Gaussian Process

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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:

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

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

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

Proof:

The moment-generating function of random vector x is

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

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

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

The moment-generating function of the multivariate normal distribution is

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

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

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

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:

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

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

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

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,

$$x_s = Sx \tag{9}$$

and we can apply the linear transformation theorem to give

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

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

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

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

$$\mu_{1|2} = \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)$$
$$\Sigma_{1|2} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} \tag{12}$$

with block-wise mean and covariance defined as:

$$\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$$
$$\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \tag{13}$$

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

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \tag{14}$$

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

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

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

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

According to conditional probability, it holds that

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

Using the probability density of multivariate-normal, this becomes

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

Writing the inverse Σ as

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

and applying 13 to 18, we obtain:

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

$$
+ \frac{1}{2}(x-\mu_2)^\top \Sigma_{22}^{-1}(x-\mu_2))
$$

Multiplying within 20, we have

$$
p(x_1|x_2) = 1/\sqrt{(2\pi)^{n-n_2}}\sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}}\exp(-\frac{1}{2}((x_1-\mu_1)^\top \Sigma^{11}(x_1-\mu_1) + 2(x_1-\mu_1)\Sigma^{12}(x_2-\mu_2)
$$

$$
+ (x_2-\mu_2)^\top \Sigma^{22}(x_2-\mu_2)) + \frac{1}{2}(x-\mu_2)^\top \Sigma_{22}^{-1}(x-\mu_2)) \tag{21}
$$

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

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

Thus, the inverse of Σ^{-1} in 19 is

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

Plugging this into 20, we have

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

Eliminating some terms, we have

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

Rearranging the terms, we have

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

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

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

such that we have for Σ that

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

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

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

which is the pdf of a multivariate normal distribution

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

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

2 The Marginal Likelihood

- Occam's razor: "When you have two competing models that produce similar predictions, the simpler, the better." The same concept goes for GP.

- The marginal likelihood $p(\mathbf{y}|\boldsymbol{\theta})$ implements a version of Occam's razor.

- Marginal likelihood for Gaussian likelihood

$$p(\mathbf{y}|\boldsymbol{\theta}) = \int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\boldsymbol{\theta})d\mathbf{f}$$
$$= \int \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2\mathbf{I})\mathcal{N}(\mathbf{f}|0, \mathbf{K})d\mathbf{f}$$
$$= \mathcal{N}(\mathbf{y}|0, \sigma^2\mathbf{I} + \mathbf{K})$$

- Then

$$\log p(\mathbf{y}|\boldsymbol{\theta}) = \underbrace{-\frac{N}{2}\log(2\pi)}_{\text{constant}} \underbrace{-\frac{1}{2}\log|\sigma^2\mathbf{I} + \mathbf{K}|}_{\text{complexity penalty}} \underbrace{-\frac{1}{2}\mathbf{y}^\top(\sigma^2\mathbf{I} + \mathbf{K})^{-1}\mathbf{y}}_{\text{data fit}}$$

2.1 The Marginal Likelihood Computation

- In practice, we should avoid computing determinants and inverses.
- Step 1: Compute Cholesky factorization of $\mathbf{C} = \sigma^2\mathbf{I} + K$ such that $C = \mathbf{L}\mathbf{L}^\top$
- Step 2: Compute the log determinant as follows:

$$\log|\mathbf{C}| = \log|\mathbf{L}\mathbf{L}^\top| = \log|\mathbf{L}||\mathbf{L}^\top| = \log|\mathbf{L}|^2 = 2\log|\mathbf{L}| = 2\sum_{n=1}^{N}\log\mathbf{L}_{nn}$$

– Step 3: Compute quadratic term as follows

$$\mathbf{y}^\top \mathbf{C}^{-1}\mathbf{y} = \mathbf{y}^\top(\mathbf{L}\mathbf{L}^\top)^{-1}\mathbf{y} = \mathbf{y}^\top\mathbf{L}^{-\top}\mathbf{L}^{-1}\mathbf{y} = (\mathbf{L}^{-1}\mathbf{y})^\top \underbrace{(\mathbf{L}^{-1}\mathbf{y})}_{=\mathbf{v}} = \mathbf{v}^\top\mathbf{v}$$

– Step 4: Sum up components

$$\log p(\mathbf{y}|\boldsymbol{\theta}) = -\frac{N}{2}\log(2\pi) - \frac{1}{2}2\sum_{n=1}^{N}\log\mathbf{L}_{nn} - \frac{1}{2}\mathbf{v}^\top\mathbf{v}$$

- Note that we never compute the determinant or the inverse of $\mathbf{C}$ directly.

