National Economics University, Vietnam

Faculty of Mathematics Economics

Data Science in Economics and Business

Machine Learning 1

Homework Week 2: Gaussian Distribution

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1 Problem 1. Proof that:

- (a) Gaussian distribution is normalized
- (b) Expectation of Gaussian distribution is μ (mean)
- (c) Variance of Gaussian distribution is σ^2 (variance)
- (d) Multivariate Gaussian distribution is normalized

Solution.

(a) Normalization of Univariate Gaussian distribution is given by:

$$\int_{-\infty}^{\infty} p(x|\mu, \sigma^2) dx = 1$$

$$\iff \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(x-\mu)^2}{2\sigma^2}\right) dx = 1$$

We will first prove the base case when the mean equals to zero $(\mu = 0)$, which means that:

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-1}{2\sigma^2}x^2\right) dx = 1$$

$$\Longleftrightarrow \int_{-\infty}^{\infty} \exp\left(\frac{-1}{2\sigma^2}x^2\right) dx = \sqrt{2\pi\sigma^2}$$

Let:

$$I = \int_{-\infty}^{\infty} \exp\left(\frac{-1}{2\sigma^2}x^2\right) dx$$

Then we will take the square of both side:

$$I^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left(\frac{-1}{2\sigma^2}x^2\right) \exp\left(\frac{-1}{2\sigma^2}y^2\right) dx dy$$

$$\Longleftrightarrow I^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2 + y^2}{2\sigma^2}\right) dx dy$$

To conduct the integration, we will make the transformation from Cartesian coordinates (x, y) to **polar coordinates** (r, θ) by assuming:

$$x = r \cos \theta$$

$$y = r \sin \theta$$

where r and θ are arbitrary number and angle. By the trigonometric identity we also have:

$$\cos^2 \theta + \sin^2 \theta = 1$$
$$x^2 + y^2 = r^2$$

While transforming integrals between two coordinate systems, we also note that the Jacobian the change of variables is given by:

$$dxdy = |J|drd\theta$$

$$= \begin{vmatrix} \frac{\partial(x)}{\partial(r)} & \frac{\partial(x)}{\partial(\theta)} \\ \frac{\partial(y)}{\partial(r)} & \frac{\partial(y)}{\partial(\theta)} \end{vmatrix}$$

$$= \begin{vmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{vmatrix}$$

$$= r\cos^2\theta + r\sin^2\theta$$

$$= r$$

$$\implies dxdy = rdrd\theta$$

Substituting the above results to the expression of I then:

$$I^{2} = \int_{0}^{2\pi} \int_{0}^{\infty} \exp\left(-\frac{r^{2}}{2\sigma^{2}}\right) r dr d\theta$$

$$= 2\pi \int_{0}^{\infty} \exp\left(-\frac{r^{2}}{2\sigma^{2}}\right) r dr$$

$$= 2\pi\pi \int_{0}^{\infty} \exp\exp\left(-\frac{r^{2}}{2\sigma^{2}}\right) \frac{d(r^{2})}{2}$$

$$= \pi \left[\exp\left(-\frac{r^{2}}{2\sigma^{2}}\right) (-2\sigma^{2})\right]_{0}^{\infty}$$

$$= 2\pi\sigma^{2}$$

Now we have $I = \sqrt{2\pi\sigma^2}$, to prove the case when mean is non zero, we suppose $t = x - \mu$ so that:

$$\int_{-\infty}^{\infty} p(x|\mu, \sigma^2) dx = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{t^2}{2\sigma^2}\right) dt$$
$$= \frac{I}{\sqrt{2\pi\sigma^2}}$$
$$= \frac{\sqrt{2\pi\sigma^2}}{\sqrt{2\pi\sigma^2}} = 1 \quad \Box$$

(b) The formula of expected value of continuous random variable is given by:

$$E(X) = \int_{-\infty}^{\infty} x f_X(x) dx$$

Then the expectation of Univariate Gaussian Distribution is:

$$E(X) = \int_{-\infty}^{\infty} x \cdot \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx$$
$$= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} x \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx$$

To simplify the equation, let $t = \frac{x - \mu}{\sqrt{2\sigma^2}}$. Then $dt = \frac{dx}{\sqrt{2\sigma^2}}$ and $x = t\sqrt{2\sigma^2} + \mu$.

