Nonnegative Matrix Factorization

Theory and Application

Presentation for Matrix Decompositions
PhD in Statistical Sciences
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University of Bologna

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Table of contents

1. Nonnegative Matrix Factorization
   - Introduction
   - The method
   - Matrix factorization
   - An ill-posed problems
   - Extensions
2. Application to Text Mining
   - Introduction
   - Analysis
3. Conclusion

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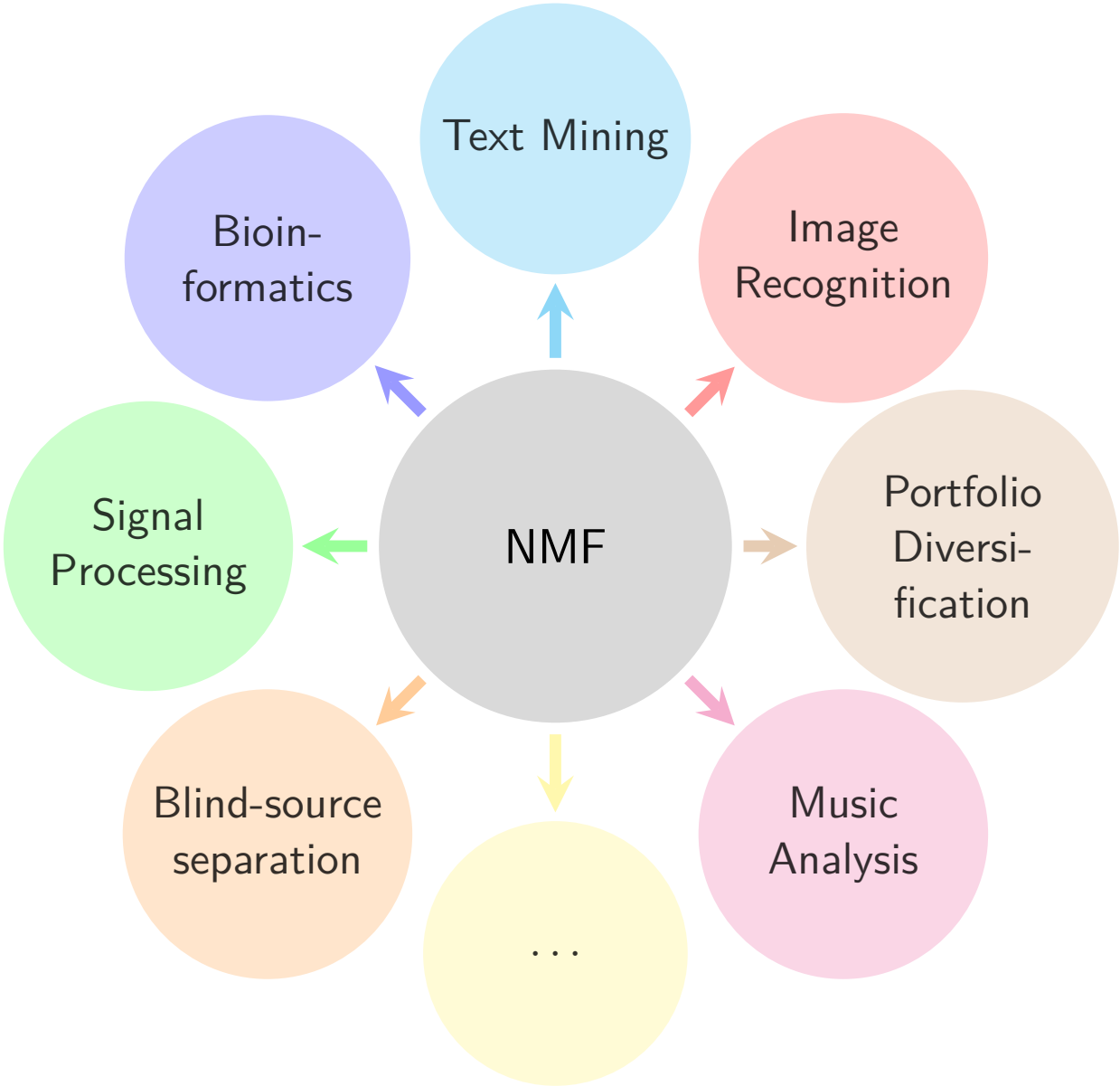
  ➜ Powerful methods for data representation and dimension reduction
- *Nonnegative data* (e.g. pixel intensities, users scores) cannot be analyzed by means of well-known techniques since they cannot guarantee to preserve nonnegativity
- **Nonnegative Matrix Factorization** (NMF; Paatero and Tapper 1994; Lee and Seung 1999) is one of the most popular low-rank approximations obtained via subspace approximation, used for compression, visualization, feature selection and noise filtering.

Fields of application



The method

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Target matrix $\boldsymbol{V}$ $(n \times m)$

	entity 1	.....	entity μ	...	entity m
variable 1	v_{11}	. . . . .	$v_{1\mu}$	. . . . .	v_{1m}
variable i	v_{i1}	. . . . .	$v_{i\mu}$	. . . . .	v_{im}
variable n	v_{n1}	. . . . .	$v_{n\mu}$	. . . . .	v_{nm}

$\boldsymbol{V}$

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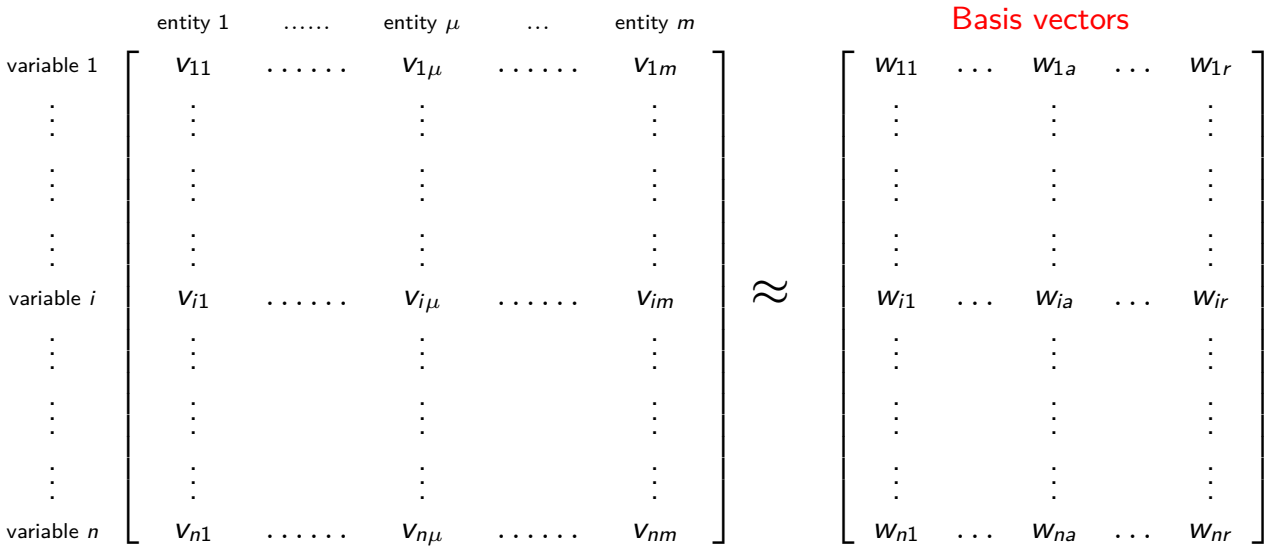

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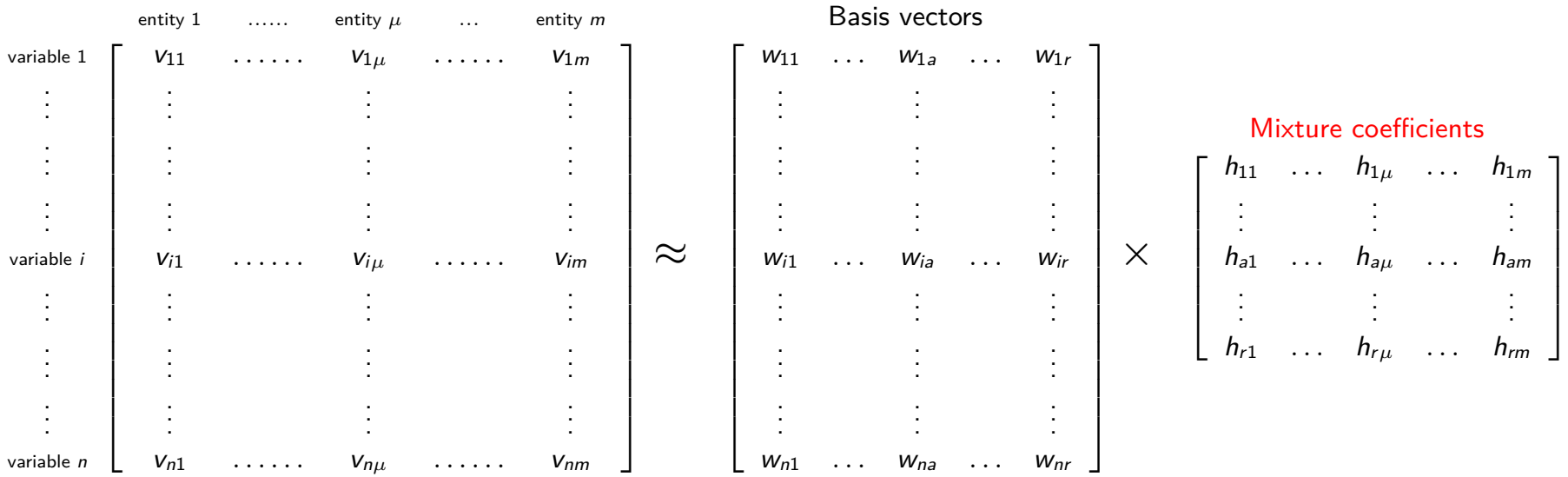

$$\boldsymbol{V} \approx \boldsymbol{W}\boldsymbol{H} \qquad \text{with } (\boldsymbol{W}, \boldsymbol{H}) \geq 0$$

