Statistical Machine Learning

Distributions

Lecture Notes 5: Jacobian and Wedge

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5.1 More About Mixture Distribution

Theorem 5.1. Let X be an $m \times 1$ random vector having a density function $f_{\mathbf{X}}(\mathbf{x})$, which is positive on a set $\mathcal{X} \subset \mathbb{R}^m$. Suppose the transform $\mathbf{y} = \mathbf{y}(\mathbf{x}) = (y_1(\mathbf{x}), y_2(\mathbf{x}), \dots, y_m(\mathbf{x}))^T$ is 1-1 for some \mathcal{Y} , where \mathcal{Y} denotes the image of \mathcal{X} under \mathbf{y} , s.t. the inverse transformation $\mathbf{x} = \mathbf{x}(\mathbf{y})$ exists for $\mathbf{y} \in \mathcal{Y}$. Assuming that the partial derivatives $\frac{\partial x_i}{\partial y_j}$'s, $(i, j = 1, 2, \dots, m)$ exist and continuous on \mathcal{Y} , it is well known that the density function of random vector $\mathbf{Y} = \mathbf{y}(\mathbf{X})$ is

$$f_{\mathbf{Y}}(\mathbf{y}) = f_{\mathbf{X}}(\mathbf{x}(\mathbf{y}))|J(\mathbf{x} \to \mathbf{y})|, \ \mathbf{y} \in \mathcal{Y}$$
 (1)

where $J(\mathbf{x} \to \mathbf{y})$ is the determinant of the Jacobian of the transformation, i.e.

$$J(\mathbf{x} \to \mathbf{y}) = \det \begin{pmatrix} \frac{\partial x_1}{\partial y_1} & \frac{\partial x_1}{\partial y_2} & \dots & \frac{\partial x_1}{\partial y_m} \\ \frac{\partial x_2}{\partial y_1} & \frac{\partial x_2}{\partial y_2} & \dots & \frac{\partial x_2}{\partial y_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial x_m}{\partial y_1} & \frac{\partial x_m}{\partial y_2} & \dots & \frac{\partial x_m}{\partial y_m} \end{pmatrix}$$
(2)

Then we define the exterior product, or wedge product, which is a useful tool to calculate the determinant.

Definition 5.1 (Wedge Product). The exterior product or wedge product of dx and dy, denoted as $dx \wedge dy$, has the property that $dx \wedge dy = -dy \wedge dx$.

Therefore, it's easy to prove that when x = y, $dx \wedge dx = 0$.

Theorem 5.2. If $d\mathbf{y} = (dy_1, dy_2, \dots, dy_m)^T$ is an $m \times 1$ vector of differentials and if $d\mathbf{x} = (dx_1, dx_2, \dots, dx_m)^T = \mathbf{B}dy$, where \mathbf{B} is an $m \times m$ nonsingular matrix, then

$$\bigwedge_{i=1}^{m} dx_i = \det(\mathbf{B}) \bigwedge_{i=1}^{m} dy_i \tag{3}$$

Proof. We'll prove it by induction.

m = 2:

$$\begin{pmatrix} dx_1 \\ dx_2 \end{pmatrix} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} dy_1 \\ dy_2 \end{pmatrix} = \begin{pmatrix} B_{11}dy_1 + B_{12}dy_2 \\ B_{21}dy_1 + B_{22}dy_2 \end{pmatrix}$$
(4)

Since $dy_i \wedge dy_i = 0$ and $dy_2 \wedge dy_1 = -dy_1 \wedge dy_2$, we have

$$dx_1 \wedge dx_2 = (B_{11}dy_1 + B_{12}dy_2) \wedge (B_{21}dy_1 + B_{22}dy_2) \tag{5}$$

$$= (B_{11}B_{22} - B_{12}B_{21})dy_1 \wedge dy_2 = \det(\mathbf{B})dy_1 \wedge dy_2 \tag{6}$$

