Maths & Probability

Introduction to Machine Learning
(CSC462)

Basics of Linear Algebra

Vectors and Matrices

- Vectors (column vectors and row vectors) and their transposes

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}, \quad \mathbf{a}^\top = \begin{bmatrix} a_1 & a_2 & a_3 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 & b_2 & b_3 \end{bmatrix}, \quad \mathbf{b}^\top = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

- We will assume vectors of be column vectors (unless specified otherwise)
- Vector with all 0s except a single 1 is called elementary vector (or "one-hot" vector in ML)
- Matrix and its transpose (shown for 3×3 matrices)

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, \quad \mathbf{A}^\top = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{bmatrix}$$

- For a symmetric matrix (must be square) $\mathbf{A} = \mathbf{A}^\top$
- Diagonal and identity matrices have nonzeros only along the diagonals
- Should know the basic rules of vector addition, matrix addition, etc (won't list here)

Inner Product

- Inner product (or dot product) of two vectors $\mathbf{a} \in \mathbb{R}^D$ and $\mathbf{b} \in \mathbb{R}^D$ is a scalar

$$c = \mathbf{a}^\top \mathbf{b} = \sum_{d=1}^{D} a_d b_d$$

- Inner product is a measure of similarity of two vectors
- Inner product is zero if $\boldsymbol{a}$ and $\boldsymbol{b}$ are orthogonal to each other
- Inner product of two vector of unit length is the same as cosine similarity
- A more general form of inner product: $c = \mathbf{a}^\top \mathbf{M} \mathbf{b}$ (here $\mathbf{M}$ is $D \times D$)
    - $\mathbf{M}$ can be diagonal or full matrix
    - For identity $\mathbf{M}$, it becomes the standard inner product
- Euclidean distance between two vectors can be also written in terms of an inner product

$$d(\boldsymbol{a}, \boldsymbol{b}) = \sqrt{(\boldsymbol{a} - \boldsymbol{b})^\top (\boldsymbol{a} - \boldsymbol{b})} = \sqrt{\boldsymbol{a}^\top \boldsymbol{a} + \boldsymbol{b}^\top \boldsymbol{b} - 2\boldsymbol{a}^\top \boldsymbol{b}}$$

Orthogonal/Orthonormal Vectors and Matrices

- A set of vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_N$ is called orthogonal if

$$\boldsymbol{a}_i^\top \boldsymbol{a}_j = 0 \quad \forall i \neq j$$

- Moreover, a set of orthogonal vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_N$ is called orthonormal if

$$\boldsymbol{a}_i^\top \boldsymbol{a}_i = 1 \quad \forall i$$

- A **matrix** with orthonormal columns is called orthogonal
- For a square orthogonal matrix $\mathbf{A}$, we have $\mathbf{A}\mathbf{A}^\top = \mathbf{A}^\top\mathbf{A} = \mathbf{I}$

Matrix-Vector/Matrix-Matrix Product as Inner Product

- Important to be conversant with these. Some basic operations worth keeping in mind
  - We can 'post-mulitply' a matrix by a column vector:

$$Ax = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} a_1^T x_1 \\ a_2^T x_2 \\ a_3^T x_3 \end{bmatrix}$$

  - We can 'pre-multiply' a matrix by a row vector:

$$x^T A = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} x^T a_1 & x^T a_2 & x^T a_3 \end{bmatrix}$$

  - In general, we can multiply matrices A and B when the number of columns in A matches the number of rows in B:

$$AB = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix} = \begin{bmatrix} a_1^T b_1 & a_1^T b_2 & a_1^T b_3 \\ a_2^T b_1 & a_2^T b_2 & a_2^T b_3 \\ a_3^T b_1 & a_3^T b_2 & a_3^T b_3 \end{bmatrix}$$

- We routinely encounter such operations in many ML problems

Outer Product

- Outer product of of two vectors $\mathbf{a} \in \mathbb{R}^D$ and $\mathbf{b} \in \mathbb{R}^D$ is a matrix. For 3-dim vectors, we'll have

$$\mathbf{C} = \mathbf{a}\mathbf{b}^\top = \begin{bmatrix} a_1 b_1 & a_1 b_2 & a_1 b_3 \\ a_2 b_1 & a_2 b_2 & a_2 b_3 \\ a_3 b_1 & a_3 b_2 & a_3 b_3 \end{bmatrix} \qquad \text{(note: } \mathbf{C} \text{ is a rank-1 matrix)}$$

- Matrix rank: Linearly indep. number of rows/columns
- Matrix multiplications can also be written as a sum of outer products (sum of rank-1 matrices)

$$\mathbf{A}\mathbf{B}^\top = \sum_{k=1}^{K} \boldsymbol{a}_k \boldsymbol{b}_k^\top$$

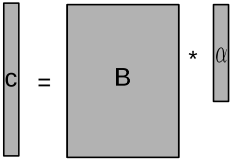
where $\boldsymbol{a}_k$ and $\boldsymbol{b}_k$ denote the k-th column of $\mathbf{A}$ (size: $D \times K$) and $\mathbf{B}$ (size: $D \times K$), respectively,

Linear Combination of Vectors as a Matrix-Vector Product

- Linear combination of a set of $D \times 1$ vectors $\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_N$ is another vector of the same size

$$\mathbf{c} = \alpha_1 \mathbf{b}_1 + \alpha_2 \mathbf{b}_2 + \ldots \alpha_N \mathbf{b}_N$$

