Exercise of Supervised Learning: Gaussian Processes 1

Yawei Li

yawei.li@stat.uni-muenchen.de

January 28, 2025

Exercise 1: Bayesian Linear Model

In the Bayesian linear model, we assume that the data follows the following law:

$$y = f(\mathbf{x}) + \epsilon = \boldsymbol{\theta}^{\top} \mathbf{x} + \epsilon,$$

where $\epsilon \sim \mathcal{N}(0, \sigma^2)$ and independent of **x**. On the data-level this corresponds to

$$y^{(i)} = f\left(\mathbf{x}^{(i)}\right) + \epsilon^{(i)} = \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)} + \epsilon^{(i)}, \text{ for } i \in [n],$$

where $\epsilon^{(i)} \in \mathcal{N}(0, \sigma^2)$ are i.i.d. and all independent of $\mathbf{x}^{(i)}$'s. In the Bayesian perspective it is assumed that the parameter vector $\boldsymbol{\theta}$ is stochastic and follows a distribution. Assume we are interested in the so-called maximum a posteriori estimate of $\boldsymbol{\theta}$, which is defined by

$$\hat{\boldsymbol{\theta}} = rg \max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathbf{X}, \mathbf{y}).$$

(a) Show that if we choose a **uniform distribution** over the parameter vector θ as the prior belief, i.e., $q(\theta) \propto 1$, then the maximum a posteriori estimate coincides with the **empirical risk minimizer** for the L2-loss (over linear models).

$$\underline{
ho(heta|\mathbf{X},\mathbf{y})} = \frac{
ho(heta,\mathbf{y}|\mathbf{X})}{
ho(\mathbf{y}|\mathbf{X})}$$

- For a linear model, $\mathbf{y}|\mathbf{X}, \boldsymbol{\theta} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \sigma^2 \mathbf{I})$. Will be computed on the next slide.
- In 1(a), we choose a **uniform prior**, indicating $q(heta) \propto 1$
- \triangleright p(y|X) does **not** depend on θ . \rightsquigarrow Treated as constant when maxing the posterior of θ .

$$egin{aligned} egin{aligned} egin{aligned\\ egin{aligned} egi$$

- For a linear model, $\mathbf{y}|\mathbf{X}, \boldsymbol{\theta} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \sigma^2 \mathbf{I})$. Will be computed on the next slide.
- In 1(a), we choose a **uniform prior**, indicating $q(\theta) \propto 1$
- \triangleright p(y|X) does **not** depend on θ . \rightsquigarrow Treated as constant when maxing the posterior of θ .

$$\underbrace{\frac{\rho(\boldsymbol{\theta}|\mathbf{X},\mathbf{y})}_{\text{posterior}} = \frac{\frac{\rho(\boldsymbol{\theta},\mathbf{y}|\mathbf{X})}{\rho(\mathbf{y}|\mathbf{X})}}_{\text{likelihood}} \underbrace{\frac{\rho(\mathbf{y}|\mathbf{X},\boldsymbol{\theta})}{\rho(\mathbf{y}|\mathbf{X})}}_{\text{marginal}}$$

- For a linear model, $\mathbf{y}|\mathbf{X}, \boldsymbol{\theta} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \sigma^2 \mathbf{I})$. Will be computed on the next slide.
- In 1(a), we choose a **uniform prior**, indicating $q(\theta) \propto 1$
- \triangleright p(y|X) does **not** depend on θ . \rightsquigarrow Treated as constant when maxing the posterior of θ .

$$\underbrace{\frac{\rho(\boldsymbol{\theta}|\mathbf{X},\mathbf{y})}_{\text{posterior}} = \frac{\frac{\rho(\boldsymbol{\theta},\mathbf{y}|\mathbf{X})}{\rho(\mathbf{y}|\mathbf{X})}}_{\text{likelihood}} \underbrace{\frac{\rho(\mathbf{y}|\mathbf{X},\boldsymbol{\theta})}{\rho(\mathbf{y}|\mathbf{X})}}_{\text{marginal}}$$

