

Multivariate normal distribution
or Gaussian Distribution

$$P(x) := N_x(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

$$X \sim N_x(\mu, \sigma^2)$$

$$E[X] = \mu$$

$$\text{Var}[X] = \sigma^2$$

Motivation: Central Limit Theorem

X_1, X_2, \dots, X_n are iid R.V. such that

$$E[X_i] = \mu \quad \text{Var}[X_i] = \sigma^2$$

$$\frac{1}{\sqrt{n}} \sum_i (X_i - \mu) \xrightarrow{d} N(0, \sigma^2)$$

$$\text{example: } y = g(x) + \underbrace{\epsilon}_{\sim N} \Rightarrow e_1 + e_2 + \dots + e_n$$

Multivariate Generalization:

$$P(x) := N_x(\mu; \Sigma) = \frac{1}{(2\pi)^{\frac{d}{2}} |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{(x-\mu)^T \Sigma^{-1} (x-\mu)}{2}\right)$$

$$\mu \in \mathbb{R}^d, \quad \Sigma \in \mathbb{R}^{d \times d}$$
$$\Sigma > 0, \text{ P.D.}$$

Geometry of MVA

unimodal, symmetric, etc.

- $(x-\mu)^T \Sigma^{-1} (x-\mu)$ determines geometry.

Mahalanobis distance.

It's a rotated and shifted Euclidean geometry.

$$- \underline{(x-\mu)^T U D U^T (x-\mu)} \quad \begin{array}{l} U \in \mathbb{R}^{d \times d} \text{ ort.} \\ D \in \mathbb{R}^{d \times d} \text{ diag.} \\ \text{diag}(D) > 0 \end{array}$$

$$y \in \mathbb{R}^d, \quad y = U^T (x-\mu) \\ y^T = (x-\mu)^T U$$



$$P(x) = \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp\left(-\frac{y^T D y}{2}\right)$$

$$= \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \prod_i \exp\left[-\frac{y_i^2}{2D_i}\right]$$

$1/D_i$ is i -th diagonal elem. of D .

$$= \prod_i \frac{1}{(2\pi)^{d/2} D_i^{1/2}} \exp\left[-\frac{y_i^2}{2D_i}\right]$$

$$P(y) = P(x) |Jac(U(x-\mu))| = \prod_i N(y_i | 0, D_i)$$

Product of d -univariate normal.

Essentially, MVN under a ^{linear} coordinate transform is a product of d univariate normal.

Normalization of MVN

$$P(y) = \prod_i N_y(0, D_i)$$

$$\text{so, } \int P(y) dy = \int \prod_i N_y(0, D_i) dy$$

$$= \prod_i \int N_y(0, D_i) dy$$

$$= 1$$

MVN is normalized under this new coord. sys.

Moments of MVN.

x is a MVN with P.D.F. $N_x(\mu, \Sigma)$

$$E[x] = \int \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp(- (x-\mu)^T \Sigma^{-1} (x-\mu) / 2) x dx$$

$$= \int \dots \exp(- z^T \Sigma^{-1} z) (z+\mu) dz$$

$$= \left(\int \dots \exp(\dots) dz \right) \mu + \underbrace{\int \dots \exp(\dots) z dz}_0$$

$$= \mu \cdot 1$$

symmetry

$$\int_{-\infty}^{\infty} \dots \exp(\dots) z_i dz_i$$

$$= \int_0^{\infty} \dots \exp(\dots) - z_i dz_i$$

$$E[x x^T] = \int \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp(- \frac{(x-\mu)^T \Sigma^{-1} (x-\mu)}{2}) x \cdot x^T$$

$$= \int \dots \exp(- \frac{z^T \Sigma^{-1} z}{2}) (z+\mu)(z+\mu)^T dz$$

$$\underline{z z^T + \mu z^T + z \mu^T + \mu \mu^T}$$

$$E[x \mu^T] = \mu \mu^T \quad E[\mu x^T] = \mu \mu^T \quad E[\mu \mu^T] = \mu \mu^T$$

$$E[Z Z^T] ?$$

$$= \int \dots \exp\left(-\frac{z^T \Sigma^{-1} z}{2}\right) z z^T dz$$

$$= \int \dots \exp\left(-\frac{z^T U D U^T z}{2}\right) z z^T dz$$

$$\begin{aligned} & \Rightarrow \square \\ z &= (U^T U^T)^T U y \\ &= \int \dots \exp\left(-\frac{y^T U^T U D U^T U y}{2}\right) U y y^T U^T dy \end{aligned}$$

$$= \int \dots \exp\left(-\frac{y^T D y}{2}\right) \sum_{i,j} u_i y_i y_j u_j^T$$

