Chapter 6 Kernel Methods

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6.1 Dual Representations

(6.3)

By setting the gradient of $J(\mathbf{w})$ with respect to \mathbf{w} to $\mathbf{0}$, it is easy to see that

$$\mathbf{w} = \arg_{\mathbf{w}} \nabla_{\mathbf{w}} J(\mathbf{w}) = \mathbf{0}$$

$$= \arg_{\mathbf{w}} \left(\sum_{n=1}^{N} \left\{ \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x}_{n}) - t_{n} \right\} + \lambda \mathbf{w} = \mathbf{0} \right)$$

$$= -\frac{1}{\lambda} \sum_{n=1}^{N} \left\{ \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x}_{n}) - t_{n} \right\} \phi(\mathbf{x}_{n})$$

$$= \mathbf{\Phi}^{\mathrm{T}} \mathbf{a}$$

where

$$\mathbf{a} = -\frac{1}{\lambda}(\mathbf{\Phi}\mathbf{w} - \mathbf{t}).$$

(6.5)

$$J(\mathbf{a}) = \frac{1}{2} \sum_{n=1}^{N} \left\{ \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_{n}) - t_{n} \right\}^{2} + \frac{\lambda}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}$$

$$= \frac{1}{2} \sum_{n=1}^{N} \left\{ \boldsymbol{\phi}(\mathbf{x}_{n})^{\mathrm{T}} \mathbf{w} - t_{n} \right\}^{2} + \frac{\lambda}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}$$

$$= \frac{1}{2} \sum_{n=1}^{N} \left\{ \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_{n}) \boldsymbol{\phi}(\mathbf{x}_{n})^{\mathrm{T}} \mathbf{w} - 2 \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_{n}) t_{n} + t_{n}^{2} \right\} + \frac{\lambda}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}$$

$$= \frac{1}{2} \mathbf{w}^{\mathrm{T}} \left(\sum_{n=1}^{N} \boldsymbol{\phi}(\mathbf{x}_{n}) \boldsymbol{\phi}(\mathbf{x}_{n})^{\mathrm{T}} \right) \mathbf{w} - \mathbf{w}^{\mathrm{T}} \sum_{n=1}^{N} \boldsymbol{\phi}(\mathbf{x}_{n}) t_{n} + \frac{1}{2} \sum_{n=1}^{N} t_{n}^{2} + \frac{\lambda}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}$$

$$= \frac{1}{2} \mathbf{a}^{\mathrm{T}} \boldsymbol{\Phi} \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{a} - \mathbf{a}^{\mathrm{T}} \boldsymbol{\Phi} \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t} + \frac{1}{2} \mathbf{t}^{\mathrm{T}} \mathbf{t} + \frac{\lambda}{2} \mathbf{a}^{\mathrm{T}} \mathbf{K} \mathbf{a}.$$

(6.8)

From the derivation of (6.3), we have

$$\begin{split} \mathbf{a} &= -\frac{1}{\lambda}(\mathbf{\Phi}\mathbf{w} - \mathbf{t}) \\ &= -\frac{1}{\lambda}(\mathbf{\Phi}\mathbf{\Phi}^{\mathrm{T}}\mathbf{a} - \mathbf{t}) \\ &= -\frac{1}{\lambda}(\mathbf{K}\mathbf{a} - \mathbf{t}). \end{split}$$

Solving for \mathbf{a} , we obtain

$$\mathbf{a} = (\mathbf{K} + \lambda \mathbf{I}_N)^{-1} \mathbf{t}.$$

(6.9)

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x}) = \mathbf{a}^{\mathrm{T}} \mathbf{\Phi} \phi(\mathbf{x}) = (\mathbf{\Phi} \phi(\mathbf{x}))^{\mathrm{T}} \mathbf{a} = \mathbf{k}(\mathbf{x})^{\mathrm{T}} (\mathbf{K} + \lambda \mathbf{I}_{N})^{-1} \mathbf{t}.$$

6.2 Constructing Kernels

(6.13)

To verify (6.13) is a valid kernel, we see that for any vector $\mathbf{u} \in \mathbb{R}^N$,

$$\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} = \mathbf{u}^{\mathrm{T}}(c\mathbf{K}_{1})\mathbf{u} = c(\mathbf{u}^{\mathrm{T}}\mathbf{K}_{1}\mathbf{u}) \geq 0,$$

which implies that $\mathbf{K} \succeq 0$.

