

Gaussian Process

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Last update: March 11, 2024

This note aims to cover some materials on the Gaussian process. The primary references are [Gaussian Process for Machine Learning](#) by C. E. Rasmussen and CS-E4895 by Arno Solin.

1 Multivariate Normal Distribution

1.1 Linear transformation theorem for the multivariate normal distribution

Let x follow a multivariate normal distribution:

$$x \sim \mathcal{N}(\mu, \Sigma) \quad (1)$$

Then, any affine transformation of x is also multivariate normally distributed:

$$y = Ax + b \sim \mathcal{N}(A\mu + b, A\Sigma A^\top) \quad (2)$$

Proof:

The moment-generating function of random vector x is

$$M_x(t) = \mathbb{E}[\exp(t^\top x)] \quad (3)$$

and therefore, the moment-generating function of the random vector y is given by

$$\begin{aligned} M_y(t) &= \mathbb{E}[\exp(t^\top (Ax + b))] \\ &= \mathbb{E}[\exp(t^\top Ax) \exp(t^\top b)] \\ &= \exp(t^\top b) \mathbb{E}[\exp(t^\top Ax)] \\ &= \exp(t^\top b) M_x(A^\top t) \end{aligned} \quad (4)$$

The moment-generating function of the multivariate normal distribution is

$$M_x(t) = \exp(t^\top \mu + \frac{1}{2} t^\top \Sigma t) \quad (5)$$

and therefore, the moment-generating function of random vector y becomes

$$M_y(t) = \exp(t^\top (A\mu + b) + \frac{1}{2} t^\top A\Sigma A^\top t) \quad (6)$$

Since the moment-generating function and the probability density function of a random variable are equivalent, this demonstrates that y follows a multivariate normal distribution with mean $A\mu + b$ and covariance $A\Sigma A^\top$.

1.2 Marginal distribution of the multivariate normal distribution

Let x follow a multivariate normal distribution:

$$x \sim \mathcal{N}(\mu, \Sigma) \quad (7)$$

Then, the marginal distribution of any subset vector x_s is also a multivariate normal distribution

$$x_s \sim \mathcal{N}(\mu_s, \Sigma_s) \quad (8)$$

where μ_s drops the irrelevant variables (the ones not in the subset, i.e., marginalized out) from the mean vector μ and Σ_s drops the corresponding rows and columns from the covariance matrix Σ .

Proof: Define an $m \times n$ subset matrix S such that $s_{ij} = 1$, if the j -th element in x_s corresponds to the i -th element in x , and $s_{ij} = 0$ otherwise. Then,

$$x_s = Sx \quad (9)$$

and we can apply the linear transformation theorem to give

$$x_s \sim \mathcal{N}(S\mu, S\Sigma S^\top) \quad (10)$$

Finally, we see that $S\mu = \mu_s$ and $S\Sigma S^\top = \Sigma_s$

1.3 Conditional distribution of the multivariate normal distribution

Let x follow a multivariate normal distribution

$$x \sim \mathcal{N}(\mu, \Sigma) \quad (11)$$

Then, the conditional distribution of any subset vector x_1 , given the complement vector x_2 , is also a multivariate normal distribution

$$\begin{aligned} \mu_{1|2} &= \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2) \\ \Sigma_{1|2} &= \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} \end{aligned} \quad (12)$$

with block-wise mean and covariance defined as:

$$\begin{aligned} \mu &= \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \\ \Sigma &= \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \end{aligned} \quad (13)$$

Proof: Without loss of generality, we assume that in parallel to 13,

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad (14)$$

where $x_1 \in \mathbb{R}^{n_1 \times 1}$, $x_2 \in \mathbb{R}^{n_2 \times 1}$, and $x \in \mathbb{R}^{n \times 1}$. The joint distribution of x_1 and x_2 is

$$x \sim \mathcal{N}(\mu, \Sigma) \quad (15)$$

Moreover, the marginal distribution of x_2 follows from 11 and 13 as

$$x_2 \sim \mathcal{N}(\mu_2, \Sigma_{22}) \quad (16)$$

According to conditional probability, it holds that

$$\begin{aligned} p(x_1|x_2) &= \frac{p(x_1, x_2)}{p(x_2)} \\ &= \frac{\mathcal{N}(\mu, \Sigma)}{\mathcal{N}(\mu_2, \Sigma_{22})} \end{aligned} \quad (17)$$

