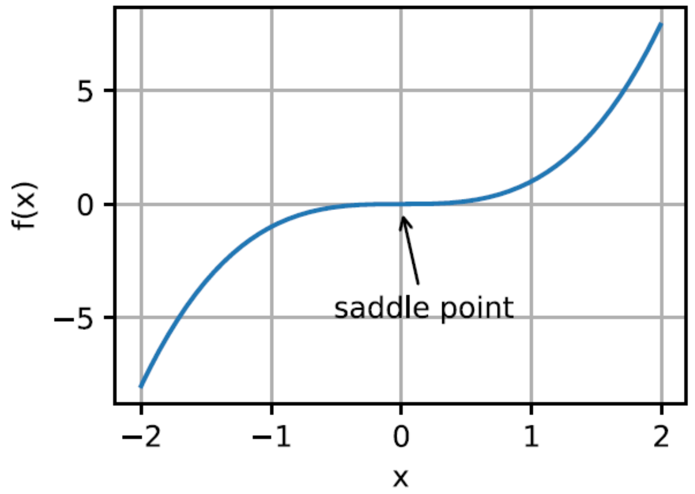


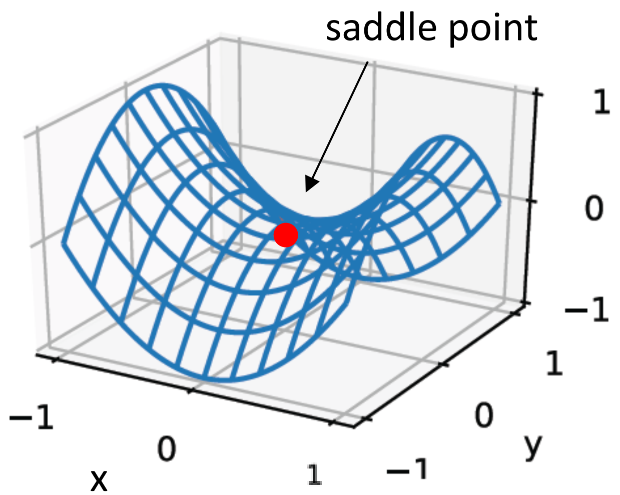
Picture from: http://d2l.ai/chapter_optimization/optimization-intro.html

Saddle Points

Optimization

- The gradient of a function $f(x)$ at a saddle point is 0, but the point is not a minimum or maximum point
  - The optimization algorithms may stall at saddle points, without reaching a minima
- Note also that the point of a function at which the sign of the curvature changes is called an inflection point
  - An inflection point ($f''(x) = 0$) can also be a saddle point, but it does not have to be
- For the 2D function (right figure), the saddle point is at (0,0)
  - The point looks like a saddle, and gives the minimum with respect to x, and the maximum with respect to y



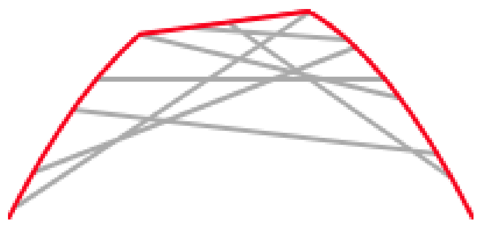


Picture from: http://d2l.ai/chapter_optimization/optimization-intro.html

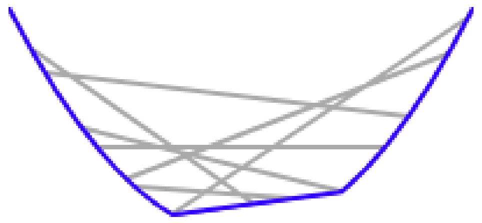
Convex Optimization

Optimization

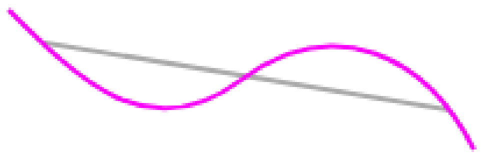
- A function of a single variable is ***concave*** if every line segment joining two points on its graph does not lie above the graph at any point
- Symmetrically, a function of a single variable is ***convex*** if every line segment joining two points on its graph does not lie below the graph at any point



A concave function: no line segment joining two points on the graph lies above the graph at any point



A convex function: no line segment joining two points on the graph lies below the graph at any point



A function that is neither concave nor convex: the line segment shown lies above the graph at some points and below it at others

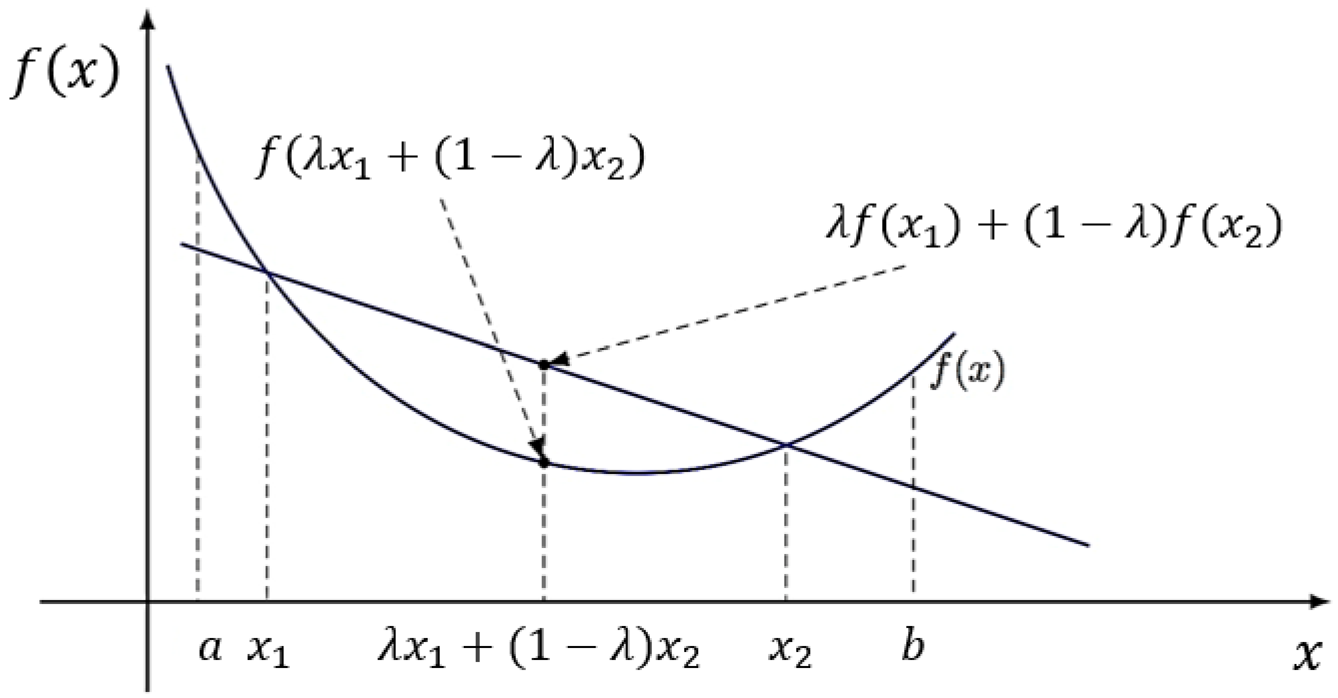
Picture from: https://mjo.osborne.economics.utoronto.ca/index.php/tutorial/index/1/cv1/t

Convex Functions

Optimization

- In mathematical terms, the function *f* is a ***convex function*** if for all points x_1, x_2 and for all $\lambda \in [0,1]$

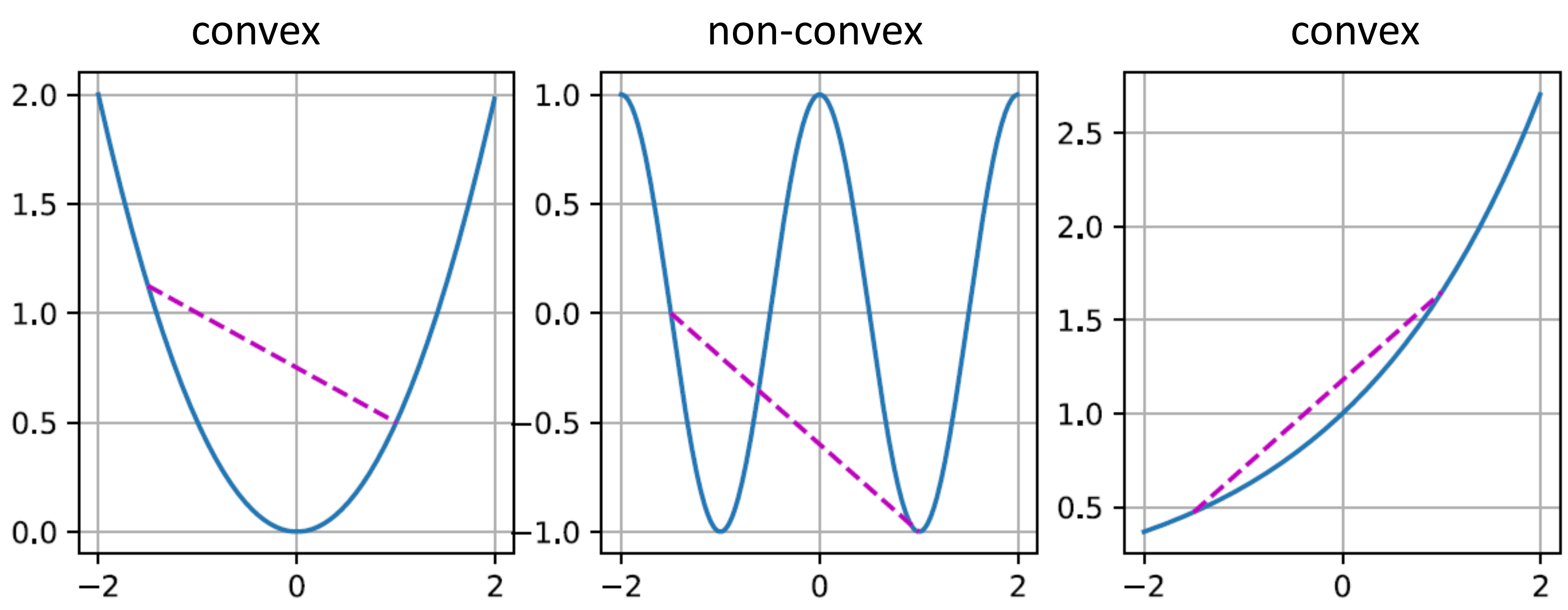
$$\lambda f(x_1) + (1-\lambda) f(x_2) \geq f(\lambda x_1 + (1-\lambda) x_2)$$