- The α_n's are scalar-valued combination weights
- The above can also be compactly written in the matrix-vector product form $\mathbf{c} = \mathbf{B}\boldsymbol{\alpha}$



where $\mathbf{B} = [\mathbf{b}_1, \mathbf{b}_2, \ldots \mathbf{b}_N]$ is a $D \times N$ matrix, and $\boldsymbol{\alpha} = [\alpha_1, \alpha_2, \ldots, \alpha_N]^\top$ is an $N \times 1$ column vector

- Note that $\boldsymbol{c}$ can be also seen as a linear transformation of $\boldsymbol{\alpha}$ using $\mathbf{B}$
- Such matrix-vector product are very common in ML problems (especially in linear models)

Vector and Matrix Norms

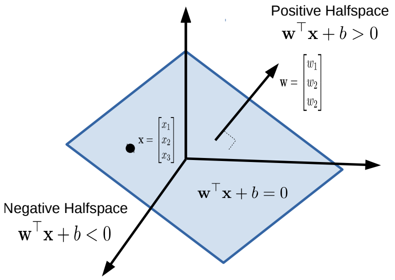
- Roughly speaking, for a vector $\boldsymbol{x}$, the norm is its "length"
- Some common norms: ℓ_2 norm (Euclidean norm), ℓ_1 form, ℓ_∞ norm, ℓ_p norm ($p \geq 1$)

$$||\boldsymbol{x}||_2 = \sqrt{\sum_{n=1}^{N} x_n^2}, \quad ||\boldsymbol{x}||_1 = \sum_{n=1}^{N} |x_n|, \quad ||\boldsymbol{x}||_\infty = \max_{1 \leq n \leq N} |x_n|, \quad ||\boldsymbol{x}||_p = \left(\sum_{n=1}^{N} |x_n|^p\right)^{1/p}$$

- Note: The square of ℓ_2 norm is the inner product of the vector with itself $||x||_2^2 = \boldsymbol{x}^\top \boldsymbol{x}$
- Note: $||\boldsymbol{x}||_p$ for $p < 1$ technically not a norm (doesn't satisfy all the formal properties of a norm)
  - Nevertheless it is often used in some ML problems (has some interesting properties)
- Norms for a matrix $\mathbf{A}$ (say of size $N \times M$) can also be defined, e.g.,
  - Frobenius norm: $||\mathbf{A}||_F = \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{M} A_{ij}^2} = \sqrt{\text{trace}(\mathbf{A}^\top \mathbf{A})}$
  - Many matrix norms can be written in terms of in terms of the singular values of $\mathbf{A}$

Hyperplanes

- An important concept in ML, especially for understanding classification problems
- Divides a vector space into two halves (positive and negative halfspaces)



- Assuming 3-dim space, it can be defined by a vector $\boldsymbol{w} = [w_1, w_2, w_3]$ and scalar b
- $\boldsymbol{w}$ is the vector pointing outward to the hyperplane
- b is the real-valued "bias" if the hyperplane doesn't pass through the origin

Some other things you should know about..

- Eigenvalues, rank, etc. for matrices
- Trace of matrix
- Determiant of matrix (and relation to eigenvalues etc)
- Inverse of matrices
- Positive definite and positive semi-definite matrices (non-negative eigenvalues)
- "Matrix Cookbook" (will provide link) is a nice source of many properties of matrices

Multivariate Calculus and Optimization

Multivariate Calculus and Optimization

- Most of ML problems boil down to solving an optimization problem
- We will usually have to optimize a function $f : \mathbb{R}^D \to \mathbb{R}$ w.r.t some variable $\boldsymbol{w} \in \mathbb{R}^D$
- Gradient of f w.r.t. $\boldsymbol{w}$ denotes the direction of steepest change at $\boldsymbol{w}$, and is defined as

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial w_1} \\ \vdots \\ \frac{\partial f}{\partial w_D} \end{bmatrix} \qquad \text{where} \quad [\nabla f]_i = \frac{\partial f}{\partial w_i}$$

- For multivariate functions $f : \mathbb{R}^D \to \mathbb{R}^M$, we can likewise define the Jacobian matrix

$$\mathbf{J}_f = \begin{bmatrix} \frac{\partial f_1}{\partial w_1} & \cdots & \frac{\partial f_1}{\partial w_D} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_M}{\partial w_1} & \cdots & \frac{\partial f_M}{\partial w_D} \end{bmatrix} \qquad \text{where} \quad [\mathbf{J}_f]_{ij} = \frac{\partial f_i}{\partial w_j}$$

- Can also define second derivatives (called Hessian): derivative of gradient/Jacobian

Taking Derivatives

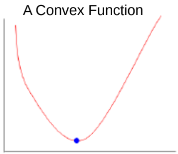
- Optimization in ML problems requires being able to take derivatives (i.e., doing Calculus)
- What makes it tricky is that usually we are no longer doing optimization w.r.t. a single scalar variable but w.r.t. vectors or sometimes even matrices (thus need vector/matrix calculus)
- For some functions, derivatives are easy (can even be done by hand)
- Perhaps the most common, easy ones include derivatives of linear and quadratic functions

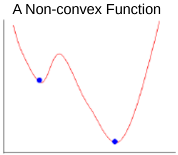
$$
\begin{aligned}
\nabla_{\boldsymbol{w}}[\boldsymbol{x}^\top \boldsymbol{w}] &= \boldsymbol{x} \\
\nabla_{\boldsymbol{w}}[\boldsymbol{w}^\top \mathbf{X} \boldsymbol{w}] &= (\mathbf{X} + \mathbf{X}^\top)\boldsymbol{w} \quad \text{(where } \mathbf{X} \text{ is } D \times D \text{ matrix)} \\
\nabla_{\boldsymbol{w}}[\boldsymbol{w}^\top \mathbf{X} \boldsymbol{w}] &= 2\mathbf{X}\boldsymbol{w} \quad \text{(if } \mathbf{X} \text{ is symmetric matrix)}
\end{aligned}
$$

