

STAT/MTHE 353: 5 – Moment Generating Functions and Multivariate Normal Distribution

Moment Generating Function

Definition Let $\mathbf{X} = (X_1, \dots, X_n)^T$ be a random vector and $\mathbf{t} = (t_1, \dots, t_n)^T \in \mathbb{R}^n$. The *moment generating function* (MGF) is defined by

$$M_{\mathbf{X}}(\mathbf{t}) = E(e^{\mathbf{t}^T \mathbf{X}})$$

for all \mathbf{t} for which the expectation exists (i.e., finite).

Remarks:

- $M_{\mathbf{X}}(\mathbf{t}) = E(e^{\sum_{i=1}^n t_i X_i})$
- For $\mathbf{0} = (0, \dots, 0)^T$, we have $M_{\mathbf{X}}(\mathbf{0}) = 1$.
- If \mathbf{X} is a discrete random variable with finitely many values, then $M_{\mathbf{X}}(\mathbf{t}) = E(e^{\mathbf{t}^T \mathbf{X}})$ is always finite for all $\mathbf{t} \in \mathbb{R}^n$.
- We will *always* assume that the distribution of \mathbf{X} is such that $M_{\mathbf{X}}(\mathbf{t})$ is finite for all $\mathbf{t} \in (-t_0, t_0)^n$ for some $t_0 > 0$.

The single most important property of the MGF is that it uniquely determines the distribution of a random vector:

Theorem 1

Assume $M_{\mathbf{X}}(\mathbf{t})$ and $M_{\mathbf{Y}}(\mathbf{t})$ are the MGFs of the random vectors \mathbf{X} and \mathbf{Y} and such that $M_{\mathbf{X}}(\mathbf{t}) = M_{\mathbf{Y}}(\mathbf{t})$ for all $\mathbf{t} \in (-t_0, t_0)^n$. Then

$$F_{\mathbf{X}}(\mathbf{z}) = F_{\mathbf{Y}}(\mathbf{z}) \text{ for all } \mathbf{z} \in \mathbb{R}^n$$

where $F_{\mathbf{X}}$ and $F_{\mathbf{Y}}$ are the joint cdfs of \mathbf{X} and \mathbf{Y} .

Remarks:

- $F_{\mathbf{X}}(\mathbf{z}) = F_{\mathbf{Y}}(\mathbf{z})$ for all $\mathbf{z} \in \mathbb{R}^n$ clearly implies $M_{\mathbf{X}}(\mathbf{t}) = M_{\mathbf{Y}}(\mathbf{t})$. Thus $M_{\mathbf{X}}(\mathbf{t}) = M_{\mathbf{Y}}(\mathbf{t}) \iff F_{\mathbf{X}}(\mathbf{z}) = F_{\mathbf{Y}}(\mathbf{z})$
- Most often we will use the theorem for random variables instead of random vectors. In this case, $M_X(t) = M_Y(t)$ for all $t \in (-t_0, t_0)$ implies $F_X(z) = F_Y(z)$ for all $z \in \mathbb{R}$.

Connection with moments

- Let k_1, \dots, k_n be nonnegative integers and $k = k_1 + \dots + k_n$. Then

$$\begin{aligned} \frac{\partial^k}{\partial t_1^{k_1} \dots \partial t_n^{k_n}} M_{\mathbf{X}}(\mathbf{t}) &= \frac{\partial^k}{\partial t_1^{k_1} \dots \partial t_n^{k_n}} E(e^{t_1 X_1 + \dots + t_n X_n}) \\ &= E\left(\frac{\partial^k}{\partial t_1^{k_1} \dots \partial t_n^{k_n}} e^{t_1 X_1 + \dots + t_n X_n}\right) \\ &= E(X_1^{k_1} \dots X_n^{k_n} (e^{t_1 X_1 + \dots + t_n X_n})) \end{aligned}$$

Setting $\mathbf{t} = \mathbf{0} = (0, \dots, 0)^T$, we get

$$\frac{\partial^k}{\partial t_1^{k_1} \dots \partial t_n^{k_n}} M_{\mathbf{X}}(\mathbf{t}) \Big|_{\mathbf{t}=\mathbf{0}} = E(X_1^{k_1} \dots X_n^{k_n})$$

- For a (scalar) random variable X we obtain the k th moment of X :

$$\frac{d^k}{dt^k} M_X(t) \Big|_{t=0} = E(X^k)$$

Theorem 2

Assume $\mathbf{X}_1, \dots, \mathbf{X}_m$ are independent random vectors in \mathbb{R}^n and let $\mathbf{X} = \mathbf{X}_1 + \dots + \mathbf{X}_m$. Then

$$M_{\mathbf{X}}(\mathbf{t}) = \prod_{i=1}^m M_{\mathbf{X}_i}(\mathbf{t})$$

Proof:

$$\begin{aligned} M_{\mathbf{X}}(\mathbf{t}) &= E(e^{\mathbf{t}^T \mathbf{X}}) = E(e^{\mathbf{t}^T (\mathbf{X}_1 + \dots + \mathbf{X}_m)}) \\ &= E(e^{\mathbf{t}^T \mathbf{X}_1} \dots e^{\mathbf{t}^T \mathbf{X}_m}) \\ &= E(e^{\mathbf{t}^T \mathbf{X}_1}) \dots E(e^{\mathbf{t}^T \mathbf{X}_m}) \\ &= M_{\mathbf{X}_1}(\mathbf{t}) \dots M_{\mathbf{X}_m}(\mathbf{t}) \quad \square \end{aligned}$$

Note: This theorem gives us a powerful tool for determining the distribution of the sum of independent random variables.