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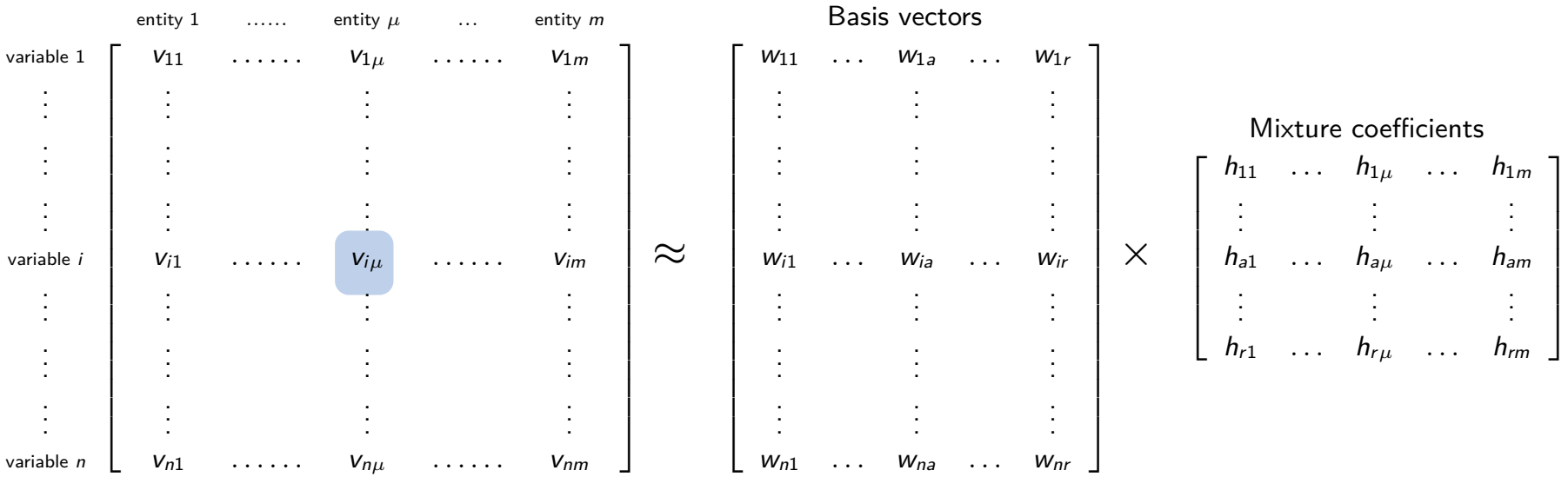

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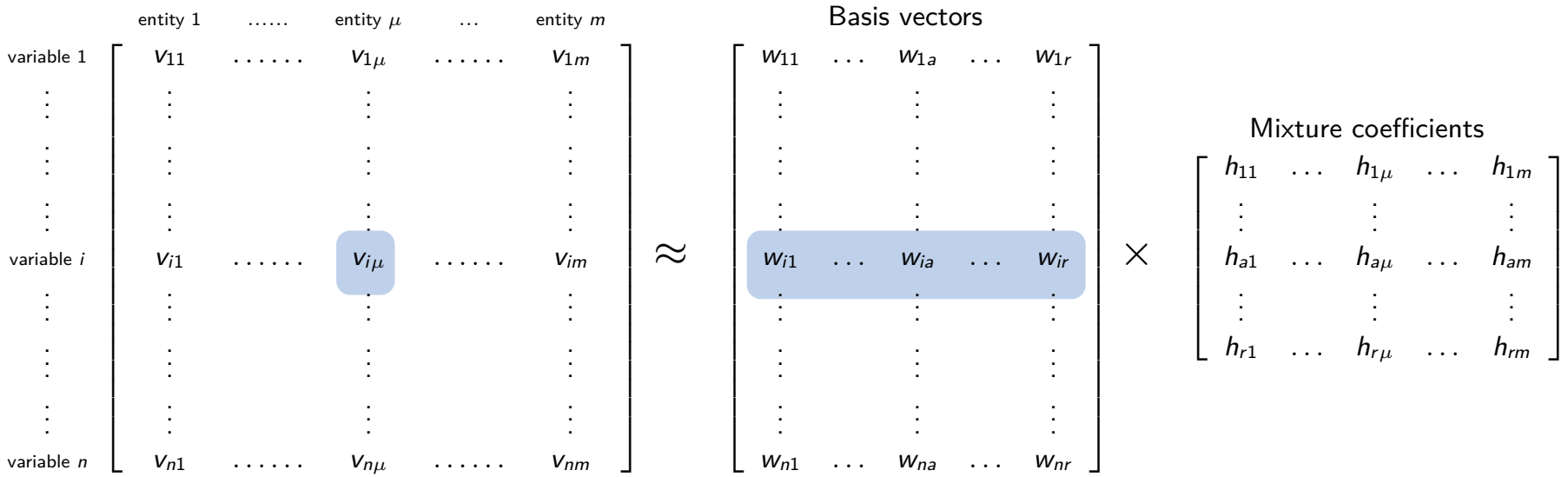

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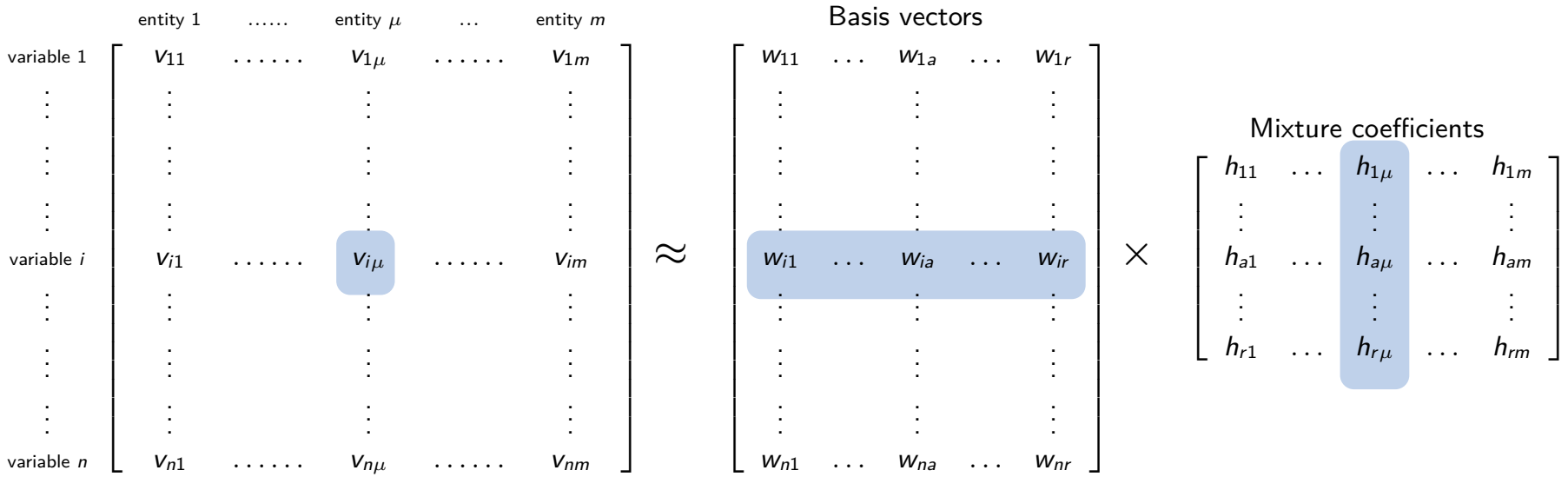

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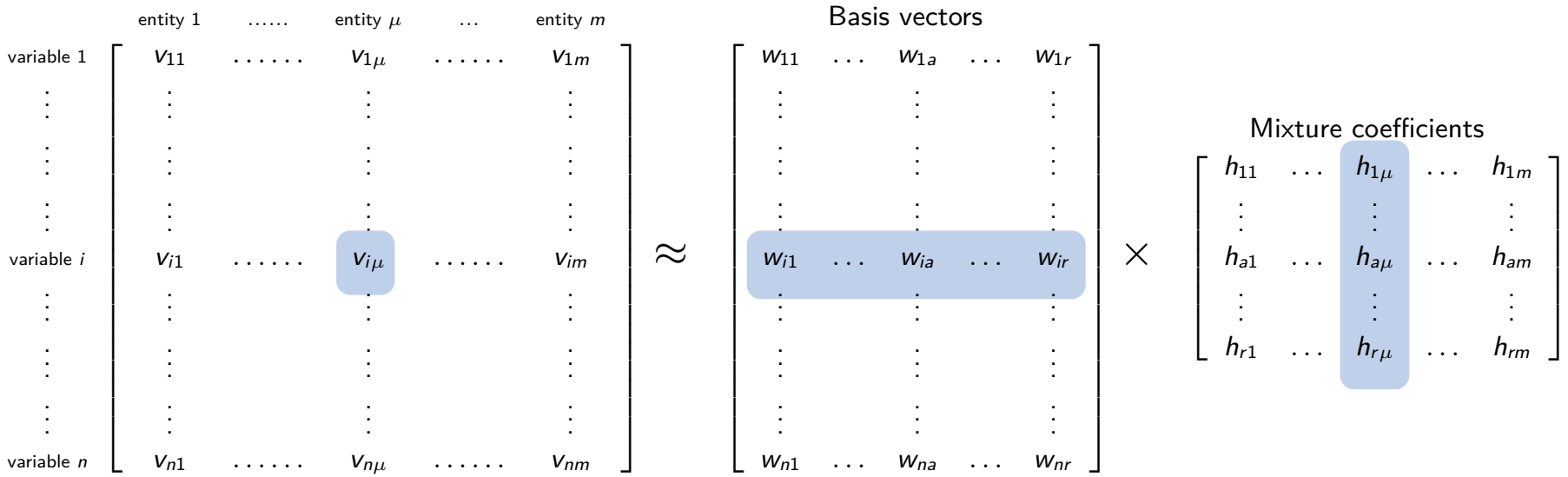

