Probability and Distributions

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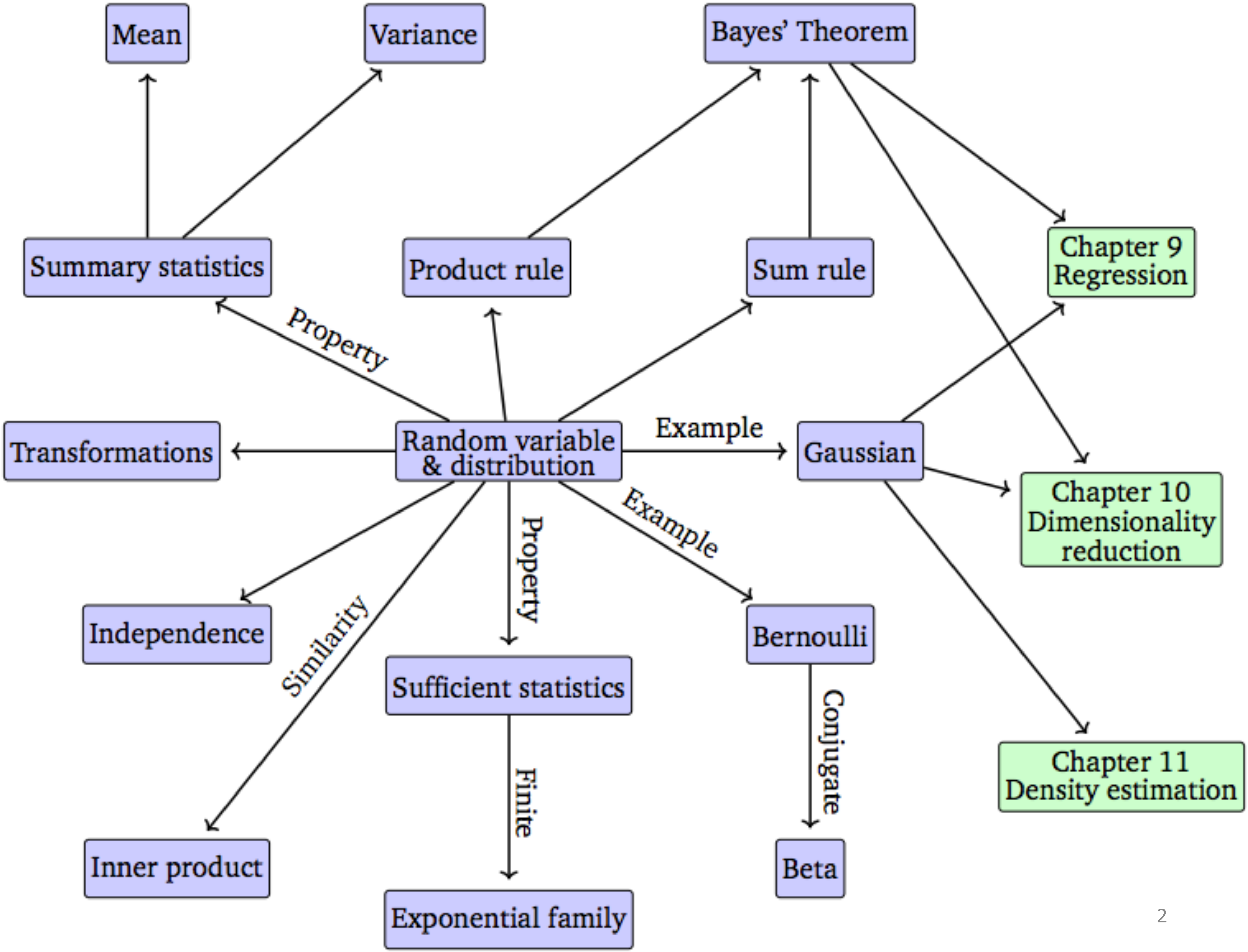
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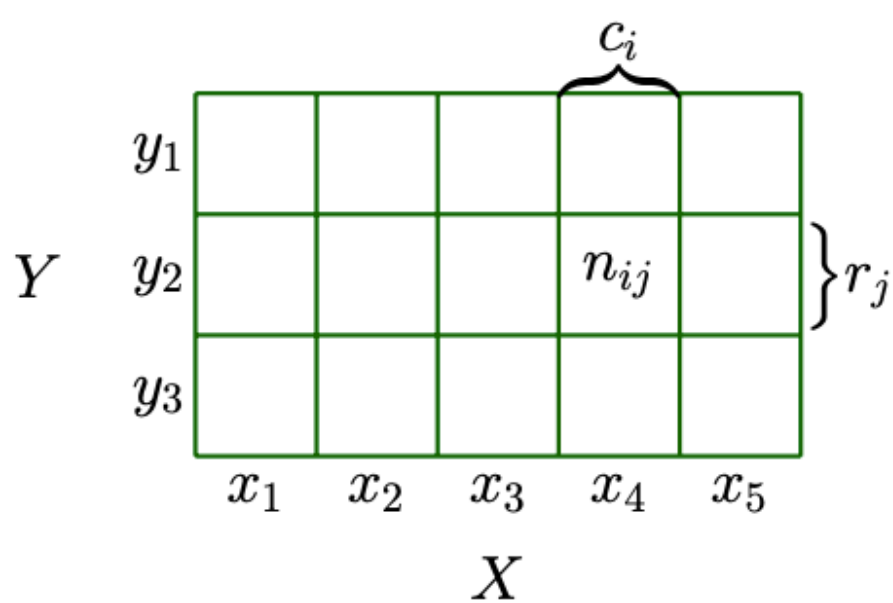
6.2.1 Discrete Probabilities

- When the target space is discrete, we can imagine the probability distribution of multiple random variables as filling out a (multidimensional) array of numbers.
- We define the joint probability as the entry of both values jointly

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

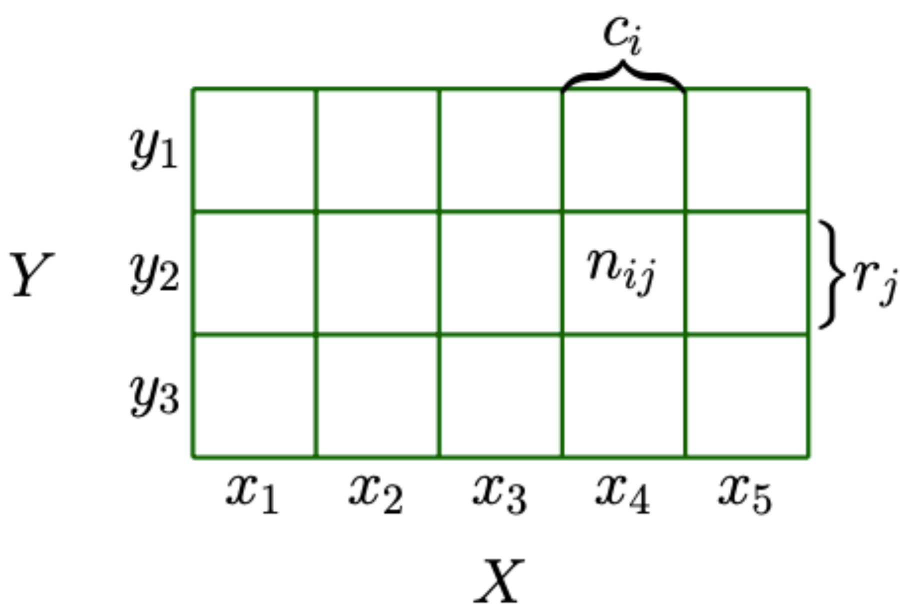
n_{ij} is the number of events with state x_i and y_j and N total number of events

- The probability that $X = x, Y = y$ is written as $p(x, y)$



6.2.1 Discrete Probabilities

- The marginal probability that $X = x$ irrespective of the value of Y is written as $p(x)$
- We write $X \sim p(x)$ to denote that the random variable X is distributed according to $p(x)$
- If we consider only the instances where $X = x$, then the fraction of instances (conditional probability) for which $Y = y$ is written as $p(y|x)$.