$$= \sum_{i,j} u_i u_j^T \int \dots \exp\left(-\frac{y^T D y}{2}\right) y_i y_j dy$$

$$\forall i \neq j \quad \int_{-\infty}^{+\infty} \dots \exp\left(-\frac{y^T D y}{2}\right) y_i y_j dy = 0$$

$$= \sum_i u_i u_i^T \left[D_i^{3/2} / 1^{1/2} \right] \quad \forall i=j \quad \int_{-\infty}^{+\infty} \dots \exp\left(-\frac{y_i^2}{2D_i}\right) y_i^2 dy$$

$$= \sum_i u_i u_i^T D_i = U(D)^{-1} U^T = D_i$$

$$= (\Sigma^{-1})^{-1} = \Sigma$$

$$\therefore E[X X^T] = \Sigma + \mu \mu^T$$

Conditional MVN.

$$P(X_a, X_b) = \mathcal{N}_X\left(\begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix}, \begin{bmatrix} \Sigma_{aa}, \Sigma_{ab} \\ \Sigma_{ba}, \Sigma_{bb} \end{bmatrix}\right)$$

$$P(X_a | X_b) ?$$

As we saw earlier, the quadratic form completely determines a MVN. Let's look for the quadratic form with respect to X_a

$$= \dots - \frac{1}{2} (x_a - \mu_a)^T \Sigma^{-1} (x_a - \mu_a) + \text{const}$$

$$\log P(x_a, x_b) = -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) + \text{const.}$$

$$\begin{aligned} \text{Let } \Theta &= \Sigma^{-1}, \quad \Theta := \begin{bmatrix} \Theta_{aa} & \Theta_{ab} \\ \Theta_{ba} & \Theta_{bb} \end{bmatrix} \\ &= - \frac{(x_a - \mu_a)^T \Theta_{aa} (x_a - \mu_a)}{2} \\ &\quad - \frac{(x_a - \mu_a)^T \Theta_{ab} (x_b - \mu_b)}{2} \\ &\quad - \frac{(x_b - \mu_b)^T \Theta_{ba} (x_a - \mu_a)}{2} \\ &\quad - \frac{(x_b - \mu_b)^T \Theta_{bb} (x_b - \mu_b)}{2} \end{aligned}$$

The only quadratic form w.r.t x_a : $-x_a^T \Theta_{aa} x_a / 2$

We know a MVN, $N_x(\mu, \Sigma)$ has an exponent:

$$-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) = -\frac{x^T \Sigma^{-1} x}{2} - x^T \Sigma^{-1} \mu + \text{const.}$$

$\Rightarrow P(x_a | x_b)$ has covariance Θ_{aa}^{-1} (NOT Σ_{aa})

Find linear terms includes x_a :

$$\begin{aligned} &- (x_a - \mu_a)^T \Theta_{ab} x_b + (x_a - \mu_a)^T \Theta_{ab} \mu_b \\ &+ (x_a - \mu_a)^T \Theta_{aa} \mu_b \quad \text{using } \Theta_{ab} = \Theta_{ba} \\ &= x_a^T [\Theta_{aa} \mu_a - \Theta_{ab} x_b + \Theta_{ab} \mu_b] \\ &= x_a^T [\Theta_{aa} \mu_a - \Theta_{aa}^{-1} \Theta_{ab} x_b + \Theta_{aa}^{-1} \Theta_{ab} \mu_b] \\ &= x_a^T \underbrace{\Theta_{aa} [\mu_a - \Theta_{aa}^{-1} \Theta_{ab} (x_b - \mu_b)]}_{\mu_{a|b}} \end{aligned}$$

Marginalization of MVN.

$$P(x_a, x_b) = N_x \left(\begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix}, \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix} \right)$$

find terms w.r.t. x_b

$$\begin{aligned} \log P(x_a, x_b) &= - \frac{(x_a - \mu_a)^T \Theta_{ab} (x_b - \mu_b)}{2} \\ &\quad - \frac{(x_b - \mu_b)^T \Theta_{ba} (x_a - \mu_a)}{2} \\ &\quad - \frac{(x_b - \mu_b)^T \Theta_{bb} (x_b - \mu_b)}{2} \end{aligned}$$

$$\begin{aligned}
& - \frac{\chi_b^T \Theta_{bb} \chi_b}{2} + \chi_b^T \Theta_{bb} \mu_b - \chi_b^T \Theta_{ba} \chi_a + \chi_b^T \Theta_{ba} \mu_a \\
& = - \frac{\chi_b^T \Theta_{bb} \chi_b}{2} + \chi_b^T (\underbrace{\Theta_{bb} \mu_b - \Theta_{ba} \chi_a + \Theta_{ba} \mu_a}_m) \\
& = \underline{-\frac{1}{2}(\chi_b - \bar{\Theta}_{bb}^{-1} m)^T \Theta_{bb} (\chi_b - \bar{\Theta}_{bb}^{-1} m) + m^T \bar{\Theta}_{bb}^{-1} m / 2} \\
& \quad \text{completing the square!!}
\end{aligned}$$

