Mathematical Background

Vahid Tarokh

ECE685D

Fall 2025

Introduction

- In order to design and implement deep networks we need to know
  - Basics of Linear Algebra
  - Basics of Multivariable Calculus
  - Basics of Probability
- For writing research papers, you may need to know more.
- Here, we will include some of the background for completeness, but will not teach them all.
- Source: **Dive into Deep Learning**
  - **Professor Smola's Slides**
  - **Professor David Carlson's Slides**
  - **Professor Lawrence Caron's slides**
  - **Professor Ruslan Salakhutdinov's slides (available online)**

Quick Review of Linear Algebra

Scalars

- **Simple operations**

$$c = a + b$$

$$c = a \cdot b$$

$$c = \sin a$$

- **Length**

$$|a| = \begin{cases} a & \text{if} a > 0 \\ -a & \text{otherwise} \end{cases}$$

$$|a + b| \leq |a| + |b|$$

$$|a \cdot b| = |a| \cdot |b|$$

Vectors

- **Simple operations**

$$c = a + b \quad \text{where } c_i = a_i + b_i$$
$$c = \alpha \cdot b \quad \text{where } c_i = \alpha b_i$$
$$c = \sin a \quad \text{where } c_i = \sin a_i$$

Definition of a vector space

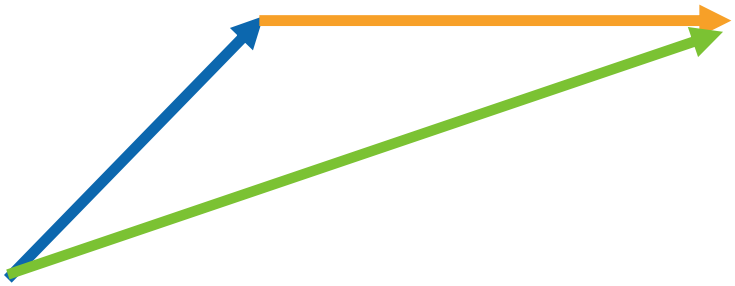
- **Length**

$$\|a\|_2 = \left[\sum_{i=1}^{m} a_i^2 \right]^{\frac{1}{2}}$$

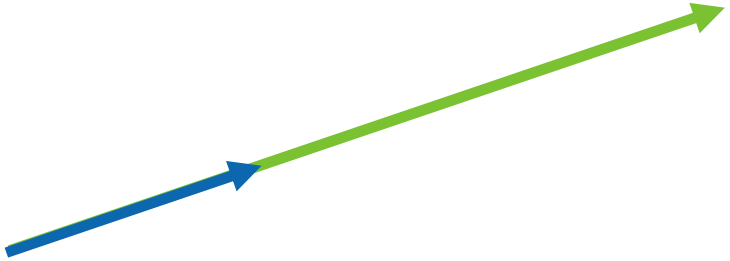
Definition of norm

$$\|a\| \geq 0 \text{ for all } a$$
$$\|a + b\| \leq \|a\| + \|b\|$$
$$\|a \cdot b\| = |a| \cdot \|b\|$$

Vectors



$$c = a + b$$



$$c = \alpha \cdot b$$

Mathematician's **'parallel for all do'**

Vectors

- **Dot product**

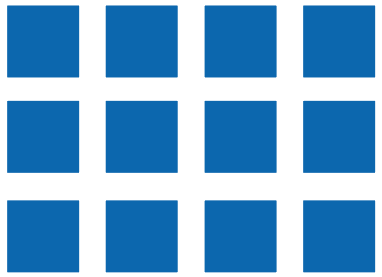
$$a^\top b = \sum_i a_i b_i$$

- **Orthogonality**

$$a^\top b = \sum_i a_i b_i = 0$$

(e.g. if we have two vectors that are orthogonal with a third, their linear combination is it, too)

Matrices



- **Simple operations**

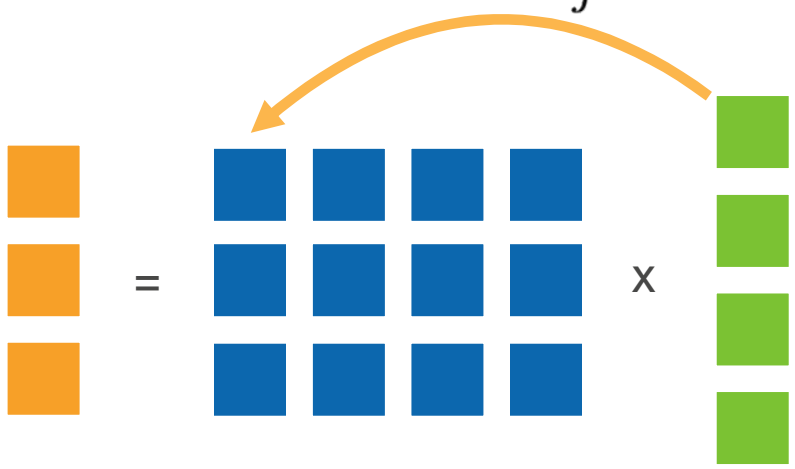
$$C = A + B \qquad \text{where } C_{ij} = A_{ij} + B_{ij}$$
$$C = \alpha \cdot B \qquad \text{where } C_{ij} = \alpha B_{ij}$$
$$C = \sin A \qquad \text{where } C_{ij} = \sin A_{ij}$$

- **Functional Analysis 101**
  vector = function, matrix = linear operator
  most theorems work sort-of in infinite dimensional spaces

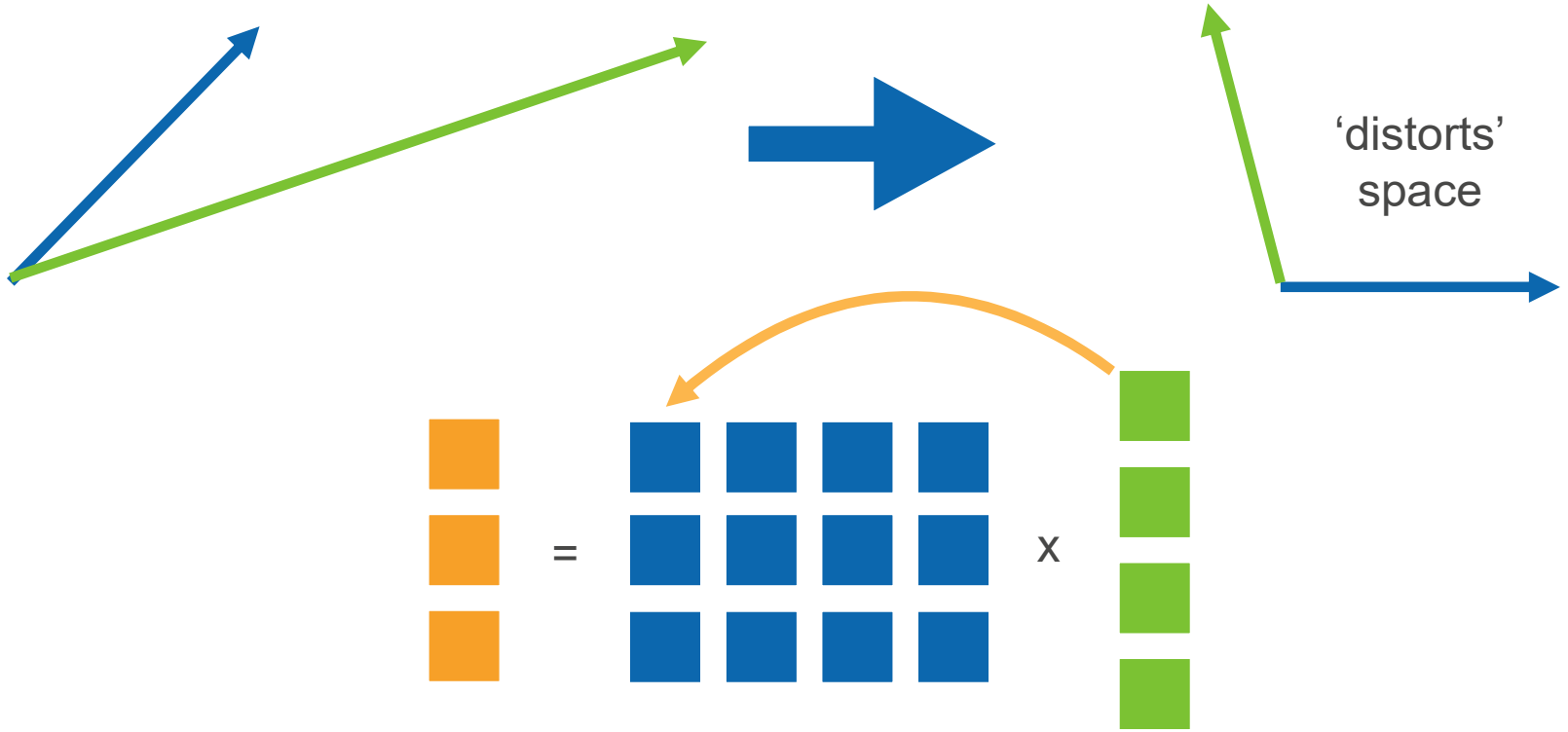
Matrices

- **Multiplications (matrix vector)**

$$c = Ab \text{ where } c_i = \sum_j A_{ij} b_j$$



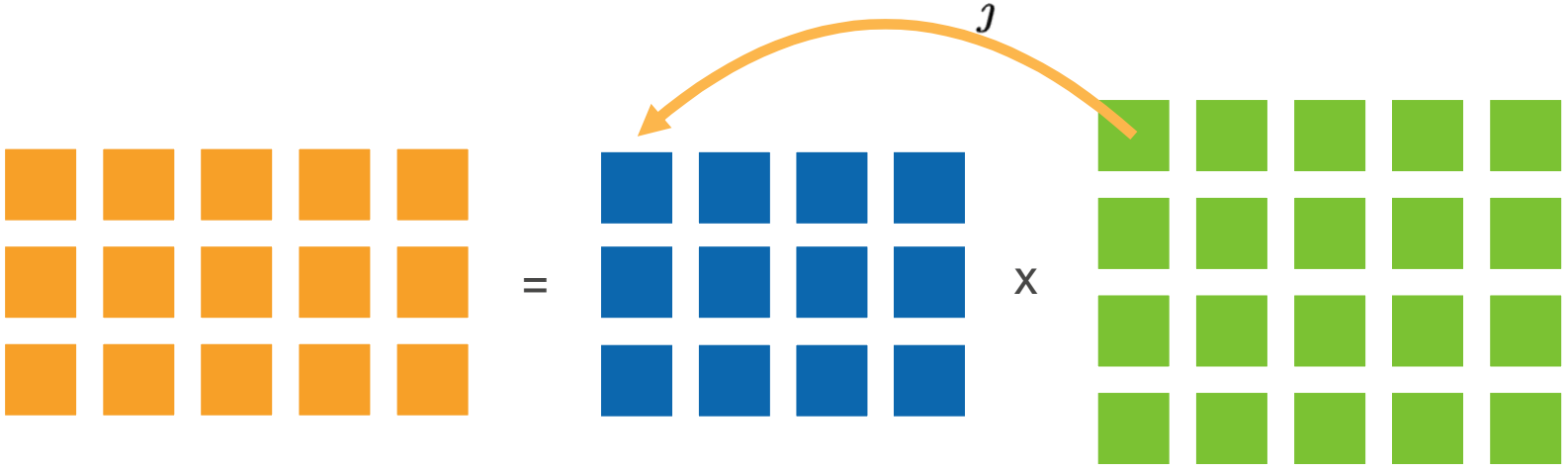
Matrices



Matrices

- **Multiplications (matrix matrix)**

$$C = AB \text{ where } C_{ik} = \sum_j A_{ij} B_{jk}$$



Matrices

- **Norms**

$$c = A \cdot b \text{ hence } \|c\| \leq \|A\| \cdot \|b\|$$

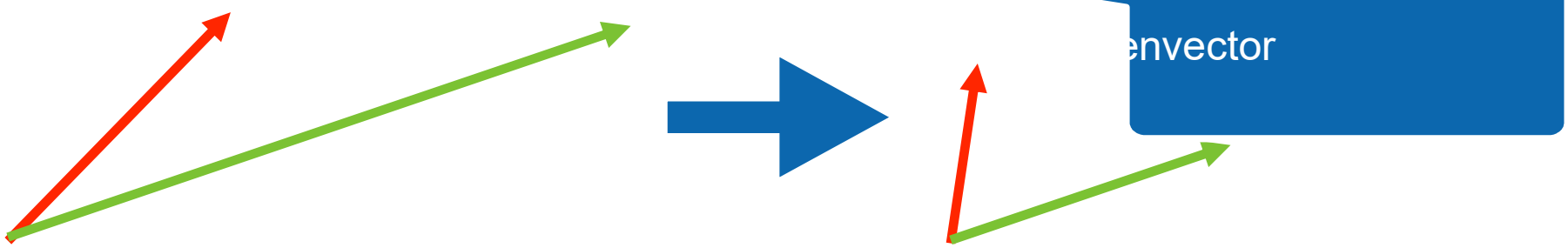
  - Choices depending on how to measure length of b and c
- **A Popular norm**
  - Frobenius norm

$$\|A\|_{\text{Frob}} = \left[\sum_{ij} A_{ij}^2 \right]^{\frac{1}{2}}$$

Matrices

- **Eigenvectors and eigenvalue**
  - Vectors that aren't changed by the matrix

$$Ax = \lambda x$$



  - For symmetric matrices we can always find this

Special Matrices

- **Symmetric, antisymmetric** $A_{ij} = A_{ji}$ and $A_{ij} = -A_{ji}$

- **Non-negative definite**

$$\|x\|^2 = x^\top x \geq 0 \text{ generalizes to } x^\top A x \geq 0$$

(all non-negative eigenvalues)

