# CS 559: Machine Learning Fundamentals & Applications

Lecture 2: Mathematics for Machine Learning
Spring 2023



### Outline



- Linear Algebra
- Analytic Geometry
- Vector Calculus
- Probability Theory



# 2.1. Linear Algebra

### 2.1.1. Basic Matrix Identities



A matrix A has elements  $A_{ij}$  where i indexes the rows, and j indexes the columns.

$$\mathbf{A} = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix}, \qquad A_{ij} \in \mathbb{R}.$$

### 2.1.2. Matrix Addition and Multiplication



The sum of two matrices  $A \in \mathbb{R}^{m \times n}$ ,  $B \in \mathbb{R}^{m \times n}$  is the element-wise sum,

$$\mathbf{C} = \mathbf{A} + \mathbf{B} = \begin{bmatrix} a_{11} + b_{11} & \cdots & a_{1n} + b_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} + b_{m1} & \cdots & a_{mn} + b_{mn} \end{bmatrix} \in \mathbb{R}^{m \times n}.$$

The product of two matrices  $A \in \mathbb{R}^{m \times n}$ ,  $B \in \mathbb{R}^{n \times k}$  is the pair-wise sum,

$$C = AB \in \mathbb{R}^{m \times k}, c_{ij} = \sum_{l=1}^{n} a_{il} b_{lj}, i = 1, ..., m, j = 1, ..., k.$$

## 2.1.2. Matrix Addition and Multiplication

#### Matrix Multiplication Properties:

- Not commutative:  $AB \neq BA$
- Associative:  $\forall A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{n \times p}, C \in \mathbb{R}^{p \times q}$ : (AB)C = A(BC)
  - o  $(\lambda \psi) \mathbf{C} = \lambda(\psi) \mathbf{C}$  where  $\lambda$  and  $\psi$  are constants.
- Distributive:  $\forall A, B \in \mathbb{R}^{m \times n}, C \in \mathbb{R}^{n \times p}$ : (A + B)C = AC + BC
  - $\circ (\lambda + \psi)\mathbf{C} = \lambda\mathbf{C} + \psi\mathbf{C}$



### 2.1.3. Inverse and Transpose



A matrix  $I_N$  is the  $N \times N$  identity matrix (also called the unit matrix)

$$I_N = \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix}.$$

The inverse of  $A \in \mathbb{R}^{n \times n}$ ,  $A^{-1}$ , satisfies

$$AA^{-1} = A^{-1}A = I.$$

If the inverse exists, **A**, is called regular/invertible/nonsingular.

Consider two matrices

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$
 and  $A' = \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}$ ,

the product of AA' is then

$$AA' = \begin{bmatrix} a_{11}a_{22} - a_{12}a_{21} & 0 \\ 0 & a_{11}a_{22} - a_{12}a_{21} \end{bmatrix} = (a_{11}a_{22} - a_{12}a_{21})I.$$

If and only if  $a_{11}a_{22} - a_{12}a_{21} \neq 0$ ,

$$A^{-1} = \frac{1}{a_{11}a_{22} - a_{12}a_{21}} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}.$$

### 2.1.3. Inverse and Transpose



Inverse Matrix Properties:

$$\bullet \quad AA^{-1} = I = A^{-1}A$$

• 
$$(AB)^{-1} = B^{-1}A^{-1}$$

• 
$$(A+B)^{-1} \neq A^{-1}+B^{-1}$$

The Woodbury identity is

$$(A+BD^{-1}C)^{-1}=A^{-1}-A^{-1}B(D+CA^{-1}B)^{-1}CA^{-1}.$$

The transpose matrix  $A^T$  has elements  $(A^T)_{ij} = A_{ji}$ . From the definition of transpose, a matrix  $A \in \mathbb{R}^{n \times n}$  is *symmetric* if  $A = A^T$ .

Transpose Properties:

$$\bullet \quad (A^T)^T = A$$

$$\bullet \quad (A+B)^T = A^T + B^T$$

$$\bullet \quad (AB)^T = B^T A^T$$

If **A** is invertible, then  $(A^{-1})^T = (A^T)^{-1} = A^{-T}$ .

## 2.1.4. Vector Spaces



**Vector**: Each row or column in a matrix A is called a *vector*. A real-valued vector  $V = (\mathcal{V}, +, \cdot)$  is a set  $\mathcal{V}$  with two operations

$$+: \mathcal{V} \times \mathcal{V} \to \mathcal{V}$$
  
 $:: \mathbb{R} \times \mathcal{V} \to \mathcal{V}$ 

where + is the vector addition and  $\cdot$  is a multiplication by a scalar.

**Vector Subspace**: Suppose V is a vector space and  $U \subseteq V$ ,  $U \neq \emptyset$ . Then U is a vector subspace of V if U is a vector subspace with the vector space operations restricted to  $U \times U$  and  $\mathbb{R} \times U$ .

Linear Combination: A vector space V and a finite number of vectors  $x_1, ..., x_k \in V$ . Then, every  $v \in V$  of the form

$$v = \sum_{i=1}^{k} \lambda_i x_i \in V$$

with  $\lambda_i \in \mathbb{R}$  is a *linear combination* of the vectors  $\mathbf{x}_1, \dots, \mathbf{x}_k$ .

#### 2.1.5. Basis and Rank



**Span:** When a set of vectors  $\mathcal{A} = \{x_1, ..., x_k\}$  is in a vector space V and if every vector can be expressible in a linear combination format,  $\mathcal{A}$  is called the *generating set* of V. The set of all linear combinations of vectors in  $\mathcal{A}$  is called the **span** of  $\mathcal{A}$ . The denotation  $V = \text{span}[\mathcal{A}]$  means  $\mathcal{A}$  spans the vector space V.

**Basis:** If there exists no smaller set  $A \subseteq V$  that spans, every linearly independent generating set of V is called a basis of V.

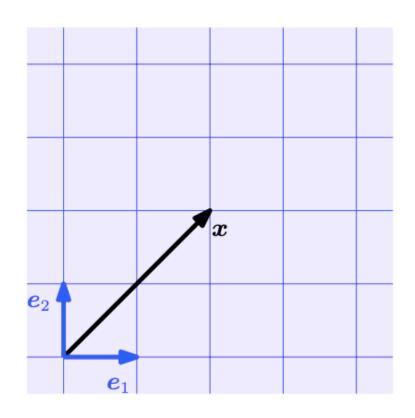
**Rank**: The number of linear independent columns of a matrix  $A \in \mathbb{R}^{m \times n}$  equals the number of linearly independent rows and is called the **rank** of A.