- The "Matrix Cookbook" contains many derivative formulas (you can use that as a reference even if you don't know how to compute derivative by hand)
- For more complicated functions, thankfully there exist tool that allow automatic differentiation
- But you should still have a good understanding of derivatives and be familiar with at least some basic results like the above (and some others from the Matrix Cookbook)

Convex Functions

- Convex functions have a unique optima



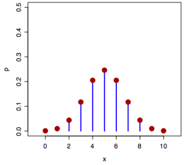


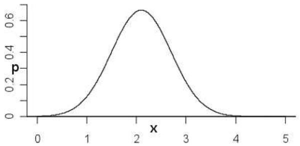
- Optimizing convex functions is usually easier than optimizing non-convex ones
- More on this when we look at optimization for ML later during the semester

Basics of Probability and Probability Distributions

Random Variables

- Informally, a random variable (r.v.) X denotes possible outcomes of an event
- Can be **discrete** (i.e., finite many possible outcomes) or **continuous**



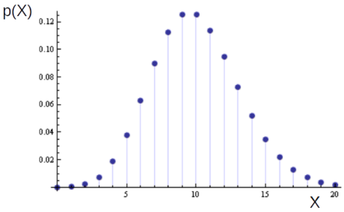


- Some examples of **discrete r.v.**
  - A random variable $X \in \{0, 1\}$ denoting outcomes of a coin-toss
  - A random variable $X \in \{1, 2, \ldots, 6\}$ denoteing outcome of a dice roll
- Some examples of **continuous r.v.**
  - A random variable $X \in (0, 1)$ denoting the bias of a coin
  - A random variable X denoting heights of students in a class
  - A random variable X denoting time to get to your hall from the department

Discrete Random Variables

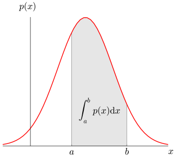
- For a discrete r.v. X, $p(x)$ denotes the probability that $p(X = x)$
- $p(x)$ is called the probability mass function (PMF)

$$\begin{aligned} p(x) &\geq 0 \\ p(x) &\leq 1 \\ \sum_x p(x) &= 1 \end{aligned}$$



Continuous Random Variables

- For a continuous r.v. X, a probability $p(X = x)$ is meaningless
- Instead we use $p(X = x)$ or $p(x)$ to denote the probability density at $X = x$
- For a continuous r.v. X, we can only talk about probability within an interval $X \in (x, x + \delta x)$
  - $p(x)\delta x$ is the probability that $X \in (x, x + \delta x)$ as $\delta x \to 0$



- The probability density $p(x)$ satisfies the following

$$p(x) \geq 0 \quad \text{and} \quad \int_x p(x)dx = 1 \qquad \text{(note: for continuous r.v., } p(x) \text{ can be } > 1)$$

A word about notation..

- $p(.)$ can mean different things depending on the context
  - $p(X)$ denotes the distribution (PMF/PDF) of an r.v. X
  - $p(X = x)$ or $p(x)$ denotes the **probability** or **probability density** at point x
- Actual meaning should be clear from the context (but be careful)
- Exercise the same care when $p(.)$ is a specific distribution (Bernoulli, Beta, Gaussian, etc.)
- The following means **drawing a random sample** from the distribution $p(X)$

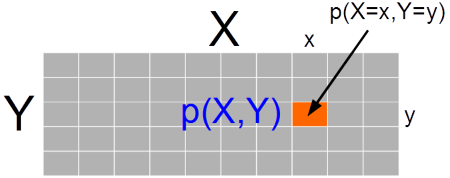
$$x \sim p(X)$$

Joint Probability Distribution

Joint probability distribution $p(X, Y)$ models probability of co-occurrence of two r.v. X, Y

For discrete r.v., the joint PMF $p(X, Y)$ is like a table (that sums to 1)

$$\sum_x \sum_y p(X = x, Y = y) = 1$$

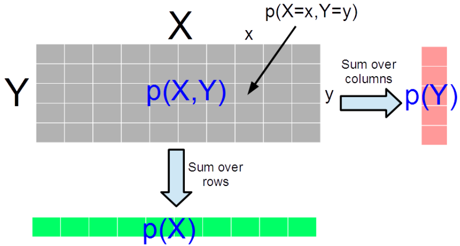


For continuous r.v., we have joint PDF $p(X, Y)$

$$\int_x \int_y p(X = x, Y = y) dx dy = 1$$

Marginal Probability Distribution

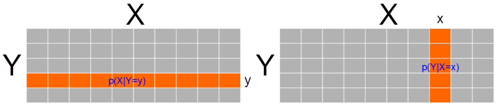
- Intuitively, the probability distribution of one r.v. regardless of the value the other r.v. takes
- For discrete r.v.'s: $p(X) = \sum_y p(X, Y = y)$, $\quad p(Y) = \sum_x p(X = x, Y)$
- For discrete r.v. it is the sum of the PMF table along the rows/columns



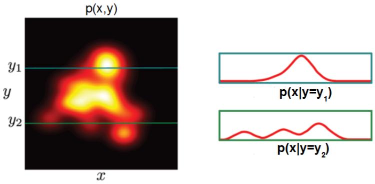
- For continuous r.v.: $p(X) = \int_y p(X, Y = y)dy$, $\quad p(Y) = \int_x p(X = x, Y)dx$
- Note: Marginalization is also called "integrating out" (especially in Bayesian learning)