(6.14)

To verify (6.14) is a valid kernel, we first notice that $k(\mathbf{x}, \mathbf{x}')$ is symmetric by

$$k(\mathbf{x}', \mathbf{x}) = ck_1(\mathbf{x}', \mathbf{x}) = ck_1(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}').$$

Also, we see that for any vector $\mathbf{u} \in \mathbb{R}^N$,

$$\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} = \sum_{i=1}^{N} \sum_{j=1}^{N} k(\mathbf{x}_{i}, \mathbf{x}_{j}) u_{i} u_{j}$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} k_{1}(\mathbf{x}_{i}, \mathbf{x}_{j}) (f(\mathbf{x}_{i}) u_{i}) (f(\mathbf{x}_{j}) u_{j})$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} k_{1}(\mathbf{x}_{i}, \mathbf{x}_{j}) v_{i} v_{j}$$

$$> 0$$

where we denote $v_i = f(\mathbf{x}_i)u_i$, implying $\mathbf{K} \succeq 0$. Therefore, (6.14) is a valid kernel.

(6.15)

To verify (6.15) is a valid kernel, let $q(k_1(\mathbf{x}, \mathbf{x}')) = \sum_m c_m k_1(\mathbf{x}, \mathbf{x}')^m$ where $c_m \geq 0$. By repeatedly applying (6.18), we see that $k_1(\mathbf{x}, \mathbf{x}')^m$ is a valid kernel. Then, according to (6.13), $c_m k_1(\mathbf{x}, \mathbf{x}')^m$ is also a valid kernel. Finally, using (6.17), we can conclude that $q(k_1(\mathbf{x}, \mathbf{x}')) = \sum_m c_m k_1(\mathbf{x}, \mathbf{x}')^m$ is a valid kernel.

(6.16)

To verify (6.16) is a valid kernel, we first notice that $k(\mathbf{x}, \mathbf{x}')$ is symmetric by

$$k(\mathbf{x}', \mathbf{x}) = \exp(k_1(\mathbf{x}', \mathbf{x})) = \exp(k_1(\mathbf{x}, \mathbf{x}')) = k(\mathbf{x}, \mathbf{x}').$$

Also, we see that for any vector $\mathbf{u} \in \mathbb{R}^N$,

$$\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} = \sum_{i=1}^{N} \sum_{j=1}^{N} k(\mathbf{x}_{i}, \mathbf{x}_{j}) u_{i} u_{j}$$
$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \exp(k_{1}(\mathbf{x}_{i}, \mathbf{x}_{j})) u_{i} u_{j}.$$

Applying the Maclaurin series for the exponential term, we have

$$\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} = \sum_{i=1}^{N} \sum_{j=1}^{N} \left(\sum_{n=0}^{\infty} \frac{k_1(\mathbf{x}_i, \mathbf{x}_j)^n}{n!} \right) u_i u_j \ge 0$$

where we made use of (6.15), implying $\mathbf{K} \succeq 0$. Therefore, (6.16) is a valid kernel.

(6.17)

To verify (6.17) is a valid kernel, we first notice that $k(\mathbf{x}, \mathbf{x}')$ is symmetric by

$$k(\mathbf{x}', \mathbf{x}) = k_1(\mathbf{x}', \mathbf{x}) + k_2(\mathbf{x}', \mathbf{x}) = k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}').$$

Also, we see that for any vector $\mathbf{u} \in \mathbb{R}^N$,

$$\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} = \sum_{i=1}^{N} \sum_{j=1}^{N} k(\mathbf{x}_{i}, \mathbf{x}_{j}) u_{i} u_{j}$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} (k_{1}(\mathbf{x}_{i}, \mathbf{x}_{j}) + k_{2}(\mathbf{x}_{i}, \mathbf{x}_{j})) u_{i} u_{j}$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} k_{1}(\mathbf{x}_{i}, \mathbf{x}_{j}) u_{i} u_{j} + \sum_{i=1}^{N} \sum_{j=1}^{N} k_{2}(\mathbf{x}_{i}, \mathbf{x}_{j}) u_{i} u_{j}$$

$$\geq 0.$$

which implies that $\mathbf{K} \succeq 0$. Therefore, (6.17) is a valid kernel.

