Random Variate Generation from Continuous Distribution Function

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References

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3.1.2.1 RVG – Principles (Inverse Transform & Rejection Methods)

Inverse Transform Method

• From a probability density function (PDF), f(x) for $a \le x \le b$, the corresponding cumulative probability density function (CDF), F(x) can be defined as

$$F(x) = \int_{a}^{x} f(x') dx'$$

• When a random variable X follows a PDF, f(x) and its corresponding CDF, F(x), it can be sampled using a random number, ξ , which is sampled from a uniform distribution in interval (0,1), as

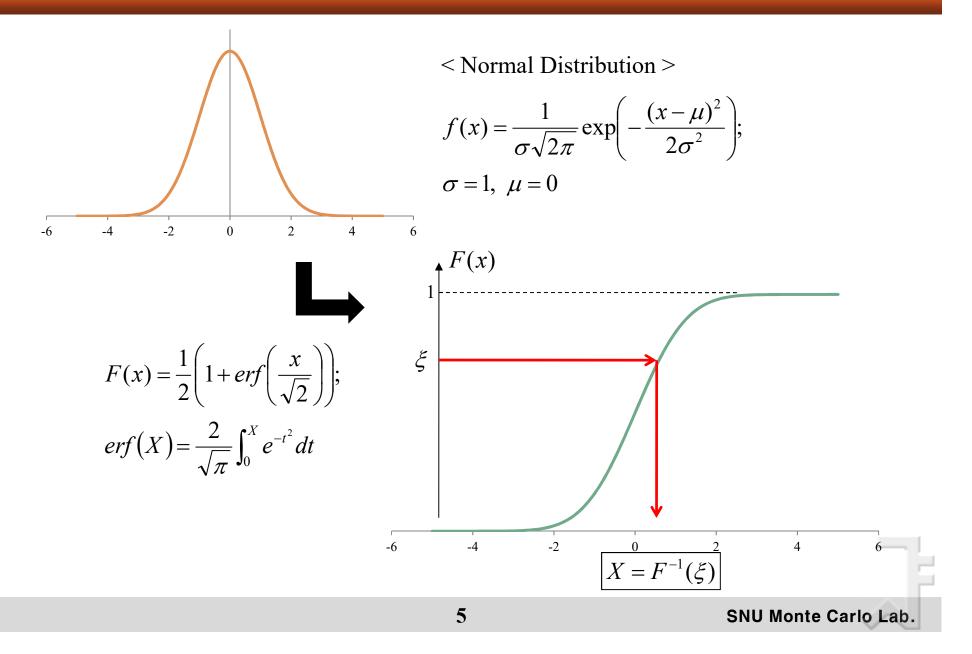
$$\xi = F(x) \implies X = F^{-1}(\xi)$$

Proof:

$$P(X \le x) = P[F^{-1}(\xi) \le x] = P[\xi \le F(x)] = F(x)$$

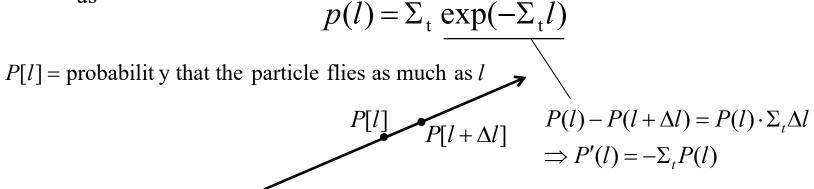


Explanatory Diagram of Inverse Transform Method



Example #1 – Sampling the flight length

A probability that a particle flies as long as l and collides with a atom can be written as

