

Chapter 18

Principal Components Analysis

Principal components analysis (PCA) is one of a family of techniques for taking high-dimensional data, and using the dependencies between the variables to represent it in a more tractable, lower-dimensional form, without losing too much information. PCA is one of the simplest and most robust ways of doing such **dimensionality reduction**. It is also one of the oldest, and has been rediscovered many times in many fields, so it is also known as the Karhunen-Loève transformation, the Hotelling transformation, the method of empirical orthogonal functions, and singular value decomposition¹. We will call it PCA.

18.1 Mathematics of Principal Components

We start with p -dimensional vectors, and want to summarize them by projecting down into a q -dimensional subspace. Our summary will be the projection of the original vectors on to q directions, the **principal components**, which span the subspace.

There are several equivalent ways of deriving the principal components mathematically. The simplest one is by finding the projections which maximize the variance. The first principal component is the direction in space along which projections have the largest variance. The second principal component is the direction which maximizes variance among all directions orthogonal to the first. The k^{th} component is the variance-maximizing direction orthogonal to the previous $k - 1$ components. There are p principal components in all.

Rather than maximizing variance, it might sound more plausible to look for the projection with the smallest average (mean-squared) distance between the original vectors and their projections on to the principal components; this turns out to be equivalent to maximizing the variance.

Throughout, assume that the data have been “centered”, so that every variable has mean 0. If we write the centered data in a matrix \mathbf{x} , where rows are objects and

¹Strictly speaking, singular value decomposition is a matrix algebra trick which is used in the most common algorithm for PCA.

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