- For a linear model, $\mathbf{y}|\mathbf{X}, \boldsymbol{\theta} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \sigma^2 \mathbf{I})$. Will be computed on the next slide.
- In 1(a), we choose a **uniform prior**, indicating $q(\theta) \propto 1$.
- \triangleright p(y|X) does **not** depend on θ . \rightsquigarrow Treated as constant when maxing the posterior of θ .

$$\underbrace{\frac{\rho(\boldsymbol{\theta}|\mathbf{X},\mathbf{y})}_{\text{posterior}} = \frac{\frac{\rho(\boldsymbol{\theta},\mathbf{y}|\mathbf{X})}{\rho(\mathbf{y}|\mathbf{X})}}_{\text{likelihood}} \underbrace{\frac{\rho(\mathbf{y}|\mathbf{X},\boldsymbol{\theta})}{\rho(\mathbf{y}|\mathbf{X})}}_{\text{marginal}}$$

- For a linear model, $\mathbf{y}|\mathbf{X}, \boldsymbol{\theta} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \sigma^2 \mathbf{I})$. Will be computed on the next slide.
- In 1(a), we choose a **uniform prior**, indicating $q(\theta) \propto 1$.
- \triangleright p(y|X) does **not** depend on θ . \rightsquigarrow Treated as constant when maxing the posterior of θ .

1 (a): The Likelihood $p(y|X, \theta)$

$$\begin{aligned} \rho(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) &\propto \exp\left[-\frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^{\top}(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})\right] \\ &= \exp\left[-\frac{||\mathbf{y} - \mathbf{X}\boldsymbol{\theta}||^2}{2\sigma^2}\right] \\ &= \exp\left[-\frac{\sum_{i=1}^{n}(\mathbf{y}^{(i)} - \boldsymbol{\theta}^{\top}\mathbf{x}^{(i)})^2}{2\sigma^2}\right]. \end{aligned}$$

In addition, recall that the prior $q(\theta) \propto 1$ and we don't care the marginal $p(\mathbf{y}|\mathbf{X})$. Now, we plug these information into $p(\theta|\mathbf{X},\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{X},\theta)q(\theta)}{p(\mathbf{y}|\mathbf{X})} \propto p(\mathbf{y}|\mathbf{X},\theta)q(\theta)$.

1 (a): The Likelihood $p(y|X, \theta)$

$$\begin{split} \rho(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) &\propto \exp\left[-\frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^{\top}(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})\right] \\ &= \exp\left[-\frac{||\mathbf{y} - \mathbf{X}\boldsymbol{\theta}||^2}{2\sigma^2}\right] \\ &= \exp\left[-\frac{\sum_{i=1}^{n}(y^{(i)} - \boldsymbol{\theta}^{\top}\mathbf{x}^{(i)})^2}{2\sigma^2}\right]. \end{split}$$

In addition, recall that the prior $q(\theta) \propto 1$ and we don't care the marginal $p(\mathbf{y}|\mathbf{X})$. Now, we plug these information into $p(\theta|\mathbf{X},\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{X},\theta)q(\theta)}{p(\mathbf{y}|\mathbf{X})} \propto p(\mathbf{y}|\mathbf{X},\theta)q(\theta)$.

1 (a): MAP Estimate

$$p(\theta|\mathbf{X},\mathbf{y}) \propto p(\mathbf{y}|\mathbf{X},\theta) \cdot q(\theta) \propto \exp\left[-\frac{\sum_{i=1}^{n} (y^{(i)} - \theta^{\top}\mathbf{x}^{(i)})^{2}}{2\sigma^{2}}\right].$$

Now we compute the maximum a posterior estimate as

$$\begin{split} \hat{\boldsymbol{\theta}} &= \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathbf{X},\mathbf{y}) \\ &= \arg\max_{\boldsymbol{\theta}} \log(p(\boldsymbol{\theta}|\mathbf{X},\mathbf{y})) \qquad \text{(log is a monotone increasing func.)} \\ &= \arg\max_{\boldsymbol{\theta}} - \frac{\sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2}}{2\sigma^{2}} \\ &= \arg\min_{\boldsymbol{\theta}} \frac{\sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2}}{2\sigma^{2}} \\ &= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2}. \end{split}$$

