# So Far…

- It's time for
  - Unsupervised learning
    - We are only given inputs
    - Goal: find "interesting patterns"

    - Discovering clusters
      - Clustering
    - Discovering latent factors
      - Dimensionality reduction
      - Topic modeling
      - Matrix factorization

# Matrix Factorization

**Deng Cai (蔡登)**

College of Computer Science
Zhejiang University

dengcai@gmail.com

# What Is Matrix Factorization?

$$X \in \mathcal{R}^{m \times n}$$

$$UV = X \qquad U \in \mathcal{R}^{m \times k}, V \in \mathcal{R}^{k \times n}$$

- Is this factorization unique?

$$\Sigma \in \mathcal{R}^{k \times k} \qquad U\Sigma\Sigma^{-1}V = X$$

$$U\Sigma V = X$$

  - Every column of $U$ and every row of $V$ are normalized

- Does this factorization always exist?

$$UV = \tilde{X} \approx X \qquad \|X - UV\|_F^2$$

# Why Matrix Factorization?

$$X = UV$$

$$\begin{bmatrix} x_{11} & x_{21} & \cdots & x_{n1} \\ x_{12} & x_{22} & \cdots & x_{n2} \\ x_{13} & x_{23} & \cdots & x_{n3} \\ \vdots & \vdots & & \vdots \\ x_{1m} & x_{2m} & \cdots & x_{nm} \end{bmatrix} = \begin{bmatrix} u_{11} & \cdots & u_{k1} \\ u_{12} & \cdots & u_{k2} \\ u_{13} & \cdots & u_{k3} \\ \vdots & & \vdots \\ u_{1m} & \cdots & u_{km} \end{bmatrix} \times \begin{bmatrix} v_{11} & v_{21} & \cdots & v_{n1} \\ \vdots & \vdots & & \vdots \\ v_{1k} & v_{2k} & \cdots & v_{nk} \end{bmatrix}$$

$$\begin{bmatrix} \\ \boldsymbol{x}_i \\ \\ \end{bmatrix} = v_{i1} \begin{bmatrix} \\ \boldsymbol{u}_1 \\ \\ \end{bmatrix} + v_{i2} \begin{bmatrix} \\ \boldsymbol{u}_2 \\ \\ \end{bmatrix} + \cdots + v_{ik} \begin{bmatrix} \\ \boldsymbol{u}_k \\ \\ \end{bmatrix}$$

- Each column vector of $X$ can be represented as a linear combination of column vectors of $U$
- Each column vector of $V$ can be regarded as a low dimensional representation of corresponding column vector of $X$

# Relation to Dimensionality Reduction

$$X = [\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots \boldsymbol{x}_n] = UV = U[\boldsymbol{v}_1, \boldsymbol{v}_2, \cdots \boldsymbol{v}_n]$$

$$\boldsymbol{x}_i = U\boldsymbol{v}_i \qquad \boldsymbol{x}_i \in \mathcal{R}^m, \boldsymbol{v}_i \in \mathcal{R}^k$$