Conditional Probability Distribution

- Probability distribution of one r.v. given the value of the other r.v.
- Conditional probability $p(X|Y = y)$ or $p(Y|X = x)$: like taking a slice of $p(X, Y)$
- For a discrete distribution:



- For a continuous distribution[1]:



[1] Picture courtesy: Computer vision: models, learning and inference (Simon Price)

Some Basic Rules

- **Sum rule:** Gives the marginal probability distribution from joint probability distribution
  - For discrete r.v.: $p(X) = \sum_Y p(X, Y)$
  - For continuous r.v.: $p(X) = \int_Y p(X, Y)dY$
- **Product rule:** $p(X, Y) = p(Y|X)p(X) = p(X|Y)p(Y)$
- **Bayes rule**: Gives conditional probability

$$\boxed{p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}}$$

  - For discrete r.v.: $p(Y|X) = \frac{p(X|Y)p(Y)}{\sum_Y p(X|Y)p(Y)}$
  - For continuous r.v.: $p(Y|X) = \frac{p(X|Y)p(Y)}{\int_Y p(X|Y)p(Y)dY}$
- Also remember the **chain rule**

$$p(X_1, X_2, \ldots, X_N) = p(X_1)p(X_2|X_1)\ldots p(X_N|X_1, \ldots, X_{N-1})$$

CDF and Quantiles

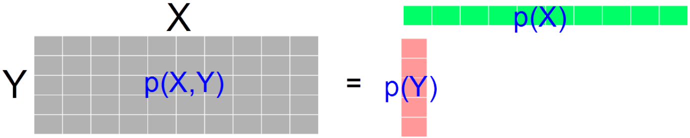
- Cumulative distribution function (CDF): $F(x) = p(X \leq x)$
- $\alpha \leq 1$ quantile is defined as the x_α s.t.

$$p(X \leq x_\alpha) = \alpha$$

Independence

- X and Y are independent ($X \perp\!\!\!\perp Y$) when knowing one tells nothing about the other

$$
\begin{aligned}
p(X|Y=y) &= p(X)\\
p(Y|X=x) &= p(Y)\\
p(X,Y) &= p(X)p(Y)
\end{aligned}
$$



- $X \perp\!\!\!\perp Y$ is also called **marginal independence**
- **Conditional independence** ($X \perp\!\!\!\perp Y|Z$): independence given the value of another r.v. Z

$$p(X,Y|Z=z) = p(X|Z=z)p(Y|Z=z)$$

Expectation

- **Expectation** or **mean** μ of an r.v. with PMF/PDF $p(X)$

$$\mathbb{E}[X] = \sum_x xp(x) \quad \text{(for discrete distributions)}$$

$$\mathbb{E}[X] = \int_x xp(x)dx \quad \text{(for continuous distributions)}$$

- **Note:** The definition applies to **functions of r.v.** too (e.g., $\mathbb{E}[f(X)]$)
- **Note:** Expectations are always w.r.t. the underlying probability distribution of the random variable involved, so sometimes we'll write this explicitly as $\mathbb{E}_{p()}[.]$, unless it is clear from the context
- **Linearity of expectation**

$$\mathbb{E}[\alpha f(X) + \beta g(Y)] = \alpha\mathbb{E}[f(X)] + \beta\mathbb{E}[g(Y)]$$

(a very useful property, true even if X and Y are not independent)

- **Rule of iterated/total expectation**

$$\mathbb{E}_{p(X)}[X] = \mathbb{E}_{p(Y)}[\mathbb{E}_{p(X|Y)}[X|Y]]$$

Variance and Covariance

- **Variance** σ^2 (or "spread" around mean μ) of an r.v. with PMF/PDF $p(X)$

$$\text{var}[X] = \mathbb{E}[(X-\mu)^2] = \mathbb{E}[X^2] - \mu^2$$

- **Standard deviation:** $\text{std}[X] = \sqrt{\text{var}[X]} = \sigma$
- For two scalar r.v.'s x and y, the **covariance** is defined by

$$\text{cov}[x, y] = \mathbb{E}\left[\{x - \mathbb{E}[x]\}\{y - \mathbb{E}[y]\}\right] = \mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y]$$

- For **vector** r.v. $\boldsymbol{x}$ and $\boldsymbol{y}$, the **covariance matrix** is defined as

$$\text{cov}[\boldsymbol{x}, \boldsymbol{y}] = \mathbb{E}\left[\{\boldsymbol{x} - \mathbb{E}[\boldsymbol{x}]\}\{\boldsymbol{y}^T - \mathbb{E}[\boldsymbol{y}^T]\}\right] = \mathbb{E}[\boldsymbol{x}\boldsymbol{y}^T] - \mathbb{E}[\boldsymbol{x}]\mathbb{E}[\boldsymbol{y}^\top]$$

- Cov. of components of a vector r.v. $\boldsymbol{x}$: $\text{cov}[\boldsymbol{x}] = \text{cov}[\boldsymbol{x}, \boldsymbol{x}]$
- **Note:** The definitions apply to functions of r.v. too (e.g., $\text{var}[f(X)]$)
- **Note:** Variance of sum of independent r.v.'s: $\text{var}[X + Y] = \text{var}[X] + \text{var}[Y]$

