Mathematics for ML

Srinivasa. R
Bangalore, India

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 $\mathcal{A}$
$\|\mathcal{A}\|$	Cardinality: number of items in set $\mathcal{A}$
$\\|\mathbf{w}\\|$	Norm of vector $\mathbf{w}$
$\mathbf{u} \cdot \mathbf{w}$ or $\langle \mathbf{u}, \mathbf{w} \rangle$	Dot product of vectors $\mathbf{u}$ and $\mathbf{w}$
$\mathbb{R}$	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
$f : \mathbb{R}^n \to \mathbb{R}$	Function (map): map an n-dimensional vector into a scalar

Notation

$\mathbf{A} \odot \mathbf{B}$	Element-wise product of matrices **A** and **B**
$\mathbf{A}$	Pseudo-inverse of matrix **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
$P(X \mid Y)$	Probability of X given Y
$\mathcal{N}(\mu, \sigma^2)$	Gaussian distribution with mean μ and variance σ^2
$\mathbb{E}_{X \sim P}[f(X)]$	Expectation of $f(X)$ with respect to $P(X)$
$\mathrm{Var}(f(X))$	Variance of $f(X)$
$\mathrm{Cov}(f(X), g(Y))$	Covariance of $f(X)$ and $g(Y)$
$\mathrm{corr}(X, Y)$	Correlation coefficient for X and Y
$D_{KL}(P \parallel Q)$	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

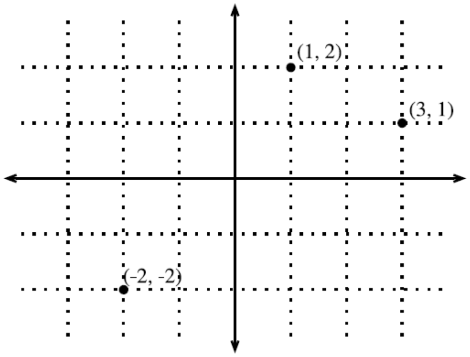
$$\mathbf{x} = \begin{bmatrix} 1 \\ 7 \\ 0 \\ 1 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} 1 & 7 & 0 & 1 \end{bmatrix}^T$$

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

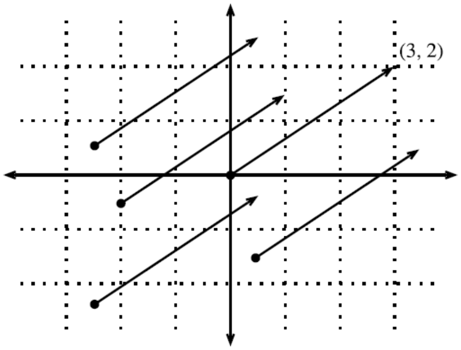
$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}$$

Geometry of Vectors

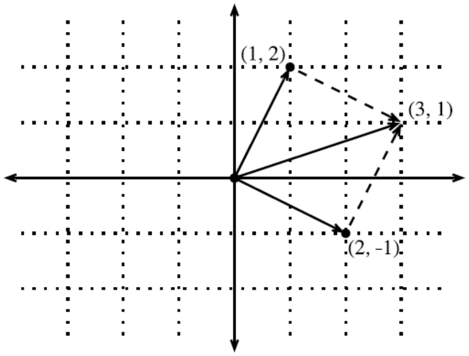
- First interpretation of a vector: point in space
  - E.g., in 2D we can visualize the data points with respect to a coordinate origin



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

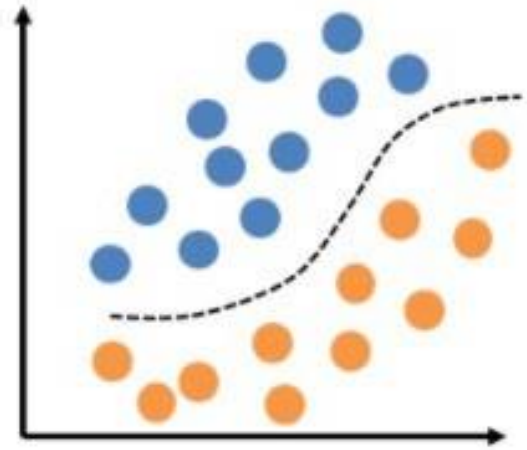


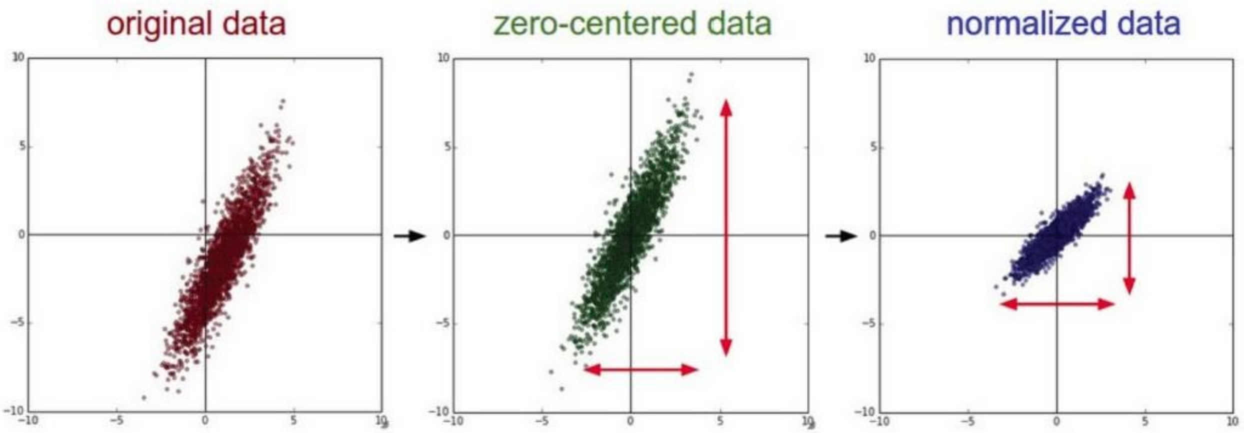
- Vector addition
  - We add the coordinates, and follow the directions given by the two vectors that are added



Contd…

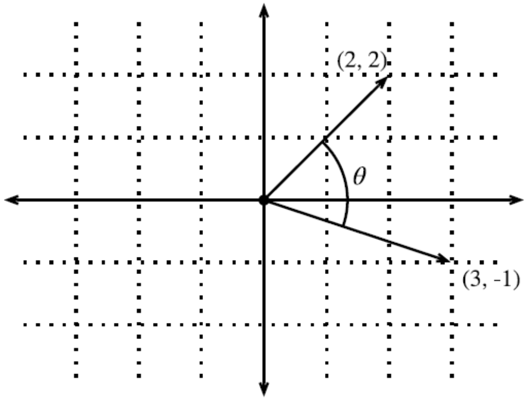
- The geometric interpretation of vectors as points in space allow us to consider a training set of input examples in ML as a collection of points in space
  - Hence, classification can be viewed as discovering how to separate two clusters of points belonging to different classes (left picture)
    -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





Dot Product and Angles

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



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

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

Norm of a Vector

Vectors

- A vector ***norm*** is a function that maps a vector to a scalar value
  - The norm is 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: $f(\mathbf{x} + \mathbf{y}) \leq f(\mathbf{x}) + f(\mathbf{y})$
  - Must be non-negative: $f(\mathbf{x}) \geq 0$
- The general ℓ_p norm of a vector $\mathbf{x}$ is obtained as: $\|\mathbf{x}\|_p = \left(\sum_{i=1}^{m} |x_i|^p\right)^{\frac{1}{p}}$
  - On next page we will review the most common norms, obtained for $p = 1, 2$, and ∞

Contd…

Vectors

- 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

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

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

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

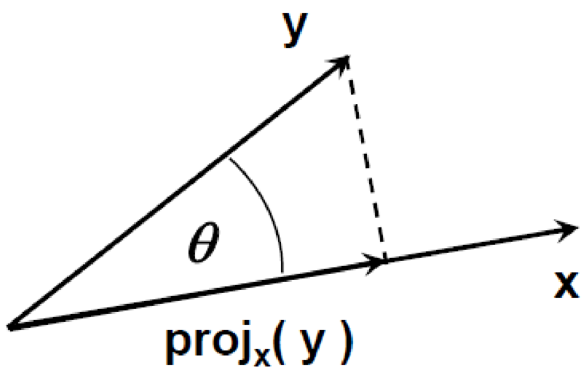
- For $p = \infty$, we have ℓ_∞ norm
  - Known as **infinity norm**, or **max norm**
  - Outputs the absolute value of the largest element

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

- 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

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



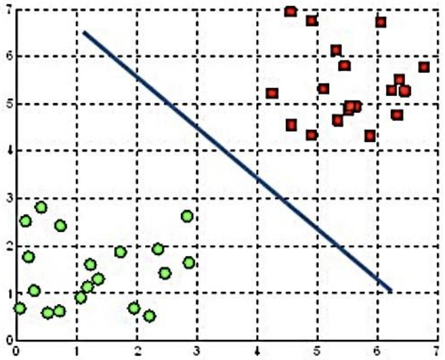
$$\mathbf{proj}_{\mathbf{x}}(\mathbf{y}) = \frac{\mathbf{x} \cdot \|\mathbf{y}\| \cdot \cos(\theta)}{\|\mathbf{x}\|}$$