Example: MGF for $X \sim \text{Gamma}(r, \lambda)$ and $X_1 + \dots + X_m$ where the X_i are independent and $X_i \sim \text{Gamma}(r_i, \lambda)$.

Example: MGF for $X \sim \text{Poisson}(\lambda)$ and $X_1 + \dots + X_m$ where the X_i are independent and $X_i \sim \text{Gamma}(\lambda_i)$. Also, use the MGF to find $E(X)$, $E(X^2)$, and $\text{Var}(X)$.

Theorem 3

Assume \mathbf{X} is a random vector in \mathbb{R}^n , \mathbf{A} is an $m \times n$ real matrix and $\mathbf{b} \in \mathbb{R}^m$. Then the MGF of $\mathbf{Y} = \mathbf{A}\mathbf{X} + \mathbf{b}$ is given at $\mathbf{t} \in \mathbb{R}^m$ by

$$M_{\mathbf{Y}}(\mathbf{t}) = e^{\mathbf{t}^T \mathbf{b}} M_{\mathbf{X}}(\mathbf{A}^T \mathbf{t})$$

Proof:

$$\begin{aligned} M_{\mathbf{Y}}(\mathbf{t}) &= E(e^{\mathbf{t}^T \mathbf{Y}}) = E(e^{\mathbf{t}^T (\mathbf{A}\mathbf{X} + \mathbf{b})}) \\ &= e^{\mathbf{t}^T \mathbf{b}} E(e^{\mathbf{t}^T \mathbf{A}\mathbf{X}}) = e^{\mathbf{t}^T \mathbf{b}} E(e^{(\mathbf{A}^T \mathbf{t})^T \mathbf{X}}) \\ &= e^{\mathbf{t}^T \mathbf{b}} M_{\mathbf{X}}(\mathbf{A}^T \mathbf{t}) \quad \square \end{aligned}$$

Note: In the scalar case $Y = aX + b$ we obtain

$$M_Y(t) = e^{tb} M_X(at)$$

Applications to Normal Distribution

Let $X \sim N(0, 1)$. Then

$$\begin{aligned} M_X(t) &= E(e^{tX}) = \int_{-\infty}^{\infty} e^{tx} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx \\ &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(x^2 - 2tx)} dx = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}[(x-t)^2 - t^2]} dx \\ &= e^{t^2/2} \int_{-\infty}^{\infty} \underbrace{\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(x-t)^2}}_{N(t,1) \text{ pdf}} dx \\ &= e^{t^2/2} \end{aligned}$$

We obtain that for all $t \in \mathbb{R}$

$$M_X(t) = e^{t^2/2}$$

Moments of a standard normal random variable

Recall the power series expansion $e^z = \sum_{k=0}^{\infty} \frac{z^k}{k!}$ valid for all $z \in \mathbb{R}$.
Apply this to $z = tX$

$$\begin{aligned} M_X(t) &= E(e^{tX}) = E\left(\sum_{k=0}^{\infty} \frac{(tX)^k}{k!}\right) \\ &= \sum_{k=0}^{\infty} \frac{E[(tX)^k]}{k!} = \sum_{k=0}^{\infty} \frac{E(X^k)}{k!} t^k \end{aligned}$$

and to $z = t^2/2$

$$M_X(t) = e^{t^2/2} = \sum_{i=0}^{\infty} \frac{(t^2/2)^i}{i!}$$

Matching the coefficient of t^k , for $k = 1, 2, \dots$ we obtain

$$E(X^k) = \begin{cases} \frac{k!}{2^{k/2}(k/2)!}, & k \text{ even,} \\ 0, & k \text{ odd.} \end{cases}$$

Sum of independent normal random variables

- Recall that if $X \sim N(0, 1)$ and $Y = \sigma X + \mu$, where $\sigma > 0$, then $Y \sim N(\mu, \sigma^2)$. Thus the MGF of a $N(\mu, \sigma^2)$ random variable is

$$\begin{aligned} M_Y(t) &= e^{t\mu} M_X(\sigma t) = e^{t\mu} e^{(\sigma t)^2/2} \\ &= \boxed{e^{t\mu + t^2\sigma^2/2}} \end{aligned}$$

- Let X_1, \dots, X_m be independent r.v.'s with $X_i \sim N(\mu_i, \sigma_i^2)$ and set $X = X_1 + \dots + X_m$. Then

$$M_X(t) = \prod_{i=1}^m M_{X_i}(t) = \prod_{i=1}^m e^{t\mu_i + t^2\sigma_i^2/2} = e^{t(\sum_{i=1}^m \mu_i) + (\sum_{i=1}^m \sigma_i^2)t^2/2}$$

This implies

$$X \sim N\left(\sum_{i=1}^m \mu_i, \sum_{i=1}^m \sigma_i^2\right)$$

i.e., $X_1 + \dots + X_m$ is normal with mean $\mu_X = \sum_{i=1}^m \mu_i$ and variance $\sigma_X^2 = \sum_{i=1}^m \sigma_i^2$.

Multivariate Normal Distributions

Linear Algebra Review

- Recall that an $n \times n$ real matrix C is called *nonnegative definite* if it is symmetric and

$$\mathbf{x}^T C \mathbf{x} \geq 0 \text{ for all } \mathbf{x} \in \mathbb{R}^n$$

and *positive definite* if it is symmetric and

$$\mathbf{x}^T C \mathbf{x} > 0 \text{ for all } \mathbf{x} \in \mathbb{R}^n \text{ such that } \mathbf{x} \neq \mathbf{0}$$

- Let A be an arbitrary $n \times n$ real matrix. Then $C = A^T A$ is nonnegative definite. If A is nonsingular (invertible), then C is positive definite.

