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The normal distribution

The multivariate normal distribution

An application PCA

The normal distribution Useful distributions

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The normal distribution

Motivation for the normal distribution is found in the central limit theorem Normal distributions provide an important family of distributions ~ Applications and inference

We first introduce the standard normal distribution

• Then, the general normal distribution

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Consider the integral



 $I = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-z^2}{2}\right) \mathrm{d}z \quad (1)$

This integral exists

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The normal distribution (cont.)

Consider the relevant part of the integrand

It is a positive continuous function bounded by an integrable function

 $\begin{array}{c} 3 \\ (\mathbb{R}) \\ 2 \\ (\mathbb{R}) \\ (\mathbb{R}$

That is,

$$0 < \exp\left(\frac{-z^2}{2}\right) < \exp(-|z|+1), \quad -\infty < z < \infty$$

and

$$\int_{-\infty}^{\infty} \exp\left(-|z|+1\right) \mathrm{d}z = 2e$$

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The normal distribution (cont.)

To evaluate the integral, we note that I > 0

We have that I^2

$$I^{2} = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z^{2}}{2}\right) \mathrm{d}x \cdot \int_{\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{w^{2}}{2}\right) \mathrm{d}w$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left(-\frac{z^{2}+w^{2}}{2}\right) \mathrm{d}z \mathrm{d}w$$

The integral can be computed by changing to polar coordinates

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The normal distribution (cont.)

Set $z = r \cos \theta$ and $w = r \sin \theta$

Then,

$$I^{2} = \frac{1}{2\pi} \int_{0}^{2\pi} \underbrace{\int_{0}^{\infty} e^{-r^{2}/2} r dr}_{\int x e^{cx^{2}} dx = 1/(2c)e^{cx^{2}} = 1} d\theta$$
$$= \frac{1}{2\pi} \int_{0}^{2\pi} d\theta$$
$$= 1$$

The integrand of Equation (1) is positive on \mathcal{R} and integrates to 1 over \mathcal{R}

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The normal distribution (cont.)

The integrand is a PDF of a continuous random variable with support \mathcal{R} Denote this random variable Z, Z has the PDF

$$f(z) = \frac{1}{\sqrt{(2\pi)}} \exp\left(\frac{-z^2}{2}\right), \text{ for } -\infty < x < \infty$$
(2)



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The normal distribution (cont.)

For $t \in \mathcal{R}$, the MGF of Z can be derived by a completion of a square

$$E[\exp(tZ)] = \int_{-\infty}^{\infty} \exp(tz) \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}z^2\right) dz$$
$$= \exp\left(\frac{1}{2}t^2\right) \int_{-\infty}^{\infty} \frac{1}{2\pi} \exp\left[-\frac{1}{2}(z-t)^2\right] dz \qquad (3)$$
$$= \exp\left(\frac{1}{2}t^2\right) \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}w^2\right] dw$$

For the last integral, we made a 1-to-1 change of variable w = z - tThe integral in Equation (3) has value 1, by the identity

$$f(z) = \frac{1}{\sqrt{(2\pi)}} \exp\left(\frac{-z^2}{2}\right), \text{ for } -\infty < x < \infty,$$

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The normal distribution (cont.)

Thus, the MGF of ${\cal Z}$

$$M_Z(t) = e^{(1/2t^2)}, \text{ for } -\infty < x < \infty$$
 (4)

The first two derivative of $M_Z(t)$ are

$$M'_Z(t) = te^{(1/2t^2)}$$
$$M''_Z(t) = e^{(1/2t^2)} + t^2 e^{(1/2t^2)}$$

Upon evaluating these derivatives at t = 0, the mean and variance of Z

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The normal distribution (cont.)

Define the continuous random variable X = bZ + a, for b > 0• This is a 1-to-1 transformation

We want to derive the PDF of X

- The inverse of the transformation is $z = b^{-1}(x a)$
- The Jacobian is $J = b^{-1}$

Because b > 0, the PDF of X

$$f_X(x) = \frac{1}{\sqrt{2\pi}} \frac{1}{b} \exp\left[-\frac{1}{2} \left(\frac{x-a}{b}\right)^2\right], \text{ for } -\infty < x < \infty$$

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The normal distribution (cont.)

By Equation (5), we have

$$\ \, \rightsquigarrow \quad E(X) = a \\ \ \, \rightsquigarrow \quad \operatorname{Var}(X) = b^2$$

The PDF of X can be written using those quantities $\rightsquigarrow a$ can be replaced by $\mu = E(X)$ $\rightsquigarrow b^2$ can be replaced by $\sigma^2 = \operatorname{Var}(X)$

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The normal distribution (cont.)

Definition 1.1

Normal distribution

A random variable X has a normal distribution if its PDF is

$$f(x) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)\right], \quad x \in (-\infty, +\infty)$$
(6)

The parameters μ and σ^2 are the mean and the variance of X We often write that X has a $N(\mu, \sigma^2)$ distribution

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The normal distribution (cont.)

Remark

Consider the random variable ${\cal Z}$ with the PDF

$$f(z) = \frac{1}{\sqrt{(2\pi)}} \exp\left(\frac{-z^2}{2}\right), \text{ for } -\infty < x < \infty$$

The RV Z is said to have a N(0, 1) distribution

• We call Z a standard normal RV

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The normal distribution (cont)

Consider the calculation of the MGF of \boldsymbol{X}

We use the relationship

$$X = \underbrace{\sigma}_{b} Z + \underbrace{\mu}_{a}$$

Remember that the MGF of ${\cal Z}$

$$M_Z(t) = e^{(1/2t^2)}$$
, for $-\infty < x < \infty$

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The normal distribution (cont)

We obtain,

$$E\left[\exp\left(tX\right)\right] = E\left\{\exp\left[t(\sigma Z + \mu)\right]\right\} = \exp\left(\mu t\right)E\left[\exp\left(t\sigma Z\right)\right]$$
$$= \exp\left(\mu t\right)\exp\left(\frac{1}{2}\sigma^{2}t^{2}\right) = \exp\left(\mu t + \frac{1}{2}\sigma^{2}t^{2}\right)$$

for
$$-\infty < t < +\infty$$

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An application PCA

The normal distribution (cont)

Remarl

Consider the relationship between Z and X

 $\rightsquigarrow X \sim N(\mu, \sigma^2)$ if and only if $Z = (X - \mu)/\sigma \sim N(0, 1)$

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The normal distribution (cont.)

Example

Consider the random variable X with the MGF



X has a normal distribution with $\mu = 2$ and $\sigma^2 = 64$, N(2, 54)The random variable Z = (X - 2)/8 has a N(0, 1) distribution

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An application PCA

The normal distribution (cont.)

