# Pattern Recognition and Machine Learning
# Cristopher Bishop

# Exercise Solutions

Stefan Stefanache

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# Chapter 1

# Kernel Methods

## Exercise 6.1 ⋆⋆

Consider the dual formulation of the least squares linear regression problem given in Section 6.1. Show that the solution for the components $a_n$ of the vector $\mathbf{a}$ can be expressed as a linear combination of the elements of the vector $\boldsymbol{\phi}(\mathbf{x}_n)$. Denoting these coefficients by the vector $\mathbf{w}$, show that the dual of the dual formulation is given by the original representation in terms of the parameter vector $\mathbf{w}$.

*Proof.* By rewriting (6.4), one has that

$$\begin{aligned} a_n &= -\frac{1}{\lambda}\{\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n) - t_n\} \\ &= -\frac{1}{\lambda}\left\{\sum_{i=1}^{M} w_i\phi_i(\mathbf{x}_n) - \frac{t_n}{\sum_{i=1}^{M}\phi_i(\mathbf{x}_n)}\sum_{i=1}^{M}\phi_i(\mathbf{x}_n)\right\} \\ &= \sum_{i=1}^{M}\left(\frac{t_n}{\lambda\sum_{i=1}^{M}\phi_i(\mathbf{x}_n)} - \frac{w_i}{\lambda}\right)\phi_i(\mathbf{x}_n) \\ &= \sum_{i=1}^{M}\Omega_{ni}\phi_i(\mathbf{x}_n) \\ &= \boldsymbol{\Omega}_n^T\boldsymbol{\phi}(\mathbf{x}_n) \end{aligned}$$

where

$$\Omega_{ni} = \frac{t_n}{\lambda\sum_{i=1}^{M}\phi_i(\mathbf{x}_n)} - \frac{w_i}{\lambda}$$

Therefore, $a_n$ can be written as a linear combination of the elements of $\boldsymbol{\phi}(\mathbf{x}_n)$ and

$$\mathbf{a} = \mathrm{diag}(\boldsymbol{\Omega}\boldsymbol{\Phi})$$

□

## Exercise 6.3 ⋆

The nearest-neighbour classifier (Section 2.5.2) assigns a new input vector $\mathbf{x}$ to the same class as that of the nearest input vector $\mathbf{x}_n$ from the training set, where in the simple case, the distance

is defined by the Euclidean metric $\|\mathbf{x} - \mathbf{x}_n\|^2$. By expressing this rule in terms of scalar product and then making use of kernel substitution, formulate the nearest-neighbour classifier for a general nonlinear kernel.

*Proof.* Since we're dealing with inner products over $\mathbb{R}$, the Euclidian metric can be rewritten as

$$\|\mathbf{x} - \mathbf{x}_n\|^2 = \langle \mathbf{x} - \mathbf{x}_n, \mathbf{x} - \mathbf{x}_n \rangle = \langle \mathbf{x}, \mathbf{x} \rangle - 2\langle \mathbf{x}, \mathbf{x}_n \rangle + \langle \mathbf{x}_n \mathbf{x}_n \rangle$$

Similarly to what happens in Section 6.2, using kernel substitution above to replace $\langle \mathbf{x}, \mathbf{x}' \rangle$ with a nonlinear kernel $\kappa(\mathbf{x}, \mathbf{x}')$ yields the nearest-neighbour classifier for a general nonlinear kernel:

$$k(\mathbf{x}, \mathbf{x}') = \kappa(\mathbf{x}, \mathbf{x}) - 2\kappa(\mathbf{x}, \mathbf{x}_n) + \kappa(\mathbf{x}_n, \mathbf{x}_n)$$

□

# Exercise 6.4 ⋆

In Appendix C, we give an example of a matrix that has positive elements but that ahas a negative eigenvalue and hence that is not positive definite. Find an example of the converse property, namely a $2 \times 2$ matrix with positive eigenvalues that has at least one negative element.

*Proof.* Consider the matrix

$$A = \begin{bmatrix} 2 & 1 \\ -1 & 2 \end{bmatrix}$$

$A$ contains one negative element and the eigenvalues of $A$ are $\lambda_1 = 1$ and $\lambda_2 = 3$, which proves that a matrix can be positive definite and have negative elements. □

# Exercise 6.5 ⋆

Verify the results (6.13) and (6.14) for constructing valid kernels.