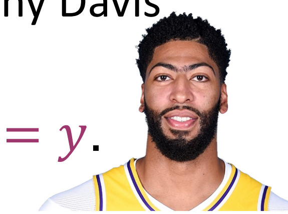


Example

Lebron James

	< 30	≥ 30
≥ 30	13	6
< 30	4	17

Anthony Davis



- X: AD scoring. Y: LBJ scoring.
- X has two possible states; Y has two possible states
- We use n_{ij} to denote the number of events with state $X = x$ and $Y = y$.
- Total number of events $N = 13 + 6 + 4 + 17 = 40$
- Value c_i is the event sum of the ith column, i.e., $c_i = \sum_{j=1}^{2} n_{ij}$
- r_j is the row sum, i.e., $r_j = \sum_{i=1}^{2} n_{ij}$
- The probability distribution of each random variable, the marginal probability, can be seen as the sum over a row or column

$$P(X = x_i) = \frac{c_i}{N} = \frac{\sum_{j=1}^{2} n_{ij}}{N}$$

and

$$P(Y = y_j) = \frac{r_j}{N} = \frac{\sum_{i=1}^{2} n_{ij}}{N}$$

$$P(LBJ\ scores\ at\ least\ 30\ pts) = \frac{13+6}{40}$$

Example

- For discrete random variables with a finite number of events, we assume that probabilities sum up to one, that is

$$\sum_{i=1}^{2} P(X = x_i) = 1 \text{ and } \sum_{j=1}^{2} P\left(Y = y_j\right) = 1$$

- The conditional probability is the fraction of a row or column in a particular cell. For example, the conditional probability of Y given X is

$$P\left(Y = y_j \mid X = x_i\right) = \frac{n_{ij}}{c_i}$$

- and the conditional probability of X given Y is

$$P\left(X = x_i \mid Y = y_j\right) = \frac{n_{ij}}{r_j}$$

Lebron James		
≥ 30	13	6
< 30	4	17
	< 30	≥ 30
	Anthony Davis	

- $P(LBJ < 30 | \, AD \geq 30) = \frac{n_{12}}{c_2} = \frac{17}{6+17}$

6.2.2 Continuous Probabilities

- A function $f\colon \mathbb{R}^D \longrightarrow \mathbb{R}$ is called a probability density function (pdf) if
$$\forall \boldsymbol{x} \in \mathbb{R}^D : f(\boldsymbol{x}) \geq 0$$
- Its integral exists and
$$\int_{\mathbb{R}^D} f(\boldsymbol{x}) d\boldsymbol{x} = 1.$$
- Observe that the probability density function is any function f that is non-negative and integrates to one. We associate a random variable X with this function f by
$$P(a \leq X \leq b) = \int_a^b f(x) dx$$

where $a, b \in \mathbb{R}$; $x \in \mathbb{R}$ are outcomes of the continuous random variable X. This association is called the distribution of the random variable X.

- Note: the probability of a continuous random variable X taking a particular value $P(X = x)$ is zero. This is to specify an interval where $a = b$

6.2.2 Continuous Probabilities

- A cumulative distribution function (cdf) of a multivariate real-valued random variable X with states $\boldsymbol{x} \in \mathbb{R}^{\mathrm{D}}$ is given by

$$F_X(\boldsymbol{x}) = P(X_1 \leq x_1, \cdots, X_D \leq x_D).$$

where $X = [X_1, \cdots, X_D]^{\mathrm{T}}, \boldsymbol{x} = [x_1, \cdots, x_D]^{\mathrm{T}}$, and the right-hand side represents the probability that random variable X_i takes the value smaller than or equal to x_i .

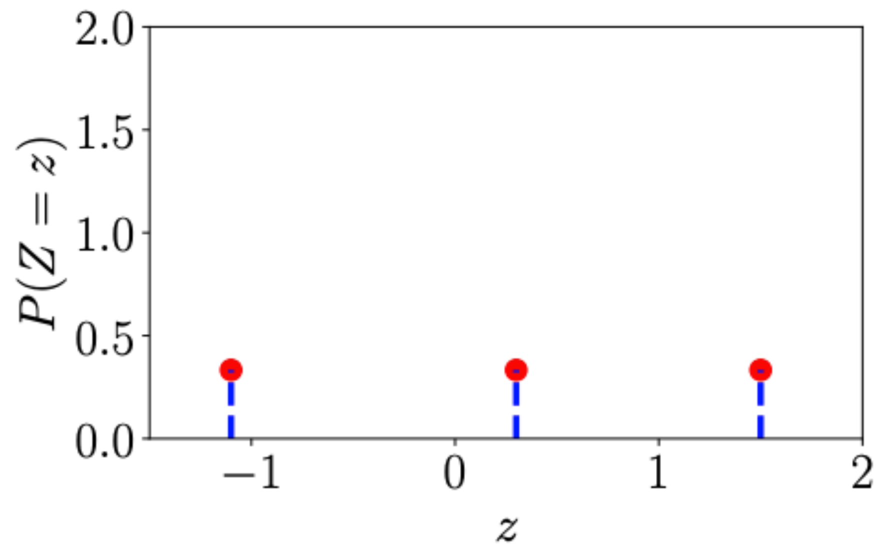
- The cdf can be expressed also as the integral of the probability density function $f(\boldsymbol{x})$ so that

$$F_X(\boldsymbol{x}) = \int_{-\infty}^{x_1} \cdots \int_{-\infty}^{x_D} f(z_1, \cdots, z_D) dz_1 \cdots dz_D$$

6.2.3 Contrasting Discrete and Continuous Distributions

- Let Z be a discrete uniform random variable with three states $\{z = -1.1, z = 0.3, z = 1.5\}$. The probability mass function can be represented as a table of probability values:

z	-1.1	0.3	1.5
$P(Z = z)$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$



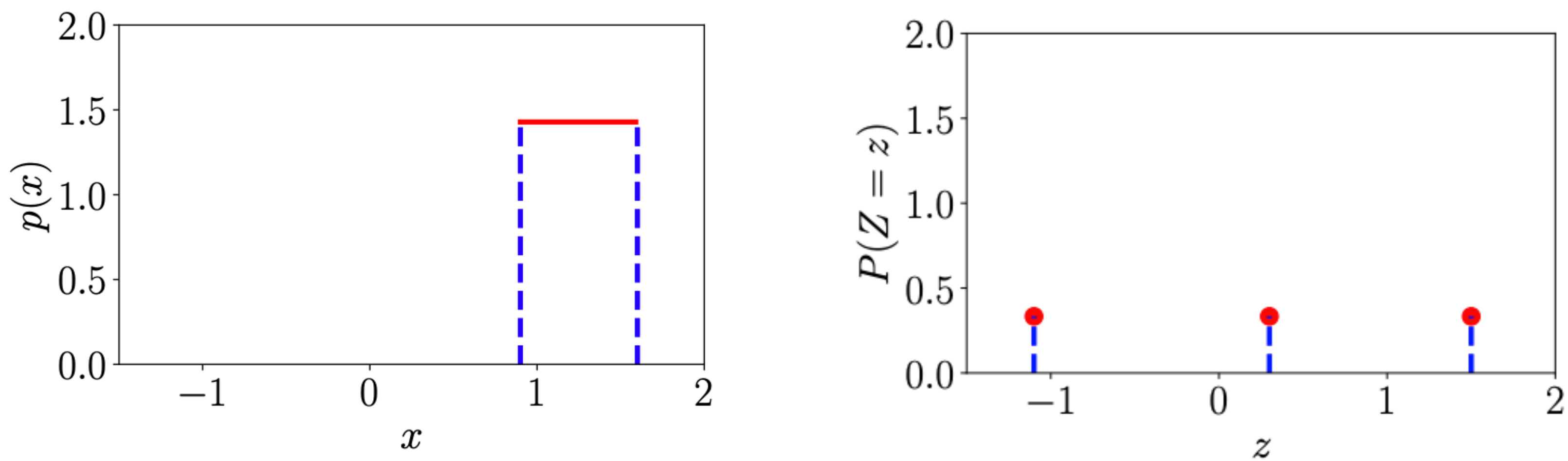
- States can be located on the x-axis, and the y-axis represents the probability of a particular state

Uniform distribution (discrete): a finite number of values are equally likely to be observed; every one of n values has equal probability $1/n$

6.2.3 Contrasting Discrete and Continuous Distributions

- Let X be a continuous random variable taking values in range $0.9 \leq X \leq 1.6$
- Observe that the height of the density can be greater than 1. However, it needs to hold that

$$\int_{0.9}^{1.6} p(x)dx = 1$$



Uniform distribution (continuous): denoted as $U(a, b)$

$$f(x) = \begin{cases} \dfrac{1}{b-a} & \text{for } a \leq x \leq b \\ 0 & \text{otherwise} \end{cases}$$

6.3 Sum Rule, Product Rule, and Bayes' Theorem

- $p(\boldsymbol{x}, \boldsymbol{y})$ is the joint distribution of the two random variables $\boldsymbol{x}, \boldsymbol{y}$
- $p(\boldsymbol{x})$ and $p(\boldsymbol{y})$ are the marginal distributions
- $p(\boldsymbol{y}|\boldsymbol{x})$ is the conditional distribution of $\boldsymbol{y}$ given $\boldsymbol{x}$
- The sum rule states that

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

where $\mathcal{Y}$ are the states of the target space of random variable Y.