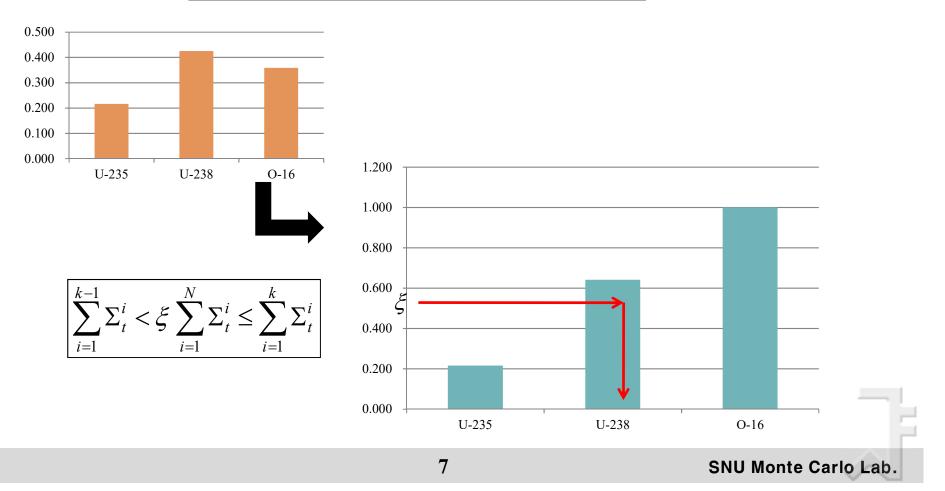


• Then, the flight length can be sampled by

$$\xi = \int_0^x \Sigma_t \exp(-\Sigma_t l) dl$$
$$\mathbf{I}$$
$$\mathbf{I}$$
$$x = -\frac{\ln(1-\xi)}{\Sigma_t} = -\frac{\ln\xi'}{\Sigma_t}$$

Example #2 – Selection of a Collided Nuclide

Nuclide	Σ_{t}	PDF	CDF
U-235	0.107	0.216	0.216
U-238	0.211	0.425	0.641
O-16	0.178	0.359	1.000

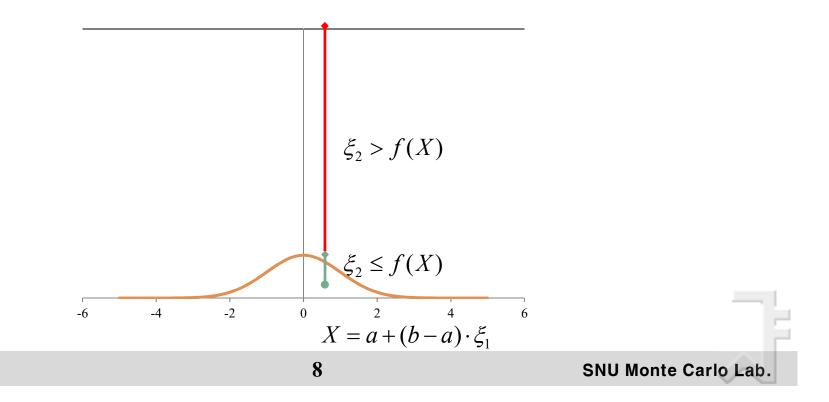


Acceptance – Rejection Method – 1/2

- It is common that the CDF and its inverse function for a random variable cannot be analytically obtained.
- A random variable X, which follows the PDF, f(x) in interval [a,b] can be sampled by trial and error as

① Sample *X* by $X = a + (b - a) \cdot \xi_1$ using a random number ξ_1 .

② From another random number ξ_2 , accept *X* if $\xi_2 \leq f(X)$ and return to ① elsewhere.



Acceptance – Rejection Method – 2/2

• In order to enhance the sampling efficiency, the PDF f(x) can be represented as

$$f(x) = Ch(x)g(x)$$

where $C \ge 1$, h(x) is also a PDF, and $0 < g(x) \le 1$.

- Then X can be sampled as
 - (1) Sample X from the PDF of h(x).
 - ② Using a random number ξ , accept X if $\xi \leq g(X)$ and reject elsewhere.