Special Matrices

- **Orthogonal Matrices**
  - All rows of the matrix are orthogonal to each other
  - All rows of the matrix have unit length

$$U \text{ with } \sum_j U_{ij} U_{kj} = \delta_{ik}$$

Show that $U^\top U = \mathbf{1}$

  - Rewrite in matrix form

$$UU^\top = \mathbf{1}$$

- **Permutation Matrices**

Show that P is orthogonal

$$P \text{ where } P_{ij} = 1 \text{ if and only if } j = \pi(i)$$

Multidimensional Arrays

N-dimensional Array Examples

N-dimensional array, short for ndarray, is the main data structure for machine learning and neural networks

0-d (scalar)

1.0

A class label

1-d (vector)

[1.0, 2.7, 3.4]

A feature vector

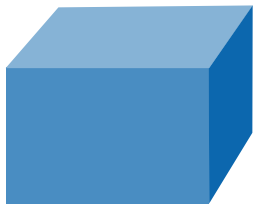
2-d (matrix)

[[1.0, 2.7, 3.4]
[5.0, 0.2, 4.6]
[4.3, 8.5, 0.2]]

A example-by-feature matrix

ND Array Examples, cont

3-d



```
[[[0.1, 2.7, 3.4]
  [5.0, 0.2, 4.6]
  [4.3, 8.5, 0.2]]
 [[3.2, 5.7, 3.4]
  [5.4, 6.2, 3.2]
  [4.1, 3.5, 6.2]]]
```

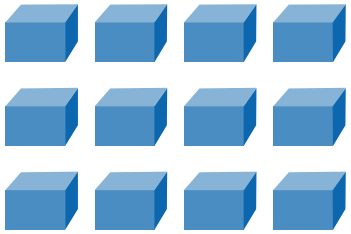
A RGB image (width x height x channels)

4-d

```
[[[[. . .
   . . .
   . . .]]]
```

A batch of RGB images (batch-size x width x height x channels)

5-d

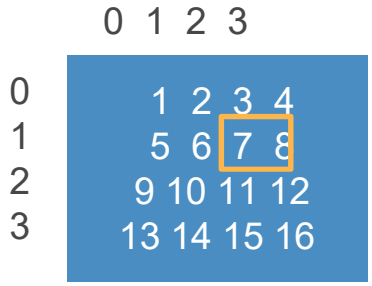


```
[[[[. . .
   . . .
   . . .]]]
```

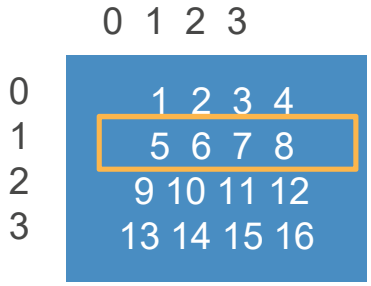
A batch of videos (batch-size x time x width x height x channels)

Access Elements

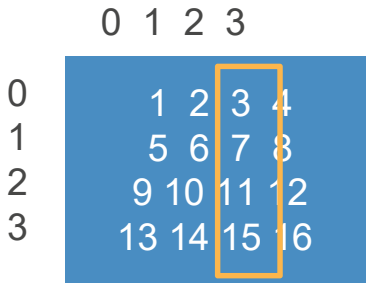
An element: [1, 2]

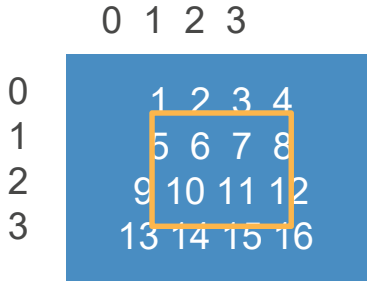


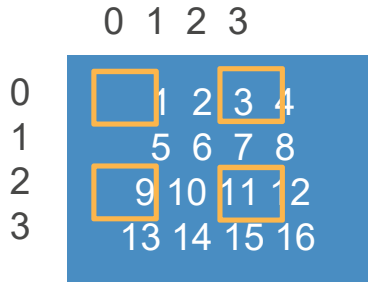
A row: [1, :]



A column: [1, :]







Review of Basic Probability

Probability

Space of events X

- server working; slow response; server broken
- income of the user (e.g. $95,000)
- query text for search (e.g. “statistics tutorial”)

Probability axioms

$$\Pr(X) \in [0,1],\ \Pr(\mathcal{X}) = 1$$
$$\Pr(\cup_i X_i) = \sum_i \Pr(X_i) \text{ if } X_i \cap X_j = \emptyset$$

Example queries

- P(server working) = 0.999 — discrete
- P(90,000 < income < 100,000) = 0.1 — continuous

What you must know

- Definitions of random variable and random vector
- Conditional probability, Independence, and dependence
- Law of Total Probability
- Definition of PMF, PDF, and CDF
- Generation of an arbitrary random variable with a given pdf from the uniform random variable
- PMF and PDF of transforms of random vectors
- Mathematical Expectation
- Variance, Covariance, correlation, etc.
- Multivariable Calculus and Lagrange's multiplier method

(In)dependence

Independence

- Login behavior of two users (approximately)
- Disk crash in different colos (approximately)

$$\Pr(x, y) = \Pr(x) \cdot \Pr(y)$$

independent events

- Emails
- Queries
- News stream / Buzz / Tweets
- IM communication
- Russian Roulette

Everywhere

$$\Pr(x, y) \neq \Pr(x) \cdot \Pr(y)$$

Weak Low of Large Numbers

Let $X_1, X_2, \cdots X_n$ be i.i.d. random variable with mean μ. Then for any $\epsilon > 0$

$$P[\ |(X_1 + X_2 + \cdots + X_n)/n\ \ - \mu| > \epsilon\ ] \to 0$$

as $n \to \infty$.

Order Statistics

For $X_1, X_2, \ldots, X_n$ iid random variables X_k is the kth smallest X, usually called the kth order statistic.

$X_{(1)}$ is therefore the smallest X and

$$X_{(1)} = \min(X_1, \ldots, X_n)$$

Similarly, $X_{(n)}$ is the largest X and

$$X_{(n)} = \max(X_1, \ldots, X_n)$$

Order Statistics (density of maximum)

For $X_1, X_2, \ldots, X_n$ iid continuous random variables with pdf f and cdf F the density of the maximum is

$$
\begin{aligned}
P(X_{(n)} \in [x, x+\epsilon]) &= P(\text{one of the } X\text{'s} \in [x, x+\epsilon] \text{ and all others} < x) \\
&= \sum_{i=1}^{n} P(X_i \in [x, x+\epsilon] \text{ and all others} < x) \\
&= nP(X_1 \in [x, x+\epsilon] \text{ and all others} < x) \\
&= nP(X_1 \in [x, x+\epsilon])P(\text{all others} < x) \\
&= nP(X_1 \in [x, x+\epsilon])P(X_2 < x) \cdots P(X_n < x) \\
&= nf(x)\epsilon F(x)^{n-1}
\end{aligned}
$$

$$
f_{(n)}(x) = nf(x)F(x)^{n-1}
$$

Order Statistics (density of minimum)

For $X_1, X_2, \ldots, X_n$ iid continuous random variables with pdf f and cdf F the density of the minimum is

$$\begin{aligned}
P(X_{(1)} \in [x, x+\epsilon]) &= P(\text{one of the } X\text{'s} \in [x, x+\epsilon] \text{ and all others} > x) \\
&= \sum_{i=1}^{n} P(X_i \in [x, x+\epsilon] \text{ and all others} > x) \\
&= nP(X_1 \in [x, x+\epsilon] \text{ and all others} > x) \\
&= nP(X_1 \in [x, x+\epsilon])P(\text{all others} > x) \\
&= nP(X_1 \in [x, x+\epsilon])P(X_2 > x) \cdots P(X_n > x) \\
&= nf(x)\epsilon(1 - F(x))^{n-1}
\end{aligned}$$

$$f_{(1)}(x) = nf(x)(1 - F(x))^{n-1}$$

Order Statistics (density of k-th)

For $X_1, X_2, \ldots, X_n$ iid continuous random variables with pdf f and cdf F the density of the kth order statistic is

$$
\begin{aligned}
P(X_{(k)} \in [x, x+\epsilon]) &= P(\text{one of the } X\text{'s} \in [x, x+\epsilon] \text{ and exactly } k-1 \text{ of the others} < x) \\
&= \sum_{i=1}^{n} P(X_i \in [x, x+\epsilon] \text{ and exactly } k-1 \text{ of the others} < x) \\
&= nP(X_1 \in [x, x+\epsilon] \text{ and exactly } k-1 \text{ of the others} < x) \\
&= nP(X_1 \in [x, x+\epsilon])P(\text{exactly } k-1 \text{ of the others} < x) \\
&= nP(X_1 \in [x, x+\epsilon]) \left(\binom{n-1}{k-1} P(X < x)^{k-1} P(X > x)^{n-k} \right)
\end{aligned}
$$

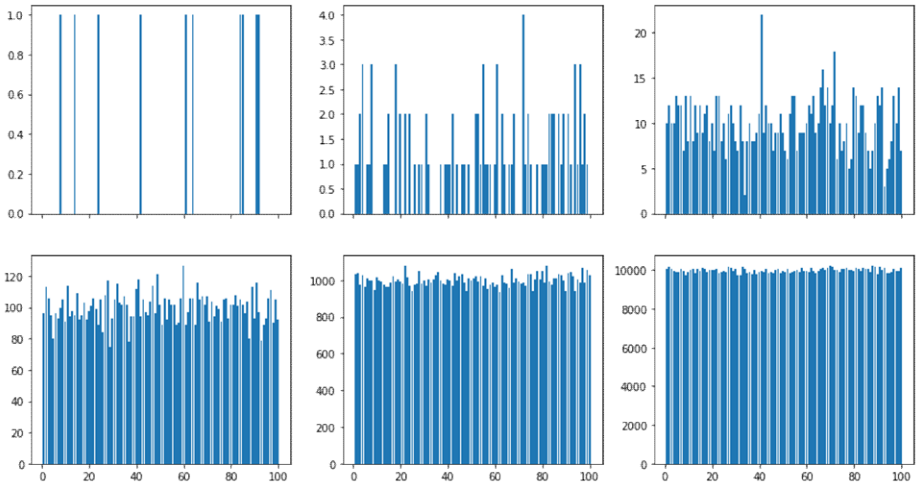
$$
f_{(k)}(x) = nf(x) \binom{n-1}{k-1} F(x)^{k-1} (1 - F(x))^{n-k}
$$