Substituting t in E(X):

$$\begin{split} E(X) &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} (t\sqrt{2\sigma^2} + \mu) \exp(-t^2) \sqrt{2\sigma^2} dt \\ &= \frac{\sqrt{2\sigma^2}}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} (t\sqrt{2\sigma^2} + \mu) \exp(-t^2) dt \\ &= \frac{1}{\sqrt{\pi}} \left(\sqrt{2\sigma^2} \int_{-\infty}^{\infty} t \exp(-t^2) dt + \mu \int_{-\infty}^{\infty} \exp(-t^2) dt \right) \end{split}$$

Let $A = \sqrt{2\sigma^2} \int_{-\infty}^{\infty} t \exp(-t^2) dt$ and $B = \mu \int_{-\infty}^{\infty} \exp(-t^2) dt$. Then:

$$\begin{split} A &= \sqrt{2\sigma^2} \int_{-\infty}^{\infty} \exp(-t^2) t d(t) \\ &= \sqrt{2\sigma^2} \int_{-\infty}^{\infty} -\frac{1}{2} \exp(-t^2) d(-t^2) \\ &= \sqrt{2\sigma^2} \left[-\frac{1}{2} \exp(-t^2) \right]_{-\infty}^{\infty} \\ &= 0 \ (1) \end{split}$$

$$B^{2} = \mu^{2} \int_{-\infty}^{\infty} \exp(-t^{2}) dt \int_{-\infty}^{\infty} \exp(-u^{2}) du$$
$$= \mu^{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp(-t^{2} - u^{2}) du dt$$

At this step, we will calculate B using polar transformation just like how the expression of I was calculated in part (a) of this problem. The final result is $B = \mu \sqrt{\pi}$ (2)

From (1) and (2) we have:

$$E(X) = \frac{\mu\sqrt{\pi}}{\sqrt{pi}} = \mu \quad \Box$$

(c) By definition, the formula of the variance in Gaussian distribution is given by:

$$\begin{split} V(X) &= E[(X - E(X))^2] \\ &= \int_{-\infty}^{\infty} (x - \mu)^2 f_X(x) dx \\ &= \int_{-\infty}^{\infty} (x - \mu)^2 \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right) dx \\ &= \int_{-\infty}^{\infty} x^2 \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right) dx \\ &= \int_{-\infty}^{\infty} (\sqrt{2\sigma^2}x)^2 \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\sqrt{2\sigma^2}x)^2}{2\sigma^2}\right) d(\sqrt{2\sigma^2}x) \\ &= \sigma^2 \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} x^2 e^{-x^2} dx \\ &= \sigma^2 \frac{4}{\sqrt{\pi}} \int_0^{\infty} x^2 e^{-x^2} dx \end{split}$$

Let $t = x^2 \Rightarrow x = \sqrt{t}$ and $dt = 2xdx = 2\sqrt{t}dx = (2\sqrt{t})^{-1}dt$. Substituting to V(X):

$$V(X) = \sigma^2 \frac{4}{\sqrt{\pi}} \int_0^\infty t e^{-t} (2\sqrt{t})^{-1} dt = \sigma^2 \frac{2}{\sqrt{\pi}} \int_0^\infty t^{1/2} e^{-t} dt$$

Note that
$$\int_0^\infty t^{1/2}e^{-t}dt = \int_0^\infty t^{\frac{3}{2}-1}e^{-t}dt = \Gamma(\frac{3}{2}) = \frac{\sqrt{\pi}}{2} \text{ (Gamma function)}$$

The result of $\Gamma(\frac{3}{2})$ can be calculated manually using Legendre duplication formula, a property of Gamma function that allows the calculation of half-integer entry. Substituting to V(X):

$$V(X) = \sigma^2 \frac{2}{\sqrt{\pi}} \frac{\sqrt{\pi}}{2} = \sigma^2 \quad \Box$$

(d) Multivariate Gaussian distribution is normalized

We have

$$\Delta^2 = (x - \mu)^T \Sigma^{-1} (x - \mu)$$
$$= \sum_{i=1}^D \frac{1}{\lambda_i} (x - \mu)^T (x - \mu)$$
$$= \sum_{i=1}^D \frac{y_i^2}{\lambda_i}$$

with $y_i = u_i^T(x - \mu)$ We also have $|\Sigma|^{\frac{1}{2}} = \prod_{i=1}^D \lambda_i^{\frac{1}{2}}$. For a D-dimensional vector x, the multivariate Gaussian distribution takes the form

$$p(x \mid \mu, \Sigma) = \frac{1}{(2\pi)^{\frac{D}{2}} |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu)\right)$$