Example #1 – Sampling from Normal Distribution

• The standard normal distribution can be expressed as

$$f(x) = \sqrt{\frac{2}{\pi}} \exp\left(-\frac{x^2}{2}\right) = Ch(x)g(x), \ x \ge 0;$$
$$C = \sqrt{\frac{2e}{\pi}}, \ h(x) = e^{-x}, \ g(x) = \exp\left[-\frac{(x-1)^2}{2}\right]$$

Then X can be sampled by
 ① Sample X from h(x).

$$\int_0^x e^{-x'} dx' = 1 - e^{-x} = \xi \Longrightarrow X = -\ln(1 - \xi) \Longrightarrow X = -\ln\xi$$

(2) If the below condition is satisfies, accept X. The condition is violated, go to step (1).

$$\xi \le \exp\left[-\frac{(X-1)^2}{2}\right] \Rightarrow -\ln\xi \le \frac{(X-1)^2}{2}$$

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Example #2 – Sampling from Isotropic Distribution

• Method 1

```
phi=2*PI*RNG->GetRN();
sinP=sin(phi); cosP=cos(phi);
```

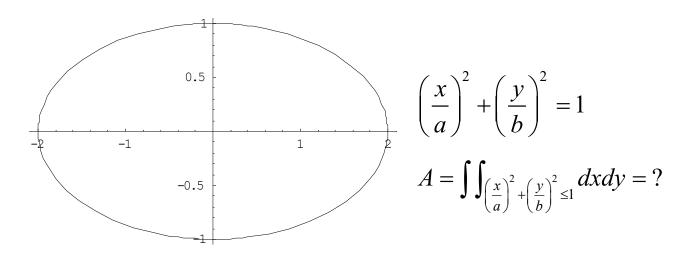
• Method 2

```
do {
   C1=2.*RNG->GetRN()-1.;
   C2=2.*RNG->GetRN()-1.;
   C3=C1*C1+C2*C2;
}while(C3>1.);
C4=sqrt(C3); sinP=C1/C4; cosP=C2/C4;
```

3.1.2.2 Substitution of Variables in Multiple Integration



Compute the Area of an Ellipse



• By substituting *x* and *y* as

$$u = \frac{x}{a}, v = \frac{y}{b} \implies dx = adu, dy = bdv$$

the double integrals can be computed by

$$A = \iint_{\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 \le 1} dx dy$$
$$= \iint_{u^2 + v^2 \le 1} ab du dv = \pi ab$$

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Integration by Linear Transformation

In the double integrations, we are going to change the original set of variables (x,y) to a set of other variables (u,v).

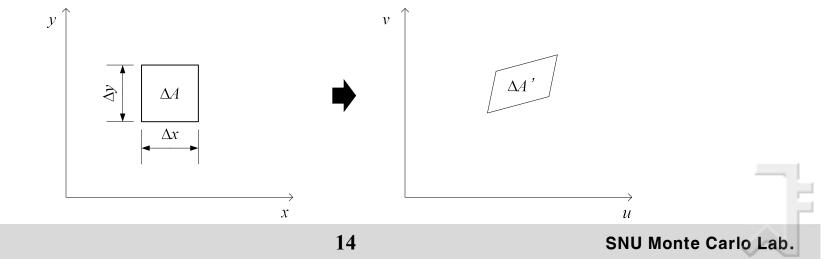
$$\iint \cdots dx dy = \iint \cdots du dv$$

- Then our problem becomes how to convert a small area of $\Delta A = \Delta x \Delta y$ to the corresponding area of $\Delta A' = \Delta u \Delta v$.
- Consider the two-dimensional linear transformation as

 $u = a_{11}x + a_{12}y,$

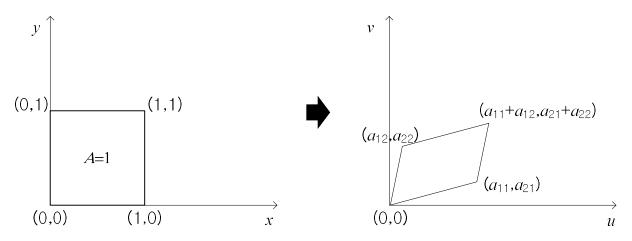
 $v = a_{21}x + a_{22}y$

• Then the rectangular area is converted to the area of a parallelogram as



Integration by Linear Transformation (Contd.)