Proof: $A^T A$ is symmetric since $(A^T A)^T = (A^T)(A)^T = A^T A$. Thus it is nonnegative definite since

$$\mathbf{x}^T (A^T A) \mathbf{x} = \mathbf{x}^T A^T A \mathbf{x} = (A \mathbf{x})^T (A \mathbf{x}) = \|A \mathbf{x}\|^2 \geq 0 \quad \square$$

For any nonnegative definite $n \times n$ matrix C the following hold:

- C has n *nonnegative* eigenvalues $\lambda_1, \dots, \lambda_n$ (counting multiplicities) and corresponding n *orthogonal* unit-length eigenvectors $\mathbf{b}_1, \dots, \mathbf{b}_n$:

$$C \mathbf{b}_i = \lambda_i \mathbf{b}_i, \quad i = 1, \dots, n$$

where $\mathbf{b}_i^T \mathbf{b}_i = 1$, $i = 1, \dots, n$ and $\mathbf{b}_i^T \mathbf{b}_j = 0$ if $i \neq j$.

- (Spectral decomposition) C can be written as

$$C = B D B^T$$

where $D = \text{diag}(\lambda_1, \dots, \lambda_n)$ is the diagonal matrix of the eigenvalues of C , and B is the orthogonal matrix whose i th column is \mathbf{b}_i , i.e., $B = [\mathbf{b}_1 \dots \mathbf{b}_n]$.

- C is *positive definite* $\iff C$ is *nonsingular* \iff all the eigenvalues λ_i are *positive*

- (4) C has a unique nonnegative definite square root $C^{1/2}$, i.e., there exists a unique nonnegative definite A such that

$$C = AA$$

Proof: We only prove the existence of A . Let $D^{1/2} = \text{diag}(\lambda_1^{1/2}, \dots, \lambda_n^{1/2})$ and note that $D^{1/2}D^{1/2} = D$. Let $A = BD^{1/2}B^T$. Then A is nonnegative definite and

$$\begin{aligned} A^2 &= AA = (BD^{1/2}B^T)(BD^{1/2}B^T) \\ &= BD^{1/2}B^TBD^{1/2}B^T = BD^{1/2}D^{1/2}B^T \\ &= C \quad \square \end{aligned}$$

Remarks:

- If C is positive definite, then so is A .
- If we don't require that A be nonnegative definite, then in general there are infinitely many solutions A for $AA^T = C$.

Lemma 4

If Σ is the covariance matrix of some random vector

$\mathbf{X} = (X_1, \dots, X_n)^T$, then it is nonnegative definite.

Proof: We know that $\Sigma = \text{Cov}(\mathbf{X})$ is symmetric. Let $\mathbf{b} \in \mathbb{R}^n$ be arbitrary. Then

$$\mathbf{b}^T \Sigma \mathbf{b} = \mathbf{b}^T \text{Cov}(\mathbf{X}) \mathbf{b} = \text{Cov}(\mathbf{b}^T \mathbf{X}) = \text{Var}(\mathbf{b}^T \mathbf{X}) \geq 0$$

so Σ is nonnegative definite

Remark: It can be shown that an $n \times n$ matrix Σ is nonnegative definite if and only if there exists a random vector $\mathbf{X} = (X_1, \dots, X_n)^T$ such that $\text{Cov}(\mathbf{X}) = \Sigma$.

Defining the Multivariate Normal Distribution

Let Z_1, \dots, Z_n be independent r.v.'s with $Z_i \sim N(0, 1)$. The multivariate MGF of $\mathbf{Z} = (Z_1, \dots, Z_n)^T$ is

$$\begin{aligned} M_{\mathbf{Z}}(\mathbf{t}) &= E(e^{\mathbf{t}^T \mathbf{Z}}) = E(e^{\sum_{i=1}^n t_i Z_i}) = \prod_{i=1}^n E(e^{t_i Z_i}) \\ &= \prod_{i=1}^n e^{t_i^2/2} = e^{\sum_{i=1}^n t_i^2/2} = \boxed{e^{\frac{1}{2} \mathbf{t}^T \mathbf{t}}} \end{aligned}$$

Now let $\boldsymbol{\mu} \in \mathbb{R}^n$ and \mathbf{A} an $n \times n$ real matrix. Then the MGF of $\mathbf{X} = \mathbf{AZ} + \boldsymbol{\mu}$ is

$$\begin{aligned} M_{\mathbf{X}}(\mathbf{t}) &= e^{\mathbf{t}^T \boldsymbol{\mu}} M_{\mathbf{Z}}(\mathbf{A}^T \mathbf{t}) = e^{\mathbf{t}^T \boldsymbol{\mu}} e^{\frac{1}{2} (\mathbf{A}^T \mathbf{t})^T (\mathbf{A}^T \mathbf{t})} \\ &= e^{\mathbf{t}^T \boldsymbol{\mu}} e^{\frac{1}{2} \mathbf{t}^T \mathbf{A} \mathbf{A}^T \mathbf{t}} = \boxed{e^{\mathbf{t}^T \boldsymbol{\mu} + \frac{1}{2} \mathbf{t}^T \Sigma \mathbf{t}}} \end{aligned}$$

where $\Sigma = \mathbf{A} \mathbf{A}^T$. Note that Σ is nonnegative definite.