We replace $y_i = u_i^T(x - \mu)$ into the equation, we have

$$p(y) = \frac{1}{(2\pi)^{\frac{D}{2}} \left(\prod_{i=1}^{D} \lambda_i\right)^{\frac{1}{2}}} \exp\left(-\frac{1}{2} \sum_{i=1}^{D} \frac{y_i^2}{\lambda_i}\right)$$

$$= \frac{1}{(2\pi)^{\frac{D}{2}} \left(\prod_{i=1}^{D} \lambda_i\right)^{\frac{1}{2}}} \prod_{i=1}^{D} \exp\left(-\frac{1}{2} \frac{y_i^2}{\lambda_i}\right)$$

$$= \prod_{j=1}^{D} \frac{1}{(2\pi\lambda_i)^{\frac{1}{2}}} \exp\left(-\frac{y_j^2}{2\lambda_j}\right)$$

$$\Longrightarrow \int_{-\infty}^{\infty} p(y) dy = \prod_{j=1}^{D} \int_{-\infty}^{\infty} \frac{1}{(2\pi\lambda_i)^{\frac{1}{2}}} \exp\left(-\frac{y_j^2}{2\lambda_j}\right) dy_j$$

$$= 1$$

2 Problem 2. Calculate:

- (a) The marginal of Gaussian distribution
- (b) The conditional of Gaussian distribution

Solution. Before jumping in the solution for each part, there will be some useful results that would help later. Given $x \in \mathbb{R}^n$:

$$\int p(x;\mu;\Sigma)dx = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} p(x;\mu;\Sigma)dx_1...dx_n = 1$$
(1)

$$\int x_i p(x; \mu; \sigma^2) dx = \mu_i \tag{2}$$

$$\int (x_i - \mu_i)(x_j - \mu_j)p(x; \mu, \sigma^2)dx = \Sigma_{ij}$$
(3)

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} M^{-1} & -M^{-1}BD^{-1} \\ -D^{-1}CM^{-1} & D^{-1} + D^{-1}CM^{-1}BD^{-1} \end{bmatrix} \text{ where } M = A - BD^{-1}C$$
 (4)

(Schur complement)

(a) Suppose that

$$\left[\begin{array}{c} x_A \\ x_B \end{array}\right] \sim \mathcal{N}\left(\left[\begin{array}{c} \mu_A \\ \mu_B \end{array}\right], \left[\begin{array}{cc} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{array}\right]\right)$$

where $x_A \in \mathbb{R}^m$, $x_B \in \mathbb{R}^n$. The marginal PDF for x_A (calculation of marginal distribution for x_B is similar) is:

$$p(x_A) = \int p(x_A, x_B; \mu, \Sigma) dx_B$$

$$= \frac{1}{(2\pi)^{\frac{m+n}{2}} |\Sigma|^{1/2}} \int \exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu)\right) dx_B$$

$$= \frac{1}{(2\pi)^{\frac{m+n}{2}}} \left| \begin{array}{cc} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{array} \right|^{1/2} \int \exp\left(-\frac{1}{2} \begin{bmatrix} x_A - \mu_A \\ x_B - \mu_B \end{bmatrix}^T \begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix}^{-1} \begin{bmatrix} x_A - \mu_A \\ x_B - \mu_B \end{bmatrix} \right)$$

Denote:

$$V = \begin{bmatrix} V_{AA} & V_{AB} \\ V_{BA} & V_{BB} \end{bmatrix} = \Sigma^{-1}$$

Let $Z = \frac{1}{(2\pi)^{\frac{m+n}{2}}|\Sigma|^{1/2}}$ be a constant that its value does not depend on x_A . Substituting to the marginal distribution expression:

$$p(x_A) = \frac{1}{Z} \int \exp\left(-\frac{1}{2}(x_A - \mu_A)^T V_{AA}(x_A - \mu_A) - \frac{1}{2}(x_A - \mu_A)^T V_{AB}(x_B - \mu_B)\right) dx_B$$
$$\cdot \int \exp\left(-\frac{1}{2}(x_B - \mu_B)^T V_{BA}(x_A - \mu_A) - \frac{1}{2}(x_B - \mu_B)^T V_{BB}(x_B - \mu_B)\right) dx_B$$