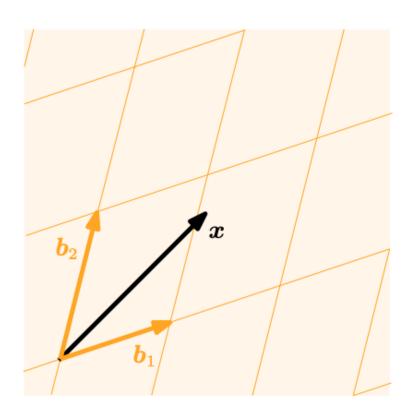
### 2.1.6. Linear Mapping

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**Linear Mapping:** For vector spaces V, W, a mapping  $\Phi: V \to W$  is called a **linear mapping** if  $\forall x, y \in V, \forall \lambda, \psi \in \mathbb{R}: \Phi(\lambda x + \psi y) = \lambda \Phi(x) + \psi \Phi(y)$ .

ο If  $\Phi: V \to W$ ,  $\Psi: V \to W$  are linear, then  $\Phi + \Psi$  and  $\lambda \Phi$ ,  $\lambda \in \mathbb{R}$ , are linear, too.





### 2.1.6. Linear Mapping



In a vector space V, an ordered basis  $B = (\boldsymbol{b}_1, ..., \boldsymbol{b}_n)$  of V, a unique linear combination of  $\boldsymbol{x} \in V$  is formulated:  $\boldsymbol{x} = \alpha_1 \boldsymbol{b}_1 + \cdots + \alpha_n \boldsymbol{b}_n$ 

where  $\boldsymbol{\alpha} = [\alpha_1, ..., \alpha_n] \in \mathbb{R}^n$  are coordinates of  $\boldsymbol{x}$  w.r.t. B.

Consider vector spaces V, W with corresponding bases  $B = (b_1, ..., b_n)$  and  $C = (c_1, ..., c_m)$ . The linear mapping  $\Phi: V \to W$  for  $j \in \{1, ..., n\}$  is

$$\Phi(\boldsymbol{b}_j) = \sum_{i=1}^m \alpha_{ij} \boldsymbol{c}_i.$$

The  $m \times n$  matrix  $A_{\Phi}$  is a transformation matrix of  $\Phi$ .



## 2.2. Analytic Geometry

#### 2.2.2. Norms



**Norm**: A **norm** on a vector space *V* is a function

$$||\cdot||:V\to\mathbb{R},$$

$$x\mapsto ||x||,$$

which assigns each vector x its length  $||x|| \in \mathbb{R}$ , such that for all  $\lambda \in \mathbb{R}$  and  $x, y \in V$  the following hold:

- Absolutely homogeneous:  $||\lambda x|| = |\lambda|||x||$
- Triangle inequality:  $||x + y|| \le ||x|| + ||y||$
- Positive definite:  $||x|| \ge 0$  and  $||x|| = 0 \Leftrightarrow x = 0$ .

### 2.2.2. Norms

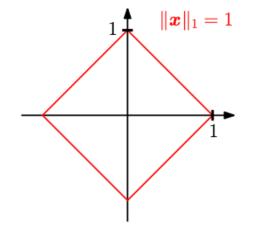


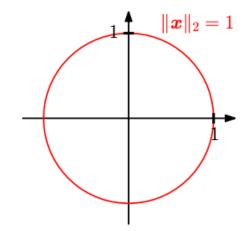
**Manhattan Norm:** The **Manhattan norm** (also called  $l_1$ ) on  $\mathbb{R}^n$  is defined for  $x \in \mathbb{R}^n$  as

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

**Euclidean Norm**: The **Euclidean norm** (also called  $l_2$ ) of  $x \in \mathbb{R}^n$  is defined as

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





#### 2.2.2. Inner Product



**Dot Product:** The dot product takes two equal-length sequences of numbers or vectors and returns a single number as follow

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

A bilinear mapping  $\Omega$  is a mapping with two arguments, and it is linear in each argument that holds for all x, y,  $z \in V$ ,  $\lambda$ ,  $\psi \in \mathbb{R}$  such that

$$\Omega(\lambda x + \psi y, z) = \lambda \Omega(x, z) + \psi \Omega(y, z)$$
  
$$\Omega(x, \lambda y + \psi z) = \lambda \Omega(x, y) + \psi \Omega(x, z)$$

- $\Omega$  is called *symmetric* if  $\Omega(x, y) = \Omega(y, x)$  for all  $x, y \in V$ , i.e., the order of the argument does not matter.
- $\Omega$  is called *positive definite* if

$$\forall x \in V \setminus \{\mathbf{0}\} : \Omega(x, x) > 0, \Omega(\mathbf{0}, \mathbf{0}) = 0.$$

- A positive definite, symmetric bilinear mapping  $\Omega: V \times V \to \mathbb{R}$  is an *inner product* on V.
- The denotation of inner product is  $\langle x, y \rangle$ .
- An inner product is not always the dot product! For example, we define the inner product in  $\mathbb{R}^2$  is

$$\langle x, y \rangle = x_1 y_1 - (x_1 y_2 + x_2 y_1) + 2x_2 y_2,$$

it is different from  $\mathbf{x}^T \mathbf{y} = x_1 y_1 + x_2 y_2$ .

• The inner product of two vectors

$$\sqrt{\langle x-y,x-y\rangle}=\big||x-y|\big|$$

is the *distance* between two vectors.

#### 2.2.2. Inner Product



Consider an *n*-dimensional vector space *V* with an inner product and an ordered basis  $B = (\boldsymbol{b}_1, ..., \boldsymbol{b}_n)$  of *V*. Any vectors  $\boldsymbol{x}, \boldsymbol{y} \in V$  form as linear combinations  $\boldsymbol{x} = \sum_{i=1}^n \psi_i \boldsymbol{b}_i \in V$  and  $\boldsymbol{y} = \sum_{j=1}^n \lambda_i \boldsymbol{b}_j \in V$  where  $\forall \lambda_j, \psi_i \in \mathbb{R}$ . The inner product is

$$\forall \boldsymbol{x}, \boldsymbol{y}: \langle \boldsymbol{x}, \boldsymbol{y} \rangle = \left( \sum_{i=1}^{n} \psi_{i} \boldsymbol{b}_{i}, \sum_{j=1}^{n} \lambda_{j} \boldsymbol{b}_{j} \right) = \sum_{i=1}^{n} \sum_{j=1}^{n} \psi_{i} \langle \boldsymbol{b}_{i}, \boldsymbol{b}_{j} \rangle \lambda_{j} = \widehat{\boldsymbol{x}}^{T} A \widehat{\boldsymbol{y}},$$

where  $A_{ij} = \langle \boldsymbol{b}_i, \boldsymbol{b}_j \rangle$  and  $\widehat{\boldsymbol{x}}, \widehat{\boldsymbol{y}}$  are unit vectors  $\left(\widehat{\boldsymbol{x}} = \frac{x}{||\boldsymbol{x}||}, \widehat{\boldsymbol{y}} = \frac{y}{||\boldsymbol{y}||}\right)$  with respect to B.