(6.18)

To verify (6.18) is a valid kernel, we first notice that $k(\mathbf{x}, \mathbf{x}')$ is symmetric by

$$k(\mathbf{x}', \mathbf{x}) = k_1(\mathbf{x}', \mathbf{x})k_2(\mathbf{x}', \mathbf{x}) = k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}').$$

Also, we see that for any vector $\mathbf{u} \in \mathbb{R}^N$,

$$\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} = \sum_{i=1}^{N} \sum_{j=1}^{N} k(\mathbf{x}_{i}, \mathbf{x}_{j}) u_{i} u_{j}$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} k_{1}(\mathbf{x}_{i}, \mathbf{x}_{j}) k_{2}(\mathbf{x}_{i}, \mathbf{x}_{j}) u_{i} u_{j}$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \phi_{1}(\mathbf{x}_{i})^{\mathrm{T}} \phi_{1}(\mathbf{x}_{j}) \phi_{2}(\mathbf{x}_{i})^{\mathrm{T}} \phi_{2}(\mathbf{x}_{j}) u_{i} u_{j}$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \left(\sum_{l=1}^{M} \phi_{1l}(\mathbf{x}_{i}) \phi_{1l}(\mathbf{x}_{j}) \right) \left(\sum_{m=1}^{M} \phi_{2m}(\mathbf{x}_{i}) \phi_{2m}(\mathbf{x}_{j}) \right) u_{i} u_{j}$$

$$= \sum_{l=1}^{M} \sum_{m=1}^{M} \left(\sum_{i=1}^{N} \phi_{1l}(\mathbf{x}_{i}) \phi_{2m}(\mathbf{x}_{i}) u_{i} \right)^{2}$$

$$> 0.$$

which implies that $\mathbf{K} \succeq 0$. Therefore, (6.18) is a valid kernel.

(6.20)

To verify (6.20) is a valid kernel, recall that any symmetric matrix S can be diagonalized by $S = Q\Lambda Q^T$ where the columns of Q are orthogonal eigenvectors. Hence,

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x}' = \mathbf{x}^{\mathrm{T}} \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{\mathrm{T}} \mathbf{x}' = (\mathbf{Q}^{\mathrm{T}} \mathbf{x})^{\mathrm{T}} \mathbf{\Lambda} (\mathbf{Q}^{\mathrm{T}} \mathbf{x}').$$

Denoting $\mathbf{v} = \mathbf{Q}^{\mathrm{T}} \mathbf{x}$ and $\mathbf{v}' = \mathbf{Q}^{\mathrm{T}} \mathbf{x}'$,

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{v}^{\mathrm{T}} \mathbf{\Lambda} \mathbf{v}' = \sum_{i=1}^{N} \Lambda_{ii} v_i v_i' = \sum_{i=1}^{N} (\sqrt{\Lambda_{ii}} v_i) (\sqrt{\Lambda_{ii}} v_j) = \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}') = k'(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}'))$$

where k' is the linear kernel, and the square roots exist because the eigenvalues for a positive semidefinite matrix are non-negative. Therefore, according to (6.19), $k(\mathbf{x}, \mathbf{x}')$ is a valid kernel.

(6.21)

$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b)$$

$$= \sum_{s=1}^{S} \phi_{as}(\mathbf{x}_a) \phi_{as}(\mathbf{x}'_a) + \sum_{t=1}^{T} \phi_{bt}(\mathbf{x}_b) \phi_{bt}(\mathbf{x}'_b)$$

$$= \sum_{i=1}^{S+T} \phi_i(\mathbf{x}) \phi_i(\mathbf{x}'),$$

which is a valid kernel.

(6.22) – To be updated

$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a) k_b(\mathbf{x}_b, \mathbf{x}'_b)$$

$$= \sum_{s=1}^{S} \phi_{as}(\mathbf{x}_a) \phi_{as}(\mathbf{x}'_a) \sum_{t=1}^{T} \phi_{bt}(\mathbf{x}_b) \phi_{bt}(\mathbf{x}'_b)$$

$$= \sum_{s=1}^{S} \sum_{t=1}^{T} \left\{ \phi_{as}(\mathbf{x}_a) \phi_{bt}(\mathbf{x}_b) \right\} \left\{ \phi_{as}(\mathbf{x}'_a) \phi_{bt}(\mathbf{x}'_b) \right\}$$

6.3 Radial Basis Function Networks

Skipped reading.