Example

We can derive all the moments of the standard normal RV using its MGF \rightsquigarrow We can do the same for a general normal RV

Let $X \sim N(\mu, \sigma^2)$

Hence, for all nonnegative integers k, by the binomial theorem¹

$$E(X^{k}) = E[(\sigma Z + \mu)^{k}] = \sum_{j=0}^{k} {\binom{k}{j}} \sigma^{j} E(Z^{j}) \mu^{k-j}$$
(7)

 \rightsquigarrow All the odd moments of Z are zero \rightsquigarrow All even moments can be calculated

$${}^{1}(x+y)^{k} = \sum_{k=0}^{n} \binom{n}{k} x^{n-k} y^{k} = \sum_{k=0}^{n} \binom{n}{k} x^{k} y^{n-k}$$

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An application PCA

The normal distribution (cont.)



→ The graph is symmetric about a vertical axis at $x = \mu$ → The graph has its maximum of $1/(\sigma\sqrt{2\pi})$ at $x = \mu$ → The graph has the *x*-axis as horizontal asymptote → The points of inflection are at $x = \mu \pm \sigma$

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An application PCA

The normal distribution (cont)

There are many practical applications that involve normal distributions \rightsquigarrow We need to be able to readily calculate probabilities

Normal PDFs contain a factor of the form $\exp(-s^2)$

- Antiderivatives are not in closed-form
- Numerical integration must be used

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An application PCA

The normal distribution (cont)

We can use the relation between normal and standard normal variables $\rightarrow X \sim N(\mu, \sigma^2)$ if and only if $Z = (X - \mu)/\sigma \sim N(0, 1)$

Thus, we need only calculate probabilities for standard normal RVs

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The normal distribution (cont)

Consider the CDF of a standard normal random variables ${\cal Z}$

$$\Phi(z) = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-w^2}{2}\right) \mathrm{d}w \tag{8}$$

Let $X \sim N(\mu, \sigma^2)$

Suppose that we want to compute $F_X(x) = P(X \le x)$ for some xThen, for $Z = (X - \mu)/\sigma$

$$F_X(x) = P(X \le x) = P\left(Z \le \frac{x-\mu}{\sigma}\right) = \Phi\left(\frac{x-u}{\sigma}\right)$$

Thus, only integration for $\Phi(z)$ is needed

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The normal distribution

Suppose we are interested in the value x_p such that $p = F_X(x_p)$ for some pTake $z_p = \Phi^{-1}(p)$, then $x_p = \sigma z_p + \mu$

Consider the standard normal density



The area to the left of z_p is p

• $\Phi(z_p) = p$

We can use an abbreviated table of probability

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The normal distribution

Suppose we are interested in $\Phi(-z)$, for some z > 0Since the PDF is symmetric,

$$\rightsquigarrow \quad \Phi(-z) = 1 - \Phi(z) \tag{9}$$

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The normal distribution

The multivariate normal distribution

An application PCA

The normal distribution (cont.)

Consider a random variable $X \sim N(a, b)$

- pnorm(x,a,b), $P(X \le x)$
- dnorm(x,a,b), the PDF of X at x

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The normal distribution (cont.)

Exampl

Let the random variable $X \sim N(2, 25)$



Using abbreviated tables of probabilities

$$P(0 < X < 10) = \Phi\left(\frac{10-2}{5}\right) - \Phi\left(\frac{0-2}{5}\right)$$
$$= \Phi(1.6) - \Phi(-0.4)$$
$$= 0.945 - (1 - 0.655) = 0.600$$

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The normal distribution (cont.)

$$P(-8 < X < 1) = \Phi\left(\frac{1-2}{5}\right) - \Phi\left(\frac{-8-2}{5}\right)$$
$$= \Phi(-0.2) - \Phi(-2)$$
$$= (1 - 0.579) - (1 - 0.977) = 0.398$$

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The normal distribution (cont.)

Example

Let the random variable $X \sim N(\mu, \sigma^2)$

$$P(\mu - 2\sigma < X < \mu + 2\sigma) = \Phi\left(\frac{\mu + 2\sigma - \mu}{\sigma}\right) - \Phi\left(\frac{\mu - 2\sigma - \mu}{\sigma}\right)$$

= $\Phi(2) - \Phi(-2)$
= $0.977 - (1 - 0.977) = 0.954$ (10)

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The normal distribution

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An application PCA

The normal distribution (cont.)

Theorem 1.

Consider a random variable $X \sim N(\mu, \sigma^2)$ with $\sigma^2 > 0$

The random variable $V = (X - \mu)^2 / \sigma^2$ is $\chi^2(1)$

Proof

The random variable $V = W^2$, with $W = (X - \mu)/\sigma \sim N(0, 1)$

The CDF G(v) for V

$$G(v) = P(W^2 \le v) = P(-\sqrt{v} \le W \le \sqrt{v}), \quad \text{for } v \ge 0$$

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The normal distribution (cont.)

That is,

$$G(v) = 2 \int_0^{\sqrt{v}} \frac{1}{\sqrt{2\pi}} e^{(-w^2/2)} \mathrm{d}w, \text{ for } 0 \le v$$

Moreover,

G(v) = 0, for v < 0

Consider a change of the integration variable, $w = \sqrt{y}$

$$\rightsquigarrow \quad G(v) = \int_0^v \frac{1}{\sqrt{2\pi}\sqrt{y}} e^{(-y/2)} \mathrm{d}y, \text{ for } 0 \le v$$

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The normal distribution (cont.)

Hence, the PDF g(v) = G'(v) of random variable V of the continuous type

$$g(v) = \begin{cases} \frac{1}{\sqrt{\pi}\sqrt{2}} v^{(1/2-1)} e^{(-v/2)}, & 0 < v < \infty \\ 0, & \text{elsewhere} \end{cases}$$

Since g(v) is a PDF,

$$\int_0^\infty g(v) \mathrm{d}v = 1,$$

Then, it must be $\Gamma(1/2) = \sqrt{\pi}$ and therefore $V \sim \chi^2(1)$

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The normal distribution (cont.)

A main property of the normal distribution is additivity under independence

Theorem 1.2

Let X_1, \ldots, X_n be independent random variables Suppose that $X_i \sim N(\mu_i, \sigma_i^2)$, for $i = 1, \ldots, n$,

Let $Y = \sum_{i=1}^{n} a_i X_i$, for some constants a_1, \ldots, a_n Then, the distribution of Y is $N(\sum_{i=1}^{n} a_i \mu_i, \sum_{i=1}^{n} a_i^2 \sigma_i^2)$

Proof

For $t \in \mathcal{R}$, the MGF of Y

$$M_Y(t) = \prod_{i=1}^n \exp\left[ta_i\mu_i + (1/2)t^2 a_i^2 \sigma_i^2\right]$$

= $\exp\left[t\sum_{i=1}^n a_i\mu_i + (1/2)t^2\sum_{i=1}^n a_i^2 \sigma_i^2\right]$

This is the MGF of a $N(\sum_{i=1}^{n} a_i \mu_i, \sum_{i=1}^{n} a_i^2 \sigma_i^2)$ distribution

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The normal distribution (cont.)

