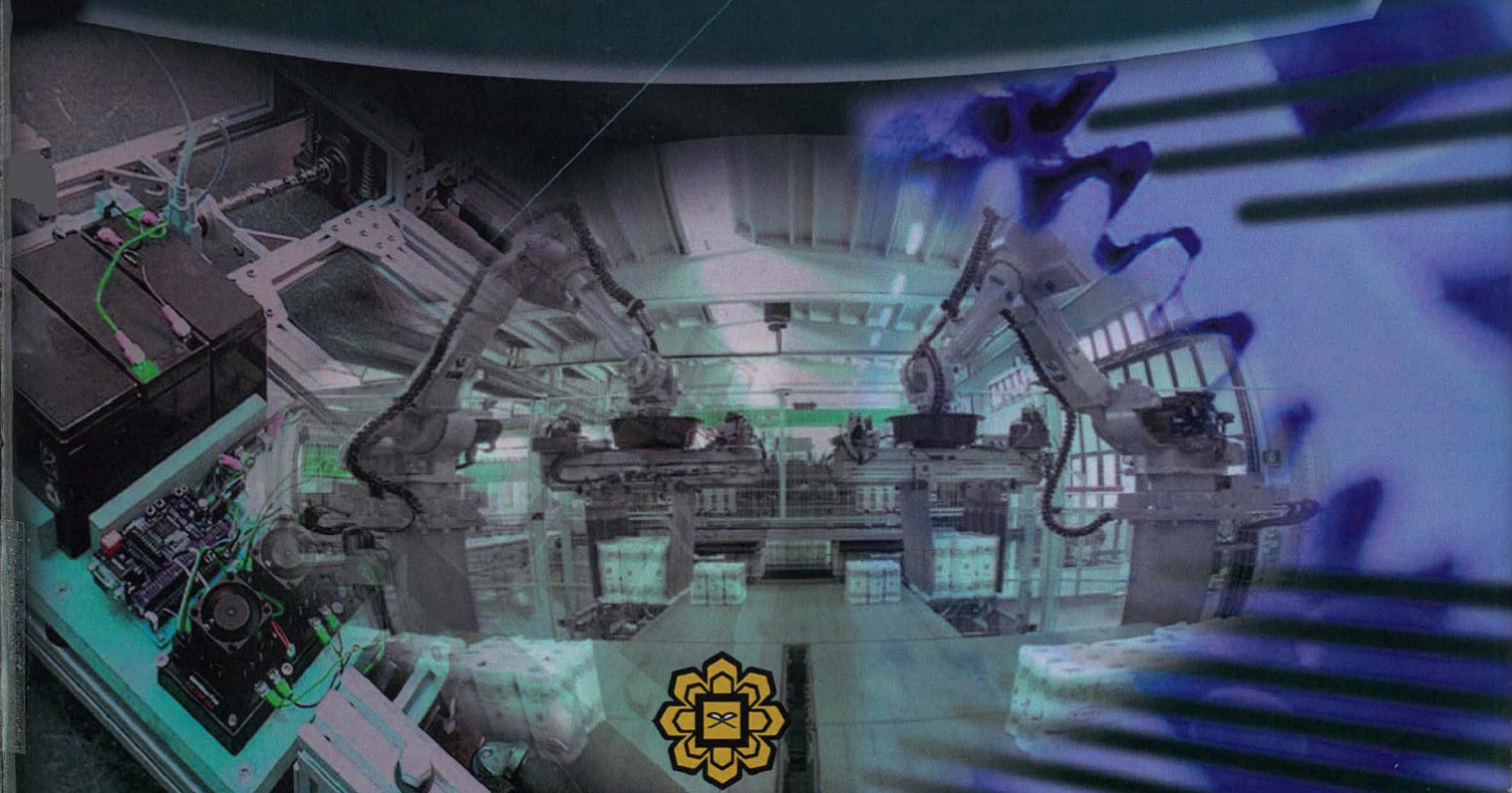
MECHATRONICS BOOK SERIES

CONTROL AND INTELLIGENT SYSTEMS

Momoh Jimoh E. Salami
Abiodun Musa Aibinu
Yasir Mohd Mustafah



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Chapter 37
Kernel PCA – An Introduction

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37.1 Introduction

The last decade has seen a huge development in data mining algorithms. Kernel methods such support vector machine, kernel fisher analysis, kernel PCA are probably the most important [1-6]. These techniques have become widely used in different areas and many open source implementations of these algorithms are available. The aim of this chapter is to give an introduction to kernel PCA along with linear PCA and other main ideas in kernel methods.

37.2 Principal Component Analysis

Principal component analysis (PCA) is a dimensionality reduction technique aimed at finding the subspace in which the data approximately lies [6,8]. It has been successively applied to many areas including data classification, compression, noise reduction, etc. We are interested in finding the directions (u_i) that maximize variance:

$$\begin{aligned} &maximize \quad Var(u^T x) && subject\ to \quad 1 - u^T u = 0 \\ \Leftrightarrow\ &maximize \quad \mathrm{E}[(u^T x)^T (u^T x)] && subject\ to \quad 1 - u^T u = 0 \\ \Leftrightarrow\ &maximize \quad u^T \mathrm{E}[x x^T] u && subject\ to \quad 1 - u^T u = 0 \\ \Leftrightarrow\ &maximize \quad u^T C u && subject\ to \quad 1 - u^T u = 0 \end{aligned} \tag{37.1}$$

Here we have assumed that the data is centred (zero mean). The covariance matrix C is symmetric with real eigenvalues and orthonormal eigenvectors. This constrained optimization problem can be solved using the Lagrangian defined as:

$$\mathrm{L}(u^T, \lambda) = u^T C u + \lambda(1 - u^T u), \tag{37.2}$$

where λ is the Lagrange multiplier associated with the constraint. In order to maximize L over u, we simply set the gradient equal to zero:

$$\frac{\partial \mathrm{L}}{\partial u} = 0 \implies 2Cu - 2\lambda u = 0 \qquad \text{or} \qquad Cu = \lambda u \tag{37.3}$$

The problem is brought forward to find the eigenvectors of the covariance matrix and their related eigenvalues. In practice we are not interested in all the eigenvectors (principal components) but only the top once ,i.e., first eigenvectors related to the largest eigenvalues. These eigenvectors can be efficiently computed using the Singular Value Decomposition (SVD) of the data matrix (design matrix). The final step of the PCA is to project the data onto the principal components [8].

37.3 Kernel PCA