Feature Selection and Representation

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Contents

Notation

symbol	meaning
$a, b, c, N \dots$	scalar number
$\boldsymbol{w}, \boldsymbol{v}, \boldsymbol{x}, \boldsymbol{y} \dots$	column vector
$\boldsymbol{X}, \boldsymbol{Y} \dots$	matrix
$\mathbb{R}$	set of real numbers
$\mathbb{Z}$	set of integer numbers
$\mathbb{N}$	set of natural numbers
$\mathbb{R}^D$	set of vectors
$\mathcal{X}, \mathcal{Y}, \dots$	set
$\mathcal{A}$	algorithm

operator	meaning
$\boldsymbol{w}^\intercal$	transpose
$\boldsymbol{X}\boldsymbol{Y}$	matrix multiplication
$\boldsymbol{X}^{-1}$	inverse

Motivation

Why Should We Select Features?

- Some problems are defined by **100 or even 1000 input features**
- Most Machine Learning models have to attribute parameters to handle these features (often at least linearly as much)
- Hence, **capacity** is determined by the number of features
- If most features are **noise**, then most of the parameters will be useless $\rightarrow$ capacity is wasted
- Worse, the algorithm might find **false regularities** in the input features of the training data and use the wasted capacity to represent them!
- Other problem: **curse of dimensionality**.
- Finally: for more **interpretability** and **efficiency**.

Classes of Feature Selection Methods

Broad classes of feature selection methods:

- **Filter Methods**:
  - Select the best features according to a **reasonable criterion**
  - The criterion is **independent** of the real problem
- **Wrapper Methods**:
  - Select the best features according to the **final criterion**
  - For each subset of features, try to solve the problem
- In any case, there are

$$\sum_{p=1}^{N} \binom{p}{N} = \sum_{p=1}^{N} \frac{N!}{p!(N-p)!} \textbf{ combinations}$$

- Alternative: **weighting methods**.

Filters

Filter Methods

- **Basic idea**: select the best features according to some prior knowledge
- **Examples** of prior knowledge:
  - if we accept to **transform** the features...
  - features should be **uncorrelated** $\rightarrow$ perform a **PCA** and keep only the eigenvectors corresponding to $x\%$ of the variance.
  - similar ideas: linear discriminant analysis (**LDA**), independent component analysis (**ICA**)
  - features should have **strong correlation with the target** $\rightarrow$ select the k features most linearly correlated to the target
  - select the k features with highest mutual information with the target:

$$I(x,y) = \sum_i \sum_j p(x=i, y=j) \log \left[\frac{p(x=i, y=j)}{p(x=i)p(y=j)} \right]$$

Wrappers

Wrapper Methods

- Basic (**naive**) algorithm:
  - For each subset of features, solve the problem.
  - Select the best subset.
- Impossible because the problem is exponentially long!
- Alternatives: **greedy** heuristics such as **forward** selection or **backward** elimination

Forward Selection

1. let $\mathcal{P} = \emptyset$ be the **current** set of selected features
2. let $\mathcal{Q}$ be the **full** set of features
3. while size of $\mathcal{P}$ smaller than a given constant
   3.1 for each $v \in \mathcal{Q}$
      - set $\mathcal{P}' \leftarrow \{v\} \cup \mathcal{P}$
      - train the model with $\mathcal{P}'$ and keep the **validation** performance

   3.2 set $\mathcal{P}' \leftarrow \{v^*\} \cup \mathcal{P}$ where v^* corresponds to the **best** validation performance obtained in step 3.1
   3.3 set $\mathcal{Q} \leftarrow \mathcal{Q} \setminus \{v^*\}$
   3.4 keep the validation performance obtained with current $\mathcal{P}$
4. return the **best set** $\mathcal{P}$

Backward Elimination

1. let $\mathcal{P}$ be the **full** set of features
2. while size of $\mathcal{P}$ smaller than a given constant
   2.1 for each $v \in \mathcal{P}$
   - set $\mathcal{P}' \leftarrow \mathcal{P} \setminus \{v\}$
   - train the model with $\mathcal{P}'$ and keep the **validation** performance

