Lecture 11: Data representations - Linear methods

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Goals of data representation

Dimension reduction while retaining important aspects of the data

Goals can be

- Visualisation
- Interpretability/Variable selection
- Data compression
- Finding a representation of the data that is more suitable to the posed question

Let us start with **linear dimension reduction**.

Re-cap: SVD

The **singular value decomposition (SVD)** of a matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$, $n \geq p$, is

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$$

where $\mathbf{U} \in \mathbb{R}^{n \times p}$ and $\mathbf{V} \in \mathbb{R}^{p \times p}$ with

$$\mathbf{U}^\top\mathbf{U} = \mathbf{I}_p \quad \text{and} \quad \mathbf{V}^\top\mathbf{V} = \mathbf{V}\mathbf{V}^\top = \mathbf{I}_p$$

and $\mathbf{D} \in \mathbb{R}^{p \times p}$ is diagonal.

Usually the diagonal elements of $\mathbf{D}$ are sorted such that

$$d_{11} \geq d_{22} \geq \ldots \geq d_{pp}.$$

SVD and best rank-q-approximation (I)

Write $\mathbf{u}_j$ and $\mathbf{v}_j$ for the columns of $\mathbf{U}$ and $\mathbf{V}$, respectively. Then

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top = \sum_{j=1}^{p} d_{jj} \underbrace{\mathbf{u}_j\mathbf{v}_j^\top}_{\text{rank-1-matrix}}$$

Best rank-q-approximation: For $q < p$

$$\mathbf{X}_{q} = \sum_{j=1}^{q} d_{jj}\mathbf{u}_j\mathbf{v}_j^\top$$

approximates $\mathbf{X}$ as a **sum of layers** with **approximation error**

$$\left\|\mathbf{X} - \mathbf{X}_q\right\|_F^2 = \left\|\sum_{j=q+1}^{p} d_{jj}\mathbf{u}_j\mathbf{v}_j^\top\right\|_F^2 = \sum_{j=q+1}^{p} d_{jj}^2$$

Alternative view of best rank-q-approximation

Using only the first $q < \min(p, n)$ columns of $\mathbf{V}$ and $\mathbf{U}$, and the first q rows and columns of $\mathbf{D}$, leads to

$$\mathbf{X}_q = \mathbf{U}_q \mathbf{D}_q \mathbf{V}_q^\top.$$

According to the **Eckart-Young-Mirsky theorem**, the matrix $\mathbf{X}_q$ is a solution to the following minimization problem (see website for proof)

$$\underset{\mathrm{rank}(\mathbf{M})=q}{\arg\min} \; ||\mathbf{X} - \mathbf{M}||_F^2.$$

The solution is unique if the $q+1$-th singular value is different from the the q-th singular value.

Alternative view of the Eckart-Young-Mirsky problem

For $q < \min(p, n)$, set $\mathbf{L} := \mathbf{U}_q\mathbf{D}_q \in \mathbb{R}^{n\times q}$ and $\mathbf{F} = \mathbf{V}_q^\top \in \mathbb{R}^{q\times p}$.

Then $\mathbf{X}_q = \mathbf{LF}$ is a solution of

$$\underset{\mathbf{L}\in\mathbb{R}^{n\times q},\mathbf{F}\in\mathbb{R}^{q\times p}}{\arg\min} ||\mathbf{X} - \mathbf{LF}||_F^2$$

Notes:

- Whereas $\mathbf{X}_q$ can be the unique minimizer for the original minimisation problem, the matrices $\mathbf{F}$ and $\mathbf{L}$ are not unique.
- **This is just PCA:** When using SVD to compute the PCA of $\mathbf{X}$, then the columns of $\mathbf{V}$ contain the PC directions and the rows of $\mathbf{F}$ the first q of them. Projecting the data onto the PCs but then reconstructing it means to compute $(\mathbf{X}\mathbf{V}_q)\mathbf{V}_q^\top = (\mathbf{U}\mathbf{D}\mathbf{V}^\top\mathbf{V}_q)\mathbf{V}_q^\top = (\mathbf{U}\mathbf{D}\mathbf{I}_{p\times q})\mathbf{V}_q^\top = (\mathbf{U}_q\mathbf{D}_q)\mathbf{V}_q^\top = \mathbf{LF}$.