Using the probability density of multivariate-normal, this becomes

$$\begin{aligned} p(x_1|x_2) &= \frac{1/\sqrt{(2\pi)^n |\Sigma|} \exp\left(-\frac{1}{2}(x - \mu)^\top \Sigma^{-1}(x - \mu)\right)}{1/\sqrt{(2\pi)^{n_2} |\Sigma_{22}|} \exp\left(-\frac{1}{2}(x - \mu_2)^\top \Sigma_{22}^{-1}(x - \mu_2)\right)} \\ &= 1/\sqrt{(2\pi)^{n-n_2}} \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \exp\left(-\frac{1}{2}(x - \mu)^\top \Sigma^{-1}(x - \mu) + \frac{1}{2}(x - \mu_2)^\top \Sigma_{22}^{-1}(x - \mu_2)\right) \end{aligned} \quad (18)$$

Writing the inverse Σ as

$$\Sigma^{-1} = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \quad (19)$$

and applying 13 to 18, we obtain:

$$\begin{aligned} p(x_1|x_2) &= 1/\sqrt{(2\pi)^{n-n_2}} \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \exp\left(-\frac{1}{2} \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \right)^\top \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \right) \right) \\ &\quad + \frac{1}{2}(x - \mu_2)^\top \Sigma_{22}^{-1}(x - \mu_2)) \end{aligned} \quad (20)$$

Multiplying within 20, we have

$$\begin{aligned} p(x_1|x_2) &= 1/\sqrt{(2\pi)^{n-n_2}} \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \exp\left(-\frac{1}{2}((x_1 - \mu_1)^\top \Sigma^{11}(x_1 - \mu_1) + 2(x_1 - \mu_1)^\top \Sigma^{12}(x_2 - \mu_2) \right. \\ &\quad \left. + (x_2 - \mu_2)^\top \Sigma^{22}(x_2 - \mu_2)) + \frac{1}{2}(x - \mu_2)^\top \Sigma_{22}^{-1}(x - \mu_2)) \right) \end{aligned} \quad (21)$$

where we have used the fact that $\Sigma^{12} = \Sigma^{21^\top}$, because Σ^{-1} is symmetric. The inverse of a block matrix is

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1} \end{bmatrix} \quad (22)$$

Thus, the inverse of Σ^{-1} in 19 is

$$\begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}^{-1} = \begin{bmatrix} (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} & -(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1}\Sigma_{12}\Sigma_{22}^{-1} \\ -\Sigma_{22}^{-1}\Sigma_{21}(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} & \Sigma_{22}^{-1} + \Sigma_{22}^{-1}\Sigma_{21}(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1}\Sigma_{12}\Sigma_{22}^{-1} \end{bmatrix} \quad (23)$$

Plugging this into 20, we have

$$\begin{aligned} p(x_1|x_2) = & \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \\ & \exp \left[-\frac{1}{2} \left((x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} (x_1 - \mu_1) - \right. \right. \\ & \quad 2(x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \Sigma_{12}\Sigma_{22}^{-1} (x_2 - \mu_2) + \\ & \quad (x_2 - \mu_2)^T [\Sigma_{22}^{-1} + \Sigma_{22}^{-1}\Sigma_{21}(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1}\Sigma_{12}\Sigma_{22}^{-1}] (x_2 - \mu_2)) \\ & \quad \left. \left. + \frac{1}{2} ((x_2 - \mu_2)^T \Sigma_{22}^{-1} (x_2 - \mu_2)) \right) \right]. \end{aligned} \quad (24)$$

