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

$$\begin{aligned}\mathbf{w} &= \arg_{\mathbf{w}} \nabla_{\mathbf{w}} J(\mathbf{w}) = \mathbf{0} \\ &= \arg_{\mathbf{w}} \left(\sum_{n=1}^{N} \left\{ \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) - t_n \right\} + \lambda \mathbf{w} = \mathbf{0} \right) \\ &= -\frac{1}{\lambda} \sum_{n=1}^{N} \left\{ \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) - t_n \right\} \boldsymbol{\phi}(\mathbf{x}_n) \\ &= \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{a}\end{aligned}$$

where

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

(6.5)

$$\begin{aligned}J(\mathbf{a}) &= \frac{1}{2} \sum_{n=1}^{N} \left\{ \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) - t_n \right\}^2 + \frac{\lambda}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} \\ &= \frac{1}{2} \sum_{n=1}^{N} \left\{ \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}} \mathbf{w} - t_n \right\}^2 + \frac{\lambda}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} \\ &= \frac{1}{2} \sum_{n=1}^{N} \left\{ \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}} \mathbf{w} - 2 \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) t_n + t_n^2 \right\} + \frac{\lambda}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} \\ &= \frac{1}{2} \mathbf{w}^{\mathrm{T}} \left(\sum_{n=1}^{N} \boldsymbol{\phi}(\mathbf{x}_n) \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}} \right) \mathbf{w} - \mathbf{w}^{\mathrm{T}} \sum_{n=1}^{N} \boldsymbol{\phi}(\mathbf{x}_n) t_n + \frac{1}{2} \sum_{n=1}^{N} t_n^2 + \frac{\lambda}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} \\ &= \frac{1}{2} \mathbf{a}^{\mathrm{T}} \boldsymbol{\Phi} \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{a} - \mathbf{a}^{\mathrm{T}} \boldsymbol{\Phi} \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t} + \frac{1}{2} \mathbf{t}^{\mathrm{T}} \mathbf{t} + \frac{\lambda}{2} \mathbf{a}^{\mathrm{T}} \mathbf{K} \mathbf{a}.\end{aligned}$$

(6.8)

From the derivation of (6.3), we have

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

Solving for $\mathbf{a}$, we obtain

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

(6.9)

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

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 $\mathbf{u} \in \mathbb{R}^N$,

$$\begin{aligned}
\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} &= \sum_{i=1}^{N}\sum_{j=1}^{N} k(\mathbf{x}_i, \mathbf{x}_j)u_i u_j \\
&= \sum_{i=1}^{N}\sum_{j=1}^{N} k_1(\mathbf{x}_i, \mathbf{x}_j)(f(\mathbf{x}_i)u_i)(f(\mathbf{x}_j)u_j) \\
&= \sum_{i=1}^{N}\sum_{j=1}^{N} k_1(\mathbf{x}_i, \mathbf{x}_j)v_i v_j \\
&\geq 0
\end{aligned}$$

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 $\mathbf{u} \in \mathbb{R}^N$,

$$\begin{aligned}
\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} &= \sum_{i=1}^{N}\sum_{j=1}^{N} k(\mathbf{x}_i, \mathbf{x}_j)u_i u_j \\
&= \sum_{i=1}^{N}\sum_{j=1}^{N} \exp(k_1(\mathbf{x}_i, \mathbf{x}_j))u_i u_j.
\end{aligned}$$

Applying the Maclaurin series for the exponential term, we have

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

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 $\mathbf{u} \in \mathbb{R}^N$,

$$\begin{aligned}
\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} &= \sum_{i=1}^{N}\sum_{j=1}^{N} k(\mathbf{x}_i,\mathbf{x}_j)u_i u_j \\
&= \sum_{i=1}^{N}\sum_{j=1}^{N}(k_1(\mathbf{x}_i,\mathbf{x}_j) + k_2(\mathbf{x}_i,\mathbf{x}_j))u_i u_j \\
&= \sum_{i=1}^{N}\sum_{j=1}^{N} k_1(\mathbf{x}_i,\mathbf{x}_j)u_i u_j + \sum_{i=1}^{N}\sum_{j=1}^{N} k_2(\mathbf{x}_i,\mathbf{x}_j)u_i u_j \\
&\geq 0,
\end{aligned}$$