Therefore, in 1 (a), maximum a posteriori estimate ⇔ ERM for the L2-loss

1 (a): MAP Estimate

$$p(\theta|\mathbf{X},\mathbf{y}) \propto p(\mathbf{y}|\mathbf{X},\theta) \cdot q(\theta) \propto \exp\left[-\frac{\sum_{i=1}^{n} (y^{(i)} - \theta^{\top}\mathbf{x}^{(i)})^{2}}{2\sigma^{2}}\right].$$

Now we compute the maximum a posterior estimate as:

$$\begin{split} \hat{\boldsymbol{\theta}} &= \arg\max_{\boldsymbol{\theta}} \rho(\boldsymbol{\theta}|\mathbf{X},\mathbf{y}) \\ &= \arg\max_{\boldsymbol{\theta}} \log(p(\boldsymbol{\theta}|\mathbf{X},\mathbf{y})) \qquad \text{(log is a monotone increasing func.)} \\ &= \arg\max_{\boldsymbol{\theta}} -\frac{\sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2}}{2\sigma^{2}} \\ &= \arg\min_{\boldsymbol{\theta}} \frac{\sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2}}{2\sigma^{2}} \\ &= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2}. \end{split}$$

Therefore, in 1 (a), maximum a posteriori estimate ⇔ ERM for the L2-loss.

Exercise 1(b)

Show that if we choose a **Gaussian distribution** over the parameter vectors θ as the prior belief, i.e.,

$$q(oldsymbol{ heta}) \propto \exp\left[-rac{1}{2 au^2}oldsymbol{ heta}^ op oldsymbol{ heta}
ight], \quad au>0,$$

then the maximum a posteriori estimate coincides for a specific choice of τ with the **regularized** empirical risk miminizer for the L2-loss with L2 penalty (over the linear models), i.e., the Ridge regression.

1 (b): Posterior with A Gaussian Prior

$$\begin{split} \rho(\boldsymbol{\theta}|\mathbf{X},\mathbf{y}) &\propto \rho(\mathbf{y}|\mathbf{X},\boldsymbol{\theta})q(\boldsymbol{\theta}) \\ &\propto \exp\left[-\frac{\sum_{i=1}^{n}(y^{(i)}-\boldsymbol{\theta}^{\top}\mathbf{x}^{(i)})^{2}}{2\sigma^{2}}-\frac{1}{2\tau^{2}}\boldsymbol{\theta}^{\top}\boldsymbol{\theta}\right] \\ &\propto \exp\left[-\frac{\sum_{i=1}^{n}(y^{(i)}-\boldsymbol{\theta}^{\top}\mathbf{x}^{(i)})^{2}}{2\sigma^{2}}-\frac{||\boldsymbol{\theta}||_{2}^{2}}{2\tau^{2}}\right]. \end{split}$$

Next, we compute $\arg \max_{\theta} \rho(\theta | \mathbf{X}, \mathbf{y})$. That is, $\arg \max_{\theta} \log \rho(\theta | \mathbf{X}, \mathbf{y})$.

1 (b): MAP Estimate

$$\begin{split} \hat{\boldsymbol{\theta}} &= \operatorname*{arg\,max} \log \rho(\boldsymbol{\theta} | \mathbf{X}, \mathbf{y}) \\ &= \operatorname*{arg\,max} - \frac{\sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2}}{2\sigma^{2}} - \frac{||\boldsymbol{\theta}||_{2}^{2}}{2\tau^{2}} \\ &= \operatorname*{arg\,min} \frac{\sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2}}{2\sigma^{2}} + \frac{||\boldsymbol{\theta}||_{2}^{2}}{2\tau^{2}} \\ &= \operatorname*{arg\,min} \sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2} + \frac{\sigma^{2}}{\tau^{2}} ||\boldsymbol{\theta}||_{2}^{2}. \end{split} \tag{Because} \times \sigma^{2} \text{ doesn't change the argmin)}$$

We define $\lambda = \frac{\sigma^2}{\tau^2}$, then the maximum a posteriori \Leftrightarrow L2-loss with L2 penalty.