Uniform Distribution

- Constant within an interval, zero outside

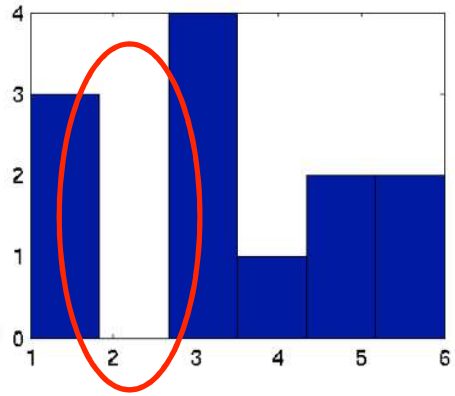
$$p(x) = \frac{1}{U - L} \text{ if } L \leq x \leq U$$

- Useful for initializing parameters or for load distribution

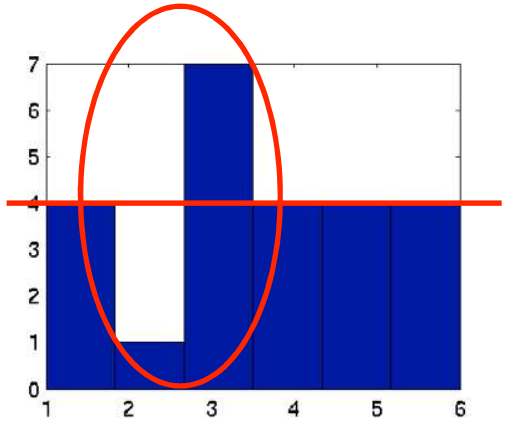


Tossing a Fair Dice

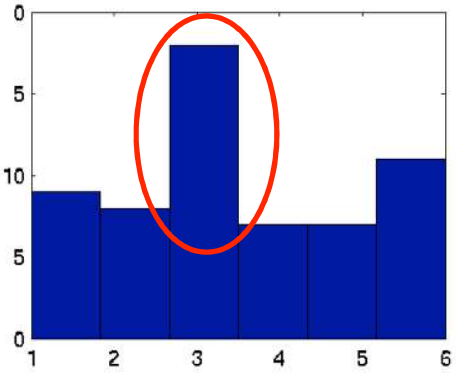
12



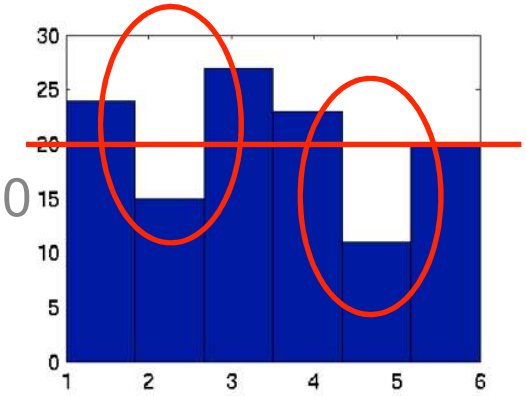
24



60



120



Euler's Gamma Function

For $x > 0$ The Euler's gamma function is defined as:

$$\Gamma(x) \equiv \int_0^\infty u^{x-1} e^{-u} du.$$

- The value $\Gamma(n) = (n-1)!$ When n > 0 is a positive integer.

- Show that $\Gamma(x) = (x-1)\Gamma(x-1)$ for $x > 1$.
- Calculate $\Gamma(3/2)$
- Calculate $\Gamma(1/2)$

Beta Distribution

- We define a distribution for a parameter $\mu \in [0, 1]$

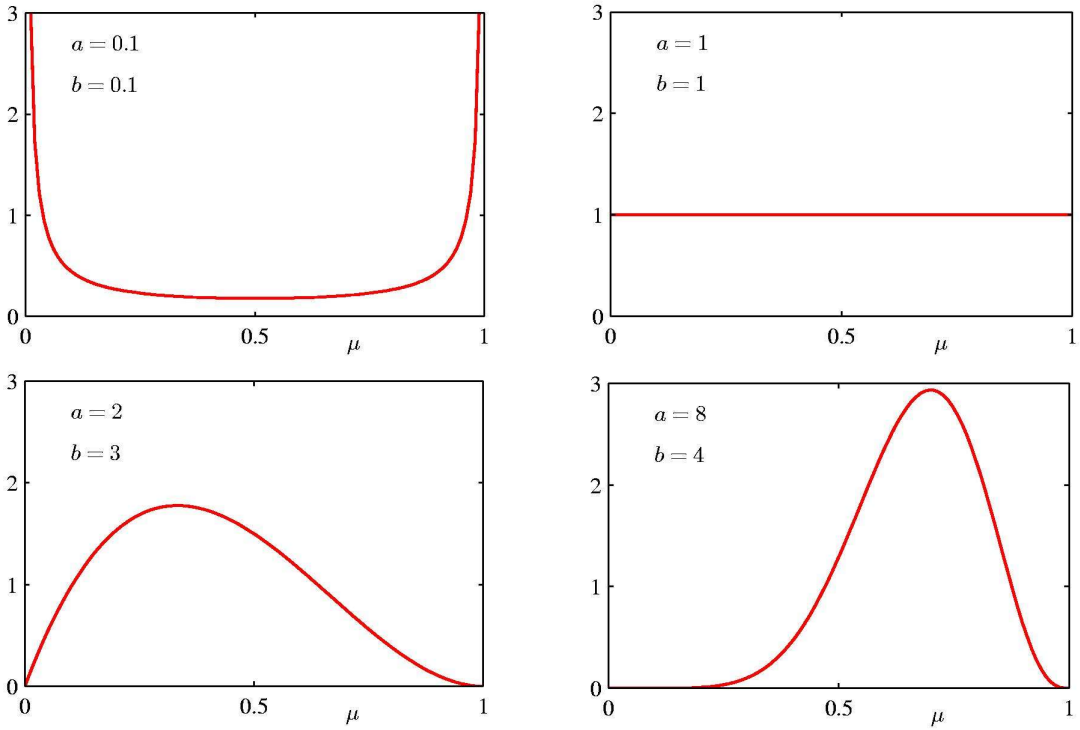
$$\begin{aligned} \text{Beta}(\mu|a,b) &= \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\mu^{a-1}(1-\mu)^{b-1} \\ \mathbb{E}[\mu] &= \frac{a}{a+b} \\ \text{var}[\mu] &= \frac{ab}{(a+b)^2(a+b+1)} \end{aligned}$$

where the Euler's gamma function is defined as:

$$\Gamma(x) \equiv \int_0^\infty u^{x-1}e^{-u}du.$$

and ensures that the Beta distribution is normalized.

Beta Distribution



Relationship Between Beta and Uniform

Let $X_1, X_2, \ldots, X_n \overset{iid}{\sim} \text{Unif}(0,1)$ then the density of $X_{(n)}$ is given by

$$f_{(k)}(x) = nf(x)\binom{n-1}{k-1}F(x)^{k-1}(1-F(x))^{n-k}$$

$$= \begin{cases} n\binom{n-1}{k-1}x^{k-1}(1-x)^{n-k} & \text{if } 0 < x < 1 \\ 0 & \text{otherwise} \end{cases}$$

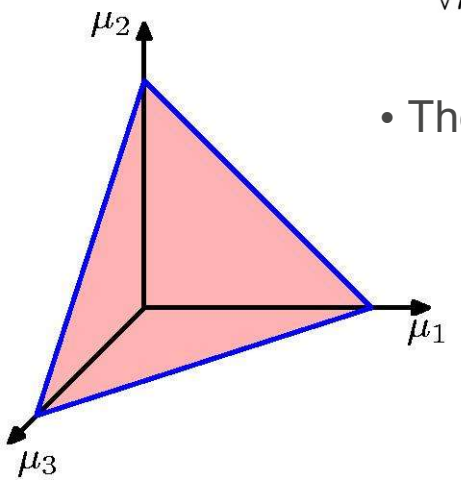
This is an example of the Beta distribution where $r = k$ and $s = n - k + 1$.

$$X_{(k)} \sim \text{Beta}(k, n-k+1)$$

Dirichlet Distribution

• Consider a distribution over the K-dimensional simplex, subject to constraints:

$$\forall k : \mu_k \geqslant 0 \quad \text{and} \quad \sum_{k=1}^{K} \mu_k = 1$$



• The Dirichlet distribution is defined as:

$$\mathrm{Dir}(\boldsymbol{\mu}|\boldsymbol{\alpha}) = \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_1)\cdots\Gamma(\alpha_K)} \prod_{k=1}^{K} \mu_k^{\alpha_k - 1}$$

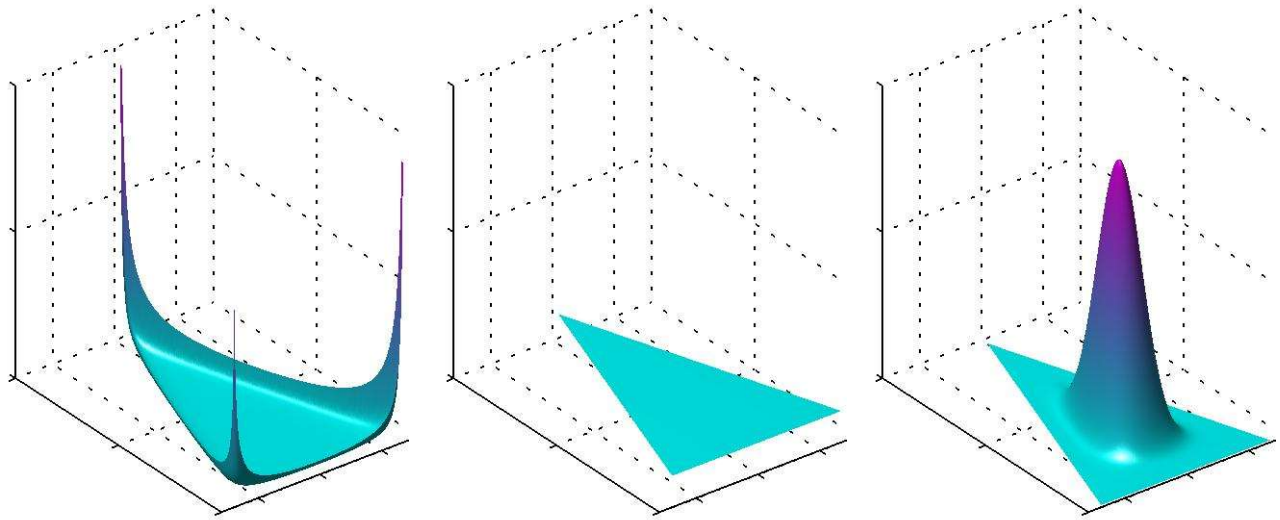
$$\alpha_0 = \sum_{k=1}^{K} \alpha_k$$

where $\alpha_{11},\ldots, \alpha_k$ are the parameters of the distribution, and $\Gamma(x)$ is the gamma function.

• The Dirichlet distribution is confined to a simplex as a consequence of the constraints.

Dirichlet Distribution

- Plots of the Dirichlet distribution over three variables.



$\alpha_k = 10^{-1}$ $\alpha_k = 10^{0}$ $\alpha_k = 10^{1}$

Generation of Dirichlet from Beta

- Consider a Stick of length 1.

Simulate a random variate $X_j \sim Beta(\alpha_j, \sum_{i=j+1}^{k} \alpha_i)$, where $j = 1, \ldots, k-1$. When $j = 1$, we have $X_1 \sim Beta(\alpha_1, \sum_{i=2}^{k} \alpha_i)$. The first piece of the stick has length $1 \cdot X_1$, such that the length of the remaining stick is $1 - X_1$. Also, set $Y_1 = X_1$.

Generation of Dirichlet from Beta

When $j = 2$, we have $X_2 \sim Beta(\alpha_2, \sum_{i=3}^{k} \alpha_i)$. The second piece of the stick has length $(1 - X_1)X_2$, such that the length of the remaining stick is $(1 - X_1) - (1 - X_1)X_2 = (1 - X_1)(1 - X_2)$. Also, set $Y_2 = (1 - X_1)X_2$.