Let X_1, X_2, \ldots, X_n be random sample from a $N(\mu, \sigma^2)$

A corollary gives the distribution of the sample mean

$$\Rightarrow \quad \overline{X} = \frac{1}{n} \sum_{i=1}^{n} X_i$$

Corollary

Let X_1, \ldots, X_n be IID random variables with common $N(\mu, \sigma^2)$ distribution Let $\overline{X} = \frac{1}{n} \sum_{i=1}^{n} X_i$

Then, \overline{X} has a $N(\mu, \sigma^2/n)$ distribution

Proof

In Theorem 1.2, take $a_i = (1/n)$, $\mu_i = \mu$ and $\sigma_i^2 = \sigma^2$, for $i = 1, 2, \ldots, n$

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The multivariate normal distribution

The multivariate normal distribution for a n-dimensional random vector

• Examples for the bivariate case, n = 2

The derivation is simplified by first discussing the standard case

• Then, we proceed with the general cases
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The multivariate normal distribution (cont.)

Consider the random vector $\mathbf{Z} = (Z_1, \dots, Z_n)'$ • Z_1, \dots, Z_n are IID N(0, 1) random variables

Then, the density of ${\bf Z}$

$$f_{\mathbf{Z}}(\mathbf{z}) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}z_{i}^{2}\right\} = \left(\frac{1}{2\pi}\right)^{n/2} \exp\left\{-\frac{1}{2}\sum_{i=1}^{n} z_{i}^{2}\right\}$$
$$= \left(\frac{1}{2\pi}\right)^{n/2} \exp\left\{-\frac{1}{2}\mathbf{z}'\mathbf{z}\right\}, \text{ for } \mathbf{z} \in \mathcal{R}^{n}$$
(11)

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The multivariate normal distribution (cont.)

Consider the random vector $\mathbf{Z} = (Z_1, Z_2)'$

Since n = 2, we have

$$f_{\mathbf{Z}}(\mathbf{z}) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}z_{i}^{2}\right\} = \left(\frac{1}{2\pi}\right)^{n/2} \exp\left\{-\frac{1}{2}\sum_{i=1}^{n} z_{i}^{2}\right\},\$$
$$= 1/(2\pi) \exp\left\{-1/2\sum_{i=1}^{2} z_{i}^{2}\right\} = 1/(2\pi) \exp\left\{-1/2(z_{1}^{2}+z_{2}^{2})\right\}$$



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The multivariate normal distribution (cont.)

The Z_i s have mean zero, unit variance and they are uncorrelated Then, the mean and covariance matrix of \mathbf{Z}

$$E(\mathbf{Z}) = \mathbf{0}$$

$$Cov(\mathbf{Z}) = \mathbf{I}_n$$
(12)

• \mathbf{I}_n indicates an identity matrix of order n

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The multivariate normal distribution

The MGF of each of the Z_i s evaluated at t_i is $e^{(t_i^2/2)}$

As the Z_i s are independent, the MGF of \mathbf{Z}

$$M_{\mathbf{Z}}(\mathbf{t}) = E\left[\prod_{i=1}^{n} \exp\left\{t_{i} Z_{i}\right\}\right] = \prod_{i=1}^{n} E\left[\exp\left\{t_{i} Z_{i}\right\}\right]$$

$$= \exp\left\{\frac{1}{2} \sum_{i=1}^{n} t_{i}^{2}\right\} = \exp\left\{\frac{1}{2} \mathbf{t}' \mathbf{t}\right\}, \text{ for all } \mathbf{t} \in \mathcal{R}^{n}$$
(13)

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Consider the random vector $\mathbf{Z} = (Z_1, Z_2)'$

Since n = 2, we have

$$M_{\mathbf{Z}}(\mathbf{t}) = E\left[\prod_{i=1}^{n} \exp\left\{t_{i} Z_{i}\right\}\right] = \prod_{i=1}^{n} E\left[\exp\left\{t_{i} Z_{i}\right\}\right]$$
$$= \exp\left\{\frac{1}{2} \sum_{i=1}^{2} t_{i}^{2}\right\} = \exp\left\{1/2(t_{1}^{2} + t_{2}^{2})\right\}, \text{ for all } (t_{1}, t_{2}) \in \mathcal{R}^{2}$$



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The multivariate normal distribution (cont.)

${\bf Z}$ is said to have a multivariate normal distribution

 \mathbf{Z} has a $N_n(\mathbf{0}, \mathbf{I}_n)$ distribution, mean $\mathbf{0}$, covariance matrix \mathbf{I}_n

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The multivariate normal distribution (cont.)

Let Σ be a $n \times n$, symmetric and positive-definite matrix $(\mathbf{z}' \Sigma \mathbf{z} > 0, \forall \mathbf{z})$

From linear algebra, we can always decompose Σ

$$\Sigma = \Gamma' \Lambda \Gamma \tag{14}$$

 Λ is the diagonal matrix $\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$

$$\mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}$$

 $\rightsquigarrow \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$ are the eigenvalues of Σ

The columns of Γ' , $\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_n$, are the corresponding eigenvectors

$$\mathbf{\Gamma}' = \begin{bmatrix} v_{1,1} & v_{2,1} & \cdots & v_{n,1} \\ v_{1,2} & v_{2,2} & \cdots & v_{n,2} \\ \vdots & \vdots & & \vdots \\ v_{1,n} & v_{2,n} & \cdots & v_{n,n} \end{bmatrix}$$

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The multivariate normal distribution (cont.)

$\boldsymbol{\Sigma} = \boldsymbol{\Gamma}' \boldsymbol{\Lambda} \boldsymbol{\Gamma}$

The factorisation is called the spectral decomposition of $\pmb{\Sigma}$

• Matrix Γ is orthogonal ($\Gamma^{-1} = \Gamma'$, thus $\Gamma\Gamma' = \mathbf{I}$)

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The multivariate normal distribution (cont.)