Exercise 1(c)

Show that if we choose a **Laplace distribution** over the parameter vectors θ as the prior belief, i.e.,

$$q(oldsymbol{ heta}) \propto \exp\left[-rac{\sum_{i}^{oldsymbol{
ho}}|oldsymbol{ heta}_{i}|}{ au}
ight], \quad au>0,$$

then the maximum a posteriori estimate coincides for a specific choice of τ with the regularized empirical risk minimizer for the L2-loss with L1 penalty (over the linear models), i.e., the Lasso regression.

1 (c): Posterior with A Laplace Prior

$$p(\theta|\mathbf{X},\mathbf{y}) \propto p(\mathbf{y}|\mathbf{X},\theta)q(\theta)$$

 $\propto \exp\left[-\frac{\sum_{i=1}^{n}(y^{(i)}-\theta^{\top}\mathbf{x}^{(i)})^{2}}{2\sigma^{2}}-\frac{||\theta||_{1}}{\tau}\right].$

1 (c): MAP Estimate

$$\begin{split} \hat{\boldsymbol{\theta}} &= \operatorname*{arg\,max} \log p(\boldsymbol{\theta}|\mathbf{X},\mathbf{y}) \\ &= \operatorname*{arg\,max} - \frac{\sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2}}{2\sigma^{2}} - \frac{||\boldsymbol{\theta}||_{1}}{\tau} \\ &= \operatorname*{arg\,min} \frac{\sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2}}{2\sigma^{2}} + \frac{||\boldsymbol{\theta}||_{1}}{\tau} \\ &= \operatorname*{arg\,min} \sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^{\top} \mathbf{x}^{(i)})^{2} + \frac{2\sigma^{2}}{\tau} ||\boldsymbol{\theta}||_{1} \quad \text{(Because } \times \sigma^{2} \text{ doesn't change the argmin)} \end{split}$$

We define $\lambda = \frac{2\sigma^2}{\tau}$, and then the MAP estimate \Leftrightarrow L2-loss with L1 penalty.

Exercise 2: Covariance Functions

Consider the commonly used covariance functions mentioned in the lecture slides: constant, linear, polynomial, squared exponential, Matern, exponential covariance functions.

- (a) Show that they are valid covariance functions. (**Proofs for Matern and exp. cov. functions are out of scope and omitted.**) You may use the following composition rules. In these rules we assume that $k_0(\cdot,\cdot)$ and $k_1(\cdot,\cdot)$ are valid covariance functions.
 - 1. $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^{\top} \mathbf{x}'$ is a valid covariance function;
 - 2. $k(\mathbf{x}, \mathbf{x}') = c \cdot k_0(\mathbf{x}, \mathbf{x}')$ is a valid covariance function if $c \ge 0$ is constant.
 - 3. $k(\mathbf{x}, \mathbf{x}') = k_0(\mathbf{x}, \mathbf{x}') + k_1(\mathbf{x}, \mathbf{x}')$ is a valid covariance function;
 - 4. $k(\mathbf{x}, \mathbf{x}') = k_0(\mathbf{x}, \mathbf{x}') \cdot k_1(\mathbf{x}, \mathbf{x}')$ is a valid covariance function;
 - 5. $k(\mathbf{x}, \mathbf{x}') = g(k_0(\mathbf{x}, \mathbf{x}'))$ is a valid cov. func. if g is a polynomial function with **pos.** coefficients;
 - 6. $k(\mathbf{x}, \mathbf{x}') = t(\mathbf{x}) \cdot k_0(\mathbf{x}, \mathbf{x}') \cdot t(\mathbf{x}')$ is a valid cov. function, where t is any **continuous** function;
 - 7. $k(\mathbf{x}, \mathbf{x}') = \exp(k_1(\mathbf{x}, \mathbf{x}'))$ is a valid covariance function;
 - 8. $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^{\top} \mathbf{A} \mathbf{x}'$ is a valid covariance function if $\mathbf{A} \succeq 0$.