*Proof.* Since $k_1$ is a valid kernel, let $\boldsymbol{\alpha}$ be a feature mapping such that

$$k_1(\mathbf{x}, \mathbf{x}') = \langle \boldsymbol{\alpha}(\mathbf{x}), \boldsymbol{\alpha}(\mathbf{x}') \rangle$$

Using the fact that an inner product on a real vector space is a positive-definite symmetric bilinear form, we have that

$$ck_1(\mathbf{x}, \mathbf{x}') = c\langle \boldsymbol{\alpha}(\mathbf{x}), \boldsymbol{\alpha}(\mathbf{x}') \rangle = \langle \sqrt{c}\boldsymbol{\alpha}(\mathbf{x}), \sqrt{c}\boldsymbol{\alpha}(\mathbf{x}') \rangle = \langle \boldsymbol{\beta}(\mathbf{x}), \boldsymbol{\beta}(\mathbf{x}') \rangle$$

where $c > 0$ is a constant and $\boldsymbol{\beta}(\mathbf{x}) = \sqrt{c}\boldsymbol{\alpha}(\mathbf{x})$. Therefore, the new kernel

$$k(\mathbf{x}, \mathbf{x}') = ck_1(\mathbf{x}, \mathbf{x}') \tag{6.13}$$

is valid. Analogously, since $f(\cdot)$ is a real-valued function,

$$f(\mathbf{x})k_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}') = f(\mathbf{x})\langle \boldsymbol{\alpha}(\mathbf{x}), \boldsymbol{\alpha}(\mathbf{x}') \rangle f(\mathbf{x}') = \langle f(\mathbf{x})\boldsymbol{\alpha}(\mathbf{x}), f(\mathbf{x}')\boldsymbol{\alpha}(\mathbf{x}') \rangle = \langle \boldsymbol{\gamma}(\mathbf{x}), \boldsymbol{\gamma}(\mathbf{x}') \rangle$$

where $\boldsymbol{\gamma}(\mathbf{x}) = f(\mathbf{x})\boldsymbol{\alpha}(\mathbf{x})$. As a result, the kernel

$$k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x})k_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}') \tag{6.14}$$

will also be valid. □

## Exercise 6.6 ⋆

Verify the results (6.15) and (6.16) for constructing valid kernels.

*Proof.* Let $q(\cdot)$ be a polynomial with nonnegative coefficients. Since in the polynomial kernels are summed and multiplied by nonnegative constants or other kernels, combining (6.13), (6.17) and (6.18) proves that the kernel

$$k(\mathbf{x}, \mathbf{x}') = q\big(k_1(\mathbf{x}, \mathbf{x}')\big) \tag{6.15}$$

is valid. Now, the exponential function is defined as

$$\exp(x) \coloneqq \sum_{i=0}^{\infty} \frac{x^i}{i!}$$

, so

$$\exp\big(k_1(\mathbf{x}, \mathbf{x}')\big) = \sum_{i=0}^{\infty} \frac{k_1(\mathbf{x}, \mathbf{x}')^i}{i!}$$

Note that the exponential of a kernel is an infinite sequence of kernel sums and products (with itself or nonnegative constants), so by using (6.13), (6.17), (6.18) again, one has that the new kernel

$$k(\mathbf{x}, \mathbf{x}') = \exp\big(k_1(\mathbf{x}, \mathbf{x}')\big) \tag{6.16}$$

is valid. □

## Exercise 6.7 ⋆

Verify the results (6.17) and (6.18) for constructing valid kernels.

*Proof.* Let $K_1$ and $K_2$ be the Gram matrices corresponding to the kernels $k_1$ and $k_2$. Therefore, they are positive semidefinite matrices, so for any $\mathbf{a} \in \mathbb{R}^n$, one has that

$$\mathbf{a}^T\mathbf{H}\mathbf{a} = \mathbf{a}^T\big(\mathbf{H}_1 + \mathbf{H}_2\big)\mathbf{a} = \mathbf{a}^T\mathbf{H}_1\mathbf{a} + \mathbf{a}^T\mathbf{H}_2\mathbf{a} > 0$$

Since $\mathbf{H} = \mathbf{H}_1 + \mathbf{H}_2$ is positive semidefinite and corresponds to the Gram matrix of the kernel $k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}')$, one has that the kernel