KL Divergence

- KullbackLeibler divergence between two probability distributions $p(X)$ and $q(X)$

$$
\begin{aligned}
KL(p||q) &= \int p(X) \log \frac{p(X)}{q(X)} dX = -\int p(X) \log \frac{q(X)}{p(X)} dX \qquad \text{(for continuous distributions)} \\
KL(p||q) &= \sum_{k=1}^{K} p(X=k) \log \frac{p(X=k)}{q(X=k)} \qquad \text{(for discrete distributions)}
\end{aligned}
$$

- It is non-negative, i.e., $KL(p||q) \geq 0$, and zero if and only if $p(X)$ and $q(X)$ are the same
- For some distributions, e.g., Gaussians, KL divergence has a closed form expression
- KL divergence is not symmetric, i.e., $KL(p||q) \neq KL(q||p)$

Entropy

- Entropy of a continuous/discrete distribution $p(X)$

$$
\begin{aligned}
H(p) &= -\int p(X)\log p(X)dX \\
H(p) &= -\sum_{k=1}^{K} p(X=k)\log p(X=k)
\end{aligned}
$$

- In general, a peaky distribution would have a smaller entropy than a flat distribution
- Note that the KL divergence can be written in terms of expetation and entropy terms

$$KL(p||q) = \mathbb{E}_{p(X)}[-\log q(X)] - H(p)$$

- Some other definition to keep in mind: conditional entropy, joint entropy, mutual information, etc.

Transformation of Random Variables

Suppose $\boldsymbol{y} = f(\boldsymbol{x}) = \mathbf{A}\boldsymbol{x} + \mathbf{b}$ be a linear function of an r.v. $\boldsymbol{x}$

Suppose $\mathbb{E}[\boldsymbol{x}] = \boldsymbol{\mu}$ and $\text{cov}[\boldsymbol{x}] = \boldsymbol{\Sigma}$

- Expectation of $\boldsymbol{y}$
$$\mathbb{E}[\boldsymbol{y}] = \mathbb{E}[\mathbf{A}\boldsymbol{x} + \mathbf{b}] = \mathbf{A}\boldsymbol{\mu} + \mathbf{b}$$
- Covariance of $\boldsymbol{y}$
$$\text{cov}[\boldsymbol{y}] = \text{cov}[\mathbf{A}\boldsymbol{x} + \mathbf{b}] = \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T$$

Likewise if $y = f(\boldsymbol{x}) = \boldsymbol{a}^T\boldsymbol{x} + b$ is a scalar-valued linear function of an r.v. $\boldsymbol{x}$:

- $\mathbb{E}[y] = \mathbb{E}[\boldsymbol{a}^T\boldsymbol{x} + b] = \boldsymbol{a}^T\boldsymbol{\mu} + b$
- $\text{var}[y] = \text{var}[\boldsymbol{a}^T\boldsymbol{x} + b] = \boldsymbol{a}^T\boldsymbol{\Sigma}\boldsymbol{a}$

Another very useful property worth remembering

Common Probability Distributions

Important: We will use these extensively to model **data** as well as **parameters**

Some **discrete distributions** and what they can model:

- **Bernoulli:** Binary numbers, e.g., outcome (head/tail, 0/1) of a coin toss
- **Binomial:** Bounded non-negative integers, e.g., # of heads in n coin tosses
- **Multinomial:** One of K (>2) possibilities, e.g., outcome of a dice roll
- **Poisson:** Non-negative integers, e.g., # of words in a document
- .. and many others

Some **continuous distributions** and what they can model:

- **Uniform:** numbers defined over a fixed range
- **Beta:** numbers between 0 and 1, e.g., probability of head for a biased coin
- **Gamma:** Positive unbounded real numbers
- **Dirichlet:** vectors that sum of 1 (fraction of data points in different clusters)
- **Gaussian:** real-valued numbers or real-valued vectors
- .. and many others

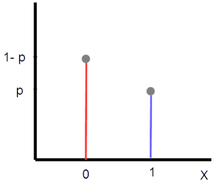
Discrete Distributions

Bernoulli Distribution

- Distribution over a binary r.v. $x \in \{0, 1\}$, like a coin-toss outcome
- Defined by a probability parameter $p \in (0, 1)$

$$P(x = 1) = p$$

- Distribution defined as: $\text{Bernoulli}(x; p) = p^x(1 - p)^{1-x}$

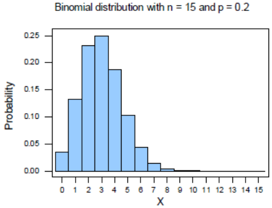


- Mean: $\mathbb{E}[x] = p$
- Variance: $\text{var}[x] = p(1 - p)$

Binomial Distribution

- Distribution over number of successes m (an r.v.) in a number of trials
- Defined by two parameters: total number of trials (N) and probability of each success $p \in (0, 1)$
- Can think of Binomial as multiple independent Bernoulli trials
- Distribution defined as

$$\text{Binomial}(m; N, p) = \binom{N}{m} p^m (1-p)^{N-m}$$



- Mean: $\mathbb{E}[m] = Np$
- Variance: $\text{var}[m] = Np(1-p)$

Multinoulli Distribution

- Also known as the **categorical distribution** (models categorical variables)
- Think of a random assignment of an item to one of K bins - a K dim. binary r.v. $\boldsymbol{x}$ with single 1 (i.e., $\sum_{k=1}^{K} x_k = 1$): **Modeled by a multinoulli**

$$\underbrace{[0 \quad 0 \quad 0 \quad \ldots 0 \quad 1 \quad 0 \quad 0]}_{\text{length} = K}$$