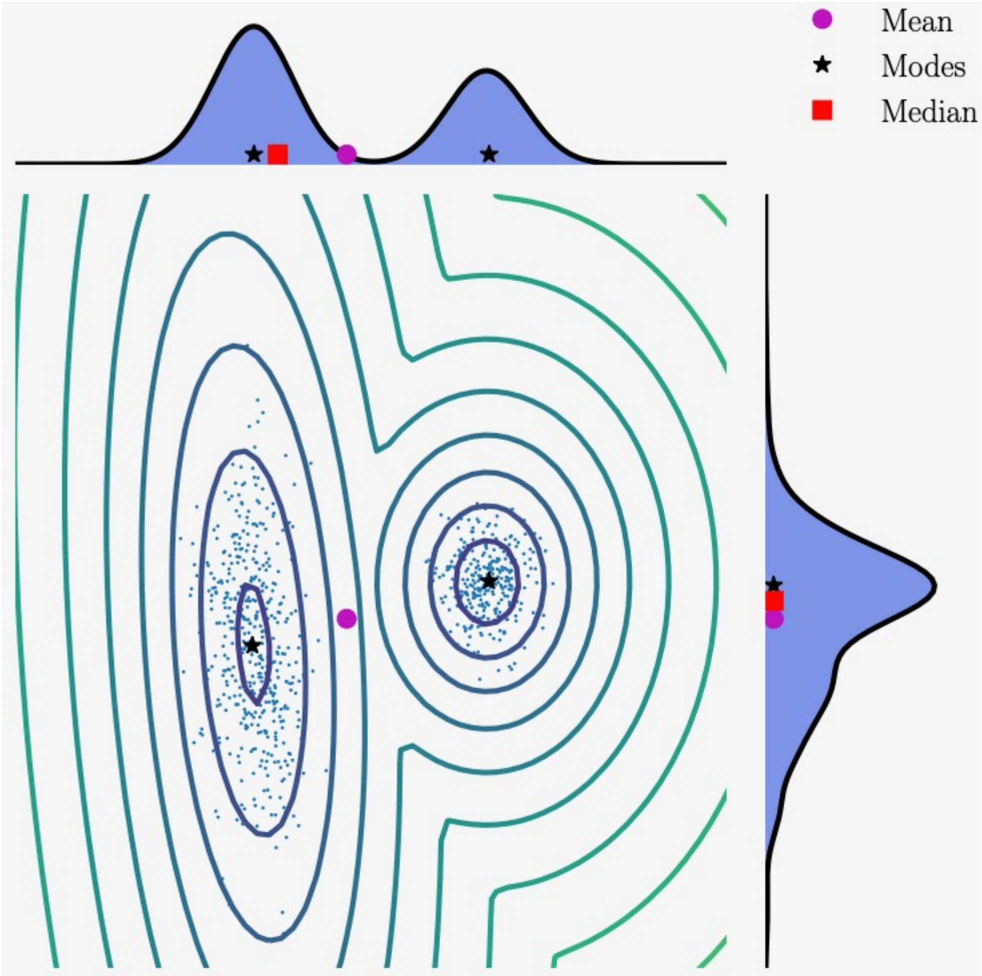
- We sum out (or integrate out) the set of states $\boldsymbol{y}$ of the random Y
- The sum rule is also known as the marginalization property.
- If $\boldsymbol{x} = [x_1, \cdots, x_D]^{\mathrm{T}}$, we obtain the marginal

$$p(x_i) = \int p(x_1, \cdots, x_D)\mathrm{d}\boldsymbol{x}_{\backslash i}$$

by repeated application of the sum rule where we integrate/sum out all random variables except x_i, which is indicated by \i, which reads all "except *i*."

$$p(x) = 0.4\mathcal{N}\left(\boldsymbol{x} \;\middle|\; \begin{bmatrix} 10 \\ 2 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right) + 0.6\mathcal{N}\left(\boldsymbol{x} \;\middle|\; \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 8.4 & 2.0 \\ 2.0 & 1.7 \end{bmatrix}\right)$$

- The distribution is bimodal (has two peaks)
- One of marginal distributions is unimodal (has one peak)



6.3 Sum Rule, Product Rule, and Bayes' Theorem

- The product rule relates the joint distribution to the conditional distribution

$$p(\boldsymbol{x}, \boldsymbol{y}) = p(\boldsymbol{y} \mid \boldsymbol{x})p(\boldsymbol{x})$$

- Every joint distribution of two random variables can be factorized (written as a product) of two other distributions

- The product rule also implies

$$p(\boldsymbol{x}, \boldsymbol{y}) = p(\boldsymbol{x} \mid \boldsymbol{y})p(\boldsymbol{y})$$

6.3 Sum Rule, Product Rule, and Bayes' Theorem

- Let us assume we have some prior knowledge $p(\boldsymbol{x})$ about an unobserved random variable $\boldsymbol{x}$ and some relationship $p(\boldsymbol{y} \mid \boldsymbol{x})$ between $\boldsymbol{x}$ and a second random variable $\boldsymbol{y}$, which we can observe. If we observe $\boldsymbol{y}$, we can use Bayes' theorem (also *Bayes' rule* or *Bayes' law*) to draw some conclusions about $\boldsymbol{x}$ given the observed values of $\boldsymbol{y}$.

$$\underbrace{p(\boldsymbol{x} \mid \boldsymbol{y})}_{\text{posterior}} = \frac{\overbrace{p(\boldsymbol{y} \mid \boldsymbol{x})}^{\text{likelihood}} \; \overbrace{p(\boldsymbol{x})}^{\text{prior}}}{\underbrace{p(\boldsymbol{y})}_{\text{evidence}}}$$

is a direct consequence of the product rule, since

$$p(\boldsymbol{x}, \boldsymbol{y}) = p(\boldsymbol{x} \mid \boldsymbol{y}) p(\boldsymbol{y})$$

and

$$p(\boldsymbol{x}, \boldsymbol{y}) = p(\boldsymbol{y} \mid \boldsymbol{x}) p(\boldsymbol{x})$$

so that

$$p(\boldsymbol{x} \mid \boldsymbol{y}) p(\boldsymbol{y}) = p(\boldsymbol{y} \mid \boldsymbol{x}) p(\boldsymbol{x}) \Leftrightarrow p(\boldsymbol{x} \mid \boldsymbol{y}) = \frac{p(\boldsymbol{y} \mid \boldsymbol{x}) p(\boldsymbol{x})}{p(\boldsymbol{y})}$$

$$p(\boldsymbol{x} \mid \boldsymbol{y}) = \frac{p(\boldsymbol{y} \mid \boldsymbol{x})p(\boldsymbol{x})}{p(\boldsymbol{y})}$$

$$p(LBJ < 30 \mid AD \geq 30) = \frac{p(AD \geq 30|LBJ < 30)p(LBJ < 30)}{p(AD \geq 30)} = \frac{\frac{17}{21} \cdot \frac{21}{40}}{\frac{23}{40}} = \frac{17}{23}$$

Lebron James	Anthony Davis < 30	Anthony Davis ≥ 30
≥ 30	13	6
< 30	4	17

6.3 Sum Rule, Product Rule, and Bayes' Theorem

Linear regression: $p(y|\boldsymbol{x}, \boldsymbol{\theta})$

$$\underbrace{p(\boldsymbol{x} \mid \boldsymbol{y})}_{\text{posterior}} = \frac{\overbrace{p(\boldsymbol{y} \mid \boldsymbol{x})}^{\text{likelihood}} \; \overbrace{p(\boldsymbol{x})}^{\text{prior}}}{\underbrace{p(\boldsymbol{y})}_{\text{evidence}}}$$

- $p(\boldsymbol{x})$ is the prior, which encapsulates our subjective prior knowledge of the unobserved (latent) variable $\boldsymbol{x}$ before observing any data
- $p(\boldsymbol{y} \mid \boldsymbol{x})$, the likelihood, describes how $\boldsymbol{x}$ and $\boldsymbol{y}$ are related
- $p(\boldsymbol{y} \mid \boldsymbol{x})$ is the probability of the data $\boldsymbol{y}$ if we were to know the latent variable $\boldsymbol{x}$
- We call $p(\boldsymbol{y} \mid \boldsymbol{x})$ either the "likelihood of $\boldsymbol{x}$ (given $\boldsymbol{y}$)" or the "probability of $\boldsymbol{y}$ given $\boldsymbol{x}$" ($\boldsymbol{y}$ is observed; $\boldsymbol{x}$ is latent)
- $p(\boldsymbol{x} \mid \boldsymbol{y})$, the posterior, is the quantity of interest in Bayesian statistics because it expresses exactly what we are interested in, i.e., what we know about $\boldsymbol{x}$ after having observed $\boldsymbol{y}$ (e.g., linear regression or Gaussian mixture models)

6.3 Sum Rule, Product Rule, and Bayes' Theorem

$$\underbrace{p(\boldsymbol{x} \mid \boldsymbol{y})}_{\text{posterior}} = \frac{\overbrace{p(\boldsymbol{y} \mid \boldsymbol{x})}^{\text{likelihood}} \; \overbrace{p(\boldsymbol{x})}^{\text{prior}}}{\underbrace{p(\boldsymbol{y})}_{\text{evidence}}}$$

- The quantity

$$p(\boldsymbol{y}) := \int p(\boldsymbol{y} \mid \boldsymbol{x}) p(\boldsymbol{x}) \, d\boldsymbol{x} = \mathbb{E}_X[p(\boldsymbol{y} \mid \boldsymbol{x})]$$

- is the *marginal likelihood/evidence*.
- The marginal likelihood integrates the numerator with respect to the latent variable $\boldsymbol{x}$