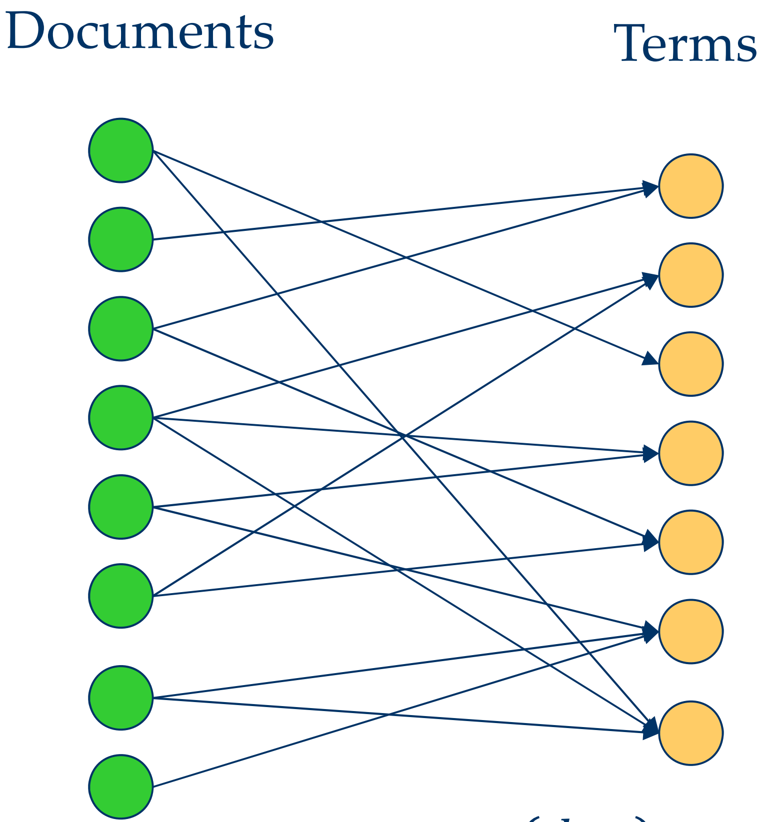
- If there is a matrix $A \in \mathcal{R}^{k\times m}$ which satisfies:

$$AU = I$$

$$A\boldsymbol{x}_i = \boldsymbol{v}_i$$

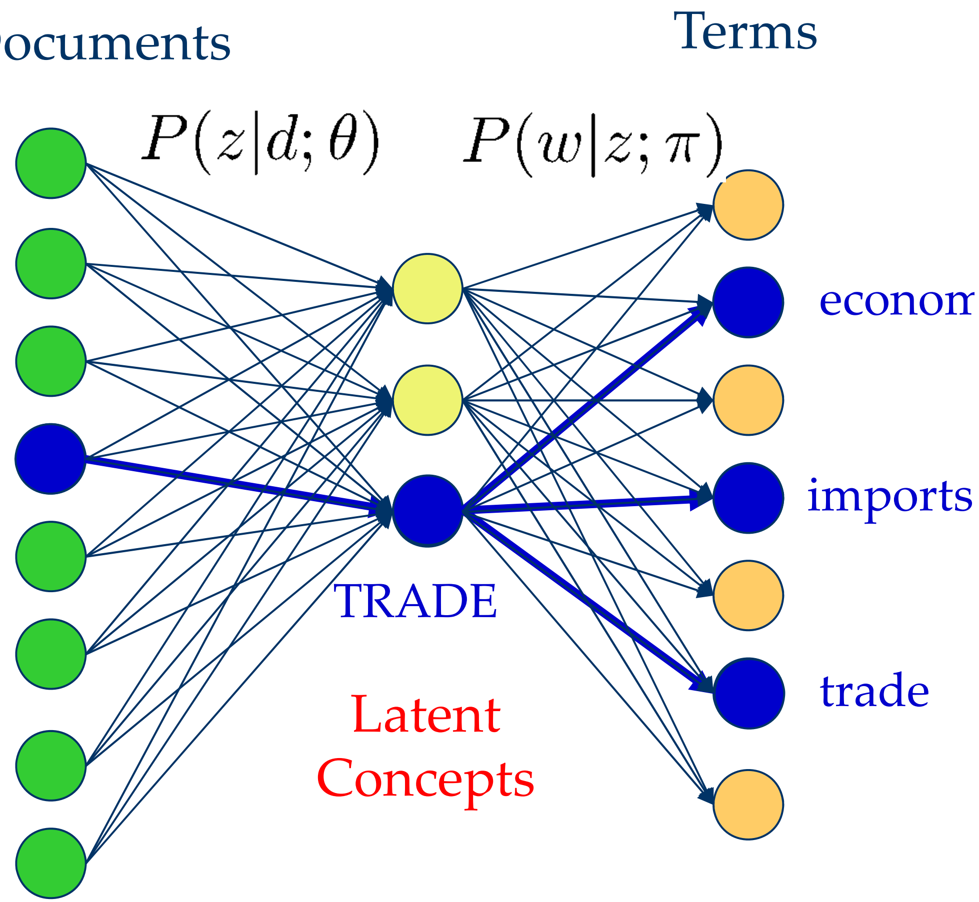
- In DR, we learn the transformation matrix
- In MF, we learn the basis matrix

