Machine Learning for Networks: Dimensionality reduction

Andrea Araldo

December 10, 2025
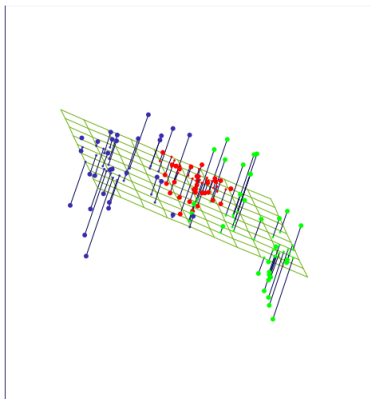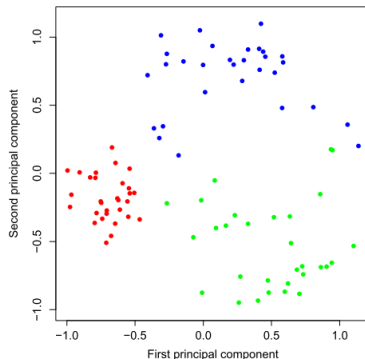
From Source:https://www.alimentipedia.it/come-si-fa-il-formaggio.html

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.
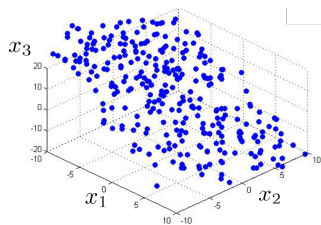- Project the samples in the new reduced space.

Advantages:

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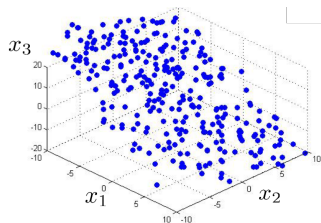- Smaller dataset
  $\Rightarrow$ Faster model runs

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

x_3

x_1 x_2

From [5]

The "best space"

x_3

x_1

x_2

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.
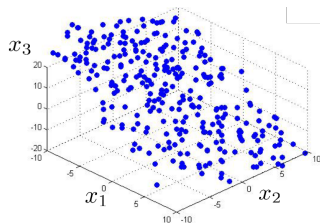
The "best space"

3 / 25

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!

- Change of basis
- Singular Value Decomposition
- Dimensionality Reduction
- Application to supervised learning
- Application to anomaly detection
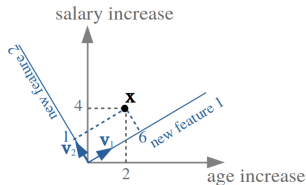
Section 1

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 $1, \ldots,$ feature $j, \ldots,$ 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

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

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

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

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:

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

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
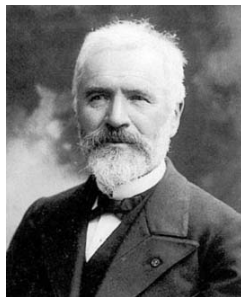
From [2]

> *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.

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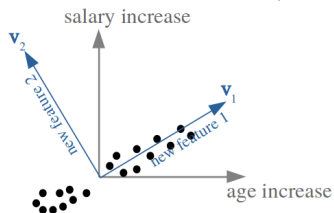you find the "best" basis $\mathbf{v}_1, \mathbf{v}_2$?

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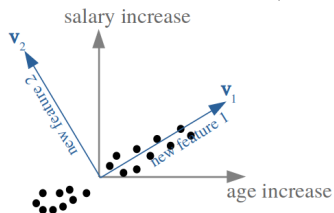
Best new feature space

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

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

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

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

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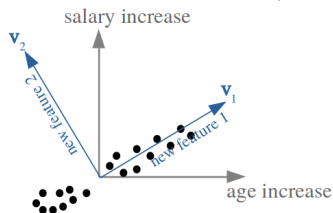
Find $\mathbf{v}_1$ such that the projection captures most of the variance:

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

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

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

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

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

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

$$\mathbf{v}^T \cdot \mathbf{v}_1 = 0$$
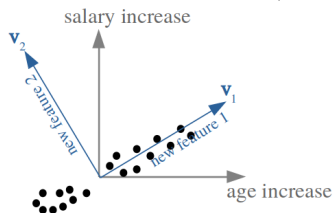
Best new feature space

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

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

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

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

Then, find $\mathbf{v}_2$:
$$\mathbf{v}_2 = \arg\max_{\mathbf{v}} \mathbf{v}^T \cdot \mathbf{X}^T \mathbf{X} \cdot \mathbf{v}$$
$$\text{s.t. } \mathbf{v}^T \cdot \mathbf{v} = 1$$
$$\mathbf{v}^T \cdot \mathbf{v}_1 = 0$$

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])

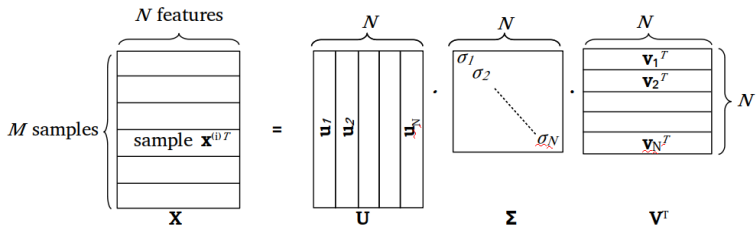*Any matrix $\mathbf{X}$ can be decomposed as follows*

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

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

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

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 $\sum_{j=1}^{N} \sigma_j^2/(M-1)$ (independent of the basis).

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

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

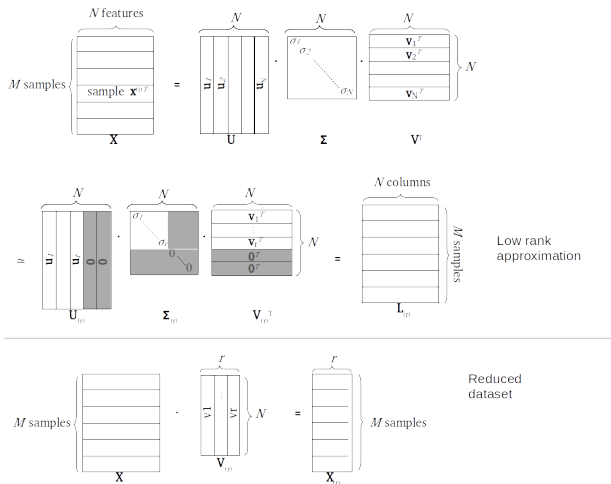where $\mathbf{e}_j$ is a vector having a 1 in the *j*-th position and 0 everywhere else.

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 $\frac{\sigma_j^2}{\Sigma_{j'=1}^r \sigma_{j'}^2}$.

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

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).

- 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)

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

Directly in the code

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

Principal Component Analysis

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

- 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.

[1] Singular Value Decomposition.
In *STAT 555 - Penn State University - Lecture Notes*, chapter 16.1.

[2] Samuel Chowning.
The singular value decomposition, 2020.

[3] Trevor Hastie, Robert Tibshirani, and Jerome Friedman.
The Elements of Statistical Learning, volume 1.
Springer, 2nd edition, 2009.
URL: http://www.springerlink.com/index/10.1007/b94608,
arXiv:1010.3003, doi:10.1007/b94608.

[4] Kevin P. Murphy.
Machine learning: A Probabilistic Perspective, chapter 12.2.3.
MIT Press, 2012.

References II

[5] Fereshteh Sadeghi.
    Dimensionality Reduction.
    Lecture notes - CSEP 546.
    URL: https://courses.cs.washington.edu/courses/csep546/16sp/slides/PCA_csep546.pdf.