Low-rank matrix factorisation

Let $q < \min(p, n)$

$$\underset{\mathbf{L} \in \mathbb{R}^{n \times q}, \mathbf{F} \in \mathbb{R}^{q \times p}}{\arg\min} ||\mathbf{X} - \mathbf{LF}||_F^2$$

Interpretation

- The rows of $\mathbf{F}$ can be seen as **basis vectors** or **coordinates** of a subspace in feature space
- The rows of $\mathbf{L}$ provide **coefficients** that combine the basis vectors in $\mathbf{F}$ to the closest q-dimensional approximation of the respective observation
- In the framework of **factor analysis** the rows of $\mathbf{F}$ are called **factors** and the rows of $\mathbf{L}$ are called **(latent) loadings**

Notes on factor analysis

- Originated in psychometrics with the idea that factors could describe unobservable (latent) properties (e.g. intelligence)
- A typical assumption is that the rows of $\mathbf{F}$ are orthogonal, i.e. $\mathbf{F}\mathbf{F}^\top = \mathbf{I}_q$
- But even row orthogonality of $\mathbf{F}$ does not ensure **identifiability** (uniqueness of the solution) since for a orthogonal matrix $\mathbf{R} \in \mathbb{R}^{q \times q}$

  $$\mathbf{L}'\mathbf{F}' := (\mathbf{L}\mathbf{R})(\mathbf{R}^\top\mathbf{F}) = \mathbf{L}\mathbf{F}$$

  and $\mathbf{F}'$ is orthogonal if $\mathbf{F}$ is
- Every orthogonal matrix describes a rotation and when applied to factors and loadings it is called a **factor rotation**
- Through optimization of $\mathbf{R}$, we can make either factors (**varimax rotation**) or loadings (**quartimax rotation**) sparse

Conclusions from Factor Analysis/SVD-based approach

- The SVD-based approach is provably best in the Frobenius norm
- Best q can be easily chosen by observing the approximation error

However:

- Interpretation is difficult since layers both add and subtract information

$$(d_{ii}\mathbf{u}_i\mathbf{v}_i^\top)^{(r,s)} = d_{ii}\mathbf{u}_i^{(r)}\mathbf{v}_i^{(s)}$$

- $\mathbf{U}$ and $\mathbf{V}$, respectively $\mathbf{L}$ and $\mathbf{F}$, are not unique and usually dense (no zero entries)

Non-negative Matrix Factorization (NMF)

Idea: We can add constraints to the low-rank matrix factorisation problem.

Non-negative matrix factorisation (NMF): Let $q < \min(p, n)$

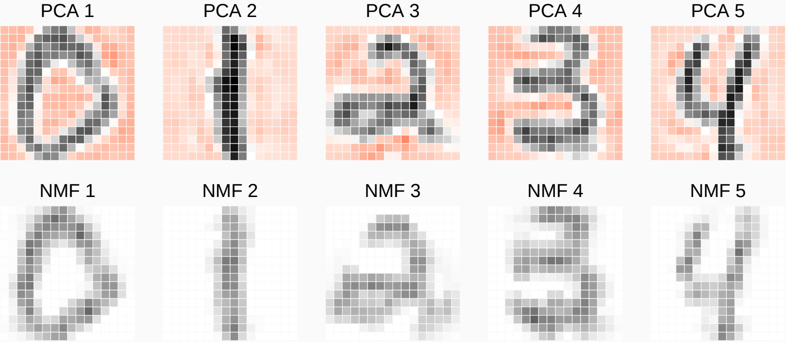
$$\underset{\mathbf{L}\in\mathbb{R}^{n\times q},\mathbf{F}\in\mathbb{R}^{q\times p}}{\arg\min} ||\mathbf{X} - \mathbf{L}\mathbf{F}||_F^2 \quad \text{such that} \quad \mathbf{L} \geq 0,\ \mathbf{F} \geq 0$$

- **Sum of positive layers:** $\mathbf{X} \approx \sum_{j=1}^{q} \mathbf{L}^{(:,j)}\mathbf{F}^{(j,:)}$
- No fast specialised algorithm or analytic solution exists (NP-hard problem)
- Requires that the data $\mathbf{X}$ has to be non-negative
- $\mathbf{L}$ and $\mathbf{F}$ are again not uniquely identifiable.
- Choice of q not as straight-forward as for SVD

SVD vs NMF – Example: Reconstruction

MNIST-derived zip code digits ($n = 1000$, $p = 256$)

100 samples are drawn randomly from each class to keep the problem balanced.



