Chapter XV

Probabilistic Kernel PCA and its Application to Statistical Modeling and Inference

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Abstract

We present a method of density estimation that is based on an extension of kernel PCA to a probabilistic framework. Given a set of sample data, we assume that this data forms a Gaussian distribution, not in the input space but upon a nonlinear mapping to an appropriate feature space. As with most kernel methods, this mapping can be carried out implicitly. Due to the strong nonlinearity, the corresponding density estimate in the input space is highly non-Gaussian. Numerical applications on 2-D data sets indicate that it is capable of approximating essentially arbitrary distributions. Beyond demonstrating applications on 2-D data sets, we apply our method to high-dimensional data given by various silhouettes of a 3-D object. The shape density estimated by our method is subsequently applied as a statistical shape prior to variational image segmentation. Experiments demonstrate that the resulting segmentation process can incorporate highly accurate knowledge on a large variety of complex real-world shapes. It makes the segmentation process robust to misleading information due to noise, clutter and occlusion.
Introduction

One of the challenges in the field of image segmentation is the incorporation of prior knowledge on the shape of the segmenting contour. A common approach is to learn the shape of an object statistically from a set of training shapes, and to then restrict the segmenting contour to a submanifold of familiar shapes during the segmentation process. For the problem of segmenting a specific known object, this approach was shown to drastically improve segmentation results (cf. Cremers, 2001; Leventon, Grimson, & Faugeras, 2000; Tsai et al., 2001).

Although the shape prior can be quite powerful in compensating for misleading information due to noise, clutter, and occlusion in the input image, most approaches are limited in their applicability to more complicated shape variations of real-world objects. Commonly, the permissible shapes are assumed to form a multivariate Gaussian distribution, which essentially means that all possible shape deformations correspond to linear combinations of a set of eigenmodes, such as those given by principal component analysis (PCA; cf. Cootes, 1999; Cremers, 2002; Kervrann & Heitz, 1998; Klassen, Srivastava, Mio, & Joshi, 2004; Leventon et al., 2000; Staib & Duncan, 1992). In particular, this means that for any two permissible shapes, the entire sequence of shapes obtained by a linear morphing of the two shapes is permissible as well. Such Gaussian shape models have recently been proposed for implicitly represented shapes as well (cf. Leventon et al., 2000; Rousson, Paragios, & Deriche, 2004; Tsai et al., 2001).\(^1\) Once the set of training shapes exhibits highly nonlinear shape deformations, such as different 2-D views of a 3-D object, one finds distinct clusters in shape space corresponding to the stable views of an object. Moreover, each of the clusters may by itself be quite non-Gaussian. The Gaussian hypothesis will then result in a mixing of the different views, and the space of accepted shapes will be far too large for the prior to sensibly restrict the contour deformation.

A number of models have been proposed to deal with nonlinear shape variation. However, they often suffer from certain drawbacks. Some involve a complicated model construction procedure (Chalmond & Girard, 1999). Some are supervised in the sense that they assume prior knowledge on the structure of the nonlinearity (Heap & Hogg, 1996). Others require prior classification with the number of classes to be estimated or specified beforehand, and each class being assumed Gaussian (Cootes, 1999; Hogg, 1998). Some cannot be easily extended to shape spaces of higher dimension (Hastie & Stuetzle, 1989).

In this chapter, we present a density-estimation approach that is based on Mercer kernels (Courant & Hilbert, 1953; Mercer, 1909) and that does not suffer from any of the mentioned drawbacks. The proposed model can be interpreted as an extension of kernel PCA (Schölkopf, 1998) to the problem of density estimation. We refer to it as probabilistic kernel PCA. This chapter comprises and extends results that were published from two conferences (Cremers, 2001; Cremers, 2002) and in a journal paper (Cremers, 2003). Then, we review the variational integration of a linear shape prior into Mumford-Shah-based segmentation. Next, we give an intuitive example for the limitations of the linear shape model. Afterward, we present the nonlinear density estimate based on probabilistic kernel PCA. We compare it to related approaches and give estimates of the involved parameters. In the next section, we illustrate its application to artificial 2-D data and to silhouettes of real objects. Then this nonlinear shape prior is integrated into segmentation. We propose a variational integration

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