Remark

Eigenvalues and eigenvectors

A $(n \times n)$ matrix **A** can be used to transform a *n*-vector **x** to another one **y**

$\mathbf{y} = \mathbf{A}\mathbf{x}$

Consider a scalar variable λ_i and a particular value of $\mathbf{x} (= \mathbf{e}_i)$ such that

$$\mathbf{y}_{\mathbf{e}_i} = \mathbf{A}\mathbf{e}_i = \lambda_i \mathbf{e}_i$$

 $\rightsquigarrow \ \lambda_i$ is often called an ${\bf eigenvalue}$ of ${\bf A}$

 \rightsquigarrow \mathbf{e}_i is the corresponding **eigenvector**

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The multivariate normal distribution (cont.)

$$\mathbf{A}\mathbf{e}_i = \lambda_i \mathbf{e}_i$$

Every $(n \times n)$ matrix has n eigenvalues and up to n eigenvectors They can be jointly specified

$$\begin{aligned} &(\lambda_1 \mathbf{I}_n - \mathbf{A}) \mathbf{e}_1 = \mathbf{0} \\ &(\lambda_2 \mathbf{I}_n - \mathbf{A}) \mathbf{e}_2 = \mathbf{0} \\ & \dots \\ &(\lambda_n \mathbf{I}_n - \mathbf{A}) \mathbf{e}_n = \mathbf{0} \end{aligned}$$

If $(\lambda_i \mathbf{I}_n - \mathbf{A}) \mathbf{e}_i = \mathbf{0}$ is satisfied, then so is $(\lambda_i \mathbf{I}_n - \mathbf{A}) \alpha \mathbf{e}_i = \mathbf{0}$ (i = 1, ..., n) \rightsquigarrow Eigenvectors are specified up to any multiplicative constant α

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The multivariate normal distribution (cont.)

The set of n vector equations can have non-trivial solutions

The *n* values of λ_i need be solutions to the scalar equation

$$|\lambda \mathbf{I}_n - \mathbf{A}| := \Delta(\lambda) = 0$$

 $\stackrel{\rightsquigarrow}{\longrightarrow} (\lambda \mathbf{I}_n - \mathbf{A}) \text{ is called the$ **characteristic matrix**of**A** $<math display="block"> \stackrel{\rightsquigarrow}{\longrightarrow} \Delta(\lambda) \text{ is the$ **characteristic polynomial**of**A** $}$

The determinant gives a *n*-degree polynomial in λ

• It can be factored as a product of n binomials

$$\Delta(\lambda) = \lambda^n + c_{n-1}\lambda^{n-1} + \dots + c_1\lambda + c_0$$

= $(\lambda - \lambda_1)(\lambda - \lambda_2) \cdots (\lambda - \lambda_n)$
= 0

• Each of the binomial roots is an eigenvalue of ${\bf A}$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

If the roots are all distinct, there will be n independent eigenvectors \rightsquigarrow If the roots are repeated, there may be fewer eigenvectors

For a distinct eigenvalue λ_i , the eigenvector \mathbf{e}_i is contained in $\operatorname{Adj}(\lambda_i \mathbf{I}_n - \mathbf{A})$

 $\operatorname{Adj}(\lambda_i \mathbf{I}_n - \mathbf{A}) = \begin{bmatrix} \alpha_1 \mathbf{e}_i & \alpha_2 \mathbf{e}_i & \cdots & \alpha_n \mathbf{e}_i \end{bmatrix}$

Since α_j are arbitrary constants, any non-zero column represents \mathbf{e}_i

 $\operatorname{Adj}(\lambda_i \mathbf{I}_n - \mathbf{A})$ is computed for each root $(i = 1, \dots, n)$

• A single eigenvector is chosen from each evaluation

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Together, the n eigenvectors form the columns of the **modal matrix E**

$$\mathbf{E} = \begin{bmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \cdots & \mathbf{e}_n \end{bmatrix}$$

Here, the eigenvectors are scaled so that $|\mathbf{e}_i| = 1$ (i = 1, ..., n)

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

The modal matrix can be used to diagonalise \mathbf{A}

To transform A into a diagonal matrix (of eigenvalues)

$$\begin{bmatrix} \mathbf{A}\mathbf{e}_1 &= \lambda_1 \mathbf{e}_1 \\ \mathbf{A}\mathbf{e}_2 &= \lambda_2 \mathbf{e}_2 \\ \vdots & \vdots \\ \mathbf{A}\mathbf{e}_n &= \lambda_n \mathbf{e}_n \end{bmatrix}, \text{ or } \mathbf{A}\mathbf{E} = \mathbf{E}\mathbf{\Lambda}$$

 Λ is a diagonal matrix of eigenvalues

$$\mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}$$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

 ${\bf E}$ is non-singular because the ${\bf e}_i$ are linearly independent

 $\mathbf{A} = \mathbf{E} \mathbf{\Lambda} \mathbf{E}^{-1}$

From the diagonal matrix of eigenvalues to the original square matrix

The inverse transformation

 $\Lambda = \mathbf{E}^{-1} \mathbf{A} \mathbf{E}$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

If A is a real, symmetric matrix, its eigenvalues are real
The eigenvectors are orthogonal to each other
There are n eigenvectors, even with repeated roots

The eigenvectors corresponding to distinct eigenvalues

$$\operatorname{Adj}(\lambda_i \mathbf{I}_n - \mathbf{A}) = \begin{bmatrix} \alpha_1 \mathbf{e}_i & \alpha_2 \mathbf{e}_i & \cdots & \alpha_n \mathbf{e}_i \end{bmatrix}$$

The eigenvectors of eigenvalues λ_i with multiplicity m

$$\frac{d^{m-1}}{d\lambda^{m-1}} \left[\operatorname{Adj}(\lambda_i \mathbf{I}_n - \mathbf{A}) \right] \Big|_{\lambda = \lambda_i} = \begin{bmatrix} \cdots & \mathbf{e}_{i_1} & \mathbf{e}_{i_2} & \cdots & \mathbf{e}_{i_m} & \cdots \end{bmatrix}$$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Rema

An alternative way to write the spectral decomposition

$$\boldsymbol{\Sigma} = \boldsymbol{\Gamma}' \boldsymbol{\Lambda} \boldsymbol{\Gamma} = \sum_{i=1}^{n} \lambda_i \mathbf{v}_i \mathbf{v}_i' \tag{15}$$

$$\underbrace{\begin{bmatrix} v_{1,1} & v_{2,1} & \cdots & v_{n,1} \\ v_{1,2} & v_{2,2} & \cdots & v_{n,2} \\ \vdots & \vdots & & \vdots \\ v_{1,n} & v_{2,n} & \cdots & v_{n,n} \end{bmatrix}}_{\lambda_2 \mathbf{v}_2} \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}} \underbrace{\begin{bmatrix} v_{1,1} & v_{1,2} & \cdots & v_{1,n} \\ v_{2,1} & v_{2,2} & \cdots & v_{2,n} \\ \vdots & \vdots & & \vdots \\ v_{n,1} & v_{n,2} & \cdots & v_{n,n} \end{bmatrix}}_{\lambda_2 \mathbf{v}_2}$$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Because the $\lambda_i s$ are non-negative, we can define the diagonal matrix

$$\boldsymbol{\Lambda}^{1/2} = \operatorname{diag}(\sqrt{\lambda_1}, \sqrt{\lambda_2}, \dots, \sqrt{\lambda_n})$$

$$= \begin{bmatrix} \lambda_1^{1/2} & 0 & \cdots & 0 \\ 0 & \lambda_2^{1/2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n^{1/2} \end{bmatrix}$$