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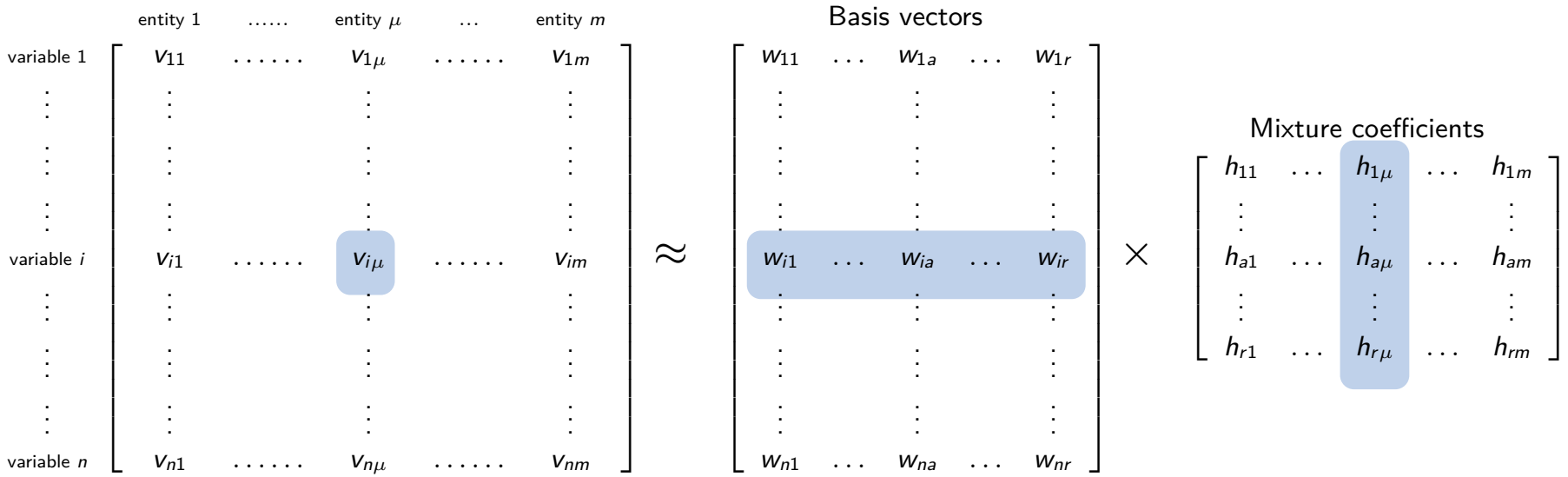

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A crucial role is played by the factorization rank $r << min(n, m)$ such that $(n+m)r < nm$.

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Nonlinear optimization problem: minimize the objective function with respect to matrix factors, subject to nonnegativity constraint:

$$\min_{\boldsymbol{W},\boldsymbol{H}\geq 0}\Big[\underbrace{L(\boldsymbol{V}, \boldsymbol{WH})}_{\textit{Loss function}} + \underbrace{R(\boldsymbol{V}, \boldsymbol{WH})}_{\textit{Regularization term}}\Big]$$

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Objective function guaranteed to monotonically decrease, but not necessarily converges to a local minimum.

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Basic ALS

1. Take $\boldsymbol{W}$ as fixed
2. Solve for $\boldsymbol{H}$ in the equation $\boldsymbol{W}^T\boldsymbol{W}\boldsymbol{H} = \boldsymbol{W}^T\boldsymbol{V}$
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Computationally demanding due to additional nonnegativity constraint on least squares.

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Several seeding methods have been proposed, based on:

- **Independent component analysis**
- **Nonnegative double singular value decomposition**
- **Clustering techniques**

In practice, one may use several different initializations via a Monte Carlo approach, and keep the best solution obtained.

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Figure 1: *Madonna del Cardellino* in grey-scale format; Target matrix rank = 400

Factorization rank

Approximated paintings with different factorization ranks: **5**, 20, 40, 80.

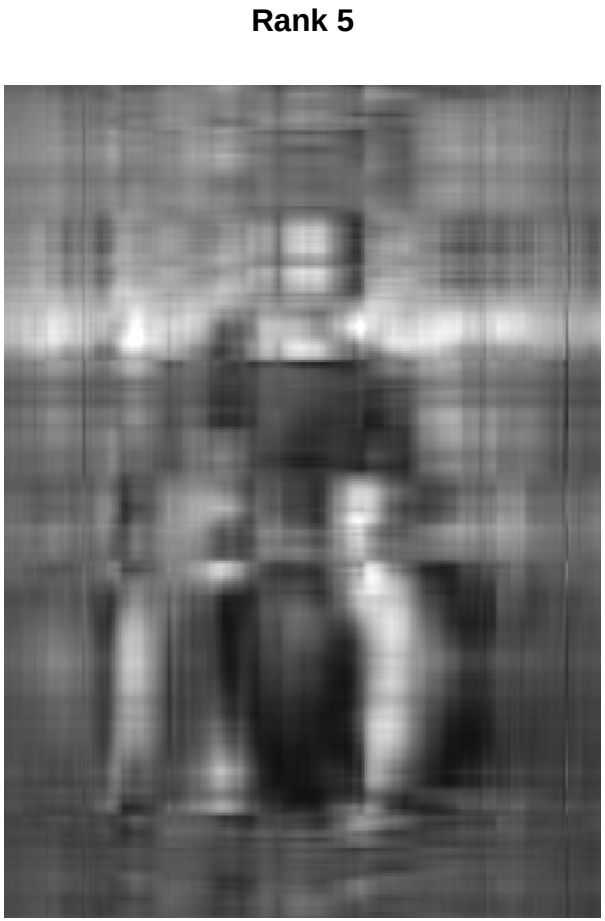

Figure 2: *Factorization rank=5*

Factorization rank

Approximated paintings with different factorization ranks: 5, **20**, 40, 80.

Figure 3: *Factorization rank=20*

Factorization rank

Approximated paintings with different factorization ranks: 5, 20, **40**, 80.

Figure 4: *Factorization rank=40*

Factorization rank

Approximated paintings with different factorization ranks: 5, 20, 40, **80**.

Figure 5: *Factorization rank=80*

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- Take the first value of r for which the **cophenetic coefficient** starts decreasing;
- Choose the first value where the **RSS curve** presents an inflection point;
- Consider smallest value at which the decrease in the **RSS** is lower than the decrease of analogous curve from **random data**.

A unique decomposition?

- *Find a simplicial convex cone* $C_{\boldsymbol{W}} = \left\{ \sum_{a=1}^{r} \lambda_a \boldsymbol{w}_a, \lambda_a \geq 0 \right\}$ *contained in the positive orthant and containing data points.*

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If data values are strictly positive:

$$v_{i\mu} \geq \epsilon \quad \forall \epsilon > 0$$

the column vectors of $\boldsymbol{V}$ are well inside the interior of positive orthant of $\mathbb{R}^n$, and there are many simplicial cones containing the data (Donoho and Stodden 2004).

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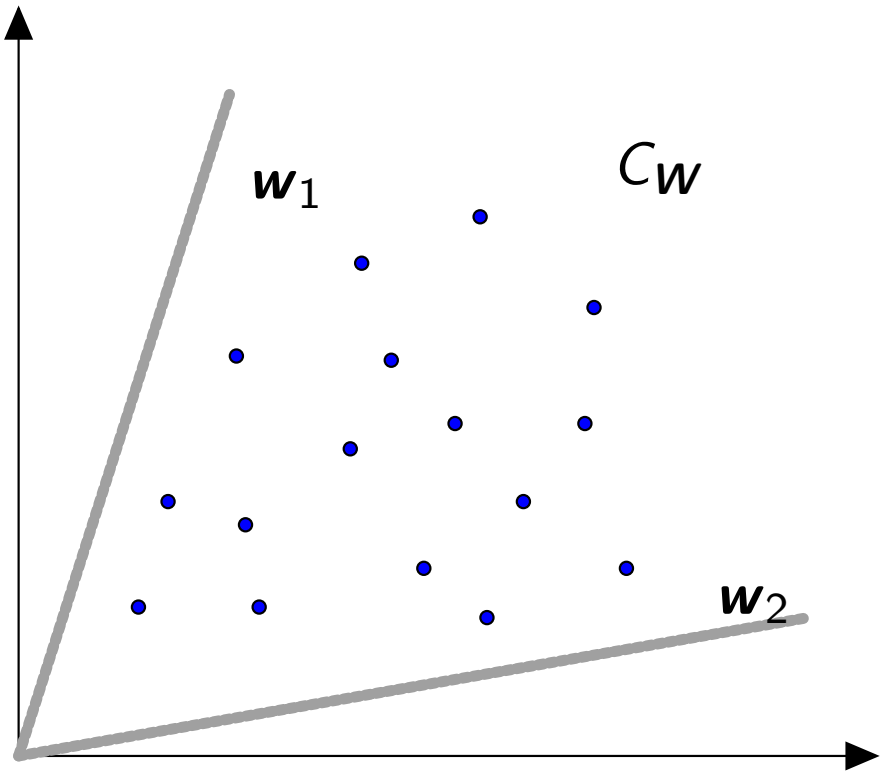

