EXAMPLES OF MULTIDIMENSIONAL PROBABILITY DISTRIBUTIONS

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In this chapter, popular multidimensional probability distributions and their properties such as the expectation, the variance, and the moment-generating functions are illustrated.

6.1 MULTINOMIAL DISTRIBUTION

The binomial distribution explained in Section 3.2 is the probability distribution of the number x of successful trials in n Bernoulli trials with the probability of success p. The *multinomial distribution* is an extension of the binomial distribution to multidimensional cases.

Let us consider a *d*-sided dice with the probability of obtaining each side $p = (p_1, \dots, p_d)^T$, where

$$p_1, \dots, p_d \ge 0$$
 and $\sum_{j=1}^d p_j = 1$.

Let $\mathbf{x} = (x^{(1)}, \dots, x^{(d)})^{\mathsf{T}}$ be the number of times each side appears when the dice is thrown n times, where

$$\mathbf{x} \in \Delta_{d,n} = \left\{ \mathbf{x} \mid x^{(1)}, \dots, x^{(d)} \ge 0, \ x^{(1)} + \dots + x^{(d)} = n \right\}.$$

The probability distribution that x follows is the multinomial distribution and is denoted by Mult(n, p).

The probability that the *j*th side appears $x^{(j)}$ times is $(p_j)^{x^{(j)}}$, and the number of combinations each of the *d* sides appears $x^{(1)}, \ldots, x^{(d)}$ times for *n* trials is given by

 $\frac{n!}{x^{(1)!\cdots x^{(d)!}}}$. Putting them together, the probability mass function of $\mathrm{Mult}(n, p)$ is given by

$$f(\mathbf{x}) = \frac{n!}{x^{(1)}! \cdots x^{(d)}!} (p_1)^{x^{(1)}} \cdots (p_d)^{x^{(d)}}.$$

When d = 2, Mult(n, p) is reduced to Bi (n, p_1) .

The binomial theorem can also be extended to multinomial theorem:

$$(p_1 + \dots + p_d)^n = \sum_{\mathbf{x} \in \Delta_{d,n}} \frac{n!}{x^{(1)!} \dots x^{(d)!}} (p_1)^{x^{(1)}} \dots (p_d)^{x^{(d)}},$$

with which the moment-generating function of Mult(n, p) can be computed as

$$M_{x}(t) = E[e^{t^{T}x}] = \sum_{x \in \Delta_{d,n}} e^{t_{1}x^{(1)}} \cdots e^{t_{d}x^{(d)}} \frac{n!}{x^{(1)!} \cdots x^{(d)!}} (p_{1})^{x^{(1)}} \cdots (p_{d})^{x^{(d)}}$$

$$= \sum_{x \in \Delta_{d,n}} \frac{n!}{x^{(1)!} \cdots x^{(d)!}} (p_{1}e^{t_{1}})^{x^{(1)}} \cdots (p_{d}e^{t_{d}})^{x^{(d)}}$$

$$= (p_{1}e^{t_{1}} + \cdots + p_{d}e^{t_{d}})^{n}.$$

From this, the expectation of and (co)variance of Mult(n, p) can be computed as

$$E[x^{(j)}] = np_j$$
 and $Cov[x^{(j)}, x^{(j')}] = \begin{cases} np_j(1 - p_j) & (j = j'), \\ -np_jp_{j'} & (j \neq j'). \end{cases}$

6.2 MULTIVARIATE NORMAL DISTRIBUTION

When random variables $y^{(1)}, \ldots, y^{(d)}$ independently follow the standard normal distribution N(0,1), the joint probability density function of $\mathbf{y}=(y^{(1)},\ldots,y^{(d)})^{\mathsf{T}}$ is given by

$$g(\mathbf{y}) = \prod_{j=1}^{d} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(\mathbf{y}^{(j)})^2}{2}\right)$$
$$= \frac{1}{(2\pi)^{d/2}} \exp\left(-\frac{1}{2}\mathbf{y}^{\mathsf{T}}\mathbf{y}\right).$$

The expectation and variance-covariance matrices of y are given by

$$E[\mathbf{v}] = \mathbf{0}$$
 and $V[\mathbf{v}] = \mathbf{I}$,

where $\mathbf{0}$ denotes the zero vector and \mathbf{I} denotes the identity matrix.

Let us transform y by $d \times d$ invertible matrix T and d-dimensional vector μ as

$$x = T y + \mu$$
.