- Let vector $\boldsymbol{p} = [p_1, p_2, \ldots, p_K]$ define the probability of going to each bin
  - $p_k \in (0, 1)$ is the probability that $x_k = 1$ (assigned to bin k)
  - $\sum_{k=1}^{K} p_k = 1$
- The multinoulli is defined as: $\text{Multinoulli}(\boldsymbol{x}; \boldsymbol{p}) = \prod_{k=1}^{K} p_k^{x_k}$
- Mean: $\mathbb{E}[x_k] = p_k$
- Variance: $\text{var}[x_k] = p_k(1 - p_k)$

Multinomial Distribution

- Think of repeating the Multinoulli N times
- Like distributing N items to K bins. Suppose x_k is count in bin k

$$0 \leq x_k \leq N \quad \forall\ k = 1, \dots, K, \qquad \sum_{k=1}^{K} x_k = N$$

- Assume probability of going to each bin: $\boldsymbol{p} = [p_1, p_2, \dots, p_K]$
- Multonomial models the bin allocations via a discrete vector $\boldsymbol{x}$ of size K

$$[x_1 \quad x_2 \quad \dots x_{k-1} \quad x_k \quad x_{k-1} \dots \quad x_K]$$

- Distribution defined as

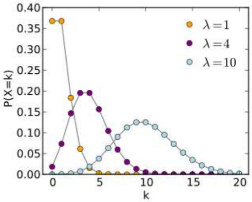
$$\text{Multinomial}(\boldsymbol{x}; N, \boldsymbol{p}) = \binom{N}{x_1 x_2 \dots x_K} \prod_{k=1}^{K} p_k^{x_k}$$

- Mean: $\mathbb{E}[x_k] = Np_k$
- Variance: $\text{var}[x_k] = Np_k(1 - p_k)$
- Note: For $N = 1$, multinomial is the same as multinoulli

Poisson Distribution

- Used to model a non-negative integer (count) r.v. k
- Examples: number of words in a document, number of events in a fixed interval of time, etc.
- Defined by a positive rate parameter λ
- Distribution defined as

$$\text{Poisson}(k;\lambda) = \frac{\lambda^k e^{-\lambda}}{k!} \qquad k = 0, 1, 2, \ldots$$



- Mean: $\mathbb{E}[k] = \lambda$
- Variance: $\text{var}[k] = \lambda$

The Empirical Distribution

- Given a set of points $\phi_1, \ldots, \phi_K$, the empirical distribution is a discrete distribution defined as

$$p_{emp}(A) = \frac{1}{K}\sum_{k=1}^{K} \delta_{\phi_k}(A)$$

where $\delta_\phi(.)$ is the **dirac function** located at ϕ, s.t.

$$\delta_\phi(A) = \begin{cases} 1 & \text{if } \phi \in A \\ 0 & \text{if } \phi \in A \end{cases}$$

- The "weighted" version of the empirical distribution is

$$p_{emp}(A) = \sum_{k=1}^{K} w_k \delta_{\phi_k}(A) \qquad \text{(where } \sum_{k=1}^{K} w_k = 1\text{)}$$

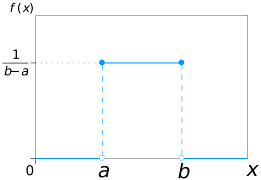
and the weights and points $(w_k, \phi_k)_{k=1}^{K}$ together define this discrete distribution

Continuous Distributions

Uniform Distribution

- Models a continuous r.v. x distributed uniformly over a finite interval $[a, b]$

$$\text{Uniform}(x; a, b) = \frac{1}{b-a}$$

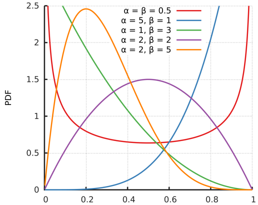


- Mean: $\mathbb{E}[x] = \frac{(b+a)}{2}$
- Variance: $\text{var}[x] = \frac{(b-a)^2}{12}$

Beta Distribution

- Used to model an r.v. p between 0 and 1 (e.g., a probability)
- Defined by two **shape parameters** α and β

$$\text{Beta}(p; \alpha, \beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{\alpha-1}(1-p)^{\beta-1}$$

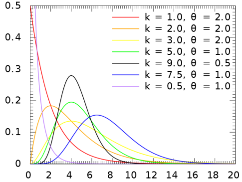


- Mean: $\mathbb{E}[p] = \frac{\alpha}{\alpha+\beta}$
- Variance: $\text{var}[p] = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$
- Often used to model the probability parameter of a Bernoulli or Binomial (also **conjugate** to these distributions)

Gamma Distribution

- Used to model positive real-valued r.v. x
- Defined by a **shape parameters** k and a **scale parameter** θ

$$\text{Gamma}(x; k, \theta) = \frac{x^{k-1} e^{-\frac{x}{\theta}}}{\theta^k \Gamma(k)}$$



- Mean: $\mathbb{E}[x] = k\theta$
- Variance: $\text{var}[x] = k\theta^2$
- Often used to model the rate parameter of Poisson or exponential distribution (conjugate to both), or to model the inverse variance (precision) of a Gaussian (conjuate to Gaussian if mean known)

Note: There is another equivalent parameterization of gamma in terms of **shape** and **rate** parameters (rate = 1/scale). Another related distribution: Inverse gamma.