:

Continue in this way.

Generation of Dirichlet from Beta

When $j = k-1$, we have $X_{k-1} \sim Beta(\alpha_{k-1}, \alpha_k)$. The $(k-1)^{th}$ piece of the stick has length $X_{k-1}\prod_{j=1}^{k-2}(1-X_j)$, such that the length of the remaining stick is $\prod_{j=1}^{k-1}(1-X_j)$. Also, set $Y_{k-1} = X_{k-1}\prod_{j=1}^{k-2}(1-X_j)$. Note that the k^{th} piece of the stick has length $\prod_{j=1}^{k-1}(1-X_j)$ and set $Y_k = \prod_{j=1}^{k-1}(1-X_j)$. We can conclude that $(Y_1, \ldots, Y_k) \sim Dir(\alpha_1, \ldots, \alpha_k)$.

Source: Bela A Frigyik, Amol Kapila, and Maya R Gupta. Introduction to the Dirichlet distribution and related processes. Technical report, UWEETR-2010-0006, 2010

Entropy

The entropy of a d-dimensional random vector $\mathbf{X} := \begin{bmatrix} X_1 & \cdots & X_d \end{bmatrix}^T$ is defined by the expectation of the self information

$$H(\mathbf{X}) := \mathbb{E}_{\mathbf{X}}\left[\log \frac{1}{p(\mathbf{X})}\right] = \sum_{\mathbf{x} \in \mathcal{X}_1 \times \cdots \times \mathcal{X}_d} p(\mathbf{x}) \log \frac{1}{p(\mathbf{x})} = H(X_1, \ldots, X_d)\,.$$

The conditional entropy of X given Y is defined by

$$H(X|\,Y) := \sum_{y \in \mathcal{Y}} p(y) H(X|\,Y = y) = \sum_{x \in \mathcal{X}, y \in \mathcal{Y}} p\,(x, y) \log \frac{1}{p_{X|\,Y}(x|y)}\,.$$

Kullback-Leibler Divergence

Let $p(\cdot)$ and $q(\cdot)$ are two p.m.f.'s of a random variable X. The relative entropy between p and q is $D(p||q) := \mathbb{E}_p\left[\log \frac{p(X)}{q(X)}\right]$

(the subscript "p" denotes that the expectation is taken over the distribution p.)

Please note that KL divergence is NOT symmetric: D (p || q) ≠ D (q || p).

Important Results:

$D(p||q) \geq 0$, *with equality iff* $p(x) = q(x)$ *for all* $x \in \mathcal{X}$.

Maximum Likelihood Estimator (MLE)

- Let $p_*(\cdot)$ be the true data generating distribution
- $E_*(\cdot)$ be expectation w.r.t. $p_*(\cdot)$
  - Suppose that iid samples (observations}

$$y_1, y_2, \cdots, y_n$$

are given.

  - Let $p \equiv p_\theta$ for $\theta \in \Theta$ denote our guesses for $p_*(\cdot)$
  - MLE: Choose the value of $\theta \in \Theta$ that achieves the maximum of

$$\frac{\Sigma_1^n \log p(y_i)}{n}$$

Maximum Likelihood Estimator (MLE)

- Why is it so popular?
  - It is an elementary function of the probability density function
  - Intimate relation with KL-divergence
  - Notice that

$$-\frac{\Sigma_1^n \log p(y_i)}{n} \rightarrow E_{p^*}[-\log\ p(y)]$$

  - Minimizing

$$-\frac{\Sigma_1^n \log p(y_i)}{n}$$

is asymptotically equivalent to minimizing

$$E_*\{-\log p(y)\} = D_{KL}(p_*||p) + \mathrm{H}(p_*)$$

or equivalently

$$D_{KL}(p_*||p).$$

Bernoulli Distribution

• Consider a single binary random variable $x \in \{0, 1\}$.

•For example, x can describe the outcome of flipping a coin:

Coin flipping: heads = 1, tails = 0.

• The probability of x=1 will be denoted by the parameter ¹, so that:

$$p(x = 1|\mu) = \mu \qquad 0 \leq \mu \leq 1.$$

• The probability distribution, known as Bernoulli distribution, can be written as:

$$\begin{aligned} \text{Bern}(x|\mu) &= \mu^x(1-\mu)^{1-x} \\ \mathbb{E}[x] &= \mu \\ \text{var}[x] &= \mu(1-\mu) \end{aligned}$$

Parameter Estimation

- Suppose we observed a data: $\mathcal{D} = \{x_1, ..., x_N\}$
- We can construct the likelihood function, which is a function of [1].

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

- Equivalently, we can maximize the log of the likelihood function:

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

- Note that the likelihood function depends on the N observations x_n only through the sum

$$\sum_n x_n$$

Sufficient Statistic

Parameter Estimation

- Suppose we observed a data: $\mathcal{D} = \{x_1, ..., x_N\}$

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

- Setting the derivative of the log-likelihood function w.r.t ¹ to zero, we obtain:

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

where m is the number of heads.

Binomial Distribution

• We can also work out the distribution of the number m of observations of x=1 (e.g. the number of heads).

• The probability of observing m heads given N coin flips and a parameter μ is given by:

$$p(m \text{ heads}|N,\mu) =$$

$$\text{Bin}(m|N,\mu) = \binom{N}{m}\mu^m(1-\mu)^{N-m}$$

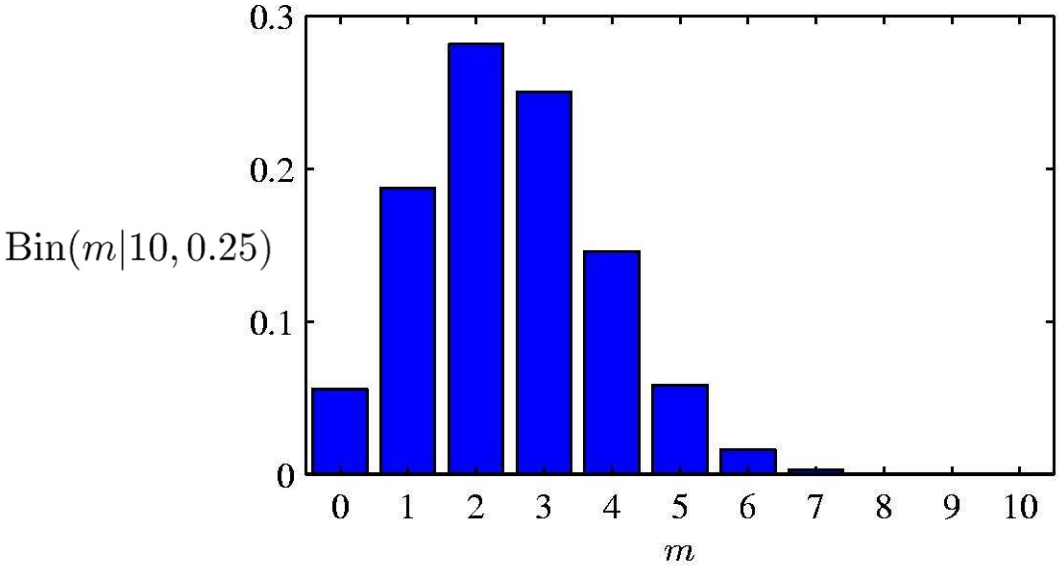
• The mean and variance can be easily derived as:

$$\mathbb{E}[m] \equiv \sum_{m=0}^{N} m\text{Bin}(m|N,\mu) = N\mu$$

$$\text{var}[m] \equiv \sum_{m=0}^{N} (m-\mathbb{E}[m])^2\,\text{Bin}(m|N,\mu) = N\mu(1-\mu)$$

Example

• Histogram plot of the Binomial distribution as a function of m for N=10 and μ = 0.25.



Multinomial Variables

• Consider a random variable that can take on one of K possible mutually exclusive states (e.g. roll of a dice).

• We will use so-called 1-of-K encoding scheme.

• If a random variable can take on K=6 states, and a particular observation of the variable corresponds to the state x_3=1, then **x** will be resented as:

1-of-K coding scheme: $$\mathbf{x} = (0, 0, 1, 0, 0, 0)^{\mathrm{T}}$$

• If we denote the probability of x_k=1 by the parameter μ_k, then the distribution over **x** is defined as:

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_k^{x_k} \qquad \forall k : \mu_k \geqslant 0 \quad \text{and} \quad \sum_{k=1}^{K} \mu_k = 1$$

Multinomial Variables

• Multinomial distribution can be viewed as a generalization of Bernoulli distribution to more than two outcomes.

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

• It is easy to see that the distribution is normalized:

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

and

$$\mathbb{E}[\mathbf{x}|\boldsymbol{\mu}] = \sum_{\mathbf{x}} p(\mathbf{x}|\boldsymbol{\mu})\mathbf{x} = (\mu_1, \ldots, \mu_K)^{\mathrm{T}} = \boldsymbol{\mu}$$

Maximum Likelihood Estimation

- Suppose we observed a data $\mathcal{D} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$
- We can construct the likelihood function, which is a function of [1].

$$p(\mathcal{D}|\boldsymbol{\mu}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \mu_k^{x_{nk}} = \prod_{k=1}^{K} \mu_k^{\left(\sum_n x_{nk}\right)} = \prod_{k=1}^{K} \mu_k^{m_k}$$

- Note that the likelihood function depends on the N data points only though the following K quantities:

$$m_k = \sum_n x_{nk}, \quad k = 1, ..., K.$$

which represents the number of observations of x_k=1.

- These are called the sufficient statistics for this distribution.

Maximum Likelihood Estimation

$$p(\mathcal{D}|\boldsymbol{\mu}) = \prod_{n=1}^{N}\prod_{k=1}^{K}\mu_k^{x_{nk}} = \prod_{k=1}^{K}\mu_k^{\left(\sum_n x_{nk}\right)} = \prod_{k=1}^{K}\mu_k^{m_k}$$

• To find a maximum likelihood solution for ¹, we need to maximize the log-likelihood taking into account the constraint that $\sum_k \mu_k = 1$

• Forming the Lagrangian:

$$\sum_{k=1}^{K} m_k \ln \mu_k + \lambda\left(\sum_{k=1}^{K}\mu_k - 1\right)$$

$$\mu_k = -m_k/\lambda \qquad \mu_k^{\mathrm{ML}} = \frac{m_k}{N} \qquad \lambda = -N$$

which is the fraction of observations for which x_k=1.

Multinomial Distribution

• We can construct the joint distribution of the quantities $\{m_1, m_2, \ldots, m_k\}$ given the parameters [1] and the total number N of observations:

$$\begin{aligned} \mathrm{Mult}(m_1, m_2, \ldots, m_K | \boldsymbol{\mu}, N) &= \binom{N}{m_1 m_2 \ldots m_K} \prod_{k=1}^{K} \mu_k^{m_k} \\ \mathbb{E}[m_k] &= N\mu_k \\ \mathrm{var}[m_k] &= N\mu_k(1-\mu_k) \\ \mathrm{cov}[m_j m_k] &= -N\mu_j\mu_k \end{aligned}$$

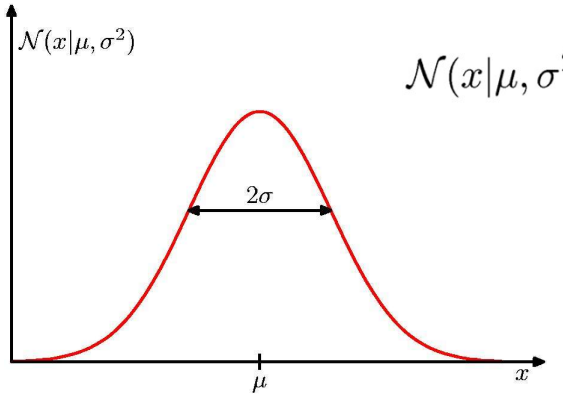
• The normalization coefficient is the number of ways of partitioning N objects into K groups of size $m_1, m_2, \ldots, m_K$.