Hyperplanes

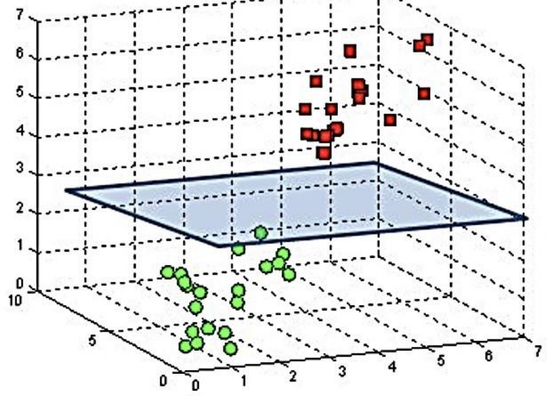
Hyperplanes

- ***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 *dd*− 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



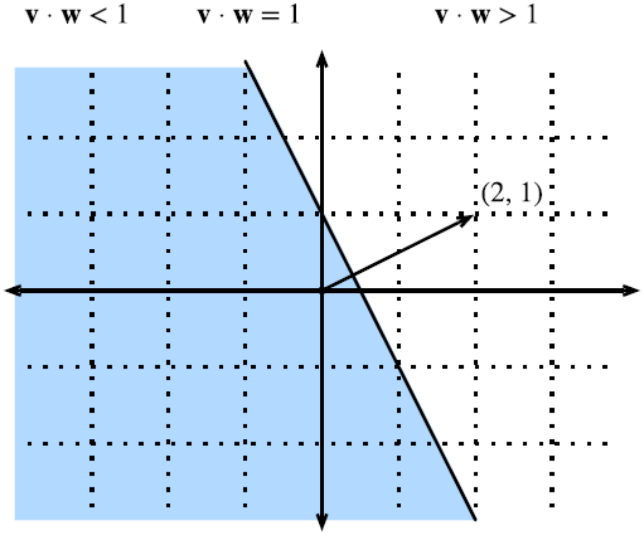
A hyperplane in $\mathbb{R}^3$ is a plane



Contd…

Hyperplanes

- For example, for a given data point **ww**= $[2,1]^{TT}$, we can use dot-product to find the hyperplane for which **ww**�**w**= 1
  - I.e., all vectors with **ww**�**w**> 1 can be classified as one class, and all vectors with **ww**�**w**< 1 can be classified as another class

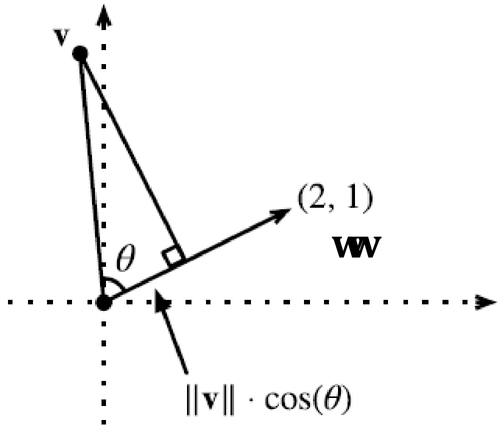


$\mathbf{v}\cdot\mathbf{w} < 1$
$\mathbf{v}\cdot\mathbf{w} = 1$
$\mathbf{v}\cdot\mathbf{w} > 1$
(2, 1)

- Solving **ww**�**w**= 1, we obtain

$$\|\mathbf{v}\|\|\mathbf{w}\|\cos(\theta) = 1 \iff \|\mathbf{v}\|\cos(\theta) = \frac{1}{\|\mathbf{w}\|} = \frac{1}{\sqrt{5}}$$

  - I.e., the solution is the set of points for which **ww**�**w**= 1 meaning the points lay on the line that is orthogonal to the vector **ww**
    - That is the line $2xx + yy = 1$
  - The orthogonal projection of **w**onto **ww**is $\|\mathbf{w}\| ccc(\theta\theta) = \frac{1}{\sqrt{5}}$

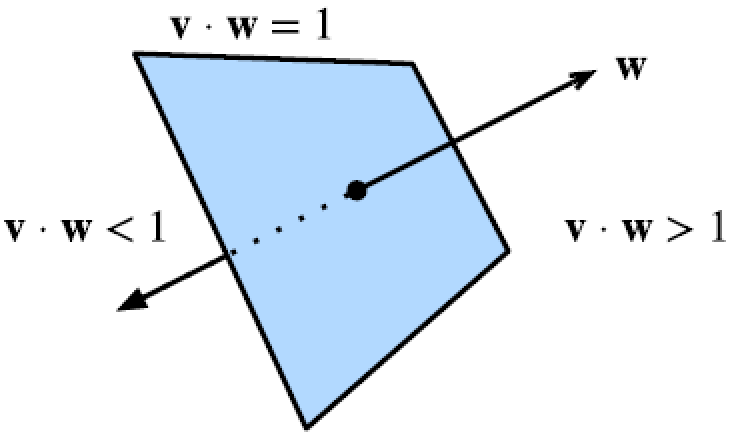


Picture from: http://d2l.ai/chapter_appendix-mathematics-for-deep-learning/geometry-linear-algebraic-ops.html#hyperplanes

Contd…

Hyperplanes

- In a 3D space, if we have a vector **ww**= $[1, 2, 3]^{TT}$ and try to find all points that satisfy **ww�w**= 1, we can obtain a plane that is orthogonal to the vector **ww**
  - The inequalities **ww�w**> 1 and **ww�w**< 1 again define the two subspaces that are created by the plane



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

- The same concept applies to high-dimensional spaces as well

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

Matrices

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 $\mathbf{A}(i,j)$

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

- 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

Contd…

Matrices

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

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

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

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

- Matrix multiplication $(\mathbf{AB})_{i,j} = \mathbf{A}_{i,1}\mathbf{B}_{1,j} + \mathbf{A}_{i,2}\mathbf{B}_{2,j} + \cdots + \mathbf{A}_{i,n}\mathbf{B}_{n,j}$
  - 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 $\mathbf{AB} \neq \mathbf{BA}$

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

Contd…

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

$$\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A} \qquad \mathbf{A}(\mathbf{B} + \mathbf{C}) = \mathbf{A}\mathbf{B} + \mathbf{A}\mathbf{C}$$

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

$$\left(\mathbf{A}^T\right)^T = \mathbf{A} \qquad (\mathbf{A}\mathbf{B})^T = \boldsymbol{B}^T\mathbf{A}^T$$

- *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 : $\mathbf{I}_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

Contd…

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

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

  - 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***

Contd…

Matrices

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

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

Matrix-Vector Products

- 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: $\mathbf{A}(m\times n)$ � $\mathbf{x}(n\times 1) = \mathbf{Ax}(m\times 1)$

Contd…

Matrices

- To multiply two matrices $\mathbf{AA} \in \mathbb{R}^{mn\times kk}$ and $\mathbf{BB} \in \mathbb{R}^{kk\times mm}$

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

- We can consider the matrix-matrix product as dot-products of rows in $\mathbf{AA}$ and columns in $\mathbf{BB}$

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

- Size: $\mathbf{AA}(m\times kk)$ �$\mathbf{BB}(kk\times mm) = \mathbf{CC}(m\times mm)$

Inverse of a Matrix

- For a square $m \times m$ matrix $\mathbf{A}$ with rank m, $\mathbf{A}^{-1}$ 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

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

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

- If $\det(A) = 0$ (i.e., $\text{rank}(A) < m$), 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 $\mathbf{A}^{\dagger} = \left(\mathbf{A}^{T}\mathbf{A}\right)^{-1}\mathbf{A}^{T}$ and $\mathbf{A}^{\dagger}\mathbf{A} = \mathbf{I}$
- If $m < n$, then the pseudo-inverse is $\mathbf{A}^{\dagger} = \mathbf{A}^{T}\left(\mathbf{A}\mathbf{A}^{T}\right)^{-1}$ and $\mathbf{A}\mathbf{A}^{\dagger} = \mathbf{I}$
  - 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 $\mathbf{X}_{2\times3}\mathbf{X}^{\dagger}_{3\times2} = \mathbf{I}_{2\times2}$

Tensors

Tensors

- *Tensors* are n-dimensional arrays of scalars
  - Vectors are first-order tensors, $\mathbf{w} \in \mathbb{R}^{nn}$
  - Matrices are second-order tensors, $\mathbf{AA} \in \mathbb{R}^{mm \times nn}$
  - E.g., a fourth-order tensor is $\mathbf{T} \in \mathbb{R}^{nn_1 \times nn_2 \times nn_3 \times nn_4}$
- 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 × 224 × 3
  - The channel axis corresponds to the color channels (red, green, and blue)