$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') \tag{6.17}$$

is valid. Now, let $\boldsymbol{\alpha}, \boldsymbol{\beta}$ be feature mappings such that

$$k_1(\mathbf{x}, \mathbf{x}') = \langle \boldsymbol{\alpha}(\mathbf{x}), \boldsymbol{\alpha}(\mathbf{x}') \rangle$$

$$k_2(\mathbf{x}, \mathbf{x}') = \langle \boldsymbol{\beta}(\mathbf{x}), \boldsymbol{\beta}(\mathbf{x}') \rangle$$

As a result,

$$\begin{aligned} k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}') &= \langle \boldsymbol{\alpha}(\mathbf{x}), \boldsymbol{\alpha}(\mathbf{x}') \rangle \langle \boldsymbol{\beta}(\mathbf{x}), \boldsymbol{\beta}(\mathbf{x}') \rangle \\ &= \boldsymbol{\alpha}(\mathbf{x})^T \boldsymbol{\alpha}(\mathbf{x}') \boldsymbol{\beta}^T(\mathbf{x}) \boldsymbol{\beta}(\mathbf{x}') \end{aligned}$$

$$
\begin{aligned}
&= \Big[\sum_{i=1}^{N} \alpha_i(\mathbf{x})\alpha_i(\mathbf{x}')\Big]\Big[\sum_{j=1}^{M} \beta_i(\mathbf{x})\beta_i(\mathbf{x}')\Big] \\
&= \sum_{i=1}^{N}\sum_{j=1}^{M} \alpha_i(\mathbf{x})\beta_j(\mathbf{x})\alpha_i(\mathbf{x}')\beta_j(\mathbf{x}') \qquad (*) \\
&= \sum_{i=1}^{N}\sum_{j=1}^{M} A_{ij}(\mathbf{x})A_{ij}(\mathbf{x}') \\
&= \langle \mathbf{A}(\mathbf{x}), \mathbf{A}(\mathbf{x}')\rangle_{\mathbf{F}}
\end{aligned}
$$

where $\mathbf{A}$ is a matrix with

$$A_{ij}(\mathbf{x}) = \alpha_i(\mathbf{x})\beta_j(\mathbf{x})$$

and $\langle \cdot, \cdot \rangle_{\mathbf{F}}$ is the Frobenius inner product. Since the product kernel can be rewritten as a valid inner product in the feature space defined by the feature mapping $\mathbf{A}(\mathbf{x})$, the new kernel

$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}') \tag{6.18}$$

is valid. Note that we can continue differently from (*), so

$$k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}') = \sum_{k=1}^{K} \phi_k(\mathbf{x})\phi_k(\mathbf{x}') = \langle \boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\rangle$$

where $K = NM$ and

$$\phi_k(\mathbf{x}) = \alpha_{((k-1)\oslash N)+1}(\mathbf{x})\beta_{((k-1)\odot N)+1}(\mathbf{x})$$

where $\oslash$ and $\odot$ denote integer division and remainder, respectively. □

# Exercise 6.8 ⋆

Verify the results (6.19) and (6.20) for constructing valid kernels.

*Proof.* Let $\boldsymbol{\psi}$ be a feature mapping such that

$$k_3(\mathbf{x}, \mathbf{x}') = \langle \boldsymbol{\psi}(\mathbf{x}), \boldsymbol{\psi}(\mathbf{x}')\rangle$$

Then,

$$
\begin{aligned}
k_3\big(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\big) &= \langle \boldsymbol{\psi}\big(\boldsymbol{\phi}(\mathbf{x})\big), \boldsymbol{\psi}\big(\boldsymbol{\phi}(\mathbf{x}')\big)\rangle \\
&= \langle \big(\boldsymbol{\psi} \circ \boldsymbol{\phi}\big)(\mathbf{x}), \big(\boldsymbol{\psi} \circ \boldsymbol{\phi}\big)(\mathbf{x}')\rangle \\
&= \langle \boldsymbol{\gamma}(\mathbf{x}), \boldsymbol{\gamma}(\mathbf{x}')\rangle
\end{aligned}
$$

where $\boldsymbol{\phi}$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$ and $\boldsymbol{\gamma} = \boldsymbol{\psi} \circ \boldsymbol{\phi}$. Therefore, the kernel

$$k(\mathbf{x}, \mathbf{x}') = k_3\big(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\big) \tag{6.19}$$