A symmetric matrix that satisfies

$$\forall \mathbf{x} \in V \setminus \{\mathbf{0}\}: \mathbf{x}^T \mathbf{A} \mathbf{x} \ge 0$$

is called *symmetric*, *positive semidefinite*.

### 2.2.3. Orthogonality



**Orthogonality**: Two vectors x and y are **orthogonal** if and only if  $\langle x, y \rangle = 0$  and its denotation is  $x \perp y$ . That is the angle between x and y is 0,

$$\cos \omega = \frac{\langle x, y \rangle}{\sqrt{\langle x, x \rangle \langle y, y \rangle}} = \frac{x^T y}{\sqrt{x^T x y^T y}} = 0.$$

A square matrix  $A \in \mathbb{R}^{n \times n}$  is an *orthogonal matrix* i.f.f. its columns are orthogonal so that

$$AA^T = I = A^T A,$$

which implies that

$$A^{-1}=A^T.$$

**Orthonormal Basis**: The basis is called an **orthonormal basis** if an *n*-dimensional vector and a basis  $\{b_1, ..., b_n\}$  hold

$$\langle \boldsymbol{b}_i, \boldsymbol{b}_j \rangle = 0 \text{ for } i \neq j \text{ and } \langle \boldsymbol{b}_i, \boldsymbol{b}_i \rangle = 1$$

for all i, j = 1, ..., n.

**Projection:** A linear mapping  $\pi: V \to U$  is called a **projection** if  $\pi^2 = \pi \circ \pi = \pi$  where  $U \subseteq V$ . The *projection matrices*  $P_{\pi}$  exhibit the property that  $P_{\pi}^2 = P_{\pi}$ .

### 2.2.3. Orthogonality

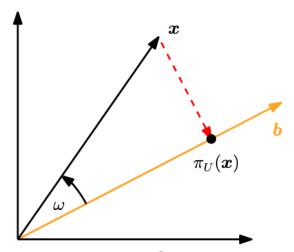


- The segment  $\pi_U(\mathbf{x}) \mathbf{x}$  is orthogonal to U and therefore the basis vector  $\mathbf{b}$  of U,  $\langle \pi_U(\mathbf{x}) \mathbf{x}, \mathbf{b} \rangle = 0$ .
- The projection  $\pi_U(\mathbf{x})$  of  $\mathbf{x}$  onto U must be an element of U and, therefore,  $\mathbf{b}$  spans U,  $\pi_U(\mathbf{x}) = \lambda \mathbf{b}$  where  $\lambda$  is the coordinate

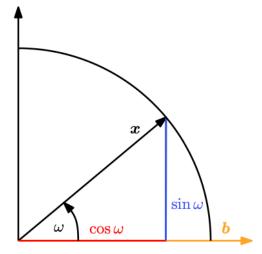
$$\lambda = \frac{\boldsymbol{b}^T \boldsymbol{x}}{\boldsymbol{b}^T \boldsymbol{b}} = \frac{\boldsymbol{b}^T \boldsymbol{x}}{||\boldsymbol{b}||^2}$$

and

$$\pi_U(\mathbf{x}) = \lambda \mathbf{b} = \frac{\mathbf{b}^T \mathbf{x}}{||\mathbf{b}||^2} \mathbf{b}.$$



(a) Projection of  $x \in \mathbb{R}^2$  onto a subspace U with basis vector  $\mathbf{b}$ .



(b) Projection of a two-dimensional vector  $\boldsymbol{x}$  with  $\|\boldsymbol{x}\|=1$  onto a one-dimensional subspace spanned by  $\boldsymbol{b}$ .

#### 2.2.4. Determinant and Trace



**Determinant**: A **determinant** is a mathematical object in the analysis and solution of systems of linear equations. It is only defined for *square matrices* and it maps a square matrix onto a real number. Recall the inverse matrix of  $A \in \mathbb{R}^{2 \times 2}$ ,  $A^{-1}$ ,

$$A^{-1} = \frac{1}{a_{11}a_{22} - a_{12}a_{21}} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}$$

can be expressed using the determination as following

$$A^{-1} = \frac{1}{\det(A)} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}$$

where

$$\det(\mathbf{A}) = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}.$$

If n = 3,

$$\det(\mathbf{A}) = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11}(a_{22}a_{33} - a_{23}a_{32})$$
$$-a_{12}(a_{21}a_{33} - a_{23}a_{31}) + a_{13}(a_{21}a_{32} - a_{22}a_{31})$$

#### 2.2.4. Determinant and Trace

For any  $A \in \mathbb{R}^{n \times n}$ , det(A) also can be computed as

• Expansion along column *j*:

$$\det(\mathbf{A}) = \sum_{k=1}^{n} (-1)^{k+j} a_{kj} \det(\mathbf{A}_{kj}).$$

• Expansion along row *j*:

$$\det(\mathbf{A}) = \sum_{k=1}^{n} (-1)^{k+j} a_{jk} \det(\mathbf{A}_{jk}).$$

where  $A_{kj} \in \mathbb{R}^{(n-1)\times (n-1)}$  is the *submatrix* of A that is obtained when row k and column j are deleted. For example,

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{21} & a_{22} & a_{23} \end{vmatrix} = (-1)^{1+1} a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} + (-1)^{1+2} a_{12} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + (-1)^{1+3} a_{13} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}.$$

The determinant exhibits the following properties:

- det(AB) = det(A) det(B)
- If **A** is invertible, then  $det(\mathbf{A}^{-1}) = \frac{1}{det(\mathbf{A})}$
- Adding a multiple of a column/row to another one does not change det(A).
- Multiplication of a column/row with  $\lambda \in \mathbb{R}$  scales  $\det(\mathbf{A})$  by  $\lambda$ :  $\det(\mathbf{A}) = \lambda^n \det(\mathbf{A})$ .
- Swapping two rows/columns changes the sign of det(A).