Then the joint probability density function of x is given by

$$f(\mathbf{x}) = g(\mathbf{y})|\det(\mathbf{T})|^{-1}$$

$$= \frac{1}{(2\pi)^{d/2}\det(\mathbf{\Sigma})^{1/2}}\exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}}\mathbf{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right),$$

where det(T) is the Jacobian (Fig. 4.2), and

$$\Sigma = TT^{\top}$$
.

This is the general form of the *multivariate normal distribution* and is denoted by $N(\mu, \Sigma)$. The expectation and variance-covariance matrices of $N(\mu, \Sigma)$ are given by

$$E[x] = TE[y] + \mu = \mu,$$

$$V[x] = V[Ty + \mu] = TV[y]T^{\top} = \Sigma.$$

Probability density functions of two-dimensional normal distribution $N(\mu, \Sigma)$ are illustrated in Fig. 6.1. The contour lines of two-dimensional normal distributions are *elliptic*, and their *principal axes* agree with the coordinate axes if the variance-covariance matrix is diagonal. Furthermore, the elliptic contour lines become spherical if all diagonal elements are equal (i.e., the variance-covariance matrix is proportional to the identity matrix).

Eigendecomposition of variance-covariance matrix Σ (see Fig. 6.2) shows that the principal axes of the ellipse are parallel to the eigenvectors of Σ , and their length is proportional to the square root of the eigenvalues (Fig. 6.3).

6.3 DIRICHLET DISTRIBUTION

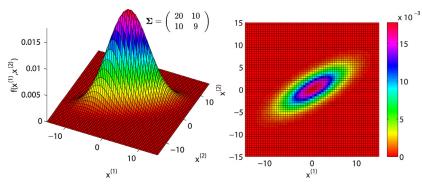
Let $\alpha = (\alpha_1, \dots, \alpha_d)^{\mathsf{T}}$ be a d-dimensional vector with positive entries and let $y^{(1)}, \dots, y^{(d)}$ be random variables that independently follow the gamma distribution $\mathrm{Ga}(\alpha_j, \lambda)$. For $V = \sum_{j=1}^d y^{(j)}$, let

$$\mathbf{x} = (x^{(1)}, \dots, x^{(d)})^{\top} = \left(\frac{y^{(1)}}{V}, \dots, \frac{y^{(d)}}{V}\right)^{\top}.$$

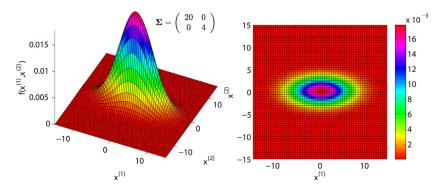
Then the distribution that the above d-dimensional vector x follows is called the *Dirichlet distribution* and is denoted by $Dir(\alpha)$. The domain of x is given by

$$\Delta_d = \{ \boldsymbol{x} \mid x^{(1)}, \dots, x^{(d)} \ge 0, \ x^{(1)} + \dots + x^{(d)} = 1 \}.$$

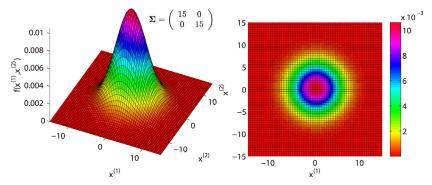
Drawing a value from a Dirichlet distribution corresponds to generating a (unfair) d-sided die.



(a) When Σ is generic, the contour lines are elliptic



(b) When Σ is diagonal, the principal axes of the elliptic contour lines agree with the coordinate axes



(c) When $\boldsymbol{\Sigma}$ is proportional to identity, the contour lines are spherical

FIGURE 6.1

Probability density functions of two-dimensional normal distribution $N(\mu, \Sigma)$ with $\mu = (0, 0)^{T}$.

For $d \times d$ matrix A, a nonzero vector ϕ and a scalar λ that satisfy

$$A\phi = \lambda \phi$$

are called an *eigenvector* and an *eigenvalue* of A, respectively. Generally, there exist d eigenvalues $\lambda_1, \ldots, \lambda_d$ and they are all real when A is symmetric. A matrix whose eigenvalues are all positive is called a *positive definite matrix*, and a matrix whose eigenvalues are all non-negative is called a *positive semidefinite matrix*. Eigenvectors ϕ_1, \ldots, ϕ_d corresponding to eigenvalues $\lambda_1, \ldots, \lambda_d$ are orthogonal and are usually normalized, i.e., they are *orthonormal* as

$$\boldsymbol{\phi}_j^{\mathsf{T}} \boldsymbol{\phi}_{j'} = \begin{cases} 1 & (j = j'), \\ 0 & (j \neq j'). \end{cases}$$