is valid. For the second part, since $\mathbf{A}$ is a symmetric, positive semidefinite matrix, one can use the Cholesky decomposition to obtain a matrix $\mathbf{L}$ such that

$$\mathbf{A} = \mathbf{L}\mathbf{L}^T$$

As a result, one can show that

$$\mathbf{x}^T\mathbf{A}\mathbf{x} = \mathbf{x}^T\mathbf{L}\mathbf{L}^T\mathbf{x} = \big(\mathbf{L}^T\mathbf{x}\big)^T\big(\mathbf{L}^T\mathbf{x}\big) = \langle \boldsymbol{\zeta}(\mathbf{x}), \boldsymbol{\zeta}(\mathbf{x}')\rangle$$

where $\boldsymbol{\zeta}(\mathbf{x}) = \mathbf{L}^T\mathbf{x}$. Hence, the kernel

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T\mathbf{A}\mathbf{x} \tag{6.20}$$

is valid. □

# Exercise 6.9 ⋆

Verify the results (6.21) and (6.22) for constructing valid kernels.

*Proof.* Let $\boldsymbol{\phi}_a$ and $\boldsymbol{\phi}_b$ be feature mappings so that

$$k_a(\mathbf{x}, \mathbf{x}') = \langle \boldsymbol{\phi}_a(\mathbf{x}), \boldsymbol{\phi}_a(\mathbf{x}')\rangle$$
$$k_b(\mathbf{x}, \mathbf{x}') = \langle \boldsymbol{\phi}_b(\mathbf{x}), \boldsymbol{\phi}_b(\mathbf{x}')\rangle$$

Therefore, since the inner product becomes a bilinear form on $\mathbb{R}$,

$$\begin{aligned} k_a(\mathbf{x}_a, \mathbf{x'}_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b) &= \langle \boldsymbol{\phi}_a(\mathbf{x}_a), \boldsymbol{\phi}_a(\mathbf{x}'_a)\rangle + \langle \boldsymbol{\phi}_b(\mathbf{x}_b), \boldsymbol{\phi}_b(\mathbf{x}'_b)\rangle \\ &= \langle \big(\boldsymbol{\phi}_a(\mathbf{x}_a), \boldsymbol{\phi}_a(\mathbf{x}'_a)\big), \big(\boldsymbol{\phi}_b(\mathbf{x}_b), \boldsymbol{\phi}_b(\mathbf{x}'_b)\big)\rangle \\ &= \langle \boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\rangle \end{aligned}$$

where

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} \boldsymbol{\phi}_a(\mathbf{x}_a) \\ \boldsymbol{\phi}_b(\mathbf{x}_b) \end{bmatrix}$$

Hence, the kernel

$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b) \tag{6.21}$$

is valid. The product identity is obtained similarly to what we do in Exercise 6.7. One has that

$$\begin{aligned} k_a(\mathbf{x}_a, \mathbf{x}'_a)k_b(\mathbf{x}_b, \mathbf{x}'_b) &= \langle \boldsymbol{\phi}_a(\mathbf{x}_a), \boldsymbol{\phi}_a(\mathbf{x}'_a)\rangle\langle \boldsymbol{\phi}_b(\mathbf{x}_b), \boldsymbol{\phi}_b(\mathbf{x}'_b)\rangle \\ &= \left[\sum_{i=1}^{N_a} \phi_{ai}(\mathbf{x}_a)\phi_{ai}(\mathbf{x}'_a)\right]\left[\sum_{j=1}^{N_b} \phi_{bj}(\mathbf{x}_b)\phi_{bj}(\mathbf{x}'_b)\right] \\ &= \sum_{i=1}^{N_a}\sum_{j=1}^{N_b} \phi_{ai}(\mathbf{x}_a)\phi_{bj}(\mathbf{x}_b)\phi_{ai}(\mathbf{x}'_a)\phi_{bj}(\mathbf{x}'_b) \\ &= \sum_{i=1}^{N_a}\sum_{j=1}^{N_b} A_{ij}(\mathbf{x})A_{ij}(\mathbf{x}') \\ &= \langle \mathbf{A}(\mathbf{x}), \mathbf{A}(\mathbf{x}')\rangle_{\boldsymbol{F}} \end{aligned}$$

where $\langle \cdot, \cdot \rangle_{\boldsymbol{F}}$ is the Frobenius inner product, $\phi_{ai}(\mathbf{x})$ is the $i$-th element of $\boldsymbol{\phi}_a(\mathbf{x})$ and