$f(x)$
$f(\lambda x_1 + (1-\lambda)x_2)$
$\lambda f(x_1) + (1-\lambda) f(x_2)$
$f(x)$
a
x_1
$\lambda x_1 + (1-\lambda)x_2$
x_2
b
x

Convex Functions

Optimization

- One important property of convex functions is that they do not have local minima
  - Every local minimum of a convex function is a global minimum
  - I.e., every point at which the gradient of a convex function = 0 is the global minimum
  - The figure below illustrates two convex functions, and one nonconvex function



Picture from: http://d2l.ai/chapter_optimization/convexity.html

Convex Functions

- Another important property of convex functions is stated by the ***Jensen's inequality***
- Namely, if we let $\alpha_1 = \lambda$ and $\alpha_2 = 1 - \lambda$, the definition of convex function becomes

$$\alpha_1 f(x_1) + \alpha_2 f(x_2) \geq f(\alpha_1 x_1 + \alpha_2 x_2)$$

- The Danish mathematician Johan Jensen showed that this can be generalized for all α_i that are non-negative real numbers and $\sum_i \alpha_i$=1, to the following:

$$\alpha_1 f(x_1) + \alpha_2 f(x_2) + \cdots + \alpha_n f(x_n) \geq f(\alpha_1 x_1 + \alpha_2 x_2 + \cdots + \alpha_n x_n)$$

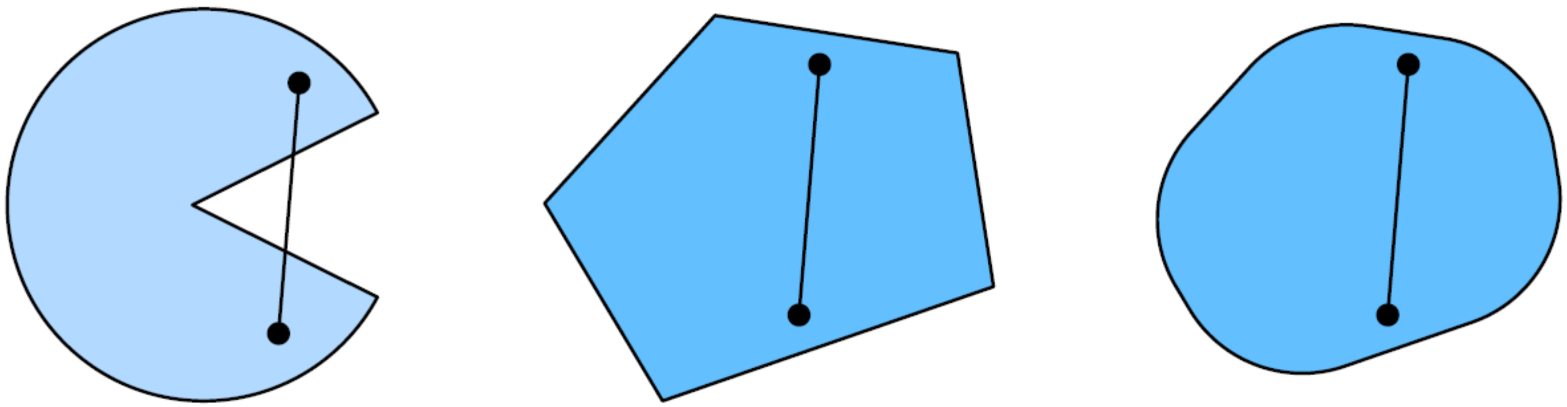
Convex Sets

Optimization

- A set $\mathcal{X}$ in a vector space is a ***convex set*** if for any $a, b \in \mathcal{X}$ the line segment connecting a and b is also in $\mathcal{X}$
- For all $\lambda \in [0,1]$, we have

$$\lambda \cdot a + (1 - \lambda) \cdot b \in \mathcal{X} \text{ for all } a, b \in \mathcal{X}$$

- In the figure, each point represents a 2D vector
  - The left set is nonconvex, and the other two sets are convex
- Properties of convex sets include:
  - If $\mathcal{X}$ and $\mathcal{Y}$ are convex sets, then $\mathcal{X} \cap \mathcal{Y}$ is also convex
  - If $\mathcal{X}$ and $\mathcal{Y}$ are convex sets, then $\mathcal{X} \cup \mathcal{Y}$ is not necessarily convex



Picture from: http://d2l.ai/chapter_optimization/convexity.html

Derivatives and Convexity

Optimization

- A twice-differentiable function of a single variable $f: \mathbb{R} \rightarrow \mathbb{R}$ is convex if and only if its second derivative is non-negative everywhere
  - Or, we can write, $\frac{d^2 f}{dx^2} \geq 0$
  - For example, $f(x) = x^2$ is convex, since $f'(x) = 2x$, and $f''(x) = 2$, meaning that $f''(x) \geq 0$
- A twice-differentiable function of many variables $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is convex if and only if its Hessian matrix is positive semi-definite everywhere
  - Or, we can write, $\mathbf{H}_f \succcurlyeq 0$
  - This is equivalent to stating that all eigenvalues of the Hessian matrix are non-negative (i.e., ≥ 0)

Constrained Optimization

- The optimization problem that involves a set of constraints which need to be satisfied to optimize the objective function is called ***constrained optimization***
- E.g., for a given objective function $f(\mathbf{x})$ and a set of constraint functions $c_i(\mathbf{x})$

$$\underset{\mathbf{x}}{\text{minimize}}\, f(\mathbf{x})$$
$$\text{subject to } c_i(\mathbf{x}) \leq 0 \;\; \text{for all} \;\; i \in \{1, 2, \dots, N\}$$

- The points that satisfy the constraints form the feasible region
- Various optimization algorithms have been developed for handling optimization problems based on whether the constraints are equalities, inequalities, or a combination of equalities and inequalities

Lagrange Multipliers

- One approach to solving optimization problems is to substitute the initial problem with optimizing another related function
- The Lagrange function for optimization of the constrained problem on the previous page is defined as

$$L(\mathbf{x}, \alpha) = f(\mathbf{x}) + \textstyle\sum_i \alpha_i c_i(\mathbf{x}) \quad \text{where} \quad \alpha_i \geq 0$$

- The variables α_i are called ***Lagrange multipliers*** and ensure that the constraints are properly enforced
  - They are chosen to ensure that $c_i(\mathbf{x}) \leq 0$ for all $i \in \{1, 2, \dots, N\}$
- This is a saddle-point optimization problem where one wants to **minimize** $L(\mathbf{x}, \alpha)$ with respect to **x** and simultaneously **maximize** $L(\mathbf{x}, \alpha)$ with respect to α_i
  - The saddle point of $L(\mathbf{x}, \alpha)$ gives the optimal solution to the original constrained optimization problem

Projections

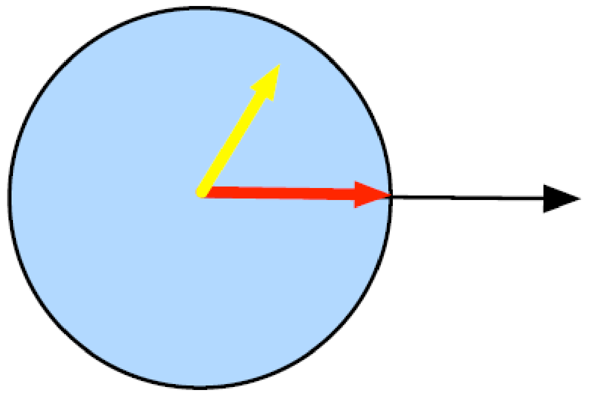
- An alternative strategy for satisfying constraints are projections
- E.g., ***gradient clipping*** in NNs can require that the norm of the gradient is bounded by a constant value *c*
- Approach:
  - At each iteration during training
  - If the norm of the gradient $\|g\| \geq$ c, then the update is $g^{new} \leftarrow c \cdot \frac{g^{old}}{\|g^{old}\|}$
  - If the norm of the gradient $\|g\| <$ c, then the update is $g^{new} \leftarrow g^{old}$
- Note that since $\frac{g^{old}}{\|g^{old}\|}$ is a unit vector (i.e., it has a norm = 1), then the vector $c \cdot \frac{g^{old}}{\|g^{old}\|}$ has a norm = *c*
- Such clipping is the projection of the gradient *g* onto the ball of radius *c*
  - For $c = 1$, it is a projection on the unit ball (i.e., ball with radius 1)