6.4 Summary Statistics and Independence
6.4.1 Means and Covariances

- The expected value of a function $g:\mathbb{R}\longrightarrow\mathbb{R}$ of a univariate continuous random variable $X \sim p(x)$ is given by

$$\mathbb{E}_X[g(x)] = \int_{\mathcal{X}} g(x)p(x)dx$$

- Correspondingly, the expected value of a function g of a discrete random variable $X \sim p(x)$ is given by

$$\mathbb{E}_X[g(x)] = \sum_{x\in\mathcal{X}} g(x)p(x)$$

where $\mathcal{X}$ is the set of possible outcomes (the target space) of the random variable X

- We consider multivariate random variables X as a finite vector of univariate random variables $[X_1,\cdots,X_n]^{\mathrm{T}}$. For multivariate random variables, we define the expected value element wise

$$\mathbb{E}_X[g(\boldsymbol{x})] = \begin{bmatrix} \mathbb{E}_{X_1}[g(x_1)] \\ \vdots \\ \mathbb{E}_{X_D}[g(x_D)] \end{bmatrix} \in \mathbb{R}^D$$

where the subscript $\mathbb{E}_{X_d}$ indicates that we are taking the expected value with respect to the dth element of the vector $\boldsymbol{x}$

6.4.1 Means and Covariances

- The mean of a random variable X with states $\boldsymbol{x} \in \mathbb{R}^D$ is an average and is defined as

$$\mathbb{E}_X[\boldsymbol{x}] = \begin{bmatrix} \mathbb{E}_{X_1}[x_1] \\ \vdots \\ \mathbb{E}_{X_D}[x_D] \end{bmatrix} \in \mathbb{R}^D$$

where

$$\mathbb{E}_{X_d}[x_d] := \begin{cases} \displaystyle\int_{\mathcal{X}} x_d p(x_d) \mathrm{d}x_d & \text{if } X \text{ is a continuous random variable} \\ \displaystyle\sum_{x_i \in \mathcal{X}} x_i p(x_d = x_i) & \text{if } X \text{ is a discrete random variable} \end{cases}$$

for $d = 1, \ldots, D$, where the subscript d indicates the corresponding dimension of $\boldsymbol{x}$. The integral and sum are over the states $\mathcal{X}$ of the target space of the random variable X.

6.4.1 Means and Covariances

- The expected value is a linear operator. For example, given a real-valued function $f(\boldsymbol{x}) = ag(\boldsymbol{x}) + bh(\boldsymbol{x})$ where $a, b \in \mathbb{R}$ and $\boldsymbol{x} \in \mathbb{R}^D$, we obtain

$$\mathbb{E}_X[f(\boldsymbol{x})] = \int f(\boldsymbol{x})p(\boldsymbol{x})\mathrm{d}\boldsymbol{x}$$

$$= \int [ag(\boldsymbol{x}) + bh(\boldsymbol{x})]p(\boldsymbol{x})\mathrm{d}\boldsymbol{x}$$

$$= a\int g(\boldsymbol{x})p(\boldsymbol{x})\mathrm{d}\boldsymbol{x} + b\int h(\boldsymbol{x})p(\boldsymbol{x})\mathrm{d}\boldsymbol{x}$$

$$= a\mathbb{E}_X[g(\boldsymbol{x})] + b\mathbb{E}_X[h(\boldsymbol{x})]$$

6.4.1 Means and Covariances

- The covariance between two univariate random variables $X, Y \in \mathbb{R}$ is given by the expected product of their deviations from their respective means, i.e.,
$$Cov_{X,Y}[x, y] \coloneqq \mathbb{E}_{X,Y}[(x - \mathbb{E}_X[x])(y - \mathbb{E}_Y[y])]$$
- By using the linearity of expectations, It can be rewritten as the expected value of the product minus the product of the expected values, i.e.,
$$Cov[x, y] = \mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y]$$
- The covariance of a variable with itself $Cov[x, x]$ is called the variance and is denoted by $\mathbb{V}_X[x]$.
- The square root of the variance is called the standard deviation and is often denoted by $\sigma(x)$.

- If we consider two multivariate random variables X and Y with states $\boldsymbol{x} \in \mathbb{R}^D$ and $\boldsymbol{y} \in \mathbb{R}^E$ respectively, the covariance between X and Y is defined as
$$\mathrm{Cov}[\boldsymbol{x}, \boldsymbol{y}] = \mathbb{E}[\boldsymbol{x}\boldsymbol{y}^\mathrm{T}] - \mathbb{E}[\boldsymbol{x}]\mathbb{E}[\boldsymbol{y}]^\mathrm{T} = Cov[\boldsymbol{y}, \boldsymbol{x}]^\mathrm{T} \in \mathbb{R}^{D \times E}$$

6.4.1 Means and Covariances

- The variance of a random variable X with states $\boldsymbol{x} \in \mathbb{R}^D$ and a mean vector $\boldsymbol{\mu} \in \mathbb{R}^D$ is defined as

$$\mathbb{V}_X[\boldsymbol{x}] = \mathrm{Cov}_X[\boldsymbol{x}, \boldsymbol{x}]$$
$$= \mathbb{E}_X[(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^{\mathrm{T}}] = \mathbb{E}_X[\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}}] - \mathbb{E}_X[\boldsymbol{x}]\mathbb{E}_X[\boldsymbol{x}]^{\mathrm{T}}$$

$$= \begin{bmatrix} Cov[x_1, x_1] & Cov[x_1, x_2] & \cdots & Cov[x_1, x_D] \\ Cov[x_2, x_1] & Cov[x_2, x_2] & \cdots & Cov[x_2, x_D] \\ \vdots & \vdots & \ddots & \vdots \\ Cov[x_D, x_1] & \cdots & \cdots & Cov[x_D, x_D] \end{bmatrix}$$

- The $D \times D$ matrix is called the covariance matrix of the multivariate random variable X. The covariance matrix is symmetric and positive definite and tells us something about the spread of the data.

- On its diagonal, the covariance matrix contains the variances of x_i

Example - Computation of covariance matrix

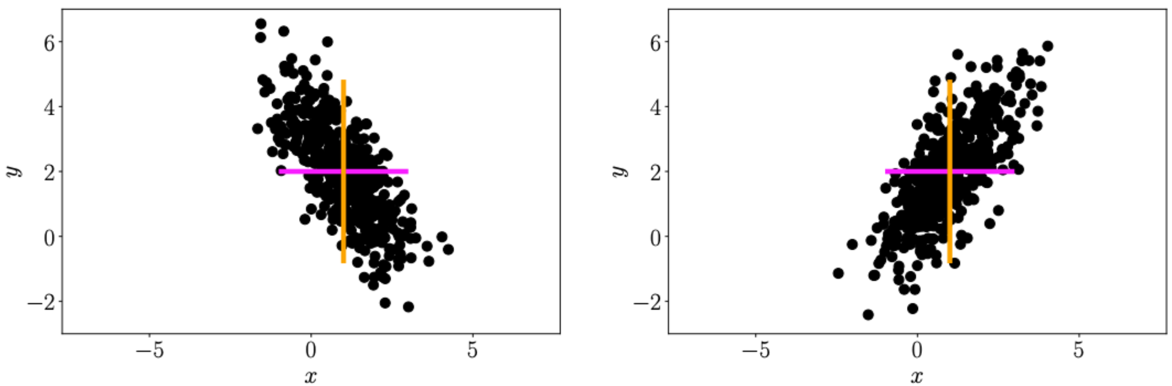
- $X = [\boldsymbol{x}_1, \boldsymbol{x}_2] = \begin{array}{cc} \begin{bmatrix} 1 & 3 \\ 2 & 1 \\ 3 & 1 \end{bmatrix} & \begin{matrix} x_1 \\ x_2 \\ x_3 \end{matrix} \end{array}$
- $\boldsymbol{\mu} = \begin{bmatrix} 2 \\ 1.5 \\ 2 \end{bmatrix}$;
- $X - \boldsymbol{\mu} = \begin{bmatrix} -1 & 1 \\ 0.5 & -0.5 \\ 1 & -1 \end{bmatrix}$
- $\sum = \frac{1}{2}(X - \boldsymbol{\mu})(X - \boldsymbol{\mu})^T = \frac{1}{2} \begin{array}{cc} \begin{matrix} x_1 & x_2 & x_3 \end{matrix} & \\ \begin{bmatrix} 2 & -1 & -2 \\ -1 & 0.5 & 1 \\ -2 & 1 & 2 \end{bmatrix} & \begin{matrix} x_1 \\ x_2 \\ x_3 \end{matrix} \end{array}$

6.4.1 Means and Covariances

- The correlation between two random variables X, Y is given by

$$\mathrm{corr}[x,y] = \frac{\mathrm{Cov}[x,y]}{\sqrt{\mathbb{V}[x]\mathbb{V}[y]}} \in [-1,1]$$

- The covariance (and correlation) indicate how two random variables are related;
- Positive correlation $\mathrm{corr}[x,y]$ means that when x grows, then y is also expected to grow. Negative correlation means that as x increases, then y decreases



(a) x and y are negatively correlated. (b) x and y are positively correlated.