Here we will apply a mathematical trick known as "completion of squares" to transform $p(X_A)$ to an expression including quadratic form. Consider the quadratic function $z^T A z + b^T z + c$ where A is a symmetric, non singular matrix. Then:

$$\frac{1}{2}z^TAz + b^Tz + c = \frac{1}{2}(z + A^{-1}b)^TA(z + A^{-1}b) + c - \frac{1}{2}b^TA^{-1}b$$

In our case:

$$z = x_B - \mu_B$$

$$A = V_{BB}$$

$$b = V_{BA}(x_A - \mu_A)$$

$$c = \frac{1}{2}(x_A - \mu_A)^T V_{AA}(x_A - \mu_A)$$

Then:

$$p(x_A) = \frac{1}{Z} \exp\left(-\frac{1}{2}(x_A - \mu_A)^T V_{AA}(x_A - \mu_A) + \frac{1}{2}(x_A - \mu_A)^T V_{AB} V_{BB}^{-1} V_{BA}(x_A - \mu_A)\right)$$

$$\cdot \int \exp\left[-\frac{1}{2}\left(x_B - \mu_B + V_{BB}^{-1} V_{BA}(x_A - \mu_A)\right)^T V_{BB}\left(x_B - \mu_B + V_{BB}^{-1} V_{BA}(x_A - \mu_A)\right)\right] dx_B$$

$$= \frac{1}{Z} \exp\left(-\frac{1}{2}(x_A - \mu_A)^T (V_{AA} - V_{AB} V_{BB}^{-1} V_{BA})(x_A - \mu_A)\right)$$

$$\cdot \int \exp\left[-\frac{1}{2}(x_B - \mu_B)^T V_{BB}(x_B - \mu_B)\right] dx_B$$

Recall the result (1) in the useful result section I have listed at the beginning of this problem:

$$p(x) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} \int \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right) dx = 1$$

Then:

$$\frac{1}{(2\pi)^{n/2}|V_{BB}|^{1/2}} \int \exp\left[-\frac{1}{2} (x_B - \mu_B)^T V_{BB} (x_B - \mu_B)\right] dx_B = 1$$

Now we have eliminated the integral part in the expression of $p(x_A)$, the remainder will be:

$$p(x_A) = \frac{1}{Z} (2\pi)^{n/2} |V_{BB}|^{1/2} \exp\left(-\frac{1}{2} (x_A - \mu_A)^T (V_{AA} - V_{AB} V_{BB}^{-1} V_{BA})(x_A - \mu_A)\right)$$

Applying Schur complement knowing that:

$$\begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix}^{-1} = \begin{bmatrix} V_{AA} & V_{AB} \\ V_{BA} & V_{BB} \end{bmatrix}$$

$$= \begin{bmatrix} (V_{AA} - V_{AB}V_{BB}^{-1}V_{BA})^{-1} & V_{AB}V_{BB}^{-1}V_{BA})^{-1} V_{AB}V_{BB}^{-1} \\ -V_{BB}V_{BA}(V_{AA} - V_{AB}V_{BB}^{-1}V_{BA})^{-1} & (V_{BB} - V_{BA}V_{AA}^{-1}V_{AB})^{-1} \end{bmatrix}$$

Then we can see that $(V_{AA} - V_{AB}VBB^{-1}V_{BA})^{-1} = \Sigma_{AA}$. The formula for marginal distribution $p(x_A)$ will be:

$$p(\mathbf{x_A}) = \frac{1}{Z} (2\pi)^{\mathbf{n/2}} |\mathbf{V_{BB}}|^{1/2} \exp\left(-\frac{1}{2} (\mathbf{x_A} - \mu_{\mathbf{A}})^{\mathbf{T}} \boldsymbol{\Sigma_{AA}} (\mathbf{x_A} - \mu_{\mathbf{A}})\right)$$

(b) Suppose that

$$\left[\begin{array}{c} x_A \\ x_B \end{array}\right] \sim \mathcal{N} \left(\left[\begin{array}{c} \mu_A \\ \mu_B \end{array}\right], \left[\begin{array}{cc} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{array}\right]\right)$$

where $x_A \in \mathbb{R}^m$, $x_B \in \mathbb{R}^n$. The conditional PDF $p(x_A|x_B)$ is:

$$p(x_A|x_B) = \frac{p(x_A, x_B; \mu, \sigma)}{p(x_A)}$$
$$= \frac{p(x_A, x_B; \mu, \sigma)}{\int p(x_A, x_B; \mu, \sigma) dx_A}$$