$$\therefore \int P(\chi_a, \chi_b) d\chi_b = \frac{1}{2\pi^{d/2} |\Sigma|^{d/2}} \exp\left(t + \frac{m^T \bar{\Theta}_{bb}^{-1} m}{2}\right) \cdot \text{const}$$

$$t = - \frac{\chi_a^T \Theta_{aa} \chi_a}{2} + \chi_a^T \Theta_{aa} \mu_a + \chi_a^T \Theta_{ab} \mu_b + \text{const.}$$

$$m = (\Theta_{bb} \mu_b - \Theta_{ba} \chi_a + \Theta_{ba} \mu_a)$$

Hint: look for quadratic and linear terms w.r.t. χ_a , other terms does not matter

$$\begin{aligned}
t + m^T \bar{\Theta}_{bb}^{-1} m &= - \frac{\chi_a^T \Theta_{aa} \chi_a}{2} + \frac{\chi_a^T \Theta_{ab} \bar{\Theta}_{bb}^{-1} \Theta_{ba} \chi_a}{2} \\
&+ \chi_a^T \Theta_{aa} \mu_a + \chi_a^T \Theta_{ab} \mu_b - \frac{\chi_a^T \Theta_{ab} \bar{\Theta}_{bb}^{-1} \Theta_{bb} \mu_b}{2} - \chi_a^T \Theta_{ab} \bar{\Theta}_{bb}^{-1} \Theta_{ba} \mu_a \\
&= - \frac{\chi_a^T (\Theta_{aa} - \Theta_{ab} \bar{\Theta}_{bb}^{-1} \Theta_{ba}) \chi_a}{2} + \chi_a^T (\Theta_{aa} - \Theta_{ab} \bar{\Theta}_{bb}^{-1} \Theta_{ba}) \mu_a \\
&= - (\chi_a - \mu_a)^T \underbrace{(\Theta_{aa} - \Theta_{ab} \bar{\Theta}_{bb}^{-1} \Theta_{ba})}_{\Sigma_{aa}^{-1}} (\chi_a - \mu_a) + \text{const} \\
\text{so, } \int P(\chi_a, \chi_b) d\chi_b &\propto \exp\left[- \frac{(\chi_a - \mu_a)^T \Sigma_{aa}^{-1} (\chi_a - \mu_a)}{2}\right]
\end{aligned}$$

is a MVN, with mean μ , cov Σ

MLE of MVN. given $x_1 \dots x_n$

$$\max_{\mu, \Sigma} L(x_1 \dots x_n, \mu, \Sigma)$$

$$L = \text{const} - \frac{N}{2} \log |\Sigma| - \frac{1}{2} \sum_{i=1}^n (x_i - \mu)^T \Sigma^{-1} (x_i - \mu)$$

$$\frac{\partial L}{\partial \mu} = - \sum_{i=1}^n \Sigma^{-1} (x_i - \mu)$$

$$\text{set } \frac{\partial L}{\partial \mu} = 0 \Rightarrow 0 = - \sum_{i=1}^n \Sigma^{-1} (x_i - \mu)$$

$$n\mu = \sum_{i=1}^n x_i$$

$$\mu = \frac{1}{n} \sum_{i=1}^n x_i$$

$$\frac{\partial L}{\partial \Sigma} = - \frac{n}{2} \Sigma^{-1} - \frac{\partial \text{tr}[\bar{X} \Sigma^{-1} \bar{X}^T]}{\partial \Sigma} / 2$$

$$\frac{\partial \log |X|}{\partial X} = X^{-1}$$

$$\bar{X} = [x_1 \dots x_n] - \mu \in \mathbb{R}^{d \times n}$$

$$\begin{aligned} \frac{\partial \text{tr}[X \Sigma^{-1} X]}{\partial \Sigma} &= -(\Sigma^{-1} \bar{X} \bar{X}^T \Sigma^{-1})^T / 2 \\ &= -\Sigma^{-1} \bar{X} \bar{X}^T \Sigma^{-1} / 2 \end{aligned}$$

$$\text{set } \frac{\partial L}{\partial \Sigma} = 0 \Rightarrow - \frac{n}{2} \Sigma^{-1} = - \Sigma^{-1} \bar{X} \bar{X}^T \Sigma^{-1} / 2$$

$$n \Sigma = \bar{X} \bar{X}^T$$

$$\Sigma = \bar{X} \bar{X}^T / n$$