Two-dimensional datasets with identical means and variances along each axis (colored lines) but with different covariances.

6.4.2 Empirical Means and Covariances

- In 6.4.1 we defined population mean and covariance, as it refers to the true statistics for the population
- In machine learning, we have a finite dataset of size N
- The empirical mean vector is the arithmetic average of the observations for each variable, and it is defined as

$$\bar{\boldsymbol{x}} := \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{x}_n$$

Where $\boldsymbol{x}_n \in \mathbb{R}^D$.

- The empirical covariance matrix is a $D \times D$ matrix

$$\sum := \frac{1}{N}\sum_{n=1}^{N} (\boldsymbol{x}_n - \bar{\boldsymbol{x}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^{\mathrm{T}}$$

- To compute the statistics for a particular dataset, we would use the observations $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ and use the two equations above.

6.4.3 Three Expressions for the Variance

- The standard definition of variance is the expectation of the squared deviation of a random variable X from its expected value μ, i.e.,
$$\mathbb{V}_X[x] := \mathbb{E}_X[(x - \mu)^2]$$
- This is equivalent to the mean of a new random variable $Z := (X - \mu)^2$.
- We use a two-pass algorithm: one pass through the data to calculate μ, and then a second pass using this estimate $\hat{\mu}$ to calculate the variance.
- It can be converted to the so-called raw-score formula for variance:
$$\mathbb{V}_X[x] = \mathbb{E}_X[x^2] - (\mathbb{E}_X[x])^2$$
- The mean of the square minus the square of the mean. It can be calculated empirically in one pass
- A third way to understand the variance is that it is a sum of pairwise differences between all pairs of observations. Consider a sample $x_1, \ldots, x_N$ of realizations of random variable X, and we compute the squared difference between pairs of x_i and x_j. By expanding the square, we can show that the sum of N^2 pairwise differences is the empirical variance of the observations:
$$\frac{1}{N^2}\sum_{i,j=1}^{N}(x_i - x_j)^2 = \cdots = 2\left[\frac{1}{N}\sum_{i=1}^{N}{x_i}^2 - \left(\frac{1}{N}\sum_{i=1}^{N}x_i\right)^2\right]$$

6.4.4 Sums and Transformations of Random Variables

- Consider two random variables X, Y with states $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^D$. Then:
- $\mathbb{E}[\boldsymbol{x}+\boldsymbol{y}] = \mathbb{E}[\boldsymbol{x}] + \mathbb{E}[\boldsymbol{y}]$
- $\mathbb{E}[\boldsymbol{x}-\boldsymbol{y}] = \mathbb{E}[\boldsymbol{x}] - \mathbb{E}[\boldsymbol{y}]$
- $\mathbb{V}[\boldsymbol{x}+\boldsymbol{y}] = \mathbb{V}[\boldsymbol{x}] + \mathbb{V}[\boldsymbol{y}] + \mathrm{Cov}[\boldsymbol{x},\boldsymbol{y}] + \mathrm{Cov}[\boldsymbol{y},\boldsymbol{x}]$
- $\mathbb{V}[\boldsymbol{x}-\boldsymbol{y}] = \mathbb{V}[\boldsymbol{x}] + \mathbb{V}[\boldsymbol{y}] - \mathrm{Cov}[\boldsymbol{x},\boldsymbol{y}] - \mathrm{Cov}[\boldsymbol{y},\boldsymbol{x}]$
- Mean and (co)variance have useful properties when it comes to affine transformation of random variables. Consider a random variable X with mean $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$ and an affine transformation $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}$ of $\boldsymbol{x}$. Then $\boldsymbol{y}$ is itself a random variable whose mean vector and covariance matrix are given by
- $\mathbb{E}_Y[\boldsymbol{y}] = \mathbb{E}_X[\boldsymbol{A}\boldsymbol{x}+\boldsymbol{b}] = \boldsymbol{A}\mathbb{E}_X[\boldsymbol{x}] + \boldsymbol{b} = \boldsymbol{A}\boldsymbol{\mu} + \boldsymbol{b}$
- $\mathbb{V}_Y[\boldsymbol{y}] = \mathbb{V}_X[\boldsymbol{A}\boldsymbol{x}+\boldsymbol{b}] = \mathbb{V}_X[\boldsymbol{A}\boldsymbol{x}] = \boldsymbol{A}\mathbb{V}_X[\boldsymbol{x}]\boldsymbol{A}^{\mathrm{T}} = \boldsymbol{A}\boldsymbol{\Sigma}\boldsymbol{A}^{\mathrm{T}}$
- Furthermore,
- $\mathrm{Cov}[\boldsymbol{x},\boldsymbol{y}] = \mathbb{E}[\boldsymbol{x}(\boldsymbol{A}\boldsymbol{x}+\boldsymbol{b})^{\mathrm{T}}] - \mathbb{E}[\boldsymbol{x}]\mathbb{E}[\boldsymbol{A}\boldsymbol{x}+\boldsymbol{b}]^{\mathrm{T}}$
- $= \mathbb{E}[\boldsymbol{x}]\boldsymbol{b}^{\mathrm{T}} + \mathbb{E}[\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}}]\boldsymbol{A}^{\mathrm{T}} - \boldsymbol{\mu}\boldsymbol{b}^{\mathrm{T}} - \boldsymbol{\mu}\boldsymbol{\mu}^{\mathrm{T}}\boldsymbol{A}^{\mathrm{T}}$
- $= \boldsymbol{\mu}\boldsymbol{b}^{\mathrm{T}} - \boldsymbol{\mu}\boldsymbol{b}^{\mathrm{T}} + \left(\mathbb{E}[\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}}] - \boldsymbol{\mu}\boldsymbol{\mu}^{\mathrm{T}}\right)\boldsymbol{A}^{\mathrm{T}}$
- $= \boldsymbol{\Sigma}\boldsymbol{A}^{\mathrm{T}}$
- where $\Sigma = \mathbb{E}[\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}}] - \boldsymbol{\mu}\boldsymbol{\mu}^{\mathrm{T}}$ is the covariance of X.

6.4.5 Statistical Independence

- Two random variables X, Y are statistically independent if and only if
$$p(\boldsymbol{x}, \boldsymbol{y}) = p(\boldsymbol{x})p(\boldsymbol{y})$$
- Intuitively, two random variables X and Y are independent if the value of $\boldsymbol{y}$ (once known) does not add any additional information about $\boldsymbol{x}$ (and vice versa). If X, Y are (statistically) independent, then
$$p(\boldsymbol{y} \mid \boldsymbol{x}) = p(\boldsymbol{y})$$
$$p(\boldsymbol{x} \mid \boldsymbol{y}) = p(\boldsymbol{x})$$
$$\mathrm{Cov}_{X,Y}[\boldsymbol{x}, \boldsymbol{y}] = \boldsymbol{0}$$
$$\mathbb{V}_{X,Y}[\boldsymbol{x} + \boldsymbol{y}] = \mathbb{V}_X[\boldsymbol{x}] + \mathbb{V}_Y[\boldsymbol{y}]$$
- The last point may not hold in converse, i.e., two random variables can have covariance zero but are not statistically independent.
- covariance measures only linear dependence. Therefore, random variables that are nonlinearly dependent could have covariance zero.
- **Example**. Consider a random variable X with zero mean ($\mathbb{E}_X[x] = 0$) and also $\mathbb{E}_X[x^3] = 0$. Let $y = x^2$ (hence, Y is dependent on X) and consider the covariance between X and Y. But this gives
$$\mathrm{Cov}[x, y] = \mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y] = \mathbb{E}[x^3] = 0$$

6.5 Gaussian Distribution

- The Gaussian distribution is the most well-studied probability distribution for continuous-valued random variables.
- It is also referred to as the normal distribution.
- For a univariate random variable, the Gaussian distribution has a density that is given by

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

- The multivariate Gaussian distribution is fully characterized by a mean vector $\boldsymbol{\mu}$ and a covariance matrix $\boldsymbol{\Sigma}$ and defined as

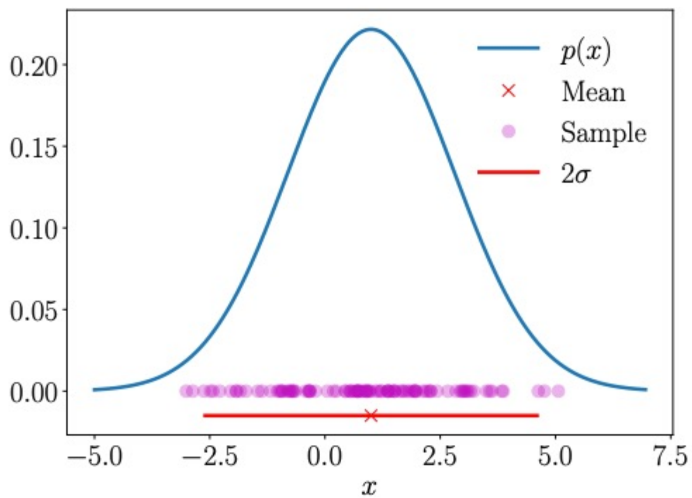
$$p(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}}|\boldsymbol{\Sigma}|^{-\frac{1}{2}}\exp(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}))$$

where $\boldsymbol{x} \in \mathbb{R}^{\mathrm{D}}$. We write $p(x) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})$ or $X \sim \mathcal{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})$.