#### 2.2.4. Determinant and Trace



**Trace**: The **trace** of a square matrix  $A \in \mathbb{R}^{n \times n}$  is defined as

$$\operatorname{tr}(A) = \sum_{i=1}^{n} a_{ii}$$

and satisfies the following properties:

- $\operatorname{tr}(\boldsymbol{A} + \boldsymbol{B}) = \operatorname{tr}(\boldsymbol{A}) + \operatorname{tr}(\boldsymbol{B}) \text{ for } \boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{n \times n}.$
- $\operatorname{tr}(\alpha A) = \alpha \operatorname{tr}(A), \alpha \in \mathbb{R} \text{ for } A \in \mathbb{R}^{n \times n}.$
- $\operatorname{tr}(\boldsymbol{I}_n) = n$ .
- $\operatorname{tr}(\boldsymbol{A}\boldsymbol{B}) = \operatorname{tr}(\boldsymbol{B}\boldsymbol{A}) \text{ for } \boldsymbol{A} \in \mathbb{R}^{n \times k}, \boldsymbol{B} \in \mathbb{R}^{k \times n}.$
- For vectors, x, y,  $\operatorname{tr}(xy^T) = y^T x \in \mathbb{R}$ .

### 2.2.5. Eigenvalues and Eigenvectors



Eigenvalues and Eigenvector: Let  $A \in \mathbb{R}^{n \times n}$  be a square matrix. Then  $\lambda \in \mathbb{R}$  is an eigenvalue of A and  $x \in \mathbb{R}^n \setminus \{0\}$  is the corresponding eigenvector of A if

$$Ax = \lambda x$$

where  $\lambda$  is eigenvalue of  $A \in \mathbb{R}^{n \times n}$ . It is equivalent to

$$(A - \lambda I_n) = 0$$

and therefore

$$\det(\boldsymbol{A} - \lambda \boldsymbol{I}_n) = 0.$$



### 2.3. Vector Calculus

### 2.3.2. Differentiation of Univariate Functions



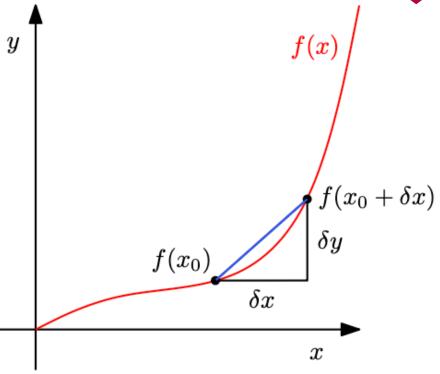
**Derivative:** The **derivative** of a function f at x is defined as the limit

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

and it points in the direction of steepest ascent of f.

#### Differentiation rules are

- Product rule: (f(x)g(x))' = f'(x)g(x) + f(x)g'(x)
- Quotient rule:  $\left(\frac{f(x)}{g(x)}\right)' = \frac{f'(x)g(x) f(x)g(x)}{\left(g(x)\right)^2}$
- Sum rule: (f(x) + g(x))' = f'(x) + g'(x)
- Chain rule:



### 2.3.2. Partial Differentiation and Gradients



**Partial derivatives and Gradient**: For a function  $f: \mathbb{R}^n \to \mathbb{R}$ ,  $x \mapsto f(x)$ ,  $x \in \mathbb{R}^n$  of n variables  $x_1, \dots, x_n$ , the **partial derivatives** are defined as

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

$$\vdots$$

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

and collect them in the row vector

$$\nabla_{x} f = \frac{df}{dx} = \left[ \frac{\partial f(x)}{\partial x_{1}}, \cdots, \frac{\partial f(x)}{\partial x_{n}} \right] \in \mathbb{R}^{1 \times n}$$

#### 2.3.3. Matrix Derivatives



The derivative of a vector **a** w.r.t. a scalar x is itself a vector whose components are given by

$$\left(\frac{\partial \mathbf{a}}{\partial x}\right)_i = \frac{\partial a_i}{\partial x}.$$

Similarly,

$$\left(\frac{\partial x}{\partial \boldsymbol{a}}\right)_i = \frac{\partial x}{\partial a_i} \text{ and } \left(\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{b}}\right)_{ij} = \frac{\partial a_i}{\partial b_i}.$$

Furthermore,

$$\frac{\partial}{\partial x}(x^T a) = \frac{\partial}{\partial x}(a^T x) = a$$

$$\frac{\partial}{\partial x}(AB) = \frac{\partial A}{\partial x}B + A\frac{\partial B}{\partial x}$$

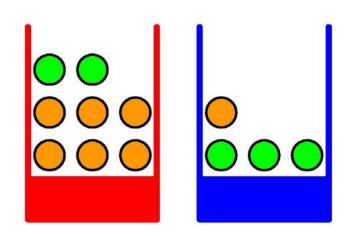
$$\frac{\partial}{\partial x}(A^{-1}) = -A^{-1}\frac{\partial A}{\partial x}A^{-1}$$



# 2.4. Probability Theory

### 2.4.0. – Motivation: Probability Theory

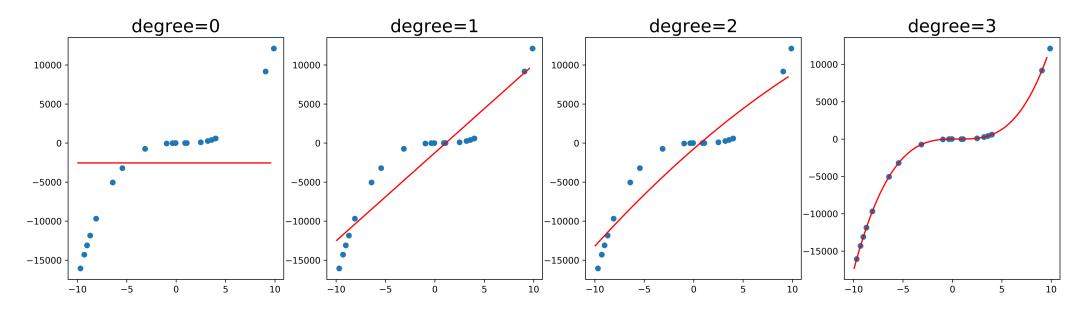




- Let us look at the following example:
  - We have two boxes, one red and one blue
  - Red box: 2 apples and 6 oranges
  - Blue box: 3 apples and 1 orange
  - Pick red box 40% of the time and blue box 60% of the time, then pick one item of fruit
  - Question 1: what is the overall probability that the selection procedure will pick an apple?
  - Question 2: given that we have chosen an orange, what is the probability that the box we chose was the blue one?