Then, the orthogonality of Γ implies

$$\Sigma = \Gamma' \underbrace{\Lambda^{1/2} \underbrace{\Gamma \Gamma'}_{I} \Lambda^{1/2} \Gamma}_{\Lambda}$$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

$$\boldsymbol{\Sigma} = \boldsymbol{\Gamma}' \underbrace{\boldsymbol{\Lambda}^{1/2} \underbrace{\boldsymbol{\Gamma} \boldsymbol{\Gamma}'}_{\mathbf{I}} \boldsymbol{\Lambda}^{1/2} \boldsymbol{\Gamma}}_{\mathbf{\Lambda}}$$

Define the square root of the positive semi-definite matrix Σ

$$\Sigma^{1/2} = \Gamma' \Lambda^{1/2} \Gamma \tag{16}$$

 $\rightsquigarrow~\boldsymbol{\Sigma}^{1/2}$ is symmetric and positive semi-definite

Suppose Σ is positive definite and all its eigenvalues are strictly positive. Then, we have

$$(\mathbf{\Sigma}^{1/2})^{-1} = \mathbf{\Gamma}' \mathbf{\Lambda}^{-1} \mathbf{\Gamma} = \mathbf{\Sigma}^{-1/2}$$
(17)

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Let **Z** have a $N_n(\mathbf{0}, \mathbf{I}_n)$ distribution

Let $\pmb{\Sigma}$ be a positive semi-definite symmetric matrix

Let μ be a $n \times 1$ vector of constants

Define the random vector ${\bf X}$

$$\mathbf{X} = \mathbf{\Sigma}^{1/2} \mathbf{Z} + \boldsymbol{\mu} \tag{18}$$

By Equation (12), we have

$$E[\mathbf{X}] = \boldsymbol{\mu}$$

Cov $[\mathbf{X}] = \boldsymbol{\Sigma}^{1/2} \boldsymbol{\Sigma}^{1/2} = \boldsymbol{\Sigma}$ (19)

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

The MGF of ${\bf X}$

$$M_{\mathbf{X}}(\mathbf{t}) = E\left[\exp\left\{\mathbf{t}'\mathbf{X}\right\}\right] = E\left[\exp\left\{\mathbf{t}'\boldsymbol{\Sigma}^{1/2}\mathbf{Z} + \mathbf{t}'\boldsymbol{\mu}\right\}\right]$$

$$= \exp\left(\mathbf{t}'\boldsymbol{\mu}\right) E\left\{\exp\left[\left(\boldsymbol{\Sigma}^{1/2}\mathbf{t}\right)'\mathbf{Z}\right]\right\}$$

$$= \exp\left(\mathbf{t}'\boldsymbol{\mu}\right)\exp\left[\left(1/2\right)\left(\boldsymbol{\Sigma}^{1/2}\mathbf{t}\right)'\boldsymbol{\Sigma}^{1/2}\mathbf{t}\right]$$

$$= \exp\left(\mathbf{t}'\boldsymbol{\mu}\right)\exp\left[\left(1/2\right)\mathbf{t}'\boldsymbol{\Sigma}\mathbf{t}\right]$$

(20)

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Definition

Multivariate normal

A n-dimensional random vector \mathbf{X} has a multivariate normal distribution if its MGF is

$$M_{\mathbf{X}}(\mathbf{t}) = \exp\left[\mathbf{t}'\boldsymbol{\mu} + (1/2)\mathbf{t}'\boldsymbol{\Sigma}\mathbf{t}\right]$$
(21)

for all $\mathbf{t} \in \mathcal{R}^n$

Σ is a symmetric, positive semi-definite matrix
 μ ∈ Rⁿ

We say that **X** has a $N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ distribution

1

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The normal distribution

The multivariate normal distribution

An applicatio PCA

The multivariate normal distribution (cont.)

The definition is for positive semi-definite positive matrices $\pmb{\Sigma}$

- Σ is usually positive definite
- \leadsto We can get the density of ${\bf X}$

If Σ is positive definite, then so is $\Sigma^{1/2}$

• Its inverse is $(\Sigma^{1/2})^{-1} = \Gamma' \Lambda^{-1} \Gamma = \Sigma^{-1/2}$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

$$\mathbf{X} = \mathbf{\Sigma}^{1/2} \mathbf{Z} + \boldsymbol{\mu}$$

The transformation between ${\bf X}$ and ${\bf Z}$ is 1-to-1

The inverse transformation

$$\mathbf{Z} = \mathbf{\Sigma}^{-1/2} (\mathbf{X} - \boldsymbol{\mu})$$

The Jacobian

$$\left|\boldsymbol{\Sigma}^{-1/2}\right| = \left|\boldsymbol{\Sigma}\right|^{-1/2}$$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Hence, upon simplification, the PDF of ${\bf X}$

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{1}{(2\pi)^{n/2} |\mathbf{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})' \mathbf{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right], \text{ for } \mathbf{x} \in \mathcal{R}^n \quad (22)$$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Γheorem 2.1

Suppose **X** has a $N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ distribution

Let $\mathbf{Y} = \mathbf{A}\mathbf{X} + \mathbf{b}$, where \mathbf{A} is a $m \times n$ matrix and $\mathbf{b} \in \mathcal{R}^m$

Then, **Y** has a $N_m(\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}')$ distribution

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Proof

From $M_{\mathbf{X}}(\mathbf{t}) \exp \left[\mathbf{t}'\boldsymbol{\mu} + (1/2)\mathbf{t}'\boldsymbol{\Sigma}\mathbf{t}\right]$, for all $\mathbf{t} \in \mathcal{R}^m$ The MGF of \mathbf{Y} $M_{\mathbf{Y}}(\mathbf{t}) = E\left[\exp \left(\mathbf{t}'\mathbf{Y}\right)\right]$ $= E\left\{\exp \left[\mathbf{t}'(\mathbf{A}\mathbf{X} + \mathbf{b})\right]\right\}$ $= \exp \left(\mathbf{t}'\mathbf{b}\right)E\left\{\exp \left[\left(\mathbf{A}'\mathbf{t}\right)'\mathbf{X}\right]\right\}$ $= \exp \left(\mathbf{t}'\mathbf{b}\right)\exp \left[\left(\mathbf{A}'\mathbf{t}\right)'\boldsymbol{\mu} + (1/2)\left(\mathbf{A}'\mathbf{t}\right)'\boldsymbol{\Sigma}\left(\mathbf{A}'\mathbf{t}\right)\right]$ $= \exp \left[\mathbf{t}'\left(\mathbf{A}\boldsymbol{\mu} + \mathbf{b}\right) + (1/2)\mathbf{t}'\mathbf{A}\boldsymbol{\Sigma}\mathbf{A}'\mathbf{t}\right]$

