Dimension Reduction

March 18th, 2019

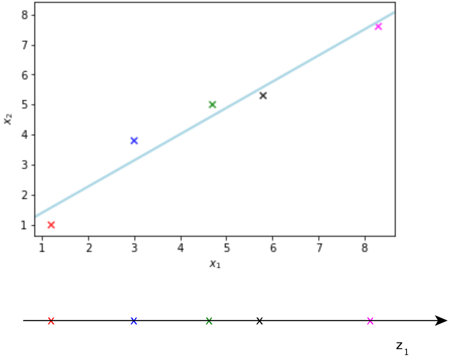
Introduction & Motivation

What is dimensionality reduction?

Dimensionality reduction is the process of taking data in a ***high dimensional*** space and mapping them into a ***new space*** whose dimensionality is much smaller.

What are the reasons to reduce data dimensionality?

Data compression



- **Reduce data** from 2D to 1D

$$
\begin{aligned}
x^1 &\in \mathbb{R} \mapsto z^1 \in \mathbb{R}\\
x^2 &\in \mathbb{R} \mapsto z^2 \in \mathbb{R}\\
&\vdots\\
x^n &\in \mathbb{R} \mapsto z^n \in \mathbb{R}
\end{aligned}
$$

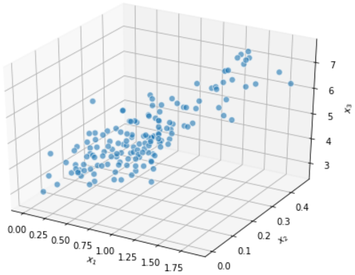
What are the reasons to reduce data dimensionality?

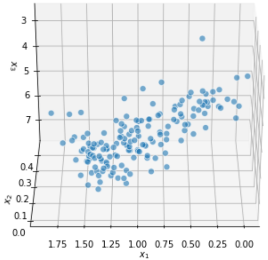
Table 1: World Happiness Report

CR	HR	HS	WH	WL	GDP	FM	LE	FR	GE	TGC	DY
Norway	1	7.5	7.59	7.47	1.61	1.53	0.79	0.63	0.36	0.31	2.27
Denmark	2	7.52	7.58	7.46	1.48	1.55	0.79	0.62	0.35	0.40	2.31
Iceland	3	7.50	7.62	7.38	1.48	1.61	0.83	0.62	0.475	0.15	2.32
Switzerland	4	7.494	7.56	7.42	1.56	1.51	0.85	0.62	0.29	0.36	2.27
Finland	5	7.46	7.52	7.41	1.44	1.54	0.80	0.61	0.24	0.38	2.43
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

What are the reasons to reduce data dimensionality?

Data visualization





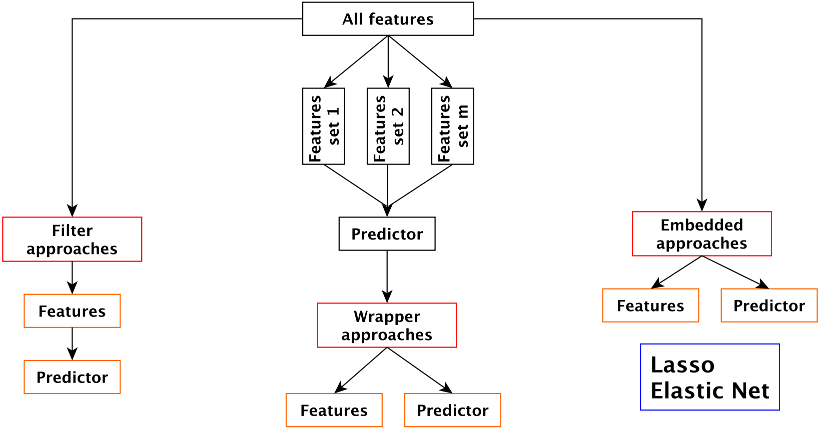
What are the reasons to reduce data dimensionality?