Projections

- More generally, a ***projection*** of a vector $\mathbf{x}$ onto a set $\mathcal{X}$ is defined as

$$\mathrm{Proj}_{\mathcal{X}}(\mathbf{x}) = \underset{\mathbf{x}'\in\mathcal{X}}{\mathrm{argmin}} \|\mathbf{x} - \mathbf{x}'\|_2$$

- This means that the vector $\mathbf{x}$ is projected onto the closest vector $\mathbf{x}'$ that belongs to the set $\mathcal{X}$
- For example, in the figure, the blue circle represents a convex set $\mathcal{X}$
  - The points inside the circle project to itself
    - E.g., if $\mathbf{x}$ is the yellow vector, its closest point $\mathbf{x}'$ in the set $\mathcal{X}$ is itself: the distance between $\mathbf{x}$ and $\mathbf{x}'$ is $\|\mathbf{x} - \mathbf{x}'\|_2 = 0$
  - The points outside the circle project to the closest point inside the circle
    - E.g., if $\mathbf{x}$ is the black vector, its closest point $\mathbf{x}'$ in the set $\mathcal{X}$ is the red vector
    - Among all vectors in the set $\mathcal{X}$, the red vector $\mathbf{x}'$ has the smallest distance to $\mathbf{x}$, i.e., $\|\mathbf{x} - \mathbf{x}'\|_2$



Picture from: http://d2l.ai/chapter_optimization/convexity.html

First-order vs Second-order Optimization

Optimization

- ***First-order optimization algorithms*** use the gradient of a function for finding the extrema points
  - Methods: gradient descent, proximal algorithms, optimal gradient schemes
  - The disadvantage is that they can be slow and inefficient
- ***Second-order optimization algorithms*** use the Hessian matrix of a function for finding the extrema points
  - This is since the Hessian matrix holds the second-order partial derivatives
  - Methods: Newton's method, conjugate gradient method, Quasi-Newton method, Gauss-Newton method, BFGS (Broyden-Fletcher-Goldfarb-Shanno) method, Levenberg-Marquardt method, Hessian-free method
  - The second-order derivatives can be thought of as measuring the curvature of the loss function
  - Recall also that the second-order derivative can be used to determine whether a stationary points is a maximum ($f''(x) < 0$), minimum ($f''(x) > 0$)
  - This information is richer than the information provided by the gradient
  - Disadvantage: computing the Hessian matrix is computationally expensive, and even prohibitive for high-dimensional data

Lower Bound and Infimum

- ***Lower bound*** of a subset $\mathcal{S}$ from a partially ordered set $\mathcal{X}$ is an element a of $\mathcal{X}$, such that $a \leq s$ for all $s \in \mathcal{S}$
  - E.g., for the subset $\mathcal{S} = \{3, 4, 6, 8\}$ from the natural numbers $\mathbb{N}$, lower bounds are the numbers 3, 2, and 1, i.e., all natural numbers ≤ 3
- ***Infimum*** of a subset $\mathcal{S}$ from a partially ordered set $\mathcal{X}$ is the greatest lower bound in $\mathcal{X}$, denoted $\inf_{s \in \mathcal{S}} s$
  - It is the maximal quantity h such that $h \leq s$ for all $s \in \mathcal{S}$
  - E.g., the infimum of the set $\mathcal{S} = \{3, 4, 6, 8\}$ is h =3, since it is the greatest lower bound
- Example: consider the subset of positive real numbers (excluding zero) $\mathbb{R}_{\geq 0}$=$\{x \in \mathbb{R}: x \geq 0\}$
  - The subset $\mathbb{R}_{\geq 0}$ does not have a minimum, because for every small positive number, there is a another even smaller positive number
  - On the other hand, all real negative numbers and 0 are lower bounds on the subset $\mathbb{R}_{\geq 0}$
  - 0 is the greatest lower bound of all lower bounds, and therefore, the infimum of $\mathbb{R}_{\geq 0}$ is 0

Upper Bound and Supremum

- *Upper bound* of a subset $\mathcal{S}$ from a partially ordered set $\mathcal{X}$ is an element b of $\mathcal{X}$, such that $b \geq s$ for all $s \in \mathcal{S}$
  - E.g., for the subset $\mathcal{S} = \{3, 4, 6, 8\}$ from the natural numbers $\mathbb{N}$, upper bounds are the numbers 8, 9, 40, and all other natural numbers ≥ 8
- *Supremum* of a subset $\mathcal{S}$ from a partially ordered set $\mathcal{X}$ is the least upper bound in $\mathcal{X}$, denoted $\sup_{s \in \mathcal{S}} s$
  - It is the minimal quantity g such that g $\geq s$ for all $s \in \mathcal{S}$
  - E.g., the supremum of the subset $\mathcal{S} = \{3, 4, 6, 8\}$ is $g = 8$, since it is the least upper bound
- Example: for the subset of negative real numbers (excluding zero) $\mathbb{R}_{\leq 0}$=$\{x \in \mathbb{R}: x \leq 0\}$
  - All real positive numbers and 0 are upper bounds
  - 0 is the least upper bound, and therefore, the supremum of $\mathbb{R}_{\leq 0}$

Lipschitz Function

- A function $f(x)$ is a ***Lipschitz continuous function*** if a constant $\rho > 0$ exists, such that for all points x_1, x_2

$$\|f(x_1) - f(x_2)\| \leq \rho\|x_1 - x_2\|$$

- Such function is also called a ρ-Lipschitz function
- Intuitively, a Lipschitz function cannot change too fast
  - I.e., if the points x_1 and x_2 are close (i.e., the distance $\|x_1 - x_2\|$ is small), that means that the $f(x_1)$ and $f(x_2)$ are also close (i.e., the distance $\|f(x_1) - f(x_2)\|$ is also small)
    - The smallest real number that bounds the change of $\|f(x_1) - f(x_2)\|$ for all points x_1, x_2 is the Lipschitz constant ρ of the function $f(x)$
  - For a ρ-Lipschitz function $f(x)$, the first derivative $f'(x)$ is bounded everywhere by ρ
- E.g., the function $f(x) = log(1 + e^x)$ is 1-Lipschitz over $\mathbb{R}$
  - Since $\|f'(x)\| = \left\|\frac{e^x}{1+e^x}\right\| = \left\|\frac{1}{e^{-x}+1}\right\| = \frac{\mathbf{1}}{\|e^{-x}+1\|} \leq 1$
  - I.e., $\rho = 1$

Lipschitz Continuous Gradient

Optimization

- A differentiable function $f(x)$ has a ***Lipschitz continuous gradient*** if a constant $\rho > 0$ exists, such that for all points x_1, x_2

$$\|\nabla f(x_1) - \nabla f(x_2)\| \leq \rho \|x_1 - x_2\|$$

- For a function $f(x)$ with a ρ-Lipschitz gradient, the second derivative $f''(x)$ is bounded everywhere by ρ
- E.g., consider the function $f(x) = x^2$
  - $f(x) = x^2$ is not a Lipschitz continuous function, since $f'(x) = 2x$, so when $x \to \infty$ then $f'(x) \to \infty$, i.e., the derivative is not bounded everywhere
  - Since $f''(x) = 2$, therefore the gradient $f'(x)$ is 2-Lipschitz everywhere, since the second derivative is bounded everywhere by 2

Probability

- Intuition:
  - In a process, several outcomes are possible
  - When the process is repeated a large number of times, each outcome occurs with a ***relative frequency***, or ***probability***
  - If a particular outcome occurs more often, we say it is more probable
- Probability arises in two contexts
  - In actual repeated experiments
    - Example: You record the color of 1,000 cars driving by. 57 of them are green. You estimate the probability of a car being green as 57/1,000 = 0.057.
  - In idealized conceptions of a repeated process
    - Example: You consider the behavior of an unbiased six-sided die. The expected probability of rolling a 5 is 1/6 = 0.1667.
    - Example: You need a model for how people's heights are distributed. You choose a normal distribution to represent the expected relative probabilities.

Probability

Probability

- Solving machine learning problems requires to deal with uncertain quantities, as well as with stochastic (non-deterministic) quantities
  - Probability theory provides a mathematical framework for representing and quantifying uncertain quantities
- There are different sources of uncertainty:
  - Inherent stochasticity in the system being modeled
    - For example, most interpretations of quantum mechanics describe the dynamics of subatomic particles as being probabilistic
  - Incomplete observability
    - Even deterministic systems can appear stochastic when we cannot observe all of the variables that drive the behavior of the system
  - Incomplete modeling
    - When we use a model that must discard some of the information we have observed, the discarded information results in uncertainty in the model's predictions
    - E.g., discretization of real-numbered values, dimensionality reduction, etc.

