

Machine Learning for Networks: Dimensionality reduction

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February 6, 2023

Retrieve most the most important information

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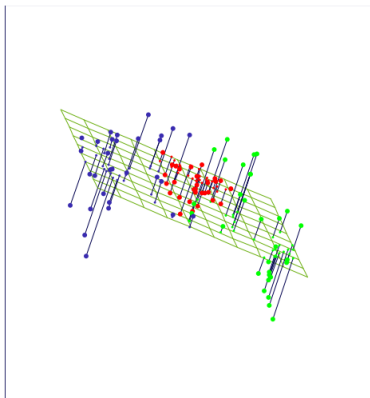


From [Source:https://www.alimentipedia.it/come-si-fa-il-formaggio.html](https://www.alimentipedia.it/come-si-fa-il-formaggio.html)

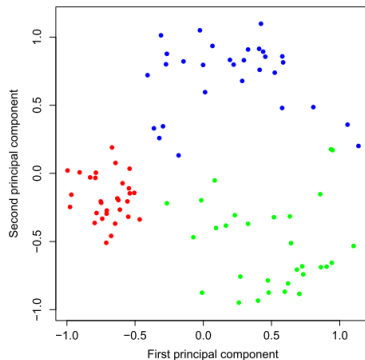
- Singular value decomposition
- Select the number of components
- Application to anomaly detection
- Application to supervised learning

Why dimensionality reduction

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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.

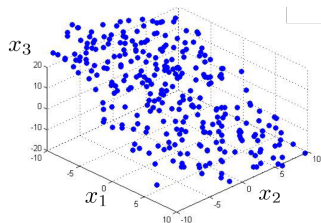
Advantages:

- Easier to visualize
- Smaller dataset
⇒ Faster model runs

The “best space”

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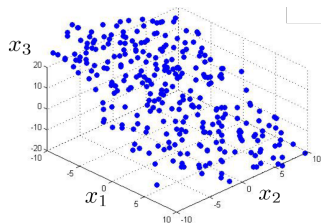
- Which 2D space would you choose?
- Any mathematical argument for your choice?



From [5]

The “best space”

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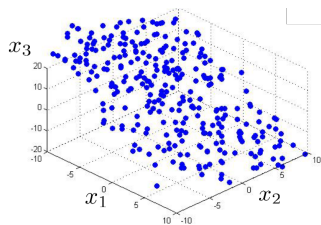


From [5]

- 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”

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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!

Section 1

Change of basis

Change of basis

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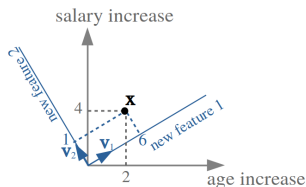
Consider data matrix \mathbf{X} , already standardized. Sample $\mathbf{x}^{(i)}$ is a vector of space \mathbb{R}^N . The dimensions of such a space are feature 1, ..., feature j , ..., feature N .

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

$$\mathbf{v}_z^T \cdot \mathbf{v}_z = 1;$$

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

They are a new basis of space \mathbb{R}^N . Each new feature is a combination of the original features.



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

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

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 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

We know that

$$(1, \dots, 1) \cdot \mathbf{X} = (0, \dots, 0).$$

Let us compute the mean of the new features:

$$(1, \dots, 1) \cdot \mathbf{X} \cdot \mathbf{v}_j = (0, \dots, 0).$$

Proposition

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

$$\begin{aligned} \sum_{j=1}^N \text{Var}_j &= \sum_{j=1}^N \mathbf{x}_j^T \cdot \mathbf{x}_j = \sum_{j=1}^N \sum_{i=1}^M x_j^{(i)} \cdot x_j^{(i)} \\ &= \sum_{i=1}^M \sum_{j=1}^N x_j^{(i)} \cdot x_j^{(i)} = \sum_{i=1}^M \mathbf{x}^{(i)T} \cdot \mathbf{x}^{(i)} \end{aligned}$$

Similarly, the total variance of the transformed dataset is:

$$\begin{aligned} \sum_{j=1}^N \text{Var}'_j &= \sum_{i=1}^M \tilde{\mathbf{x}}^{(i)T} \cdot \tilde{\mathbf{x}}^{(i)} = \sum_{i=1}^M \mathbf{x}^{(i)T} \cdot \mathbf{V} \cdot \mathbf{V}^T \mathbf{x}^{(i)} \\ &\stackrel{\text{orthonormal}}{=} \sum_{i=1}^M \mathbf{x}^{(i)T} \cdot \mathbf{x}^{(i)} \end{aligned}$$

Section 2

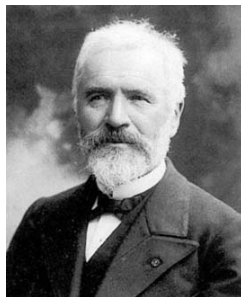
Singular Value Decomposition

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

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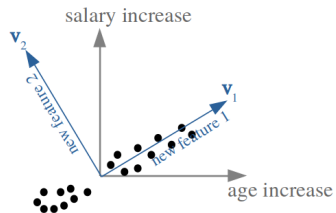
With the following dataset, can you find the “best” basis $\mathbf{v}_1, \mathbf{v}_2$?