A matrix A can be expressed by using its eigenvectors and eigenvalues as

$$A = \sum_{j=1}^{d} \lambda_j \boldsymbol{\phi}_j \boldsymbol{\phi}_j^{\mathsf{T}} = \mathbf{\Phi} \mathbf{\Lambda} \mathbf{\Phi}^{\mathsf{T}},$$

where $\Phi = (\phi_1, \dots, \phi_d)$ and Λ is the diagonal matrix with diagonal elements $\lambda_1, \dots, \lambda_d$. This is called *eigenvalue decomposition* of A. In MATLAB, eigenvalue decomposition can be performed by the eig function. When all eigenvalues are nonzero, the inverse of A can be expressed as

$$A^{-1} = \sum_{j=1}^{d} \lambda_j^{-1} \boldsymbol{\phi}_j \boldsymbol{\phi}_j^{\top} = \mathbf{\Phi} \boldsymbol{\Lambda}^{-1} \mathbf{\Phi}^{\top}.$$

For $d \times d$ matrix A and $d \times d$ positive symmetric matrix B, a nonzero vector ϕ and a scalar λ that satisfy

$$A\phi = \lambda B\phi$$

are called a generalized eigenvector and a generalized eigenvalue of A, respectively.

FIGURE 6.2

Eigenvalue decomposition.

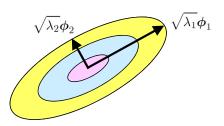


FIGURE 6.3

Contour lines of the normal density. The principal axes of the ellipse are parallel to the eigenvectors of variance-covariance matrix Σ , and their length is proportional to the square root of the eigenvalues.

The probability density function of $Dir(\alpha)$ is given by

$$f(\mathbf{x}) = \frac{\prod_{j=1}^{d} (x^{(j)})^{\alpha_j - 1}}{B_d(\alpha)},$$

where

$$B_d(\boldsymbol{\alpha}) = \int_{\Delta_d} \prod_{j=1}^d (x^{(j)})^{\alpha_j - 1} d\boldsymbol{x}$$
 (6.1)

is the *d*-dimensional *beta function*.

For $x = (\sqrt{p} \sin \theta)^2$ with $0 \le p \le 1$, Eq. (4.6) implies

$$\int_0^p x^{\alpha-1} (p-x)^{\beta-1} dx$$

$$= \int_0^{\frac{\pi}{2}} (\sqrt{p} \sin \theta)^{2(\alpha-1)} \left(p - (\sqrt{p} \sin \theta)^2 \right)^{\beta-1} \frac{dx}{d\theta} d\theta$$

$$= \int_0^{\frac{\pi}{2}} p^{\alpha-1} (\sin \theta)^{2(\alpha-1)} p^{\beta-1} (\cos \theta)^{2(\beta-1)} \cdot 2p \sin \theta \cos \theta d\theta$$

$$= p^{\alpha+\beta-1} \left(2 \int_0^{\frac{\pi}{2}} (\sin \theta)^{2\alpha-1} (\cos \theta)^{2\beta-1} d\theta \right)$$

$$= p^{\alpha+\beta-1} B(\alpha, \beta).$$

Letting $p = 1 - \sum_{j=1}^{d-2} x^{(j)}$, the integration with respect to $x^{(d-1)}$ in

$$B_{d}(\alpha) = \int_{0}^{1} (x^{(1)})^{\alpha_{1}-1} \times \int_{0}^{1-x^{(1)}} (x^{(2)})^{\alpha_{2}-1} \times \cdots \times \int_{0}^{1-\sum_{j=1}^{d-2} x^{(j)}} (x^{(d-1)})^{\alpha_{d-1}-1} \times \left(1 - \sum_{j=1}^{d-1} x^{(j)}\right)^{\alpha_{d}-1} dx^{(1)} dx^{(2)} \cdots dx^{(d-1)}$$

can be computed as

$$\int_{0}^{1-\sum_{j=1}^{d-2} x^{(j)}} (x^{(d-1)})^{\alpha_{d-1}-1} \left(1 - \sum_{j=1}^{d-1} x^{(j)}\right)^{\alpha_{d}-1} dx^{(d-1)}$$

$$= \left(1 - \sum_{j=1}^{d-2} x^{(j)}\right)^{\sum_{j=d-1}^{d} \alpha_{j}-1} B(\alpha_{d-1}, \alpha_{d}).$$