   2.2 set $\mathcal{P}' \leftarrow \mathcal{P} \setminus \{v^*\}$ where v^* corresponds to the **worst** validation performance obtained in step 2.1
   2.3 keep the validation performance obtained with current $\mathcal{P}$
3. return the **best set** $\mathcal{P}$

Feature Weighting

Feature Weighting Methods

- Instead of **selecting** a subset of features, which is a **combinatorial** problem, why not simply **weight** them?
- Most feature weighting methods are based on the **wrapper** approach
- **Heuristics** for feature weighting:
  - **gradient descent** on the input space $\rightarrow$ train with all features, then fix the parameters and estimate the importance of each input, and loop
  - **AdaBoost** when each model is trained on one feature only ($\rightarrow$ final solution is a linear combination)

Principal Component Analysis

Introduction

Concept 1

Principal Component Analysis (PCA) is an **unsupervised** dimension-reduction tool that can be used to reduce a large set of variables to a small set that still contains most of the information in the large set.

Algorithm

- **Input**: Data $\mathcal{D} = \{\boldsymbol{x}_1, ..., \boldsymbol{x}_n\}, \boldsymbol{x}_i \in \mathbb{R}^D$
- **Output**: projection matrix W

1. Construct the mean vector $\boldsymbol{\mu}$

$$\boldsymbol{\mu} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}_i$$

2. Construct the covariance matrix S.

$$S = \frac{1}{n} \sum_{i=1}^{n} (\boldsymbol{x}_i - \boldsymbol{\mu}_i)(\boldsymbol{x}_i - \boldsymbol{\mu}_i)^\mathsf{T}$$

Algorithm (cont.)

3. Decompose the covariance matrix into its eigenvectors and eigenvalues.

$$\{\boldsymbol{w}_1, ..., \boldsymbol{w}_D\} \text{ and } \{\lambda_1, ..., \lambda_D\}$$

4. Sort the eigenvalues by decreasing order to rank the corresponding eigenvectors.

$$\{\boldsymbol{w}_1, ..., \boldsymbol{w}_D\} \text{ where } \lambda_1 \geq ... \geq \lambda_D$$

5. Select k eigenvectors which correspond to the k largest eigenvalues, where k is the dimensionality of the new feature subspace ($k \leq D$).

$$\{\boldsymbol{w}_1, ..., \boldsymbol{w}_k\} \text{ where } \lambda_1 \geq ... \geq \lambda_k$$

6. Construct a projection matrix W from the "top" k eigenvectors.

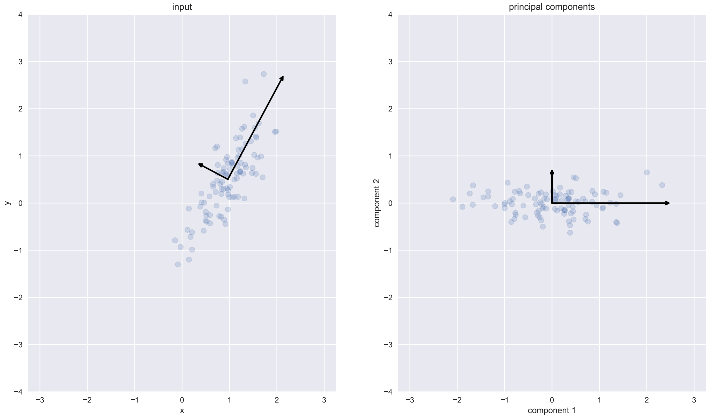
$$W = \begin{bmatrix} \boldsymbol{w}_1 & \dots & \boldsymbol{w}_k \end{bmatrix}^\intercal$$

Algorithm (cont.)

- Transform the D-dimensional input dataset $\mathcal{D}$ using the projection matrix W to obtain the new k-dimensional feature subspace.