Suppose eq. 3 holds for
$$m-1$$
. Now consider the case of m . Let $\mathbf{B} = \begin{pmatrix} \mathbf{A}_{(m-1)\times(m-1)} & \mathbf{b} \\ \mathbf{a}^T & B_{mm} \end{pmatrix}$ and $\mathbf{Q} = \begin{pmatrix} \mathbf{I}_{(m-1)\times(m-1)} & -\mathbf{b}B_{mm}^{-1} \\ 0 & 1 \end{pmatrix}$.

$$d\mathbf{x} = \begin{pmatrix} \mathbf{A}_{(m-1)\times(m-1)} & \mathbf{b} \\ \mathbf{a}^T & B_{mm} \end{pmatrix} d\mathbf{y}$$

$$\implies \mathbf{Q}d\mathbf{x} = \mathbf{Q}\mathbf{B}d\mathbf{y}$$

$$\implies \begin{pmatrix} d\mathbf{x}_{1:(m-1)} - B_{mm}^{-1}\mathbf{b}dx_m \\ dx_m \end{pmatrix} = \begin{pmatrix} (\mathbf{A} - B_{mm}^{-1}\mathbf{b}\mathbf{a}^T)d\mathbf{y}_{1:(m-1)} \\ \mathbf{a}^T d\mathbf{y}_{1:(m-1)} + B_{mm}dy_m \end{pmatrix}$$

where $d\mathbf{x}_{1:(m-1)} = (dx_1, \dots, dx_{m-1})$ and $d\mathbf{y}_{1:(m-1)}$ is defined similarly. Calculating the wedge for both sides, we have

$$\bigwedge_{i=1}^{m} dx_{i} = \bigwedge ((\mathbf{A} - B_{mm}^{-1} \mathbf{b} \mathbf{a}^{T}) d\mathbf{y}_{1:(m-1)}) \bigwedge (B_{mm} dy_{m})$$

$$= B_{mm} \det(\mathbf{A} - B_{mm}^{-1} \mathbf{b} \mathbf{a}^{T}) \bigwedge_{i=1}^{m} dy_{i}$$

$$= \det \begin{pmatrix} \mathbf{A} - B_{mm}^{-1} \mathbf{b} \mathbf{a}^{T} & \mathbf{0} \\ \mathbf{a}^{T} & B_{mm} \end{pmatrix} \bigwedge_{i=1}^{m} dy_{i}$$

$$= \det(\mathbf{Q}\mathbf{B}) \bigwedge_{i=1}^{m} dy_{i} = \det(\mathbf{Q}) \det(\mathbf{B}) \bigwedge_{i=1}^{m} dy_{i} = \det(\mathbf{B}) \bigwedge_{i=1}^{m} dy_{i}$$

Example 5.1. Convert rectangular coordinates x_1, x_2, \ldots, x_m to polar coordinates $r, \theta_1, \theta_2, \ldots, \theta_{m-1}$, where

$$x_1 = r sin\theta_1 sin\theta_2 \cdots sin\theta_{m-2} sin\theta_{m-1} \tag{7}$$

$$x_2 = r sin\theta_1 sin\theta_2 \cdots sin\theta_{m-2} cos\theta_{m-1} \tag{8}$$

$$\vdots$$
 (9)

$$x_{m-1} = rsin\theta_1 cos\theta_2 \tag{10}$$

$$x_m = rcos\theta_1 \tag{11}$$

$$(r > 0, 0 < \theta_i \le \pi (i = 1, 2, \dots, m - 2), 0 < \theta_{m-1} \le 2\pi).$$
 (12)

Then

$$J(\mathbf{x} \to r, \theta_1, \dots, \theta_{m-1}) = r^{m-1} sin^{m-2} \theta_1 sin^{m-3} \theta_2 \cdots sin\theta_{m-2}.$$
(13)

Proof.