Note that the integral in the denominator does not depend on x_A because it is the marginal distribution over x_B . Then, to simplify, we will denote M including all the factors that does not depend on x_A and the denominator as well. The expression for $p(x_A|x_B)$ will be:

$$p(x_A|x_B) = \frac{1}{M} \exp(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu))$$

$$= \frac{1}{M} \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right) dx_B$$

$$= \exp\left(-\frac{1}{2} \begin{bmatrix} x_A - \mu_A \\ x_B - \mu_B \end{bmatrix}^T \begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix}^{-1} \begin{bmatrix} x_A - \mu_A \\ x_B - \mu_B \end{bmatrix}\right)$$

$$= \frac{1}{M} \exp\left(-\frac{1}{2}(x_A - \mu_A)^T V_{AA}(x_A - \mu_A) - \frac{1}{2}(x_A - \mu_A)^T V_{AB}(x_B - \mu_B)\right)$$

$$\cdot \exp\left(-\frac{1}{2}(x_B - \mu_B)^T V_{BA}(x_A - \mu_A) - \frac{1}{2}(x_B - \mu_B)^T V_{BB}(x_B - \mu_B)\right)$$

Applying complement square again, in this case:

$$z = x_A - \mu_A$$

$$A = V_{AA}$$

$$b = V_{AB}(x_B - \mu_B)$$

$$c = \frac{1}{2}(x_B - \mu_B)^T V_{BB}(x_B - \mu_B)$$

Then the new expression for $p(x_A|x_B)$ will be:

$$p(x_A|x_B) = \frac{1}{M} \exp\left[-\frac{1}{2}(x_A - \mu_A + V_{AA}^{-1}V_{AB}(x_A - \mu_A))^T V_{AA}(x_A - \mu_A + V_{AA}^{-1}V_{AB}(x_B - \mu_B))\right] \cdot \exp\left[-\frac{1}{2}(x_B - \mu_B)^T V_{BB}(x_B - \mu_B) + \frac{1}{2}(x_B - \mu_B)^T V_{BA}V_{AA}^{-1}V_{AB}(x_B - \mu_B)\right]$$
(*)

The second exp factor in (*) does not depend on x_A so we can include it and M in a normalization constant M'. Then:

$$p(x_A|x_B) = \frac{1}{M'} \exp\left[-\frac{1}{2}(x_A - \mu_A + V_{AA}^{-1}V_{AB}(x_A - \mu_A))^T V_{AA}(x_A - \mu_A + V_{AA}^{-1}V_{AB}(x_B - \mu_B))\right]$$

Applying Schur complement knowing that:

$$\begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix}^{-1} = \begin{bmatrix} V_{AA} & V_{AB} \\ V_{BA} & V_{BB} \end{bmatrix}$$

$$= \begin{bmatrix} (V_{AA} - V_{AB}V_{BB}^{-1}V_{BA})^{-1} & V_{AB}V_{BB}^{-1}V_{BA})^{-1} & V_{AB}V_{BB}^{-1}V_{BB} & V_{AB}V_{BB}^{-1}V_{BB} & V_{AB}V_{AA}^{-1}V_{AB}V_{AB}^{-1} & V_{AB}V_{AA}^{-1}V_{AB}V_{AA}^{-1}V_{AB}V_{AA}^{-1} & V_{AB}V_{AA}^{-1}V_{AB}V_{AA}^{-1}V_{AB}V_{AA}^{-1} & V_{AB}V_{AA}^{-1}V$$

Then we have:

$$\mu_{A|B} = \mu_A - V_{AA}^{-1} V_{AB} (x_B - \mu_B) = \mu_A + \Sigma_{AB} \Sigma_{BB} (x_B - \mu_B)$$

Conversely, we can also derive $V_{AA}^{-1} = \Sigma_{AA} - \Sigma_{AB} \Sigma_{BB}^{-1} \Sigma_{BA})^{-1}$ then

$$\Sigma_{A|B} = V_{AA}^{-1} = \Sigma_{AA} - \Sigma_{AB} \Sigma_{BB}^{-1} \Sigma_{BA})^{-1}$$
$$\Rightarrow p(x_A|x_B) \sim \mathbb{N}(\mu_{A|B}; \Sigma_{A|B})$$

with mean and variance are calculated above.