2 (a): Proof via Kernel Matrix

Construct of the kernel matrix $\mathbf{K} \in \mathbb{R}^{n \times n}$ from $\mathcal{D} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\}$. Each element $K_{i,j} = k(\mathbf{x}, \mathbf{x}')$. In the current case $k(\mathbf{x}, \mathbf{x}') = \sigma_0^2$, we have $K_{i,j} = \sigma_0^2$. In other words,

$$\mathbf{K} = \begin{pmatrix} \sigma_0^2 & \dots & \sigma_0^2 \\ \vdots & \ddots & \vdots \\ \sigma_0^2 & \dots & \sigma_0^2 \end{pmatrix}$$

Note: kernel matrix **K** is NOT kernel function $k(\cdot, \cdot)$. Don't claim " $k(\cdot, \cdot)$ is P.S.D." in the exam. Now, We need to prove that **K** is P.S.D.

- 1. Prove K is symmetric.
- 2. Prove that $\forall v \in \mathbb{R}^n, v^\top K v \geq 0$.

- 1. Since $K_{i,j} = \sigma_0^2$ for all i, j, we have $\mathbf{K}^{\top} = \mathbf{K}$, thus \mathbf{K} is symmetric.
- 2. For any $\mathbf{v} = (v_1, v_2, \dots, v_n)^\top$, we need to prove $\mathbf{v}^\top \mathbf{K} \mathbf{v} \ge 0$.
 - 2.1 Naive way: First compute (Kv) and then $v^{\perp}(Kv)$.

$$\mathbf{K}\mathbf{v} = \sigma_0^2 (\sum_{i} v_i, \sum_{i} v_i, \dots, \sum_{i} v_i)^{\top}$$

$$\mathbf{v}^{\top} \mathbf{K}\mathbf{v} = \sigma_0^2 [v_1(\sum_{i} v_i) + v_2(\sum_{i} v_i) + \dots + v_n(\sum_{i} v_i)] = \sigma_0^2 (v_1 + v_2 + \dots + v_n)(\sum_{i} v_i)$$

$$= \sigma_0^2 (v_1 + \dots + v_n)(\sum_{i} v_i) = \sigma_0^2 (\sum_{i} v_i)(\sum_{i} v_i) = \sigma_0^2 (\sum_{i} v_i)^2 \ge 0.$$

2.2 Faster way: $\mathbf{K} = \sigma_0^2 \mathbf{I} \mathbf{I}^{\top}$, where $\mathbf{I} = (1, 1, ..., 1)^{\top}$. So $\mathbf{v}^{\top} \mathbf{K} \mathbf{v} = \sigma_0^2 \mathbf{v}^{\top} \mathbf{I}^{\top} \mathbf{v} = \sigma_0^2 (\mathbf{I}^{\top} \mathbf{v})^2 \ge 0$.

- 1. Since $K_{i,j} = \sigma_0^2$ for all i, j, we have $\mathbf{K}^{\top} = \mathbf{K}$, thus \mathbf{K} is symmetric.
- 2. For any $\mathbf{v} = (v_1, v_2, \dots, v_n)^{\top}$, we need to prove $\mathbf{v}^{\top} \mathbf{K} \mathbf{v} \geq 0$.
 - 2.1 Naive way: First compute $(K\nu)$ and then $\nu^{\top}(K\nu)$.

$$\mathbf{K}\mathbf{v} = \sigma_0^2 (\sum_i v_i, \sum_i v_i, \dots, \sum_i v_i)^{\top}$$

$$\mathbf{v}^{\top} \mathbf{K}\mathbf{v} = \sigma_0^2 [v_1(\sum_i v_i) + v_2(\sum_i v_i) + \dots + v_n(\sum_i v_i)] = \sigma_0^2 (v_1 + v_2 + \dots + v_n)(\sum_i v_i)$$

$$= \sigma_0^2 (v_1 + \dots + v_n)(\sum_i v_i) = \sigma_0^2 (\sum_i v_i)(\sum_i v_i) = \sigma_0^2 (\sum_i v_i)^2 \ge 0.$$

2.2 Faster way:
$$\mathbf{K} = \sigma_0^2 \mathbf{I} \mathbf{I}^{\top}$$
, where $\mathbf{I} = (1, 1, \dots, 1)^{\top}$. So, $\mathbf{v}^{\top} \mathbf{K} \mathbf{v} = \sigma_0^2 \mathbf{v}^{\top} \mathbf{I} \mathbf{I}^{\top} \mathbf{v} = \sigma_0^2 (\mathbf{I}^{\top} \mathbf{v})^2 \geq 0$.

