Machine Learning for Networks: Dimensionality reduction

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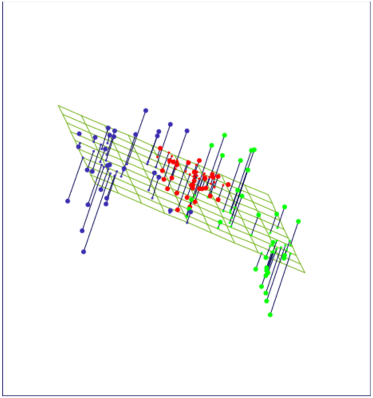
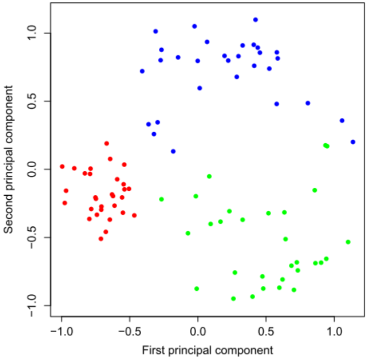
Retrieve most the most important information

From Source:https://www.alimentipedia.it/come-si-fa-il-formaggio.html

Why dimensionality reduction





From [3]

Main idea:

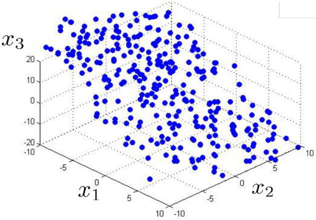
- Sample = Vector of a vectorial space (each feature is a dimension)
- Find the "best" space for your data
- Keep few "most important" dimensions only.
- Project the samples in the new reduced space.

Advantages:

- Easier to visualize
- Smaller dataset
  $\Rightarrow$ Faster model runs

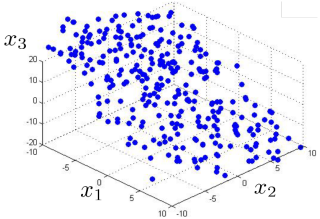
The "best space"

- Which 2D space would you choose?
- Any mathematical argument for your choice?



From [5]

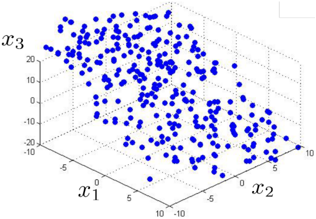
The “best space”



From [5]

- Which 2D space would you choose?
- Any mathematical argument for your choice?
- Hyperplane capturing most of the variation of data
- *Most important dimension*:
  the one along which data have the largest variance.

The “best space”



From [5]

- Which 2D space would you choose?
- Any mathematical argument for your choice?
- Hyperplane capturing most of the variation of data
- *Most important dimension*:
  the one along which data have the largest variance.
- “Best space”:
  Dimensions are ordered from the most to the least important.
- **Singular Value Decomposition (SVD)**
  finds this space!

Outline

- Change of basis
- Singular Value Decomposition
- Dimensionality Reduction
- Application to supervised learning
- Application to anomaly detection

Section 1

Change of basis

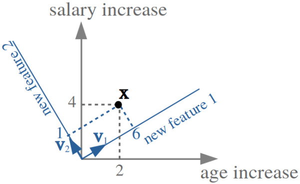
Change of basis

Consider data matrix $\mathbf{X}$, already standardized. Sample $\mathbf{x}^{(i)}$ is a vector of space $\mathbb{R}^N$. The dimensions of such a space are feature *1*, ..., feature *j*, ..., feature *N*.

Take any set of N orthonormal vectors $\mathbf{v}_1, \ldots, \mathbf{v}_N$:

$$\mathbf{v}_z^T \cdot \mathbf{v}_z = 1;$$
$$\mathbf{v}_z^T \cdot \mathbf{v}_{z'} = 0 \quad \text{for } z' \neq z.$$

They are a new basis of space $\mathbb{R}^N$.



The projection of $\mathbf{x}^{(i)}$ over the j-th new feature is

$$\tilde{x_j^{(i)}} = {\mathbf{x}^{(i)}}^T \cdot \mathbf{v}_j.$$

The projection of $\mathbf{x}^{(i)}$ over the new space is

$$\tilde{\mathbf{x}^{(i)}}^T = {\mathbf{x}^{(i)}}^T \cdot \underbrace{[\mathbf{v}_1 | \ldots | \mathbf{v}_N]}_{\mathbf{V}} = {\mathbf{x}^{(i)}}^T \cdot \mathbf{V}.$$

The projections of all samples on the j-th new feature (the j-th column of the transformed dataset) is

$$\mathbf{X} \cdot \mathbf{v}_j.$$

The projection of all samples on all the new features is:

$$\mathbf{X} \cdot \mathbf{V}.$$

Properties of change of basis

Proposition

If all features of $\mathbf{X}$ have zero-mean, after changing bases, the new features have also zero-mean

Proof

The mean is:

$$\frac{1}{M} \cdot (1, \ldots, 1) \cdot \mathbf{X} = (0, \ldots, 0).$$

Let us compute the mean of the new features:

$$\frac{1}{M} \cdot (1, \ldots, 1) \cdot \mathbf{X} \cdot \mathbf{V} = (0, \ldots, 0).$$

Proposition

If all features of $\mathbf{X}$ have zero-mean, the total variance of $\mathbf{X}$ does not change when changing basis.