### 2.4.0. Motivation: Curve Fit





## 2.4.2. Probability and Random Variables

- Sample Space  $\Omega$ : the set of all possible outcomes of the experiment.
- Event Space: the space of potential results of the experiment. A subset of sample space is in the event space.
- **Probability**: measurements the probability or degree of belief that the event will occur.

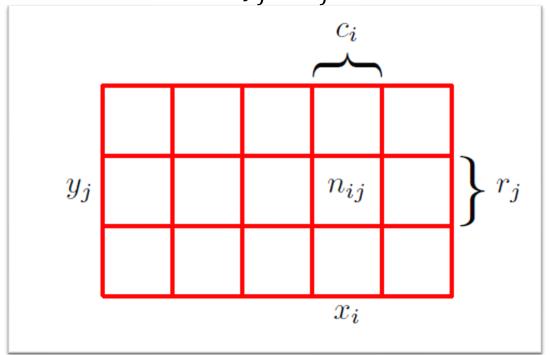
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When the target space is *discrete*, the probability distribution of multiple random variables as filling out a (multidimensional) array of numbers.

**Probability mass function:** If x is a discrete variable, then p(x) is sometimes called a *probability mass function* which implies as a set of probability masses concentrated at the allowed values of x.

#### Consider

- X can take any of the values  $x_i$  where i = 1, ..., M.
- Y can take the values  $y_j$  where j = 1, ..., L.
- A total of *N* trials in both of the variables *X* and *Y*.
- Let the number of trials for  $X = x_i$ ,  $Y = y_j$  be  $n_{ij}$ .
- Let the number of trials in which X takes the value  $x_i$  (irrespective of the value that Y takes) be denoted by  $c_i$ , and let the number of trials in which Y takes the value  $y_i$  be  $r_i$ .





• The probability that X will take the value of  $x_i$  and Y will take the value  $y_j$ ,  $p(X = x_i, Y = y_j)$ , is called the *joint probability* of  $X = x_i$  and  $Y = y_i$ .

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}.$$

• The probability that X takes the value  $x_i$  irrespective of the value of Y is

$$p(X=x_i)=\frac{c_i}{N}.$$

• Sum Rule: We have  $c_i = \sum_i n_{ij}$  and therefore,

$$p(X = x_i) = \sum_{i=1}^{L} p(X = x_i, Y = y_j).$$

• Similarly, the probability that Y takes the value  $y_i$  irrespective of the value of X is

$$p(Y = y_j) = \frac{r_j}{N} = \sum_{i=1}^{M} p(X = x_i, Y = y_j).$$

•  $p(X = x_i)$  and  $p(Y = y_i)$  are sometimes called the *marginal* probability.



- Consider for which  $X = x_i$ , the fraction of instances for which  $Y = y_j$  is  $p(Y = y_j | X = x_i)$  called the *conditional* probability of  $Y = y_j$  given  $X = x_i$ .
- It is obtained by finding the fraction of those points in i fall in (i, j):

$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{c_i}.$$

• The conditional probability of *X* given *Y* is

$$p(X = x_i | Y = y_j) = \frac{n_{ij}}{r_j}.$$

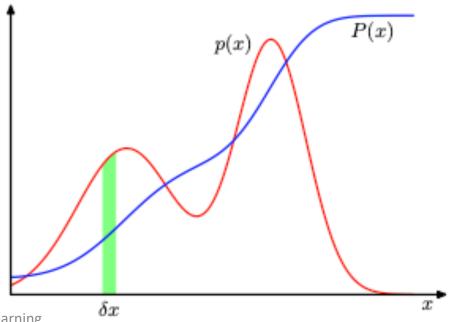
## 2.4.3. Continuous Probability

- Consider the target space with real continuous numbers  $\mathbb{R}$ .
- Most often, we pretend that we perform operations as we have discrete probability spaces with finite spaces. However, the simplification is not precise when
  - o if operations were infinitely repeated. or
  - o if a single point were drawn from an interval.
- **Probability Density Function** (pdf): If the probability of a real-valued variable x falling in the interval  $(x, x + \delta x)$  is given by  $p(x)\delta x$  for  $\delta x \to 0$ , then p(x) is called the *probability density* over x.
- The probability that x will lie in an interval (a, b) is then given by

$$p(x \in (a,b)) = \int_a^b p(x) dx.$$

• The probability density p(x) must satisfy the two conditions:

$$p(x) \ge 0$$
$$\int_{-\infty}^{\infty} p(x)dx = 2.$$



# 2.4.3. Continuous Probability

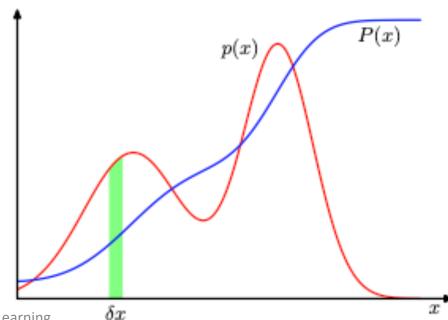
• If we consider a change variable x = g(y), then a function f(x) becomes f(g(y)). This means that a probability density  $p_x(x)$  that corresponds to a density  $p_y(y)$  with respect to the new variable y, where the suffixes denote the fact that  $p_x(x)$  and  $p_y(y)$  are different densities. The observation then transforms into the range  $(y, y + \delta y)$  where  $p_x(x)\delta x \sim p_y(y)\delta y$  and

$$p_{y}(y) = p_{x}(x) \left| \frac{dx}{dy} \right| = p_{x}(g(y))|g'(y)|.$$

• Cumulative distribution function (cdf): The probability that x lies in the interval  $(-\infty, z)$  is given by the cumulative distribution function defined by

$$P(z) = \int_{-\infty}^{z} p(x) dx$$

Which satisfies P'(z) = p(x).