- 1. Since $K_{i,j} = \sigma_0^2$ for all i, j, we have $\mathbf{K}^{\top} = \mathbf{K}$, thus \mathbf{K} is symmetric.
- 2. For any $\mathbf{v} = (v_1, v_2, \dots, v_n)^{\top}$, we need to prove $\mathbf{v}^{\top} \mathbf{K} \mathbf{v} \geq 0$.
 - 2.1 Naive way: First compute $(\mathbf{K}\mathbf{v})$ and then $\mathbf{v}^{\top}(\mathbf{K}\mathbf{v})$.

$$\mathbf{K}\mathbf{v} = \sigma_0^2 (\sum_i v_i, \sum_i v_i, \dots, \sum_i v_i)^{\top}$$

$$\mathbf{v}^{\top} \mathbf{K}\mathbf{v} = \sigma_0^2 [v_1(\sum_i v_i) + v_2(\sum_i v_i) + \dots + v_n(\sum_i v_i)] = \sigma_0^2 (v_1 + v_2 + \dots + v_n)(\sum_i v_i)$$

$$= \sigma_0^2 (v_1 + \dots + v_n)(\sum_i v_i) = \sigma_0^2 (\sum_i v_i)(\sum_i v_i) = \sigma_0^2 (\sum_i v_i)^2 \ge 0.$$

2.2 Faster way:
$$\mathbf{K} = \sigma_0^2 \mathbf{I} \mathbf{I}^{\top}$$
, where $\mathbf{I} = (1, 1, \dots, 1)^{\top}$. So, $\mathbf{v}^{\top} \mathbf{K} \mathbf{v} = \sigma_0^2 \mathbf{v}^{\top} \mathbf{I} \mathbf{I}^{\top} \mathbf{v} = \sigma_0^2 (\mathbf{I}^{\top} \mathbf{v})^2 \geq 0$.

- 1. Since $K_{i,j} = \sigma_0^2$ for all i, j, we have $\mathbf{K}^{\top} = \mathbf{K}$, thus \mathbf{K} is symmetric.
- 2. For any $\mathbf{v} = (v_1, v_2, \dots, v_n)^{\top}$, we need to prove $\mathbf{v}^{\top} \mathbf{K} \mathbf{v} \geq 0$.
 - 2.1 Naive way: First compute $(\mathbf{K}\mathbf{v})$ and then $\mathbf{v}^{\top}(\mathbf{K}\mathbf{v})$.

$$\mathbf{K}\mathbf{v} = \sigma_0^2 (\sum_i v_i, \sum_i v_i, \dots, \sum_i v_i)^{\top}$$

$$\mathbf{v}^{\top} \mathbf{K}\mathbf{v} = \sigma_0^2 [v_1(\sum_i v_i) + v_2(\sum_i v_i) + \dots + v_n(\sum_i v_i)] = \sigma_0^2 (v_1 + v_2 + \dots + v_n)(\sum_i v_i)$$

$$= \sigma_0^2 (v_1 + \dots + v_n)(\sum_i v_i) = \sigma_0^2 (\sum_i v_i)(\sum_i v_i) = \sigma_0^2 (\sum_i v_i)^2 \ge 0.$$

2.2 Faster way:
$$\mathbf{K} = \sigma_0^2 \mathbf{I} \mathbf{I}^{\top}$$
, where $\mathbf{I} = (1, 1, ..., 1)^{\top}$. So, $\mathbf{v}^{\top} \mathbf{K} \mathbf{v} = \sigma_0^2 \mathbf{v}^{\top} \mathbf{I} \mathbf{I}^{\top} \mathbf{v} = \sigma_0^2 (\mathbf{I}^{\top} \mathbf{v})^2 \ge 0$.

2 (a): Proof via Transformed Feature Map

Alternatively, we can prove $k(\mathbf{x}, \mathbf{x}') = \sigma_0^2$ is a valid cov. func. via writing $k(\mathbf{x}, \mathbf{x}')$ as an inner product of two transformed feature maps.