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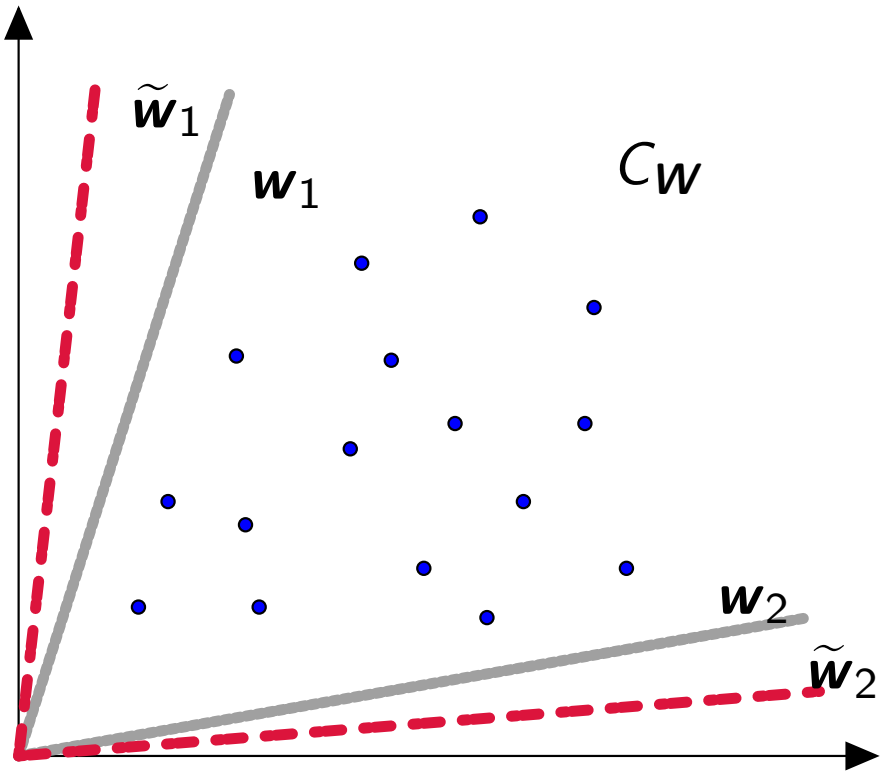

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➜ Impose additional constraints to confine the feasible solution set.

Extensions

Over the years, the standard NMF model has been extended to explicitly include auxiliary constraints (incorporated in the objective function) on $\boldsymbol{W}$ and/or $\boldsymbol{H}$ to improve the factorization.

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Some other extensions of standard NMF include:

1. *Non-smooth NMF (nsNMF);*
2. *NMF with offset;*
3. *Pattern-expression NMF*

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Term-document matrix

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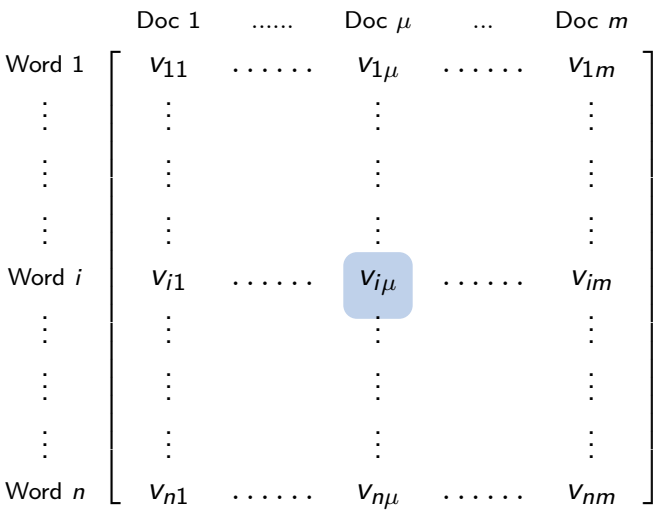

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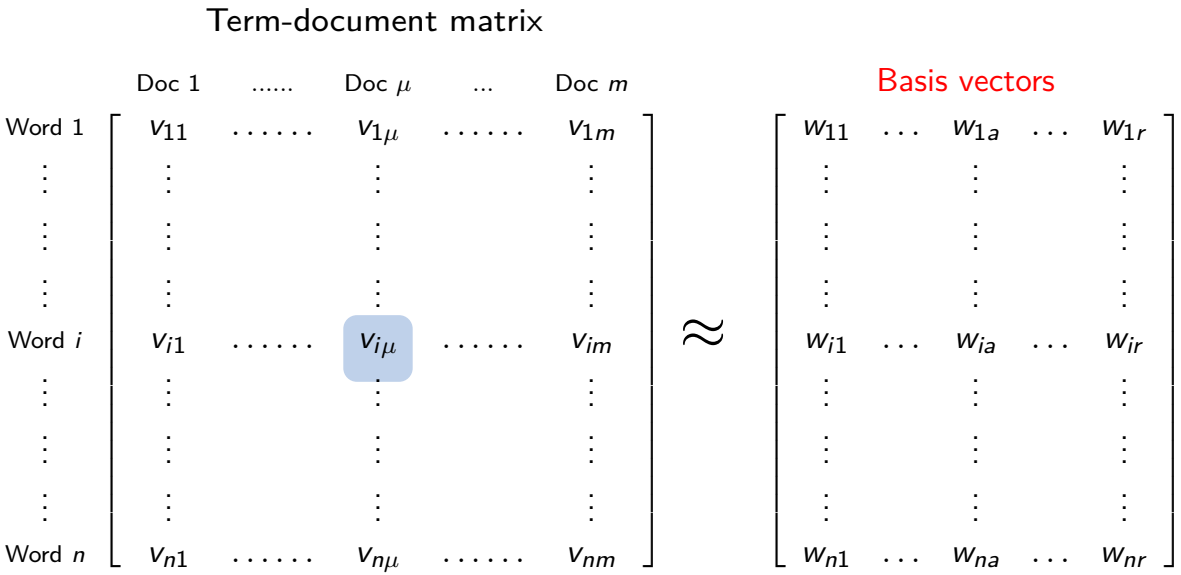

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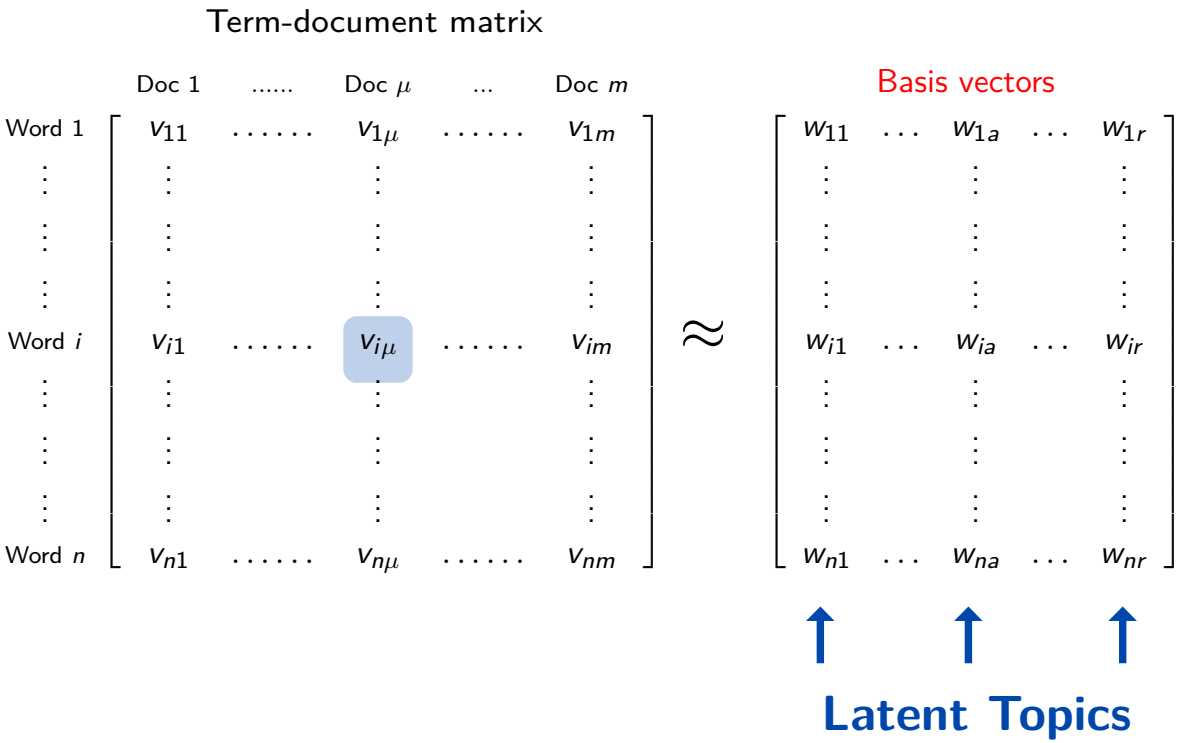