3 Kernel Theory

3.1 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 $\|.\|_\mathcal{V} \in \mathbb{R}$, it is a norm space.

- A Hilbert space $\mathcal{H}$ is a complete inner product space, with inner product $\langle.\rangle_\mathcal{H}$ and induced norm $\|x\| = \sqrt{\langle x, x\rangle_\mathcal{H}}$.

3.2 Kernel Function and Reproducing Kernel Hilbert Space (RKHS)

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

$$k(x, y) = \langle\phi(x), \phi(y)\rangle \tag{31}$$

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

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

$$k_x := \phi(x) = k(x, .) \tag{32}$$

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.,

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

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

$$\langle k_x, k_y\rangle := k(x, y) \tag{34}$$

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

- 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:

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

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

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

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

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 $\langle ., . \rangle_\mathcal{H}$ if there exists a kernel function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ with the following properties:*

1. *For every $x \in \mathcal{X}, k_x(y) = k(x, y)$ as function of $y \in \mathcal{X}$ belongs to $\mathcal{H}$, and*

2. *k has the reproducing property.*

- Reproducing property:

$$\langle k_x, f \rangle = \langle k_x, \sum_i \alpha_i k_{x_i} \rangle \tag{38}$$

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

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

3.3 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:*

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

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

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

4 Spectral Kernel

4.1 Fourier Transforms

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

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

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

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

- Euler's identity:

$$\exp(ix) = \cos x + i \sin x \tag{44}$$

Hence

$$\exp(\pm 2\pi i x \omega) = \cos(2\pi x \omega) \pm i \sin(2\pi x \omega) \tag{45}$$

4.2 Fourier Duals

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

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

$$S(\omega) = \int_{-\infty}^{\infty} k(\tau) \exp(-2\pi i x \omega^\top \tau) d\tau$$

5 Marginal Likelihood via Laplace Approximation

- Marginal likelihood to do model selection:

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

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

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

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

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

- Substituting back

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

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

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

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

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

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

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

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

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

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

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

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

6 Multi-output GP

6.1 Intrinsic coregionalization model (ICM): two-outputs

- Consider two output $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$ with $\mathbf{x} \in \mathbb{R}^d$

- Assume the following generative model:

  1. Sample from a GP $u(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$ to obtain $u^1(\mathbf{x})$
  2. Obtain $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$ by linearly transforming $u^1(\mathbf{x})$

$$f_1(\mathbf{x}) = a_1^1 u(\mathbf{x})$$
$$f_2(\mathbf{x}) = a_2^1 u(\mathbf{x})$$

6.2 ICM: covariance

- For a fixed value $\mathbf{x}$, we can group $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$ in a vector $\mathbf{f}(\mathbf{x})$

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{bmatrix}$$

  We refer to this as a vector-valued function.

- The covariance for $\mathbf{f}(\mathbf{x})$ is computed as

$$cov(\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x})) = \mathbb{E}[\mathbf{f}(\mathbf{x})\mathbf{f}(\mathbf{x}')^\top] - \mathbb{E}[\mathbf{f}(\mathbf{x})]\mathbb{E}[\mathbf{f}(\mathbf{x}')]^\top$$