This requires to explicitly construct the feature map $\phi(\mathbf{x}) \in \mathbb{R}^d$ for some d. In the current case, we can write

$$\phi(\mathbf{x}) = \sigma_0.$$

So that

$$k (\mathbf{x}, \mathbf{x}') = \sigma_0^2$$

= $\langle \sigma_0, \sigma_0 \rangle$
= $\langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$

2 (a): Proof of $k(\mathbf{x}, \mathbf{x}') = \sigma_0^2 + \mathbf{x}^{\top} \mathbf{x}'$

$$k\left(\mathbf{x},\mathbf{x}'\right) = \underbrace{\sigma_0^2}_{:=k_0(\mathbf{x},\mathbf{x}')} + \underbrace{\mathbf{x}^\top\mathbf{x}'}_{:=k_1(\mathbf{x},\mathbf{x}')}$$

- 1. We have shown that k_0 is a valid cov. func.
- 2. k_1 is a inner product $\langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$, where $\phi(\mathbf{x}) := \mathbf{x}$. So, k_1 is a valid cov. func.
- 3. Their sum $k_0 + k_1$ is also a cov. func.

2 (a): Proof of
$$k(\mathbf{x}, \mathbf{x}') = (\sigma_0^2 + \mathbf{x}^{\top} \mathbf{x})^p$$

We define
$$k_2(\mathbf{x}, \mathbf{x}') = \sigma_0^2 + \mathbf{x}^\top \mathbf{x}$$
, so $k_3 = (\sigma_0^2 + \mathbf{x}^\top \mathbf{x})^p = k_2^p$.

- 1. We have shown that k_2 is a cov. func.
- 2. $k_3 = k_2^p$ is a polynomial of k_2 with only one p-order item k_2^p , and the polynomial coefficient 1 is positive. So $k_3 = k_2^p$ is a cov. func.

2 (a): Proof of $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||_2^2}{2\ell^2}\right)$

We can write

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||_{2}^{2}}{2\ell^{2}}\right)$$

$$= \exp\left(-\frac{\mathbf{x}^{\top}\mathbf{x} - 2\mathbf{x}^{\top}\mathbf{x}' + \mathbf{x}'^{\top}\mathbf{x}'}{2\ell^{2}}\right)$$

$$= \exp\left(-\frac{\mathbf{x}^{\top}\mathbf{x}}{2\ell^{2}}\right) \cdot \exp\left(\frac{\mathbf{x}^{\top}\mathbf{x}'}{\ell^{2}}\right) \cdot \exp\left(-\frac{\mathbf{x}'^{\top}\mathbf{x}'}{2\ell^{2}}\right).$$

$$:= t(\mathbf{x})$$

$$:= t(\mathbf{x})$$

where we defined a function $t(\cdot)$.

Furthermore, $\mathbf{x}^{\top}\mathbf{x}'$ is cov. func., so $\frac{\mathbf{x}^{\top}\mathbf{x}'}{\ell^2}$ is a kernel, so $\exp(\frac{\mathbf{x}^{\top}\mathbf{x}'}{\ell^2})$ is a cov. func.

Therefore, $k(\mathbf{x}, \mathbf{x}') = t(\mathbf{x}) \cdot k_4(\mathbf{x}, \mathbf{x}') \cdot t(\mathbf{x}')$ is a cov. func.

Exercise 2 (b)

(b): Are these covariance functions stationary or isotropic? Justify your answer.

2 (b): Stationary and Isotropic

- 1. $k(\cdot, \cdot)$ is stationary if $k(\mathbf{x}, \mathbf{x} + \mathbf{d}) = k(\mathbf{0}, \mathbf{d})$.
- 2. $k(\cdot, \cdot)$ is isotropic if it is a function of $||\mathbf{x} \mathbf{x}'||$.

2 (b): Constant functions

1.
$$k(\mathbf{x}, \mathbf{x}') = \sigma_0^2$$
 is stationary since $k(\mathbf{x}, \mathbf{x} + \mathbf{d}) = \sigma_0^2 = k(\mathbf{0}, \mathbf{d})$.

2.
$$k(\mathbf{x}, \mathbf{x}') = \sigma_0^2$$
 is isotropic since $k(\mathbf{x}, \mathbf{x}') = \sigma_0^2 ||\mathbf{x} - \mathbf{x}'||^0$.