$$A_{ij}(\mathbf{x}) = \phi_{ai}(\mathbf{x}_a)\phi_{bj}(\mathbf{x}_b)$$

Therefore, the new kernel

$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a)k_b(\mathbf{x}_b, \mathbf{x}'_b) \tag{6.22}$$

will also be valid. □

## Exercise 6.10 ⋆

Show that an excellent choice of kernel for learning a function $f(\mathbf{x})$ is given by $k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x})f(\mathbf{x}')$ by showing that a linear learning machine-based on this kernel will always find a solution proportional to $f(\mathbf{x})$.

*Proof.* By substituting the kernel and (6.8) into (6.9), one has that

$$y(\mathbf{x}) = \mathbf{k}(\mathbf{x})^T(\mathbf{K} + \lambda \mathbf{I}_N)^{-1}\mathbf{t} = \mathbf{k}(\mathbf{x})^T\mathbf{a} = \sum_{n=1}^{N} k(\mathbf{x}, \mathbf{x}_n)a_n = f(\mathbf{x})\left[\sum_{n=1}^{N} f(\mathbf{x}_n)a_n\right]$$

which shows that the prediction function will always be proportional to $f(\mathbf{x})$. □

## Exercise 6.11 ⋆

By making use of the expansion (6.25), and then expanding the middle factor as a power series, show that the Gaussian kernel (6.23) can be expressed as the inner product of an infinite-dimensional feature vector.

*Proof.* We've seen in Section 6.2 that the Gaussian kernel can be expanded as

$$k(\mathbf{x}, \mathbf{x}') = \exp\left\{-\frac{\|\mathbf{x}\|^2}{2\sigma^2}\right\}\exp\left\{\frac{\langle \mathbf{x}, \mathbf{x}'\rangle}{\sigma^2}\right\}\exp\left\{-\frac{\|\mathbf{x}'\|^2}{2\sigma^2}\right\} \tag{6.25}$$

In Exercise 6.7 we proved that if $\boldsymbol{\alpha}, \boldsymbol{\beta}$ are feature maps, there exists a feature map $\boldsymbol{\psi}$ such that

$$\langle \boldsymbol{\alpha}(\mathbf{x}), \boldsymbol{\alpha}(\mathbf{x}')\rangle\langle \boldsymbol{\beta}(\mathbf{x}), \boldsymbol{\beta}(\mathbf{x}')\rangle = \langle \boldsymbol{\psi}(\mathbf{x}), \boldsymbol{\psi}(\mathbf{x}')\rangle$$

Therefore, one can prove using induction that there exists a feature map $\boldsymbol{\zeta}$ such that for $n \in \mathbb{N}$,

$$\langle \boldsymbol{\alpha}(\mathbf{x}), \boldsymbol{\alpha}(\mathbf{x}')\rangle^n = \langle \boldsymbol{\zeta}(\mathbf{x}), \boldsymbol{\zeta}(\mathbf{x}')\rangle$$

Now, using the definition of the exponential function for the middle term gives

$$\exp\left\{\frac{\langle \mathbf{x}, \mathbf{x}'\rangle}{\sigma^2}\right\} = \sum_{i=0}^{\infty}\frac{1}{i!\sigma^{2i}}\langle \mathbf{x}, \mathbf{x}'\rangle^i = \sum_{i=0}^{\infty}\frac{1}{i!\sigma^{2i}}\langle \boldsymbol{\Psi}_i(\mathbf{x}), \boldsymbol{\Psi}_i(\mathbf{x}')\rangle = \sum_{i=0}^{\infty}\left\langle \frac{1}{\sigma}\sqrt{\frac{1}{i!}}\boldsymbol{\Psi}_i(\mathbf{x}), \frac{1}{\sigma}\sqrt{\frac{1}{i!}}\boldsymbol{\Psi}_i(\mathbf{x}')\right\rangle$$

where $\boldsymbol{\Psi}_i$ are feature maps such that

$$\langle \mathbf{x}, \mathbf{x}'\rangle^i = \langle \boldsymbol{\Psi}_i(\mathbf{x}), \boldsymbol{\Psi}_i(\mathbf{x}')\rangle$$