Manifolds

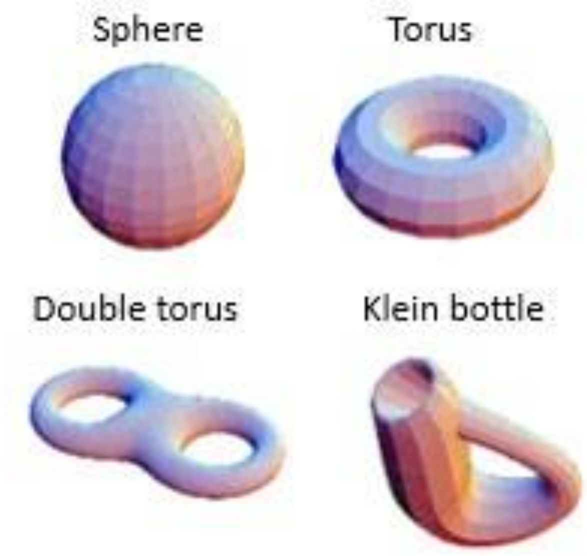
Manifolds

- 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

Contd…

Manifolds

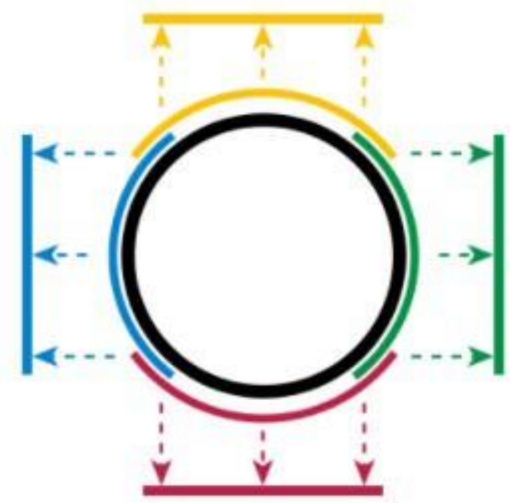
- Manifolds are studied in mathematics under topological spaces
- An n-dimensional ***manifold*** is defined as a topological space with the property that each point has a neighborhood that is homeomorphic to the Euclidean space of dimension n
  - This means that a manifold locally resembles Euclidean 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

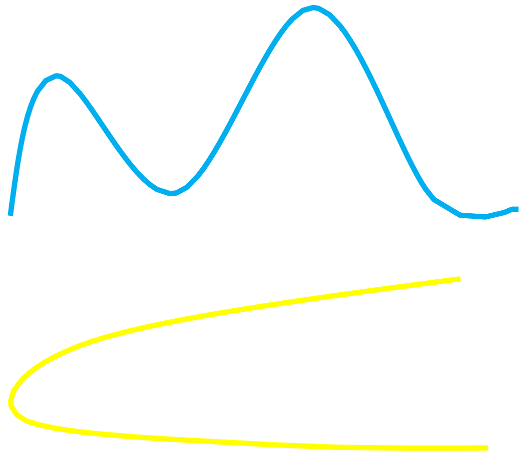


Contd…

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

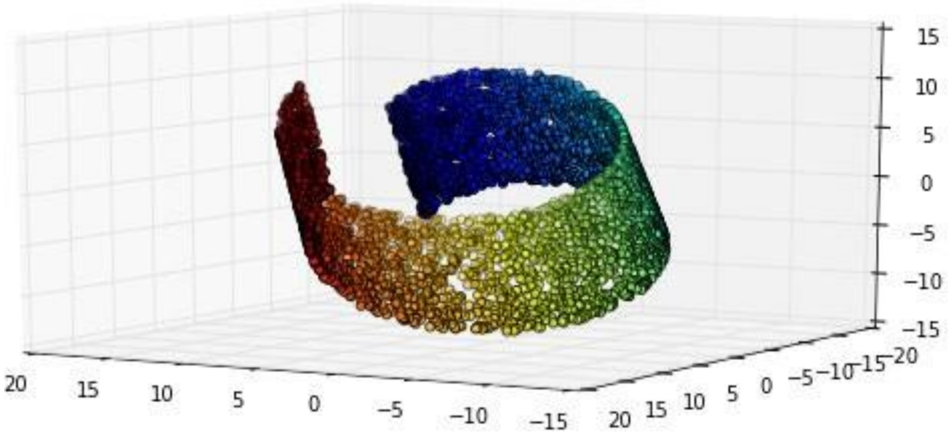


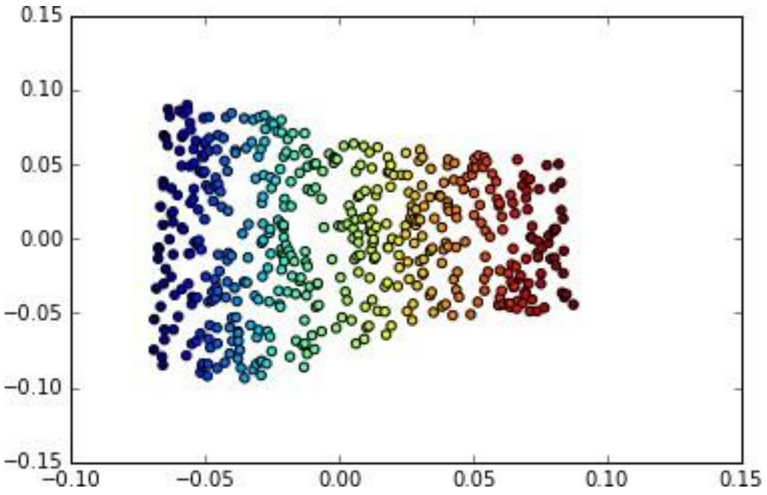


Manifolds

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

- *Eigen decomposition* is decomposing a matrix into a set of eigenvalues and eigenvectors
- *Eigenvalues* of a square matrix $\mathbf{A}$ are scalars λ and *eigenvectors* are non-zero vectors $\mathbf{w}$ that satisfy

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

- Eigenvalues are found by solving the following equation

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

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

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

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

Contd…

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

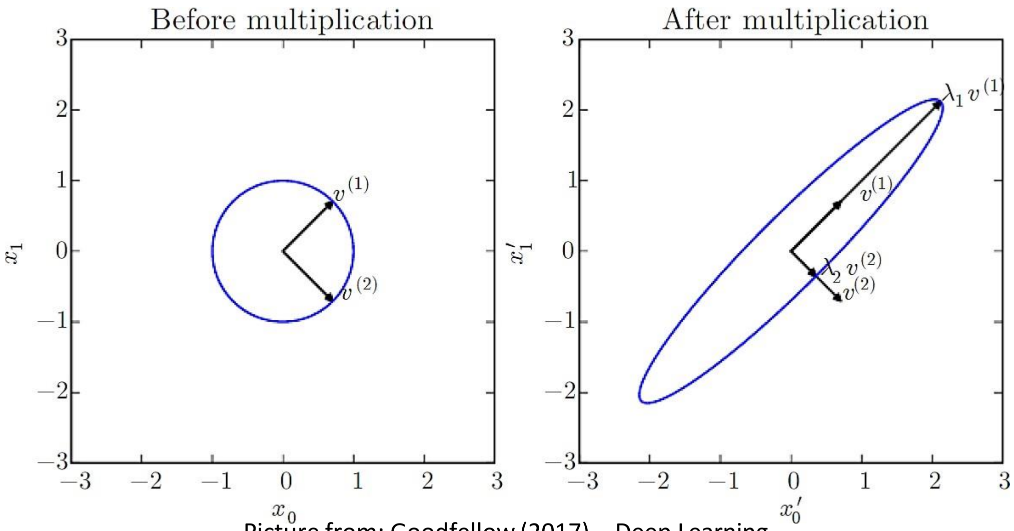
$$\det(\mathbf{A}) = \lambda_1 \text{�} \lambda_2 \cdots \lambda_n$$

  - If any of the eigenvalues are zero, the matrix is singular (it does not have an inverse)
- However, not every matrix can be decomposed into eigenvalues and eigenvectors
  - Also, in some cases the decomposition may involve complex numbers
  - Still, every real symmetric matrix is guaranteed to have an eigen decomposition according to $\mathbf{A} = \mathbf{W}\boldsymbol{\Lambda}\mathbf{W}^{-1}$, where $\mathbf{W}$ is an orthogonal matrix

Contd…

Eigen Decomposition

- Geometric interpretation of the eigenvalues and eigenvectors is that they allow to stretch the space in specific directions
  - Left figure: the two eigenvectors $\mathbf{w}^1$ and $\mathbf{w}^2$ are shown for a matrix, where the two vectors are unit vectors (i.e., they have a length of 1)
  - Right figure: the vectors $\mathbf{w}^1$ and $\mathbf{w}^2$ 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

Differential Calculus

Differential Calculus

- For a function $f: \mathbb{R} \to \mathbb{R}$, 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:

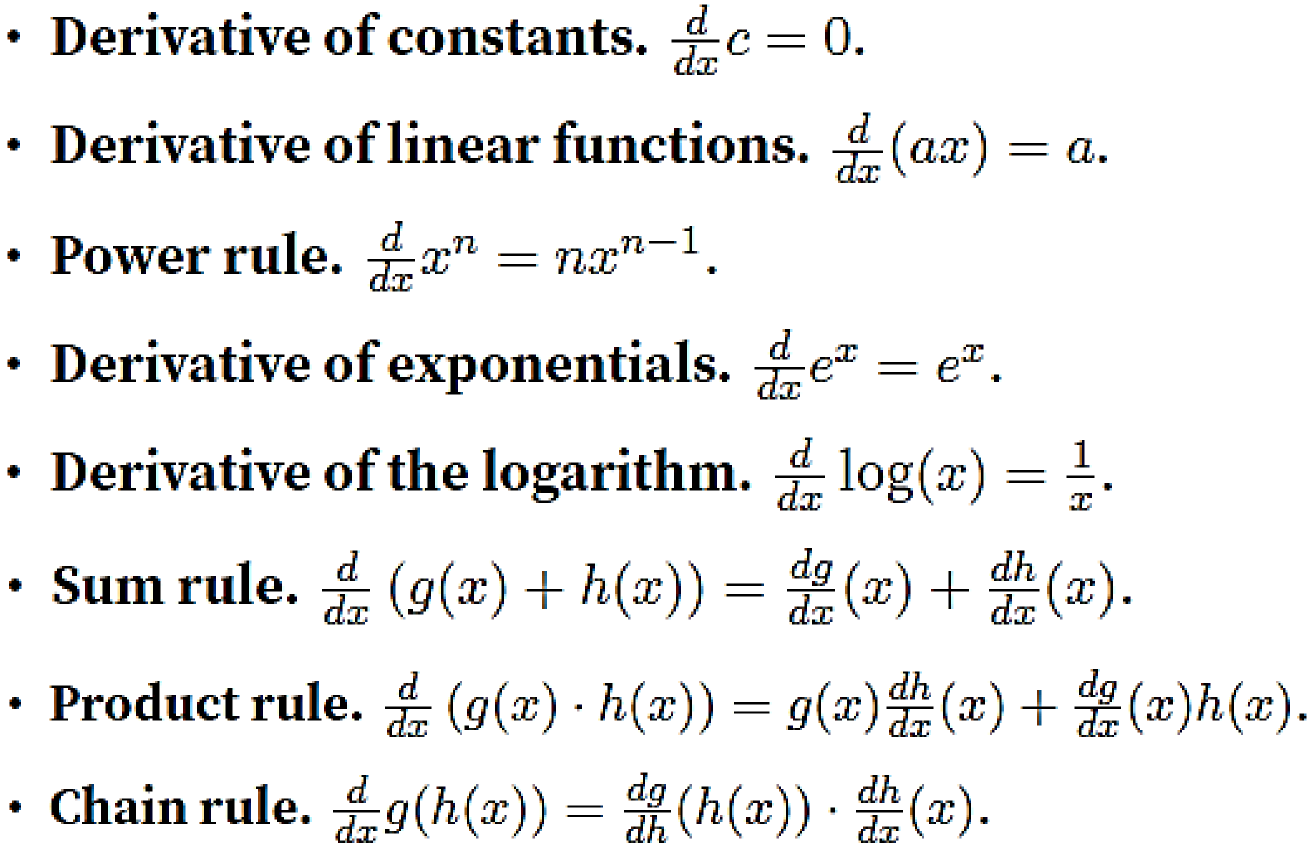
$$f'(x) = f' = \frac{dy}{dx} = \frac{df}{dx} = \frac{d}{dx} f(x) = Df(x) = D_x f(x)$$

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

Contd…

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.** $\frac{d}{dx}\left(g(x) + h(x)\right) = \frac{dg}{dx}(x) + \frac{dh}{dx}(x).$
- **Product rule.** $\frac{d}{dx}\left(g(x) \cdot h(x)\right) = g(x)\frac{dh}{dx}(x) + \frac{dg}{dx}(x)h(x).$
- **Chain rule.** $\frac{d}{dx}g(h(x)) = \frac{dg}{dh}(h(x)) \cdot \frac{dh}{dx}(x).$

Contd…

Differential Calculus

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

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

- 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 $f(x)$

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

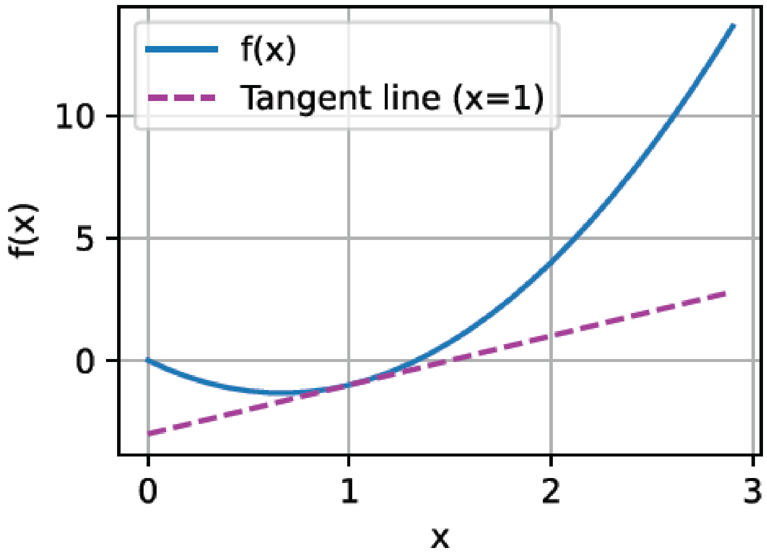
Geometric Interpretation

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

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

- The expression approximates the function $f(x)$ by a line which passes through the point $\big(x_0, f(x_0)\big)$ and has slope $\frac{df}{dx}\big|_{x_0}$ (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



Partial Derivatives

Differential Calculus

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

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

- To calculate $\frac{\partial y}{\partial x_i}$ (∂ pronounced "del" or we can just say "partial derivative"), we can treat $x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n$ 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 $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$, is a vector of n partial derivatives

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

- 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 **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

Optimization

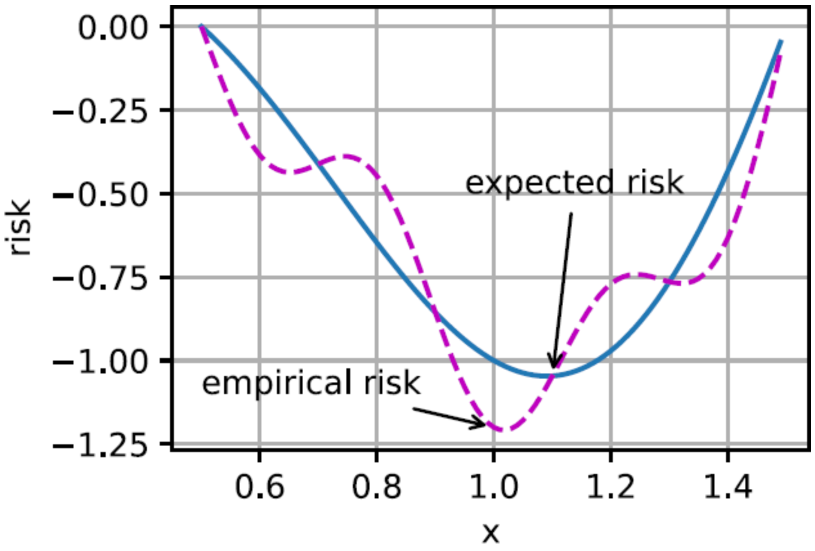
Optimization

- ***Optimization*** is concerned with optimizing an objective function — finding the value of an argument that minimizes or maximizes the function
  - Most optimization algorithms are formulated in terms of minimizing a function $ff(xx)$
  - Maximization is accomplished vie minimizing the negative of an objective function (e.g., minimize $-ff(xx)$)
  - 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

Contd…

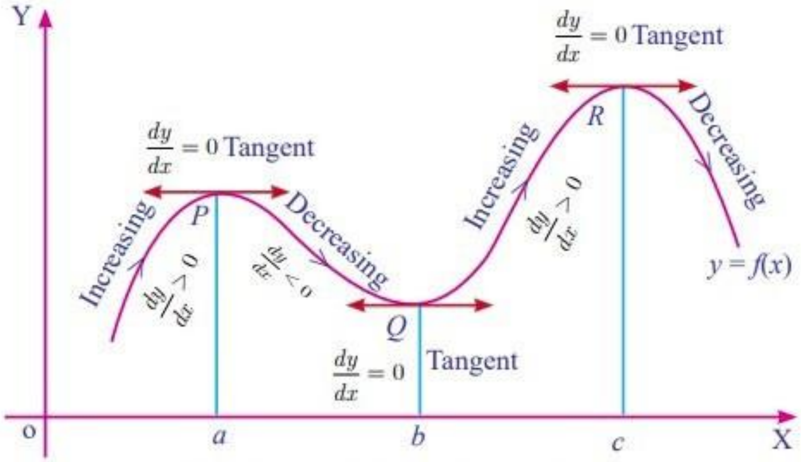
Optimization

- 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
- The expected function *f* (blue curve) is obtained given a limited amount of training data examples
- ML algorithms attempt to find the point of minimum expected risk, based on minimizing the error on a set of testing examples
    - Which may be at a different location than the minimum of the training examples
    - And which may not be minimal in a formal sense