Random variables

- A ***random variable*** X is a variable that can take on different values
  - Example: X = rolling a die
    - Possible values of X comprise the **sample space**, or **outcome space**, $\mathcal{S} = \{1, 2, 3, 4, 5, 6\}$
    - We denote the event of "seeing a 5" as $\{X = 5\}$ or $X = 5$
    - The probability of the event is $P(\{X = 5\})$ or $P(X = 5)$
    - Also, $P(5)$ can be used to denote the probability that X takes the value of 5
- A ***probability distribution*** is a description of how likely a random variable is to take on each of its possible states
  - A compact notation is common, where $P(X)$ is the probability distribution over the random variable X
    - Also, the notation $\mathrm{X}{\sim}P(X)$ can be used to denote that the random variable X has probability distribution $P(X)$
- Random variables can be discrete or continuous
  - Discrete random variables have finite number of states: e.g., the sides of a die
  - Continuous random variables have infinite number of states: e.g., the height of a person

Axioms of probability

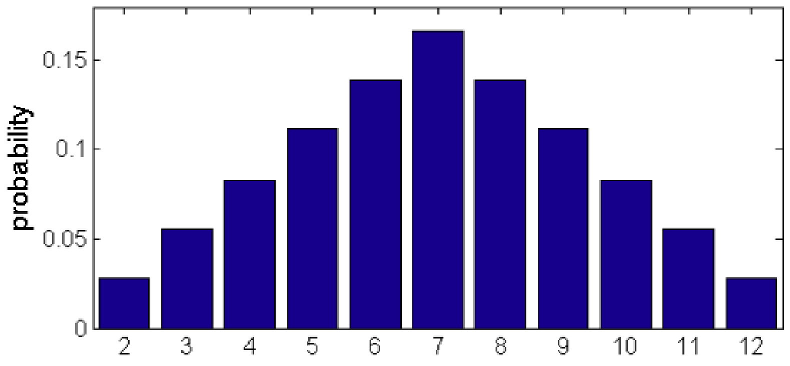
- The probability of an event $\mathcal{A}$ in the given sample space $\mathcal{S}$, denoted as $P(\mathcal{A})$, must satisfies the following properties:
  - Non-negativity
    - For any event $\mathcal{A} \in \mathcal{S}$, $P(\mathcal{A}) \geq 0$
  - All possible outcomes
    - Probability of the entire sample space is 1, $P(\mathcal{S}) = 1$
  - Additivity of disjoint events
    - For all events $\mathcal{A}_1, \mathcal{A}_2 \in \mathcal{S}$ that are mutually exclusive ($\mathcal{A}_1 \cap \mathcal{A}_2 = \emptyset$), the probability that both events happen is equal to the sum of their individual probabilities, $P(\mathcal{A}_1 \cup \mathcal{A}_2) = P(\mathcal{A}_1) + P(\mathcal{A}_2)$

- The probability of a random variable $P(X)$ must obey the axioms of probability over the possible values in the sample space $\mathcal{S}$

Discrete Variables

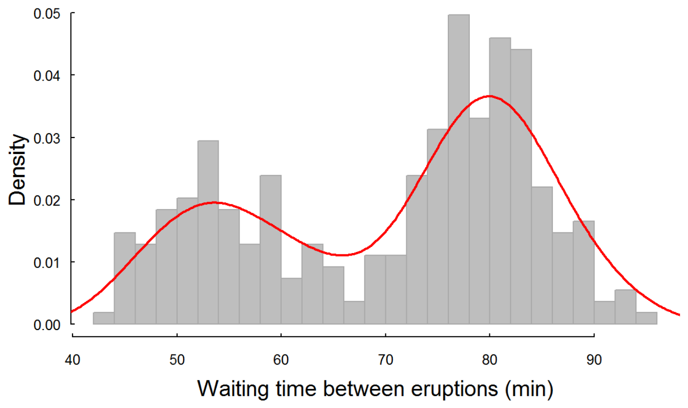
Probability

- A probability distribution over discrete variables may be described using a *probability mass function* (PMF)
  - E.g., sum of two dice



- A probability distribution over continuous variables may be described using a *probability density function* (PDF)
  - E.g., waiting time between eruptions of Old Faithful
  - A PDF gives the probability of an infinitesimal region with volume δX
  - To find the probability over an interval $[a, b]$, we can integrate the PDF as follows:

$$P(X \in [a, b]) = \int_a^b P(X)dX$$



Picture from: Jeff Howbert — Machine Learning Math Essentials

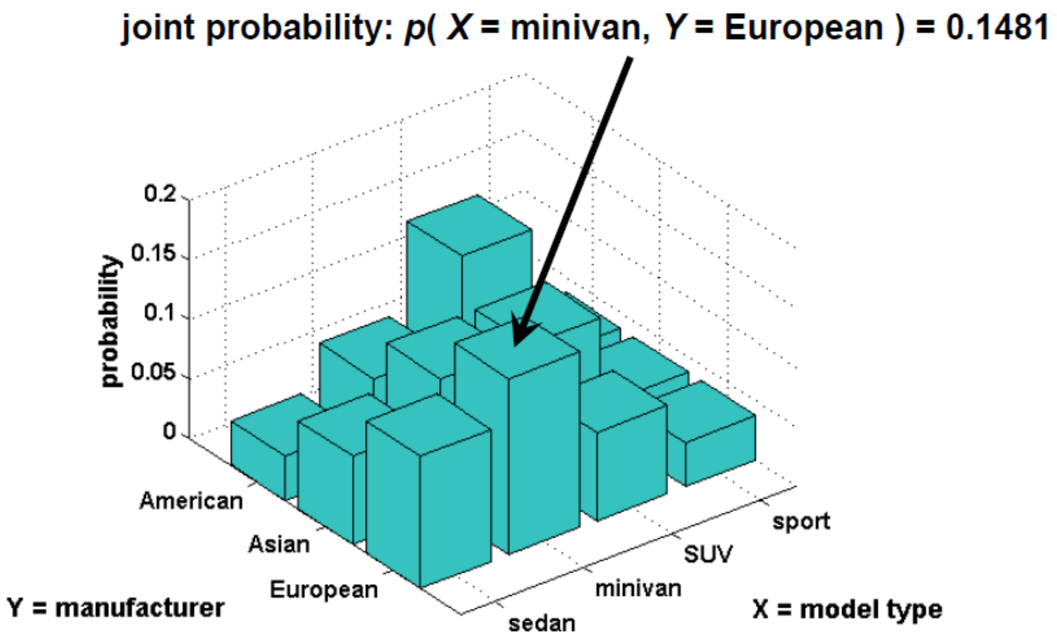
Multivariate Random Variables

- We may need to consider several random variables at a time
  - If several random processes occur in parallel or in sequence
  - E.g., to model the relationship between several diseases and symptoms
  - E.g., to process images with millions of pixels (each pixel is one random variable)
- Next, we will study probability distributions defined over multiple random variables
  - These include joint, conditional, and marginal probability distributions
- The individual random variables can also be grouped together into a random vector, because they represent different properties of an individual statistical unit
- A ***multivariate random variable*** is a vector of multiple random variables $\mathbf{X} = (X_1, X_2, \dots, X_n)^T$
  - It is also referred to as a ***random vector***

Joint Probability Distribution

Probability

- Probability distribution that acts on many variables at the same time is known as a ***joint probability distribution***
- Given any values x and y of two random variables X and Y, what is the probability that $X = x$ and $Y = y$ simultaneously?
  - $P(X = x, Y = y)$ denotes the joint probability
  - We may also write $P(x, y)$ for brevity



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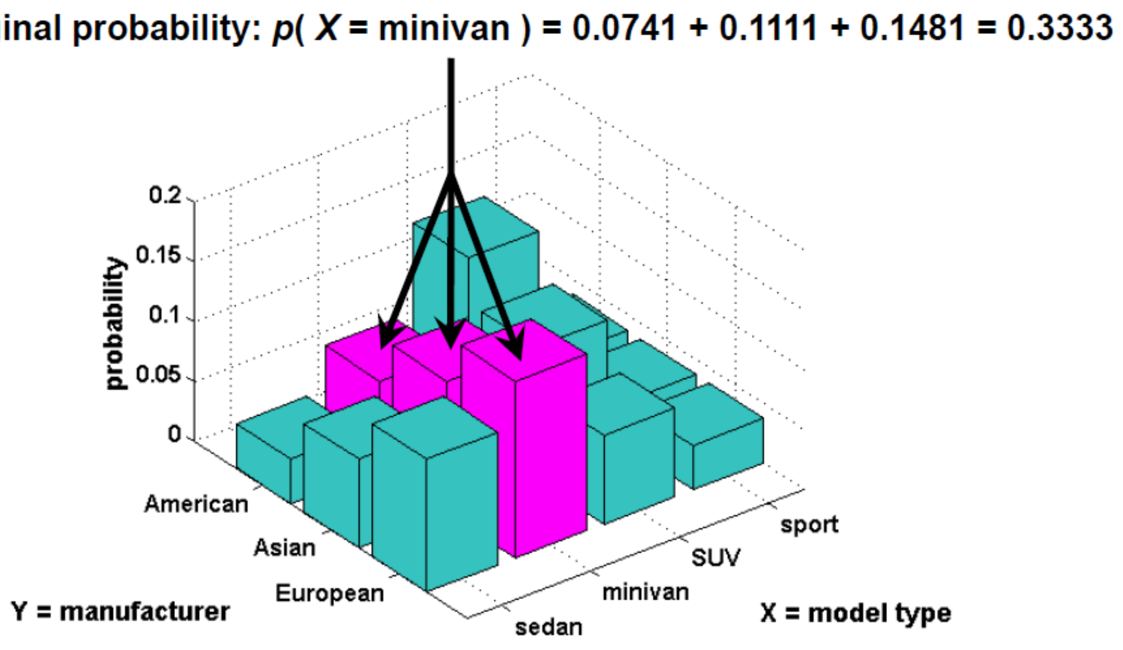
Marginal Probability Distribution

Probability

- ***Marginal probability distribution*** is the probability distribution of a single variable
  - It is calculated based on the joint probability distribution $P(X, Y)$
  - I.e., using the sum rule: $P(X = x) = \sum_y P(X = x, Y = y)$
    - For continuous random variables, the summation is replaced with integration, $P(X = x) = \int P(X = x, Y = y)\, dy$
  - This process is called marginalization