Definition Let $\boldsymbol{\mu} \in \mathbb{R}^n$ and let Σ be an $n \times n$ nonnegative definite matrix. A random vector $\mathbf{X} = (X_1, \dots, X_n)$ is said to have a *multivariate normal* distribution with parameters $\boldsymbol{\mu}$ and Σ if its multivariate MGF is

$$M_{\mathbf{X}}(\mathbf{t}) = e^{\mathbf{t}^T \boldsymbol{\mu} + \frac{1}{2} \mathbf{t}^T \Sigma \mathbf{t}}$$

Notation: $\mathbf{X} \sim N(\boldsymbol{\mu}, \Sigma)$.

Remarks:

- If $\mathbf{Z} = (Z_1, \dots, Z_n)^T$ with $Z_i \sim N(0, 1)$, $i = 1, \dots, n$, then $\mathbf{Z} \sim N(\mathbf{0}, \mathbf{I})$, where \mathbf{I} is the $n \times n$ identity matrix.
- We saw that if $\mathbf{Z} \sim N(\mathbf{0}, \mathbf{I})$, then $\mathbf{X} = \mathbf{AZ} + \boldsymbol{\mu} \sim N(\boldsymbol{\mu}, \Sigma)$, where $\Sigma = \mathbf{A} \mathbf{A}^T$. One can show the following:

$\mathbf{X} \sim N(\boldsymbol{\mu}, \Sigma)$ if and only if $\mathbf{X} = \mathbf{AZ} + \boldsymbol{\mu}$ for a random n -vector $\mathbf{Z} \sim N(\mathbf{0}, \mathbf{I})$ and some $n \times n$ matrix \mathbf{A} with $\Sigma = \mathbf{A} \mathbf{A}^T$.

Mean and covariance for multivariate normal distribution

Consider first $\mathbf{Z} \sim N(\mathbf{0}, \mathbf{I})$, i.e., $\mathbf{Z} = (Z_1, \dots, Z_n)^T$, where the Z_i are independent $N(0, 1)$ random variables. Then

$$E(\mathbf{Z}) = (E(Z_1), \dots, E(Z_n))^T = (0, \dots, 0)^T$$

and

$$E((Z_i - E(Z_i))(Z_j - E(Z_j))) = E(Z_i Z_j) = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j \end{cases}$$

Thus

$$E(\mathbf{Z}) = \mathbf{0}, \quad \text{Cov}(\mathbf{Z}) = \mathbf{I}$$

If $\mathbf{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, then $\mathbf{X} = \mathbf{AZ} + \boldsymbol{\mu}$ for a random n -vector $\mathbf{Z} \sim N(\mathbf{0}, \mathbf{I})$ and some $n \times n$ matrix \mathbf{A} with $\boldsymbol{\Sigma} = \mathbf{AA}^T$.

We have

$$E(\mathbf{AZ} + \boldsymbol{\mu}) = \mathbf{A}E(\mathbf{Z}) + \boldsymbol{\mu} = \boldsymbol{\mu}$$

Also,

$$\text{Cov}(\mathbf{AZ} + \boldsymbol{\mu}) = \text{Cov}(\mathbf{AZ}) = \mathbf{A} \text{Cov}(\mathbf{Z}) \mathbf{A}^T = \mathbf{AA}^T = \boldsymbol{\Sigma}$$

Thus

$$E(\mathbf{X}) = \boldsymbol{\mu}, \quad \text{Cov}(\mathbf{X}) = \boldsymbol{\Sigma}$$

Joint pdf for multivariate normal distribution

Lemma 5

If a random vector $\mathbf{X} = (X_1, \dots, X_n)^T$ has covariance matrix $\boldsymbol{\Sigma}$ that is not of full rank (i.e., singular), then \mathbf{X} does not have a joint pdf.

Proof sketch: If $\boldsymbol{\Sigma}$ is singular, then there exists $\mathbf{b} \in \mathbb{R}^n$ such that $\mathbf{b} \neq \mathbf{0}$ and $\boldsymbol{\Sigma}\mathbf{b} = \mathbf{0}$. Consider the random variable $\mathbf{b}^T \mathbf{X} = \sum_{i=1}^n b_i X_i$:

$$\text{Var}(\mathbf{b}^T \mathbf{X}) = \text{Cov}(\mathbf{b}^T \mathbf{X}) = \mathbf{b}^T \text{Cov}(\mathbf{X}) \mathbf{b} = \mathbf{b}^T \boldsymbol{\Sigma} \mathbf{b} = 0$$

Therefore $P(\mathbf{b}^T \mathbf{X} = c) = 1$ for some constant c . If \mathbf{X} had a joint pdf $f(\mathbf{x})$, then for $B = \{\mathbf{x} : \mathbf{b}^T \mathbf{x} = c\}$ we should have

$$1 = P(\mathbf{b}^T \mathbf{X} = c) = P(\mathbf{X} \in B) = \int \cdots \int_B f(x_1, \dots, x_n) dx_1 \cdots dx_n$$

But this is impossible since B is an $(n - 1)$ -dimensional hyperplane whose n -dimensional volume is zero, so the integral must be zero. \square

Theorem 6

If $\mathbf{X} = (X_1, \dots, X_n)^T \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, where $\boldsymbol{\Sigma}$ is nonsingular, then it has a joint pdf given by

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^n \det \boldsymbol{\Sigma}}} e^{-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})}, \quad \mathbf{x} \in \mathbb{R}^n$$