**Sum Rule**: The sum ule is the *marginalization property*. It relates the joint distribution to a marginal distribution via

$$p(\mathbf{x}) = \begin{cases} \sum_{\mathbf{y} \in Y} p(\mathbf{x}, \mathbf{y}), & \text{if } \mathbf{y} \text{ is discrete} \\ \int_{Y} p(\mathbf{x}, \mathbf{y}) d\mathbf{y}, & \text{if } \mathbf{y} \text{ is continuous} \end{cases}$$

**Product Rule**: It relates the joint distribution to the conditional distribution via p(x, y) = p(y|x)p(x).

- Every joint distribution of two random variables can be factorized of two other distributions.
- The ordering of random variables is arbitrary, p(x, y) = p(x|y)p(y).

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- In machine learning and Bayesian statistics, we are often interested in making inferences of unobserved random variables given that we have observed other random variables.
- Assume some prior knowledge p(Y) about an observed random variable Y and some relationship p(X|Y) between X and a second random variable Y, which we can observe.
- **Bayes' Theorem (rule or law)**: From the product rule, together with the symmetry property p(X,Y) = p(Y,X), we can build the following relationship called *Bayes' theorem* between conditional probabilities

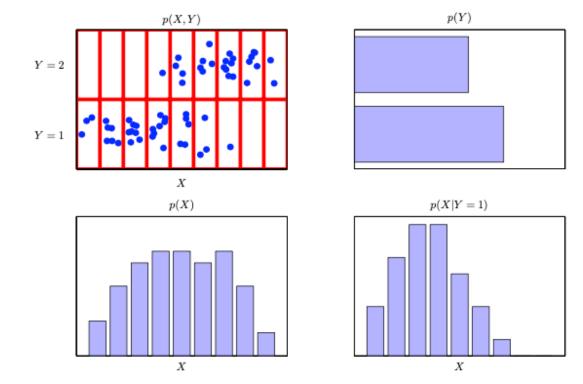
Posterior = Likelihood 
$$\cdot \frac{\text{Prior}}{\text{Event}} \to p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$
.

• We can view the denominator as the normalizer

$$p(X) = \sum_{V} p(X|Y)p(Y)$$

using the sum rule.

- The prior P(X) probability encapsulates the subjective prior knowledge of the unobserved variable before observing any data.
- The *likelihood* p(X|Y) describes how X and Y are related. It is the probability of the data X if the latent variable Y were to know. The likelihood is not a distribution in Y, but only in X.
- The posterior P(Y|X) is the quantity of interest in Bayesian statistics.





- From a Bayesian perspective, probability provides a quantification of uncertainty.
- Considering the curve-fit example, we can use the probability theory to describe the uncertainty in model parameters and the models.
- Let the function be  $t(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3$ .
  - Assume we know the prior probability of  $\mathbf{w} = [w_0, w_1, w_2, w_3], p(\mathbf{w}).$
  - The effect of the observed data  $\mathcal{D} = \{t_1, \dots, t_N\}$  is expressed through the conditional probability  $p(\mathcal{D}|\mathbf{w})$ .
  - Then the uncertainty in **w** after we have observed  $\mathcal{D}$  in the form of the posterior probability  $p(\mathbf{w}|\mathcal{D})$ :

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}.$$

- $p(\mathcal{D}|\mathbf{w})$  is a function of parameter vector  $\mathbf{w}$  called the *likelihood function* expressing how probable the observed data set is for different settings of the parameter vector  $\mathbf{w}$ .
- The denominator  $p(\mathcal{D})$  is

$$p(\mathcal{D}) = \int p(\mathcal{D}|\mathbf{w})p(\mathbf{w}) d\mathbf{w}.$$



- Given the definition of likelihood, we can state Bayes' theorem in words

  Posterior  $\propto$  likelihood  $\times$  prior

  where all of these quantities are viewed as functions of  $\boldsymbol{w}$ .
- In the sum and product rule approach, w is considered to be a fixed parameter found by some 'estimator' and errors are obtained by considering the distribution of possible data sets  $\mathcal{D}$ .
- The common estimator is *maximum likelihood* in which w is set to the value that maximizes  $p(\mathcal{D}|w)$ . In ML, we use the negative log of the likelihood function and call it the *error function* it is a monotonically decreasing function. Maximizing the likelihood is equivalent to minimizing the error.
- In Bayesian approach, the uncertainty in the parameters is expressed through the probability distribution over  $\mathbf{w}$  in a single data set  $\mathcal{D}$ . Therefore, the inclusion of prior knowledge arises naturally.
- Example: Suppose that a fair-coin is tossed three times and lands heads each time. What is the probability of landing heads?



Question 1: What is the probability of picking an apple?

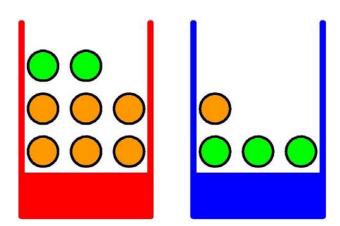
$$p(F = a) = p(F = a|B = r)p(B = r) + p(F = a|B = b)p(B = b)$$

$$= \frac{2}{8} \left(\frac{4}{10}\right) + \frac{3}{4} \left(\frac{6}{10}\right) = \frac{11}{20}.$$

$$p(F = o) = 1 - p(F = a) = 1 - \frac{11}{20} = \frac{9}{20}.$$

Question 2: What is the probability of picking an orange from the blue box?

$$p(B = b|F = o) = \frac{p(F = o|B = b)p(B = b)}{p(F = o)} = 1 - p(r|o) = 1 - \frac{p(F = o|B = r)p(B = r)}{p(F = o)}$$



$$= 1 - \left(\frac{3}{4} \left(\frac{4}{10}\right) \left(\frac{20}{9}\right)\right) = \frac{1}{3}$$



- **Prior and Posterior Probability**: The probability available before we observe the identity is called the prior probability and the probability after the observation is called the posterior probability. In this example, p(B) is the prior probability and p(B|F) is the posterior probability.
- **Independent**: If the joint distribution of two variables factorizes into the product of the marginals, so that

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

then, X and Y are *independent*. If each box had the same fraction of apples and oranges, then p(F|B) = p(F).

## 2.4.5. Expectations and Covariances

• The average value of some function f(x) under a probability distribution p(x) is called the *expectation* f(x) and will be denoted as  $\mathbb{E}(f)$ 

$$\mathbb{E}(f) = \sum_{x} p(x)f(x)$$

• So that the average is weighted by the relative probabilities of the different values of x. In the case of continuous variables, expectations are expressed in terms of an integration w.r.t. the corresponding probability density

$$\mathbb{E}(f) = \int p(x)f(x)dx.$$

• For a case of several variables,

$$\mathbb{E}_{x}(f(x,y))$$

where the subscript x is the variable being averaged over and f(x, y) is the function w.r.t. the distribution of x.