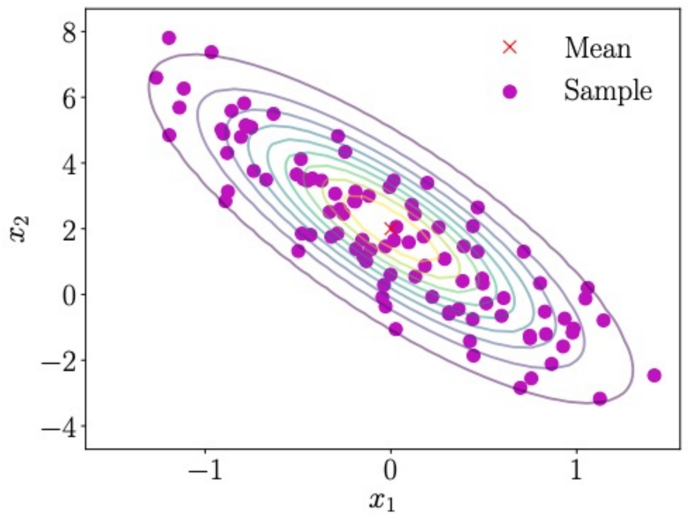
- The special case of the Gaussian with zero mean and identity covariance, that is, $\boldsymbol{\mu} = \mathbf{0}$ and $\boldsymbol{\Sigma} = \boldsymbol{I}$, is referred to as the standard normal distribution.

6.5 Gaussian Distribution

- Figure below shows a univariate Gaussian and a bivariate Gaussian with corresponding samples.



(a) Univariate (one-dimensional) Gaussian; The red cross shows the mean and the red line shows the extent of the variance.



(b) Multivariate (two-dimensional) Gaussian, viewed from top. The red cross shows the mean and the colored lines show the contour lines of the density.

Spherical Gaussian

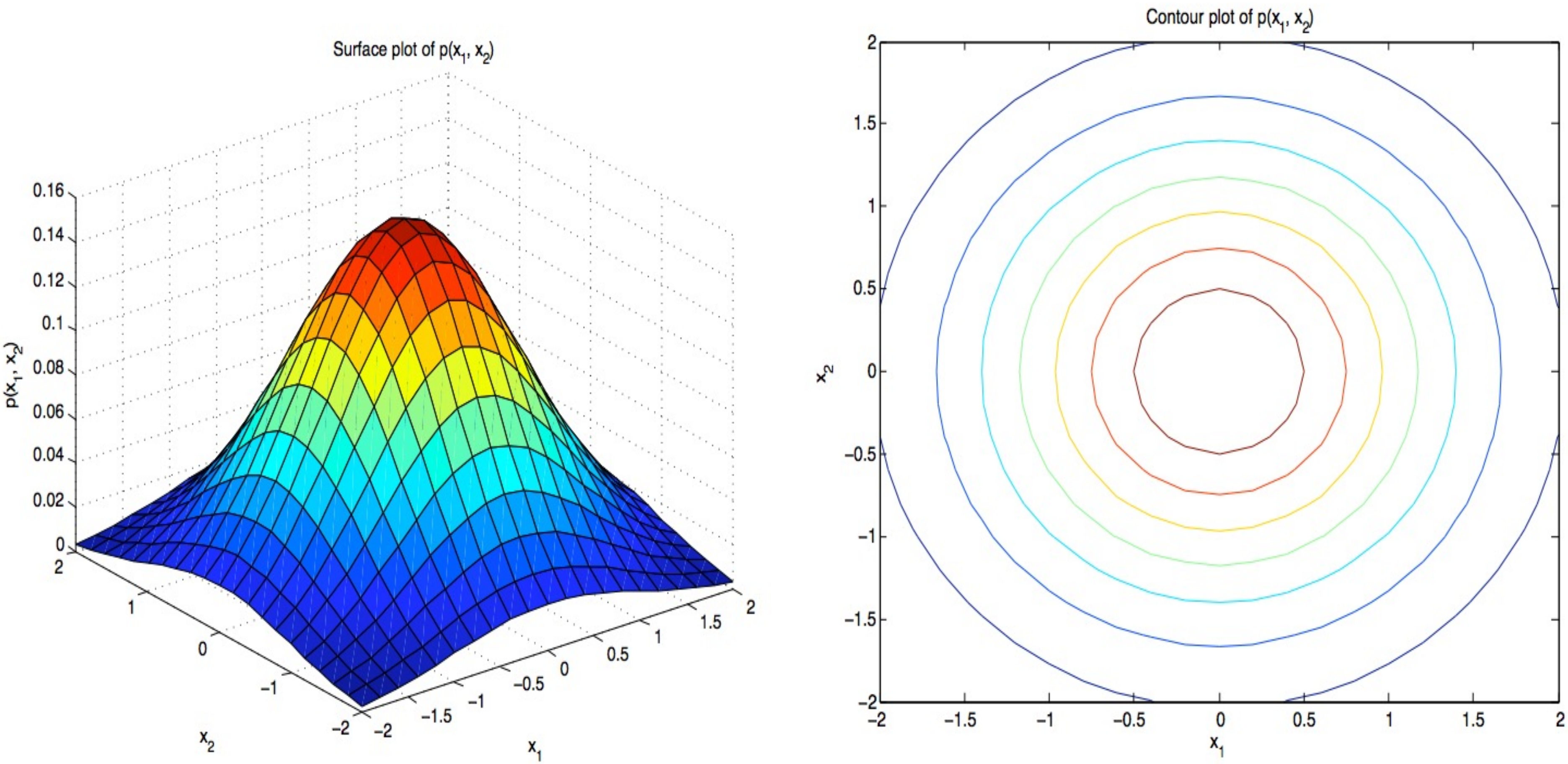
- General probability density function

$$p(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}}|\boldsymbol{\Sigma}|^{-\frac{1}{2}}\exp(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}))$$

- Spherical Gaussian
- $p(\boldsymbol{x} \mid \boldsymbol{\mu}, \sigma^2) = (2\pi\sigma^2)^{-D/2} \exp\left\{-\frac{1}{2\sigma^2}\|\boldsymbol{x}-\boldsymbol{\mu}\|^2\right\}, \qquad \boldsymbol{\mu} \in \mathbb{R}^D, \sigma \in \mathbb{R}.$

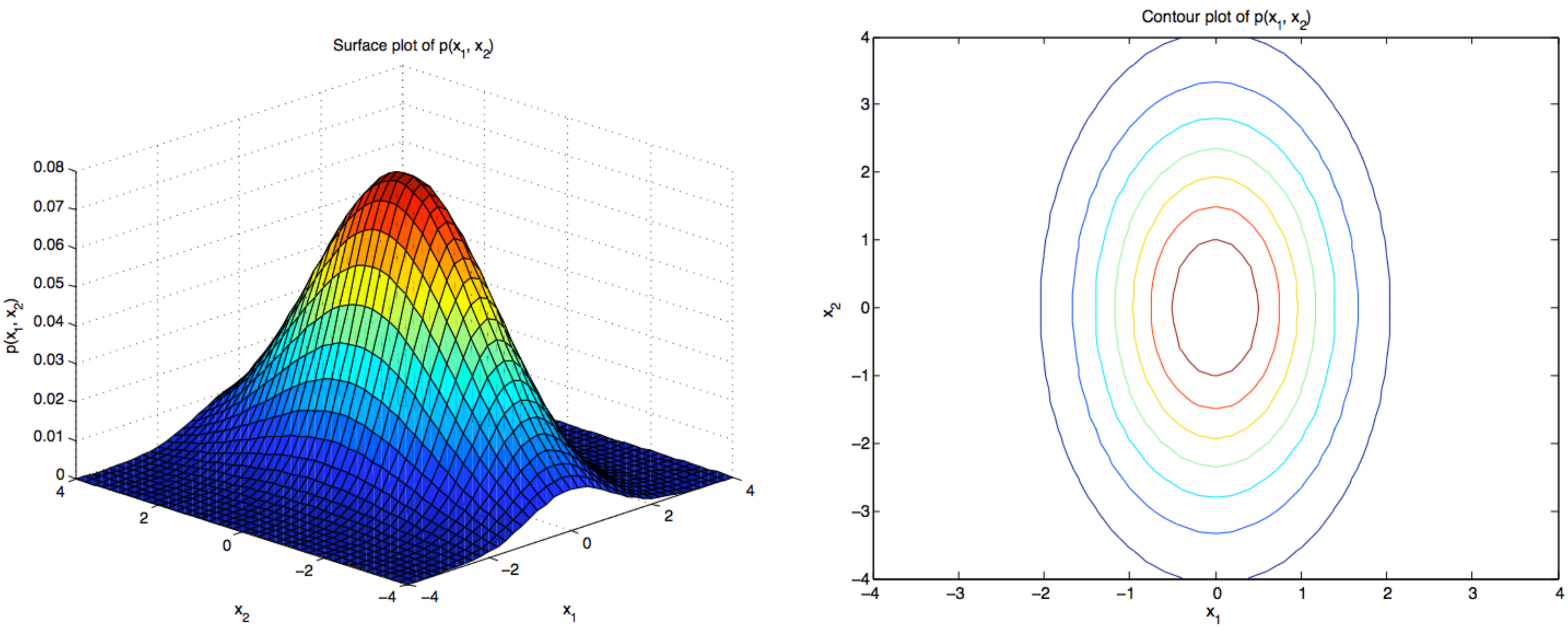
$$\sum = \begin{bmatrix} \sigma^2 & 0 & 0 \\ 0 & \sigma^2 & 0 \\ 0 & 0 & \sigma^2 \end{bmatrix}$$ diagonal covariance, equal variances