• From the property of the linear transformation, the scaling factor F in $\Delta A' = F \Delta A$ is independent of its location and size.



• The scaling factor *F* becomes the area of the parallelogram:

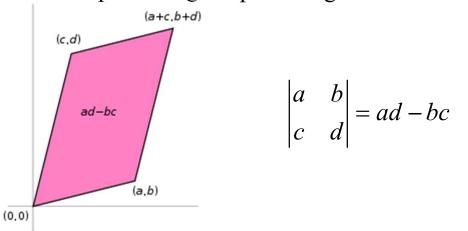
$$F = A' = a_{11}a_{22} - a_{12}a_{21}$$

Therefore the integration becomes

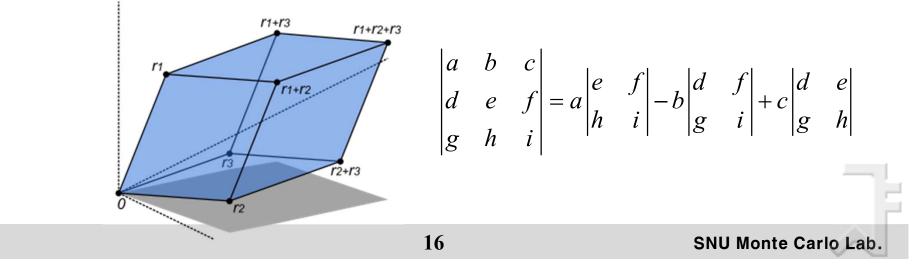
$$\iint \cdots dx dy = \iint \cdots F^{-1} du dv$$

Meaning of Determinant

• The area of the parallelogram is the absolute value of the determinant of the matrix formed by the vectors representing the parallelogram's sides.



• The volume of the parallelepiped is the absolute value of the determinant of the matrix formed by the rows *r*1, *r*2, and *r*3.



Properties of Determinant

$$\det(A^T) = \det(A)$$

$$\det(A^{-1}) = 1/\det(A)$$

 $\det(AB) = \det(A)\det(B)$

General Transformation

• When the variable *x* and *y* are transformed to *u* and *v* as

```
u \equiv u(x, y),v \equiv v(x, y)
```

• Then, by the linear approximation Δx and Δy can be written as

$$\Delta u \cong u_x \Delta x + u_y \Delta y, \ \Delta v \cong v_x \Delta x + v_y \Delta y;$$

$$f_\alpha = \frac{\partial f}{\partial \alpha} \ (f = u \text{ or } v, \ \alpha = x \text{ or } y)$$

$$\begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix} = \begin{pmatrix} u_x & u_y \\ v_x & v_y \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix}$$

In the same way to the linear transformation, the small rectangular area in *x-y* coordinate becomes a small area of the corresponding parallelogram in *u-v* coordinate.

$$(\Delta x, 0) \Rightarrow (u_x \Delta x, v_x \Delta x)$$

(0, Δy) $\Rightarrow (u_y \Delta y, v_y \Delta y)$ \blacktriangleright $Area' = \begin{vmatrix} u_x & u_y \\ v_x & v_y \end{vmatrix} \Delta x \Delta y$

Jacobian Matrix

 In vector calculus, the Jacobian matrix is the matrix of all first-order partial derivatives of a vector- or scalar-valued function with respect to another vector.

$$J = \begin{pmatrix} \frac{\partial F_1}{\partial x_1} & \cdots & \frac{\partial F_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_m}{\partial x_1} & \cdots & \frac{\partial F_m}{\partial x_n} \end{pmatrix} \equiv \frac{\partial (F_1, \cdots, \partial F_m)}{\partial (x_1, \cdots, x_n)}$$

• According to the inverse function theorem, the matrix inverse of the Jacobian matrix of an invertible function is the Jacobian matrix of the *inverse* function.