Eliminating some terms, we have

$$\begin{aligned} p(x_1|x_2) = & \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \\ & \exp \left[-\frac{1}{2} \left((x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} (x_1 - \mu_1) - \right. \right. \\ & \quad 2(x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \Sigma_{12}\Sigma_{22}^{-1} (x_2 - \mu_2) + \\ & \quad \left. \left. (x_2 - \mu_2)^T \Sigma_{22}^{-1} \Sigma_{21} (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \Sigma_{12}\Sigma_{22}^{-1} (x_2 - \mu_2) \right) \right]. \end{aligned} \quad (25)$$

Rearranging the terms, we have

$$\begin{aligned} p(x_1|x_2) = & \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \exp \left[-\frac{1}{2} \cdot \right. \\ & \left. [(x_1 - \mu_1) - \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)]^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} [(x_1 - \mu_1) - \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)] \right] \\ = & \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \exp \left[-\frac{1}{2} \cdot \right. \\ & \left. [x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2))]^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} [x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2))] \right] \end{aligned} \quad (26)$$

where we used the fact that $\Sigma_{21} = \Sigma_{12}^T$. The determinant of a block matrix is

$$\begin{vmatrix} A & B \\ C & D \end{vmatrix} = |D| \cdot |A - BD^{-1}C|, \quad (27)$$

such that we have for Σ that

$$\begin{vmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{vmatrix} = |\Sigma_{22}| \cdot |\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}| \quad (28)$$

with this and $n - n_2 = n_1$, we finally arrive at

$$p(x_1|x_2) = \frac{1}{\sqrt{(2\pi)^{n_1} |\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}|}} \cdot \exp \left[-\frac{1}{2} \cdot \left[x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)) \right]^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \left[x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)) \right] \right] \quad (29)$$

which is the pdf of a multivariate normal distribution

$$p(x_1|x_2) = \mathcal{N}(x_1; \mu_{1|2}, \Sigma_{1|2}) \quad (30)$$

with mean $\mu_{1|2}$ and covariance $\Sigma_{1|2}$ given by 12.

2 Kernel Theory

2.1 Hilbert Space

- A vector space \mathcal{V} is a set of closed vectors under addition and scalar multiplication.
- If \mathcal{V} is equipped with a norm $\|\cdot\|_{\mathcal{V}} \in \mathbb{R}$, it is a norm space.
- A Hilbert space \mathcal{H} is a complete inner product space, with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ and induced norm $\|x\| = \sqrt{\langle x, x \rangle_{\mathcal{H}}}$.

2.2 Kernel Function and Reproducing Kernel Hilbert Space (RKHS)

- A function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a kernel function if and only if there exists a Hilbert space \mathcal{H} and a map $\phi : \mathcal{X} \rightarrow \mathcal{H}$ such that:

$$k(x, y) = \langle \phi(x), \phi(y) \rangle \quad (31)$$

for all $x, y \in \mathcal{X}$.

- Let $\phi : \mathcal{X} \rightarrow \mathbb{R}^{\mathcal{X}}$ and let us define:

$$k_x := \phi(x) = k(x, \cdot) \quad (32)$$

Therefore, we have $k_x(y) = k(x, y)$.

- Let \mathcal{G} denote a vector space with span based on the images $\{k_x | x \in \mathcal{X}\}$, i.e.,

$$\{\mathcal{G} := \sum_{i=1}^m \alpha_i k_{x_i} | \alpha_i \in \mathbb{R}, m \in \mathbb{N}, x_i \in \mathcal{X}\} \quad (33)$$

- By the definition of the kernel function, the inner product on \mathcal{G} is defined as follows:

$$\langle k_x, k_y \rangle := k(x, y) \quad (34)$$

Recall that $k_x = k(x, \cdot)$, hence, $\langle k_x, k_y \rangle = \langle k(x, \cdot), k(y, \cdot) \rangle$.