• The *conditional expectation* w.r.t. a conditional distribution is

$$\mathbb{E}_{x}(f|y) = \sum_{x} p(x|y)f(x).$$

## 2.4.5. Expectations and Covariances



• The *variance* of f(x) is defined by

$$var(f) = \mathbb{E}\left[\left(f(x) - \mathbb{E}(f(x))\right)^{2}\right]$$

• And provides a measure of how much variability there is in f(x) around its  $\mathbb{E}(f(x))$ . The variance also can be written as  $\mathbb{E}(f(x)^2) - \mathbb{E}(f(x))^2$ :

$$\mathbb{E}\left[\left(f(x) - \mathbb{E}(f(x))\right)^{2}\right] = \mathbb{E}\left[f(x)^{2} - 2f(x)\mathbb{E}(f(x)) + \mathbb{E}(f(x))^{2}\right]$$

$$= \mathbb{E}[f(x)^{2}] - 2\mathbb{E}(f(x))\mathbb{E}(f(x)) + \mathbb{E}\left[\mathbb{E}(f(x))^{2}\right]$$

$$= \mathbb{E}[f(x)^{2}] - \mathbb{E}[f(x)]^{2}.$$

• For two random variables x and y, the *covariance* is the product of their deviations from their respective means,

$$cov[x,y] = \mathbb{E}_{x,y}[\{x - \mathbb{E}[x]\}\{y - \mathbb{E}[y]\}] = \mathbb{E}_{x,y}[xy] - \mathbb{E}[x]\mathbb{E}[y]$$

when x and y vary together. Otherwise, the covariance vanishes. We also can consider cov(x) = cov[x, x].

# 2.4.5. Expectations and Covariances



• The *correlation* between two random variables is the normalized covariance between them via

$$corr(x,y) = \frac{cov[x,y]}{\sqrt{var(x)var(y)}}.$$

• The *empirical mean* vector is the arithmetic average of the observation for each variable and is defined as

$$\mu = \overline{x} = \frac{1}{N} \sum_{n=1}^{N} x_n.$$

• The *empirical covariance* is

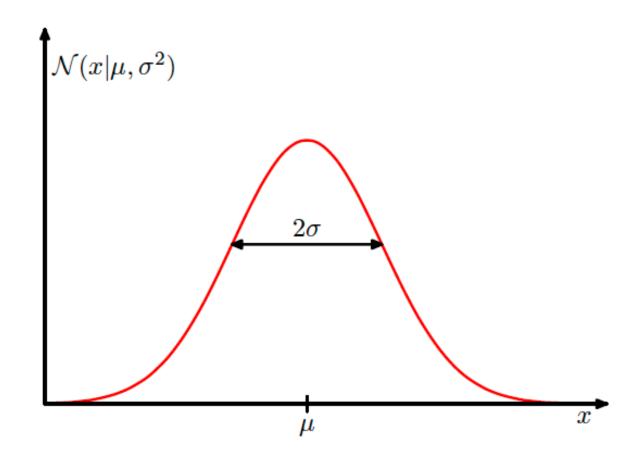
$$\Sigma = \frac{1}{N} \sum_{n=1}^{N} (x_n - \overline{x})(x_n - \overline{x})^T.$$



For the case of a single real-valued variable x, the Gaussian distribution is defined by

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

where  $\mu$  is the mean and  $\sigma^2$  is the variance ( $\sqrt{\sigma^2}$  is the standard deviation). Sometimes, we use  $\beta = 1/\sigma^2$  and it is called the precision.



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#### Properties:

• Condition

$$\mathcal{N}(x|\mu,\sigma^2) > 0$$

Normalization

$$\int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) \ dx = 1$$

• Expectation value

$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x \ dx = \mu$$

Variance

$$var[x] = \sigma^2$$

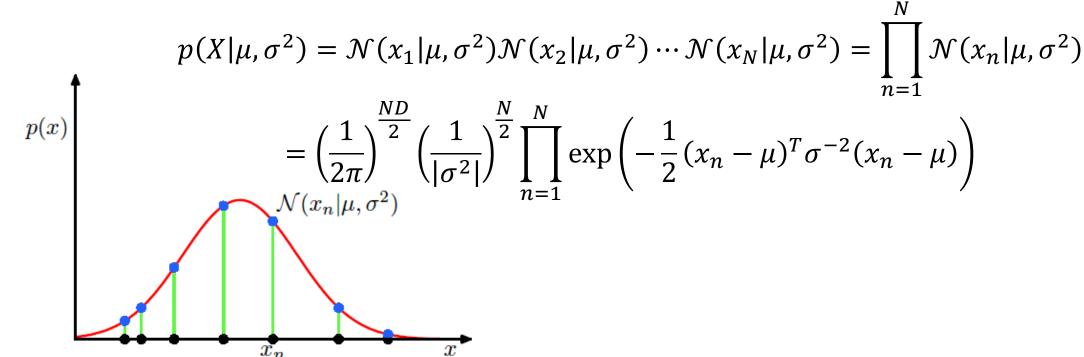
• The maximum of a distribution is the mode that is coincides with the mean.



• The Gaussian distribution over a D-dimensional vector x of continuous variables is given by

$$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \left(\frac{1}{2\pi}\right)^{\frac{D}{2}} \left(\frac{1}{|\boldsymbol{\Sigma}|}\right)^{\frac{1}{2}} \exp\left\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x}-\boldsymbol{\mu})\right\}.$$

• Suppose we have a data set of observations  $X = (x_1, ..., x_N)^T$  and the observations are drawn independently from a Gaussian distribution from unknown  $\mu$  and  $\sigma^2$ . We call this situation independent and identically distributed (i.i.d.). The probability of the data set is then



We can determine values for the unknown parameters by maximizing the log-likelihood function

$$\ln p(X|\mu,\sigma^2) = -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu)^2 - \frac{N}{2} \ln \sigma^2 - \frac{N}{2} \ln(2\pi).$$

$$\mu_{ML} = \frac{1}{N} \sum_{n=1}^{N} x_n$$

$$\sigma_{ML}^2 = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu_{ML})^2$$

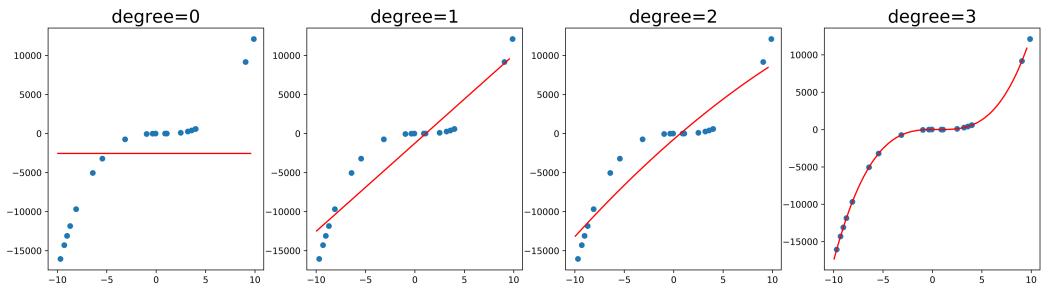
which are the *sample mean* and *sample variance*, respectively. The maximum likelihood approach systematically underestimates the variance of the distribution.