This is the MGF of a $N_m(\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}')$ distribution

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

A corollary gives us the marginal distributions of a multivariate normal RV Let \mathbf{X}_1 be any sub-vector of \mathbf{X} of dimension m < nWe can always rearrange means and correlations

There is no loss in writing

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{bmatrix}$$
(23)

 \mathbf{X}_2 is of dimension p = n - m

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

In the same way, we partition mean and covariance matrix of ${\bf X}$

$$\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix}$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix}$$
(24)

- Σ_{11} is the covariance matrix of \mathbf{X}_1
- Σ_{12} contains all covariances between the components of X_1 and X_2

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

We define \mathbf{A} to be the matrix

$$\mathbf{A} = \begin{bmatrix} [\mathbf{I}_m] & | [\mathbf{0}_{mp}] \end{bmatrix}$$

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

 \rightsquigarrow **I**_m indicates a $m \times m$ identity matrix

 \rightsquigarrow **0**_{mp} indicates a $m \times p$ matrix of zeros

Then, $\mathbf{X}_1 = \mathbf{A}\mathbf{X}$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

We apply Theorem 2.1 to the transformation $\mathbf{X}_1 = \mathbf{A}\mathbf{X}$

We have the following corollary

Corollary 2.1

Suppose **X** has a $N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ distribution, partitioned as in Equation (23-24)

$$egin{aligned} \mu &= egin{bmatrix} \mu_1 \ \mu_2 \end{bmatrix} \ \Sigma &= egin{bmatrix} \Sigma_{11} & \Sigma_{12} \ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \end{aligned}$$

Then, \mathbf{X}_1 has a $N_m(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11})$ distribution

This is a useful result

The corollary shows that any marginal distribution of \mathbf{X} is also normal \rightsquigarrow Mean and covariance matrix are those from the partial vector

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Example

Consider the multivariate normal in the case when n=2 \rightsquigarrow The bivariate normal

We use common notation (X, Y) rather than (X_1, X_2) Suppose that $(X, Y) \sim N_2(\mu, \Sigma)$

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$$
$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_2^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{bmatrix}$$

(25)

 $\rightsquigarrow \mu_1$ and σ_1^2 are the mean and variance of X $\rightsquigarrow \mu_2$ and σ_2^2 are the mean and variance of Y

 $\sigma_{12} = \rho(\sigma_1 \sigma_2)$ is the covariance between X and Y $\rightsquigarrow \rho$ is the correlation coefficient between X and Y

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Substituting $\rho \sigma_1 \sigma_2$ for σ_{12} in Σ

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

The determinant of Σ is σ₁²σ₂²(1 − ρ²) (remember that ρ² ≤ 1)
Suppose that ρ² < 1, so that Σ is invertible

The inverse of Σ

$$\boldsymbol{\Sigma}^{-1} = \frac{1}{\sigma_1^2 \sigma_2^2 (1 - \rho^2)} \begin{bmatrix} \sigma_2^2 & -\rho \sigma_1 \sigma_2 \\ -\rho \sigma_2 \sigma_1 & \sigma_1^2 \end{bmatrix}$$
(26)

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

From this expression, the PDF of (X, Y)

$$f(x,y) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}}e^{(-q/2)}, \quad -\infty < x, y < \infty$$
(27)

with

$$q = \frac{1}{1 - \rho^2} \left[\left(\frac{x - \mu_1}{\sigma_1} \right)^2 - 2\rho \left(\frac{x - \mu_1}{\sigma_1} \right) \left(\frac{x - \mu_2}{\sigma_2} \right) + \left(\frac{y - \mu_2}{\sigma^2} \right)^2 \right]$$
(28)

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

In general, if X and Y are independent RVs, correlation coefficient is zero If they are normal, then $X \sim N(\mu_1, \sigma_1^2)$ and $Y \sim N(\mu_2, \sigma_2^2)$ • (by Corollary 2.1)

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

$$f(x,y) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}}e^{(-q/2)}, \quad -\infty < x, y < \infty$$
$$q = \left[\left(\frac{x-\mu_1}{\sigma_1}\right)^2 + \left(\frac{y-\mu_2}{\sigma^2}\right)^2\right]$$

From the joint PDF of (X, Y), let the correlation coefficient be zero

• X and Y are independent

For the bivariate normal, independence corresponds to $\rho=0$

The generalisation to the multivariate case also holds true
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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

If two random variables are independent their covariance is zero

• The converse is not necessarily true

Yet, it can be shown that this is true for the multivariate normal

Theorem 2.2

Suppose that $\mathbf{X} \sim N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

 $Suppose \ the \ partitioning$

$$egin{aligned} \mu &= egin{bmatrix} \mu_1 \ \mu_2 \end{bmatrix} \ \Sigma &= egin{bmatrix} \Sigma_{11} & \Sigma_{12} \ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \end{aligned}$$

Then, \mathbf{X}_1 and \mathbf{X}_2 are independent if and only if $\mathbf{\Sigma}_{12} = \mathbf{0}$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Proof

Note that $\Sigma_{12} = \Sigma'_{21}$

The joint MGF of \mathbf{X}_1 and \mathbf{X}_2

 $M_{\mathbf{x}_{1},\mathbf{x}_{2}}(\mathbf{t}_{1},\mathbf{t}_{2}) = \exp\left\{\mathbf{t}_{1}'\mu_{1} + \mathbf{t}_{2}'\mu_{2} + \frac{1}{2}\left(\mathbf{t}_{1}'\boldsymbol{\Sigma}_{11}\mathbf{t}_{1} + \mathbf{t}_{2}'\boldsymbol{\Sigma}_{22}\mathbf{t}_{2} + \mathbf{t}_{2}'\boldsymbol{\Sigma}_{21}\mathbf{t}_{1} + \mathbf{t}_{1}'\boldsymbol{\Sigma}_{12}\mathbf{t}_{2}\right)\right\}$ (29) We used

 $\mathbf{t}' = (\mathbf{t}_1', \mathbf{t}_2')$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

By Corollary (2.1),

- $\mathbf{X}_1 \sim N_m(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11})$
- $\mathbf{X}_2 \sim N_p(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_{22})$