$$J(\mathbf{F}^{-1}(p)) = \left[J(\mathbf{F}(p))\right]^{-1}$$

If *m=n*, then F is a function from *n*-space to *n*-space and the Jacobian matrix is a square matrix. We can then form its determinant, known as the Jacobian determinant. <u>The Jacobian determinant is sometimes simply called "the Jacobian."</u>

$$J = \begin{vmatrix} \frac{\partial F_1}{\partial x_1} & \cdots & \frac{\partial F_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_m}{\partial x_1} & \cdots & \frac{\partial F_m}{\partial x_n} \end{vmatrix} = \frac{\partial (F_1, \cdots, \partial F_m)}{\partial (x_1, \cdots, x_n)}$$
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Change of Variables in Double Integrals

- Sometimes, it is often advantageous to evaluate $\iint_{R} f(x, y) dx dy$ in a coordinate system other than the *xy*-coordinate system.
- The formula for change of variables is given by

$$\iint_{R} f(x, y) dx dy = \iint_{S} f\left[x(u, v), y(u, v)\right] \left| \frac{\partial(x, y)}{\partial(u, v)} \right| du dv$$

where $|\ldots|$ means the absolute value.

Example 1 of Transformation to Polar Coordinates

• Let *R* be the disc of radius 2 centered at the origin. Calculate

$$\iint_R \sin(x^2 + y^2) dx dy = ?$$

• Solution:

$$\int \sin(x^2 + y^2) dx dy = \iint_S \sin r \left\| \begin{array}{c} \cos \theta & -r \sin \theta \\ \sin \theta & r \cos \theta \end{array} \right\| dr d\theta$$

$$\boxed{x = r \cos \theta, \quad y = r \sin \theta}$$

$$= 2\pi \int_0^2 r \sin r^2 dr$$

$$\boxed{r^2 = t \Rightarrow 2r dr = dt}$$

$$= \pi \int_0^4 \sin t dt$$

$$= \pi \left(-\cos t \right) \Big|_0^4 = \pi (1 - \cos 4)$$

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Example 2

• Evaluate

$$\iint_{R} e^{x^2 + y^2} dx dy$$

where *R* is the region between the two circles $x^2+y^2=1$ and $x^2+y^2=4$.

• Solution:

$$\iint_{R} e^{x^{2} + y^{2}} dx dy = \int_{0}^{2\pi} \int_{1}^{2} e^{-r^{2}} r dr d\theta$$
$$= \int_{0}^{2\pi} \left[-\frac{1}{2} e^{-r^{2}} \right]_{1}^{2} d\theta$$
$$= \pi (e^{-1} - e^{-4})$$

Example 3

• The function $\exp(-x^2)$ has no elementary anti-derivative. But we can evaluate $\int_{-\infty}^{\infty} e^{-x^2} dx$ by using the theory of double integrals.

$$\left(\int_{-\infty}^{\infty} e^{-x^2} dx\right)^2 = \left(\int_{-\infty}^{\infty} e^{-x^2} dx\right) \left(\int_{-\infty}^{\infty} e^{-x^2} dx\right) = \left(\int_{-\infty}^{\infty} e^{-x^2} dx\right) \left(\int_{-\infty}^{\infty} e^{-y^2} dy\right)$$
$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^2+y^2)} dx dy$$

• Now transform to polar coordinates $x=r\cos\theta$, $y=r\sin\theta$.

$$\int_{-\infty}^{\infty} e^{-x^2} dx \Big)^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^2 + y^2)} dx dy$$
$$= \int_{0}^{2\pi} \int_{0}^{\infty} e^{-r^2} r dr d\theta$$
$$= \int_{0}^{2\pi} \left[-\frac{1}{2} e^{-r^2} \right]_{0}^{\infty} d\theta = \pi$$

Hence

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

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3.1.2.3 Generations of Continuous Random Variables

Normal (Gaussian) Distribution

• If $Z \sim N(\mu, \sigma^2)$, its pdf is given by

$$f(z) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{(z-\mu)^2}{2\sigma^2}\right\}, \quad -\infty < z < \infty$$

where μ is the mean and σ^2 the variance of the distribution.