- Therefore, for any $f, g \in \mathcal{G}$, with $f = \sum_i \alpha_i k_{x_i}$ and $g = \sum_j \beta_j k_{y_j}$, we have:

$$\langle f, g \rangle = \langle \sum_i \alpha_i k_{x_i}, \sum_j \beta_j k_{y_j} \rangle \quad (35)$$

$$= \sum_{ij} \alpha_i \beta_j \langle k_{x_i}, k_{y_j} \rangle \quad (36)$$

$$= \sum_{ij} \alpha_i \beta_j k(x_i, y_j) \quad (37)$$

- To make \mathcal{G} a Hilbert space, we need to make it complete, i.e., ensure all Cauchy sequences converge.

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Definition 1. Let \mathcal{H} be a Hilbert space of real function f defined on an index set \mathcal{X} . Then \mathcal{H} is called a reproducing kernel Hilbert space endowed with an inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ if there exists a kernel function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ with the following properties:

- For every $x \in \mathcal{X}$, $k_x(y) = k(x, y)$ as function of $y \in \mathcal{X}$ belongs to \mathcal{H} , and
- k has the reproducing property.

- Reproducing property:

$$\langle k_x, f \rangle = \langle k_x, \sum_i \alpha_i k_{x_i} \rangle \quad (38)$$

$$= \sum_i \alpha_i \langle k_x, k_{x_i} \rangle = \sum_i \alpha_i k(x, x_i) = f(x) \quad (39)$$

- Moore-Aronszajn theorem: Given a kernel, there is a unique RKHS, Given an RKHS, there is a unique kernel.

2.3 Representer Theorem

Settings:

- We are given kernel k and denote the corresponding RKHS at \mathcal{H} .
- We want to learn a linear function $f(\mathbf{x})$ from a finite data set $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$

Theorem 1. Consider the risk minimization problem of the form:

$$\min_{f \in \mathcal{H}} \underbrace{R_n(\mathbf{y}, \mathbf{f})}_{\text{Empirical Risk}} + \underbrace{\lambda \Omega(\|f\|_{\mathcal{H}})}_{\text{Regularizer}} \quad (40)$$

where $\mathbf{f} = \{f(\mathbf{x}_1), \dots, f(\mathbf{x}_n)\}$, $\mathbf{y} = \{y_1, \dots, y_n\}$, and λ is a scaling parameter. Then 40 always has an optimal solution of the form:

$$f(\mathbf{x}) = \sum_{i=1}^n \alpha_i k(\mathbf{x}_i, \mathbf{x}) \quad (41)$$

3 Spectral Kernel

3.1 Fourier Transforms

- Fourier transform $S(\omega)$ of a function $f(x)$,

$$S(\omega) = \int_{-\infty}^{\infty} f(x) \exp(-2\pi i x \omega) dx \quad (42)$$

- Inverse Fourier transform $f(x)$ of a spectral density $S(\omega)$

$$f(x) = \int_{-\infty}^{\infty} S(\omega) \exp(2\pi i x \omega) d\omega \quad (43)$$

- Euler's identity:

$$\exp(ix) = \cos x + i \sin x \quad (44)$$

Hence

$$\exp(\pm 2\pi i x \omega) = \cos(2\pi x \omega) \pm i \sin(2\pi x \omega) \quad (45)$$

3.2 Fourier Duals

Theorem 2. Bochner's theorem: Any stationary kernel $k : \mathbb{R}^D \rightarrow \mathbb{R}$ and its spectral density $S : \mathbb{R}^D \rightarrow \mathbb{R}$ are Fourier duals

$$\begin{aligned} k(x - x') &\equiv k(\tau) = \int_{-\infty}^{\infty} S(\omega) \exp(2\pi i x \omega^\top \tau) d\omega \\ S(\omega) &= \int_{-\infty}^{\infty} k(\tau) \exp(-2\pi i x \omega^\top \tau) d\tau \end{aligned}$$

4 Marginal Likelihood via Laplace Approximation

- Marginal likelihood to do model selection:

$$p(\mathbf{y}) = \int p(\mathbf{y}|\mathbf{f}) p(\mathbf{f}) d\mathbf{f} \quad (46)$$