6.4 Gaussian Processes

(6.52)

$$\mathbb{E}[\mathbf{y}] = \mathbb{E}[\mathbf{\Phi}\mathbf{w}] = \mathbf{\Phi}\mathbb{E}[\mathbf{w}] = \mathbf{0}.$$

(6.53)

$$cov[\mathbf{y}] = \mathbb{E}[\mathbf{y}\mathbf{y}^{\mathrm{T}}] - \mathbb{E}[\mathbf{y}]\mathbb{E}[\mathbf{y}^{\mathrm{T}}] = \mathbb{E}[\mathbf{y}\mathbf{y}^{\mathrm{T}}] = \mathbb{E}[\mathbf{\Phi}\mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{\Phi}^{\mathrm{T}}] = \mathbf{\Phi}\mathbb{E}[\mathbf{w}\mathbf{w}^{\mathrm{T}}]\mathbf{\Phi}^{\mathrm{T}} = \mathbf{\Phi}cov[\mathbf{w}]\mathbf{\Phi}^{\mathrm{T}} = \frac{1}{\alpha}\mathbf{\Phi}\mathbf{\Phi}^{\mathrm{T}} = \mathbf{K}$$
where

$$K_{nm} = k(\mathbf{x}_n, \mathbf{x}_m) = \frac{1}{\alpha} \phi(\mathbf{x}_n)^{\mathrm{T}} \phi(\mathbf{x}_m).$$

(6.61)

We use the property that if $p(\mathbf{x})$ and $p(\mathbf{y}|\mathbf{x})$ are Gaussian, p(y) is also a Gaussian. Plugging the equations

$$egin{aligned} oldsymbol{\mu} &= \mathbf{0} \ oldsymbol{\Lambda}^{-1} &= \mathbf{K} \ \mathbf{A}\mathbf{x} + \mathbf{b} &= \mathbf{y} \ \mathbf{L}^{-1} &= eta^{-1}\mathbf{I}_N \end{aligned}$$

into (2.115), we obtain

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{y})p(\mathbf{y}) d\mathbf{y} = \mathcal{N}(\mathbf{0}, \mathbf{C})$$

where

$$\mathbf{C} = \mathbf{K} + \beta^{-1} \mathbf{I}_N.$$

$$(6.66) - (6.67)$$

Using the property that if two sets of variables are jointly Gaussian, the conditional distribution of one on the other is also Gaussian, we have

$$\mu_{t_{N+1}|\mathbf{t}} = \mu_{t_{N+1}} + \mathbf{\Sigma}_{t_{N+1}\mathbf{t}} \mathbf{\Sigma}_{\mathbf{tt}}^{-1} (\mathbf{t} - \boldsymbol{\mu}_{\mathbf{t}})$$

$$= 0 + \mathbf{k}^{\mathrm{T}} \mathbf{C}^{-1} (\mathbf{t} - \mathbf{0})$$

$$= \mathbf{k}^{\mathrm{T}} \mathbf{C}_{N}^{-1} \mathbf{t}$$

$$\sigma_{t_{N+1}|\mathbf{t}}^{2} = \sigma_{t_{N+1}t_{N+1}}^{2} - \mathbf{\Sigma}_{t_{N+1}\mathbf{t}} \mathbf{\Sigma}_{\mathbf{tt}}^{-1} \mathbf{\Sigma}_{\mathbf{t}t_{N+1}}$$

$$= c - \mathbf{k}^{\mathrm{T}} \mathbf{C}_{N}^{-1} \mathbf{k}.$$

(6.79)

$$p(\mathbf{t}_N|\mathbf{a}_N) = \prod_{n=1}^N \sigma(a_n)^{t_n} (1 - \sigma(a_n))^{1 - t_n}$$

$$= \prod_{n=1}^N \left(\frac{1}{1 + \exp(-a_n)}\right)^{t_n} \left(\frac{\exp(-a_n)}{1 + \exp(-a_n)}\right)^{1 - t_n}$$

$$= \prod_{n=1}^N \left(\frac{1}{1 + \exp(-a_n)} \frac{1 + \exp(-a_n)}{\exp(-a_n)}\right)^{t_n} \exp(-a_n)$$

$$= \prod_{n=1}^N e^{a_n t_n} \sigma(-a_n).$$

(6.81)

Here, $-\boldsymbol{\sigma}_N$ is derived from

$$\nabla \left(-\sum_{n=1}^{N} \ln(1 + e^{a_n}) \right) = \left[\frac{\partial f}{\partial a_1}, \dots, \frac{\partial f}{\partial a_N} \right]^{\mathrm{T}}$$
$$= [\sigma(a_1), \dots, \sigma(a_N)]^{\mathrm{T}}$$
$$= -\boldsymbol{\sigma}_N.$$

(6.82)