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 $\mathbf{u} \in \mathbb{R}^N$,

$$\begin{aligned}
\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} &= \sum_{i=1}^{N}\sum_{j=1}^{N} k(\mathbf{x}_i,\mathbf{x}_j)u_i u_j \\
&= \sum_{i=1}^{N}\sum_{j=1}^{N} k_1(\mathbf{x}_i,\mathbf{x}_j)k_2(\mathbf{x}_i,\mathbf{x}_j)u_i u_j \\
&= \sum_{i=1}^{N}\sum_{j=1}^{N} \boldsymbol{\phi}_1(\mathbf{x}_i)^{\mathrm{T}}\boldsymbol{\phi}_1(\mathbf{x}_j)\boldsymbol{\phi}_2(\mathbf{x}_i)^{\mathrm{T}}\boldsymbol{\phi}_2(\mathbf{x}_j)u_i u_j \\
&= \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\sum_{l=1}^{M}\phi_{1l}(\mathbf{x}_i)\phi_{1l}(\mathbf{x}_j)\right)\left(\sum_{m=1}^{M}\phi_{2m}(\mathbf{x}_i)\phi_{2m}(\mathbf{x}_j)\right)u_i u_j \\
&= \sum_{l=1}^{M}\sum_{m=1}^{M}\left(\sum_{i=1}^{N}\phi_{1l}(\mathbf{x}_i)\phi_{2m}(\mathbf{x}_i)u_i\right)^2 \\
&\geq 0,
\end{aligned}$$

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 $\mathbf{S}$ can be diagonalized by $\mathbf{S} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^{\mathrm{T}}$ where the columns of $\mathbf{Q}$ 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)

$$\begin{aligned} k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}_a') + k_b(\mathbf{x}_b, \mathbf{x}_b') \\ &= \sum_{s=1}^{S} \phi_{as}(\mathbf{x}_a)\phi_{as}(\mathbf{x}_a') + \sum_{t=1}^{T} \phi_{bt}(\mathbf{x}_b)\phi_{bt}(\mathbf{x}_b') \\ &= \sum_{i=1}^{S+T} \phi_i(\mathbf{x})\phi_i(\mathbf{x}'), \end{aligned}$$

which is a valid kernel.

(6.22) – To be updated

$$\begin{aligned} k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}_a')k_b(\mathbf{x}_b, \mathbf{x}_b') \\ &= \sum_{s=1}^{S} \phi_{as}(\mathbf{x}_a)\phi_{as}(\mathbf{x}_a') \sum_{t=1}^{T} \phi_{bt}(\mathbf{x}_b)\phi_{bt}(\mathbf{x}_b') \\ &= \sum_{s=1}^{S}\sum_{t=1}^{T} \big\{\phi_{as}(\mathbf{x}_a)\phi_{bt}(\mathbf{x}_b)\big\}\big\{\phi_{as}(\mathbf{x}_a')\phi_{bt}(\mathbf{x}_b')\big\} \end{aligned}$$

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)

$$\begin{aligned}
\text{cov}[\mathbf{y}] &= \mathbb{E}[\mathbf{y}\mathbf{y}^{\mathrm{T}}] - \mathbb{E}[\mathbf{y}]\mathbb{E}[\mathbf{y}^{\mathrm{T}}] \\
&= \mathbb{E}[\mathbf{y}\mathbf{y}^{\mathrm{T}}] \\
&= \mathbb{E}[\boldsymbol{\Phi}\mathbf{w}\mathbf{w}^{\mathrm{T}}\boldsymbol{\Phi}^{\mathrm{T}}] \\
&= \boldsymbol{\Phi}\mathbb{E}[\mathbf{w}\mathbf{w}^{\mathrm{T}}]\boldsymbol{\Phi}^{\mathrm{T}} \\
&= \boldsymbol{\Phi}\text{cov}[\mathbf{w}]\boldsymbol{\Phi}^{\mathrm{T}} \\
&= \frac{1}{\alpha}\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} \\
&= \mathbf{K}
\end{aligned}$$

where

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

(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

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

into (2.115), we obtain

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

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

$$\begin{aligned}
\mu_{t_{N+1}|\mathbf{t}} &= \mu_{t_{N+1}} + \boldsymbol{\Sigma}_{t_{N+1}\mathbf{t}}\boldsymbol{\Sigma}_{\mathbf{tt}}^{-1}(\mathbf{t} - \boldsymbol{\mu}_{\mathbf{t}}) \\
&= 0 + \mathbf{k}^{\mathrm{T}}\mathbf{C}^{-1}(\mathbf{t} - \mathbf{0}) \\
&= \mathbf{k}^{\mathrm{T}}\mathbf{C}_N^{-1}\mathbf{t} \\
\sigma^2_{t_{N+1}|\mathbf{t}} &= \sigma^2_{t_{N+1}t_{N+1}} - \boldsymbol{\Sigma}_{t_{N+1}\mathbf{t}}\boldsymbol{\Sigma}_{\mathbf{tt}}^{-\mathbf{1}}\boldsymbol{\Sigma}_{\mathbf{t}t_{N+1}} \\
&= c - \mathbf{k}^{\mathrm{T}}\mathbf{C}_N^{-1}\mathbf{k}.
\end{aligned}$$