Similarly, letting $p = 1 - \sum_{j=1}^{d-3} x^{(j)}$, the integration with respect to $x^{(d-2)}$ in the above equation can be computed as

$$\begin{split} & \int_0^{1-\sum_{j=1}^{d-3} x^{(j)}} (x^{(d-2)})^{\alpha_{d-2}-1} \left(1-\sum_{j=1}^{d-2} x^{(j)}\right)^{\sum_{j=d-1}^{d} \alpha_j-1} \mathrm{d}x^{(d-2)} \\ & = \left(1-\sum_{j=1}^{d-3} x^{(j)}\right)^{\sum_{j=d-2}^{d} \alpha_j-1} B\left(\alpha_{d-2}, \sum_{j=d-1}^{d} \alpha_j\right). \end{split}$$

Repeating this computation yields

$$B_d(\alpha) = \prod_{j=1}^{d-1} B\left(\alpha_j, \sum_{j'=j+1}^d \alpha_{j'}\right).$$

Applying

$$B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)}$$

given in Eq. (4.7) to the above equation, the *d*-dimensional beta function can be expressed by using the gamma function as

$$B_d(\alpha) = \prod_{j=1}^{d-1} \frac{\Gamma(\alpha_j) \Gamma\left(\sum_{j'=j+1}^d \alpha_{j'}\right)}{\Gamma\left(\sum_{j'=j}^d \alpha_{j'}\right)} = \frac{\prod_{j=1}^d \Gamma(\alpha_j)}{\Gamma(\alpha_0)},$$

where

$$\alpha_0 = \sum_{j=1}^d \alpha_j.$$

When d = 2, $x^{(2)} = 1 - x^{(1)}$ holds and thus the Dirichlet distribution is reduced to the beta distribution shown in Section 4.4:

$$f(x) = \frac{x^{\alpha_1 - 1} (1 - x)^{\alpha_2 - 1}}{B(\alpha_1, \alpha_2)}.$$

Thus, the Dirichlet distribution can be regarded as a multidimensional extension of the beta distribution.

The expectation of $Dir(\alpha)$ is given by

$$\begin{split} E[x^{(j)}] &= \frac{\int x^{(j)} \prod_{j'=1}^{d} (x^{(j')})^{\alpha_{j'}-1} \mathrm{d}x^{(j)}}{B_d(\alpha)} \\ &= \frac{B_d(\alpha_1, \dots, \alpha_{j-1}, \alpha_j + 1, \alpha_{j+1}, \dots, \alpha_d)}{B_d(\alpha_1, \dots, \alpha_{j-1}, \alpha_j, \alpha_{j+1}, \dots, \alpha_d)} \\ &= \frac{\Gamma(\alpha_1) \cdots \Gamma(\alpha_{j-1}) \Gamma(\alpha_j + 1) \Gamma(\alpha_{j+1}) \cdots \Gamma(\alpha_d) \times \Gamma(\alpha_0)}{\Gamma(\alpha_0 + 1) \times \Gamma(\alpha_1) \cdots \Gamma(\alpha_{j-1}) \Gamma(\alpha_j) \Gamma(\alpha_j) \Gamma(\alpha_{j+1}) \cdots \Gamma(\alpha_d)} \\ &= \frac{\Gamma(\alpha_j + 1) \Gamma(\alpha_0)}{\Gamma(\alpha_0 + 1) \Gamma(\alpha_j)} = \frac{\alpha_j \Gamma(\alpha_j) \Gamma(\alpha_0)}{\alpha_0 \Gamma(\alpha_0) \Gamma(\alpha_j)} \\ &= \frac{\alpha_j}{\alpha_0}. \end{split}$$

The variance and covariance of $Dir(\alpha)$ can also be obtained similarly as

$$\operatorname{Cov}[x^{(j)}, x^{(j')}] = \begin{cases} \frac{\alpha_j(\alpha_0 - \alpha_j)}{\alpha_0^2(\alpha_0 + 1)} & (j = j'), \\ -\frac{\alpha_j \alpha_{j'}}{\alpha_0^2(\alpha_0 + 1)} & (j \neq j'). \end{cases}$$

Probability density functions of $Dir(\alpha)$ when d=3 are illustrated in Fig. 6.4. When $\alpha_1=\alpha_2=\alpha_3=\alpha$, the probability density takes larger values around the corners of the triangle if each $\alpha<1$, the probability density is uniform if each $\alpha=1$, and the probability density takes larger values around the center if each $\alpha>1$. When $\alpha_1,\alpha_2,\alpha_3$ are nonuniform, the probability density tends to take large values around the corners of the triangle with large α_i .