Noticing that

$$\frac{\mathrm{d}\sigma(a_i)}{\mathrm{d}a_j} = \begin{cases} \sigma(a_i)(1 - \sigma(a_i)) & \text{if } i = j\\ 0 & \text{if } i \neq j, \end{cases}$$

and \mathbf{C}_N is symmetric, it is easy to see that

$$\nabla \nabla \Psi(\mathbf{a}_N) = -\mathbf{W}_N - \mathbf{C}_N^{-1}.$$

For any diagonal element, we have

$$\sigma(a_i)(1 - \sigma(a_i)) = -\left(\sigma(a_i) - \frac{1}{2}\right)^2 + \frac{1}{4} \le \frac{1}{4},$$

which implies that \mathbf{W}_N is positive definite.

(6.83)

According to the Newton-Raphson formula, we have

$$\begin{split} \mathbf{a}_N^{\text{new}} &= \mathbf{a}_N - \mathbf{H}^{-1} \nabla \Psi(\mathbf{a}_N) \\ &= \mathbf{a}_N - (-\mathbf{W}_N - \mathbf{C}_N^{-1})^{-1} \{ \mathbf{t}_N - \boldsymbol{\sigma}_N - \mathbf{C}_N^{-1} \mathbf{a}_N \} \\ &= \mathbf{a}_N + (\mathbf{W}_N + \mathbf{C}_N^{-1})^{-1} \{ \mathbf{t}_N - \boldsymbol{\sigma}_N - \mathbf{C}_N^{-1} \mathbf{a}_N \} \\ &= (\mathbf{W}_N + \mathbf{C}_N^{-1})^{-1} \{ (\mathbf{W}_N + \mathbf{C}_N^{-1}) \mathbf{a}_N + \mathbf{t}_N - \boldsymbol{\sigma}_N - \mathbf{C}_N^{-1} \mathbf{a}_N \} \\ &= \mathbf{C}_N (\mathbf{I} + \mathbf{W}_N \mathbf{C}_N)^{-1} \{ \mathbf{t}_N - \boldsymbol{\sigma}_N + \mathbf{W}_N \mathbf{a}_N \}. \end{split}$$

(6.84)

At the mode, the gradient $\nabla \Psi(\mathbf{a}_N)$ vanishes, that is

$$\nabla \Psi(\mathbf{a}_N) = \mathbf{t}_N - \boldsymbol{\sigma}_N - \mathbf{C}_N^{-1} \mathbf{a}_N = \mathbf{0}.$$

Solving for \mathbf{a}_N , we obtain

$$\mathbf{a}_N = \mathbf{C}_N(\mathbf{t}_N - \boldsymbol{\sigma}_N).$$

Therefore,

$$\mathbf{a}_N^* = \mathbf{a}_N - \mathbf{H}^{-1} \nabla \Psi(\mathbf{a}_N) = \mathbf{a}_N = \mathbf{C}_N (\mathbf{t}_N - \boldsymbol{\sigma}_N).$$

$$(6.87) - (6.88)$$

Let

$$\begin{split} p(\mathbf{a}_N|\mathbf{t}_N) &= \mathcal{N}(\mathbf{a}_N|\mathbf{a}_N^*, \mathbf{H}^{-1}) = \mathcal{N}(\mathbf{a}_N|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}) \\ p(a_{N+1}|\mathbf{a}_N) &= \mathcal{N}(a_{N+1}|\mathbf{k}^{\mathrm{T}}\mathbf{C}_N^{-1}\mathbf{a}_N, c - \mathbf{k}^{\mathrm{T}}\mathbf{C}_N^{-1}\mathbf{k}) = \mathcal{N}(a_{N+1}|\mathbf{A}\mathbf{a}_N + \mathbf{b}, \mathbf{L}^{-1}), \end{split}$$

we have

$$\begin{split} \boldsymbol{\mu} &= \mathbf{a}_N^* \\ \boldsymbol{\Lambda}^{-1} &= \mathbf{H}^{-1} \\ \mathbf{A} &= \mathbf{k}^{\mathrm{T}} \mathbf{C}_N^{-1} \\ \mathbf{b} &= \mathbf{0} \\ \mathbf{L}^{-1} &= c - \mathbf{k}^{\mathrm{T}} \mathbf{C}_N^{-1} \mathbf{k}. \end{split}$$