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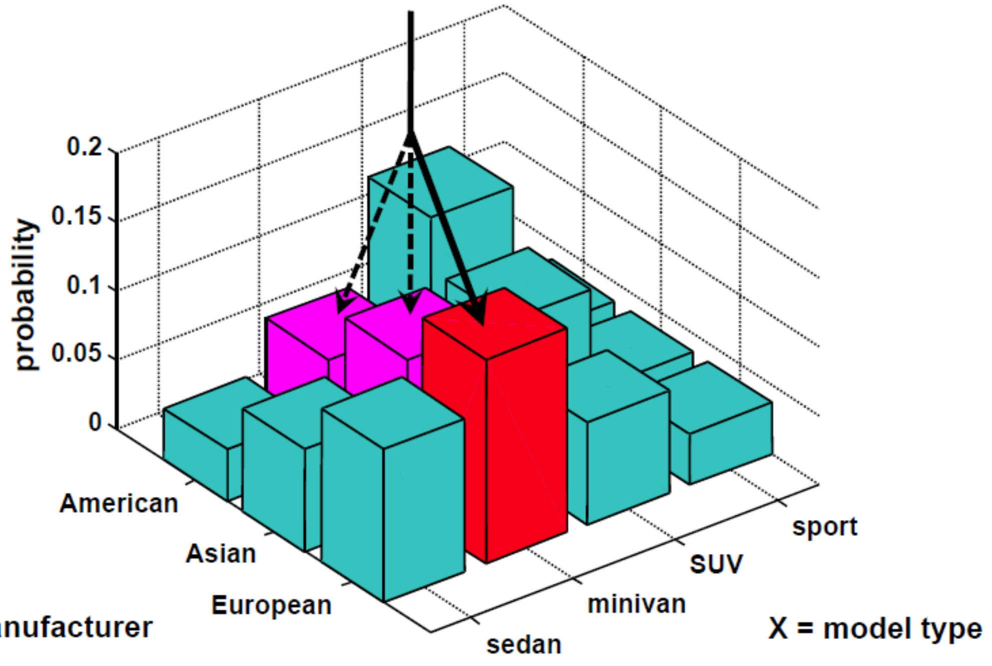
Conditional Probability Distribution

Probability

- ***Conditional probability distribution*** is the probability distribution of one variable provided that another variable has taken a certain value
  - Denoted $P(Y = y|\, X = x)$
- Note that: $P(Y = y|\, X = x) = \frac{P(Y=y,\, X=x)}{P(X=x)}$

conditional probability: $p(\ Y = \text{European}\ |\ X = \text{minivan}\ ) =$
$0.1481\ /\ (\ 0.0741 + 0.1111 + 0.1481\ ) = 0.4433$



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Bayes' Theorem

- ***Bayes' theorem*** – allows to calculate conditional probabilities for one variable when conditional probabilities for another variable are known

$$P(X|Y) = \frac{P(Y|X)P(X)}{P(Y)}$$

- Also known as Bayes' rule
- Multiplication rule for the joint distribution is used: $P(X,Y) = P(Y|X)P(X)$
- By symmetry, we also have: $P(Y,X) = P(X|Y)P(Y)$

- The terms are referred to as:
  - $P(X)$, the prior probability, the initial degree of belief for X
  - $P(X|Y)$, the posterior probability, the degree of belief after incorporating the knowledge of Y
  - $P(Y|X)$, the likelihood of Y given X
  - P(Y), the evidence

  - Bayes' theorem: $\textbf{posterior probability} = \frac{\textbf{likelihood} \times \textbf{prior probability}}{\textbf{evidence}}$

Independence

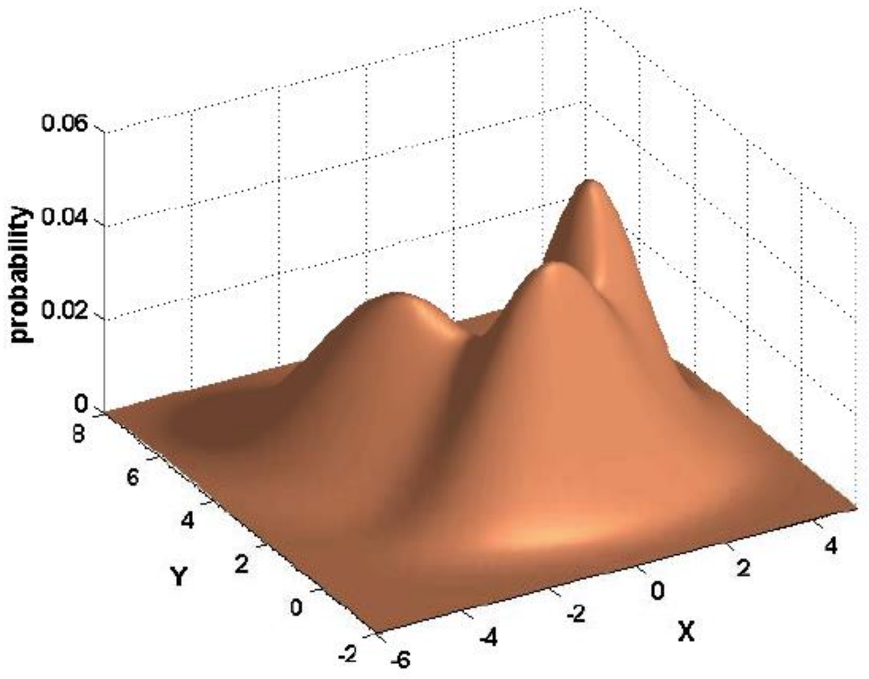
- Two random variables X and Y are ***independent*** if the occurrence of Y does not reveal any information about the occurrence of X
  - E.g., two successive rolls of a die are independent
- Therefore, we can write: $P(X|\,Y) = P(X)$
  - The following notation is used: $X \perp Y$
  - Also note that for independent random variables: $P(X, Y) = P(X)P(Y)$
- In all other cases, the random variables are ***dependent***
  - E.g., duration of successive eruptions of Old Faithful
  - Getting a king on successive draws form a deck (the drawn card is not replaced)

- Two random variables X and Y are ***conditionally independent*** given another random variable Z if and only if $P(X, Y|Z) = P(X|Z)P(Y|Z)$
  - This is denoted as $X \perp Y|Z$

Continuous Multivariate Distributions

Probability

- Same concepts of joint, marginal, and conditional probabilities apply for continuous random variables
- The probability distributions use integration of continuous random variables, instead of summation of discrete random variables
  - Example: a three-component Gaussian mixture probability distribution in two dimensions



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Expected Value

Probability

- The ***expected value*** or ***expectation*** of a random variable X drawn from a probability distribution $P(X)$ is the average (mean) value of all possible outcomes
  - For a discrete random variable X, it is calculated as

$$\mathbb{E}_{X\sim P}[X] = \sum_X X\,P(X)$$

  - For a continuous random variable X, it is calculated as

$$\mathbb{E}_{X\sim P}[X] = \int X\,P(X)\,dX$$

  - When the identity of the distribution is clear from the context, we can write $\mathbb{E}[X]$
  - E.g., for a sample of observations: $\mu = \mathbb{E}[X] = \sum_i P(X_i) \cdot X_i = \frac{1}{N} \sum_i X_i$
- Mean is the most common measure of central tendency of a distribution
  - Other measures of central tendency: median, mode
- By analogy, the ***expected value of a function*** $f(X)$ of a discrete random variable X with respect to a probability distribution $P(X)$ is:

$$\mathbb{E}_{X\sim P}[f(X)] = \sum_X f(X)\,P(X)$$

Variance

- ***Variance*** of a random variable X gives the measure of how much the values of X deviate from the expected value as we sample X from $P(X)$

$$\mathrm{Var}(X) = \mathbb{E}[(X - \mathbb{E}[X])^2]$$

- When the variance is low, the values of X cluster near the expected value
- Variance is commonly denoted with σ^2
  - The above equation is similar to an expected value of a function $f(X) = (X_i - \mu)^2$
  - We can write:

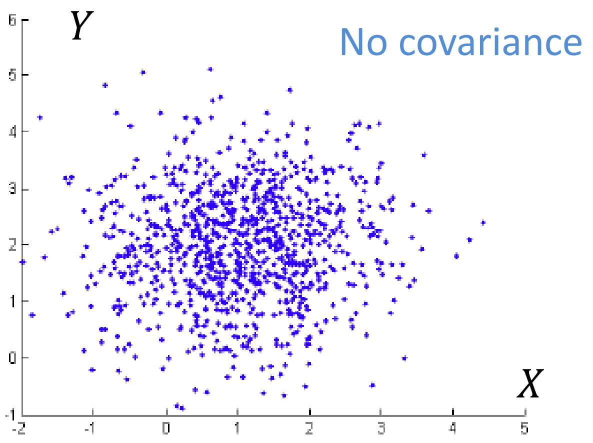
$$\sigma^2 = \mathbb{E}[(X_i - \mu)^2] = \sum_i (X_i - \mu)^2 \cdot P(X_i)$$