$$\begin{array}{lll} x_1^2 & = r^2 sin^2 \theta_1 sin^2 \theta_2 \cdots sin^2 \theta_{m-2} sin^2 \theta_{m-1} \\ x_1^2 + x_2^2 & = r^2 sin^2 \theta_1 sin^2 \theta_2 \cdots sin^2 \theta_{m-2} \\ \vdots & \vdots & \vdots \\ x_1^2 + \cdots + x_{m-1}^2 & = r^2 sin^2 \theta_1 \\ x_1^2 + \cdots + x_{m-1}^2 + x_m^2 & = r^2 \\ \Longrightarrow 2x_1 dx_1 & = 2r^2 sin^2 \theta_1 \cdots sin^2 \theta_{m-2} sin \theta_{m-1} cos \theta_{m-1} d\theta_{m-1} + \text{terms of } dr, d\theta_1, \dots, d\theta_{m-2} \\ 2x_1 dx_1 + 2x_2 dx_2 & = 2r^2 sin^2 \theta_1 \cdots sin^2 \theta_{m-3} sin \theta_{m-2} cos \theta_{m-2} d\theta_{m-2} + \text{terms of } dr, d\theta_1, \dots, d\theta_{m-3} \\ \vdots & \vdots & \vdots \\ 2x_1 dx_1 + \cdots + 2x_m dx_m = 2r dr \end{array}$$

Take wedge product for LHS and RHS simultaneously. we have

$$2^{m} \prod_{i=1}^{m} x_{i} \bigwedge_{i=1}^{m} dx_{i} = 2^{m} r^{2m-1} sin^{2m-3} \theta_{1} \cdots sin\theta_{m-1} \prod_{i=1}^{m-1} cos\theta_{i} dr \bigwedge (\bigwedge_{i=1}^{m-1} d\theta_{i})$$
 (14)

where

$$\prod_{i=1}^{m} x_i = r^m sin^{m-1} \theta_1 \cdots sin\theta_{m-1} \prod_{i=1}^{m-1} cos\theta_i.$$

$$\tag{15}$$

Then we can prove eq. 13 easily.

Definition 5.2. For any matrix $\mathbf{X} = (x_{ij})_{n \times m}$, $d\mathbf{X} \stackrel{def}{=} (dx_{ij})$, $d(\mathbf{XY}) = \mathbf{X}d\mathbf{Y} + d\mathbf{XY}$, where the symbol $(d\mathbf{X}) = \bigwedge_{i=1}^{n} \bigwedge_{j=1}^{m} dx_{ij}$.

If **X** is a symmetric $m \times m$ matrix, the symbol $(d\mathbf{X}) = \bigwedge_{1 \le i \le j \le m} dx_{ij}$.

Theorem 5.3. Let \mathbf{X} and \mathbf{Y} be two $n \times m$ matrix, and $\mathbf{X} = \mathbf{BYC}$ where $B_{n \times n}$ and $C_{m \times m}$ are nonsingular. Then we have

$$(d\mathbf{X}) = (\det \mathbf{B})^m (\det \mathbf{C})^n (d\mathbf{Y}), \ i.e. J(\mathbf{X} \to \mathbf{Y}) = (\det \mathbf{B})^m (\det \mathbf{C})^n$$
 (16)

Proof.

$$vec(\mathbf{X}) = vec(\mathbf{BYC})$$
 (17)

$$= (\mathbf{C}^T \otimes \mathbf{B}) vec(\mathbf{Y}), \tag{18}$$

where $\mathbf{A} \otimes \mathbf{B} = (a_{ij}\mathbf{B})$ is the Kronecker product of \mathbf{A} and \mathbf{B} and $vec(\mathbf{A})$ is the result of concatenating the columns of \mathbf{A} .

$$(d\mathbf{X}) = \det(\mathbf{C}^T \otimes \mathbf{B})(d\mathbf{Y}) \tag{19}$$

$$= (\det \mathbf{C})^n (\det \mathbf{B})^m (d\mathbf{Y}) \tag{20}$$

(21)

Consider the symmetric case, we have the following.

Theorem 5.4. If $X = BYB^T$ where X and Y are $m \times m$ symmetric matrices and B is a nonsingular matrix, then

$$(d\mathbf{X}) = (\det \mathbf{B})^{m+1}(d\mathbf{Y}), J(\mathbf{X} \to \mathbf{Y}) = (\det \mathbf{B})^{m+1}$$
(22)

Proof.

$$d\mathbf{X} = \mathbf{B}d\mathbf{Y}\mathbf{B}^T \Rightarrow (d\mathbf{X}) = (\mathbf{B}d\mathbf{Y}\mathbf{B}^T) = \rho(\mathbf{B})(d\mathbf{Y})$$
(23)

where $\rho(\mathbf{B})$ is a polynomial of elements of \mathbf{B} .