According to (2.115), we obtain

$$\begin{split} \mathbb{E}[a_{N+1}|\mathbf{t}_{N}] &= \mathbf{A}\boldsymbol{\mu} + \mathbf{b} \\ &= \mathbf{k}^{\mathrm{T}}\mathbf{C}_{N}^{-1}\mathbf{a}_{N}^{*} + \mathbf{0} \\ &= \mathbf{k}^{\mathrm{T}}\mathbf{C}_{N}^{-1}\mathbf{C}_{N}(\mathbf{t}_{N} - \boldsymbol{\sigma}_{N}) \\ &= \mathbf{k}^{\mathrm{T}}(\mathbf{t}_{N} - \boldsymbol{\sigma}_{N}) \\ \mathrm{var}[a_{N+1}|\mathbf{t}_{N}] &= \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\mathrm{T}} \\ &= c - \mathbf{k}^{\mathrm{T}}\mathbf{C}_{N}^{-1}\mathbf{k} + \mathbf{k}^{\mathrm{T}}\mathbf{C}_{N}^{-1}\mathbf{H}^{-1}(\mathbf{k}^{\mathrm{T}}\mathbf{C}_{N}^{-1})^{\mathrm{T}} \\ &= c - \mathbf{k}^{\mathrm{T}}\mathbf{C}_{N}^{-1}\mathbf{k} + \mathbf{k}^{\mathrm{T}}\mathbf{C}_{N}^{-1}(\mathbf{W}_{N} + \mathbf{C}_{N}^{-1})^{-1}\mathbf{C}_{N}^{-1}\mathbf{k} \\ &= c - \mathbf{k}^{\mathrm{T}}\mathbf{C}_{N}^{-1}(\mathbf{W}_{N} + \mathbf{C}_{N}^{-1})^{-1}(\mathbf{W}_{N} + \mathbf{C}_{N}^{-1})\mathbf{k} + \mathbf{k}^{\mathrm{T}}\mathbf{C}_{N}^{-1}(\mathbf{W}_{N} + \mathbf{C}_{N}^{-1})^{-1}\mathbf{C}_{N}^{-1}\mathbf{k} \\ &= c - \mathbf{k}^{\mathrm{T}}\mathbf{C}_{N}^{-1}(\mathbf{W}_{N} + \mathbf{C}_{N}^{-1})^{-1}((\mathbf{W}_{N} + \mathbf{C}_{N}^{-1} - \mathbf{C}_{N}^{-1})\mathbf{k} \\ &= c - \mathbf{k}^{\mathrm{T}}\mathbf{C}_{N}^{-1}(\mathbf{W}_{N} + \mathbf{C}_{N}^{-1})^{-1}\mathbf{W}_{N}\mathbf{k} \\ &= c - \mathbf{k}^{\mathrm{T}}(\mathbf{W}_{N}^{-1}(\mathbf{W}_{N} + \mathbf{C}_{N}^{-1})\mathbf{C}_{N})^{-1}\mathbf{k} \\ &= c - \mathbf{k}^{\mathrm{T}}((\mathbf{I} + \mathbf{W}_{N}^{-1}\mathbf{C}_{N}^{-1})\mathbf{C}_{N})^{-1}\mathbf{k} \\ &= c - \mathbf{k}^{\mathrm{T}}(\mathbf{W}_{N}^{-1} + \mathbf{C}_{N})^{-1}\mathbf{k}. \end{split}$$

(6.90)

Identifying $f(\mathbf{a}_N) = p(\mathbf{t}_N | \mathbf{a}_N) p(\mathbf{a}_N | \boldsymbol{\theta})$ and $Z = p(\mathbf{t}_N | \boldsymbol{\theta})$ and applying the Laplace approximation, we obtain

$$\ln p(\mathbf{t}_N|\boldsymbol{\theta}) = \ln \left(f(\mathbf{a}_N^*) \frac{(2\pi)^{N/2}}{|\mathbf{H}|^{1/2}} \right)$$

$$= \ln(p(\mathbf{t}_N|\mathbf{a}_N)p(\mathbf{a}_N|\boldsymbol{\theta})) - \frac{1}{2} \ln |\mathbf{W}_N + \mathbf{C}_N^{-1}| + \frac{N}{2} \ln(2\pi)$$

$$= \Psi(\mathbf{a}_N^*) - \frac{1}{2} \ln |\mathbf{W}_N + \mathbf{C}_N^{-1}| + \frac{N}{2} \ln(2\pi)$$

where we made use of (4.135), (6.80) and (6.85).

(6.91) - (6.94) - To be updated