Proof: We know that $\mathbf{X} = \mathbf{AZ} + \boldsymbol{\mu}$ where $\mathbf{Z} = (Z_1, \dots, Z_n)^T \sim N(\mathbf{0}, \mathbf{I})$ and \mathbf{A} is an $n \times n$ matrix such that $\mathbf{AA}^T = \boldsymbol{\Sigma}$. Since $\boldsymbol{\Sigma}$ is nonsingular, \mathbf{A} must be nonsingular with inverse \mathbf{A}^{-1} . Thus the mapping

$$h(\mathbf{z}) = \mathbf{Az} + \boldsymbol{\mu}$$

is invertible with inverse $g(\mathbf{x}) = \mathbf{A}^{-1}(\mathbf{x} - \boldsymbol{\mu})$ whose Jacobian is

$$J_g(\mathbf{x}) = \det \mathbf{A}^{-1}$$

By the multivariate transformation theorem

$$f_{\mathbf{X}}(\mathbf{x}) = f_{\mathbf{Z}}(g(\mathbf{x})) |J_g(\mathbf{x})| = f_{\mathbf{Z}}(\mathbf{A}^{-1}(\mathbf{x} - \boldsymbol{\mu})) |\det \mathbf{A}^{-1}|$$

Proof cont'd: Since $\mathbf{Z} = (Z_1, \dots, Z_n)^T$, where the Z_i are independent $N(0, 1)$ random variables, we have

$$f_{\mathbf{Z}}(\mathbf{z}) = \prod_{i=1}^n \left(\frac{1}{\sqrt{2\pi}} \right) e^{-z_i^2/2} = \frac{1}{\sqrt{(2\pi)^n}} e^{-\frac{1}{2} \sum_{i=1}^n z_i^2} = \boxed{\frac{1}{\sqrt{(2\pi)^n}} e^{-\frac{1}{2} \mathbf{z}^T \mathbf{z}}}$$

so we get

$$\begin{aligned} f_{\mathbf{X}}(\mathbf{x}) &= f_{\mathbf{Z}}(\mathbf{A}^{-1}(\mathbf{x} - \boldsymbol{\mu})) |\det \mathbf{A}^{-1}| \\ &= \frac{1}{\sqrt{(2\pi)^n}} e^{-\frac{1}{2} (\mathbf{A}^{-1}(\mathbf{x} - \boldsymbol{\mu}))^T (\mathbf{A}^{-1}(\mathbf{x} - \boldsymbol{\mu}))} |\det \mathbf{A}^{-1}| \\ &= \frac{1}{\sqrt{(2\pi)^n}} e^{-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T (\mathbf{A}^{-1})^T \mathbf{A}^{-1} (\mathbf{x} - \boldsymbol{\mu})} |\det \mathbf{A}^{-1}| \\ &= \frac{1}{\sqrt{(2\pi)^n \det \boldsymbol{\Sigma}}} e^{-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})} \end{aligned}$$

since $|\det \mathbf{A}^{-1}| = \frac{1}{\sqrt{\det \boldsymbol{\Sigma}}}$ and $(\mathbf{A}^{-1})^T \mathbf{A}^{-1} = \boldsymbol{\Sigma}^{-1}$ (exercise!) \square

Special case: bivariate normal

For $n = 2$ we have

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \quad \text{and} \quad \boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}$$

where $\mu_i = E(X_i)$, $\sigma_i^2 = \text{Var}(X_i)$, $i = 1, 2$, and

$$\rho = \rho(X_1, X_2) = \frac{\text{Cov}(X_1, X_2)}{\sigma_1\sigma_2}$$

Thus the bivariate normal distribution is determined by five scalar parameters μ_1 , μ_2 , σ_1^2 , σ_2^2 , and ρ .

$\boldsymbol{\Sigma}$ is positive definite $\iff \boldsymbol{\Sigma}$ is invertible $\iff \det \boldsymbol{\Sigma} > 0$:

$$\det \boldsymbol{\Sigma} = (1 - \rho^2)\sigma_1^2\sigma_2^2 > 0 \iff |\rho| < 1 \text{ and } \sigma_1^2\sigma_2^2 > 0$$

so a bivariate normal random variable (X_1, X_2) has a pdf if and only if the components X_1 and X_2 have positive variances and $|\rho| < 1$.

We have

$$\boldsymbol{\Sigma}^{-1} = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}^{-1} = \frac{1}{\det \boldsymbol{\Sigma}} \begin{bmatrix} \sigma_2^2 & -\rho\sigma_1\sigma_2 \\ -\rho\sigma_1\sigma_2 & \sigma_1^2 \end{bmatrix}$$

and

$$\begin{aligned} (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) &= \begin{bmatrix} x_1 - \mu_1 & x_2 - \mu_2 \end{bmatrix} \frac{1}{(1 - \rho^2)\sigma_1^2\sigma_2^2} \begin{bmatrix} \sigma_2^2 & -\rho\sigma_1\sigma_2 \\ -\rho\sigma_1\sigma_2 & \sigma_1^2 \end{bmatrix} \begin{bmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{bmatrix} \\ &= \frac{1}{(1 - \rho^2)\sigma_1^2\sigma_2^2} \begin{bmatrix} x_1 - \mu_1 & x_2 - \mu_2 \end{bmatrix} \begin{bmatrix} \sigma_2^2(x_1 - \mu_1) - \rho\sigma_1\sigma_2(x_2 - \mu_2) \\ \sigma_1^2(x_2 - \mu_2) - \rho\sigma_1\sigma_2(x_1 - \mu_1) \end{bmatrix} \\ &= \frac{1}{(1 - \rho^2)\sigma_1^2\sigma_2^2} (\sigma_2^2(x_1 - \mu_1)^2 - 2\rho\sigma_1\sigma_2(x_1 - \mu_1)(x_2 - \mu_2) + \sigma_1^2(x_2 - \mu_2)^2) \\ &= \frac{1}{(1 - \rho^2)} \left(\frac{(x_1 - \mu_1)^2}{\sigma_1^2} + \frac{(x_2 - \mu_2)^2}{\sigma_2^2} - \frac{2\rho(x_1 - \mu_1)(x_2 - \mu_2)}{\sigma_1\sigma_2} \right) \end{aligned}$$