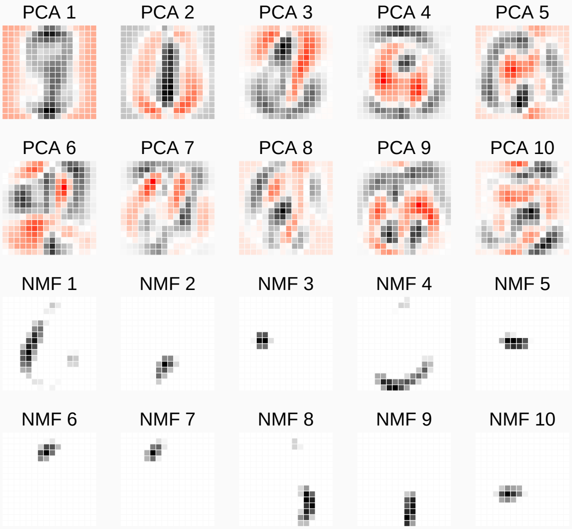
Red-ish colours are for negative values, white is around zero and dark stands for positive values. Reconstructions are done using 50 first PCs / $q = 50$.

SVD vs NMF – Example: Basis Components

Large difference between principal components (columns of $\mathbf{V}$) and NMF basis components (rows of $\mathbf{F}$)

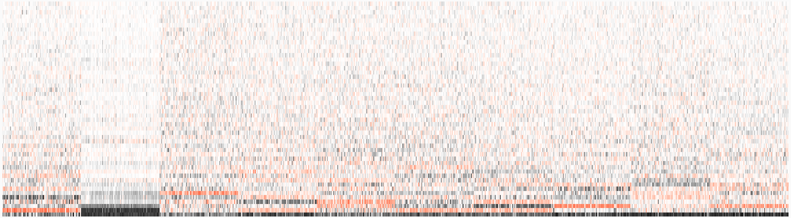
The non-negativity constraint leads to **sparsity** in the **basis** (in $\mathbf{F}$) and **coefficients** (in $\mathbf{L}$, next slide).

Therefore, NMF captures **sparse characteristic parts** while PCA components capture more global features.

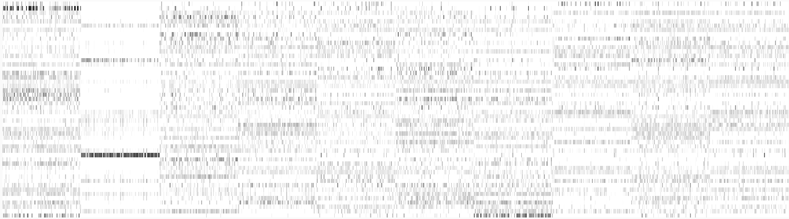


SVD vs NMF – Example: Coefficients ()

SVD coefficients



NMF coefficients



Note the additional **sparsity** in the NMF coefficients.

How to solve the NMF problem?

The NMF problem is

$$\underset{\mathbf{L}\in\mathbb{R}^{n\times q},\mathbf{F}\in\mathbb{R}^{q\times p}}{\arg\min} ||\mathbf{X}-\mathbf{L}\mathbf{F}||_F^2 \quad \text{such that} \quad \mathbf{L}\geq 0, \mathbf{F}\geq 0$$

Most algorithms use **two-block coordinate descent** and solve

$$\mathbf{L}^{[t]} = \underset{\mathbf{L}\geq 0}{\arg\min} ||\mathbf{X}-\mathbf{L}\mathbf{F}^{[t-1]}||_F^2 \quad \text{and} \quad \mathbf{F}^{[t]} = \underset{\mathbf{F}\geq 0}{\arg\min} ||\mathbf{X}-\mathbf{L}^{[t]}\mathbf{F}||_F^2$$

iteratively.