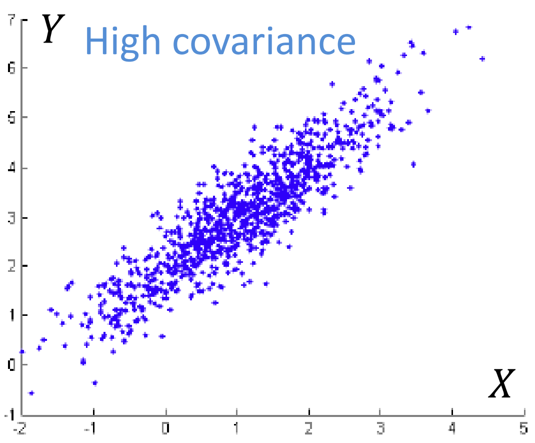
  - Similarly, the variance of a sample of observations can be calculated as:
  - $\sigma^2 = \frac{1}{N}\sum_i (X_i - \mu)^2$
- The square root of the variance is the ***standard deviation***
  - $\sigma = \sqrt{\mathrm{Var}(X)}$

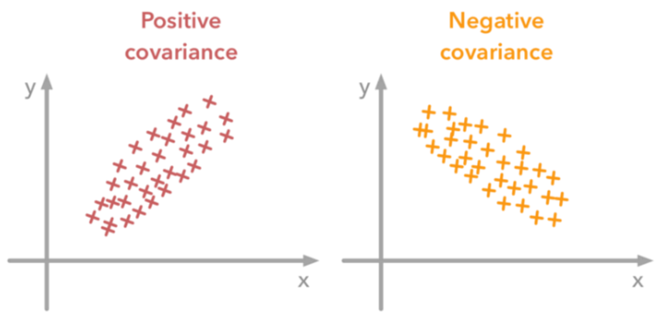
Covariance

Probability

- *Covariance* is a measure of the joint variability of two random variables X and Y from their means
$$\mathrm{Cov}(X, Y) = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])]$$
- If $f(X) = X_i - \mu_X$ and $g(Y) = Y_i - \mu_Y$
  - Then, the covariance is: $\mathrm{Cov}(X_i, Y_i) = \mathbb{E}[f(X)g(Y)] = \sum_i P(X_i, Y_i) \cdot (X_i - \mu_X) \cdot (Y_i - \mu_Y)$
  - Covariance of samples of observations is: $\mathrm{Cov}(X, Y) = \frac{1}{N}\sum_i (Y_i - \mu_X)(Y_i - \mu_Y)$
- The covariance measures the tendency for X and Y to deviate from their means in the same (or opposite) directions at same time







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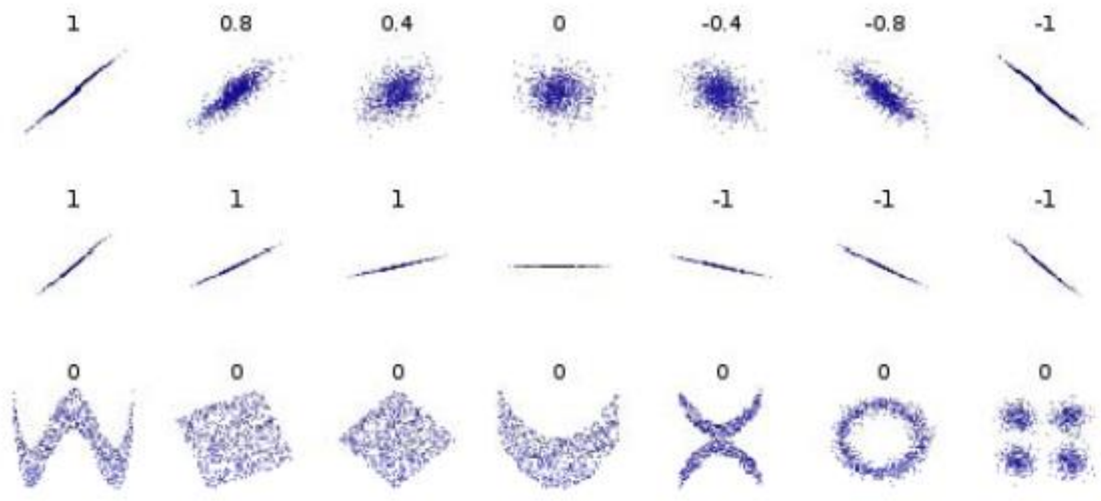
Correlation

- *Correlation coefficient* is the covariance normalized by the standard deviations of the two variables

$$\text{corr}(X, Y) = \frac{\text{Cov}(X, Y)}{\sigma_X \cdot \sigma_Y}$$

  - It is also called Pearson's correlation coefficient and it is denoted $\rho(X, Y)$
  - The values are in the interval $[-1, 1]$
  - It only reflects linear dependence between variables, and it does not measure non-linear dependencies between the variables



Linear dependence with noise

Linear dependence without noise

Various nonlinear dependencies

Picture from: Jeff Howbert — Machine Learning Math Essentials

Covariance Matrix

- ***Covariance matrix*** of a multivariate random variable $\mathbf{X} = (X_1, X_2, \dots, X_n)^T$ is an $n \times n$ matrix, such that

$$\mathrm{Cov}(\mathbf{X})_{i,j} = \mathrm{Cov}(X_i, X_j)$$

- I.e.,

$$\mathrm{Cov}(\mathbf{X}) = \begin{bmatrix} \mathrm{Cov}(X_1, X_1) & \mathrm{Cov}(X_1, X_2) & \cdots & \mathrm{Cov}(X_1, X_n) \\ \mathrm{Cov}(X_2, X_1) & \ddots & & \mathrm{Cov}(X_2, X_n) \\ \vdots & & & \vdots \\ \mathrm{Cov}(X_n, X_1) & \mathrm{Cov}(X_n, X_2) & \cdots & \mathrm{Cov}(X_n, X_n) \end{bmatrix}$$

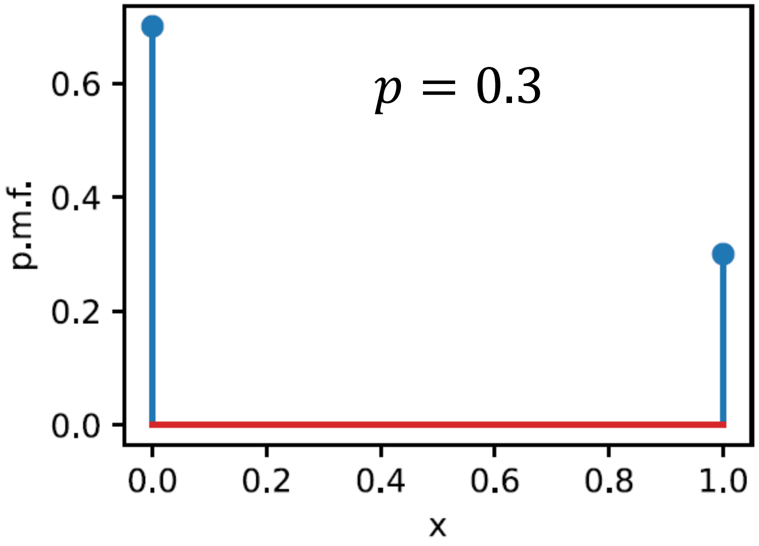
- The diagonal elements of the covariance matrix are the variances of the elements of the random vector $\mathbf{X}$

$$\mathrm{Cov}(X_i, X_i) = \mathrm{Var}(X_i)$$

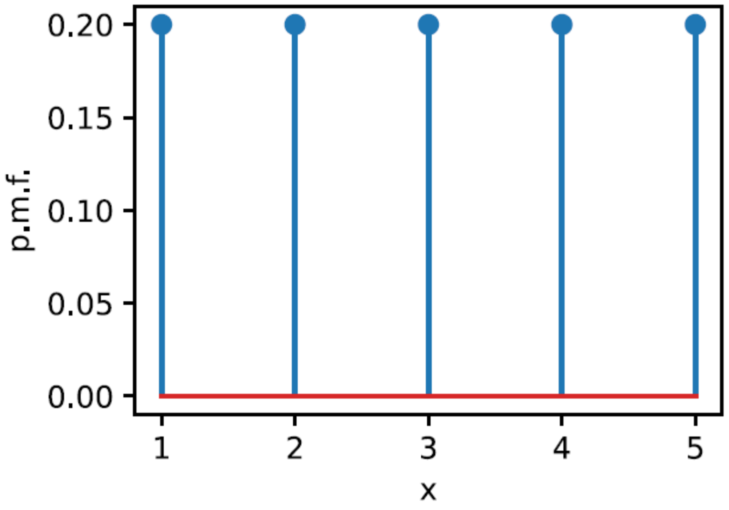
- Also note that the covariance matrix is symmetric, since $\mathrm{Cov}(X_i, X_j) = \mathrm{Cov}(X_j, X_i)$

Probability Distributions

- ***Bernoulli distribution***
  - Binary random variable X with states $\{0, 1\}$
  - E.g., the random variable can encode a coin flip which comes up 1 with probability p and 0 with probability $1 - p$
  - Notation: $X \sim Bernoulli(p)$