- Dimensionality reduction can be used to:
  - reduce storage and computing time
  - help us on understanding a model (e.g., ***interpretability***)
  - find meaningful structure of the data
  - visualize the data (e.g., in 2 or 3 dimensions)
  - ***remove irrelevant features*** that can lead a model to have difficulty in learning
  - reduce the cost of ***data acquisition***

There are different strategies to reduce data dimensionality

- ***Feature selection***: select m features $m < p$, ignoring the remaining ones
- ***Approaches***:
  - ***Filtering***: applies a statistical measure to assign a score to each feature (e.g., correlation, χ^2-test)
  - ***subset selection***: finds the best set of features for a specific predictive model
  - ***Embedded***: simultaneously fits a model and learn which features should be included

Overview of feature selection strategies



Subset selection:

forward selection
backward selection
floating selection

Subset selection

- It aims to find the subset of features that leads to the best-performing model
- Therefore, a brute force strategy needs to deal with 2^p subsets
- We can embrace a ***forward search*** strategy
  - at each step, we add the best feature to train a predictor
- Given a dataset $\mathcal{D} = (\mathcal{X}, \hat{y})$, where $\mathcal{X} \in \mathbb{R}^{n,p}$, a subset of variables $\varepsilon \subset \{1, \ldots, p\}$, and a $\mathcal{E}(\mathcal{F})$ the error of a predictor trained only using the features in $\mathcal{F}$.

Subset selection

- ***Forward search*** algorithm
  1. $\mathcal{F} \leftarrow \emptyset$
  2. Find new best feature to include in $\mathcal{F}$:
  $$j^* = \arg\min_{j \in \{1,\ldots,p\}} \mathcal{E}(\mathcal{F} \cup \{j\})$$
  3. stop if $\mathcal{E}(\mathcal{F}) < \mathcal{E}(\mathcal{F} \cup \{j\})$
  4. else $\mathcal{F} \leftarrow \mathcal{F} \cup \{j\}$; go to step 2;
- **What is the complexity?**
  - In the worst case ($\mathcal{F} = \{1, \ldots, p\}$), it's $\mathcal{O}(p^2)$
- Other alternative strategies include:
  - ***Backward search***: starting from $\{1, \ldots, p\}$, eliminate the feature $\mathcal{E}(\mathcal{F} \setminus \{j\}) \geq \mathcal{E}(\mathcal{F})$
  - ***Floating search***: add q features and remove r features

Feature extraction

- Project p features on $m < p$ new dimensions
- There are different methods for linear and non-linear problems, and most of them are ***unsupervised methods***
- Linear methods
  - Principal Component Analysis (PCA)
  - Factor Analysis (FA)
  - Non-negative Matrix Factorization (NMF)
  - Linear Discriminant Analysis (LDA)
- Non-linear methods
  - Multidimensional scaling (MDS)
  - Isometric feature mapping (Isomap)
  - Locally Linear Embedding (LLE)
  - Autoencoders

Linear feature extraction: Principal Component Analysis (PCA)

What is principal component analysis?

Principal component analysis (PCA)

- It is a mathematical procedure that transforms a number of possibly correlated variables into a smaller number of uncorrelated variables called ***principal components***
- The ***first principal component*** accounts for the maximum variability of the data, and each succeeding component accounts for as much of the remaining variability
- PCA aims to find a low-dimensional space such that ***variance*** is ***maximized*** when the data are projected on that space.
- It is an ***unsupervised method***, as we look only at the data and not on any label.
- This method requires ***feature standardization***

Feature standardization

1. ***Variance*** of feature j in dataset $\mathcal{D}$,
   $\mathcal{D} = \{x^1, \ldots, x^p\}$ $x \in \mathbb{R}^{nxp}$

$$\sigma_j^2 = \frac{1}{n} \sum_{i=1}^{n} (x_j^i - \mu_j)^2$$

$$\mu_j = \frac{1}{n} \sum_{i=1}^{n} x_j^i$$

2. Data normalization:
   - ***mean centering***: give each feature a mean of 0
   - ***variance scaling***: give each feature a variance of 1

$$x_j^i \hookleftarrow \frac{x_j^i - \mu_j}{\sigma_j}$$

Principal component analysis: algorithm

PCA

Principal components are features constructed as linear combinations of given features. In this case, the ***first principal component*** is given by the direction of the **maximum variance** in the data. The **second principal component** is the direction of maximum variance orthogonal to the first component, and so on.