Note that the problem is **symmetric** in $\mathbf{L}$ and $\mathbf{F}$ since

$$||\mathbf{X}-\mathbf{L}\mathbf{F}||_F^2 = ||\mathbf{X}^\top-\mathbf{F}^\top\mathbf{L}^\top||_F^2.$$

No separate algorithms needed for $\mathbf{L}$ and $\mathbf{F}$.

Short note on cost functions

Our derviation was based on Frobenius norm and inspired by the SVD-based approach of the best rank-q approximation. However, other cost functions are possible.

- **Note:** Cost functions determine the distribution of noise
- Frobenius norm implies Gaussian distribution
- An alternative for Poisson distributed data (count data)

$$D(\mathbf{X}||\mathbf{LF}) = \sum_{i=1}^{p} \sum_{j=1}^{n} \left(\mathbf{X}^{(i,j)} \log \frac{\mathbf{X}^{(i,j)}}{(\mathbf{LF})^{(i,j)}} - \mathbf{X}^{(i,j)} + (\mathbf{LF})^{(i,j)} \right)$$

Resembles the **Kullback-Leibler divergence** and the **log-likelihood of Poisson-distributed data** with mean $(\mathbf{LF})^{(i,j)}$ for $\mathbf{X}^{(i,j)}$.

Alternating least squares updates for NMF

A simple update rule is **alternating least squares (ALS)**: Solve the unconstrained least squares problem

$$\mathbf{Z}^{[t]} = \underset{\mathbf{Z} \in \mathbb{R}^{q \times p}}{\arg\min} ||\mathbf{X} - \mathbf{L}^{[t-1]}\mathbf{Z}||_F^2$$

and set elementwise $\mathbf{F}^{[t]} = \max(\mathbf{Z}^{[t]}, 0)$. Analogous for $\mathbf{L}^{[t]}$.

- The method is cheap but can have convergence issues.
- Can be useful for initialisation (some steps of ALS first, then another algorithm)

Alternating non-negative least squares updates for NMF

It holds that

$$\begin{aligned} \|\mathbf{X} - \mathbf{L}\mathbf{F}\|_F^2 &= \sum_{i=1}^{p} \|\mathbf{X}^{(:,i)} - \mathbf{L}\mathbf{F}^{(:,i)}\|_2^2 \\ &= \sum_{i=1}^{p} \mathbf{F}^{(:,i)^\top}(\underbrace{\mathbf{L}^\top\mathbf{L}}_{=\mathbf{Q}})\mathbf{F}^{(:,i)} + (\underbrace{-\mathbf{L}^\top\mathbf{X}^{(:,i)}}_{=\mathbf{c}})^\top\mathbf{F}^{(:,i)} + \|\mathbf{X}^{(:,i)}\|_2^2 \end{aligned}$$

Minimizing over $\mathbf{F}^{(:,i)} \geq 0$, this is a sum of p independent **non-negative least squares (NNLS)** problems. The resulting update rule is called **alternating NNLS**.

NNLS problems are equivalent to quadratic programming problems of the form

$$\arg\min_{\mathbf{x}\geq 0} \frac{1}{2}\mathbf{x}^\top\mathbf{Q}\mathbf{x} + \mathbf{c}^\top\mathbf{x}$$

for positive semi-definite $\mathbf{Q}$.

Multiplicative updates for NMF

Multiplicative updates (MU) have been popularized by Lee and Seung (1999). Their form depends on the cost function. In the following $\mathbf{A} \circ \mathbf{B}$ denotes elementwise multiplication of matrices and division is also meant elementwise.