2 (b): Constant functions

1.
$$k(\mathbf{x}, \mathbf{x}') = \sigma_0^2$$
 is stationary since $k(\mathbf{x}, \mathbf{x} + \mathbf{d}) = \sigma_0^2 = k(\mathbf{0}, \mathbf{d})$.

2.
$$k(\mathbf{x}, \mathbf{x}') = \sigma_0^2$$
 is isotropic since $k(\mathbf{x}, \mathbf{x}') = \sigma_0^2 ||\mathbf{x} - \mathbf{x}'||^0$.

2 (b):
$$k(\mathbf{x}, \mathbf{x}') = \sigma_0^2 + \mathbf{x}^{\top} \mathbf{x}'$$

1. $k(\mathbf{x}, \mathbf{x}') = \sigma_0^2 + \mathbf{x}^\top \mathbf{x}'$ is NOT stationary, since

$$k(\mathbf{x}, \mathbf{x} + \mathbf{d}) = \sigma_0^2 + \mathbf{x}^{\top} \mathbf{x} + \mathbf{x}^{\top} \mathbf{d}$$

 $k(\mathbf{0}, \mathbf{d}) = \sigma_0^2.$

2. It is NOT isotropic, since it cannot be written as a func. of $||\mathbf{x} - \mathbf{x}'||$.

2 (b):
$$k(\mathbf{x}, \mathbf{x}') = \sigma_0^2 + \mathbf{x}^{\top} \mathbf{x}'$$

1. $k(\mathbf{x}, \mathbf{x}') = \sigma_0^2 + \mathbf{x}^{\top} \mathbf{x}'$ is NOT stationary, since

$$k(\mathbf{x}, \mathbf{x} + \mathbf{d}) = \sigma_0^2 + \mathbf{x}^{\top} \mathbf{x} + \mathbf{x}^{\top} \mathbf{d}$$

 $k(\mathbf{0}, \mathbf{d}) = \sigma_0^2.$

2. It is NOT isotropic, since it cannot be written as a func. of $||\mathbf{x} - \mathbf{x}'||$.

2 (b): Polynomial Cov. Func.

Similar to linear covariance functions, the polynomial covariance function is NOT stationary and NOT isotropic. (Prove this on your own.)

2 (b):
$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||_2^2}{2\ell^2}\right)$$

- 1. $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} \mathbf{x}'||_2^2}{2\ell^2}\right)$ is stationary, since $k(\mathbf{x}, \mathbf{x} + \mathbf{d}) = \exp\left(-\frac{||\mathbf{d}||_2^2}{2\ell^2}\right) = k(\mathbf{0}, \mathbf{d}).$
- 2. It is isotropic, since it is a function of $||\mathbf{x} \mathbf{x}'||$.

2 (b):
$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||_2^2}{2\ell^2}\right)$$

- 1. $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} \mathbf{x}'||_2^2}{2\ell^2}\right)$ is stationary, since $k(\mathbf{x}, \mathbf{x} + \mathbf{d}) = \exp\left(-\frac{||\mathbf{d}||_2^2}{2\ell^2}\right) = k(\mathbf{0}, \mathbf{d}).$
- 2. It is isotropic, since it is a function of $||\mathbf{x} \mathbf{x}'||$.

2 (b): Matern and Exponential Cov. Func.

Similar to the argument of squared exponential conv. func. $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||_2^2}{2\ell^2}\right)$.

1. Matern cov. func. is stationary and isotropic.

$$k\left(\mathbf{x},\mathbf{x}'
ight) = rac{1}{2^{
u}} \left(rac{\sqrt{2
u}}{\ell}||\mathbf{x}-\mathbf{x}'||
ight)^{
u} \mathcal{K}_{
u} \left(rac{\sqrt{2
u}}{\ell}||\mathbf{x}-\mathbf{x}'||
ight)$$

2. Exponential cov. func. is stationary and isotropic.

$$k\left(\mathbf{x},\mathbf{x}'\right) = \exp\left(-\frac{||\mathbf{x}-\mathbf{x}'||}{\ell}\right)$$