• Note that

$$\sum_k m_k = N.$$

Gaussian Univariate Distribution

• In the case of a single variable x, the Gaussian distribution takes form:



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

which is governed by two parameters:

- μ (mean)
- σ^2 (variance)

- The Gaussian distribution satisfies:

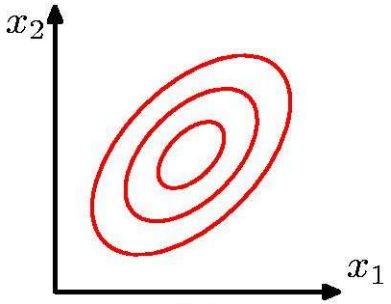
$$\mathcal{N}(x|\mu,\sigma^2) > 0$$

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

Multivariate Gaussian Distribution

• For a D-dimensional vector **x**, the Gaussian distribution takes form:

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



which is governed by two parameters:

- μ is a D-dimensional mean vector.
- Σ is a D by D covariance matrix.

and $|\Sigma|$ denotes the determinant of Σ.

- Note that the covariance matrix is a symmetric positive definite matrix.

Central Limit Theorem

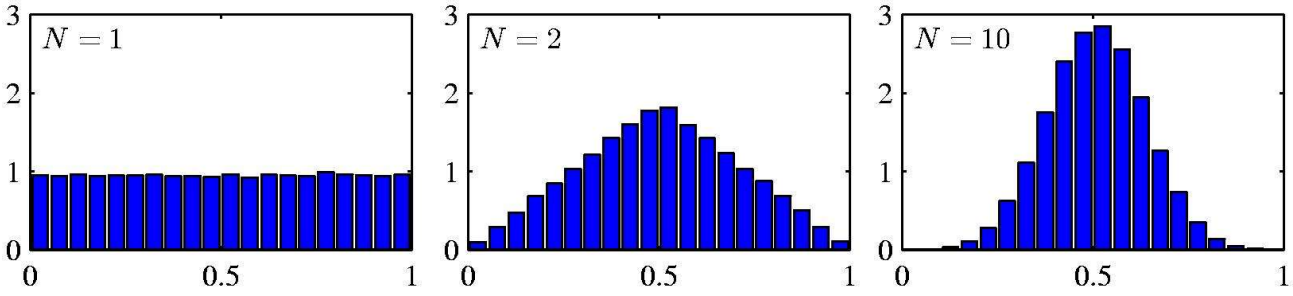
• The distribution of the sum of N i.i.d. random variables becomes increasingly Gaussian as N grows.

• Consider N variables, each of which has a uniform distribution over the interval [0,1].

• Let us look at the distribution over the mean:

$$\frac{x_1 + x_2 + ... + x_N}{N}.$$

• As N increases, the distribution tends towards a Gaussian distribution.



Moments of the Gaussian Distribution

- The expectation of **x** under the Gaussian distribution:

$$\begin{aligned}\mathbb{E}[\mathbf{x}] &= \frac{1}{(2\pi)^{D/2}}\frac{1}{|\boldsymbol{\Sigma}|^{1/2}}\int \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}\mathbf{x}\,\mathrm{d}\mathbf{x} \\ &= \frac{1}{(2\pi)^{D/2}}\frac{1}{|\boldsymbol{\Sigma}|^{1/2}}\int \exp\left\{-\frac{1}{2}\mathbf{z}^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}\mathbf{z}\right\}(\mathbf{z}+\boldsymbol{\mu})\,\mathrm{d}\mathbf{z}\end{aligned}$$

The term in z in the factor $(z+^{1})$ will vanish by symmetry.

$$\mathbb{E}[\mathbf{x}] = \boldsymbol{\mu}$$

Moments of the Gaussian Distribution

- The second order moments of the Gaussian distribution:

$$\mathbb{E}[\mathbf{x}\mathbf{x}^{\mathrm{T}}] = \boldsymbol{\mu}\boldsymbol{\mu}^{\mathrm{T}} + \boldsymbol{\Sigma}$$

- The covariance is given by:

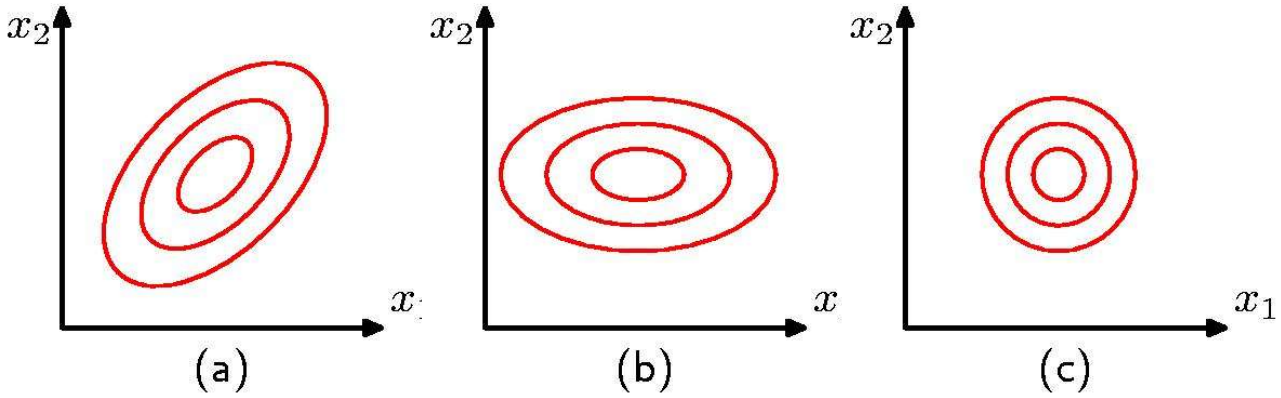
$$\mathrm{cov}[\mathbf{x}] = \mathbb{E}\left[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^{\mathrm{T}}\right] = \boldsymbol{\Sigma}$$

$$\mathbb{E}[\mathbf{x}] = \boldsymbol{\mu}$$

- Because the parameter matrix § governs the covariance of x under the Gaussian distribution, it is called the covariance matrix.

Moments of the Gaussian Distribution

- Contours of constant probability density:



Covariance matrix is of general form.

Diagonal, axis-aligned covariance matrix.

Spherical (proportional to identity) covariance matrix.

Partitioned Gaussian Distribution

- Consider a D-dimensional Gaussian distribution: $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- Let us partition **x** into two disjoint subsets x_a and x_b:

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix} \qquad \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{pmatrix}$$

- In many situations, it will be more convenient to work with the precision matrix (inverse of the covariance matrix):

$$\boldsymbol{\Lambda} \equiv \boldsymbol{\Sigma}^{-1} \qquad \boldsymbol{\Lambda} = \begin{pmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{pmatrix}$$

- Note that Λ_{aa} is not given by the inverse of Σ_{aa}.

Marginal Distribution

• It turns out that the marginal distribution is also a Gaussian distribution:

$$\begin{aligned} p(\mathbf{x}_a) &= \int p(\mathbf{x}_a, \mathbf{x}_b)\, \mathrm{d}\mathbf{x}_b \\ &= \mathcal{N}(\mathbf{x}_a | \boldsymbol{\mu}_a, \boldsymbol{\Sigma}_{aa}) \end{aligned}$$

• For a marginal distribution, the mean and covariance are most simply expressed in terms of partitioned covariance matrix.

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix} \qquad \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{pmatrix}$$

Conditional Distribution

- It turns out that the conditional distribution is also a Gaussian distribution:

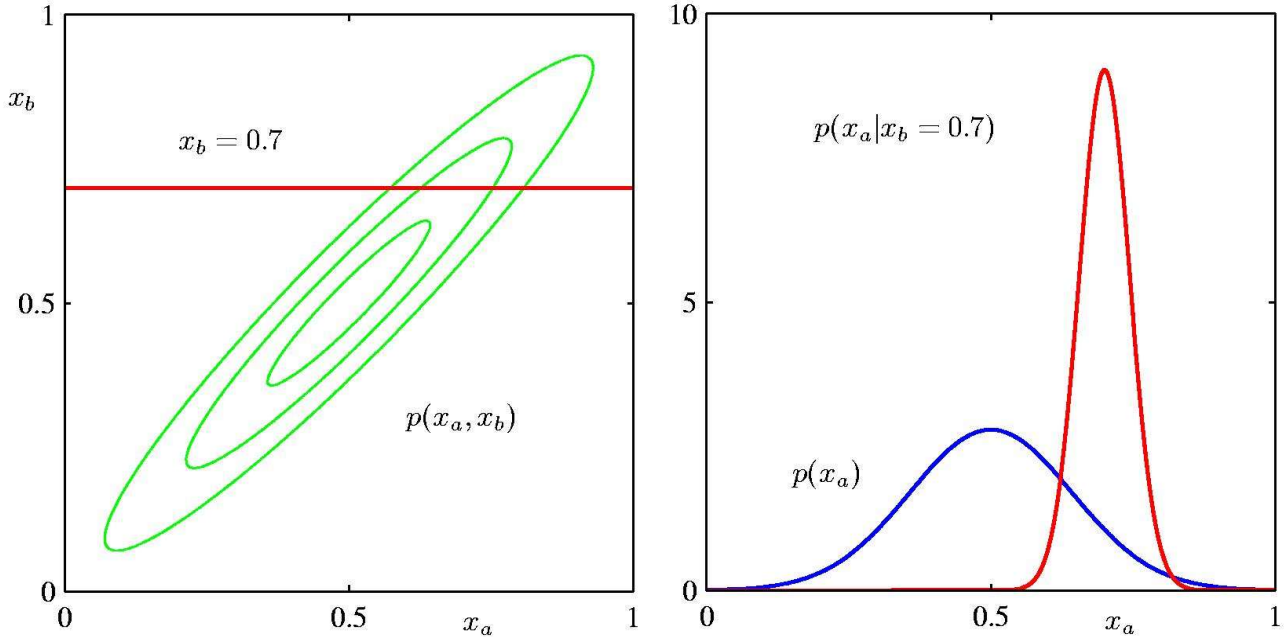
$$p(\mathbf{x}_a|\mathbf{x}_b) = \mathcal{N}(\mathbf{x}_a|\boldsymbol{\mu}_{a|b}, \boldsymbol{\Sigma}_{a|b})$$

Covariance does not depend on x_b.

$$\begin{aligned}
\boldsymbol{\Sigma}_{a|b} &= \boldsymbol{\Lambda}_{aa}^{-1} = \boldsymbol{\Sigma}_{aa} - \boldsymbol{\Sigma}_{ab}\boldsymbol{\Sigma}_{bb}^{-1}\boldsymbol{\Sigma}_{ba} \\
\boldsymbol{\mu}_{a|b} &= \boldsymbol{\Sigma}_{a|b}\{\boldsymbol{\Lambda}_{aa}\boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{ab}(\mathbf{x}_b - \boldsymbol{\mu}_b)\} \\
&= \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ab}(\mathbf{x}_b - \boldsymbol{\mu}_b) \\
&= \boldsymbol{\mu}_a + \boldsymbol{\Sigma}_{ab}\boldsymbol{\Sigma}_{bb}^{-1}(\mathbf{x}_b - \boldsymbol{\mu}_b)
\end{aligned}$$

Linear function of x_b.

Conditional and Marginal Distributions



Maximum Likelihood Estimation

• To find a maximum likelihood estimate of the mean, we set the derivative of the log-likelihood function to zero:

$$\frac{\partial}{\partial \boldsymbol{\mu}} \ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \boldsymbol{\Sigma}^{-1}(\mathbf{x}_n - \boldsymbol{\mu}) = 0$$

and solve to obtain:

$$\boldsymbol{\mu}_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n.$$

• Similarly, we can find the ML estimate of Σ :

$$\boldsymbol{\Sigma}_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})(\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})^{\mathrm{T}}.$$

Maximum Likelihood Estimation

• Evaluating the expectation of the ML estimates under the true distribution, we obtain:

Unbiased estimate

$$\mathbb{E}[\boldsymbol{\mu}_{\mathrm{ML}}] = \boldsymbol{\mu}$$

$$\mathbb{E}[\boldsymbol{\Sigma}_{\mathrm{ML}}] = \frac{N-1}{N}\boldsymbol{\Sigma}.$$

Biased estimate

• Note that the maximum likelihood estimate of § is biased.