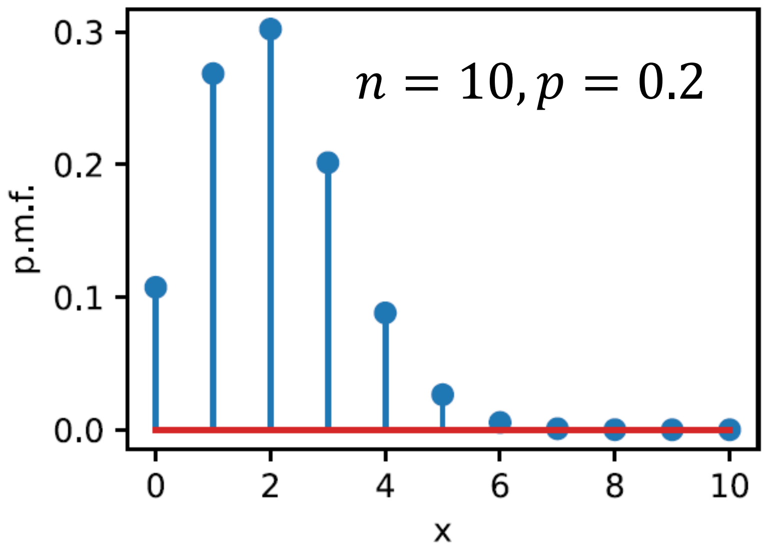
- ***Uniform distribution***
  - The probability of each value $i \in \{1,2, \dots, n\}$ is $p_i = \frac{1}{n}$
  - Notation: $X \sim U(n)$
  - Figure: $n = 5,\ p = 0.2$



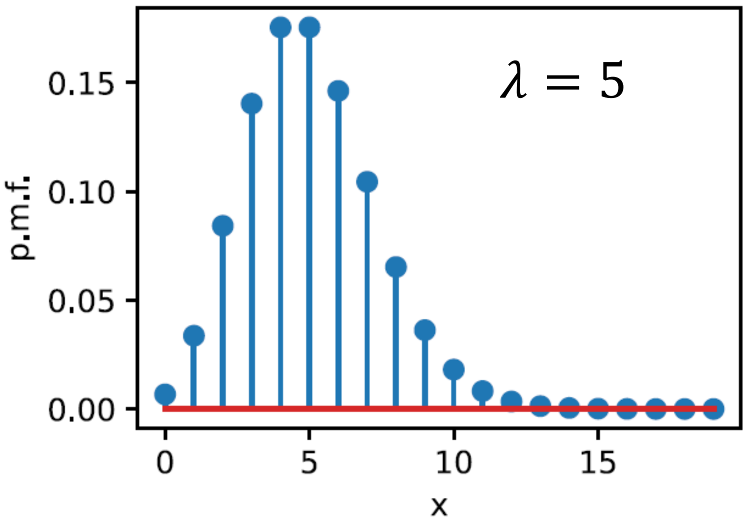
Picture from: http://d2l.ai/chapter_appendix-mathematics-for-deep-learning/distributions.html

Probability Distributions

- ***Binomial distribution***
  - Performing a sequence of n independent experiments, each of which has probability p of succeeding, where $p \in \{0, 1\}$
    - E.g., tossing a coin 100 times, head probability is 0.5
  - The probability of getting k successes in n trials is $P(X = k) = \binom{n}{k} p^k (1-p)^{n-k}$
  - Notation: $X \sim Binomial(n, p)$



- ***Poisson distribution***
  - A number of events occurring independently in a fixed interval of time with a known rate λ
    - E.g., number of arriving patients in ER
  - A discrete random variable X with states $k \in \{0, 1, 2, \dots\}$ has probability $P(X = k) = \frac{\lambda^k \cdot e^{-\lambda}}{k!}$
  - The rate λ is the average number of occurrences of the event
  - Notation: $X \sim Poisson(\lambda)$



Picture from: http://d2l.ai/chapter_appendix-mathematics-for-deep-learning/distributions.html

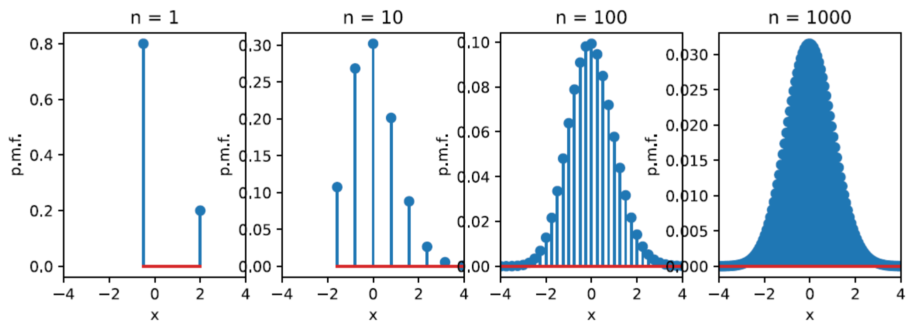
Probability Distributions

Probability

- ***Gaussian distribution***
  - The most well-studied distribution
    - Referred to as normal distribution or informally bell-shaped distribution
  - Defined with the mean μ and variance σ^2
    - Notation: $X \sim \mathcal{N}(\mu, \sigma^2)$
  - For a random variable X with n independent measurements, the density is

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

  - E.g., shown below is a Binomial distribution; as the number of experiments increases from 1 to 1000, it yields a Gaussian distribution
    - ***Central limit theorem***: the distribution of the mean of samples approximates a normal distribution as the sample size becomes larger



Picture from: http://d2l.ai/chapter_appendix-mathematics-for-deep-learning/distributions.html

Probability Distributions

Probability

- ***Multinoulli distribution***
  - It is an extension of the Bernoulli distribution, from binary class to multi-class
  - Multinoulli distribution is also called categorical distribution or generalized Bernoulli distribution
  - Multinoulli is a discrete probability distribution that describes the possible results of a random variable that can take on one of k possible categories
    - A categorical random variable is a discrete variable with more than two possible outcomes (such as the roll of a die)
  - For example, in multi-class classification in machine learning, we have a set of data examples $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$, and corresponding to the data example $\mathbf{x}_i$ is a k-class label $\mathbf{y}_i = \{y_{i1}, y_{i2}, \dots, y_{ik}\}$ representing one-hot encoding
    - One-hot encoding is also called 1-of-k vector, where one element has the value 1 and all other elements have the value 0
    - Let's denote the probabilities for assigning the class labels to a data example by $\{p_1, p_2, \dots, p_k\}$
    - We know that $0 \le p_j \le 1$ and $\sum p_j = 1$ for the different classes $j = 1, 2, \dots, k$
    - The multinoulli probability of the data example $\mathbf{x}_i$ is $P(\mathbf{x}_i) = {p_1}^{y_{i1}} \cdot {p_2}^{y_{i2}} \cdots {p_k}^{y_{ik}} = \prod_j {p_j}^{y_{ij}}$
    - Similarly, we can calculate the probability of all data examples as $\prod_i \prod_j {p_j}^{y_{ij}}$

Information Theory

- ***Information theory*** studies encoding, decoding, transmitting, and manipulating information
  - It is a branch of applied mathematics that revolves around quantifying how much information is present in different signals
- As such, information theory provides fundamental language for discussing the information processing in computer systems
  - E.g., machine learning applications use the cross-entropy loss, derived from information theoretic considerations
- A seminal work in this field is the paper *A Mathematical Theory of Communication* by Clause E. Shannon, which introduced the concept of information entropy for the first time
  - Information theory was originally invented to study sending messages over a noisy channel, such as communication via radio transmission

Self-information

Information Theory

- The basic intuition behind information theory is that learning that an unlikely event has occurred is more informative than learning that a likely event has occurred
  - E.g., a message saying "the sun rose this morning" is so uninformative that it is unnecessary to be sent
  - But, a message saying "there was a solar eclipse this morning" is very informative
- Based on that intuition, Shannon defined the ***self-information*** of an event X as

$$I(X) = -\log\big(P(X)\big)$$

  - $I(X)$ is the self-information, and$P(X)$ is the probability of the event X
- The self-information outputs the bits of information received for the event X
  - For example, if we want to send the code "0010" over a channel
  - The event "0010" is a series of codes of length n (in this case, the length is n =4)
  - Each code is a bit (0 or 1), and occurs with probability of $\frac{1}{2}$; for this event $P = \frac{1}{2^n}$

$$I(\text{"0010"}) = -\log\big(P(\text{"0010"})\big) = -\log\left(\frac{1}{2^4}\right) = -\log_2(1) + \log_2(2^4) = 0 + 4 = 4 \text{ bits}$$

Entropy

Information Theory

- For a discrete random variable X that follows a probability distribution P with a probability mass function $P(X)$, the expected amount of information through ***entropy*** (or Shannon entropy) is

$$H(X) = \mathbb{E}_{X\sim P}[I(X)] = -\mathbb{E}_{X\sim P}\,[\log P(X)]$$

- Based on the expectation definition $\mathbb{E}_{X\sim P}[f(X)] = \sum_X P(X) f(X)$, we can rewrite the entropy as

$$H(X) = -\sum_X P(X) \log P(X)$$

- If X is a continuous random variable that follows a probability distribution P with a probability density function $P(X)$, the entropy is