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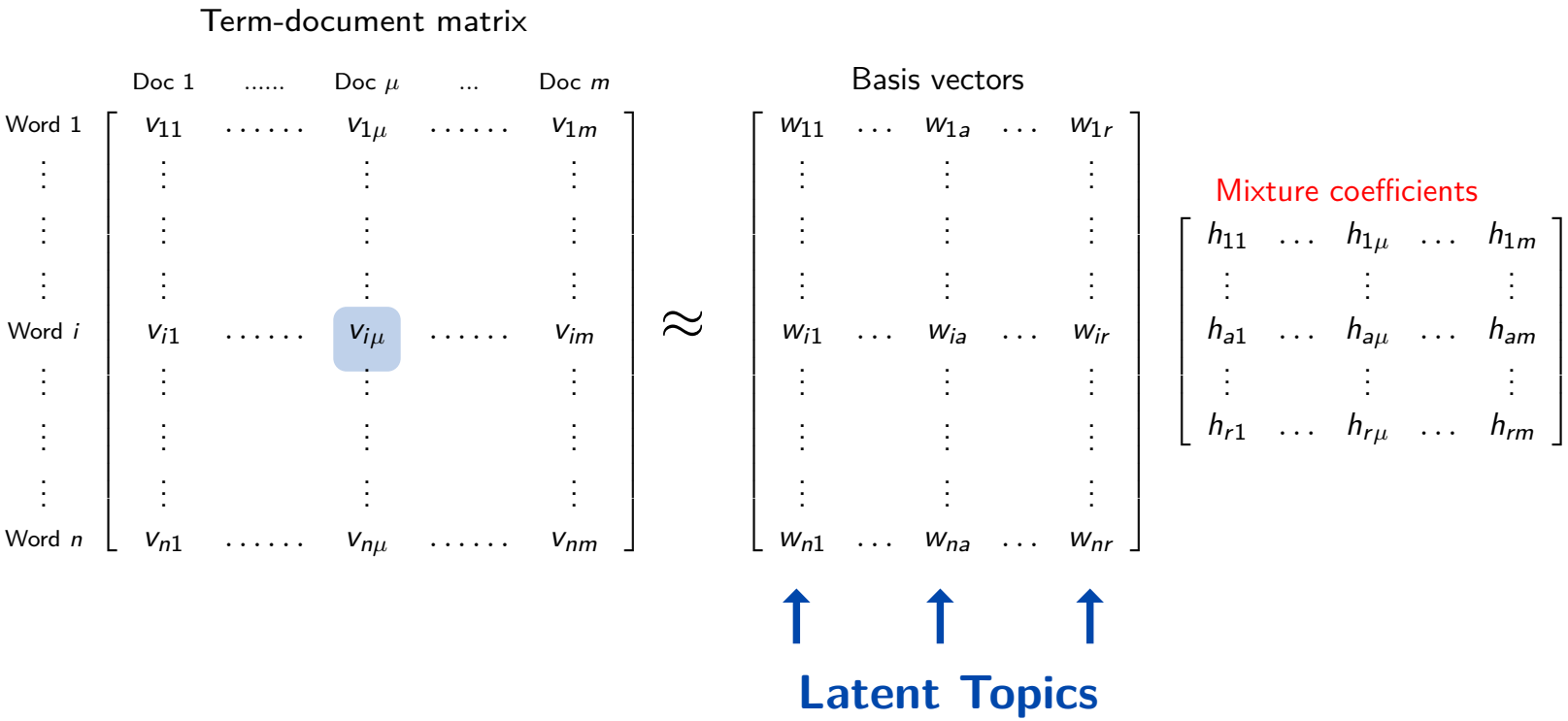

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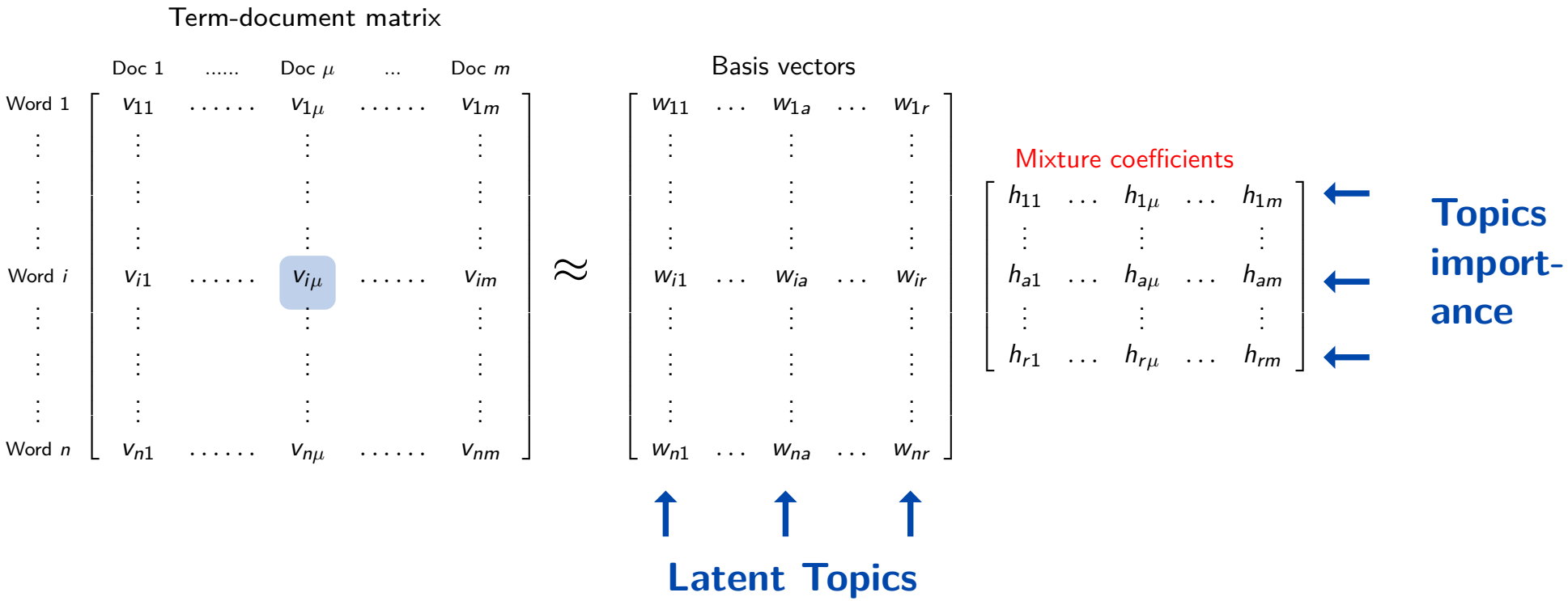

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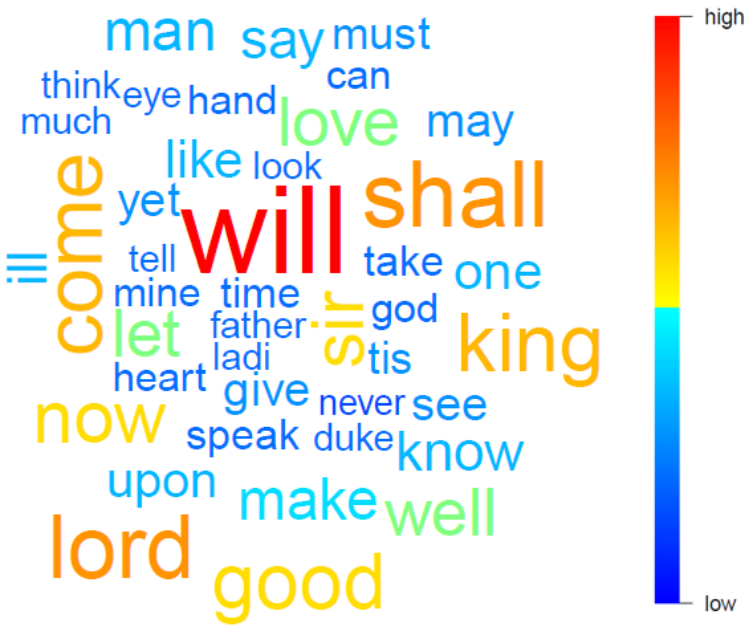

Figure 7: Word cloud (words occurring more than 1000 times)

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6. Factor matrices explored by means of heatmaps.

Topic recovery

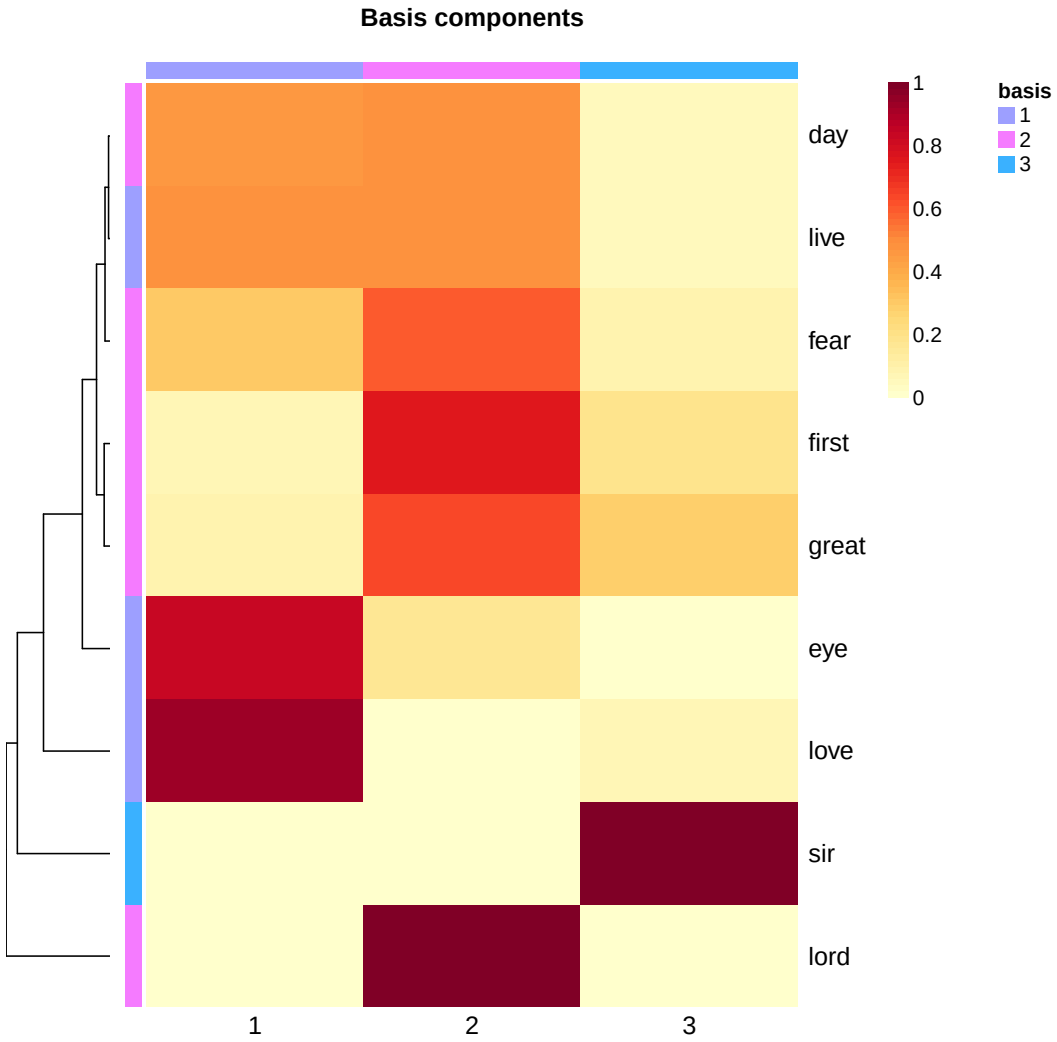

Figure 7: Heatmap of basis matrix (only relevant rows selected)

