2.5 Summary

The crucial ingredient of SVMs and other kernel methods is the so-called kernel trick (see (2.7) and Remark 2.8), which permits the computation of dot products in high-dimensional feature spaces, using simple functions defined on pairs of input patterns. This trick allows the formulation of nonlinear variants of any algorithm that can be cast in terms of dot products, SVMs being but the most prominent example. The mathematical result underlying the kernel trick is almost a century old [359]. Nevertheless, it was only much later that it was exploited by the machine learning community for the analysis [4] and construction of algorithms [62], and that it was described as a general method for constructing nonlinear generalizations of dot product algorithms [480].

The present chapter has reviewed the mathematical theory of kernels. We started with the class of polynomial kernels, which can be motivated as computing a combinatorially large number of monomial features rather efficiently. This led to the general question of which kernel can be used, or: which kernel can be represented as a dot product in a linear feature space. We defined this class and discussed some of its properties. We described several ways how, given such a kernel, one can construct a representation in a feature space. The most well-known representation employs Mercer's theorem, and represents the feature space as an ℓ_2 space defined in terms of the eigenfunctions of an integral operator associated with the kernel. An alternative representation uses elements of the theory of reproducing kernel Hilbert spaces, and yields additional insights, representing the linear space as a space of functions written as kernel expansions. We gave an indepth discussion of the kernel trick in its general form, including the case where we are interested in dissimilarities rather than similarities; that is, when we want to come up with nonlinear generalizations of distance-based algorithms rather than dot-product-based algorithms.

In both cases, the underlying philosophy is the same: we are trying to express a complex nonlinear algorithm in terms of simple geometrical concepts, and we are then dealing with it in a linear space. This linear space may not always be readily available; in some cases, it may even be hard to construct explicitly. Nevertheless, for the sake of design and analysis of the algorithms, it is sufficient to know that the linear space exists, empowering us to use the full potential of geometry, linear algebra and functional analysis.

2.6 Problems

2.1 (Monomial Features in $\mathbb{R}^2 \bullet$) *Verify the second equality in (2.9).*

2.2 (Multiplicity of Monomial Features in \mathbb{R}^N [515] ••) *Consider the monomial kernel* $k(x, x') = \langle x, x' \rangle^d$ (where $x, x' \in \mathbb{R}^N$), generating monomial features of order d. Prove