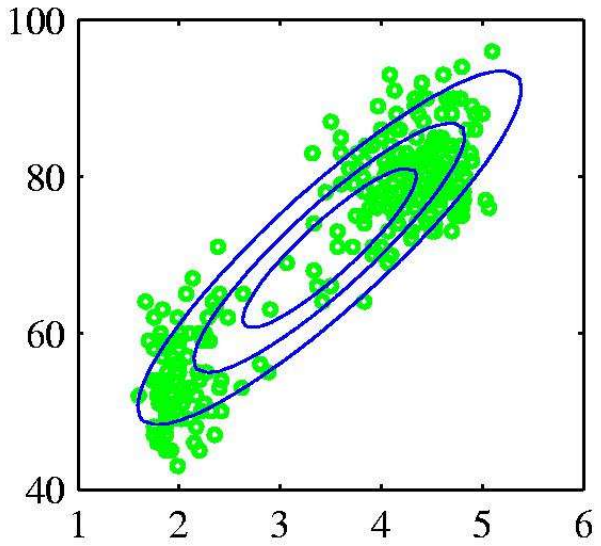
• We can correct the bias by defining a different estimator:

$$\widetilde{\boldsymbol{\Sigma}} = \frac{1}{N-1}\sum_{n=1}^{N}(\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})(\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})^{\mathrm{T}}.$$

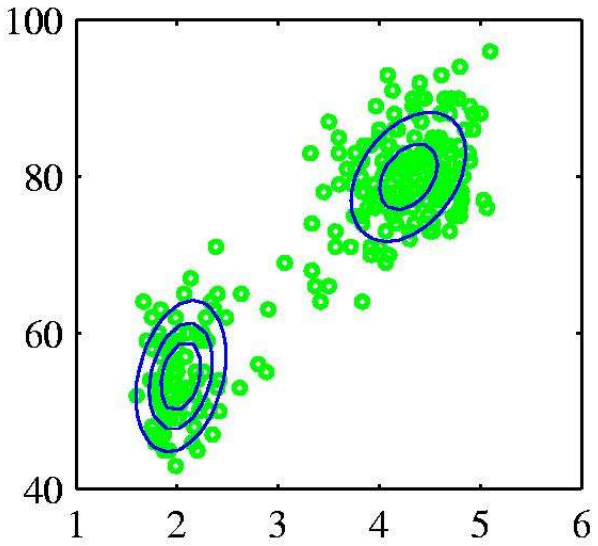
Mixture of Gaussians

- When modeling real-world data, Gaussian assumption may not be appropriate.

- Consider the following example: Old Faithful Dataset



Single Gaussian



Mixture of two Gaussians

Mixture of Gaussians

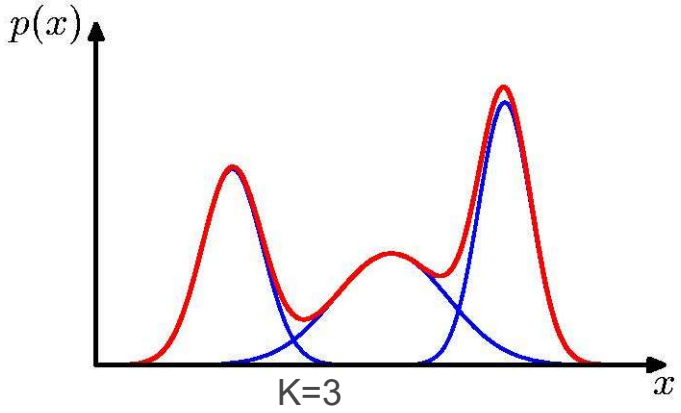
• We can combine simple models into a complex model by defining a superposition of K Gaussian densities of the form:

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Component

Mixing coefficient

$$\forall k : \pi_k \geqslant 0 \qquad \sum_{k=1}^{K} \pi_k = 1$$

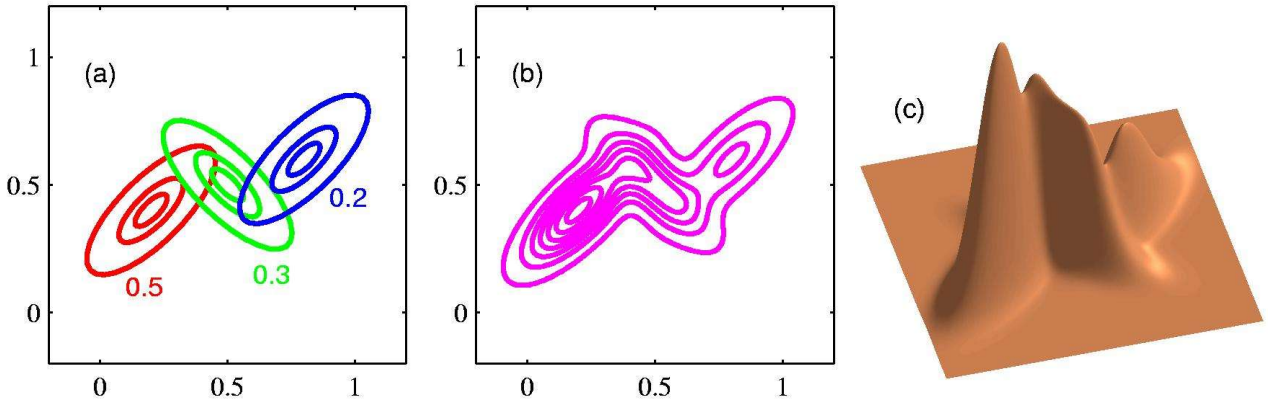


• Note that each Gaussian component has its own mean μ_k and covariance Σ_k. The parameters π_k are called mixing coefficients.

• More generally, mixture models can comprise linear combinations of other distributions.

Mixture of Gaussians

• Illustration of a mixture of 3 Gaussians in a 2-dimensional space:



(a) Contours of constant density of each of the mixture components, along with the mixing coefficients

(b) Contours of marginal probability density $p(\mathbf{x})$

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

(c) A surface plot of the distribution p(x).

Maximum Likelihood Estimation

• Given a dataset D, we can determine model parameters by maximizing the log-likelihood function:

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

Log of a sum: no closed form solution

• **Solution**: use standard, iterative, numeric optimization methods or the Expectation Maximization algorithm.

The Exponential Distribution

The family of exponential distribution provides probability models that are very widely used.

Definition

X is said to have an **exponential distribution** with parameter $\lambda > 0$ if the pdf of *X* is

$$f(x;\lambda) = \begin{cases} \lambda e^{-\lambda x} & x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

The Gamma Distribution

Definition

A continuous random variable *X* is said to have a **gamma distribution** if the pdf of *X* is

$$f(x;\alpha,\beta) = \begin{cases} \dfrac{1}{\beta^{\alpha}\Gamma(\alpha)} x^{\alpha-1} e^{-x/\beta} & x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

where the parameters α and β satisfy $\alpha > 0$, $\beta > 0$. The **standard gamma distribution** has $\beta = 1$.

We may be lazy and write Gam(x| α , β) for the above pdf instead.

Generation of Dirichlet from Gamma

- Take $Y_1 \sim \mathrm{Gam}(\mathrm{x}|\ \alpha_1\ , \beta)$, $Y_2 \sim \mathrm{Gam}(\mathrm{x}|\ \alpha_2\ , \beta)$, $\cdots\ \ Y_n \sim \mathrm{Gam}(\mathrm{x}|\ \alpha_n\ , \beta)$,
- Let $V = \sum_1^n Y_i$.
- Let

$$X_i = \frac{Y_i}{V}$$

- Then $(X_1, \cdots, X_n)$ are distributed according to Dirichlet with parameters $\alpha_1, \cdots\ \alpha_n$.

Student's t-Distribution

- Consider Student's t-Distribution

$$
\begin{aligned}
p(x|\mu,a,b) &= \int_0^\infty \mathcal{N}(x|\mu,\tau^{-1})\mathrm{Gam}(\tau|a,b)\,\mathrm{d}\tau \\
&= \int_0^\infty \mathcal{N}\left(x|\mu,(\eta\lambda)^{-1}\right)\mathrm{Gam}(\eta|\nu/2,\nu/2)\,\mathrm{d}\eta \\
&= \frac{\Gamma(\nu/2+1/2)}{\Gamma(\nu/2)}\left(\frac{\lambda}{\pi\nu}\right)^{1/2}\left[1+\frac{\lambda(x-\mu)^2}{\nu}\right]^{-\nu/2-1/2} \\
&= \mathrm{St}(x|\mu,\lambda,\nu)
\end{aligned}
$$

Infinite mixture of Gaussians

where

$$\lambda = a/b \qquad \eta = \tau b/a \qquad \nu = 2a.$$

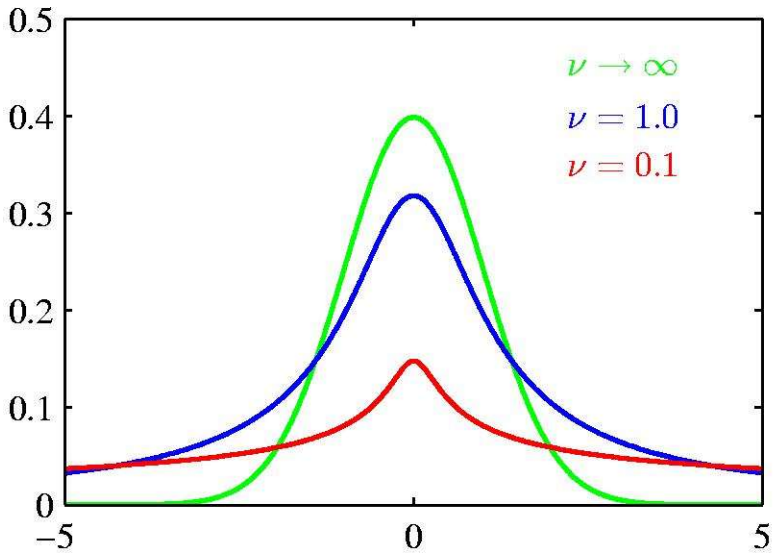
Sometimes called the precision parameter.

Degrees of freedom

Student's t-Distribution

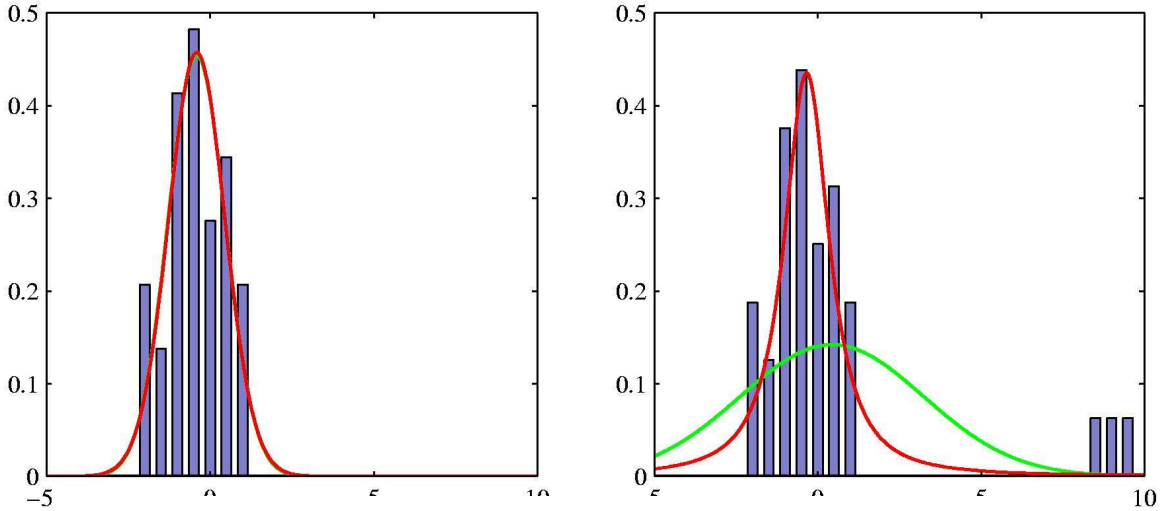
- Setting $\nu = 1$ recovers Cauchy distribution
- The limit $\nu \to \infty$ corresponds to a Gaussian distribution.