Stationary Points

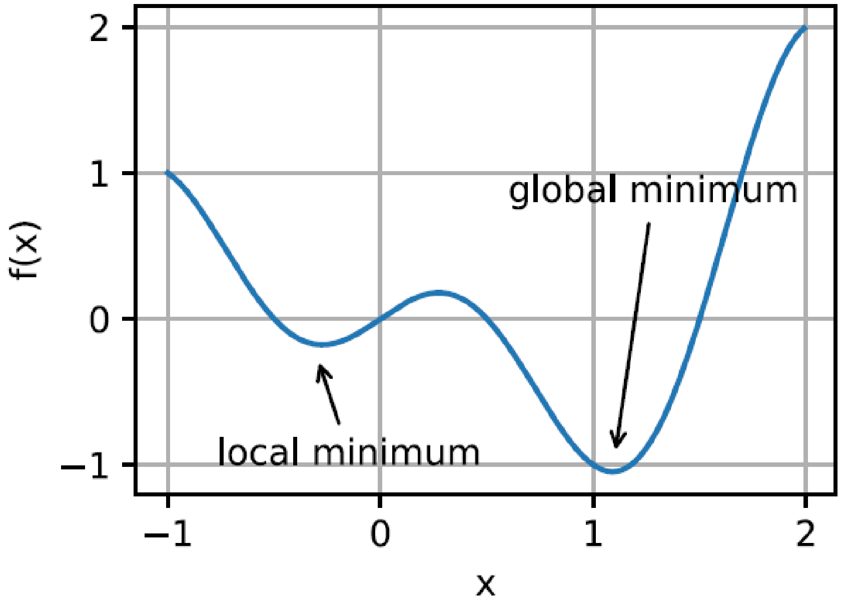
- ***Stationary points*** (or critical points) of a differentiable function $ff(xx)$ of one variable are the points where the derivative of the function is zero, i.e., $fff(xx) = 0$
- The stationary points can be:
  - ***Minimum***, a point where the derivative changes from negative to positive
  - ***Maximum***, 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 $ff(xx)$ at the point
  - If $ff''(xx) > 0$, the point is a minimum
  - If $ff''(xx) < 0$, the point is a maximum
  - If $ff''(xx) = 0$, 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

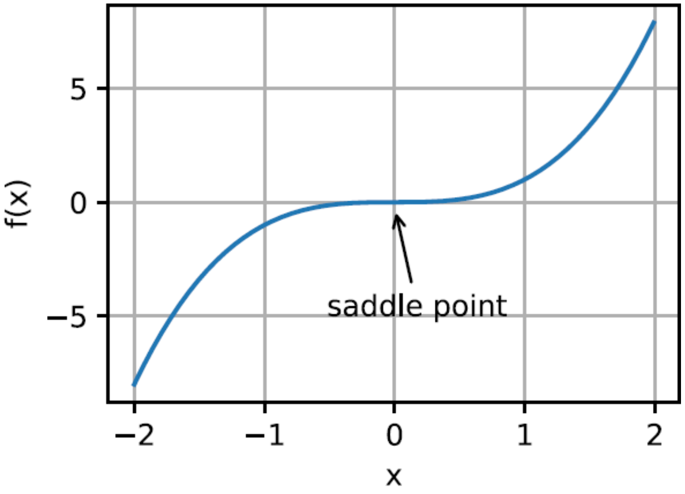
Local Minima

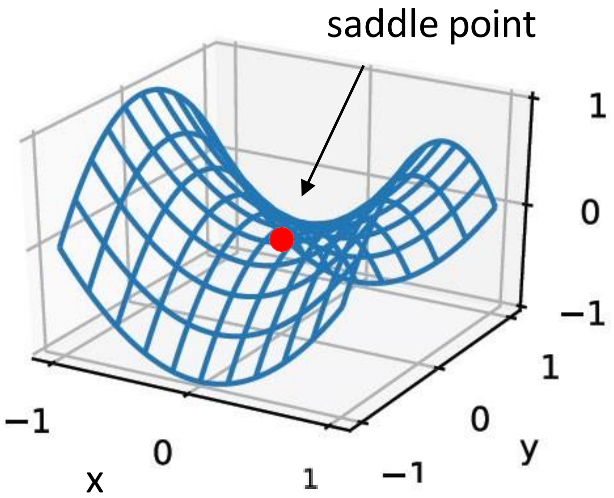
- Among the challenges in optimization of model's parameters in ML involve local minima, saddle points, vanishing gradients
- For an objective function $ff(xx)$, if the value at a point x is the minimum of the objective function over the entire domain of x, then it is the ***global minimum***
- If the value of $ff(xx)$ 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



Saddle Points

- The gradient of a function $ff(xx)$ 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 ($ffff(xx) = 0$) 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

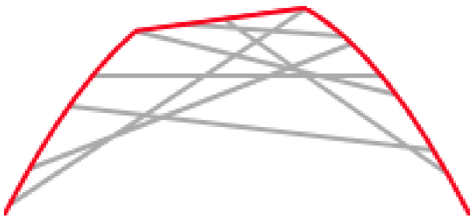




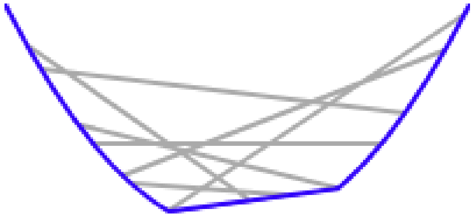
Convex Optimization

Optimization

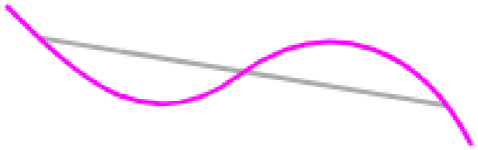
- A function of a single variable is ***concave*** if every line segment joining two points on its graph does not lie above the graph at any point
- Symmetrically, a function of a single variable is ***convex*** if every line segment joining two points on its graph does not lie below the graph at any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

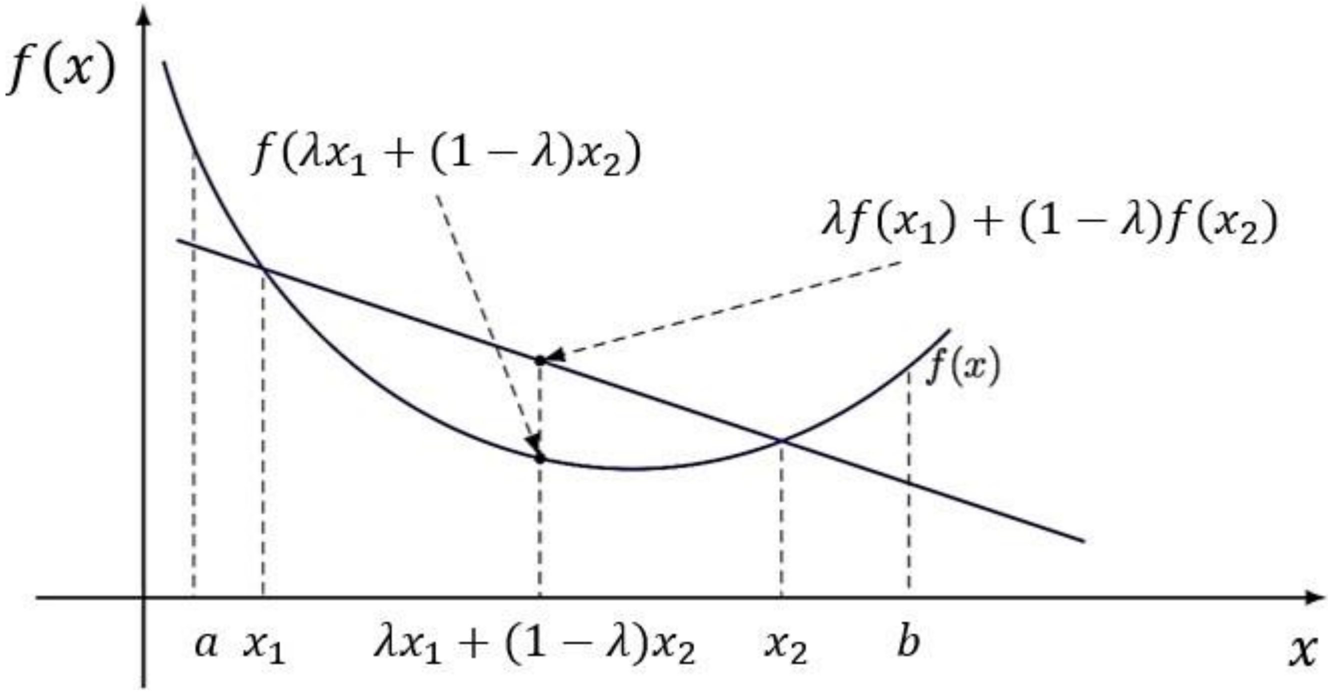


A function that is neither
concave nor convex:
the line segment shown lies
above the graph at some
points and below it at others

