Principal Component Analysis

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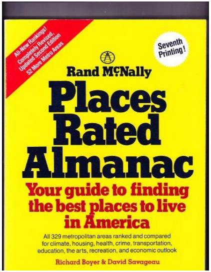
Example: Places Rated

Boyer and Savageau rated 329 communities according to 9 criteria:

1. Climate
2. Housing Cost
3. Health Care
4. Crime Rate
5. Transportation
6. Education
7. The Arts
8. Recreation
9. Economics



Question: Are all those criteria super important? Or are some more important than others?

Learning Objectives

Principal component analysis (PCA) is a data reduction technique.

- reduce the number of possibly correlated variables of interest into a smaller set of uncorrelated components
- a useful tool in exploratory data analysis and for predictive modeling

Outline:

1. Understand PCA procedure
2. Assess how many principal components should be considered in an analysis

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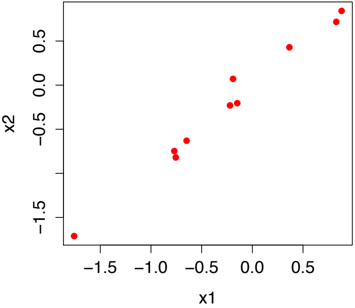
Why It May Be Possible to Reduce Dimensions?

When we have correlations between the variables, the data may more or less fall on a line or plane in a lower number of dimensions.



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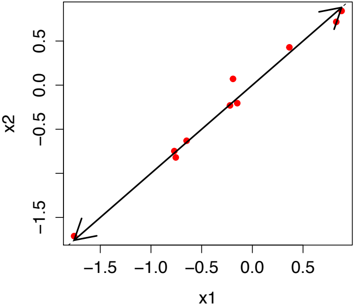

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PCA Procedure

Question: Can we reduce the large number of correlated variables to a few uncorrelated linear combinations of them?

Suppose that we have a random vector $\mathbf{X} = (X_1, X_2, \ldots, X_p)'$ with $p \times p$ variance-covariance matrix Σ.

Consider the linear combinations

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\begin{aligned}
Y_1 &= e_{11}X_1 + e_{12}X_2 + \cdots + e_{1p}X_p \\
Y_2 &= e_{21}X_1 + e_{22}X_2 + \cdots + e_{2p}X_p \\
&\vdots \\
Y_p &= e_{p1}X_1 + e_{p2}X_2 + \cdots + e_{pp}X_p
\end{aligned}
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- Let $\mathbf{e}_i = (e_{i1}, \ldots, e_{ip})'$, $i = 1, 2, \ldots, p$.

$$\operatorname{var}(Y_i) = \mathbf{e}_i'\Sigma\mathbf{e}_i \qquad \operatorname{cov}(Y_i, Y_j) = \mathbf{e}_i'\Sigma\mathbf{e}_j$$

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Principal Components

- ***First Principal Component (PC1):*** Y_1
  - PC1 is the linear combination of X-variables that has maximum variance among all linear combinations.
  - Select $\mathbf{e}_1 = (e_{11}, e_{12}, \ldots, e_{1p})'$ that maximizes

$$\text{var}(Y_1) = \mathbf{e}_1' \Sigma \mathbf{e}_1 \quad s.t. \quad \mathbf{e}_1' \mathbf{e}_1 = 1.$$

- ***Second Principal Component (PC2):*** Y_2
  - PC2 is the linear combination of X-variables that accounts for as much of the remaining variation as possible
  - the correlation between PC1 and PC2 is 0.
  - select $\mathbf{e}_2 = (e_{21}, e_{22}, \ldots, e_{2p})'$ that maximizes $\text{var}(Y_2) = \mathbf{e}_2' \Sigma \mathbf{e}_2$

$$\text{s.t. } \mathbf{e}_2' \mathbf{e}_2 = 1 \quad \text{and} \quad \text{cov}(Y_1, Y_2) = \mathbf{e}_1' \Sigma \mathbf{e}_2 = 0.$$

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Principal Components

All subsequent principal components have the same properties:

- linear combinations that account for as much of the remaining variation as possible
- not correlated with the other principal components

Question: How do we obtain the coefficients e_{ij} ?

Eigenvalue decomposition for Real Symmetric Matrices

Every $p \times p$ real symmetric matrix Σ can be decomposed as

$$\Sigma = Q \Lambda Q^T$$

where Λ is a $p \times p$ diagonal matrix whose entries are the eigenvalues of Σ and Q is a $p \times p$ orthogonal matrix whose columns are the corresponding eigenvectors.

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Solution of coefficients e_{ij}

- Let λ_1 through λ_p denote the eigenvalues of the variance-covariance matrix Σ which are ordered such that

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0.$$

- Let vectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_p$ denote the corresponding orthogonal eigenvectors. Then $\mathbf{e}_i$ will be the coefficients of i^{th} principal component, $i = 1, 2, \ldots, p$.

Discuss:

1. Why are all the principal components obtained in this way uncorrelated with one another?
2. What is the variance for i^{th} principal component, $i = 1, \ldots, p$?
3. * Why this is a valid solution?

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Interpretation of Principal Components (I)

- The variance for the i^{th} principal component is

$$\mathrm{var}(Y_i) = \mathrm{var}(\mathbf{e}_i' X_i) = \mathbf{e}_i' \Sigma \mathbf{e}_i = \lambda_i, \;\; i = 1, 2, \ldots, p.$$

- The total variation of $\mathbf{X}$ is defined as the trace of Σ.

$$\begin{aligned} \mathrm{trace}(\Sigma) &= \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_p^2 \\ &= \lambda_1 + \lambda_2 + \cdots + \lambda_p \end{aligned}$$

- The i^{th} principal component explains the following proportion of the total variation:

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How many PCs should be considered?

- A related quantity is the proportion of variation explained by the first k principal components:

$$\frac{\lambda_1 + \lambda_2 + \cdots + \lambda_k}{\lambda_1 + \lambda_2 + \cdots + \lambda_p}$$

- If this quantity is large, not much information is lost by considering only the first k principal components.

Eigenvalues of $\hat{\Sigma}$ in the Places Rated data (Boyer and Savageau)

PC	Eigen	Prop	Cumu
1	0.3775	0.7227	0.7227
2	0.0511	0.0977	0.8204
3	0.0279	0.0525	0.8739
4	0.0230	0.0440	0.9178
5	0.0168	0.0321	0.9500
6	0.0120	0.0229	0.9728
7	0.0085	0.0162	0.9890
8	0.0039	0.0075	0.9966
9	0.0018	0.0034	1.0000
Total	0.5225		

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- An alternative method is to look at a Scree Plot – The number of components can be determined at the point beyond which the remaining eigenvalues are all relatively small.