- We consider only generation from N(0,1) (standard normal variables), since any random $Z \sim N(\mu, \sigma^2)$ can be represented as $Z = \mu + \sigma X$, where X is from N(0,1).
- Box and Müller Algorithm:
 - Let *X* and *Y* be two independent standard normal random variables, so (*X*,*Y*) is a random point in the plane.
 - Then the pdf of the two random variable, f(x,y) can be expressed as

$$f(x, y) = \left(\frac{1}{\sqrt{2\pi}}e^{-x^2/2}\right) \left(\frac{1}{\sqrt{2\pi}}e^{-y^2/2}\right)$$
$$= \frac{1}{2\pi}e^{-(x^2+y^2)/2}$$

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Box and Müller Algorithm (Contd.)

• When $x = r\cos\theta$ and $y = r\sin\theta$, the pdf, $f(r, \theta)$ becomes

$$f(x, y)dxdy = f(r\cos\theta, r\sin\theta) \left| \frac{\partial(r\cos\theta, r\sin\theta)}{\partial(r, \theta)} \right| drd\theta$$
$$= e^{-r^2/2} r dr d\theta$$
$$f(r, \theta) = f_R(r) f_{\Theta}(\theta);$$
$$f_R(r) = e^{-r^2/2} r, f_{\Theta}(\theta) = \frac{1}{2\pi}$$

• Then *r* can be sampled by

$$F(r) = \int_0^r e^{-r'^2/2} r' dr' = \left[-e^{-r'^2/2} \right]_0^r = 1 - e^{-r^2/2} = \xi'$$

$$\Rightarrow e^{-r^2/2} = \xi_1 \Rightarrow r = \sqrt{-2\ln\xi_1}$$

• Because θ can be generated from the uniform distribution over $[0,2\pi]$, X and Y can be sampled by

$$x = \sqrt{-2\ln\xi_1}\cos(2\pi\xi_2),$$

$$y = \sqrt{-2\ln\xi_1}\sin(2\pi\xi_2)$$

Example #1 – Sampling from Isotropic Distribution

• Method 1

```
phi=2*PI*RNG->GetRN();
```

```
sinP=sin(phi); cosP=cos(phi);
```

• Method 2

```
do {
```

```
C1=2.*RNG->GetRN()-1.;
```

```
C2=2.*RNG->GetRN()-1.;
```

```
C3=C1*C1+C2*C2;
```

}while(C3>1.);

```
C4=sqrt(C3); sinP=C1/C4; cosP=C2/C4;
```

Proof of Method 2 for the Isotropic Distribution

Let's consider a uniform distribution in a disc of radius of 1:

$$f(x, y) = \frac{1}{\pi}; x^2 + y^2 < 1$$

Then the corresponding pdf for the polar coordinates becomes

$$f(x, y)dxdy = \frac{1}{\pi} \left| \frac{\partial(x, y)}{\partial(r, \theta)} \right| drd\theta = \frac{1}{\pi} r drd\theta$$
$$f(r, \theta) = f_R(r) f_{\Theta}(\theta);$$
$$f_R(r) = 2r, f_{\Theta}(\theta) = \frac{1}{2\pi}, r \in [0, 1)$$

- Therefore the uniform pdf in a disc can be regarded as the multiplication of $f_R(r)$ and $f_{\Theta}(\theta)$ where $f_{\Theta}(\theta)$ follows the isotropic distribution.
- Then from the sampled X and Y in the xy-coordinates, the R and Θ can be calculated by

$$x = r \cos \theta,$$

$$y = r \sin \theta \qquad \Longrightarrow \qquad \cos \theta = \frac{X}{\sqrt{X^2 + Y^2}}, \quad \sin \theta = \frac{Y}{\sqrt{X^2 + Y^2}}$$
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3.1.2.4 Random Variate Generation from Joint Distribution



Linear Transformation

- Let $\mathbf{x} = (x_1, ..., x_n)^T$ be a column vector in \mathbb{R}^n and \mathbf{A} an $m \times n$ matrix. The mapping $\mathbf{x} \rightarrow \mathbf{z}$, with $\mathbf{z} = \mathbf{A}\mathbf{x}$, is called a linear transformation.
- Now consider a random vector $\mathbf{X} = (X_1, ..., X_n)^T$, and let

$$\mathbf{Z} = \mathbf{A}\mathbf{X}$$

Then \mathbb{Z} is a random vector in \mathbb{R}^m .

