MONASH University

ETC3250

Business Analytics

Week 5
Other dimensionality reduction methods

27 August 2015

Dimensionality reduction

- Wy dimensionality reduction?
  - Curse of dimensionality
  - Intrinsic dimensionality
  - Visualization
- Dimensionality reduction methods
  - Feature selection vs feature extraction (examples? advantages?)
  - Unsupervised vs supervised
  - Linear vs nonlinear
- Principal components analysis (PCA)
  - PCA produces a low-dimensional representation of a dataset. It finds a sequence of linear combinations of the variables that have maximal variance, and are mutually uncorrelated.
  - PCA: linear and unsupervised feature extraction

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Dimensionality reduction in regression

- How would you reduce dimensionality in linear regression?
- How would use PCA to reduce dimensionality in linear regression?
- *Principal components regression* (PCR): use PCA to construct the first M principal components, $Z_1, \ldots, Z_M$, and then fit a linear regression model using these components.
- Assumption: *the directions in which $X_1, \ldots, X_p$ show the most variation are the directions that are associated with Y*. When is PCR better than traditional least squares?

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Partial least squares

- With PCR, the components are identified in an **unsupervised way**. No guarantee that the directions that best explain the predictors will also be the best directions to use for predicting the response Y. How would you use the response Y to reduce dimensionality?
- Partial least squares (PLS) is a **supervised** alternative to PCR. Same procedure as PCR, but the new features are identified in a supervised way. Roughly speaking, PLS attempts to find directions that help explain both the response and the predictors.

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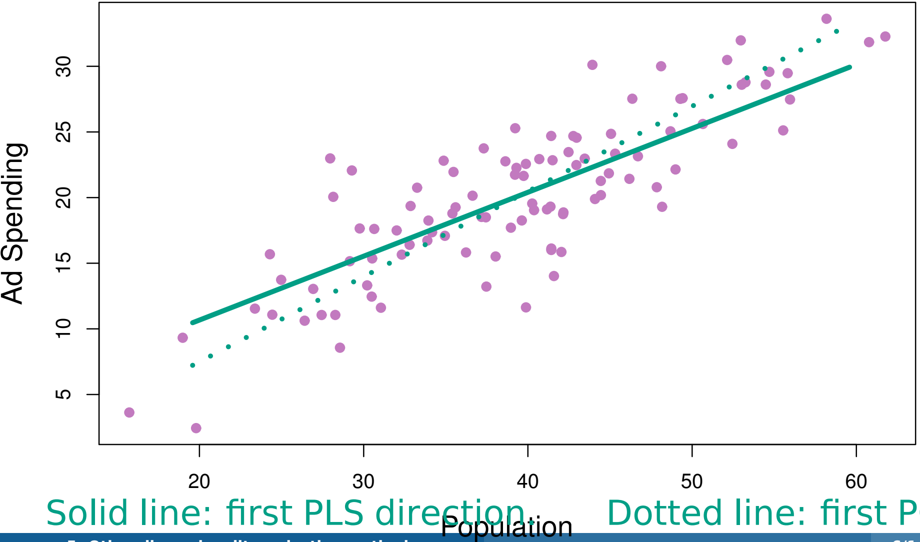
Partial least squares

1. Standardize the p predictors
2. Compute the first direction Z_1 by setting each ϕ_{j1} in $Z_1 = \sum_{j=1}^{p} \phi_{j1} X_j$ equal to the coefficient from the simple linear regression of Y onto X_j (see Figure)
3. For the second direction Z_2, we first adjust each of the variables for Z_1, by regressing each variable on Z_1, and taking residuals, say X_j'. These residuals represent the remaining information that has not been explained by the the first PLS direction Z_1. We then compute Z_2 using X_j' as Z_1 was computed from X_j
4. We can compute $Z_1, \ldots, Z_M$ iteratively. Then we use least squares to fit a linear model using $Z_1, \ldots, Z_M$ as for PCR. How to choose M?

PLS Example



Solid line: first PLS direction. Dotted line: first PC.

Partial least squares

- There are two variants of PLS: PLS1 (one response variable) and PLS2 (at least two response variables).
- In practice, PLS1 is not better than ridge regression or PCR (PLS reduces bias but can potentially increase variance).
- PLS2 is a useful tool for multiresponse regression.
- Other supervised dimensionality reduction methods: CCA, LDA, etc.

Multidimensional scaling

Suppose that instead of measuring a $n \times p$ dataset $\boldsymbol{X} = [x_{ij}]$, we were only given a pairwise distance matrix Δ where

$$\Delta_{ij} = \|x_i - x_j\|, \quad i, j = 1, \ldots, N$$

i.e. we do not know the points themselves. Can we find a lower-dimension representation $\boldsymbol{Z}$ for $\boldsymbol{X}$ from Δ? (If we have only a distance matrix, we cannot perform PCA.)