Best new feature space

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Best new feature space

11 / 25

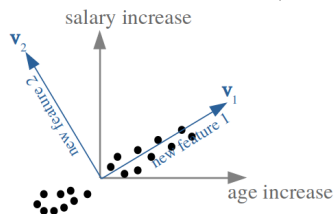
Intuitive algorithm:

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

$$\mathbf{v}_1 = \arg \max_{\mathbf{v}} \mathbf{v}^T \cdot \mathbf{X}^T \mathbf{X} \cdot \mathbf{v}$$

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

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



Best new feature space

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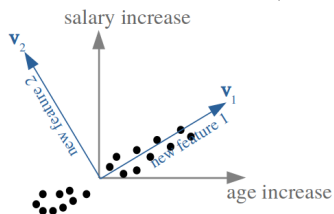
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With the following dataset, can you find the “best” basis $\mathbf{v}_1, \mathbf{v}_2$?



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

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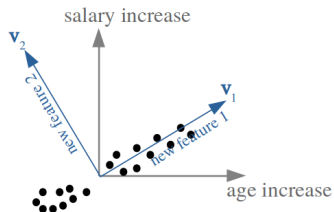
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With the following dataset, can you find the “best” basis $\mathbf{v}_1, \mathbf{v}_2$?



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 :

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

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

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

$$\mathbf{v}^T \cdot \mathbf{v}_2 = 0$$

Theorem ([4])

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

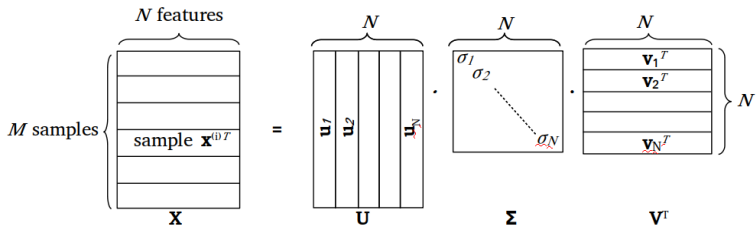
$$\mathbf{X} = \mathbf{U} \times \mathbf{\Sigma} \times \mathbf{V}^T$$

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: $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_N \geq 0$.

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



Corollary

σ_j^2 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:

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

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

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

$$\begin{array}{c}
 \begin{array}{c} N \text{ features} \\ \left\{ \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{sample } \mathbf{x}^{(i)T} \\ \text{---} \\ \text{---} \end{array} \right\} \\ \mathbf{X} \end{array} = \begin{array}{c} N \\ \left\{ \begin{array}{c} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_N \end{array} \right\} \\ \mathbf{U} \end{array} \cdot \begin{array}{c} N \\ \left\{ \begin{array}{c} \sigma_1 \\ \sigma_2 \\ \vdots \\ \sigma_N \end{array} \right\} \\ \mathbf{\Sigma} \end{array} \cdot \begin{array}{c} N \\ \left\{ \begin{array}{c} \mathbf{v}_1^T \\ \mathbf{v}_2^T \\ \vdots \\ \mathbf{v}_N^T \end{array} \right\} \\ \mathbf{V}^T \end{array} \quad \left. \vphantom{\begin{array}{c} N \\ \left\{ \begin{array}{c} \mathbf{v}_1^T \\ \mathbf{v}_2^T \\ \vdots \\ \mathbf{v}_N^T \end{array} \right\} \\ \mathbf{V}^T \end{array}} \right\} N
 \end{array}$$

$$\approx \begin{array}{c} N \\ \left\{ \begin{array}{c} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_r \\ \mathbf{0} \\ \mathbf{0} \end{array} \right\} \\ \mathbf{U}_{(r)} \end{array} \cdot \begin{array}{c} N \\ \left\{ \begin{array}{c} \sigma_1 \\ \vdots \\ \sigma_r \\ \mathbf{0} \\ \mathbf{0} \end{array} \right\} \\ \mathbf{\Sigma}_{(r)} \end{array} \cdot \begin{array}{c} N \\ \left\{ \begin{array}{c} \mathbf{v}_1^T \\ \vdots \\ \mathbf{v}_r^T \\ \mathbf{0}^T \\ \mathbf{0}^T \end{array} \right\} \\ \mathbf{V}_{(r)}^T \end{array} \quad \left. \vphantom{\begin{array}{c} N \\ \left\{ \begin{array}{c} \mathbf{v}_1^T \\ \vdots \\ \mathbf{v}_r^T \\ \mathbf{0}^T \\ \mathbf{0}^T \end{array} \right\} \\ \mathbf{V}_{(r)}^T \end{array}} \right\} N = \begin{array}{c} r \text{ features} \\ \left\{ \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \mathbf{\tilde{x}}^{(i)T} \\ \text{---} \\ \text{---} \end{array} \right\} \\ \mathbf{X}_{(r)} \end{array} \quad \left. \vphantom{\begin{array}{c} r \text{ features} \\ \left\{ \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \mathbf{\tilde{x}}^{(i)T} \\ \text{---} \\ \text{---} \end{array} \right\} \\ \mathbf{X}_{(r)} \end{array}} \right\} M \text{ samples}$$