Goal

Find a low-dimensional space such that ***variance*** is ***maximized*** when the data are projected on that space.

- ***Assumption***: data are ***centered*** (i.e., they have zero mean)

Principal component analysis: algorithm

- When they don't, we have to subtract the mean:

$$X \leftarrow X - \boldsymbol{\mu}$$

- We want to project x in the direction of a matrix $\boldsymbol{w}$, $||\boldsymbol{w}|| = 1$

$$z = X\boldsymbol{w}$$

- The dimensions of z, X, and $\boldsymbol{w}$ are: $(n, 1)$, (n, p), and $(p, 1)$, where n is the number of samples, p is the number of features.

Principal component analysis: algorithm

- We can compute $\boldsymbol{Var}(z)$ in function of $\boldsymbol{X}$ and w

$$
\begin{aligned}
Var(z) &= Var(X\mathbf{w}) \\
&= Var(X^T\mathbf{w}^T) \\
&= \mathbb{E}[((X^T\mathbf{w}^T) - \mathbb{E}[\mathbf{w}^T X^T])^2] \\
&= \mathbb{E}[(\mathbf{w}^T X^T - \mathbf{w}^T\mathbb{E}[X]^2)] \\
&= \mathbb{E}[\mathbf{w}^T X^T X\mathbf{w}] \\
&= \mathbf{w}^T\mathbb{E}[X^T X]\mathbf{w}
\end{aligned}
$$

- The dimensions are: $(1, p)$ x (p, n) x (n, p) x $(p, 1)$

Computing the principal components: algorithm

- Reducing data from *n*-dimensions to *k*-dimensions
  - Compute the covariance matrix Σ

$$\Sigma = \frac{1}{n}\sum_{i=1}^{n} x^i {x^i}^T$$

  - Compute the eigenvectors of matrix Σ

$$U, S, V = svd(\Sigma)$$

Computing the principal components: theory behind

Let $X \in \mathbb{R}^{n_x p}$ be a centered matrix of covariance $\Sigma = \frac{1}{n}X^T X$. The principal components of X are the eigenvectors of Σ, ordered by their decreasing eigenvalues.

- For all vector $\vec{w} \in \mathbb{R}^p$, the variance of the project of $X \mapsto \vec{w}$ is $\boldsymbol{w}^T \Sigma \boldsymbol{w}$
- The projection of $X \in \mathbb{R}^{n_x p}$ onto $\vec{w} \in \mathbb{R}^p$ is the vector $\vec{z}$

$$\vec{z} = X\boldsymbol{w}$$

Computing the principal components: theory behind

- X is ***centered***. It means that the ***mean*** of $\vec{z}$ is:

$$\begin{aligned} &= \frac{1}{n}\sum_{i=1}^{n} z_i \\ &= \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{p} x_j^i w_j \\ &= \frac{1}{n}\sum_{j=1}^{p} w_j \sum_{i=1}^{n} x_j^i \\ &= 0 \end{aligned}$$

- $Var[\vec{z}]$

$$\begin{aligned} Var[\vec{z}] &= \frac{1}{n}\vec{w}^T X^T X \vec{w} \\ &= \vec{w}^T \Sigma \vec{w} \end{aligned}$$

Computing the principal components: theory behind

- Let $\vec{w}_1 \in \mathbb{R}^p$ be the first principal component. Thus $\vec{w}_1$ is orthogonal in a way that the variance of $X\vec{w}_1$ is maximal

$$\vec{w}_1 = \underset{\vec{w}\in\mathbb{R}^p}{\arg\max}\, \vec{w}^T \Sigma \vec{w}$$
$$\text{subject to} ||\vec{w}_1||_2 = 1$$