• Let's see how the expectation vector and covariance matrix of **Z** are transformed.

$$\mu_{\mathbf{Z}} \equiv E[\mathbf{Z}] = E[\mathbf{A}\mathbf{X}] = \mathbf{A}E[\mathbf{X}] = \mathbf{A}\mu_{\mathbf{X}}$$
$$\mathbf{\Sigma}_{\mathbf{Z}} \equiv E[(\mathbf{Z} - \boldsymbol{\mu}_{\mathbf{Z}})(\mathbf{Z} - \boldsymbol{\mu}_{\mathbf{Z}})^{T}]$$
$$= E[(\mathbf{A}\mathbf{X} - \mathbf{A}\boldsymbol{\mu}_{\mathbf{X}})(\mathbf{A}\mathbf{X} - \mathbf{A}\boldsymbol{\mu}_{\mathbf{X}})^{T}]$$
$$= \mathbf{A}E[(\mathbf{X} - \boldsymbol{\mu}_{\mathbf{X}})(\mathbf{X} - \boldsymbol{\mu}_{\mathbf{X}})^{T}]\mathbf{A}^{T}$$
$$= \mathbf{A}\mathbf{\Sigma}_{\mathbf{X}}\mathbf{A}^{T}$$

Transformation of PDF

• For a linear transformation **z**=**Ax**,

$$f_{\mathbf{Z}}(\mathbf{z}) = \frac{f_{\mathbf{X}}(\mathbf{A}^{-1}\mathbf{z})}{|\mathbf{A}|}$$

• For general transformations

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \rightarrow \begin{pmatrix} g_1(\mathbf{x}) \\ g_2(\mathbf{x}) \\ \vdots \\ g_n(\mathbf{x}) \end{pmatrix} \text{ and } \mathbf{z} = \mathbf{g}(\mathbf{x})$$

, the pdf function for z becomes

$$f_{\mathbf{Z}}(\mathbf{z}) = f_{\mathbf{X}}(\mathbf{g}^{-1}(\mathbf{z})) \left| J_{\mathbf{Z}}(\mathbf{g}^{-1}) \right|; \quad J_{\mathbf{Z}}(\mathbf{g}^{-1}) = \begin{pmatrix} \frac{\partial g_1^{-1}}{\partial z_1} & \cdots & \frac{\partial g_1^{-1}}{\partial z_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial g_n^{-1}}{\partial z_1} & \cdots & \frac{\partial g_n^{-1}}{\partial z_n} \end{pmatrix} \equiv \frac{\partial (g_1^{-1}, \cdots, \partial g_n^{-1})}{\partial (z_1, \cdots, z_n)}$$

Standardization

• Let $X \sim N(0,1)$. Then X has density f_X given by

$$f_X(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$$

• Now consider the transformation $Z = \mu + \sigma X$. Then Z has density

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

In other words, $Z \sim N(\mu, \sigma^2)$.

• If $Z \sim N(\mu, \sigma^2)$, then $(Z - \mu) / \sigma \sim N(0, 1)$. This procedure is called *standardization*.

Standardization of Joint PDF

• We now generalize this to *n* dimensions. Let $X_1, ..., X_n$ be independent and standard normal random variables. The joint pdf of $\mathbf{X} = (X_1, ..., X_n)^T$ is given by

$$f_{\mathbf{X}}(x) = \left(\frac{1}{\sqrt{2\pi}}\right)^n e^{-\frac{1}{2}\mathbf{x}^T\mathbf{x}}$$

• Consider the affine transformation (that is, a linear transformation plus a constant).