$\mathbf{X}_{(r)}$ is a *low-rank* approximation of \mathbf{X} .

Each component j “captures” (has) a variance $\frac{\sigma_j^2}{\sum_{j'=1}^r \sigma_{j'}^2}$.

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

If you do not scale:

- The features with higher magnitude will concentrate most of the variance
- They will automatically be more present in the first principal components
 - Not because 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”.
- Supervised learning and dimensionality reduction
 - Given a dataset (already scaled) \mathbf{X} with true labels \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](#)

Unsupervised Learning: Clustering

- K-means clustering

Unsupervised Learning: Dimensionality reduction (next class)

Anomaly detection

- k-means anomaly detection
- Isolation Forests
- Neural Networks: Autoencoders

Section 4

Backup slides (you can ignore)

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:

$$\begin{aligned}
 & \begin{array}{c} N \text{ features} \\ \hline \begin{array}{c} \text{sample } \mathbf{x}^{(0)T} \\ \vdots \\ \text{sample } \mathbf{x}^{(M-1)T} \end{array} \\ \hline M \text{ samples} \end{array} = \begin{array}{c} N \\ \hline \begin{array}{c} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_N \end{array} \\ \hline \mathbf{U} \end{array} \cdot \begin{array}{c} N \\ \hline \begin{array}{c} \sigma_1 \\ \sigma_2 \\ \vdots \\ \sigma_N \end{array} \\ \hline \Sigma \end{array} \cdot \begin{array}{c} N \\ \hline \begin{array}{c} \mathbf{v}_1^T \\ \mathbf{v}_2^T \\ \vdots \\ \mathbf{v}_N^T \end{array} \\ \hline \mathbf{V}^T \end{array} \\
 \\
 & = \begin{array}{c} \begin{array}{c} \sigma_1 \cdot \mathbf{u}_1 \\ \sigma_2 \cdot \mathbf{u}_2 \\ \vdots \\ \sigma_N \cdot \mathbf{u}_N \end{array} \end{array} \cdot \begin{array}{c} N \\ \hline \begin{array}{c} \mathbf{v}_1^T \\ \mathbf{v}_2^T \\ \vdots \\ \mathbf{v}_N^T \end{array} \\ \hline \end{array} \\
 \\
 & = \begin{array}{c} \begin{array}{c} \sigma_1 \cdot \mathbf{u}_1 \\ \sigma_2 \cdot \mathbf{u}_2 \\ \vdots \\ \sigma_N \cdot \mathbf{u}_N \end{array} \end{array} \cdot \sum_{z=1}^N \begin{array}{c} \begin{array}{c} 0 \\ \vdots \\ \mathbf{v}_z^T \\ \vdots \\ 0 \end{array} \end{array} \\
 \\
 & = \sum_{z=1}^N \begin{array}{c} \begin{array}{c} \sigma_1 \cdot \mathbf{u}_1 \\ \sigma_2 \cdot \mathbf{u}_2 \\ \vdots \\ \sigma_N \cdot \mathbf{u}_N \end{array} \end{array} \cdot \begin{array}{c} \begin{array}{c} 0 \\ \vdots \\ \mathbf{v}_z^T \\ \vdots \\ 0 \end{array} \end{array} \\
 \\
 & = \sum_{z=1}^N \begin{array}{c} \begin{array}{c} \sigma_z \cdot \mathbf{u}_z \end{array} \end{array} \cdot \begin{array}{c} \begin{array}{c} \mathbf{v}_z^T \end{array} \end{array} = \sum_{z=1}^N \sigma_z \cdot \begin{array}{c} \begin{array}{c} \mathbf{u}_z \cdot \mathbf{v}_z^T \end{array} \end{array}
 \end{aligned}$$

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](https://arxiv.org/abs/1010.3003), doi:10.1007/b94608.
- [4] Kevin P. Murphy.
Machine learning: A Probabilistic Perspective, chapter 12.2.3.
MIT Press, 2012.

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