Contd…

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

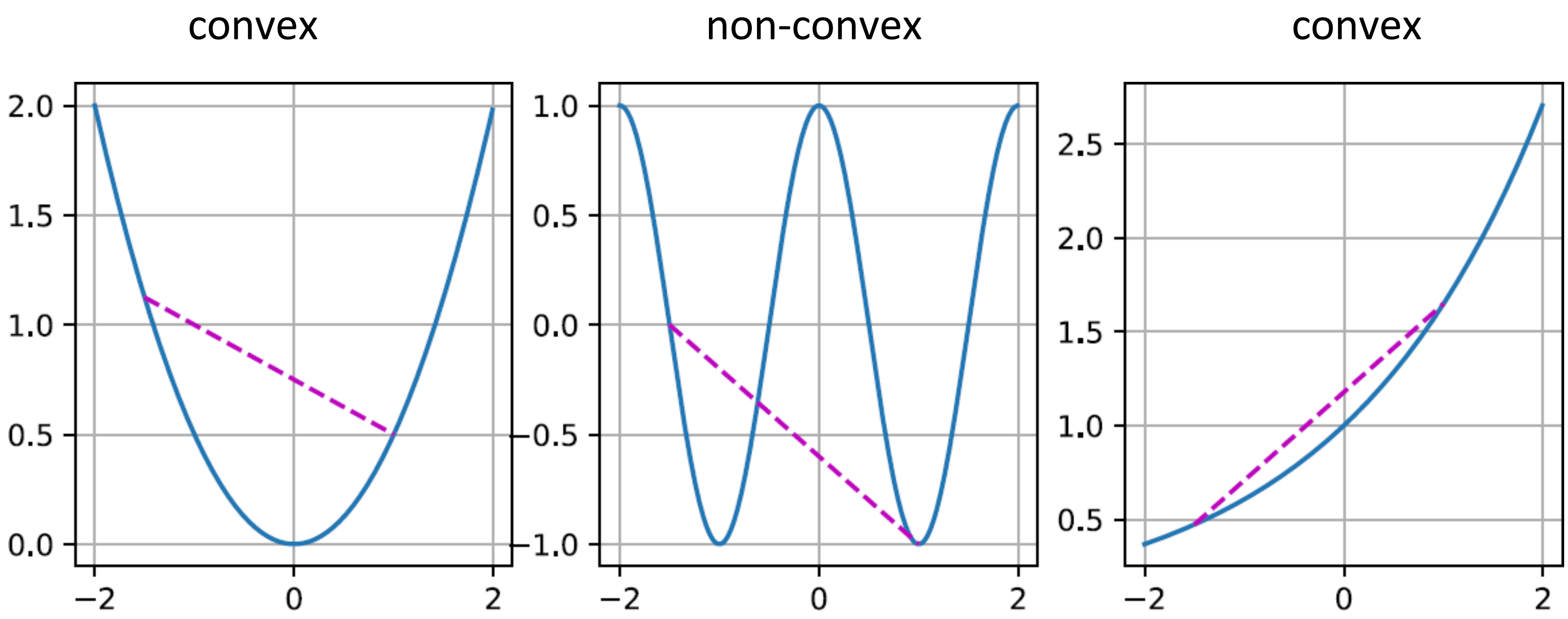
$$\lambda f(x_1) + (1-\lambda) f(x_2) \geq f(\lambda x_1 + (1-\lambda) x_2)$$


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



Probability

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.

Contd…

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**, $S = \{1, 2, 3, 4, 5, 6\}$
    - 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 $X \sim P(X)$ 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

Probability

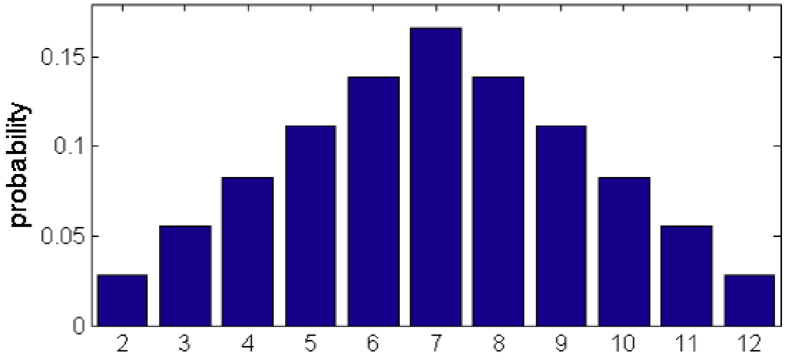
- The probability of an event A in the given sample space S, denoted as $P(A)$, must satisfies the following properties:
  - Non-negativity
    - For any event $A \in S$, $P(A) \geq 0$
  - All possible outcomes
    - Probability of the entire sample space is 1, $P(S) = 1$
  - Additivity of disjoint events
    - For all events $A_1, A_2 \in S$ that are mutually exclusive ($A_1 \cap A_2 = \emptyset$), the probability that both events happen is equal to the sum of their individual probabilities, $P(A_1 \cup A_2) = P(A_1) + P(A_2)$

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

Discrete Variables

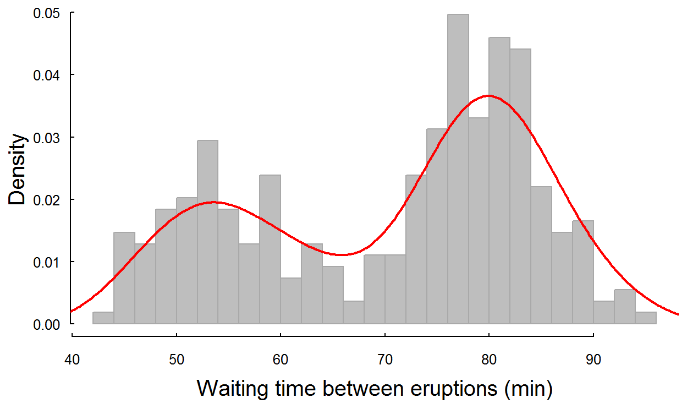
Probability

- 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:

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



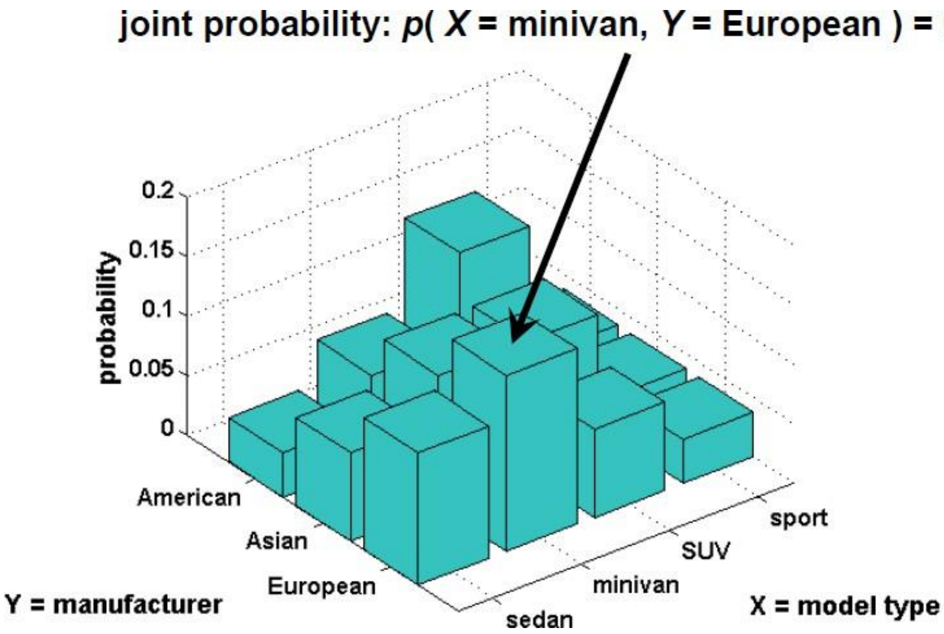
Multivariate Random Variables

- 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 $\mathbf{X} = (X_1, X_2, \ldots, X_n)^T$

Joint Probability Distribution

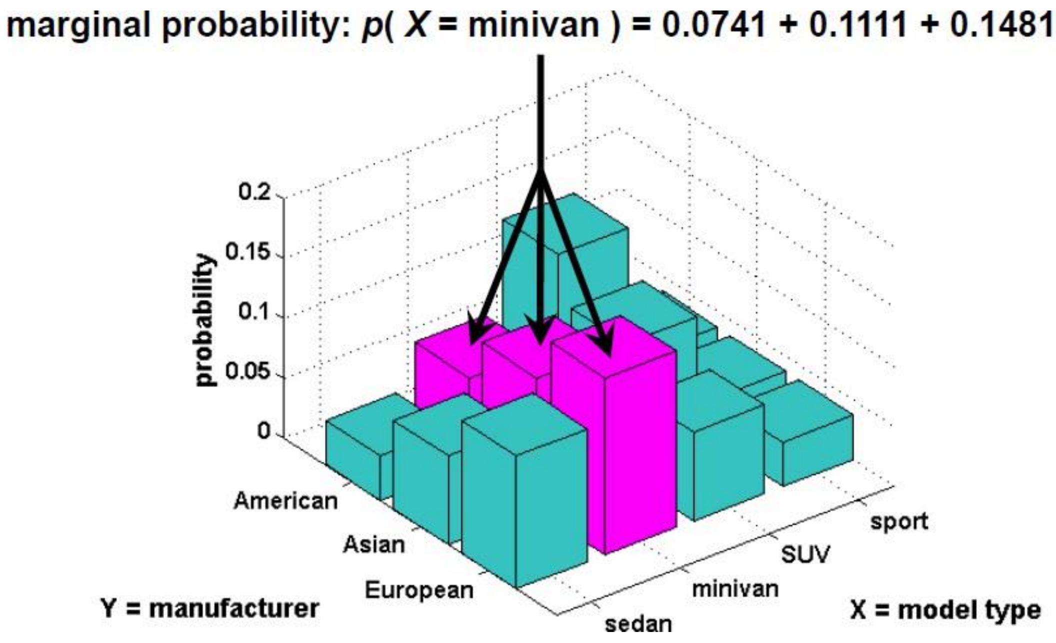
Probability

- 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 $XX$and YY, what is the probability that $XX= x$ and $YY= y$ simultaneously?
  - $PP(XX = xx, YY = yy)$ denotes the joint probability
  - We may also write $PP(xx, yy)$ for brevity