Thus the joint pdf of $(X_1, X_2)^T \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ is

$$f(x_1, x_2) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1 - \rho^2}} e^{-\frac{1}{2(1 - \rho^2)} \left(\frac{(x_1 - \mu_1)^2}{\sigma_1^2} + \frac{(x_2 - \mu_2)^2}{\sigma_2^2} - \frac{2\rho(x_1 - \mu_1)(x_2 - \mu_2)}{\sigma_1\sigma_2} \right)}$$

Remark: If $\rho = 0$, then

$$\begin{aligned} f(x_1, x_2) &= \frac{1}{2\pi\sigma_1\sigma_2} e^{-\frac{1}{2} \left(\frac{(x_1 - \mu_1)^2}{\sigma_1^2} + \frac{(x_2 - \mu_2)^2}{\sigma_2^2} \right)} \\ &= \frac{1}{\sigma_1\sqrt{2\pi}} e^{-\frac{(x_1 - \mu_1)^2}{2\sigma_1^2}} \cdot \frac{1}{\sigma_2\sqrt{2\pi}} e^{-\frac{(x_2 - \mu_2)^2}{2\sigma_2^2}} \\ &= f_{X_1}(x_1)f_{X_2}(x_2) \end{aligned}$$

Therefore X_1 and X_2 are independent. It is also easy to see that $f(x_1, x_2) = f_{X_1}(x_1)f_{X_2}(x_2)$ for all x_1 and x_2 implies $\rho = 0$. Thus we obtain

Two jointly normal random variables X_1 and X_2 are independent if and only if they are *uncorrelated*.

In general, the following important facts can be proved using the multivariate MGF:

- (i) If $\mathbf{X} = (X_1, \dots, X_n)^T \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, then X_1, X_2, \dots, X_n are independent if and only if they are uncorrelated, i.e., $\text{Cov}(X_i, X_j) = 0$ if $i \neq j$, i.e., $\boldsymbol{\Sigma}$ is a diagonal matrix.
- (ii) Assume $\mathbf{X} = (X_1, \dots, X_n)^T \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and let

$$\mathbf{X}_1 = (X_1, \dots, X_k)^T, \quad \mathbf{X}_2 = (X_{k+1}, \dots, X_n)^T$$

Then \mathbf{X}_1 and \mathbf{X}_2 are independent if and only if $\text{Cov}(\mathbf{X}_1, \mathbf{X}_2) = \mathbf{0}_{k \times (n-k)}$, the $k \times (n-k)$ matrix of zeros, i.e., $\boldsymbol{\Sigma}$ can be partitioned as

$$\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \mathbf{0}_{k \times (n-k)} \\ \mathbf{0}_{(n-k) \times k} & \boldsymbol{\Sigma}_{22} \end{bmatrix}$$

where $\boldsymbol{\Sigma}_{11} = \text{Cov}(\mathbf{X}_1)$ and $\boldsymbol{\Sigma}_{22} = \text{Cov}(\mathbf{X}_2)$.

Marginals of multivariate normal distributions

Let $\mathbf{X} = (X_1, \dots, X_n)^T \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. If \mathbf{A} is an $m \times n$ matrix and $\mathbf{b} \in \mathbb{R}^m$, then

$$\mathbf{Y} = \mathbf{A}\mathbf{X} + \mathbf{b}$$

is a random m -vector. Its MGF at $\mathbf{t} \in \mathbb{R}^m$ is

$$M_{\mathbf{Y}}(\mathbf{t}) = e^{\mathbf{t}^T \mathbf{b}} M_{\mathbf{X}}(\mathbf{A}^T \mathbf{t})$$

Since $M_{\mathbf{X}}(\boldsymbol{\tau}) = e^{\boldsymbol{\tau}^T \boldsymbol{\mu} + \frac{1}{2} \boldsymbol{\tau}^T \boldsymbol{\Sigma} \boldsymbol{\tau}}$ for all $\boldsymbol{\tau} \in \mathbb{R}^n$, we obtain

$$\begin{aligned} M_{\mathbf{Y}}(\mathbf{t}) &= e^{\mathbf{t}^T \mathbf{b}} e^{(\mathbf{A}^T \mathbf{t})^T \boldsymbol{\mu} + \frac{1}{2} (\mathbf{A}^T \mathbf{t})^T \boldsymbol{\Sigma} (\mathbf{A}^T \mathbf{t})} \\ &= e^{\mathbf{t}^T (\mathbf{b} + \mathbf{A}\boldsymbol{\mu}) + \frac{1}{2} \mathbf{t}^T \mathbf{A} \boldsymbol{\Sigma} \mathbf{A}^T \mathbf{t}} \end{aligned}$$

This means that $\mathbf{Y} \sim N(\mathbf{b} + \mathbf{A}\boldsymbol{\mu}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)$, i.e., \mathbf{Y} is multivariate normal with mean $\mathbf{b} + \mathbf{A}\boldsymbol{\mu}$ and covariance $\mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T$.

Example: Let $a_1, \dots, a_n \in \mathbb{R}$ and determine the distribution of $Y = a_1 X_1 + \dots + a_n X_n$.