Lemma 5.1. if ρ is a polynomial and has the property that $\rho(\mathbf{X}_1\mathbf{X}_2) = \rho(\mathbf{X}_1)\rho(\mathbf{X}_2)$, then $\rho(\mathbf{X}) = (\det \mathbf{X})^k$ for some k.

It's easy to show $\rho(\mathbf{B}_1\mathbf{B}_2) = \rho(\mathbf{B}_1)\rho(\mathbf{B}_2)$:

$$(\mathbf{B}_1 \mathbf{B}_2 d \mathbf{Y} \mathbf{B}_2^T \mathbf{B}_1^T) = (\mathbf{B}_1 (\mathbf{B}_2 d \mathbf{Y} \mathbf{B}_2^T) \mathbf{B}_1^T) = \rho(\mathbf{B}_1) (\mathbf{B}_2 d \mathbf{Y} \mathbf{B}_2^T) = \rho(\mathbf{B}_1) \rho(\mathbf{B}_2) (d \mathbf{Y})$$
(24)

Because of this property, we have $\rho(\mathbf{B}) = (\det \mathbf{B})^k$ for some k. To determine k, we consider a simple case where $\mathbf{B} = \operatorname{diag}(b, 1, \dots, 1)$ and let $\mathbf{Y} = (y_{ij})$. Then

$$\mathbf{BYB}^{T} = \begin{pmatrix} b^{2}y_{11} & by_{12} & \cdots & by_{1m} \\ by_{21} & y_{22} & \cdots & y_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ by_{m1} & y_{m2} & \cdots & y_{mm} \end{pmatrix}.$$

So considering the upper triangular part, we have

$$(d\mathbf{X}) = (\mathbf{B}d\mathbf{Y}\mathbf{B}^T) = b^{m+1}(d\mathbf{Y}) = (\det \mathbf{B})^{m+1}(d\mathbf{Y})$$

Therefore, k = m + 1.

Theorem 5.5. If $\mathbf{X}_{m \times m} = \mathbf{Y}^{-1}$, then

$$(d\mathbf{X}) = (\det \mathbf{Y})^{-2m} (d\mathbf{Y}).$$

Further, if Y is symmetric, then

$$(d\mathbf{X}) = (\det \mathbf{Y})^{-(m+1)}(d\mathbf{Y}).$$

Proof. Since

$$\mathbf{X} = \mathbf{Y}^{-1}\mathbf{Y}\mathbf{Y}^{-1}.$$

If Y is asymmetric, by Theorem. 5.3, we have

$$(d\mathbf{X}) = (\det \mathbf{Y}^{-1})^{2m} (d\mathbf{Y}) = (\det \mathbf{Y})^{-2m} (d\mathbf{Y}).$$

If **Y** is symmetric, by Theorem. 5.4, we have

$$(d\mathbf{X}) = (\det \mathbf{Y}^{-1})^{m+1} (d\mathbf{Y}) = (\det \mathbf{Y})^{-(m+1)} (d\mathbf{Y}).$$

Theorem 5.6. If **A** is an $m \times m$ symmetric positive definite matrix, by Cholesky decomposition, $\mathbf{A} = \mathbf{T}^T \mathbf{T}$, where $\mathbf{T} = \begin{pmatrix} t_{11} & t_{12} & \cdots & t_{1m} \\ t_{22} & \cdots & t_{2m} \\ & & \ddots & \vdots \\ & & & t_{mm} \end{pmatrix}$ is an upper triangular matrix with positive diagonal elements. Then we have

$$J(\mathbf{A} \to \mathbf{T}) = 2^m \prod_{i=1}^m t_{ii}^{m+1-i}.$$
 (25)

Proof. Let $\mathbf{A} = (a_{ij})_{m \times m}$.