- Let $\psi(\mathbf{f}) = \log h(\mathbf{f}) = \log(p(\mathbf{y}|\mathbf{f})p(\mathbf{f}))$

$$\psi(\mathbf{f}) = \log p(\mathbf{y}|\mathbf{f}) - \frac{N}{2} \log 2\pi - \frac{1}{2} \log |\mathbf{K}| - \frac{1}{2} \mathbf{f}^\top \mathbf{K}^{-1} \mathbf{f} \quad (47)$$

- Second order Taylor approximation around the mode $\hat{\mathbf{f}}$

$$\psi(\mathbf{f}) \approx \psi(\hat{\mathbf{f}}) - \frac{1}{2} (\mathbf{f} - \hat{\mathbf{f}})^\top \mathbf{A} (\mathbf{f} - \hat{\mathbf{f}}) \quad (48)$$

- Substituting back

$$p(\mathbf{y}) \approx q(\mathbf{y}) = \int \exp(\psi(\hat{\mathbf{f}}) - \frac{1}{2}(\mathbf{f} - \hat{\mathbf{f}})^\top \mathbf{A}(\mathbf{f} - \hat{\mathbf{f}})) d\mathbf{f} \quad (49)$$

$$= \exp(\psi(\hat{\mathbf{f}})) \int \exp(-\frac{1}{2}(\mathbf{f} - \hat{\mathbf{f}})^\top \mathbf{A}(\mathbf{f} - \hat{\mathbf{f}})) d\mathbf{f} \quad (50)$$

$$= \exp(\psi(\hat{\mathbf{f}})) (2\pi)^{N/2} |\mathbf{A}^{-1}|^{1/2} \quad (51)$$

$$= \exp(\log p(\mathbf{y}|\hat{\mathbf{f}}) - \frac{N}{2} \log 2\pi - \frac{1}{2} \log |\mathbf{K}| - \frac{1}{2} \hat{\mathbf{f}}^\top \mathbf{K}^{-1} \hat{\mathbf{f}}) (2\pi)^{N/2} |\mathbf{A}^{-1}|^{1/2} \quad (52)$$

- Taking the log of $q(\mathbf{y})$

$$\begin{aligned} \log q(\mathbf{y}) &= \log p(\mathbf{y}|\hat{\mathbf{f}}) - \frac{N}{2} \log 2\pi - \frac{1}{2} \log |\mathbf{K}| - \frac{1}{2} \hat{\mathbf{f}}^\top \mathbf{K}^{-1} \hat{\mathbf{f}} \\ &\quad + \frac{N}{2} \log 2\pi + \frac{1}{2} \log |\mathbf{A}|^{-1} \end{aligned} \quad (53)$$

$$= \log p(\mathbf{y}|\hat{\mathbf{f}}) - \frac{1}{2} \log |\mathbf{K}| - \frac{1}{2} \hat{\mathbf{f}}^\top \mathbf{K}^{-1} \hat{\mathbf{f}} + \frac{1}{2} |\mathbf{A}^{-1}| \quad (54)$$

- We can now use the fact that $|\mathbf{A}^{-1}| = |\mathbf{A}|^{-1}$

$$\log q(\mathbf{y}) = \log p(\mathbf{y}|\hat{\mathbf{f}}) - \frac{1}{2} \log |\mathbf{K}| - \frac{1}{2} \hat{\mathbf{f}}^\top \mathbf{K}^{-1} \hat{\mathbf{f}} - \frac{1}{2} |\mathbf{A}| \quad (55)$$

- Recall that $\mathbf{A} = \mathbf{K}^{-1} + \mathbf{W}$

$$\log q(\mathbf{y}) = \log p(\mathbf{y}|\hat{\mathbf{f}}) - \frac{1}{2} \log |\mathbf{K}| - \frac{1}{2} \hat{\mathbf{f}}^\top \mathbf{K}^{-1} \hat{\mathbf{f}} - \frac{1}{2} |\mathbf{K}^{-1} + \mathbf{W}| \quad (56)$$

- We optimize $\log q(\mathbf{y})$ using gradient based methods to choose hyperparameters.