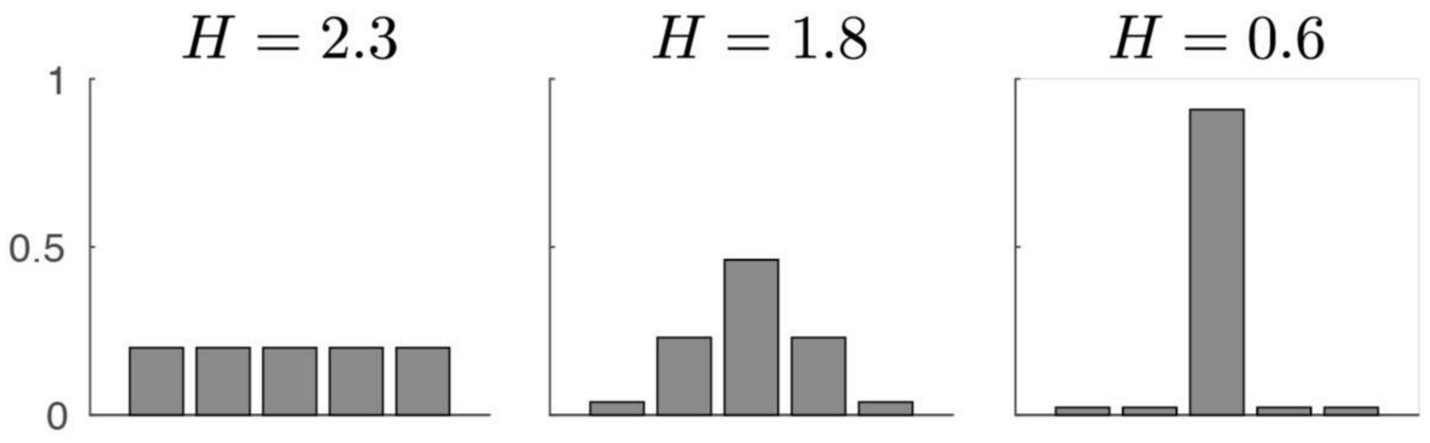
$$H(X) = -\int_X P(X) \log P(X)\, dX$$

  - For continuous random variables, the entropy is also called differential entropy

Entropy

Information Theory

- Intuitively, we can interpret the self-information ($I(X) = -\log(P(X))$) as the amount of surprise at seeing a particular outcome of X
  - We are less surprised when seeing a more frequent event
- Similarly, we can interpret the entropy ($H(X) = \mathbb{E}_{X\sim P}[I(X)]$) as the average amount of surprise from observing all possible outcomes of X
  - Therefore, distributions that are closer to a uniform distribution have high entropy
  - This is because there is more surprise (uncertainty) when we draw samples from a uniform distribution, since all outcomes are equally likely
  - High entropy = high uncertainty (surprise) = outcomes are spread over many values



Kullback–Leibler Divergence

Information Theory

- ***Kullback-Leibler (KL) divergence*** (or relative entropy) provides a measure of how different two probability distribution are
- For two probability distributions $P(X)$ and $Q(X)$ over the same random variable X, the KL divergence is

$$D_{KL}(P||Q) = \mathbb{E}_{X\sim P}\left[\log \frac{P(X)}{Q(X)}\right]$$

- For discrete random variables, this formula is equivalent to

$$D_{KL}(P||Q) = \sum_X P(X) \log \frac{P(X)}{Q(X)}$$

- KL divergence can be considered as the amount of information lost when the distribution Q is used to approximate the distribution P

Kullback–Leibler Divergence

- KL divergence is non-negative: $D_{KL}(P||Q) \geq 0$
- $D_{KL}(P||Q) = 0$ if and only if $P(X)$ and $Q(X)$ are the same distribution
- The most important property of KL divergence is that it is non-symmetric, i.e.,

$$D_{KL}(P||Q) \neq D_{KL}(Q||P)$$

- Because D_{KL} is non-negative and measures the difference between distributions, it is often considered as a "distance metric" between two distributions
  - However, KL divergence is not a true distance metric, because it is not symmetric
  - The asymmetry means that there are important consequences to the choice of whether to use $D_{KL}(P||Q)$ or $D_{KL}(Q||P)$
- An alternative divergence which is non-negative and symmetric is the ***Jensen-Shannon divergence***, defined as

$$D_{JS}(P||Q) = \frac{1}{2} D_{KL}(P||M) + \frac{1}{2} D_{KL}(Q||M)$$

  - In the above, M is the average of the two distributions, $M = \frac{1}{2}(P + Q)$

Cross-entropy

Information Theory

- *Cross-entropy* is closely related to the KL divergence, and it is defined as the summation of the entropy $H(P)$ and KL divergence $D_{KL}(P||Q)$

$$CE(P, Q) = H(P) + D_{KL}(P||Q)$$

- Alternatively, the cross-entropy can be written as

$$CE(P, Q) = -\mathbb{E}_{X\sim P}\,[\log Q(X)]$$

- In machine learning, let's assume a classification problem based on a set of data examples $\{x_1, x_2, \ldots, x_n\}$, that need to be classified into k classes
  - For each data example x_i we have a class label y_i
    - The true labels $\mathbf{y}$ follow the true distribution P
  - The goal is to train a classifier (e.g., a NN) parameterized by θ, that outputs a predicted class label $\hat{y}_i$ for each data example x_i
    - The predicted labels $\hat{\mathbf{y}}$ follow the estimated distribution Q
  - The cross-entropy loss between the true distribution P and the estimated distribution Q is calculated as: $CE(\mathbf{y}, \hat{\mathbf{y}}) = -\mathbb{E}_{X\sim P}\,[\log Q(X)] = -\sum_X P(X) \log Q(X) = -\sum_i y_i \log \hat{y}_i$
    - The further away the true and estimated distributions are, the greater the cross-entropy loss is

References

1. A. Zhang, Z. C. Lipton, M. Li, A. J. Smola, *Dive into Deep Learning*, https://d2l.ai, 2020.
2. I. Goodfellow, Y. Bengio, A. Courville, *Deep Learning*, MIT Press, 2017.
3. M. P. Deisenroth, A. A. Faisal, C. S. Ong, *Mathematics for Machine Learning*, Cambridge University Press, 2020.
4. Jeff Howbert — Machine Learning Math Essentials presentation
5. Brian Keng – Manifolds: A Gentle Introduction blog
6. Martin J. Osborne – Mathematical Methods for Economic Theory (link)

Appendix

(Not required for quizzes or assignments)

Maximum Likelihood

Information Theory

- Cross-entropy is also related to the ***maximum likelihood*** estimation
- In ML, we want to find a model with parameters θ that maximize the probability that the data is assigned the correct class, i.e., $\text{argmax}_\theta\, P(\text{model} \mid \text{data})$
  - For the classification problem from previous page, we want to find parameters θ so that for the data examples $\{x_1, x_2, \ldots, x_n\}$ the probability of outputting class labels $\{y_1, y_2, \ldots, y_n\}$ is maximized
    - I.e., for some data examples, the predicted class $\hat{y}_j$ will be different than the true class y_j, but the goal is to find θ that results in an overall maximum probability
- From Bayes' theorem, argmax $P(\text{model} \mid \text{data})$ is proportional to argmax $P(\text{data} \mid \text{model})$

$$P(\theta | x_1, x_2, \ldots, x_n) = \frac{P(x_1, x_2, \ldots, x_n | \theta)\, P(\theta)}{P(x_1, x_2, \ldots, x_n)}$$

  - This is true since $P(x_1, x_2, \ldots, x_n)$ does not depend on the parameters θ
  - Also, we can assume that we have no prior assumption on which set of parameters θ are better than any others
- Recall that $P(\text{data}|\text{model})$ is the likelihood, therefore, the maximum likelihood estimate of θ is based on solving

$$\arg\max_\theta P(x_1, x_2, \ldots, x_n | \theta)$$

Maximum Likelihood

Information Theory

- For a total number of n observed data examples $\{x_1, x_2, \dots, x_n\}$, the predicted class labels for the data example x_i is $\hat{\mathbf{y}}_i$
  - Using the multinoulli distribution, the probability of predicting the true class label $\mathbf{y}_i = \{y_{i1}, y_{i2}, \dots, y_{ik}\}$ is $\mathcal{P}(x_i \mid \theta) = \prod_j \hat{y}_{ij}{}^{y_{ij}}$, where $j \in \{1,2,\dots,k\}$
  - E.g., we have a problem with 3 classes [car, house, tree], and an image of a car x_i, the true label $\mathbf{y}_i = [1,0,0]$, and let's assume a predicted label $\hat{\mathbf{y}}_i = [0.7, 0.1, 02]$, then the probability is $\mathcal{P}(x_i \mid \theta) = \prod_j \hat{y}_{ij}{}^{y_{ij}} = 0.7^1 \cdot 0.1^0 \cdot 0.2^0 = 0.7 \cdot 1 \cdot 1 = 0.7$
- Assuming that the data examples are independent, the likelihood of the data given the model parameters θ can be written as $\mathcal{P}(x_1, x_2, \dots, x_n \mid \theta) = \mathcal{P}(x_1 \mid \theta) \cdots \mathcal{P}(x_n \mid \theta) = \prod_j \hat{y}_{1j}{}^{y_{1j}} \cdot \prod_j \hat{y}_{2j}{}^{y_{2j}} \cdots \prod_j \hat{y}_{nj}{}^{y_{nj}} = \prod_i \prod_j \hat{y}_{ij}{}^{y_{ij}}$
- Log-likelihood is often used because it simplifies numerical calculations, since it transforms a product with many terms into a summation, e.g., $\log\left(a_1{}^{b_1} \cdot a_2{}^{b_2}\right) = b_1 \log(a_1) + b_2 \log(a_2)$
  - $\log \mathcal{P}(x_1, x_2, \dots, x_n \mid \theta) = \log\left(\prod_i \prod_j \hat{y}_{ij}{}^{y_{ij}}\right) = \sum_i \sum_j y_{ij} \log \hat{y}_{ij}$
  - A negative of the log-likelihood allows us to use minimization approaches, i.e., $-\log \mathcal{P}(x_1, x_2, \dots, x_n \mid \theta) = -\sum_i \sum_j y_{ij} \log \hat{y}_{ij} = CE(\mathbf{y}, \hat{\mathbf{y}})$
- Thus, maximizing the likelihood is the same as minimizing the cross-entropy