	$\nu = 1$	$\nu \to \infty$
$\mathrm{St}(x\|\mu, \lambda, \nu)$	Cauchy	$\mathcal{N}(x\|\mu, \lambda^{-1})$



Student's t-Distribution

- Robustness to outliners: Gaussian vs. t-Distribution.



Student's t-Distribution

- The multivariate extension of the t-Distribution of dimension D:

$$\begin{aligned}\mathrm{St}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Lambda},\nu) &= \int_0^\infty \mathcal{N}(\mathbf{x}|\boldsymbol{\mu},(\eta\boldsymbol{\Lambda})^{-1})\mathrm{Gam}(\eta|\nu/2,\nu/2)\,\mathrm{d}\eta \\ &= \frac{\Gamma(D/2+\nu/2)}{\Gamma(\nu/2)}\frac{|\boldsymbol{\Lambda}|^{1/2}}{(\pi\nu)^{D/2}}\left[1+\frac{\Delta^2}{\nu}\right]^{-D/2-\nu/2}\end{aligned}$$

where $\Delta^2 = (\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})$

- Properties:

$$\begin{aligned}\mathbb{E}[\mathbf{x}] &= \boldsymbol{\mu}, && \text{if } \nu > 1 \\ \mathrm{cov}[\mathbf{x}] &= \frac{\nu}{(\nu-2)}\boldsymbol{\Lambda}^{-1}, && \text{if } \nu > 2 \\ \mathrm{mode}[\mathbf{x}] &= \boldsymbol{\mu}\end{aligned}$$

The Exponential Family

• The exponential family of distributions over **x** is defined to be a set of distributions of the form:

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}$$

where

- $\boldsymbol{\eta}$ is the vector of natural parameters
- $\mathbf{u}(\mathbf{x})$ is the vector of sufficient statistics

• The function g($\boldsymbol{\eta}$) can be iinterpreted as the coefficient that ensures that the distribution p($\mathbf{x}|\boldsymbol{\eta}$) is normalized:

$$g(\boldsymbol{\eta})\int h(\mathbf{x})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}\,\mathrm{d}\mathbf{x} = 1$$

Bernoulli Distribution

- The Bernoulli distribution is a member of the exponential family:

$$\begin{aligned} p(x|\mu) &= \text{Bern}(x|\mu) = \mu^x(1-\mu)^{1-x} \\ &= \exp\{x\ln\mu + (1-x)\ln(1-\mu)\} \\ &= (1-\mu)\exp\left\{\ln\left(\frac{\mu}{1-\mu}\right)x\right\} \end{aligned}$$

- Comparing with the general form of the exponential family:

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}$$

we see that

$$\eta = \ln\left(\frac{\mu}{1-\mu}\right) \qquad \text{and so} \qquad \underbrace{\mu = \sigma(\eta) = \frac{1}{1+\exp(-\eta)}.}_{\text{Logistic sigmoid}}$$

Bernoulli Distribution

- The Bernoulli distribution is a member of the exponential family:

$$\begin{aligned} p(x|\mu) &= \text{Bern}(x|\mu) = \mu^x(1-\mu)^{1-x} \\ &= \exp\{x\ln\mu + (1-x)\ln(1-\mu)\} \\ &= (1-\mu)\exp\left\{\ln\left(\frac{\mu}{1-\mu}\right)x\right\} \end{aligned}$$

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}$$

- The Bernoulli distribution can therefore be written as:

$$p(x|\eta) = \sigma(-\eta)\exp(\eta x)$$

where

$$\begin{aligned} u(x) &= x \\ h(x) &= 1 \\ g(\eta) &= 1 - \sigma(\eta) = \sigma(-\eta). \end{aligned}$$

Multinomial Distribution

• The Multinomial distribution is a member of the exponential family:

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^{M} \mu_k^{x_k} = \exp\left\{\sum_{k=1}^{M} x_k \ln \mu_k\right\} = h(\mathbf{x}) g(\boldsymbol{\eta}) \exp\left(\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right)$$

where $\mathbf{x} = (x_1, \ldots, x_M)^{\mathrm{T}}$ $\boldsymbol{\eta} = (\eta_1, \ldots, \eta_M)^{\mathrm{T}}$

and

$$\begin{aligned} \eta_k &= \ln \mu_k \\ \mathbf{u}(\mathbf{x}) &= \mathbf{x} \\ h(\mathbf{x}) &= 1 \\ g(\boldsymbol{\eta}) &= 1. \end{aligned}$$

NOTE: The parameters μ_k are not independent since the corresponding μ_k must satisfy

$$\sum_{k=1}^{M} \mu_k = 1.$$

• In some cases it will be convenient to remove the constraint by expressing the distribution over the M-1 parameters.

Multinomial Distribution

- The Multinomial distribution is a member of the exponential family:

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^{M} \mu_k^{x_k} = \exp\left\{\sum_{k=1}^{M} x_k \ln \mu_k\right\} = h(\mathbf{x}) g(\boldsymbol{\eta}) \exp\left(\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right)$$

- Let $\mu_M = 1 - \sum_{k=1}^{M-1} \mu_k$

- This leads to:

$$\eta_k = \ln\left(\frac{\mu_k}{1 - \sum_{j=1}^{M-1} \mu_j}\right) \quad \text{and} \quad \mu_k = \underbrace{\frac{\exp(\eta_k)}{1 + \sum_{j=1}^{M-1} \exp(\eta_j)}}_{\text{Softmax function}}.$$

- Here the parameters η_k are independent.

- Note that:

$$0 \leqslant \mu_k \leqslant 1 \quad \text{and} \quad \sum_{k=1}^{M-1} \mu_k \leqslant 1.$$

Multinomial Distribution

- The Multinomial distribution is a member of the exponential family:

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^{M} \mu_k^{x_k} = \exp\left\{\sum_{k=1}^{M} x_k \ln \mu_k\right\} = h(\mathbf{x}) g(\boldsymbol{\eta}) \exp\left(\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right)$$

- The Multinomial distribution can therefore be written as:

$$p(\mathbf{x}|\boldsymbol{\mu}) = h(\mathbf{x}) g(\boldsymbol{\eta}) \exp\left(\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right)$$

where

$$\begin{aligned} \boldsymbol{\eta} &= (\eta_1, \ldots, \eta_{M-1}, 0)^{\mathrm{T}} \\ \mathbf{u}(\mathbf{x}) &= \mathbf{x} \\ h(\mathbf{x}) &= 1 \\ g(\boldsymbol{\eta}) &= \left(1 + \sum_{k=1}^{M-1} \exp(\eta_k)\right)^{-1} . \end{aligned}$$

Gaussian Distribution

- The Gaussian distribution can be written as:

$$
\begin{aligned}
p(x|\mu,\sigma^2) &= \frac{1}{(2\pi\sigma^2)^{1/2}}\exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\} \\
&= \frac{1}{(2\pi\sigma^2)^{1/2}}\exp\left\{-\frac{1}{2\sigma^2}x^2+\frac{\mu}{\sigma^2}x-\frac{1}{2\sigma^2}\mu^2\right\} \\
&= h(x)g(\boldsymbol{\eta})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(x)\right\}
\end{aligned}
$$

where

$$
\boldsymbol{\eta} = \begin{pmatrix} \mu/\sigma^2 \\ -1/2\sigma^2 \end{pmatrix} \qquad h(\mathbf{x}) = (2\pi)^{-1/2}
$$

$$
\mathbf{u}(x) = \begin{pmatrix} x \\ x^2 \end{pmatrix} \qquad g(\boldsymbol{\eta}) = (-2\eta_2)^{1/2}\exp\left(\frac{\eta_1^2}{4\eta_2}\right).
$$

ML for the Exponential Family

- Recall the Exponential Family:

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}$$

  - From the definition of the normalizer g(´):

$$g(\boldsymbol{\eta})\int h(\mathbf{x})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}\,\mathrm{d}\mathbf{x} = 1$$

  - We can take a derivative w.r.t ´:

$$\nabla g(\boldsymbol{\eta})\underbrace{\int h(\mathbf{x})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}\,\mathrm{d}\mathbf{x}}_{1/g(\boldsymbol{\eta})} + g(\boldsymbol{\eta})\underbrace{\int h(\mathbf{x})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}\mathbf{u}(\mathbf{x})\,\mathrm{d}\mathbf{x}}_{\mathbb{E}[\mathbf{u}(\mathbf{x})]} = 0$$

  - Thus

$$-\nabla \ln g(\boldsymbol{\eta}) = \mathbb{E}[\mathbf{u}(\mathbf{x})]$$

ML for the Exponential Family

- Recall the Exponential Family:

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}$$

  - We can take a derivative w.r.t ´:

$$\nabla g(\boldsymbol{\eta}) \underbrace{\int h(\mathbf{x})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}\,\mathrm{d}\mathbf{x}}_{1/g(\boldsymbol{\eta})} + g(\boldsymbol{\eta}) \underbrace{\int h(\mathbf{x})\exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}\mathbf{u}(\mathbf{x})\,\mathrm{d}\mathbf{x}}_{\mathbb{E}[\mathbf{u}(\mathbf{x})]} = 0$$

  - Thus

$$-\nabla \ln g(\boldsymbol{\eta}) = \mathbb{E}[\mathbf{u}(\mathbf{x})]$$

  - Note that the covariance of **u**(**x**) can be expressed in terms of the second derivative of g(´), and similarly for the higher moments.

ML for the Exponential Family

• Suppose we observed i.i.d da $\mathbf{X} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$.

• We can construct the log-likelihood function, which is a function of the natural parameter ´.

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta}) \exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}$$

$$p(\mathbf{X}|\boldsymbol{\eta}) = \left(\prod_{n=1}^{N} h(\mathbf{x}_n)\right) g(\boldsymbol{\eta})^N \exp\left\{\boldsymbol{\eta}^{\mathrm{T}} \sum_{n=1}^{N} \mathbf{u}(\mathbf{x}_n)\right\}.$$

• Therefore we have

$$-\nabla \ln g(\boldsymbol{\eta}_{\mathrm{ML}}) = \underbrace{\frac{1}{N} \sum_{n=1}^{N} \mathbf{u}(\mathbf{x}_n)}$$

Sufficient Statistic

Review of Multivariable Calculus

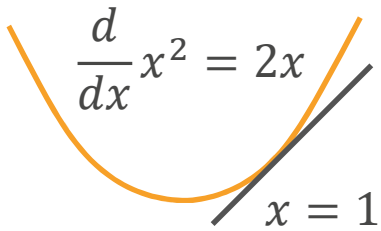
Review Scalar Derivative

y	a	x^n	$\exp(x)$	$\log(x)$	$\sin(x)$
$\frac{dy}{dx}$	0	nx^{n-1}	$\exp(x)$	$\frac{1}{x}$	$\cos(x)$

a is not a function of x

y	$u+v$	uv	$y=f(u),u=g(x)$
$\frac{dy}{dx}$	$\frac{du}{dx}+\frac{dv}{dx}$	$\frac{du}{dx}v+\frac{dv}{dx}u$	$\frac{dy}{du}\frac{du}{dx}$

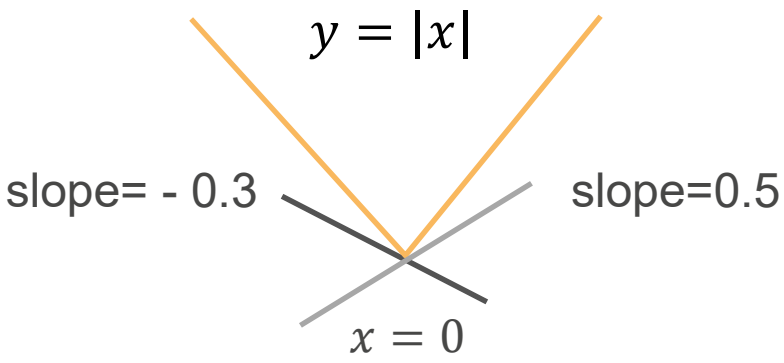
Derivative is the slope of the tangent line