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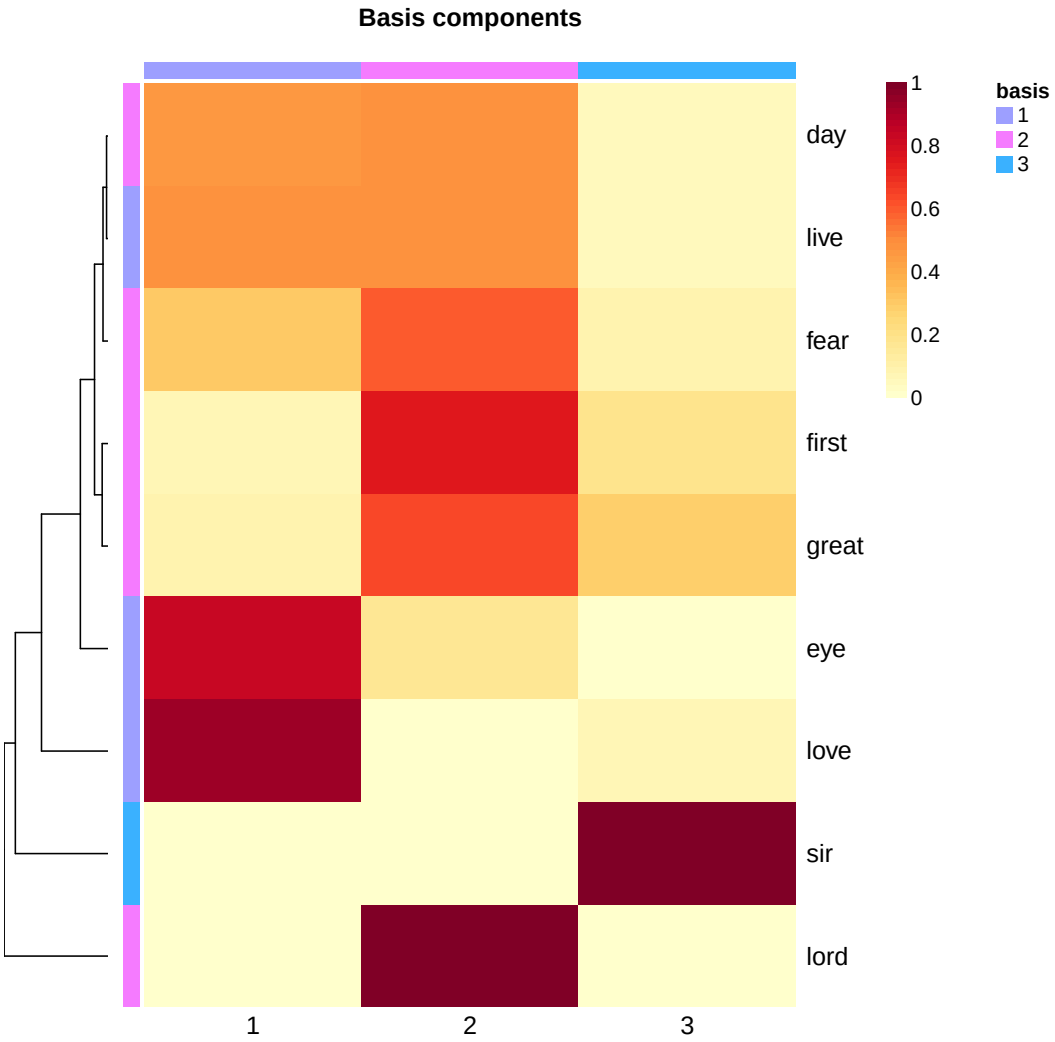

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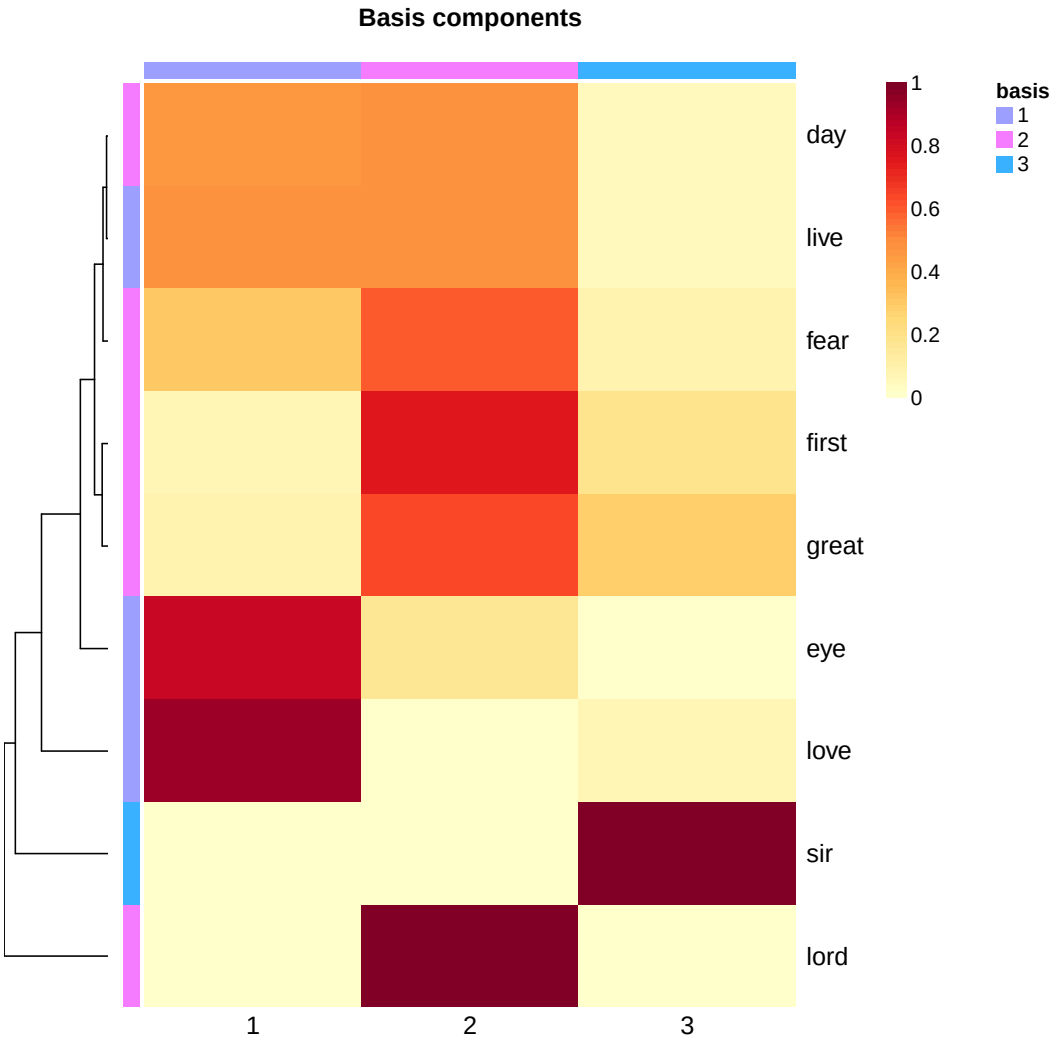