Marginal Probability Distribution

- *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

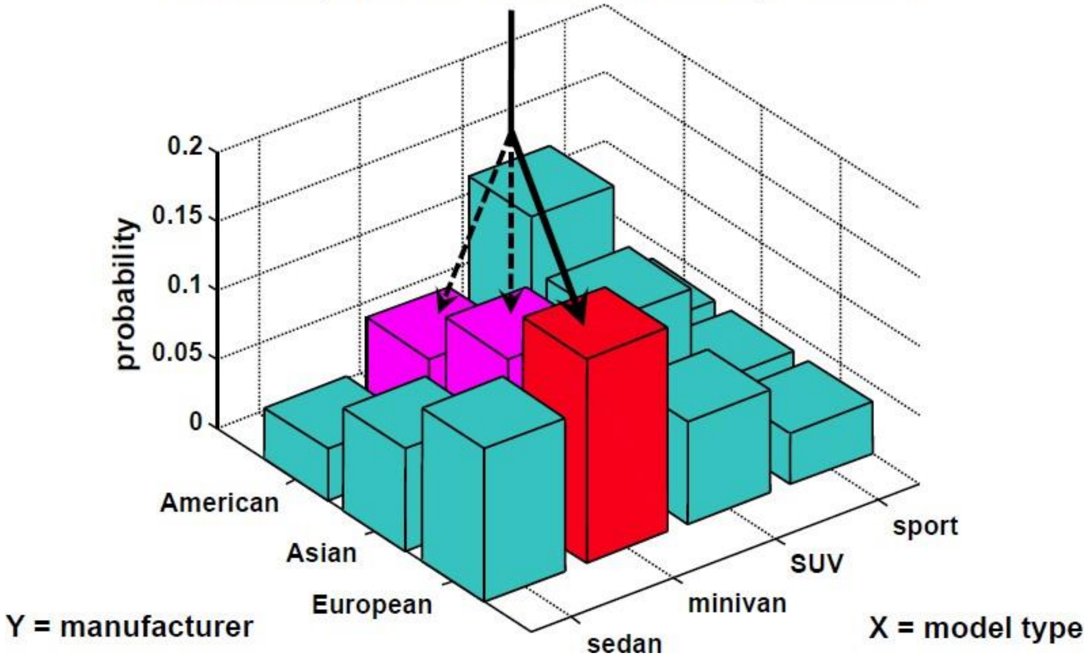


Conditional Probability Distribution

Probability

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

conditional probability: *p*(*Y* = European | *X* = minivan) =
0.1481 / (0.0741 + 0.1111 + 0.1481) = 0.4433



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: $\textbf{posterior probability} = \dfrac{\textbf{likelihood} \times \textbf{prior probability}}{\textbf{evidence}}$

Independence

Probability

- 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 $X \perp Y|Z$

Expected Value

Probability

- The ***expected value*** or ***expectation*** of a function $f(X)$ with respect to a probability distribution $P(X)$ is the average (mean) when X is drawn from $P(X)$
- For a discrete random variable X, it is calculated as

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

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

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

  - When the identity of the distribution is clear from the context, we can write $\mathbb{E}_X[f(X)]$
  - If it is clear which random variable is used, we can write just $\mathbb{E}[f(X)]$
- Mean is the most common measure of central tendency of a distribution
  - For a random variable: $f(X_i) = X_i \quad \Rightarrow \quad \mu = \mathbb{E}[X_i] = \sum_i P(X_i) \cdot X_i$
  - This is similar to the mean of a sample of observations: $\mu = \frac{1}{N} \sum_i X_i$
  - Other measures of central tendency: median, mode

Variance

Probability

- ***Variance*** gives the measure of how much the values of the function $ff(XX)$ deviate from the expected value as we sample values of X from $PP(XX)$

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

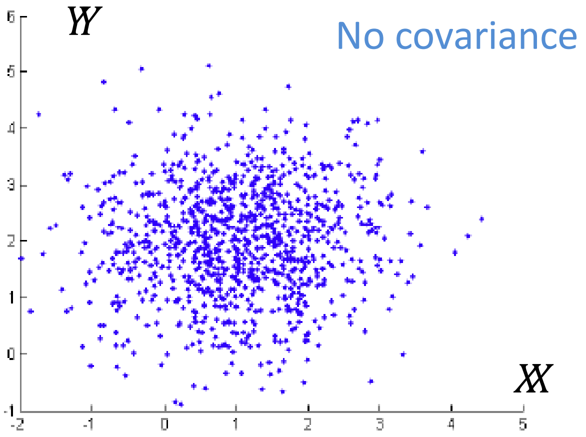
- When the variance is low, the values of $ff(XX)$ cluster near the expected value
- Variance is commonly denoted with $\sigma\sigma^2$
  - The above equation is similar to a function $ff(XX_i) = XX_i - \mu$
  - We have $\sigma\sigma^2 = \sum_{ii} PP(XX_i)$ �$XX_i - \mu)^2$
  - This is similar to the formula for calculating the variance of a sample of observations: $\sigma\sigma^2 = \frac{1}{NN-1}\sum_{ii}(XX_i - \mu)^2$
- The square root of the variance is the ***standard deviation***
  - Denoted $\sigma\sigma = \sqrt{\mathrm{Var}(XX)}$

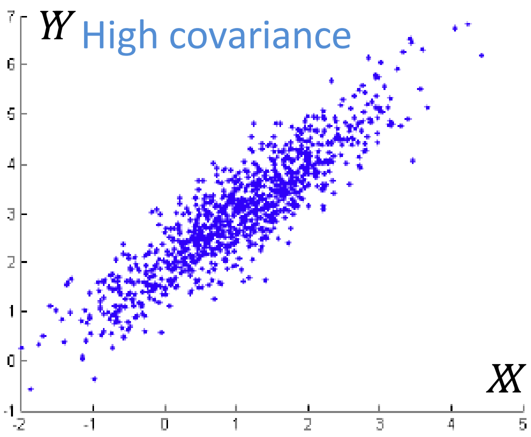
Covariance

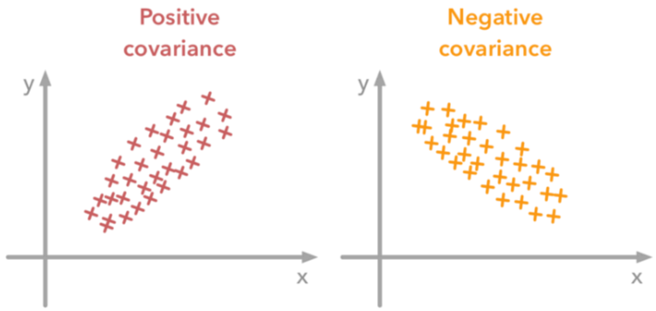
- *Covariance* gives the measure of how much two random variables are linearly related to each other

$$\mathrm{Cov}\big(f(X), g(Y)\big) = \mathbb{E}[(f(X) - \mathbb{E}[f(X)])(g(Y) - \mathbb{E}[g(Y)])]$$

- If $f(X_i) = X_i - \mu_X$ and $g(Y_i) = Y_i - \mu_Y$
  - Then, the covariance is: $\mathrm{Cov}(X,Y) = \sum_i P(X_i, Y_i) \cdot (X_i - \mu_X) \cdot (Y_i - \mu_Y)$
  - Compare to covariance of actual samples: $\mathrm{Cov}(X,Y) = \frac{1}{N-1} \sum_i (X_i - \mu_X)(Y_i - \mu_Y)$
- The covariance measures the tendency for X and Y to deviate from their means in same (or opposite) directions at same time