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Multidimensional scaling

MDS seeks values $z_1, z_2, \ldots, z_n \in \mathbb{R}^k$ that minimize the so-called stress function:

$$S_M(z_1, z_2, \ldots, z_n) = \sum_{i \neq j} (\|x_i - x_j\| - \|z_i - z_j\|)^2.$$

(least squares or *Kruskal-Shephard* scaling).

A variation on least squares scaling minimizes

$$S_{\mathrm{Sm}}(z_1, z_2, \ldots, z_n) = \sum_{i \neq j} \frac{(\|x_i - x_j\| - \|z_i - z_j\|)^2}{\|x_i - x_j\|}$$

(*Sammmon mapping*) Difference with least squares scaling?

Link between MDS and PCA

Computation of PCs in PCA:

- Singular value decomposition
  - $\boldsymbol{X} = \boldsymbol{U}\Lambda\boldsymbol{V}'$ with $\boldsymbol{U}'\boldsymbol{U} = \boldsymbol{I}$ and $\boldsymbol{V}'\boldsymbol{V} = \boldsymbol{I}$
  - $\Phi = \boldsymbol{V} \rightarrow \boldsymbol{Z} = \boldsymbol{X}\Phi$
- Eigenvalue decomposition
  - $\boldsymbol{C} = \boldsymbol{X}'\boldsymbol{X}$ where the columns of $\boldsymbol{X}$ are scaled
  - $\boldsymbol{C} = \boldsymbol{V}\boldsymbol{D}\boldsymbol{V}'$ with $\boldsymbol{V}'\boldsymbol{V} = \boldsymbol{I}$
  - $\Phi = \boldsymbol{V} \rightarrow \boldsymbol{Z} = \boldsymbol{X}\Phi$

Link between MDS and PCA

If Δ_{ij} are Euclidean distances between the rows of $\boldsymbol{X}$, then MDS is equivalent to PCA.

Given distance matrix $\Delta \in \mathbb{R}^{n\times n}$,

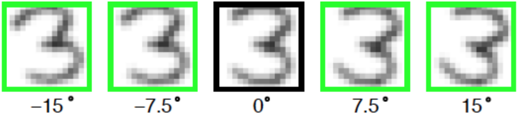
1. Recover the inner product $\boldsymbol{XX}'$ from Δ
   - Compute $A_{ij} = -\frac{1}{2}\Delta_{ij}^2$
   - Double center A to recover B:
     $B = (I - M)A(I - M)$ where $M = \frac{1}{n}\mathbb{1}\mathbb{1}' \in \mathbb{R}^{n\times n}$
2. Factorize B to gest the first k principal component scores

This is called *classical multidimensional scaling*.

$$S_C(z_1, z_2, \ldots, z_n) = \sum_{i\neq j}(\langle x_i - \bar{x}, x_j - \bar{x}\rangle - \langle z_i - \bar{z}, z_j - \bar{z}\rangle)^2$$

Multidimensional scaling

- Multidimensional scaling can be applied to any Δ_{ij}, not just Euclidean distances
- In this case, we don't compute principal component scores, and the lower-dimensional representation can be a nonlinear function of the data
- When do we need to use non-Euclidean distances?



We wish to remove the effect of rotation in measuring distances between two digits

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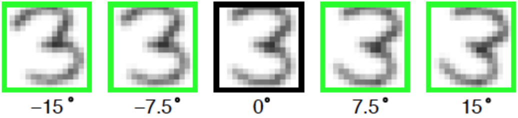

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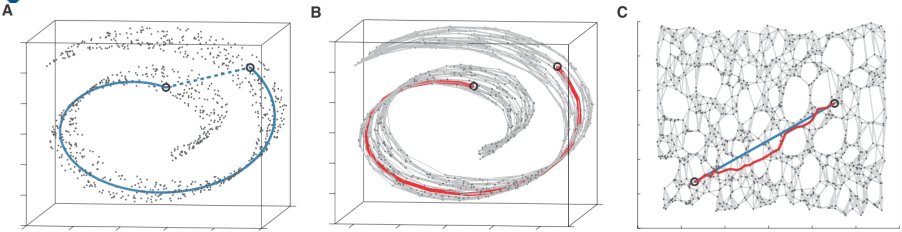
Isometric feature mapping



(From Tenenbaum et al. (2000), "A global geometric framework for nonlinear dimensionality reduction")

- Construct a graph $G = (V, E)$ based on the structure between $x_1, \ldots, x_n$.
- Then, define a graph distance $\Delta_{ij}^{\text{Isomap}}$ between i and j, and use MDS for the low-dimensional representation

Dimensionality reduction methods

- Feature selection vs feature extraction
- Linear and nonlinear
- Unsupervised and supervised
- Low-dimensional representation with maximum variance, that retains local properties of the data, etc.
- **Linear PCA**, Nonlinear PCA, Kernel PCA, Sparse PCA, etc.
- **MDS**, ICA, LDA, etc.
- **PLS**, CCA, FA, etc.
- **Isomap**, diffusion maps, MVU, LLE, t-SNE, autoencoders, etc.