

1 Multivariate Gaussians: A review

(a) Consider a two-dimensional random variable $Z \in \mathbb{R}^2$. In order for the random variable to be jointly Gaussian, a necessary and sufficient condition is that

- Z_1 and Z_2 are each marginally Gaussian, and
- $Z_1|Z_2 = z$ is Gaussian, and $Z_2|Z_1 = z$ is Gaussian.

A second characterization of a jointly Gaussian Random Variable (RV) Z is that it can be written as $Z = AX$, where X is a collection of i.i.d. standard normal RVs and $A \in \mathbb{R}^{2 \times 2}$ is a matrix.

Note that the probability density function of a Gaussian RV with mean vector μ and covariance matrix Σ is:

$$f(z) = \frac{\exp\left(-\frac{1}{2}(\mathbf{x} - \mu)^T \Sigma^{-1}(\mathbf{x} - \mu)\right)}{\sqrt{(2\pi)^k |\Sigma|}}$$

Let X_1 and X_2 be i.i.d. standard normal RVs. Let U denote a random variable uniformly distributed on $\{-1, 1\}$, independent of everything else. Verify if the conditions of the first characterization hold for the following random variables, and calculate the covariance matrix Σ_Z .

- $Z_1 = X_1$ and $Z_2 = X_2$.
 - $Z_1 = X_1$ and $Z_2 = X_1 + X_2$. (Use the second characterization to argue joint Gaussianity.)
 - $Z_1 = X_1$ and $Z_2 = -X_1$.
 - $Z_1 = X_1$ and $Z_2 = UX_1$.
- (b) Use the above example to show that two Gaussian random variables can be uncorrelated, but not independent. On the other hand, show that two uncorrelated, jointly Gaussian RVs are independent.
- (c) With the setup above, let $Z = VX$, where $V \in \mathbb{R}^{2 \times 2}$ as a fixed non-random matrix, and $Z, X \in \mathbb{R}^2$. What is the covariance matrix Σ_Z ? Is this also true for a RV other than Gaussian?
- (d) Use the above setup to show that $X_1 + X_2$ and $X_1 - X_2$ are independent. Give another example pair of linear combinations that are independent.
- (e) Given a jointly Gaussian RV $Z \in \mathbb{R}^2$ with covariance matrix $\Sigma_Z = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{12} & \Sigma_{22} \end{bmatrix}$, how would you derive the distribution of $Z_1|Z_2 = z$?

Hint: The following identity may be useful

$$\begin{bmatrix} a & b \\ b & c \end{bmatrix}^{-1} = \begin{bmatrix} 1 & 0 \\ -\frac{b}{c} & 1 \end{bmatrix} \begin{bmatrix} \left(a - \frac{b^2}{c}\right)^{-1} & 0 \\ 0 & \frac{1}{c} \end{bmatrix} \begin{bmatrix} 1 & -\frac{b}{c} \\ 0 & 1 \end{bmatrix}.$$

2 Kernel Validity

For a function $k(x_i, x_j)$ to be a valid kernel, it suffices to show either of the following conditions is true:

1. k has an inner product representation: $\exists \Phi : \mathbb{R}^d \rightarrow \mathcal{H}$, where \mathcal{H} is some (possibly infinite-dimensional) inner product space such that $\forall x_i, x_j \in \mathbb{R}^d$, $k(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle$.
2. For every sample $x_1, x_2, \dots, x_n \in \mathbb{R}^d$, the kernel matrix

$$K = \begin{bmatrix} k(x_1, x_1) & \cdots & k(x_1, x_n) \\ \vdots & k(x_i, x_j) & \vdots \\ k(x_n, x_1) & \cdots & k(x_n, x_n) \end{bmatrix}$$

is positive semidefinite. For the following parts you can use either condition (1) or (2) in your proofs.

- (a) Show that the first condition implies the second one, i.e. if $\forall x_i, x_j \in \mathbb{R}^d$, $k(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle$ then the kernel matrix K is PSD.
- (b) Given a positive semidefinite matrix $A \in \mathbb{R}^{d \times d}$, show that $k(x_i, x_j) = x_i^\top A x_j$ is a valid kernel.
- (c) Show why $k(x_i, x_j) = x_i^\top (\text{rev}(x_j))$ (where $\text{rev}(x)$ reverses the order of the components in x) is *not* a valid kernel.
- (d) Soon we will cover a regression method based on kernels called kernel ridge regression (KRR). A key intermediate step to solve KRR is the following optimization problem:

$$\operatorname{argmin}_{\alpha \in \mathbb{R}^n} \left[\frac{1}{2} \alpha^\top (K + \lambda I) \alpha - \lambda \langle \alpha, y \rangle \right]$$

where $y \in \mathbb{R}^n$, $\lambda \geq 0$, and $K \in \mathbb{R}^{n \times n}$ is the kernel matrix computed by applying a kernel function k on every sample pair: $k(x_i, x_j)$. How does the requirement that K be a kernel affect the properties of this optimization problem? You may want to consider the cases where λ is close to zero or even $\lambda = 0$?