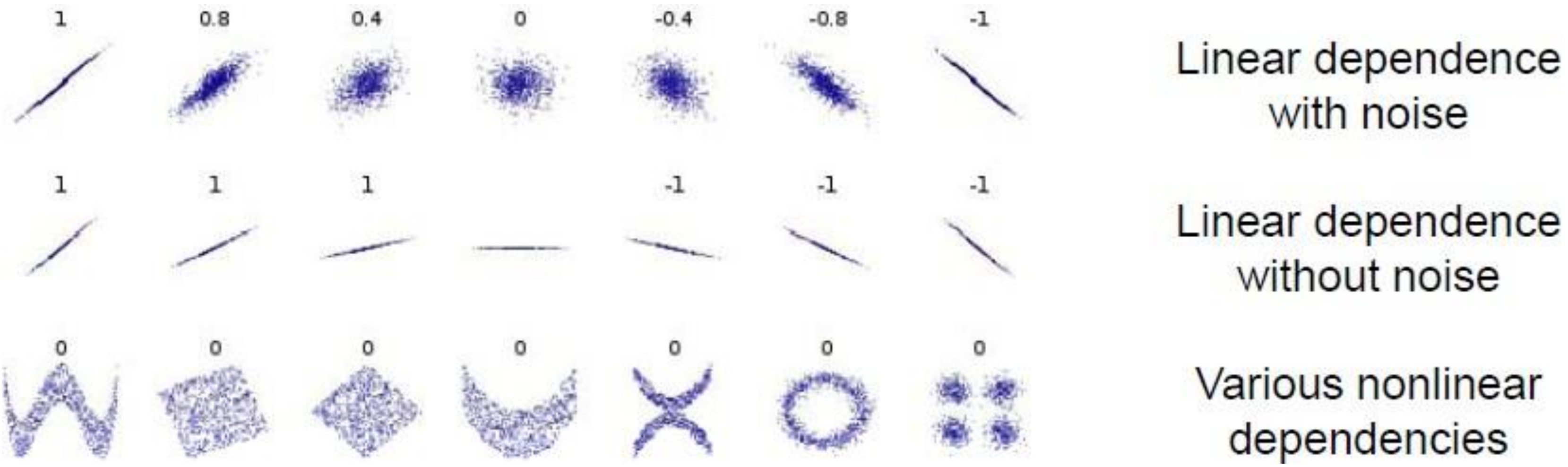


Correlation

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

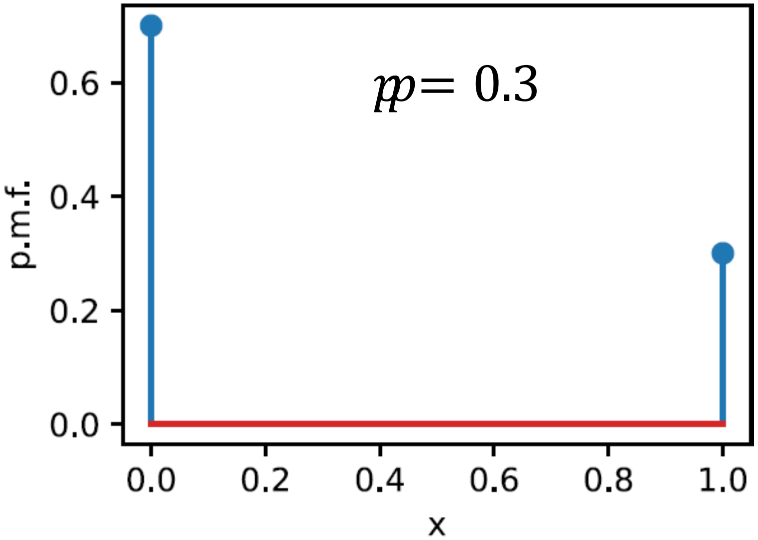
$$\mathrm{corr}(X,Y) = \frac{\mathrm{Cov}(X,Y)}{\sigma_X \cdot \sigma_Y}$$

  - 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

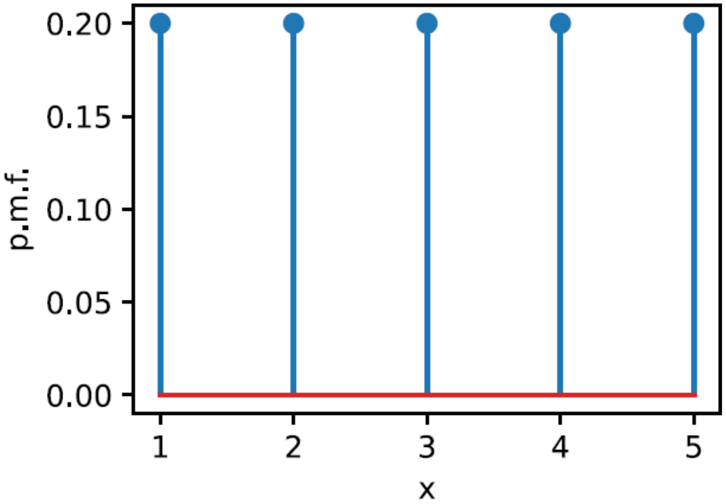


Probability Distributions

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



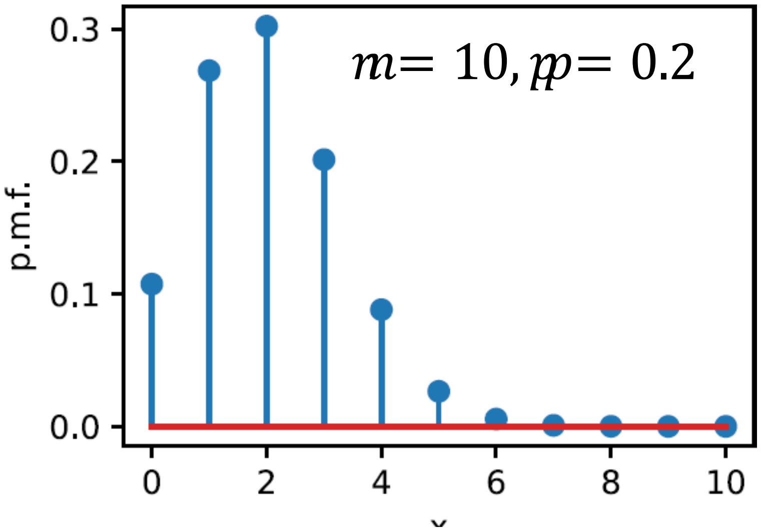
- ***Uniform distribution***
  - The probability of each value $i \in \{1,2, \dots, m\}$ is $p_i = \frac{1}{m}$
  - Notation: $X \sim U(m)$
  - Figure: $m = 5$, $p = 0.2$

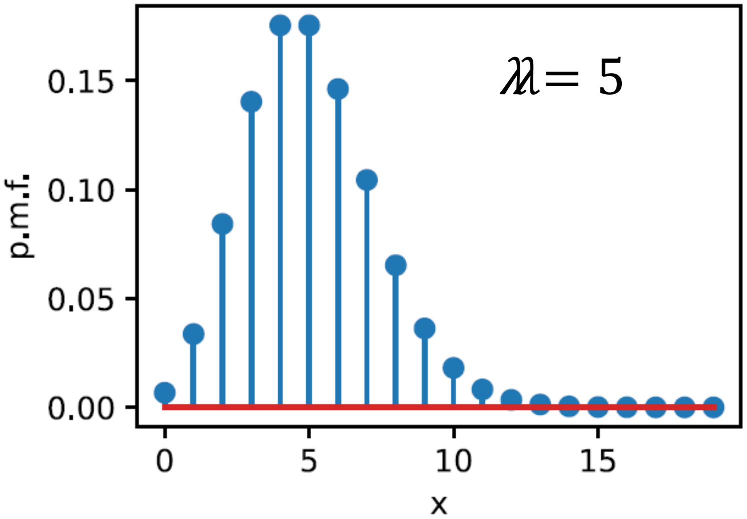


Contd…

Probability

- ***Binomial distribution***
  - Performing a sequence of *n* independent experiments, each of which has probability *p* of succeeding, where $p \in \{0, 1\}$
  - The probability of getting *k* successes in *n* trials is $P(X = k) = \binom{n}{k} p^{k} (1 - p)^{n-k}$
  - Notation: $X \sim \text{Binom}(n, p)$
- ***Poisson distribution***
  - A number of events occurring independently in a fixed interval of time with a known rate λ
  - A discrete random variable X with states $k \in \{0, 1, 2, \dots\}$ has probability $P(X = k) = \frac{\lambda^{X} e^{-\lambda}}{X!}$
  - The rate λ is the average number of occurrences of the event
  - Notation: $X \sim \text{Poisson}(\lambda)$



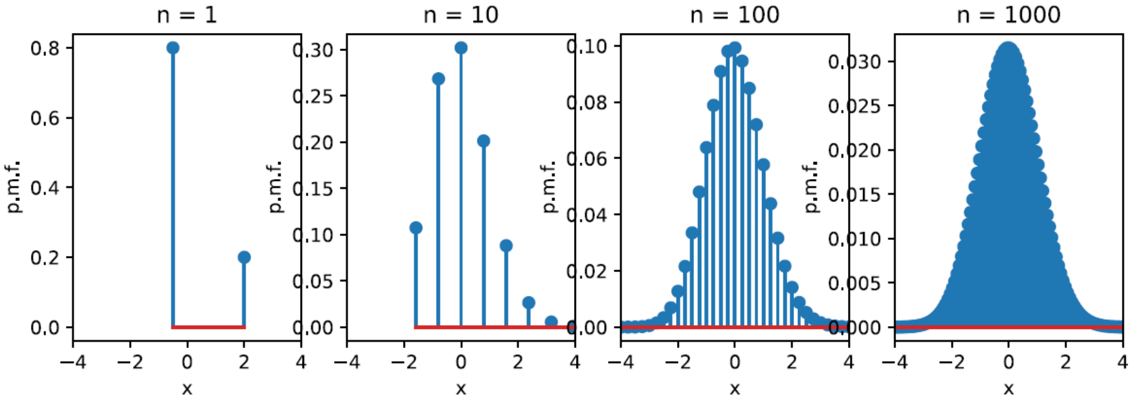


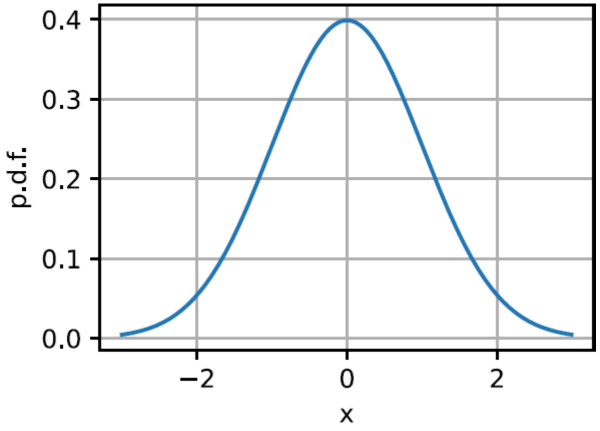
Contd…

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

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





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

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

- In machine learning, let's assume a classification problem based on a set of data examples $\{x_1, x_2, \dots, x_m\}$, 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: $CE(\mathbf{y},\hat{\mathbf{y}}) = -\mathbb{E}_{X\sim P}\left[\log Q(X)\right] = -\sum_x P(X)\log Q(X) = -\sum_i y_i \log \hat{y}_i$
    - The further away the true and estimated distributions are, the greater the cross-entropy loss is