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mm} \end{pmatrix} = \begin{pmatrix} t_{11} & & & \\ t_{12} & t_{22} & * & \\ \vdots & \vdots & \ddots & \\ t_{1m} & t_{2m} & \cdots & t_{mm} \end{pmatrix} \begin{pmatrix} t_{11} & t_{12} & \cdots & t_{1m} \\ & t_{22} & \cdots & t_{2m} \\ & * & \ddots & \vdots \\ & & & t_{mm} \end{pmatrix}$$

So

When taking wedge of both sides, we have

$$(d\mathbf{A}) = 2^m \prod_{i=1}^m t_{ii}^{m+1-i}(d\mathbf{T})$$

Homework

- 1. Compute the Laplace transforms of Gamma, Negative Binomial, Poisson distributions.
- 2. Consider that

$$w_1 = w\alpha$$
 $, w_2 = w(1 - \alpha),$
 $u_1 = u - \beta\sigma\sqrt{\frac{w_2}{w_1}}$ $, u_2 = u + \beta\sigma\sqrt{\frac{w_1}{w_2}}$
 $\sigma_1^2 = r(1 - \beta^2)\sigma^2w/w_1, \sigma_2^2 = (1 - r)(1 - \beta^2)\sigma^2w/w_2,$

where $\alpha, \beta, r \in (0, 1)$. Compute the Jacobian from $(w_1, w_2, u_1, u_2, \sigma_1^2, \sigma_2^2)$ to $(w, u, \sigma^2, \alpha, \beta, r)$

5.2 Random variables and their properties

Definition 5.3. Let random vector $\mathbf{X} = (X_1, \dots, X_m)^T$. Then mean of \mathbf{X} is

$$\mu = (\mu_1, \dots, \mu_m)^T = (\mathbb{E}[X_1], \dots, \mathbb{E}[X_m])^T.$$

The covariance matrix Σ is

$$\Sigma = Cov(\mathbf{X}) = \begin{pmatrix} Var(X_1) & Cov(X_1, X_2) & \cdots & Cov(X_1, X_m) \\ Cov(X_1, X_2) & Var(X_2) & \cdots & Cov(X_2, X_m) \\ \vdots & \vdots & \ddots & \vdots \\ Cov(X_m, X_1) & Cov(X_m, X_2) & \cdots & Var(X_m, X_m) \end{pmatrix}.$$

Lemma 5.2. If **a** is a vector and **X** is a random vector with mean μ and covariance matrix Σ , then

$$\mathbb{E}[\mathbf{a}^T \mathbf{X}] = \mathbf{a}^T \boldsymbol{\mu} \quad and \quad Var(\mathbf{a}^T \mathbf{X}) = \mathbf{a}^T \boldsymbol{\Sigma} \mathbf{a}$$

. If A is a matrix then

$$\mathbb{E}[\mathbf{AX}] = \mathbf{A}\boldsymbol{\mu}$$
 and $Cov(\mathbf{AX}) = \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T$

.

5.2.1 Examples

Definition 5.4 (The Multinomial Distribution). A discrete random vector $\mathbf{X} = (X_1, \dots, X_k)$ has Multinomial distribution of dimension k with parameters $\boldsymbol{\theta} = (\theta_1, \dots, \theta_k)$ and n $(0 \le \theta_i \le 1, \sum_{i=1}^k \theta_i \le 1, n = 1, 2, \dots)$. If it's p.d.f. is

$$Mul(\mathbf{x}|\boldsymbol{\theta}, n) = \frac{n!}{\prod_{i=1}^{k} x_i! (n - \sum_{i=1}^{k} x_i)!} \prod_{i=1}^{k} \theta_i^{x_i} (1 - \sum_{t=1}^{k} \theta_t)^{n - \sum_{j=1}^{k} x_j}.$$
 (26)

The mean vector and covariance matrix

$$\mathbb{E}[X_i] = n\theta_i \tag{27}$$

$$Var(X_i) = n\theta_i(1 - \theta_i) \tag{28}$$

$$Cov(X_i, X_j) = -n\theta_i\theta_j. (29)$$

Theorem 5.7. The marginal distribution of $\mathbf{X}^{(m)} = (X_1, \dots, X_m)^T$, (m < k) is the multinomial distribution

$$M_m(\mathbf{x}^{(m)}|(\theta_1,\ldots,\theta_m),n).$$

The conditional distribution of $\mathbf{X}^{(m)}$ given the remaining X_i 's is also Multinomial

$$f(x^{(m)}|x_{m+1},\dots,x_k) \sim M_{m-1}(\mathbf{x}^{(m)}|(\theta_1',\dots,\theta_m'),n-s),$$

where
$$\theta'_i = \frac{\theta_i}{\sum_{j=1}^m \theta_j}$$
, $(1 \le i \le m)$ and $s = \sum_{i=m+1}^k x_i$.