Spherical Gaussian



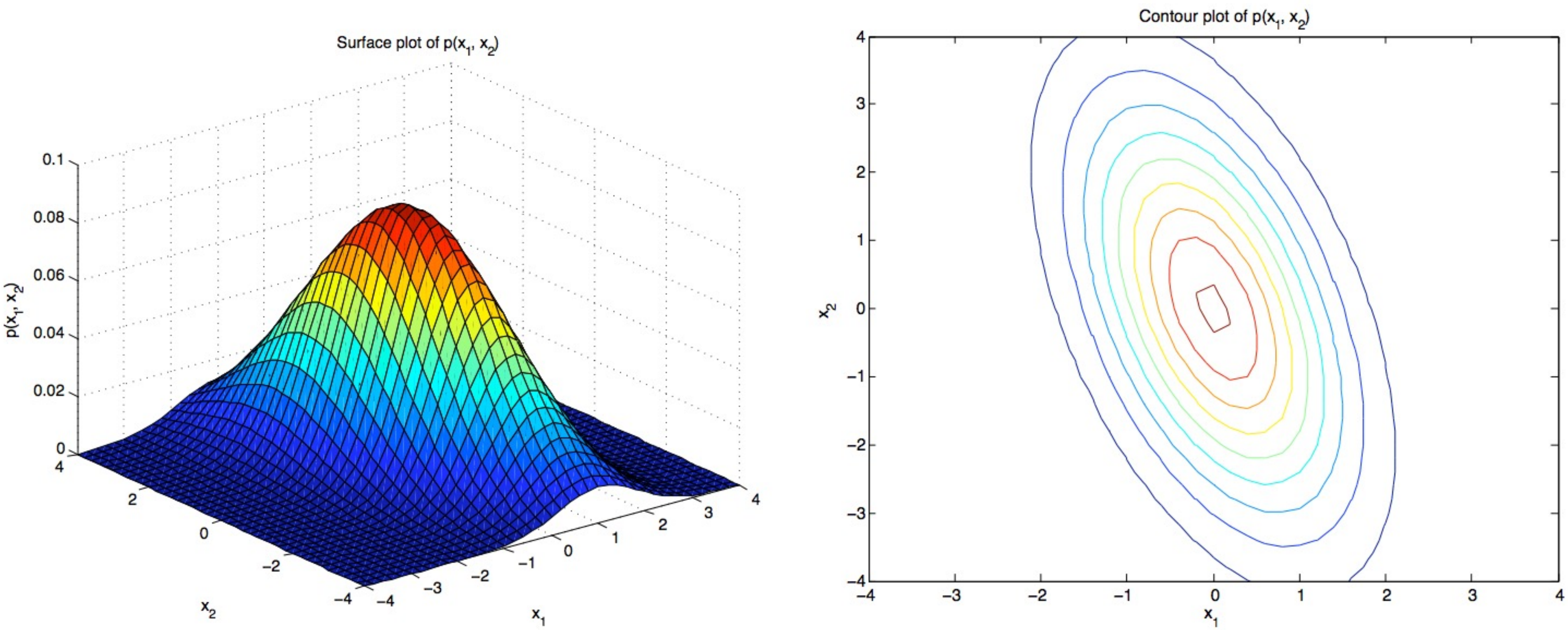
(a) Spherical Gaussian (diagonal covariance, equal variances)

Gaussian with diagonal covariance matrix (variance not equal for different x_i)



(b) Gaussian with diagonal covariance matrix

Gaussian with full covariance matrix



(c) Gaussian with full covariance matrix

6.5.1 Marginals and Conditionals of Gaussians are Gaussians

- Let X and Y be two multivariate random variables that may have different dimensions.
- We write the Gaussian distribution in terms of the concatenated states $[\boldsymbol{x};\ \boldsymbol{y}]$,

$$p(\boldsymbol{x}, \boldsymbol{y}) = \mathcal{N}\left(\begin{bmatrix}\boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y\end{bmatrix}, \begin{bmatrix}\boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy}\end{bmatrix}\right)$$

where $\boldsymbol{\Sigma}_{xx} = \mathrm{Cov}[\boldsymbol{x}, \boldsymbol{x}]$ and $\boldsymbol{\Sigma}_{yy} = \mathrm{Cov}[\boldsymbol{y}, \boldsymbol{y}]$ are the marginal covariance matrices of $\boldsymbol{x}$ and $\boldsymbol{y}$, respectively, and $\boldsymbol{\Sigma}_{xy} = \mathrm{Cov}[\boldsymbol{x}, \boldsymbol{y}]$ is the cross-covariance matrix between $\boldsymbol{x}$ and $\boldsymbol{y}$.

- The conditional distribution $p(\boldsymbol{x} \mid \boldsymbol{y})$ is also Gaussian and given by

$$p(\boldsymbol{x} \mid \boldsymbol{y}) = \mathcal{N}\left(\boldsymbol{\mu}_{x \mid y}, \boldsymbol{\Sigma}_{x \mid y}\right)$$

$$\boldsymbol{\mu}_{x \mid y} = \boldsymbol{\mu}_x + \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}(\boldsymbol{y} - \boldsymbol{\mu}_y)$$

$$\boldsymbol{\Sigma}_{x \mid y} = \boldsymbol{\Sigma}_{xx} - \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}\boldsymbol{\Sigma}_{yx}$$

- The marginal distribution $p(\boldsymbol{x})$ of a joint Gaussian distribution $p(\boldsymbol{x}, \boldsymbol{y})$ is itself Gaussian and computed by applying the sum rule and given by

$$p(\boldsymbol{x}) = \int p(\boldsymbol{x}, \boldsymbol{y})d\boldsymbol{y} = \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_x, \boldsymbol{\Sigma}_{xx})$$

- Consider the bivariate Gaussian distribution

$$p(x_1, x_2) = \mathcal{N}\left(\begin{bmatrix}0\\2\end{bmatrix}, \begin{bmatrix}0.3 & -1\\-1 & 5\end{bmatrix}\right)$$

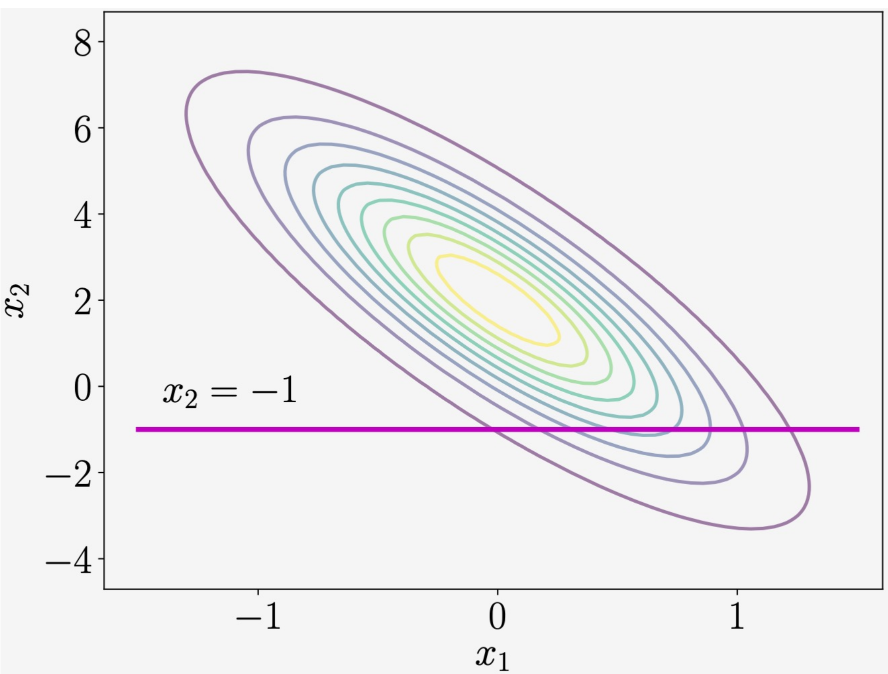
- We can compute the parameters of the univariate Gaussian, conditioned on $x_2 = -1$, to obtain the mean and variance respectively.
- Numerically, this is