When the Dirichlet parameters α are all equal, i.e.,

$$\alpha_1 = \cdots = \alpha_d = \alpha$$
,

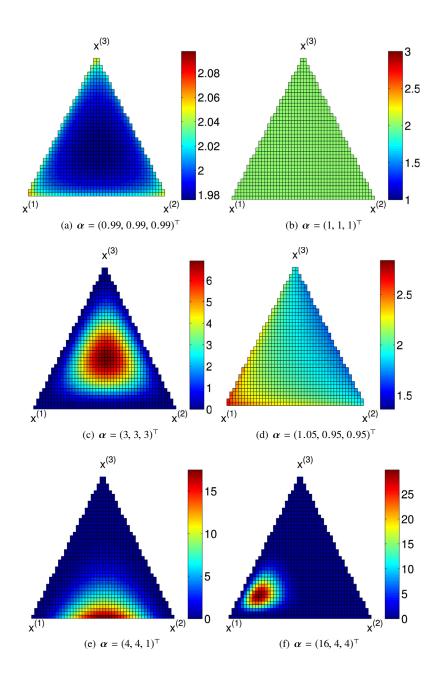


FIGURE 6.4

Probability density functions of Dirichlet distribution $Dir(\alpha)$. The center of gravity of the triangle corresponds to $x^{(1)} = x^{(2)} = x^{(3)} = 1/3$, and each vertex represents the point that the corresponding variable takes one and the others take zeros.

the probability density function is simplified as

$$f(\mathbf{x}) = \frac{\Gamma(\alpha d)}{\Gamma(\alpha)^d} \prod_{j=1}^d (x^{(j)})^{\alpha - 1}.$$

This is called *symmetric Dirichlet distribution* and is denoted by $Dir(\alpha)$. The common parameter α is often referred to as the *concentration parameter*.

6.4 WISHART DISTRIBUTION

Let $x_1, ..., x_n$ be *d*-dimensional random variables independently following the normal distribution $N(\mathbf{0}, \Sigma)$, and let

$$S = \sum_{i=1}^{n} x_i x_i^{\mathsf{T}}$$

be the *scatter matrix* which is assumed to be invertible. The probability distribution that S follows is called the *Wishart distribution* with n degrees of freedom and is denoted by $W(\Sigma, d, n)$. The probability density function of $W(\Sigma, d, n)$ is given by

$$f(S) = \frac{\det(S)^{\frac{n-d-1}{2}} \exp\left(-\frac{1}{2} \operatorname{tr}\left(\Sigma^{-1}S\right)\right)}{\det(2\Sigma)^{\frac{n}{2}} \Gamma_d(\frac{n}{2})},$$

where $\det(\cdot)$ denotes the determinant of a matrix, $\operatorname{tr}(\cdot)$ denotes the trace of a matrix, $\Gamma_d(\cdot)$ denotes the *d*-dimensional *gamma function* defined by

$$\Gamma_d(a) = \int_{\mathbf{S} \in \mathbb{S}_d^+} \det(\mathbf{S})^{a - \frac{d+1}{2}} \exp\left(-\operatorname{tr}(\mathbf{S})\right) d\mathbf{S},\tag{6.2}$$

and \mathbb{S}_d^+ denotes the set of all $d \times d$ positive symmetric matrices.

When $\Sigma = \frac{1}{2}I$, the definition of *d*-dimensional gamma function immediately yields

$$\int_{\mathbf{S} \in \mathbb{S}_d^+} f(\mathbf{S}) d\mathbf{S} = 1. \tag{6.3}$$

Since the Jacobian is given by $\det(2\Sigma)^{\frac{d+1}{2}}$ when S is transformed to $\frac{1}{2}\Sigma^{-1}S$ (Fig. 4.2), Eq. (6.3) is also satisfied for generic $\Sigma \in \mathbb{S}_d^+$.

d-dimensional gamma function $\Gamma_d(\cdot)$ can be expressed by using two-dimensional gamma function $\Gamma(\cdot)$ as

$$\Gamma_d(a) = \pi^{\frac{d(d-1)}{4}} \prod_{j=1}^d \Gamma\left(a + \frac{1-j}{2}\right)$$
$$= \pi^{\frac{d-1}{2}} \Gamma_{d-1}(a) \Gamma\left(a + \frac{1-d}{2}\right).$$