- We compute the term $\mathbb{E}[\mathbf{f}(\mathbf{x})\mathbf{f}(\mathbf{x}')^\top]$

$$\begin{aligned} \mathbb{E}\left[\begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{bmatrix} \begin{bmatrix} f_1(\mathbf{x}') & f_2(\mathbf{x}') \end{bmatrix} \right] &= \begin{bmatrix} \mathbb{E}[f_1(\mathbf{x})f_1(\mathbf{x}')] & \mathbb{E}[f_1(\mathbf{x})f_2(\mathbf{x}')] \\ \mathbb{E}[f_2(\mathbf{x})f_1(\mathbf{x}')] & \mathbb{E}[f_2(\mathbf{x})f_2(\mathbf{x}')] \end{bmatrix} \\ &= \begin{bmatrix} (a_1^1)^2\mathbb{E}[u_1(\mathbf{x})u^1(\mathbf{x}')] & a_1^1 a_2^1\mathbb{E}[u_1(\mathbf{x})u^1(\mathbf{x}')] \\ a_1^1 a_2^1\mathbb{E}[u_1(\mathbf{x})u^1(\mathbf{x}')] & (a_2^1)^2\mathbb{E}[u_1(\mathbf{x})u^1(\mathbf{x}')] \end{bmatrix} \\ &= \begin{bmatrix} (a_1^1) & a_1^1 a_2^1 \\ a_1^1 a_2^1 & (a_2^1)^2 \end{bmatrix} \mathbb{E}[u^1(\mathbf{x})u^1(\mathbf{x}')] \end{aligned}$$

- The term $\mathbb{E}[\mathbf{f}(\mathbf{x})]$ is computed as

$$\mathbb{E}\left[\begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{bmatrix} \right] = \begin{bmatrix} \mathbb{E}[f_1(\mathbf{x})] \\ \mathbb{E}[f_2(\mathbf{x})] \end{bmatrix} = \begin{bmatrix} a_1^1 \\ a_2^1 \end{bmatrix} \mathbb{E}[u^1(\mathbf{x})]$$

- Putting the terms together, the covariance for $\mathbf{f}(\mathbf{x})$ follows

$$\begin{bmatrix} (a_1^1) & a_1^1 a_2^1 \\ a_1^1 a_2^1 & (a_2^1)^2 \end{bmatrix} \mathbb{E}[u^1(\mathbf{x})u^1(\mathbf{x}')] - \begin{bmatrix} a_1^1 \\ a_2^1 \end{bmatrix} \begin{bmatrix} a_1^1 & a_2^1 \end{bmatrix} \mathbb{E}[u^1(\mathbf{x})]\mathbb{E}[u^1(\mathbf{x}')]$$

- Defining $\mathbf{a} = \begin{bmatrix} a_1^1 & a_2^1 \end{bmatrix}^\top$ and $\mathbf{B} = \mathbf{a}\mathbf{a}^\top$,

$$cov(\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')) = \mathbf{a}\mathbf{a}^\top k(\mathbf{x}, \mathbf{x}') = \mathbf{B}^\top k(\mathbf{x}, \mathbf{x}')$$

6.3 ICM: Observed data

- Given $\mathcal{D}_1 = \{(\mathbf{x}_i, f_1(\mathbf{x}_i)) | i = 1, \cdots, N\}$ and $\mathcal{D}_2 = \{(\mathbf{x}_i, f_2(\mathbf{x}_i)) | i = 1, \cdots, N\}$, then

$$\begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{bmatrix} = \begin{bmatrix} f_1(\mathbf{x}_1) \\ \vdots \\ f_1(\mathbf{x}_N) \\ f_2(\mathbf{x}_1) \\ \vdots \\ f_2(\mathbf{x}_N) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} b_{11}\mathbf{K} & b_{12}\mathbf{K} \\ b_{21}\mathbf{K} & b_{22}\mathbf{K} \end{bmatrix} \right) = \mathcal{N}(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \mathbf{B} \otimes \mathbf{K})$$

- The inversion rule: $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$

7 Computational Complexity of GP Regression

- Data set with N observations, computing posterior for 1 test point:

$$\mu_* = \mathbf{K}_{f_*f}(\mathbf{K}_{ff} + \sigma^2\mathbf{I})^{-1}\mathbf{y}$$
$$\sigma_*^2 = k_{f_*f} - \mathbf{K}_{f_*f}(\mathbf{K}_{ff} + \sigma^2 I)^{-1}\mathbf{K}_{f_*f}^\top$$