The slope of the tangent line is 2

Subderivative

Extend derivative to non-differentiable cases



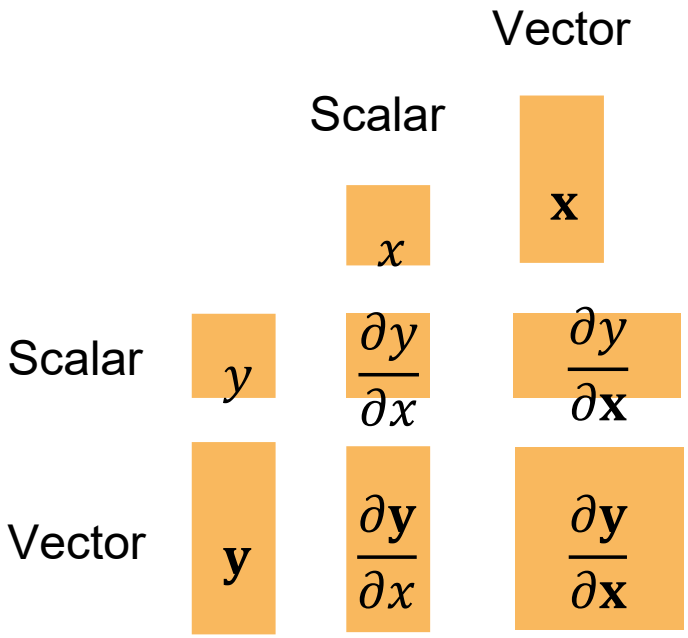
$$\frac{\partial |x|}{\partial x} = \begin{cases} 1 & if\ x > 0 \\ -1 & if\ x < 0 \\ a & if x = 0, a \in [-1,1] \end{cases}$$

Another example:

$$\frac{\partial}{\partial x} max(x, 0) = \begin{cases} 1 & if x > 0 \\ 0 & if x < 0 \\ a & if\ x = 0, a \in [0,1] \end{cases}$$

Gradients

Generalize derivatives into vectors



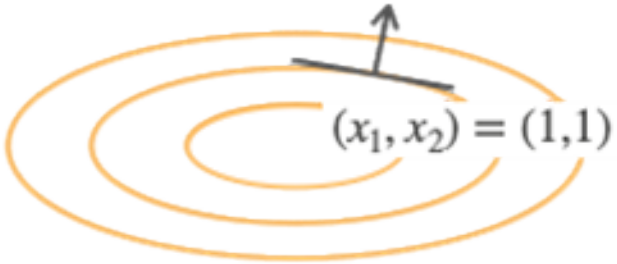
$\partial y / \partial \mathbf{x}$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \qquad \frac{\partial y}{\partial \mathbf{x}} = \left[\frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \ldots, \frac{\partial y}{\partial x_n} \right]$$

	x	$\mathbf{x}$
y	$\frac{\partial y}{\partial x}$	$\frac{\partial y}{\partial \mathbf{x}}$
$\mathbf{y}$	$\frac{\partial \mathbf{y}}{\partial x}$	$\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$

$$\frac{\partial}{\partial \mathbf{x}} x_1^2 + 2x_2^2 = [2x_1, 4x_2]$$

Direction (2, 4), perpendicular to the contour lines



Examples

y	a	au	$sum(\mathbf{x})$	$\| \mathbf{x} \|^2$
$\frac{\partial y}{\partial \mathbf{x}}$	$\mathbf{0}^T$	$a\frac{\partial u}{\partial \mathbf{x}}$	$\mathbf{1}^T$	$2\mathbf{x}^T$

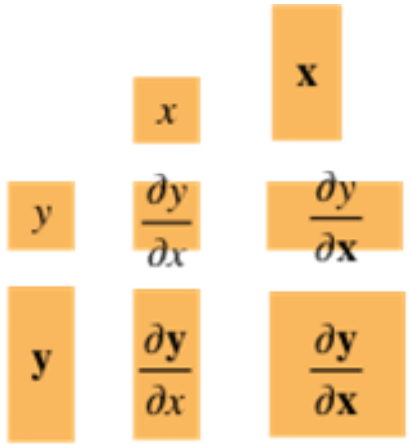
a is not a function of $\mathbf{x}$

$\mathbf{0}$ and $\mathbf{1}$ are vectors

y	$u+v$	uv	$\langle \mathbf{u}, \mathbf{v} \rangle$
$\frac{\partial y}{\partial \mathbf{x}}$	$\frac{\partial u}{\partial \mathbf{x}} + \frac{\partial v}{\partial \mathbf{x}}$	$\frac{\partial u}{\partial \mathbf{x}}v + \frac{\partial v}{\partial \mathbf{x}}u$	$\mathbf{u}^T\frac{\partial \mathbf{v}}{\partial \mathbf{x}} + \mathbf{v}^T\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$

$\partial \mathbf{y} / \partial x$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \qquad \frac{\partial \mathbf{y}}{\partial x} = \begin{bmatrix} \frac{\partial y_1}{\partial x} \\ \frac{\partial y_2}{\partial x} \\ \vdots \\ \frac{\partial y_m}{\partial x} \end{bmatrix}$$



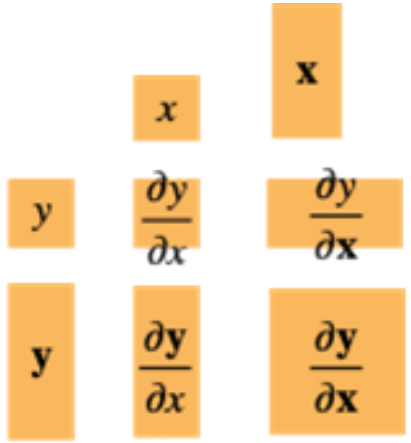
$\partial y / \partial \mathbf{x}$ is a row vector, while $\partial \mathbf{y} / \partial x$ is a column vector

It is called numerator-layout notation. The reversed version is called denominator-layout notation

$\partial \mathbf{y} / \partial \mathbf{x}$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial \mathbf{x}} \\ \frac{\partial y_2}{\partial \mathbf{x}} \\ \vdots \\ \frac{\partial y_m}{\partial \mathbf{x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1}, \frac{\partial y_1}{\partial x_2}, \ldots, \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_2}{\partial x_1}, \frac{\partial y_2}{\partial x_2}, \ldots, \frac{\partial y_2}{\partial x_n} \\ \vdots \\ \frac{\partial y_m}{\partial x_1}, \frac{\partial y_m}{\partial x_2}, \ldots, \frac{\partial y_m}{\partial x_n} \end{bmatrix}$$



Examples

$\mathbf{y}$	$\mathbf{a}$	$\mathbf{x}$	$\mathbf{Ax}$	$\mathbf{x}^T\mathbf{A}$
$\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$	$\mathbf{0}$	$\mathbf{I}$	$\mathbf{A}$	$\mathbf{A}^T$

$\mathbf{y}$	$a\mathbf{u}$	$\mathbf{Au}$	$\mathbf{u}+\mathbf{v}$
$\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\mathbf{A}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}+\frac{\partial \mathbf{v}}{\partial \mathbf{x}}$

$\mathbf{x} \in \mathbb{R}^n, \mathbf{y} \in \mathbb{R}^m, \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \in \mathbb{R}^{m \times n}$

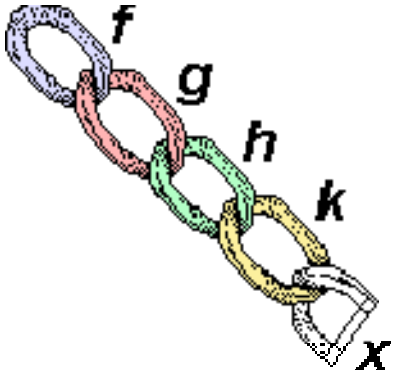
a, $\mathbf{a}$ and $\mathbf{A}$ are not functions of $\mathbf{x}$

$\mathbf{0}$ and $\mathbf{I}$ are matrices

Generalize to Matrices

	Scalar	Vector	Matrix
	x $(1,)$	$\mathbf{x}$ $(n,1)$	$\mathbf{X}$ (n,k)
Scalar	y $(1,)$	$\frac{\partial y}{\partial x}$ $(1,)$	$\frac{\partial y}{\partial \mathbf{x}}$ $(1,n)$	$\frac{\partial y}{\partial \mathbf{X}}$ (k,n)
Vector	$\mathbf{y}$ $(m,1)$	$\frac{\partial \mathbf{y}}{\partial x}$ $(m,1)$	$\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$ (m,n)	$\frac{\partial \mathbf{y}}{\partial \mathbf{X}}$ (m,k,n)
Matrix	$\mathbf{Y}$ (m,l)	$\frac{\partial \mathbf{Y}}{\partial x}$ (m,l)	$\frac{\partial \mathbf{Y}}{\partial \mathbf{x}}$ (m,l,n)	$\frac{\partial \mathbf{Y}}{\partial \mathbf{X}}$ (m,l,k,n)

Chain Rule



Generalize to Vectors

Chain rule for scalars:

$$y = f(u), u = g(x) \quad \frac{\partial y}{\partial x} = \frac{\partial y}{\partial u}\frac{\partial u}{\partial x}$$

Generalize to vectors straightforwardly

$$\frac{\partial y}{\partial \mathbf{x}} = \frac{\partial y}{\partial u}\frac{\partial u}{\partial \mathbf{x}} \qquad \frac{\partial y}{\partial \mathbf{x}} = \frac{\partial y}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{x}} \qquad \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$$

$$(1,n) \quad (1,)(1,n) \qquad (1,n) \quad (1,k)\,(k,n) \qquad (m,n)\ (m,k)(k,n)$$

Example 1

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}}$$

Assume $\mathbf{x}, \mathbf{w} \in \mathbb{R}^n, \quad y \in \mathbb{R}$

$$z = \left(\langle \mathbf{x}, \mathbf{w} \rangle - y\right)^2$$

Compute $\dfrac{\partial z}{\partial \mathbf{w}}$

$$\begin{aligned}
\frac{\partial z}{\partial \mathbf{w}} &= \frac{\partial z}{\partial b} \frac{\partial b}{\partial a} \frac{\partial a}{\partial \mathbf{w}} \\
&= \frac{\partial b^2}{\partial b} \frac{\partial a - y}{\partial a} \frac{\partial \langle \mathbf{x}, \mathbf{w} \rangle}{\partial \mathbf{w}} \\
&= 2b \cdot 1 \cdot \mathbf{x}^T \\
&= 2\left(\langle \mathbf{x}, \mathbf{w} \rangle - y\right) \mathbf{x}^T
\end{aligned}$$

Decompose

$$\begin{aligned}
a &= \langle \mathbf{x}, \mathbf{w} \rangle \\
b &= a - y \\
z &= b^2
\end{aligned}$$

Example 2

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}}$$

Assume $\mathbf{X} \in \mathbb{R}^{m \times n}, \quad \mathbf{w} \in \mathbb{R}^{n}, \quad \mathbf{y} \in \mathbb{R}^{m}$

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

Compute $\dfrac{\partial z}{\partial \mathbf{w}}$

$$\begin{aligned}
\frac{\partial z}{\partial \mathbf{w}} &= \frac{\partial z}{\partial \mathbf{b}} \frac{\partial \mathbf{b}}{\partial \mathbf{a}} \frac{\partial \mathbf{a}}{\partial \mathbf{w}} \\
&= \frac{\partial \|\mathbf{b}\|^2}{\partial \mathbf{b}} \frac{\partial \mathbf{a} - \mathbf{y}}{\partial \mathbf{a}} \frac{\partial \mathbf{X}\mathbf{w}}{\partial \mathbf{w}} \\
&= 2\mathbf{b}^T \times \mathbf{I} \times \mathbf{X} \\
&= 2\left(\mathbf{X}\mathbf{w} - \mathbf{y}\right)^T \mathbf{X}
\end{aligned}$$

Decompose

$$\begin{aligned}
\mathbf{a} &= \mathbf{X}\mathbf{w} \\
\mathbf{b} &= \mathbf{a} - \mathbf{y} \\
z &= \|\mathbf{b}\|^2
\end{aligned}$$