An operator that transforms an $m \times n$ matrix $A = (a_1, \dots, a_n)$ to the mn-dimensional vector,

$$\operatorname{vec}(A) = (a_1^\top, \dots, a_n^\top)^\top,$$

is called the *vectorization operator*. The operator that transforms an $m \times n$ matrix A and a $p \times q$ matrix B to an $mp \times nq$ matrix as

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} a_{1,1} \mathbf{B} & \cdots & a_{1,n} \mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{m,1} \mathbf{B} & \cdots & a_{m,n} \mathbf{B} \end{pmatrix}$$

is called the *Kronecker product*. The vectorization operator and the Kronecker product satisfy the following properties:

$$\operatorname{vec}(\boldsymbol{A}\boldsymbol{B}\boldsymbol{C}) = (\boldsymbol{C}^{\top} \otimes \boldsymbol{A})\operatorname{vec}(\boldsymbol{B})$$

$$= (\boldsymbol{I} \otimes \boldsymbol{A}\boldsymbol{B})\operatorname{vec}(\boldsymbol{C})$$

$$= (\boldsymbol{C}^{\top}\boldsymbol{B}^{\top} \otimes \boldsymbol{I})\operatorname{vec}(\boldsymbol{A}),$$

$$(\boldsymbol{A} \otimes \boldsymbol{B})^{-1} = \boldsymbol{A}^{-1} \otimes \boldsymbol{B}^{-1},$$

$$(\boldsymbol{A} \otimes \boldsymbol{B})(\boldsymbol{C} \otimes \boldsymbol{D}) = (\boldsymbol{A}\boldsymbol{C} \otimes \boldsymbol{B}\boldsymbol{D}),$$

$$\operatorname{tr}(\boldsymbol{A} \otimes \boldsymbol{B}) = \operatorname{tr}(\boldsymbol{A})\operatorname{tr}(\boldsymbol{B}),$$

$$\operatorname{tr}(\boldsymbol{A}\boldsymbol{B}) = \operatorname{vec}(\boldsymbol{A}^{\top})^{\top}\operatorname{vec}(\boldsymbol{B}),$$

$$\operatorname{tr}(\boldsymbol{A}\boldsymbol{B}\boldsymbol{C}\boldsymbol{D}) = \operatorname{vec}(\boldsymbol{A}^{\top})^{\top}(\boldsymbol{D}^{\top} \otimes \boldsymbol{B})\operatorname{vec}(\boldsymbol{C}).$$

These formulas allow us to compute the product of big matrices efficiently.

FIGURE 6.5

Vectorization operator and Kronecker product.

Thus, the Wishart distribution can be regarded as a multidimensional extension of the gamma distribution. When d = 1, S and Σ become scalars, and letting S = x and $\Sigma = 1$ yields

$$f(x) = \frac{x^{\frac{n}{2}-1} \exp\left(-\frac{x}{2}\right)}{2^{\frac{n}{2}} \Gamma\left(\frac{n}{2}\right)}.$$

This is equivalent to the probability density function of the chi-squared distribution with n degrees of freedom explained in Section 4.3.

The moment-generating function of $W(\Sigma, d, n)$ can be obtained by transforming S to $(\frac{1}{2}\Sigma^{-1} - T)S$ as

$$\begin{split} M_{S}(T) &= E[e^{\operatorname{tr}(TS)}] \\ &= \int_{S \in \mathbb{S}_{d}^{+}} \frac{\det(S)^{\frac{n-d-1}{2}} \exp\left(-\operatorname{tr}\left((\frac{1}{2}\Sigma^{-1} - T)S\right)\right)}{2^{\frac{dn}{2}} \det(\Sigma)^{\frac{n}{2}} \Gamma_{d}(\frac{n}{2})} \mathrm{d}S \\ &= \det(I - 2T\Sigma)^{-\frac{n}{2}}. \end{split}$$

The expectation and variance-covariance matrices of S that follows $W(\Sigma,d,n)$ are given by

$$E[S] = n\Sigma$$
 and $V[\text{vec}(S)] = 2n\Sigma \otimes \Sigma$,

where $\text{vec}(\cdot)$ is the vectorization operator and \otimes denotes the *Kronecker product* (see Fig. 6.5).