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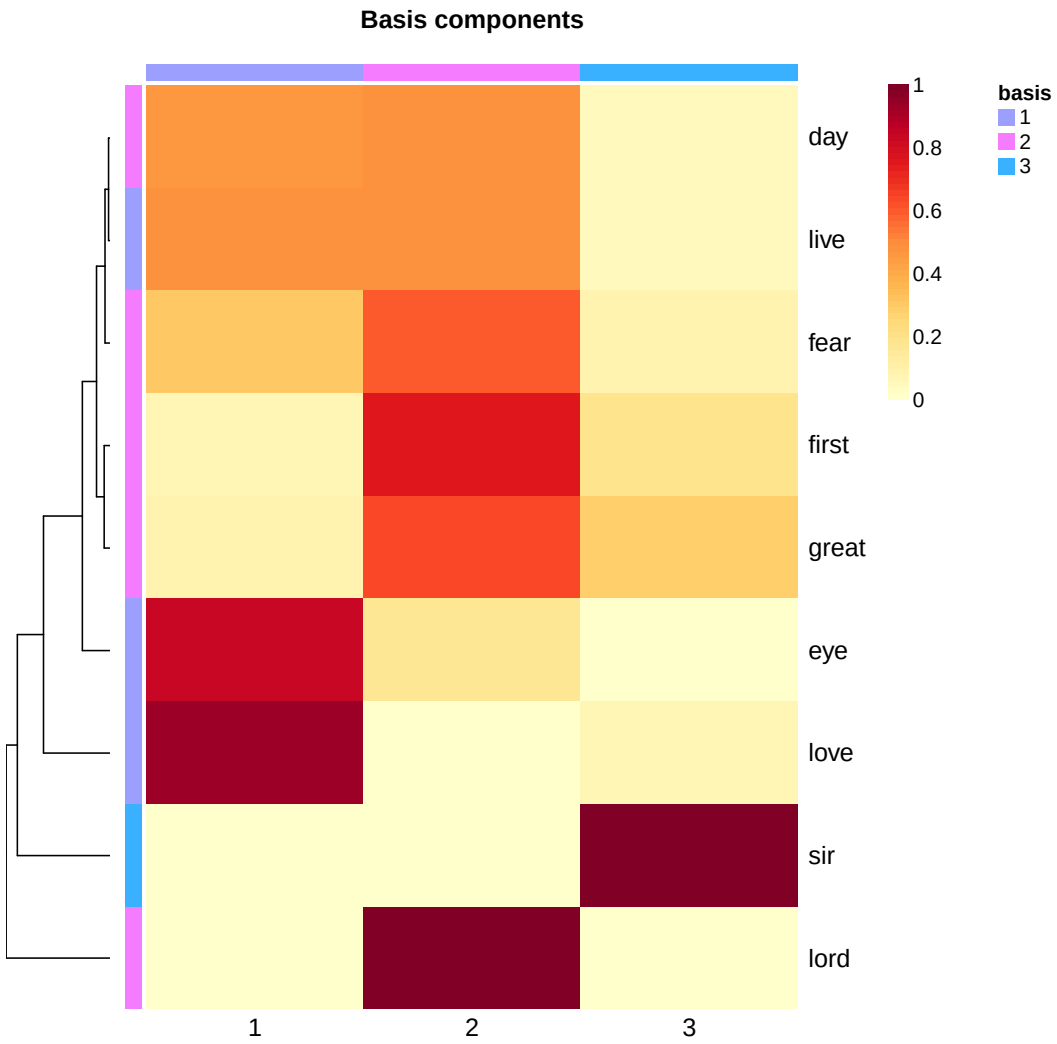

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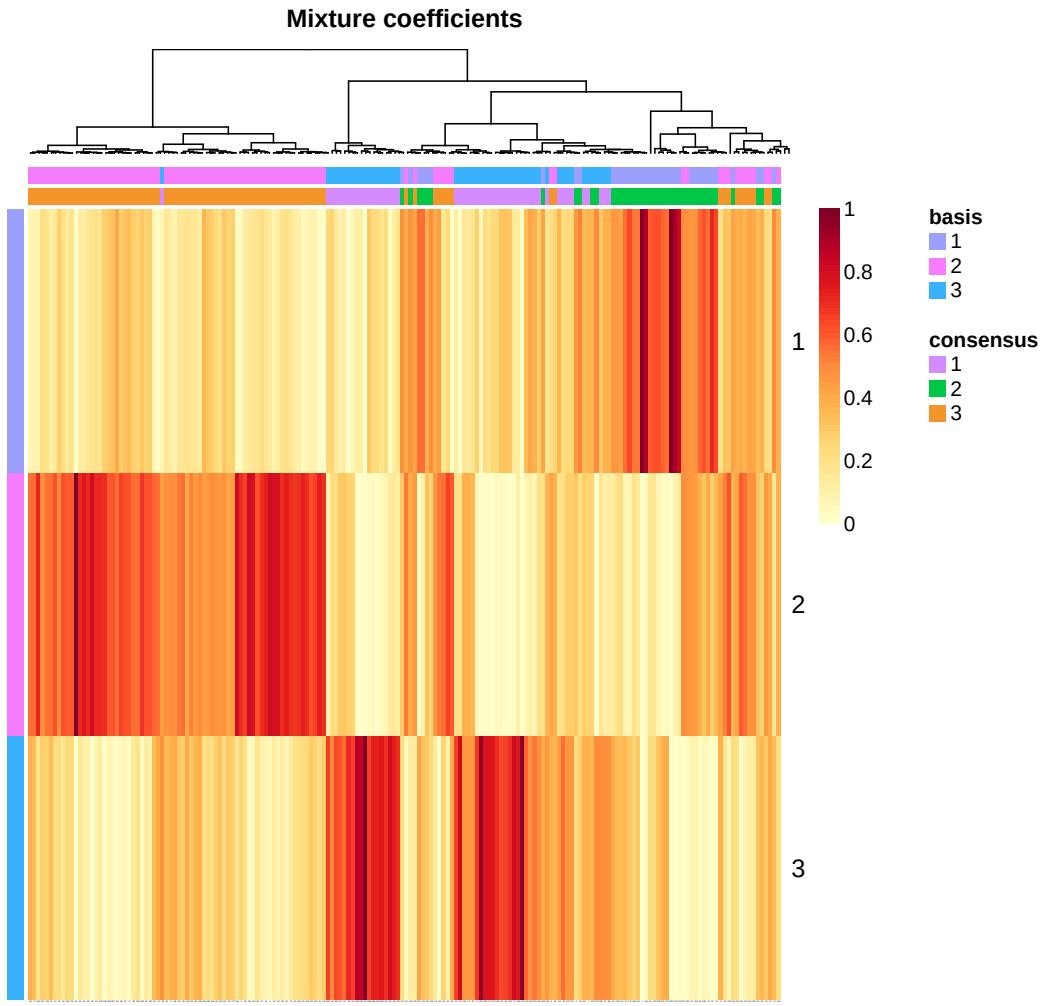

Figure 8: Mixture coefficients heatmap

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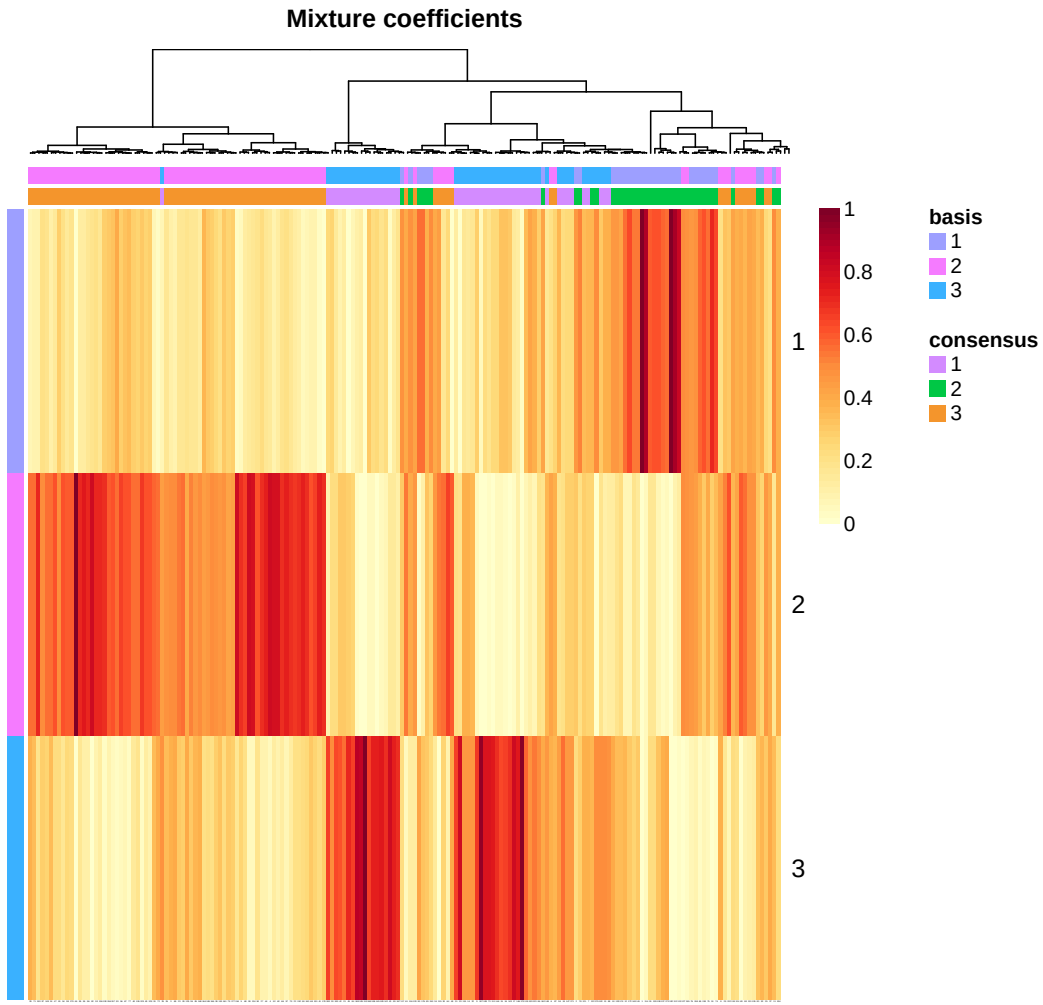
Love's Labour's Lost
A Midsummer Night's Dream
The Two Gentlemen of Verona
A Lover's Complaint
The Tempest
. . .