The expectation of these parameters is

$$\mathbb{E}[\mu_{ML}] = \mu$$
$$\mathbb{E}[\sigma_{ML}^2] = \frac{N-1}{N}\sigma^2.$$

## 2.4.7. Curve Fitting Revisit

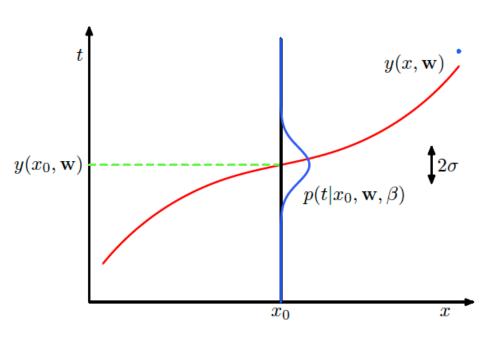




• Suppose we predict for the target variable t given some new value of the input variable x on the basis of a set of data,  $X = (x_1, ..., x_N)^T$  and  $T = (t_1, ..., t_N)^T$ . Assume that the given value of x, the corresponding value of t has a Gaussian distribution with a mean equal to the value  $y(x, \mathbf{w})$  of the polynomial curve.

$$p(t|x, \mathbf{w}, \beta) = \mathcal{N}(t|y(x, \mathbf{w}), \beta^{-1})$$

## 2.4.7. Curve Fitting Revisit



If the data are assumed to be i.i.d., then the likelihood furis

$$p(T|X, \boldsymbol{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n|y(x_n, \boldsymbol{w}), \beta^{-1})$$

and the log likelihood function is

$$\ln p(T|X, \boldsymbol{w}, \boldsymbol{\beta})$$

$$= -\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{N}{2} \ln \beta - \frac{N}{2} \ln 2\pi.$$

If w and  $\beta$  are determined, then we have a probabilistic model that are expressed in terms of the predictive distribution that gives the probability distribution over t, rather than simply a point estimate, and is obtained by substituting the maximum likelihood parameters

$$p(t|x, \mathbf{w_{ML}}, \beta_{ML}) = \mathcal{N}(t|y(x, \mathbf{w_{ML}}), \beta_{ML}^{-1}).$$

# 2.4.7. Curve Fitting Revisit



If we use Bayesian approach with a prior distribution over the polynomial coefficients w,

$$p(\boldsymbol{w}|\alpha) = \mathcal{N}(\boldsymbol{w}|\boldsymbol{0}, \alpha^{-1}\boldsymbol{I}) = \left(\frac{\alpha}{2\pi}\right)^{\frac{M+1}{2}} \exp\left\{-\frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w}\right\}$$

where  $\alpha$  is the precision of the distribution (called *hyperparameter* that controls the distribution of model parameter), and M+1 is the total number of elements in the vector w for an  $M^{th}$  order polynomial. The posterior distribution for w is

$$p(\mathbf{w}|X,T,\alpha,\beta) \propto p(T|X,\mathbf{w},\beta)p(\mathbf{w}|\alpha).$$

We can find w by maximizing the posterior distribution called *maximum posterior* (MAP) by taking the negative log. The maximum of the posterior is equivalent to the minimum of the negative log of the posterior as shown

$$-\ln p(\mathbf{w}|X,T,\alpha,\beta) = -\ln p(T|X,\mathbf{w},\beta) - \ln p(\mathbf{w}|\alpha).$$

## 2.4.8. Binary Variables



Consider a single binary random variable  $x \in \{0,1\}$ . The probability of x = 1 will be denoted by the parameter  $\mu$  so that  $p(x = 1|\mu) = \mu$ 

where  $0 \le \mu \le 1$ , from which it follows that  $p(x = 0|\mu) = 1 - \mu$ . The probability distribution (*Bernoulli* distribution) over x can therefore be written in the form

$$Bern(x|\mu) = \mu^{x}(1-\mu)^{1-x}.$$

This distribution is normalized and has mean and variance given by

$$\mathbb{E}[x] = \mu$$
$$var[x] = \mu(1 - \mu).$$

Suppose we have a data set  $D = \{x_1, ..., x_N\}$ . Assume that observations are i.i.d. from  $p(x|\mu)$ , so that

$$p(D|\mu) = \prod_{n=1}^{N} p(x_n|\mu) = \prod_{n=1}^{N} \mu^{x_n} (1-\mu)^{1-x_n} .$$

The log likelihood is

$$\ln p(D|\mu) = \sum_{n=1}^{N} \ln p(x_n|\mu) = \sum_{n=1}^{N} \{x_n \ln \mu + (1 - x_n) \ln(1 - \mu)\}.$$

### 2.4.9. Multinomial Variable



• Consider the Bernoulli distribution to an K-dimensional binary variable  $x_k \in \{0,1\}$  such that  $\sum_k x_k = 1$ . Then the distribution of **x** is given

$$p(\boldsymbol{x}|\boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_k^{x_k}$$

where  $\mu = (\mu_1, ..., \mu_K)^T$ , and the parameters  $\mu_k$  are constrained to satisfy  $\mu_k \ge 0$  and  $\sum_k \mu_k = 1$ .



## 2.5. Conclusion

### 2.5.2. Conclusion

- A brief review of Mathematics that will play central roles in Machine Learning Algorithms
  - Linear Algebra, Analytic Geometry, and Vector Calculus will help to understand the work of algorithms.
  - Probability theory will help to understand the characteristics of algorithms
  - If discussed topics are not fully digestible, it is still okay.
    - Most of the terms will be repeatedly discussed throughout the semesters.