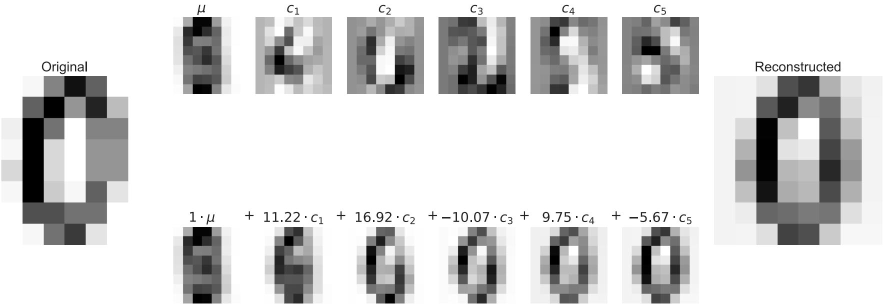
Example

- Project data

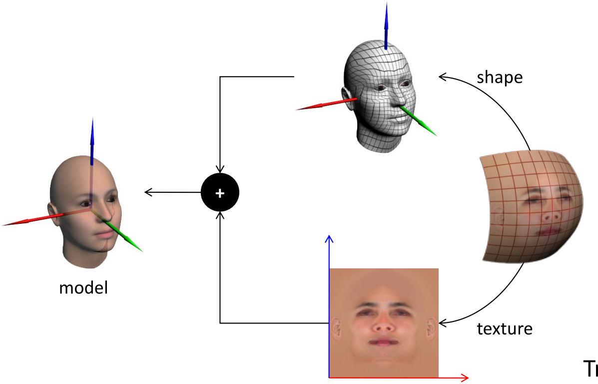


Example

- Reconstruct data



3D Head Model



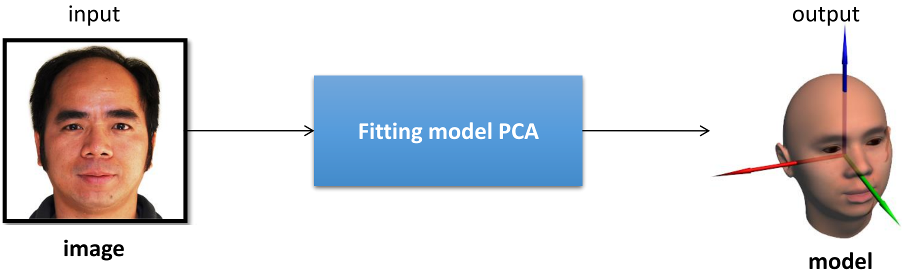
$$\text{Shape } S = \begin{pmatrix} x_1 & x_2 & \dots & x_k \\ y_1 & y_2 & \dots & y_k \\ z_1 & z_2 & \dots & z_k \end{pmatrix}$$

$$\updownarrow \quad \updownarrow \quad \updownarrow$$

$$\text{Texture } T = \begin{pmatrix} r_1 & r_2 & \dots & r_k \\ g_1 & g_2 & \dots & g_k \\ b_1 & b_2 & \dots & b_k \end{pmatrix}$$

$$\text{Triangle List } L = \{t_1, \dots, t_n\}$$

Fitting 3D Head Model



Linear Discriminant Analysis

Introduction

Concept 2

Linear Discriminant Analysis (LDA) is a **supervised** dimension-reduction tool that the goal is to find the feature subspace that optimizes class separability.

Algorithm

- **Input**: Data $\mathcal{D} = \{(\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_n, y_n)\}, \boldsymbol{x}_i \in \mathbb{R}^D, y_i \in \{c_1, ..., c_k\}$
- **Output**: projection matrix W

1. For each class, compute the D dimensional mean vector.
2. Construct the between-class scatter matrix S_B and the within-class scatter matrix S_W.
3. Compute the eigenvectors and corresponding eigenvalues of the matrix $S_W^{-1} S_B$.
4. Sort the eigenvalues by decreasing order to rank the corresponding eigenvectors.
5. Choose the k eigenvectors that correspond to the k largest eigenvalues to construct a $D \times D$-dimensional transformation matrix W; the eigenvectors are the columns of this matrix.

Algorithm (cont.)

- Transform the D-dimensional input dataset $\mathcal{D}$ using the projection matrix W to obtain the new k-dimensional feature subspace.

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