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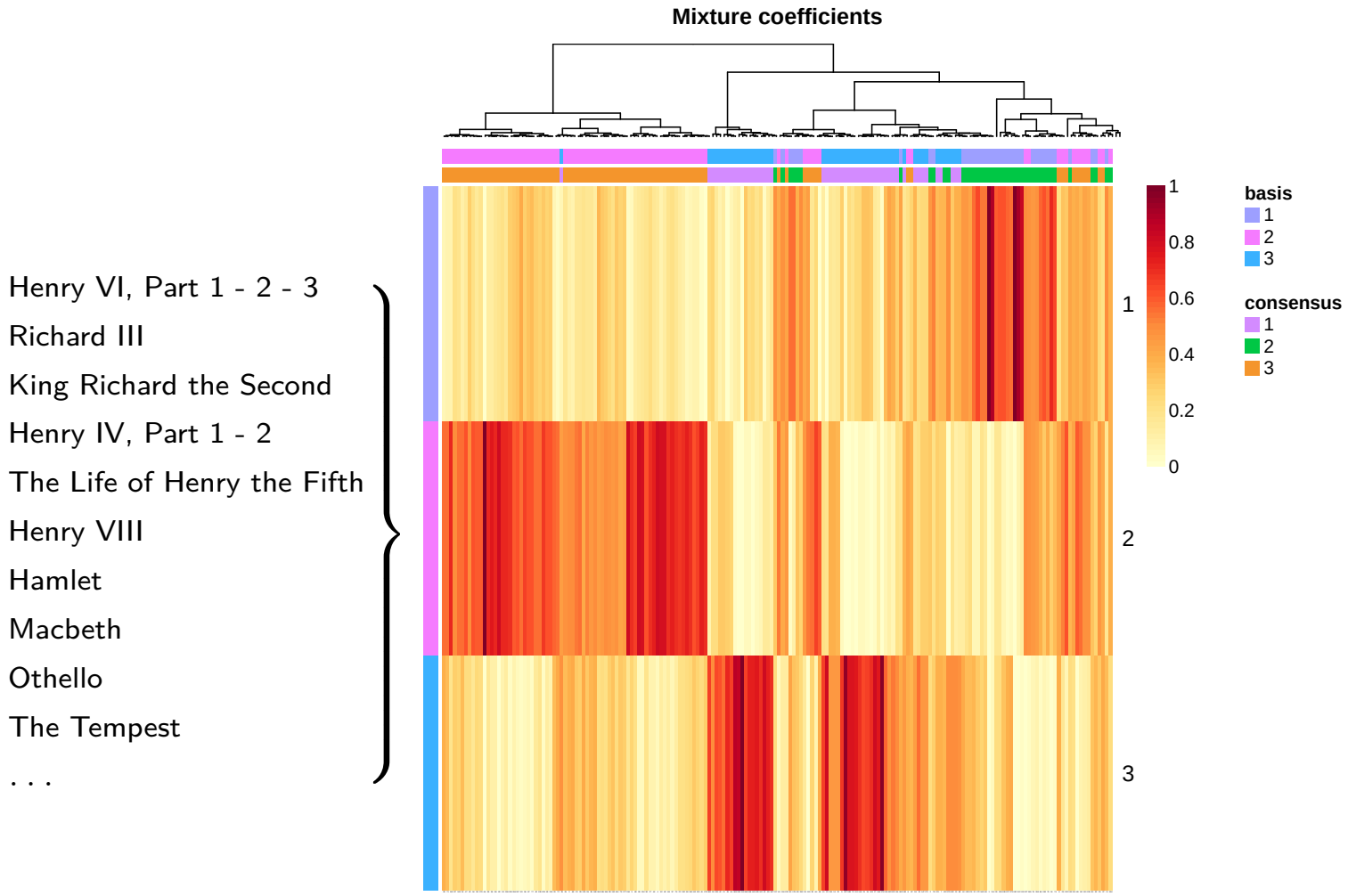

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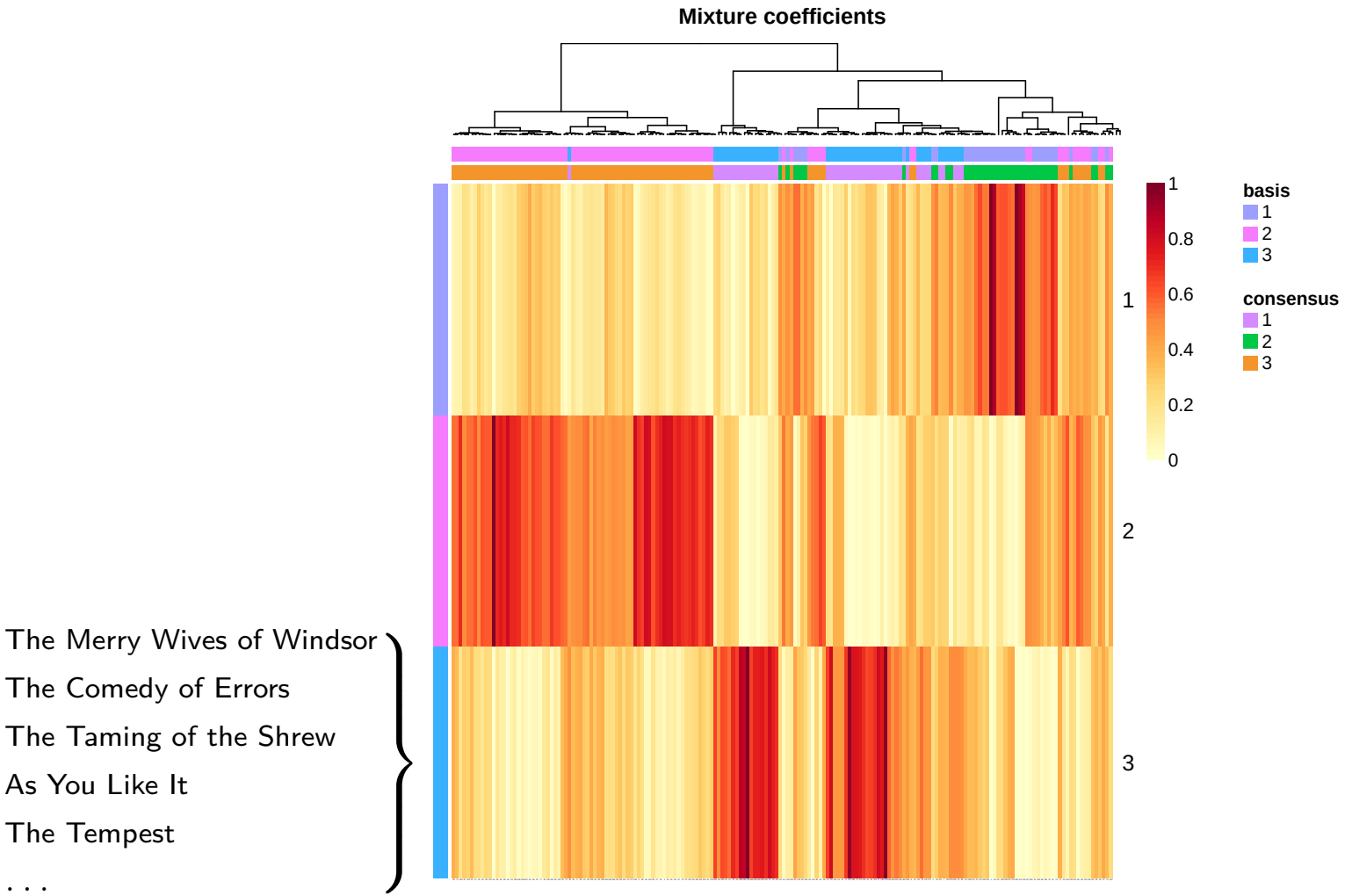

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Conclusion

NMF has made great strides and huge impact in the last few years and, by looking at the number of yearly citations received by founding paper of Lee and Seung 1999, it's very likely it will have a promising and bright future.

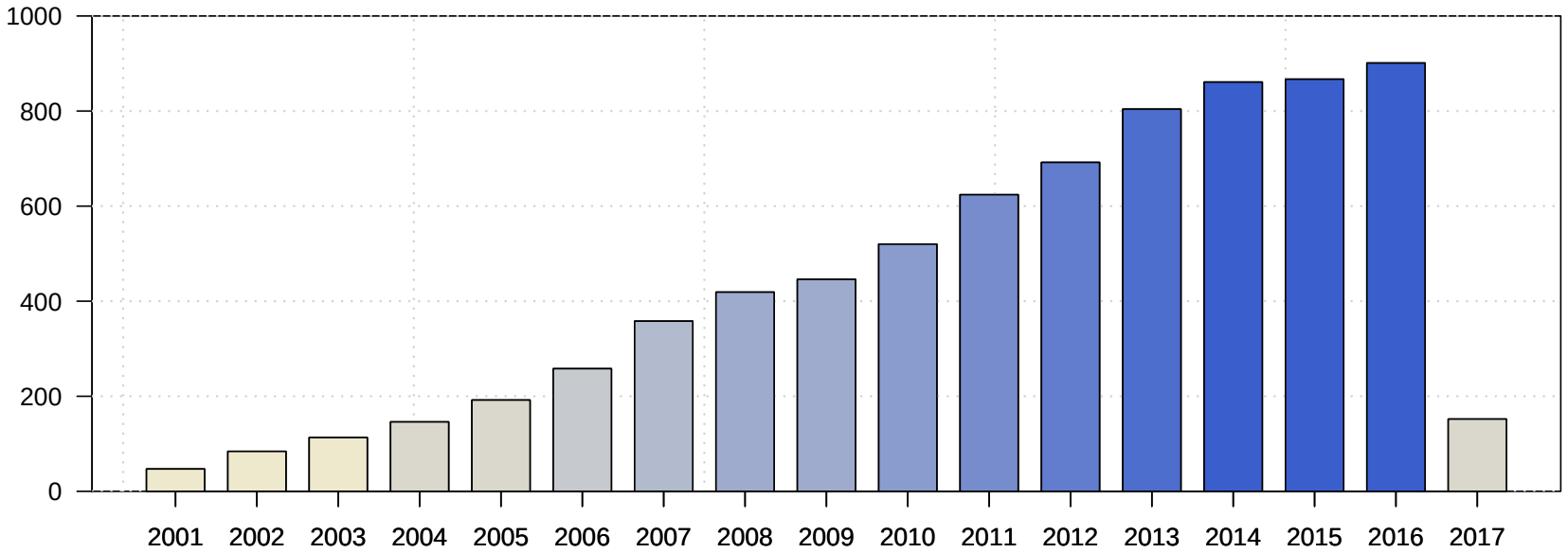

Figure 9: Citations per year of Lee and Seung 1999's paper that launched NMF

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