Substituting this result back into (6.25) yields

$$\begin{aligned} k(\mathbf{x}, \mathbf{x}') &= \exp\left\{-\frac{\|\mathbf{x}\|^2}{2\sigma^2}\right\}\exp\left\{-\frac{\|\mathbf{x}'\|^2}{2\sigma^2}\right\}\sum_{i=0}^{\infty}\left\langle \frac{1}{\sigma}\sqrt{\frac{1}{i!}}\boldsymbol{\Psi}_i(\mathbf{x}), \frac{1}{\sigma}\sqrt{\frac{1}{i!}}\boldsymbol{\Psi}_i(\mathbf{x}')\right\rangle \\ &= \sum_{i=0}^{\infty}\exp\left\{-\frac{\|\mathbf{x}\|^2}{2\sigma^2}\right\}\exp\left\{-\frac{\|\mathbf{x}'\|^2}{2\sigma^2}\right\}\left\langle \frac{1}{\sigma}\sqrt{\frac{1}{i!}}\boldsymbol{\Psi}_i(\mathbf{x}), \frac{1}{\sigma}\sqrt{\frac{1}{i!}}\boldsymbol{\Psi}_i(\mathbf{x}')\right\rangle \end{aligned}$$

$$
\begin{aligned}
&= \sum_{i=0}^{\infty} \left\langle \frac{1}{\sigma}\sqrt{\frac{1}{i!}}\mathbf{\Psi}_i(\mathbf{x}) \exp\left\{-\frac{\|\mathbf{x}\|^2}{2\sigma^2}\right\}, \frac{1}{\sigma}\sqrt{\frac{1}{i!}}\mathbf{\Psi}_i(\mathbf{x}') \exp\left\{-\frac{\|\mathbf{x}'\|^2}{2\sigma^2}\right\} \right\rangle \\
&= \sum_{i=0}^{\infty} \phi_i(\mathbf{x})\phi_i(\mathbf{x}') \\
&= \langle \boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}') \rangle
\end{aligned}
$$

where $\boldsymbol{\phi}(\mathbf{x})$ is a feature vector of infinite dimensionality with

$$
\phi_i(\mathbf{x}) = \left\langle \frac{1}{\sigma}\sqrt{\frac{1}{i!}}\mathbf{\Psi}_i(\mathbf{x}) \exp\left\{-\frac{\|\mathbf{x}\|^2}{2\sigma^2}\right\} \right\rangle
$$

□

# Exercise 6.12 ⋆⋆

Consider the space fo all possible subsets $A$ of a given fixed set $D$. Show that the kernel function (6.27) corresponds to an inner product in a feature space of dimensionality $2^{|D|}$ defined by the mapping $\boldsymbol{\phi}(A)$ where $A$ is a subset of $D$ and the element $\phi_U(\mathbf{A})$, indexed by the subset $U$, is given by

$$
\phi_U(A) = \begin{cases} 1, & \text{if } U \subseteq A \\ 0, & \text{otherwise} \end{cases} \tag{6.95}
$$

Here $U \subseteq A$ denotes that $U$ is either a subset of $A$ or is equal to $A$.

*Proof.* Using simple combinatorics, one can easily show that the number of subsets of a given fixed set $D$ is given by $2^{|D|}$. Therefore, $\boldsymbol{\phi}(A)$ will be of dimensionality $2^{|D|}$. Since the element $\phi_U(A)$ is 1 if $U \subseteq A$ and 0 otherwise, the result of the inner product $\langle \boldsymbol{\phi}(A_1), \boldsymbol{\phi}(A_2) \rangle$ will give the number of subsets of $D$ contained by both $A_1$ and $A_2$. However, since $A_1, A_2 \subseteq D$ this can also be expressed by counting the number of subsets of $A_1 \cap A_2$. This is done by the kernel

$$
k(A_1, A_2) = 2^{|A_1 \cap A_2|} \tag{6.27}
$$

Hence, the kernel can be written as an inner product in the space defined by the mapping $\boldsymbol{\phi}(A)$ since

$$
k(A_1, A_2) = 2^{|A_1 \cap A_2|} = \langle \boldsymbol{\phi}(A_1), \boldsymbol{\phi}(A_2) \rangle
$$

□

# Exercise 6.13 ⋆ TODO

Show that the Fisher kernel, defined by (6.33), remains invariant if we make a nonlinear transformation of the parameter vector $\boldsymbol{\theta} \to \boldsymbol{\psi}(\boldsymbol{\theta})$, where the function $\boldsymbol{\psi}(\cdot)$ is invertible and differentiable.