 $\mathbf{Z} = \boldsymbol{\mu} + B\mathbf{X}$

• Then the expectation and covariance becomes

$$\mathbf{u}_{\mathbf{Z}} \equiv E[\mathbf{Z}] = E[\mathbf{\mu} + \mathbf{B}\mathbf{X}] = E[\mathbf{\mu}] + \mathbf{B}E[\mathbf{X}] = \mathbf{\mu}$$
$$\mathbf{\Sigma}_{\mathbf{Z}} \equiv E[(\mathbf{Z} - \mathbf{\mu}_{\mathbf{Z}})(\mathbf{Z} - \mathbf{\mu}_{\mathbf{Z}})^{T}]$$
$$= E[(\mathbf{\mu} + \mathbf{B}\mathbf{X} - \mathbf{\mu})(\mathbf{\mu} + \mathbf{B}\mathbf{X} - \mathbf{\mu})^{T}]$$
$$= E[(\mathbf{B}\mathbf{X})(\mathbf{B}\mathbf{X})^{T}]$$
$$= \mathbf{B}E[\mathbf{X}\mathbf{X}^{T}]\mathbf{B}^{T}$$
$$= \mathbf{B}\mathbf{I}\mathbf{B}^{T} = \mathbf{B}\mathbf{B}^{T}$$

• Any random vector of the form of $\mathbf{Z} = \mathbf{\mu} + \mathbf{B}\mathbf{X}$ is said to have a jointly normal or multivariate normal distribution.

Jointly Normal Random Variables

Conversely, given a covariance matrix Σ, there exists a unique lower triangular matrix

$$B = \begin{pmatrix} b_{11} & 0 & \cdots & 0 \\ b_{21} & b_{22} & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{nn} \end{pmatrix}$$

such that $\Sigma = BB^T$. This matrix can be obtained efficiently via the Cholesky decomposition.

Cholesky Square Root Method

- Let Σ be a covariance matrix. Then we wish to find a matrix **B** such that $\Sigma = \mathbf{B}\mathbf{B}^T$.
- The *Cholesky square root method* computes a lower triangular matrix **B** via a set of recursive equations as follows:

$$\mathbf{Z} = \mathbf{\mu} + B\mathbf{X}; \ B = \begin{pmatrix} b_{11} & 0 & \cdots & 0 \\ b_{21} & b_{22} & \cdots & 0 \\ \vdots & \vdots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{nn} \end{pmatrix}$$

$$\Rightarrow Z_{1} = b_{11}X_{1} + \mu_{1} \Rightarrow \sigma^{2}[Z_{1}] = b_{11}^{2} \Rightarrow b_{11} = \sqrt{\sigma^{2}[Z_{1}]}$$

$$Z_{2} = b_{21}X_{1} + b_{22}X_{2} + \mu_{2} \Rightarrow \sigma^{2}[Z_{2}] = b_{21}^{2} + b_{22}^{2}$$

$$\operatorname{cov}[Z_{1}, Z_{2}] = E[(Z_{1} - \mu_{1})(Z_{2} - \mu_{2})]$$

$$= E[((b_{11}X_{1} + \mu_{1}) - \mu_{1})((b_{21}X_{1} + b_{22}X_{2} + \mu_{2}) - \mu_{2})]$$

$$= E[b_{11}X_{1}(b_{21}X_{1} + b_{22}X_{2})]$$

$$= b_{11}b_{21}$$

$$\Rightarrow b_{21} = \frac{\Sigma_{12}}{b_{11}} = \frac{\Sigma_{12}}{\sqrt{\Sigma_{11}}}, \ b_{22} = \sqrt{\Sigma_{22} - \frac{\Sigma_{21}^{2}}{\Sigma_{11}}}$$

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Cholesky Square Root Method (Contd.)

• Generally, the b_{ij} can be found by

$$b_{ij} = \frac{\sum_{ij} - \sum_{k=1}^{j-1} b_{ik} b_{jk}}{\sqrt{\sum_{jj} - \sum_{k=1}^{j-1} b_{jk}^{2}}}$$

where by convention,

$$\sum_{k=1}^{0} b_{ik} b_{jk} = 0, \ 1 \le j \le i \le n$$