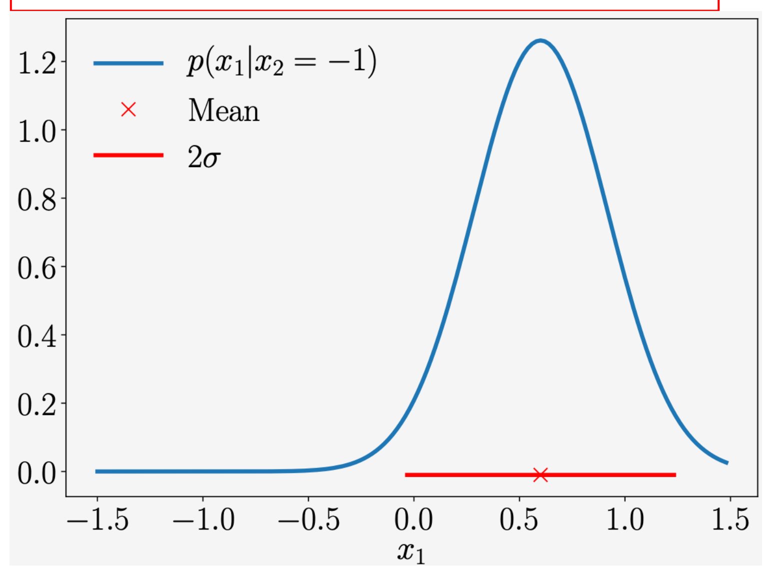
$$\mu_{x_1|x_2=-1} = 0 + (-1)(0.2)(-1-2) = 0.6$$
$${\sigma^2}_{x_1|x_2=-1} = 0.3 - (-1)(0.2)(-1) = 0.1$$

- Therefore, the conditional Gaussian is given by

$$p(x_1 | x_2 = -1) = \mathcal{N}(0.6, 0.1)$$

$$\boldsymbol{\mu}_{x|y} = \boldsymbol{\mu}_x + \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}(\boldsymbol{y} - \boldsymbol{\mu}_y)$$
$$\boldsymbol{\Sigma}_{x|y} = \boldsymbol{\Sigma}_{xx} - \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}\boldsymbol{\Sigma}_{yx}$$





- Consider the bivariate Gaussian distribution

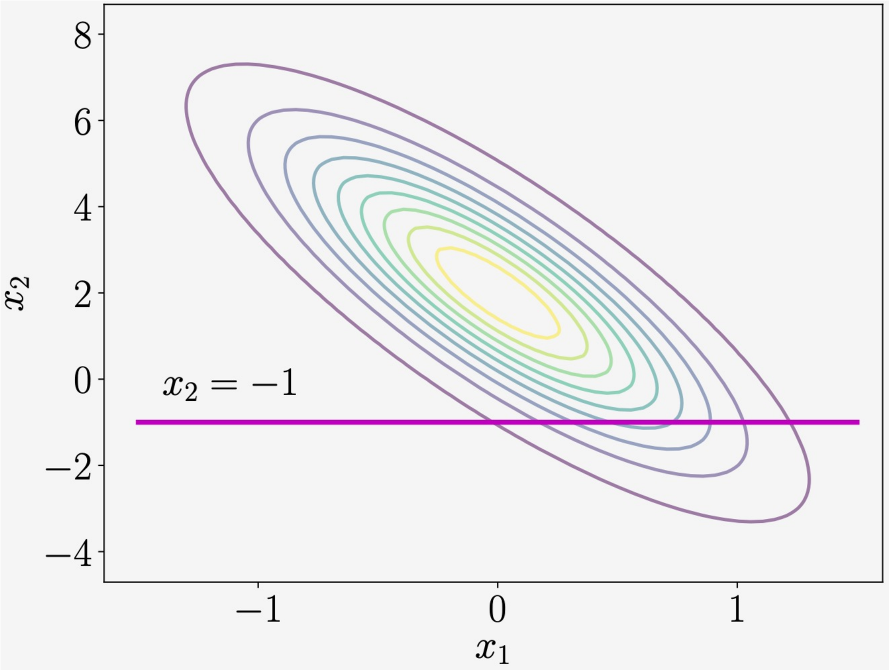
$$p(x_1, x_2) = \mathcal{N}\left(\begin{bmatrix}0\\2\end{bmatrix}, \begin{bmatrix}0.3 & -1\\-1 & 5\end{bmatrix}\right)$$

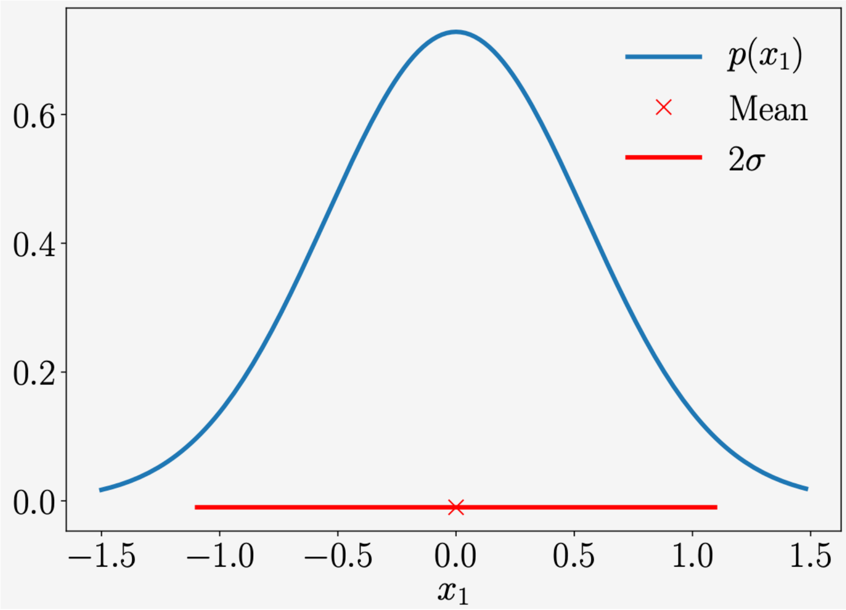
- The marginal distribution $p(x_1)$ can be obtained by

$$p(\boldsymbol{x}) = \int p(\boldsymbol{x}, \boldsymbol{y}) d\boldsymbol{y} = \mathcal{N}(\boldsymbol{x} \,|\, \boldsymbol{\mu}_x, \boldsymbol{\Sigma}_{xx})$$

which is essentially using the mean and variance of the random variable x_1. So we have,

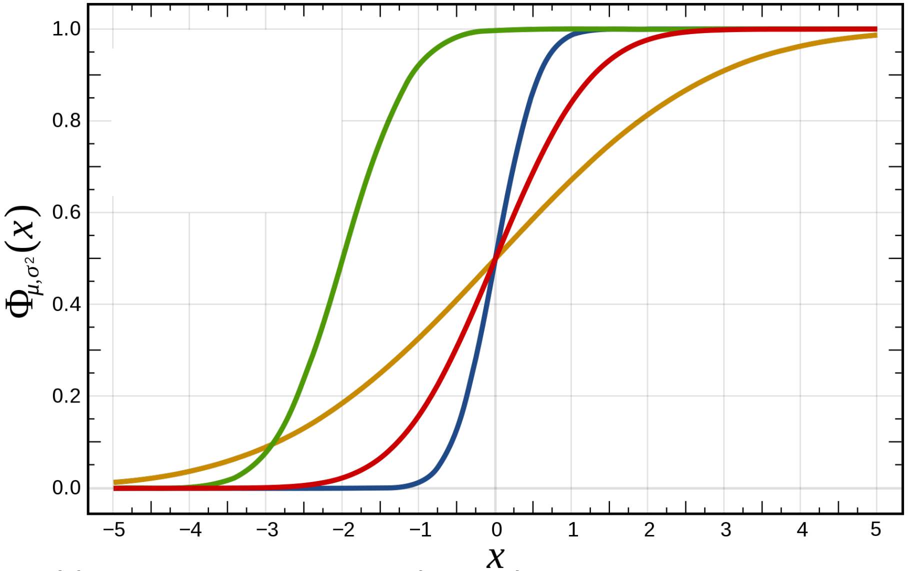
$$p(x_1) = \mathcal{N}(0, 0.3)$$





Check your understanding

- Covariance (correlation) of univariate random variables has two directions, i.e., negative and positive values have different meanings, while variance does not.
- When the covariance of two random variables equals to the sum of their individual covariances, the two variables are statistically independent.
- The empirical mean $\frac{1}{N}\sum_{n=1}^{N} \boldsymbol{x}_n$ approximates the expected value $\int_{\mathcal{X}} g(\boldsymbol{x})p(\boldsymbol{x})d\boldsymbol{x}$ of a random variable when N is large.
- In the figure (cumulative distribution function, cdf), which Gaussian has the largest variance?
    - Green? Blue? Red? Yellow?
- What is the mean of the red Gaussian?
- The cdf terminates at →1.
- The cdf starts from → 0.
- The cdf always increases.



https://en.wikipedia.org/wiki/Normal_distribution