*Proof.* The Fisher kernel is defined by

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^T \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}') \tag{6.33}$$

where

$$\mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) = \nabla_{\boldsymbol{\theta}} \ln p(\mathbf{x}|\boldsymbol{\theta}) \tag{6.32}$$

is the Fisher *score* and $\mathbf{F}$ is the Fisher *information matrix*, given by

$$\mathbf{F} = \mathbb{E}_{\mathbf{x}}\big[\mathbf{g}(\boldsymbol{\theta}, \mathbf{x})\mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^T\big] \tag{6.34}$$

□

# Exercise 6.14 ⋆

Write down the form of the Fisher kernel, defined by (6.33), for the case of a distribution $p(\mathbf{x}|\boldsymbol{\mu}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{S})$ that is Gaussian with mean $\boldsymbol{\mu}$ and fixed covariance $\mathbf{S}$.

*Proof.* We start by evaluating the Fisher *score* using (6.32):

$$\begin{aligned}
\mathbf{g}(\boldsymbol{\mu}, \mathbf{x}) &= \nabla_{\boldsymbol{\mu}} \ln p(\mathbf{x}|\boldsymbol{\mu}) \\
&= \nabla_{\boldsymbol{\mu}} \ln \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{S}) \\
&= \nabla_{\boldsymbol{\mu}} \ln \left[ \frac{1}{(2\pi)^{k/2}|\mathbf{S}|^{1/2}} \exp\left\{ -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \mathbf{S}^{-1}(\mathbf{x} - \boldsymbol{\mu}) \right\} \right] \\
&= \nabla_{\boldsymbol{\mu}} \left[ -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})\mathbf{S}^{-1}(\mathbf{x} - \boldsymbol{\mu}) \right] \\
&= \mathbf{S}^{-1}(\mathbf{x} - \boldsymbol{\mu})
\end{aligned}$$

Now, the *information matrix* will be given by (6.34):

$$\mathbf{F} = \mathbb{E}_{\mathbf{x}}\big[\mathbf{g}(\boldsymbol{\mu}, \mathbf{x})\mathbf{g}(\boldsymbol{\mu}, \mathbf{x})^T\big] = \mathbb{E}_{\mathbf{x}}\big[\mathbf{S}^{-1}(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T\mathbf{S}^{-1}\big] = \mathbf{S}^{-1}\mathbb{E}_{\mathbf{x}}\big[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T\big]\mathbf{S}^{-1}$$

Since the expectation corresponds to the covariance matrix, we have that

$$\mathbf{F} = \mathbf{S}^{-1}$$

Finally, the Fisher kernel can be obtained by substituting the obtained values into (6.33):

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{g}(\boldsymbol{\mu}, \mathbf{x})^T \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\mu}, \mathbf{x}') = (\mathbf{x} - \boldsymbol{\mu})^T \mathbf{S}^{-1}\mathbf{S}\mathbf{S}^{-1}(\mathbf{x} - \boldsymbol{\mu}) = (\mathbf{x} - \boldsymbol{\mu})^T \mathbf{S}^{-1}(\mathbf{x} - \boldsymbol{\mu})$$

which turns out to be the Mahalnobis distance. □

# Exercise 6.15 ⋆

By considering the determinant of a $2 \times 2$ Gram matrix, show that a positive definite kernel function $k(x, x')$ satisfies the Cauchy-Schwartz inequality

$$k(x_1, x_2)^2 \leq k(x_1, x_1)k(x_2, x_2) \tag{6.96}$$

*Proof.* Consider the $2 \times 2$ Gram matrix corresponding to the kernel $k$:

$$\mathbf{K} = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) \\ k(x_2, x_1) & k(x_2, x_2) \end{bmatrix}$$

Since the kernel function is symmetric, the determinant of $K$ is given by

$$|\mathbf{K}| = k(x_1, x_1)k(x_2, x_2) - k(x_1, x_2)^2$$

Now, since the Gram matrix $\mathbf{K}$ is positive definite, its eigenvalues are positive. Since the determinant of a matrix is given by the product of its eigenvalues, then the determinant of $\mathbf{K}$ must then be positive. Hence,

$$k(x_1, x_2)^2 \leq k(x_1, x_1)k(x_2, x_2) \tag{6.96}$$

□