Proof

Denote with $\mathbf{x}_j$ the j-th column of the original dataset. The total variance is

$$(M-1) \cdot \sum_{j=1}^{N} \mathrm{Var}_j = \sum_{j=1}^{N} \mathbf{x}_j^T \cdot \mathbf{x}_j = \sum_{j=1}^{N} \sum_{i=1}^{M} x_j^{(i)} \cdot x_j^{(i)}$$
$$= \sum_{i=1}^{M} \sum_{j=1}^{N} x_j^{(i)} \cdot x_j^{(i)} = \sum_{i=1}^{M} \mathbf{x}^{(i)^T} \cdot \mathbf{x}^{(i)}$$

Similarly, the total variance of the transformed dataset is:

$$(M-1) \cdot \sum_{j=1}^{N} \mathrm{Var}'_j = \sum_{i=1}^{M} \mathbf{x}^{\tilde{(i)}^T} \cdot \mathbf{x}^{\tilde{(i)}} = \sum_{i=1}^{M} \mathbf{x}^{(i)^T} \cdot \mathbf{V} \cdot \mathbf{V}^T \mathbf{x}^{(i)}$$
$$\underbrace{=}_{\mathbf{V}\text{ orthonormal}} \sum_{i=1}^{M} \mathbf{x}^{(i)^T} \cdot \mathbf{x}^{(i)}$$

Section 2

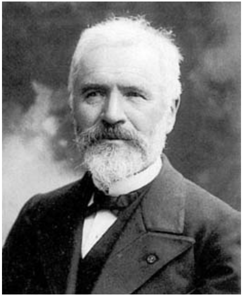
Singular Value Decomposition

An old history

From [2]

> *The Singular Value Decomposition was discovered and developed independently by a number of mathematicians. Eugenio Beltrami and Camille Jordan were the first to do so, in 1873 and 1874, respectively*

Eugenio Beltrami
Prof. at Università di Bologna.



Camille Jordan
Prof. at École Polytechnique.

Best new feature space

With the following dataset, can you find the "best" basis $\mathbf{v}_1, \mathbf{v}_2$?

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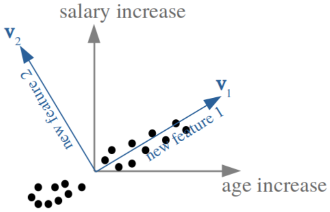

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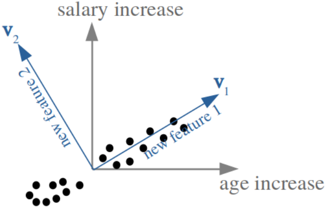

Find $\mathbf{v}_1$ such that the projection captures most of the variance:

$$\mathbf{v}_1 = \arg\max_{\mathbf{v}} \left(\mathbf{v}^T \cdot \mathbf{X}^T \cdot \underbrace{\mathbf{X} \cdot \mathbf{v}}_{\substack{\text{Proj. of all samples} \\ \text{on the new feat} \\ \text{represented by } \mathbf{v}}} \right)$$

$$\text{s.t. } \mathbf{v}^T \cdot \mathbf{v} = 1$$

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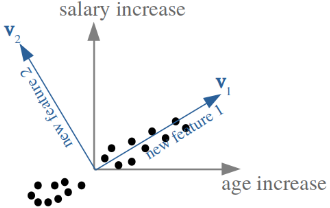

Then, find $\mathbf{v}_2$:

$$\mathbf{v}_2 = \arg\max_{\mathbf{v}} \mathbf{v}^T \cdot \mathbf{X}^T \mathbf{X} \cdot \mathbf{v}$$

$$\text{s.t. } \mathbf{v}^T \cdot \mathbf{v} = 1$$

$$\mathbf{v}^T \cdot \mathbf{v}_1 = 0$$

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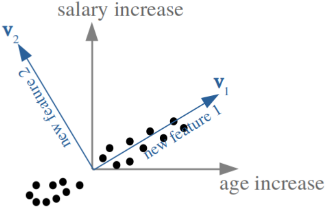

Find $\mathbf{v}_1$ such that the projection captures most of the variance:

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Then, find $\mathbf{v}_2$:

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$$\text{s.t. } \mathbf{v}^T \cdot \mathbf{v} = 1$$

$$\mathbf{v}^T \cdot \mathbf{v}_1 = 0$$

Then, find $\mathbf{v}_3$:

$$\mathbf{v}_3 = \arg\max_{\mathbf{v}} \mathbf{v}^T \cdot \mathbf{X}^T \mathbf{X} \cdot \mathbf{v}$$

$$\text{s.t. } \mathbf{v}^T \cdot \mathbf{v} = 1$$

$$\mathbf{v}^T \cdot \mathbf{v}_1 = 0$$

Singular Value Decomposition

Theorem ([4])

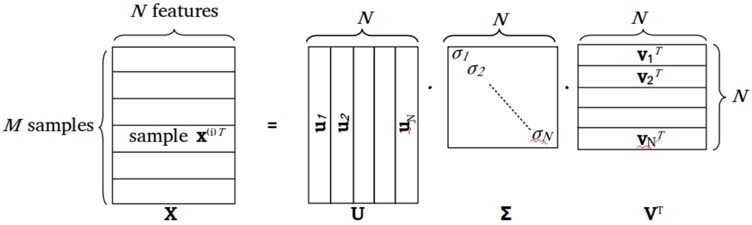
Any matrix $\mathbf{X}$ *can be decomposed as follows*

$$\mathbf{X} = \mathbf{U} \times \mathbf{\Sigma} \times \mathbf{V}^T$$

where $\mathbf{\Sigma}$ *is a diagonal matrix of dimension* $N \times N$ *and* $N = \min(N, M)$*.*
The elements on the diagonal of $\mathbf{\Sigma}$ *are the singular values of* $\mathbf{X}$ *and are ordered:* $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_N \geq 0$*.*
Denoting with $\mathbf{I}_N$ *the identity matrix of dimension* N*, we also have*

$$\mathbf{V}^T \cdot \mathbf{V} = \mathbf{V} \cdot \mathbf{V}^T = \mathbf{I}_N \textit{ and } \mathbf{U}^T \cdot \mathbf{U} = \mathbf{I}_N.$$

The columns $\mathbf{v}_1, \ldots, \mathbf{v}_N$ *are thus an orthonormal basis of* $\mathbb{R}^N$*.*



Variance of the new features

Corollary

$\sigma_j^2/(M-1)$ is the variance of the j-th new feature.
Therefore, the new features are ordered from the one with the most variance to the least.
Moreover, the total variance of the dataset is $\sum_{j=1}^{N} \sigma_j^2$ (independent of the basis).

Proof. The variance of the j-th new feature is:

$$\begin{aligned}
\frac{1}{M-1} \cdot (\mathbf{X} \cdot \mathbf{v}_j)^T \cdot (\mathbf{X} \cdot \mathbf{v}_j) &= \frac{1}{M-1} \cdot \mathbf{v}_j^T \cdot \mathbf{X}^T \mathbf{X} \cdot \mathbf{v}_j \\
&= \frac{1}{M-1} \cdot \mathbf{v}_j^T \cdot \mathbf{V} \boldsymbol{\Sigma} \mathbf{U}^T \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^T \cdot \mathbf{v}_j \\
&= \frac{1}{M-1} \cdot (\mathbf{v}_j^T \cdot \mathbf{V}) \boldsymbol{\Sigma}^2 (\mathbf{V}^T \cdot \mathbf{v}_j) \\
\text{(thanks to orthonormality of the columns of } \mathbf{V}\text{)} \quad &= \frac{1}{M-1} \cdot \mathbf{e}_j^T \cdot \boldsymbol{\Sigma}^2 \cdot \mathbf{e}_j \\
&= \frac{1}{M-1} \cdot \sigma_j^2,
\end{aligned}$$

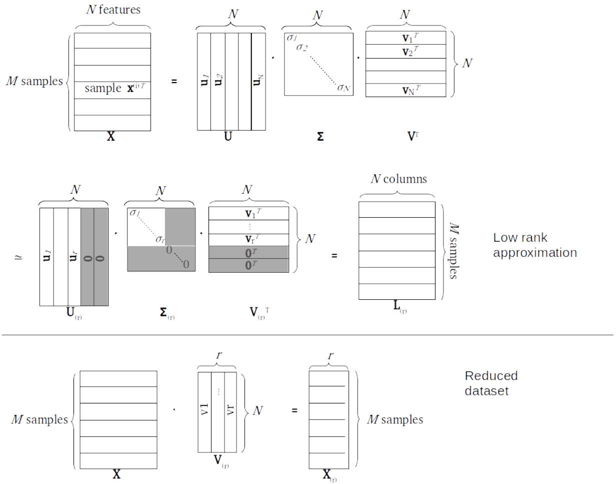
where $\mathbf{e}_j$ is a vector having a 1 in the j-th position and 0 everywhere else.