For some $1 \leq m < n$ let $\{i_1, \dots, i_m\} \subset \{1, \dots, n\}$ such that $i_1 < i_2 < \dots < i_m$. Let $\mathbf{e}_j = (0, \dots, 0, 1, 0, \dots, 0)^t$ be the j th unit vector in \mathbb{R}^n and define the $m \times n$ matrix \mathbf{A} by

$$\mathbf{A} = \begin{bmatrix} \mathbf{e}_{i_1}^T \\ \vdots \\ \mathbf{e}_{i_m}^T \end{bmatrix}$$

Then

$$\mathbf{A}\mathbf{X} = \begin{bmatrix} \mathbf{e}_{i_1}^T \\ \vdots \\ \mathbf{e}_{i_m}^T \end{bmatrix} \begin{bmatrix} X_1 \\ \vdots \\ X_n \end{bmatrix} = \begin{bmatrix} X_{i_1} \\ \vdots \\ X_{i_m} \end{bmatrix}$$

Thus $(X_{i_1}, \dots, X_{i_m})^T \sim N(\mathbf{A}\boldsymbol{\mu}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)$.

Note the following:

$$\mathbf{A}\boldsymbol{\mu} = \begin{bmatrix} \mu_{i_1} \\ \vdots \\ \mu_{i_m} \end{bmatrix}$$

and the (j, k) th entry of $\mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T$ is

$$\begin{aligned} (\mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)_{jk} &= (\mathbf{A} \times (i_k \text{th column of } \boldsymbol{\Sigma}))_j \\ &= (\boldsymbol{\Sigma})_{i_j i_k} = \text{Cov}(X_{i_j}, X_{i_k}) \end{aligned}$$

Thus if $\mathbf{X} = (X_1, \dots, X_n)^T \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, then $(X_{i_1}, \dots, X_{i_m})^T$ is multivariate normal whose mean and covariance are obtained by picking out the corresponding elements of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$.

Special case: For $m = 1$ we obtain that $X_i \sim N(\mu_i, \sigma_i^2)$, where $\mu_i = E(X_i)$ and $\sigma_i^2 = \text{Var}(X_i)$, for all $i = 1, \dots, n$.

Conditional distributions

Let $\mathbf{X} = (X_1, \dots, X_n)^T \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and for $1 \leq m < n$ define

$$\mathbf{X}_1 = (X_1, \dots, X_m)^T, \quad \mathbf{X}_2 = (X_{m+1}, \dots, X_n)^T$$

We know that $\mathbf{X}_1 \sim N(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11})$ and $\mathbf{X}_2 \sim N(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_{22})$ where $\boldsymbol{\mu}_i = E(\mathbf{X}_i)$, $\boldsymbol{\Sigma}_{ii} = \text{Cov}(\mathbf{X}_i)$, $i = 1, 2$.

Then $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ can be partitioned as

$$\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix}$$

where $\boldsymbol{\Sigma}_{ij} = \text{Cov}(\mathbf{X}_i, \mathbf{X}_j)$, $i, j = 1, 2$. Note that $\boldsymbol{\Sigma}_{11}$ is $m \times m$, $\boldsymbol{\Sigma}_{22}$ is $(n-m) \times (n-m)$, $\boldsymbol{\Sigma}_{12}$ is $m \times (n-m)$, and $\boldsymbol{\Sigma}_{21}$ is $(n-m) \times m$. Also, $\boldsymbol{\Sigma}_{21} = \boldsymbol{\Sigma}_{12}^T$.

We assume that $\boldsymbol{\Sigma}_{11}$ is *nonsingular* and we want to determine the conditional distribution of \mathbf{X}_2 given $\mathbf{X}_1 = \mathbf{x}_1$.

Recall that $\mathbf{X} = \mathbf{AZ} + \boldsymbol{\mu}$ for some $\mathbf{Z} = (Z_1, \dots, Z_n)^T$ where the Z_i are independent $N(0, 1)$ random variables and \mathbf{A} is such that $\mathbf{AA}^T = \boldsymbol{\Sigma}$.

Let $\mathbf{Z}_1 = (Z_1, \dots, Z_m)^T$ and $\mathbf{Z}_2 = (Z_{m+1}, \dots, Z_n)^T$. We want to determine such \mathbf{A} in a partitioned form with dimensions corresponding to the partitioning of $\boldsymbol{\Sigma}$:

$$\mathbf{A} = \begin{bmatrix} \mathbf{B} & \mathbf{0}_{m \times (n-m)} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}$$

We can write $\boldsymbol{\Sigma} = \mathbf{AA}^T$ as

$$\begin{aligned} \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix} &= \begin{bmatrix} \mathbf{B} & \mathbf{0}_{m \times (n-m)} \\ \mathbf{C} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \mathbf{B}^T & \mathbf{C}^T \\ \mathbf{0}_{(n-m) \times m} & \mathbf{D}^T \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{BB}^T & \mathbf{BC}^T \\ \mathbf{CB}^T & \mathbf{CC}^T + \mathbf{DD}^T \end{bmatrix} \end{aligned}$$

We want to solve for \mathbf{B} , \mathbf{C} and \mathbf{D} . First consider $\mathbf{BB}^T = \boldsymbol{\Sigma}_{11}$. We choose \mathbf{B} to be the unique positive definite square root of $\boldsymbol{\Sigma}_{11}$:

$$\mathbf{B} = \boldsymbol{\Sigma}_{11}^{1/2}$$

Recall that \mathbf{B} is symmetric and it is invertible since $\boldsymbol{\Sigma}_{11}$ is. Then $\boldsymbol{\Sigma}_{21} = \mathbf{CB}^T = \mathbf{CB}^{-1}$

$$\mathbf{C} = \boldsymbol{\Sigma}_{21}(\mathbf{B}^T)^{-1} = \boldsymbol{\Sigma}_{21}\mathbf{B}^{-1}$$

