Approximated PCA

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February 9, 2017

1 Introduction

The PCA method transforms a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components using an orthogonal transformation (rotations and reflections).

The transformation, projects the data in a new subspace, in which each new variable it's now uncorrelated. That means that the covariance of each pair of new variables is zero. To compute the transformation, different approaches can be taken. In a first attempt, the covariance matrix will be used. Let x_{ij} be the observation j of the variable i. Let n be the number of variables and m the number of observations. Each element s_{ij} in the covariance matrix S is computed by

$$s_{ij} = \frac{\sum x_{ik}x_{jk} - \sum x_{ij}x_{jk}}{n(n-1)}$$

Once the covariance matrix S in computed, it can be used to find his eigenvalues and eigenvectors. One method to compute those values, is a combination of a Householder transformation, followed by the QR transformation. The first will transform S in a product of two matrix Q and R.

$$S = QR$$

Such that R contains 3 diagonals (tridiagonal) with elements and zeros in the rest. The QR transformation then takes this two matrices, and computes iteratively a new diagonal matrix $A^{(i+1)} = R^{(i)}Q^{(i)}$. Finally, the eigenvalues are in the diagonal of A and the eigenvectors are computed from these.

2 Householder transformation

The Householder transformation of S in a tridiagonal matrix has the property that the eigenvalues are preserved.