Section 3

Dimensionality reduction

Low-rank approximation

After applying SVD, we can just consider the first r new features (or components):



Each component j of the reduced dataset "captures" a fraction of variance $\frac{\sigma_j^2}{\sum_{j'=1}^{r}\sigma_{j'}^2}$.

By taking only the first r new features, we capture a fraction $\frac{\sum_{j=1}^{r}\sigma_j^2}{\sum_{j'=1}^{N}\sigma_{j'}^2}$

Why applying standard scaler?

If you do not standardize:

- The features with higher magnitude will concentrate most of the variance
- They will automatically be more present in the first new features.
  - Not beacause they are the most important, but just because of their magnitude
- All the theory only holds if features have zero-mean (see definition of variance).

Advantages of dimensionality reduction

- Scalability: work with $r < N$ features.
- Stability: we only preserve the "important" information (by keeping the components that capture most of the variance) and remove the "details".
- Apply dimensionality reduction before doing supervised learning
  - Given a dataset (already standardized) $\mathbf{X}$ with true lables $\mathbf{y}$:
  - Partition the dataset: $(\mathbf{X}^{\text{train}}, \mathbf{y}^{\text{train}})$ and $(\mathbf{X}^{\text{test}}, \mathbf{y}^{\text{test}})$
  - Apply SVD: $\mathbf{X}^{\text{train}} = \mathbf{U} \cdot \mathbf{\Sigma} \cdot \mathbf{V}^T$
  - Keep the r most important components: $\tilde{\mathbf{X}}^{\text{train}} = \mathbf{X} \cdot \mathbf{V}_{(r)}$
  - Train your model $h(\cdot)$ on $(\tilde{\mathbf{X}}^{\text{train}}, \mathbf{y}^{\text{train}})$
  - For a new test sample $\mathbf{x}$:
    - Project it on the first r components: $\tilde{\mathbf{x}}^T = \mathbf{x} \cdot \mathbf{V}_{(r)}$.
    - The prediction is $\hat{y} = h(\tilde{\mathbf{x}})$.
  - By doing so, your predictions are usually more stable (they do not overfit on details)

Let's code ...

Go to notebook 07.dimensionality-reductuion/b.svd-and-regression.ipynb

Dimensionality reduction for anomaly detection

Directly in the code

Let's code ...

Go to notebook
07.dimensionality-reductuion/a.singular-value-decomposition.ipynb

Principal Component Analysis

- Principal Component Analysis (PCA) and Singular Value Decomponsition (SVD) are similar in spirit
- However, principal components $\neq$ most important features: good explanation here.

Recap

- Change of basis
- Singular Value Decomposition
- Dimensionality Reduction
- Application to supervised learning
- Application to anomaly detection

Section 4

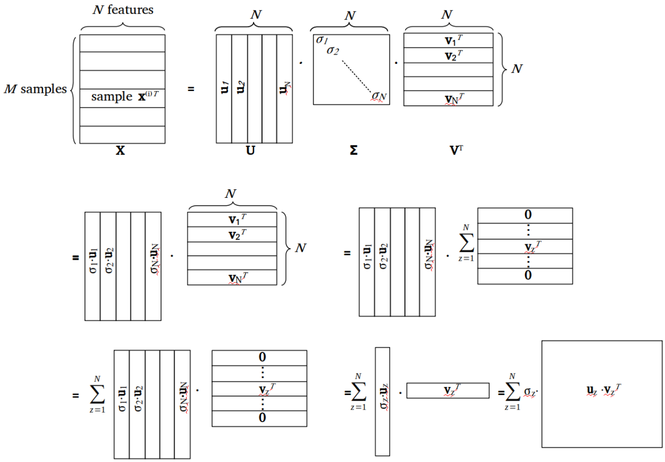
Backup slides (you can ignore)

Component matrices

Theorem ([1])

The sample matrix can be written as $\mathbf{X} = \sum_{z=0}^{N} \sigma_z \cdot \mathbf{u}_z \cdot \mathbf{v}_z^T$.
The sample matrix is thus a linear combination of component matrices $\mathbf{u}_i \cdot \mathbf{v}_i^T$ *with weights* σ_i.

Proof:



Matrix $\mathbf{u}_i \cdot \mathbf{v}_i^T$ contributes to the sample matrix for a fraction $\frac{\sigma_i}{\sum_{j=1}^{r} \sigma_j}$

The first component matrices are the most important.

References I

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In *STAT 555 - Penn State University - Lecture Notes*, chapter 16.1.

[2] Samuel Chowning.
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References II

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