Then $\boldsymbol{\Sigma}_{22} = \mathbf{CC}^T + \mathbf{DD}^T$ gives

$$\begin{aligned} \mathbf{DD}^T &= \boldsymbol{\Sigma}_{22} - \mathbf{CC}^T = \boldsymbol{\Sigma}_{22} - \boldsymbol{\Sigma}_{21}\mathbf{B}^{-1}\mathbf{B}^{-1}(\boldsymbol{\Sigma}_{21})^T \\ &= \boldsymbol{\Sigma}_{22} - \boldsymbol{\Sigma}_{21}(\mathbf{BB})^{-1}\boldsymbol{\Sigma}_{12} = \boldsymbol{\Sigma}_{22} - \boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\Sigma}_{12} \end{aligned}$$

Now note that $\mathbf{X} = \mathbf{AZ} + \boldsymbol{\mu}$ gives

$$\mathbf{X}_1 = \mathbf{BZ}_1 + \boldsymbol{\mu}_1, \quad \mathbf{X}_2 = \mathbf{CZ}_1 + \mathbf{DZ}_2 + \boldsymbol{\mu}_2$$

Since \mathbf{B} is invertible, given $\mathbf{X}_1 = \mathbf{x}_1$, we have $\mathbf{Z}_1 = \mathbf{B}^{-1}(\mathbf{x}_1 - \boldsymbol{\mu}_1)$. So given $\mathbf{X}_1 = \mathbf{x}_1$, we have that the conditional distribution of \mathbf{X}_2 and the conditional distribution of

$$\mathbf{CB}^{-1}(\mathbf{x}_1 - \boldsymbol{\mu}_1) + \mathbf{DZ}_2 + \boldsymbol{\mu}_2$$

are the same.

But \mathbf{Z}_2 is independent of \mathbf{X}_1 , so given $\mathbf{X}_1 = \mathbf{x}_1$, the conditional distribution of $\mathbf{CB}^{-1}(\mathbf{x}_1 - \boldsymbol{\mu}_1) + \mathbf{DZ}_2 + \boldsymbol{\mu}_2$ is the same as its unconditional distribution.

We conclude that the conditional distribution of \mathbf{X}_2 given $\mathbf{X}_1 = \mathbf{x}_1$ is *multivariate normal* with mean

$$\begin{aligned} E(\mathbf{X}_2 | \mathbf{X}_1 = \mathbf{x}_1) &= \boldsymbol{\mu}_2 + \mathbf{CB}^{-1}(\mathbf{x}_1 - \boldsymbol{\mu}_1) \\ &= \boldsymbol{\mu}_2 + \boldsymbol{\Sigma}_{21}\mathbf{B}^{-1}\mathbf{B}^{-1}(\mathbf{x}_1 - \boldsymbol{\mu}_1) \\ &= \boldsymbol{\mu}_2 + \boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}(\mathbf{x}_1 - \boldsymbol{\mu}_1) \end{aligned}$$

and covariance matrix $\boldsymbol{\Sigma}_{22|1} = \mathbf{DD}^T = \boldsymbol{\Sigma}_{22} - \boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\Sigma}_{12}$

Special case: bivariate normal

Suppose $\mathbf{X} = (X_1, X_2)^T \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_1 \end{bmatrix} \quad \text{and} \quad \boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}$$

We have

$$\mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(x_1 - \mu_1) = \mu_2 + \rho\frac{\sigma_2}{\sigma_1}(x_1 - \mu_1)$$

and

$$\Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12} = \sigma_2^2 - \frac{\rho^2\sigma_1^2\sigma_2^2}{\sigma_1^2} = \sigma_2^2(1 - \rho^2)$$

Thus the conditional distribution of X_2 given $X_1 = x_1$ is normal with (conditional) mean

$$E(X_2|X_1 = x_1) = \mu_2 + \rho\frac{\sigma_2}{\sigma_1}(x_1 - \mu_1)$$

and variance

$$\text{Var}(X_2|X_1 = x_1) = \sigma_2^2(1 - \rho^2)$$

Equivalently, the conditional distribution of X_2 given $X_1 = x_1$ is

$$N\left(\mu_2 + \rho\frac{\sigma_2}{\sigma_1}(x_1 - \mu_1), \sigma_2^2(1 - \rho^2)\right)$$

If $|\rho| < 1$, then the conditional pdf exists and is given by

$$f_{X_2|X_1}(x_2|x_1) = \frac{1}{\sigma_2\sqrt{2\pi(1-\rho^2)}} e^{-\frac{(x_2 - \mu_2 - \rho\frac{\sigma_2}{\sigma_1}(x_1 - \mu_1))^2}{2\sigma_2^2(1-\rho^2)}}$$

Remark: Note that $E(X_2|X_1 = x_1) = \mu_2 + \rho\frac{\sigma_2}{\sigma_1}(x_1 - \mu_1)$ is a linear (affine) function of x_1 .

Example: Recall the MMSE estimate problem for $X \sim N(0, \sigma_X^2)$ from the observation $Y = X + Z$, where $Z \sim N(0, \sigma_Z^2)$ and X and Z are independent. Use the above to find $g^*(y) = E[X|Y = y]$ and compute the minimum mean square error $E[(X - g^*(Y))^2]$.