Dirichlet Distribution

- Used to model non-negative r.v. vectors $\boldsymbol{p} = [p_1, \ldots, p_K]$ that sum to 1

$$0 \leq p_k \leq 1, \quad \forall k = 1, \ldots, K \quad \text{and} \quad \sum_{k=1}^{K} p_k = 1$$

- Equivalent to a distribution over the $K-1$ dimensional simplex
- Defined by a K size vector $\boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_K]$ of positive reals
- Distribution defined as

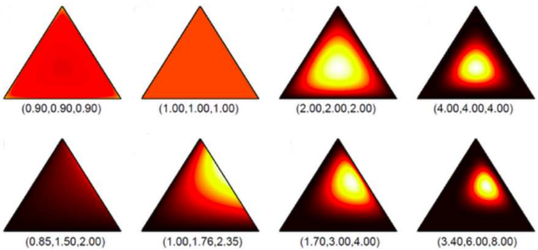
$$\text{Dirichlet}(\boldsymbol{p}; \boldsymbol{\alpha}) = \frac{\Gamma(\sum_{k=1}^{K} \alpha_k)}{\prod_{k=1}^{K} \Gamma(\alpha_k)} \prod_{k=1}^{K} p_k^{\alpha_k - 1}$$

- Often used to model the probability vector parameters of Multinoulli/Multinomial distribution
- Dirichlet is conjugate to Multinoulli/Multinomial
- **Note:** Dirichlet can be seen as a generalization of the Beta distribution. Normalizing a bunch of Gamma r.v.'s gives an r.v. that is Dirichlet distributed.

Dirichlet Distribution

- For $\boldsymbol{p} = [p_1, p_2, \ldots, p_K]$ drawn from Dirichlet$(\alpha_1, \alpha_2, \ldots, \alpha_K)$
  - Mean: $\mathbb{E}[p_k] = \frac{\alpha_k}{\sum_{k=1}^{K} \alpha_k}$
  - Variance: $\text{var}[p_k] = \frac{\alpha_k(\alpha_0 - \alpha_k}{\alpha_0^2(\alpha_0+1)}$ where $\alpha_0 = \sum_{k=1}^{K} \alpha_k$
- Note: $\boldsymbol{p}$ is a point on $(K-1)$-simplex
- Note: $\alpha_0 = \sum_{k=1}^{K} \alpha_k$ controls how peaked the distribution is
- Note: α_k's control where the peak(s) occur

Plot of a 3 dim. Dirichlet (2 dim. simplex) for various values of $\boldsymbol{\alpha}$:

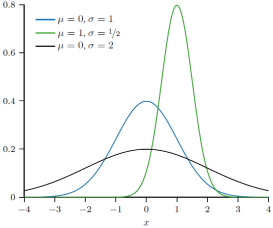


Now comes the
Gaussian (Normal) distribution..

Univariate Gaussian Distribution

- Distribution over real-valued scalar r.v. x
- Defined by a scalar **mean** μ and a scalar **variance** σ^2
- Distribution defined as

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

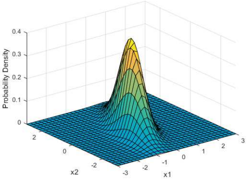


- Mean: $\mathbb{E}[x] = \mu$
- Variance: $\text{var}[x] = \sigma^2$
- Precision (inverse variance) $\beta = 1/\sigma^2$

Multivariate Gaussian Distribution

- Distribution over a multivariate r.v. vector $\boldsymbol{x} \in \mathbb{R}^D$ of real numbers
- Defined by a **mean vector** $\boldsymbol{\mu} \in \mathbb{R}^D$ and a $D \times D$ **covariance matrix** $\boldsymbol{\Sigma}$

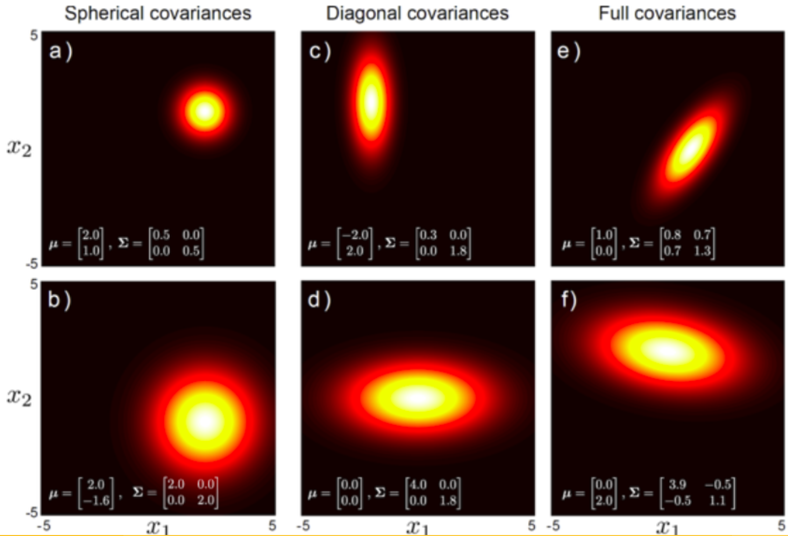
$$\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^D |\boldsymbol{\Sigma}|}} e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})}$$



- The covariance matrix $\boldsymbol{\Sigma}$ must be symmetric and positive definite
  - All eigenvalues are positive
  - $\boldsymbol{z}^\top \boldsymbol{\Sigma} \boldsymbol{z} > 0$ for any real vector $\boldsymbol{z}$
- Often we parameterize a multivariate Gaussian using the inverse of the covariance matrix, i.e., the **precision matrix** $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$

Multivariate Gaussian: The Covariance Matrix

The covariance matrix can be spherical, diagonal, or full



Some nice properties of the Gaussian distribution..