The product of their marginal MGFs

$$M_{\mathbf{x}_{1}}(\mathbf{t}_{1})M_{\mathbf{x}_{2}}(\mathbf{t}_{2}) = \exp\left\{\mathbf{t}_{1}'\boldsymbol{\mu}_{1} + \mathbf{t}_{2}'\boldsymbol{\mu}_{2} + \frac{1}{2}\left(\mathbf{t}_{1}'\boldsymbol{\Sigma}_{11}\mathbf{t}_{1} + \mathbf{t}_{2}'\boldsymbol{\Sigma}_{22}\mathbf{t}_{2}\right)\right\}$$
(30)

For \mathbf{X}_1 and \mathbf{X}_2 be independent, Equation (29) and (30) must be identical

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

$$\exp\left\{\mathbf{t}_{1}'\boldsymbol{\mu}_{1} + \mathbf{t}_{2}'\boldsymbol{\mu}_{2} + \frac{1}{2} \left(\mathbf{t}_{1}'\boldsymbol{\Sigma}_{11}\mathbf{t}_{1} + \mathbf{t}_{2}'\boldsymbol{\Sigma}_{22}\mathbf{t}_{2} + \mathbf{t}_{2}'\boldsymbol{\Sigma}_{21}\mathbf{t}_{1} + \mathbf{t}_{1}'\boldsymbol{\Sigma}_{12}\mathbf{t}_{2}\right)\right\} \\ \exp\left\{\mathbf{t}_{1}'\boldsymbol{\mu}_{1} + \mathbf{t}_{2}'\boldsymbol{\mu}_{2} + \frac{1}{2} \left(\mathbf{t}_{1}'\boldsymbol{\Sigma}_{11}\mathbf{t}_{1} + \mathbf{t}_{2}'\boldsymbol{\Sigma}_{22}\mathbf{t}_{2}\right)\right\}$$

Independence of \mathbf{X}_1 and \mathbf{X}_2 is verified when $\Sigma_{12} = \mathbf{0}'$ and hence $\Sigma_{21} = \mathbf{0}$ \rightsquigarrow The covariances between their components are all 0

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distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Theorem

Suppose **X** has a $N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ distribution, partitioned as in Equation (23-24)

$$egin{aligned} \mu &= egin{bmatrix} \mu_1 \ \mu_2 \end{bmatrix} \ \Sigma &= egin{bmatrix} \Sigma_{11} & \Sigma_{12} \ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \end{aligned}$$

Assume that Σ is positive definite

Then, the conditional distribution of $\mathbf{X}_1 | \mathbf{X}_2$

$$N_m \left[\boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} (\boldsymbol{X}_2 - \boldsymbol{\mu}_2), \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \boldsymbol{\Sigma}_{21} \right]$$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Proof

Consider the joint distribution of $\mathbf{W} = \mathbf{X}_1 - \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \mathbf{X}_2$ and \mathbf{X}_2

The joint distribution can be obtained from the transformation

$$\begin{bmatrix} \mathbf{W} \\ \mathbf{X}_2 \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbf{I}_m & -\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1} \\ \mathbf{0} & \mathbf{I}_p \end{bmatrix}}_{\mathbf{A}} \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{bmatrix}$$

This is a linear transformation

The joint distribution is multivariate normal (Theorem 2.1)

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

The means

- $E(\mathbf{W}) = \mu_1 \Sigma_{12} \Sigma_{22}^{-1} \mu_2$
- $E(\mathbf{X}_2) = \boldsymbol{\mu}_2$

The covariance matrix

$$\underbrace{\begin{bmatrix} \mathbf{I}_m & -\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1} \\ \mathbf{0} & \mathbf{I}_p \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix}}_{\mathbf{\Sigma}} \underbrace{\begin{bmatrix} \mathbf{I}_m & \mathbf{0}' \\ -\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21} & \mathbf{I}_p \end{bmatrix}}_{\mathbf{A}'} \\ = \begin{bmatrix} \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{21}^{-1}\boldsymbol{\Sigma}_{21} & \mathbf{0}' \\ \mathbf{0} & \boldsymbol{\Sigma}_{22} \end{bmatrix}}$$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

By Theorem 2.2, the random vectors \mathbf{W} and \mathbf{X}_2 are independent

• The conditional of $\mathbf{W}_2 | \mathbf{X}_2$ equals the marginal of \mathbf{W} $\mathbf{W} | \mathbf{X}_2 \sim N_m \left(\mu_1 - \Sigma_{12} \Sigma_{22}^{-1} \mu_2, \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \right)$

Because of this independence,

$$\begin{split} \mathbf{W} + \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \mathbf{X}_2 | \mathbf{X}_2 \\ & \sim N_m \big(\boldsymbol{\mu}_1 - \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \boldsymbol{\mu}_2 + \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \mathbf{X}_2, \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \boldsymbol{\Sigma}_{21} \big) \end{split}$$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Example

Suppose that $(X, Y) \sim N_2(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$$
$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_2^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{bmatrix}$$

 $\rightsquigarrow \mu_1$ and σ_1^2 are the mean and variance of $Y (= X_1)$ $\rightsquigarrow \mu_2$ and σ_2^2 are the mean and variance of $X (= X_2)$

$$N_m \left(\boldsymbol{\mu}_1 - \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \boldsymbol{\mu}_2 + \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \mathbf{X}_2, \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \boldsymbol{\Sigma}_{21} \right)$$

The expression shows the conditional distribution of Y given X = x

$$N\left[\mu_{2} + \rho \frac{\sigma_{2}}{\sigma_{1}}(x - \mu_{1}), \sigma_{2}^{2}(1 - \rho^{2})\right]$$

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An application PCA

The multivariate normal distribution (cont.)

The coefficient of x in the conditional mean of E(Y|x) is $\rho\sigma_2/\sigma_1$

$$E(Y|x) = \mu_2 + \rho \frac{\sigma_2}{\sigma_1}$$

The conditional mean of Y, given that X = x is linear in x

The σ_1 and σ_2 are the respective standard deviations

 ρ is the correlation coefficient of X and Y

Remark

This follows from the fact that the coefficient of x in a linear conditional mean E(Y|x) is the product of correlation coefficient and σ_2/σ_1

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An application PCA

The multivariate normal distribution (cont.)

The mean of the conditional distribution of Y given X = x

• It depends upon x (unless $\rho = 0$)

The variance $\sigma_2^2(1-\rho^2)$ is the same for all real values of x

Thus, given that X = x, the conditional probability that Y is within (≈ 2.57) $\sigma_2 \sqrt{(1-\rho^2)}$ units of the conditional mean is 0.99, whatever is x

Most of the probability for the distribution of (X, Y) lies within the band

$$\mu_2 + \rho \frac{\sigma_2}{\sigma_1} (x - \mu_1) \pm (\approx 2.57) \sigma_2 \sqrt{1 - \rho^2}$$

about the plot of the linear conditional mean

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The normal distribution

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An application PCA

The multivariate normal distribution (cont.)