- Matrix-vector multiplication (mvm): for $\mathbf{A} \in \mathbb{R}^{N \times M}$ and $\mathbf{b} \in \mathbb{R}^M$, computing $\mathbf{Ab}$ costs $\mathcal{O}(NM)$

- Matrix inverse: for $\mathbf{C} \in \mathbb{R}^{N \times N}$, computing $\mathbf{C}^{-1}$ costs $\mathcal{O}(N^3)$

- $(\mathbf{K}_{ff} + \sigma^2\mathbf{I})^{-1}\mathbf{y}$ scales as $\mathcal{O}(N^3)$.

8 Approximately solving linear system

8.1 Matrix inverse as quadratic optimization

- Rewrite matrix inverse

$$\mathbf{v} = \hat{\mathbf{K}}^{-1}\mathbf{y}, \qquad \hat{K} = \mathbf{K} + \sigma^2\mathbf{I}$$

as a linear system:

$$\hat{K}\mathbf{v} - \mathbf{y} = 0$$

- Solve as a quadratic optimization problem:

$$\mathbf{v}^* = \arg\min_{\mathbf{v}} \mathbf{v}^\top \hat{K}\mathbf{v} - \mathbf{v}^\top \mathbf{y}$$

8.2 Conjugate gradient

- Using conjugate gradient to solve the quadratic optimization

  1. Iterative method
  2. Each step is $\mathcal{O}(N^2)$
  3. Recovers exact solution after N steps $\rightarrow \mathcal{O}(N^3)$
  4. Approximate solution in much fewer steps: less steps.

8.3 Convergence and preconditioning

- Condition number: ratio of largest to smallest eigenvalue $\lambda_{\min}(\hat{K})/\lambda_{\max}(\hat{K})$.

- High condition numbers: numerically unstable, slow convergence.

- Improve by preconditioning: Instead of $\hat{K}\mathbf{v} - \mathbf{y} = 0$, solve

$$\mathbf{P}^{-1}\hat{K}\mathbf{v} - \mathbf{P}^{-1}\mathbf{y} = 0$$

9 Low-rank approximation

- Recall GP marginal log-likelihood:

$$\log p(\mathbf{y}|\mathbf{X}) = \log \mathcal{N}(\mathbf{y}|0, \mathbf{K} + \sigma^2 \mathbf{I})$$

Assume $\mathbf{K}$ to be low rank.

9.1 Approximation by subset

- Let's randomly pick a subset from training data: $\mathbf{Z} \in \mathbb{R}^{M \times Q}$

- Approximate the covariance matrix $\mathbf{K}$ by $\hat{K}$

$$\hat{\mathbf{K}} = \mathbf{K}_z \mathbf{K}_{zz}^{-1} \mathbf{K}_z^\top \in \mathbb{R}^{N \times N}$$
$$\mathbf{K}_z = \mathbf{K}(\mathbf{X}, \mathbf{Z}) \in \mathbb{R}^{N \times M}$$
$$\mathbf{K}_{zz} = \mathbf{K}(\mathbf{Z}, \mathbf{Z}) \in \mathbb{R}^{M \times M}$$

- The log-likelihood is approximated by

$$\log p(\mathbf{y}|\mathbf{X}) = \log \mathcal{N}(\mathbf{y}|0, \mathbf{K}_z \mathbf{K}_{zz}^{-1} \mathbf{K}_z^\top + \sigma^2 \mathbf{I})$$

- Furthermore, apply Woodbury matrix identity:

$$(UCV + A)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$
$$(\mathbf{K}_z \mathbf{K}_{zz}^{-1} \mathbf{K}_z^\top + \sigma^2 \mathbf{I})^{-1} = \sigma^{-2}\mathbf{I} - \sigma^{-4}\mathbf{K}_z(\mathbf{K}_{zz} + \sigma^{-2}\mathbf{K}_z^\top \mathbf{K}_z)^{-1}\mathbf{K}_z^\top$$

- The complexity reduces to $\mathcal{O}(NM^2)$.