1. Frobenius norm:

$$\mathbf{L} \leftarrow \mathbf{L} \circ \frac{\mathbf{X}\mathbf{F}^\top}{\mathbf{L}\mathbf{F}\mathbf{F}^\top} \quad \text{and} \quad \mathbf{F} \leftarrow \mathbf{F} \circ \frac{\mathbf{L}^\top\mathbf{X}}{\mathbf{L}^\top\mathbf{L}\mathbf{F}}$$

2. KL divergence:

$$\mathbf{L}^{(l,k)} \leftarrow \mathbf{L}^{(l,k)} \frac{\sum_{i=1}^{p} \mathbf{F}^{(k,i)}\mathbf{X}^{(l,i)}/(\mathbf{L}\mathbf{F})^{(l,i)}}{\sum_{i=1}^{p} \mathbf{F}^{(k,i)}} \quad \text{and}$$

$$\mathbf{F}^{(k,i)} \leftarrow \mathbf{F}^{(k,i)} \frac{\sum_{l=1}^{n} \mathbf{L}^{(l,k)}\mathbf{X}^{(l,i)}/(\mathbf{L}\mathbf{F})^{(l,i)}}{\sum_{l=1}^{n} \mathbf{L}^{(l,k)}}$$

Multiplicative updates for NMF and gradient descent

Multiplicative updates are a special case of **gradient descent**. Let $J(\mathbf{L},\mathbf{F}) = \frac{1}{2}||\mathbf{X}-\mathbf{LF}||_F^2$ then

$$\nabla_{\mathbf{L}} J = \mathbf{LFF}^\top - \mathbf{XF}^\top$$

$$\nabla_{\mathbf{F}} J = \mathbf{L}^\top\mathbf{LF} - \mathbf{L}^\top\mathbf{X}$$

Gradient descent in $\mathbf{L}$ for step-length α performs

$$\mathbf{L} \leftarrow \mathbf{L} - \alpha \nabla_{\mathbf{L}} J$$

It can be shown that

$$\boldsymbol{\alpha} = \frac{\mathbf{L}}{\mathbf{LFF}^\top} \in \mathbb{R}^{n\times q},$$

where division is element-wise, is an **admissible step length**. Element-wise multiplication of $\boldsymbol{\alpha}$ and $\nabla_{\mathbf{L}} J$ yields the MU for $\mathbf{L}$. Analogously for $\mathbf{F}$.

Note: Analogous results hold for the KL divergence.

Advantages of NMF

- **Interpretability:** As in the case of truncated SVD we are adding layers, but now all layers are positive and each layer adds information
- **Clustering interpretation:**
  - The rows of $\mathbf{F}$ can be interpreted as cluster centroids
  - Cluster membership of each observation is determined by the rows of $\mathbf{L}$
  - Observation j is assigned to the cluster k if $\mathbf{L}^{(j,k)} > \mathbf{L}^{(j,i)}$ for all $i \neq k$

Initialising NMF

NMF can be initialised in multiple ways

- **Random initialisation:** Uniformly distributed entries in $[0, 1]$ for $\mathbf{L}$ and $\mathbf{F}$
- **Clustering techniques:** Run k-means with q clusters on data, store cluster centroids in rows of $\mathbf{F}$ and $\mathbf{L}^{(l,k)} \neq 0 \Leftrightarrow \mathbf{X}^{(l,:)}$ belongs to cluster k
- **SVD**: Determine best rank-q-approximation $\sum_{i=1}^{q} d_{ii}\mathbf{v}_i\mathbf{u}_i^\top$, note that

$$\begin{aligned} d_{ii}\mathbf{u}_i\mathbf{v}_i^\top &= ([+d_{ii}\mathbf{u}_i]_+[+\mathbf{v}_i^\top]_+ + [-d_{ii}\mathbf{u}_i]_+[-\mathbf{v}_i^\top]_+) \\ &\quad - ([+d_{ii}\mathbf{u}_i]_+[-\mathbf{v}_i^\top]_+ + [-d_{ii}\mathbf{u}_i]_+[+\mathbf{v}_i^\top]_+) \end{aligned}$$

  and initialize NMF by summing only the positive parts or the larger of the positive parts.

Take-home message

- Linear dimension reduction approximates matrices through additive layers (hence linear).
- The SVD-based approach leads to factor analysis, built on the intuition that there are underlying factors describing the data and the intensity of their presence in a sample is quantified in the loadings
- By adding non-negativity constraints to the matrix factorisation problem, NMF creates more interpretable results and can be used for clustering at the same time