Multivariate Gaussian: Marginals and Conditionals

- Given $\boldsymbol{x}$ having multivariate Gaussian distribution $\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$. Suppose

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix}, \qquad \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{pmatrix}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{pmatrix}, \qquad \boldsymbol{\Lambda} = \begin{pmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{pmatrix}$$

- The marginal distribution is simply

$$p(\boldsymbol{x}_a) = \mathcal{N}(\boldsymbol{x}_a|\boldsymbol{\mu}_a, \boldsymbol{\Sigma}_{aa})$$

- The conditional distribution is given by

$$\begin{aligned} p(\mathbf{x}_a|\mathbf{x}_b) &= \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{a|b}, \boldsymbol{\Lambda}_{aa}^{-1}) \\ \boldsymbol{\mu}_{a|b} &= \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ab}(\mathbf{x}_b - \boldsymbol{\mu}_b) \end{aligned}$$

Thus marginals and conditionals of Gaussians are Gaussians

Multivariate Gaussian: Marginals and Conditionals

- Given the conditional of an r.v. $\boldsymbol{y}$ and marginal of r.v. $\boldsymbol{x}$, $\boldsymbol{y}$ is conditioned on

$$
\begin{aligned}
p(\mathbf{y}|\mathbf{x}) &= \mathcal{N}\left(\mathbf{y}|\mathbf{A}\mathbf{x}+\mathbf{b},\mathbf{L}^{-1}\right) \\
p(\mathbf{x}) &= \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Lambda}^{-1}\right)
\end{aligned}
$$

- Marginal of $\boldsymbol{y}$ and "reverse" conditional are given by

$$
\begin{aligned}
p(\mathbf{x}|\mathbf{y}) &= \mathcal{N}(\mathbf{x}|\boldsymbol{\Sigma}\{\mathbf{A}^{\mathrm{T}}\mathbf{L}(\mathbf{y}-\mathbf{b})+\boldsymbol{\Lambda}\boldsymbol{\mu}\},\boldsymbol{\Sigma}) \\
p(\mathbf{y}) &= \mathcal{N}(\mathbf{y}|\mathbf{A}\boldsymbol{\mu}+\mathbf{b},\mathbf{L}^{-1}+\mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\mathrm{T}})
\end{aligned}
$$

  where $\boldsymbol{\Sigma} = (\boldsymbol{\Lambda} + \mathbf{A}^\top\mathbf{L}\mathbf{A})^{-1}$

- Note that the "reverse conditional" $p(\boldsymbol{x}|\boldsymbol{y})$ is basically the posterior of $\boldsymbol{x}$ is the prior is $p(\boldsymbol{x})$
- Also note that the marginal $p(\boldsymbol{y})$ is the predictive distribution of $\boldsymbol{y}$ after integrating out $\boldsymbol{x}$
- Very useful property for probabilistic models with Gaussian likelihoods and/or priors. Also very handly for computing **marginal likelihoods**.

Gaussians: Product of Gaussians

- Pointwise multiplication of two Gaussians is another (unnormalized) Gaussian

$$\mathcal{N}(\mathrm{x};\boldsymbol{\mu},\boldsymbol{\Sigma})\mathcal{N}(\mathrm{x};\boldsymbol{\nu},\mathbf{P}) = \frac{1}{Z}\mathcal{N}(\mathrm{x};\boldsymbol{\omega},\mathbf{T}),$$

where

$$\mathbf{T} = (\boldsymbol{\Sigma}^{-1} + \mathbf{P}^{-1})^{-1}$$

$$\boldsymbol{\omega} = \mathbf{T}(\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \mathbf{P}^{-1}\boldsymbol{\nu})$$

$$Z^{-1} = \mathcal{N}(\boldsymbol{\mu};\boldsymbol{\nu},\boldsymbol{\Sigma}+\mathbf{P}) = \mathcal{N}(\boldsymbol{\nu};\boldsymbol{\mu},\boldsymbol{\Sigma}+\mathbf{P})$$

Multivariate Gaussian: Linear Transformations

- Given a $\boldsymbol{x} \in \mathbb{R}^d$ with a multivariate Gaussian distribution

$$\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- Consider a linear transform of $\boldsymbol{x}$ into $\boldsymbol{y} \in \mathbb{R}^D$

$$\boldsymbol{y} = \mathbf{A}\boldsymbol{x} + \mathbf{b}$$

  where $\mathbf{A}$ is $D \times d$ and $\mathbf{b} \in \mathbb{R}^D$

- $\boldsymbol{y} \in \mathbb{R}^D$ will have a multivariate Gaussian distribution

$$\mathcal{N}(\boldsymbol{y}; \mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^\top)$$

Some Other Important Distributions

- Wishart Distribution and Inverse Wishart (IW) Distribution: Used to model $D \times D$ p.s.d. matrices
  - Wishart often used as a conjugate prior for modeling precision matrices, IW for covariance matrices
  - For $D = 1$, Wishart is the same as gamma dist., IW is the same as inverse gamma (IG) dist.
- Normal-Wishart Distribution: Used to model mean and precision matrix of a multivar. Gaussian
  - Normal-Inverse Wishart (NIW): : Used to model mean and cov. matrix of a multivar. Gaussian
  - For $D = 1$, the corresponding distr. are Normal-Gamma and Normal-Inverse Gamma (NIG)
- Student-t Distribution (a more robust version of Normal distribution)
  - Can be thought of as a mixture of infinite many Gaussians with different precisions (or a single Gaussian with its precision/precision matrix given a gamma/Wishart prior and integrated out)

Please refer to PRML (Bishop) Chapter 2 + Appendix B, or MLAPP (Murphy) Chapter 2 for more details