Theorem

Suppose **X** has a $N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ distribution

Let Σ is positive definite

Then, the RV $W = (\mathbf{X} - \boldsymbol{\mu})' \boldsymbol{\Sigma} (\mathbf{X} - \boldsymbol{\mu})$ has a $\chi^2(n)$ distribution

Proof

Write $\Sigma = \Sigma^{1/2} \Sigma^{1/2}$, with $\Sigma^{1/2} = \Gamma' \Lambda^{1/2} \Gamma$ Then, $\mathbf{Z} = \Sigma^{-1/2} (\mathbf{X} - \mu)$ is $N_n(\mathbf{0}, \mathbf{I}_n)$

Let $W = \mathbf{Z}'\mathbf{Z} = \sum_{i=1}^{n} Z_i^2$

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The normal distribution

The multivariate normal distribution

An application PCA

The multivariate normal distribution (cont.)

Each Z_i has a N(0, 1) distribution, for i = 1, 2, ..., nFrom Theorem 1.1, it follows that Z_i^2 has a $\chi^2(1)$ distribution

Variables Z_1, \ldots, Z_n are independent standard normal RVs

- Thus, $\sum_{i=1}^{n} Z_i^2 = W$ has a $\chi^2(n)$ distribution
- (by an earlier corollary)

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PCA

Principal components analysis An application

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The multivariate normal distribution

An application $\$

PCA

Principal components analysis

We consider applications of the multivariate normal distribution

• Principal components analysis (PCA)

It results in a linear function of a multivariate normal random vector

- The function preserves the 'total variation in the problem'
- The random vector has independent components

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The normal distribution

The multivariate normal distribution

An application PCA

Principal components analysis (cont.)

Let the random vector \mathbf{X} has the multivariate normal distribution $N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

• Σ is positive definite

Consider the spectral decomposition of $\Sigma = \Gamma' \Lambda \Gamma$ \rightsquigarrow The eigenvalues form the main diagonal of Λ

 $\lambda_1, \lambda_2, \ldots, \lambda_n$

 $\rightsquigarrow\,$ The corresponding eigenvectors are the columns of Γ

 $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$

Assume without loss of generality that the eigenvalues are sorted

$$\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n > 0$$

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The normal distribution

The multivariate normal distribution

An application PCA

Principal components analysis (cont.)

Define the random vector $\mathbf{Y} = \mathbf{\Gamma}(\mathbf{X} - \boldsymbol{\mu})$

 $\Gamma \Sigma \Gamma' = \Lambda$, thus **Y** has a $N_n(\mathbf{0}, \Lambda)$ distribution (by Theorem 2.1) \rightsquigarrow The components Y_1, Y_2, \ldots, Y_n are independent RVs \rightsquigarrow Y_i has a $N(\mathbf{0}, \lambda_i)$ distribution, for $i = 1, 2, \ldots, n$

The random vector **Y** is the vector of **principal components**

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The normal distribution

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An application

PCA

Principal components analysis (cont.)

Total variation of a random vector sums the variances of its components

For a random vector \mathbf{X} , because $\mathbf{\Gamma}$ is an orthogonal matrix

$$TV(\mathbf{X}) = \sum_{i=1}^{n} \sigma_i^2 = \operatorname{Tr}(\mathbf{\Sigma}) = \operatorname{Tr}(\mathbf{\Gamma}' \mathbf{\Lambda} \mathbf{\Gamma}) = \operatorname{Tr}(\mathbf{\Lambda} \mathbf{\Gamma} \mathbf{\Gamma}') = \sum_{i=1}^{n} \lambda_i = TV(\mathbf{Y})$$

Hence, ${\bf X}$ and ${\bf Y}$ share the same total variation

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The multivariate normal distribution

An application PCA

Principal components analysis (cont.)

Consider the first component of ${\bf Y}$

$$Y_1 = \mathbf{v}_1'(\mathbf{X} - \boldsymbol{\mu})$$

- This is a linear combination of the components of $\mathbf{X}-\boldsymbol{\mu}$
- Because of orthogonality, $||\mathbf{v}_1||^2 = \sum_{j=1}^n v_{1j}^2 = 1$

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The normal distribution

The multivariate normal distribution

An application PCA

Principal components analysis (cont.)

Consider any other linear combination of $(\mathbf{X}-\boldsymbol{\mu})$

$$\mathbf{a}'(\mathbf{X} - \boldsymbol{\mu}), \text{ with } ||\mathbf{a}||^2 = 1$$

As $\mathbf{a} \in \mathcal{R}^n$ and because $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ form a basis for \mathcal{R}^n \rightsquigarrow We must have

$$\mathbf{a} = \sum_{j=1}^{n} a_j \mathbf{v}_j$$

for some set of scalars a_1, a_2, \ldots, a_n

Furthermore, the basis $\{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ is orthonormal

$$\mathbf{a}'\mathbf{v}_i = \Big(\sum_{j=1}^n a_j \mathbf{v}_j\Big)'\mathbf{v}_i = \sum_{j=1}^n a_j \mathbf{v}_j' \mathbf{v}_i = a_i$$

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An application PCA

Principal components analysis (cont.)

We have that
$$\Sigma = \Gamma' \Lambda \Gamma = \sum_{i=1}^n \lambda_i \mathbf{v}_i \mathbf{v}'_i$$
 and that $\lambda_i > 0$

Then, the inequality

$$\operatorname{Var}(\mathbf{a}'\mathbf{X}) = \mathbf{a}'\operatorname{Cov}(\mathbf{X})\mathbf{a} = \mathbf{a}'\mathbf{\Sigma}\mathbf{a} = \sum_{i=1}^{n} \lambda_{i} (\mathbf{a}'\mathbf{v}_{i})^{2}$$
$$= \sum_{i=1}^{n} \lambda_{i} a_{i}^{2} \leq \lambda_{1} \sum_{i=1}^{n} a_{i}^{2} = \lambda_{1} = \operatorname{Var}(Y_{1})$$
(31)

 Y_1 has the maximum variance of any other linear combination $\rightsquigarrow Y_1$ is called the **first principal component** of **X**

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The normal distribution

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An application PCA

Principal components analysis (cont.)

Other components Y_2, Y_3, \ldots, Y_n share a similar property Relative to the order of their associated eigenvalue \rightarrow Second, third, ..., n-th principal component

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The normal distribution

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An application PCA

Principal components analysis (cont.)

Theorem

For j = 2, ..., n and i = 1, 2, ..., j - 1,

$$Var[\mathbf{a}'\mathbf{X}] \leq \lambda_j = Var(Y_j)$$

for all vectors \mathbf{a} such that $\mathbf{a} \perp \mathbf{v}_i$ and $||\mathbf{a}|| = 1$

Proof

The proof follows the lines of that for the first principal component (\star)