Its corresponding prior is

Definition 5.5 (Dirichlet Distribution). A continuous random vector $\mathbf{X} = (X_1, \dots, X_k)$ has a Dirichlet distribution of dimension k with parameter $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_{k+1})$, $(\alpha_i > 0, i = 1, \dots, k+1)$ if its p.d.f. is

$$Dir(\mathbf{x}|\alpha) = \frac{\Gamma(\sum_{i=1}^{k+1} \alpha_i)}{\prod_{i=1}^{k+1} \Gamma(\alpha_i)} x_1^{\alpha_1 - 1} \cdots x_k^{\alpha_k - 1} (1 - \sum_{i=1}^k x_i)^{\alpha_{k+1} - 1}$$
(30)

.

The mean vector and covariance matrix

$$\mathbb{E}[X_i] = \alpha_i / \sum_{j=1}^{k+1} \alpha_j \tag{31}$$

$$Var(X_i) = \frac{\mathbb{E}[X_i](1 - \mathbb{E}[X_i])}{1 + \sum_{j=1}^{k+1} \alpha_j}$$
(32)

$$Cov(X_i, X_j) = \frac{\mathbb{E}[X_i]\mathbb{E}[X_j]}{1 + \sum_{t=1}^{k+1} \alpha_t}.$$
 (33)

Theorem 5.8. The marginal distribution of $\mathbf{X}^{(m)} = (X_1, \dots, X_m)^T$, (m < k) is the Dirichlet distribution

$$Dir(\mathbf{x}^{(m)}|(\alpha_1,\ldots,\alpha_m),\sum_{i=m+1}^{k+1}\alpha_i).$$

The conditional distribution of $\mathbf{X}^{(m)}$ given the X_{m+1}, \ldots, X_k of $Y_i = \frac{X_i}{1 - \sum_{j=m+1}^k X_j}$ is also Dirichlet

$$Dir(\mathbf{y}^{(m)}|\alpha_1,\ldots,\alpha_m,\alpha_{k+1}).$$

Theorem 5.9. A random vector $\mathbf{X} = (X_1, \dots, X_k) \sim Dir(\mathbf{x} | \boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_{k+1}))$. If $\mathbf{Z} = (Z_1, \dots, Z_t)$ satisfies

$$Z_1 = X_1 + \dots + X_{i_1} \tag{34}$$

$$Z_2 = X_{i_1+1} + \dots + X_{i_2} \tag{35}$$

$$\vdots (36)$$

$$Z_t = X_{i_{t-1}+1} + \dots + X_k, \tag{37}$$

then

$$\mathbf{Z} \sim Dir(\mathbf{z}|\boldsymbol{\beta}),$$

where $\boldsymbol{\beta} = (\beta_1, \dots, \beta_{t+1})$ and

$$\beta_1 = \alpha_1 + \dots + \alpha_{i_1}$$

$$\beta_2 = \alpha_{i_1+1} + \dots + \alpha_{i_2}$$

$$\vdots$$

$$\beta_t = \alpha_{i_{t-1}+1} + \dots + \alpha_k$$

$$\beta_{t+1} = \alpha_{k+1}.$$

${\bf Homework}$

- 1. Show the conditional distribution of multinomial distribution in Theorem 5.7.
- 2.

$$\mathbb{P}(\mathbf{X}|\boldsymbol{\theta},n) \sim Multinomial\ Distribution,$$

 $\mathbb{P}(\boldsymbol{\theta}|\boldsymbol{\alpha}) \sim Dirichlet\ Distribution.$

Compute $\mathbb{P}(\theta|\mathbf{X})$.