- This represents a quadratic optimization problem, under the constraint of $g(\vec{w}) = 0$. In that case, we can solve it introducing the Lagrange multiplier $\alpha_1 > 0$

$$L(\alpha_1, \vec{w}) = \vec{w}^T \Sigma \vec{w} - \alpha_1(||\vec{w}||_2 - 1)$$

Computing the principal components: theory behind

- Due to the strong duality, the maximum of $\vec{w}^T \Sigma \vec{w}$ subject to $||\vec{w}||_2 = 1$ is the $\min_{\alpha_1} \sup_{\vec{w} \in \mathbb{R}^p} L(\alpha_1, \vec{w})$. The *supremum* (least upper bound) of Lagrangien is achieved in the point where its gradient is null

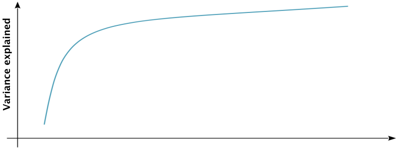
$$2\Sigma \vec{w} - 2\alpha_1 \vec{w} = 0$$

- As a result, $\Sigma \vec{w}_1 = \alpha_1 \vec{w}_1$ and $\alpha_1, \vec{w}_1$ are respectively an eigenvalue and an eigenvector of Σ. Considering all the eigenvectors of Σ, $\vec{w}_1$ is the one that maximize the variance

$$\begin{aligned} \vec{w}_1^T \Sigma \vec{w}_1 & \\ &= \alpha_1 ||\vec{w}_1||_2 \\ &= \alpha_1 \end{aligned}$$

How to choose the number of principal components?

- In principal component analysis, we take n dimensional features and reduce them to m feature representation
- Thus, m is a parameter of the PCA algorithm, which is known as the number of principal components
- Choose m in function of the ***percentage of variance explained***:
  1. Total variance in the data: $Tr(\Sigma) = \sum_{i=1}^{p} \lambda_i$
  2. The first m principal components accounts for $\frac{\sum_{i=1}^{m} \lambda_i}{\sum_{i=1}^{p} \lambda_i}$ of the total variance



Non-linear feature extraction

t-Stochastic Neighbor Embedding (t-SNE)

- It is nowadays a popular method proposed by Maaten and Hinton[1] in 2008
- It approximates the distribution of pairwise distances in the data following a t-distribution[2]

$$\arg\min_{Q} \sum_{i=1}^{n} KL(P_i|Q_i)$$

- where:
  - Q follows a t-distribution
  - KL is the *Kullback-Leibler* divergence (i.e., it measures how much P diverges from Q)
  - P_i is the distribution of the conditional probability that x^i picks x^j as a neighbor. In this case, neighbors are picked in proportion to their probability density under a Gaussian centered in x^i. $P_i = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{||x^j - x^i||^2}{s\sigma^2})$

[1] Laurens van der Maaten and Geoffrey Hinton. "Visualizing data using t-SNE". In: *Journal of machine learning research* 9.Nov (2008), pp. 2579–2605. URL: jmlr.org/papers/volume9/vandermaaten08a/

Multidimensional scaling (MDS)

Goal

Find a mapping that preserves the dissimilarities between the data points.

$$\arg\min_{Z \in \mathbb{R}^{nxm}} \sum_{t=1}^{n} \sum_{u=t+1}^{n} (||z^t - z^u|| - d_{tu})^2$$

- $d_{tu} = ||x^t - x^u||$ In Euclidean space, which is similar to PCA
- Therefore, dissimilarity can also come from other metrics $d : \mathcal{X} x \mathcal{X} \mapsto \mathbb{R}_+$
  - ***identity of indiscernibles***: $d(x, v) = 0 \Leftrightarrow x = v$
  - ***symmetry***: $d(x, v) = d(v, x)$
  - ***triangular inequalities***: $d(x, v) \leq d(x, w) + d(w, v)$

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  PCA session 14.5.1
  MDS session 14.8

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