# Relation to Topic Modeling




$$P(w|d) = \frac{n(d,w)}{\sum_{w'} n(d,w')}$$

$$X = \begin{bmatrix} P(w_1|d_1) & \cdots & P(w_1|d_n) \\ \vdots & \ddots & \vdots \\ P(w_m|d_1) & \cdots & P(w_m|d_n) \end{bmatrix}$$




$$\hat{P}(w|d) = \sum_{z} P(w|z)P(z|d)$$

# Relation to Topic Modeling

$$P(w|d) = \frac{n(d,w)}{\sum_{w'} n(d,w')}$$

$$\hat{P}(w|d) = \sum_{z} P(w|z)P(z|d)$$

$$X = \begin{bmatrix} P(w_1|d_1) & \cdots & P(w_1|d_n) \\ \vdots & \ddots & \vdots \\ P(w_m|d_1) & \cdots & P(w_m|d_n) \end{bmatrix}$$

$$U = \begin{bmatrix} \hat{P}(w_1|z_1) & \cdots & \hat{P}(w_1|z_k) \\ \vdots & \ddots & \vdots \\ \hat{P}(w_m|z_1) & \cdots & \hat{P}(w_m|z_k) \end{bmatrix}$$

$$\hat{X} = \begin{bmatrix} \hat{P}(w_1|d_1) & \cdots & \hat{P}(w_1|d_n) \\ \vdots & \ddots & \vdots \\ \hat{P}(w_m|d_1) & \cdots & \hat{P}(w_m|d_n) \end{bmatrix}$$

$$V = \begin{bmatrix} \hat{P}(z_1|d_1) & \cdots & \hat{P}(z_k|d_1) \\ \vdots & \ddots & \vdots \\ \hat{P}(z_1|d_n) & \cdots & \hat{P}(z_k|d_n) \end{bmatrix}$$

$$X \approx \hat{X} = UV^T$$

# Algorithms

- Singular Value Decomposition
- Nonnegative Matrix Factorization
- Sparse Coding

# Singular Value Decomposition (SVD)

- For an arbitrary matrix $X \in \mathcal{R}^{m\times n}$ there exists a factorization as follows:

$$X = U\Sigma V$$

- where

$$U \in \mathcal{R}^{m\times m}, V \in \mathcal{R}^{n\times n}, UU^T = U^TU = I, VV^T = V^TV = I$$

diagonal matrix $\Sigma \in \mathcal{R}^{m\times n}$

- If $rank(X) = d$

$$U \in \mathcal{R}^{m\times d}, V \in \mathcal{R}^{d\times n}, U^TU = I, \cancel{VV^T = I}$$

$$\Sigma = \text{diag}(\sigma_1, \sigma_2, \cdots \sigma_d) \quad \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_d > 0$$

# SVD: Low-rank Approximation

- SVD can be used to compute optimal **low-rank approximations**.
- Approximation problem:

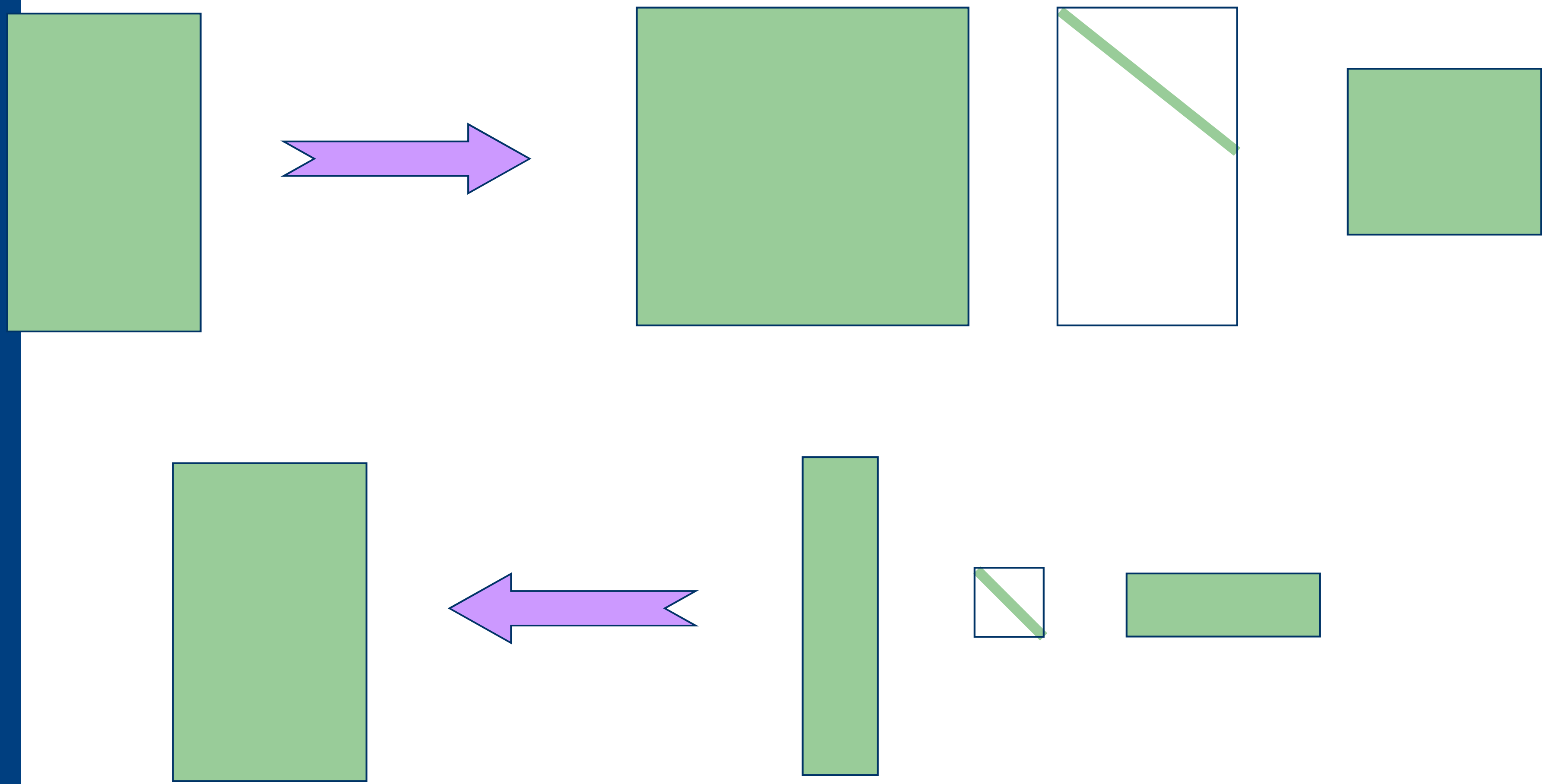
$$X^* = \underset{rank(\tilde{X})=k}{\operatorname{argmin}} \left\| X - \tilde{X} \right\|_F^2$$

- Solution via SVD

$$X^* = U\mathrm{diag}(\sigma_1, \cdots, \sigma_k, \underbrace{0, \cdots, 0}_{\text{set small singular values to zero}})V$$

C. Eckart, G. Young, The approximation of a matrix by another of lower rank. Psychometrika, 1, 211-218, 1936.

# Low rank approximation by SVD



# Relation to PCA

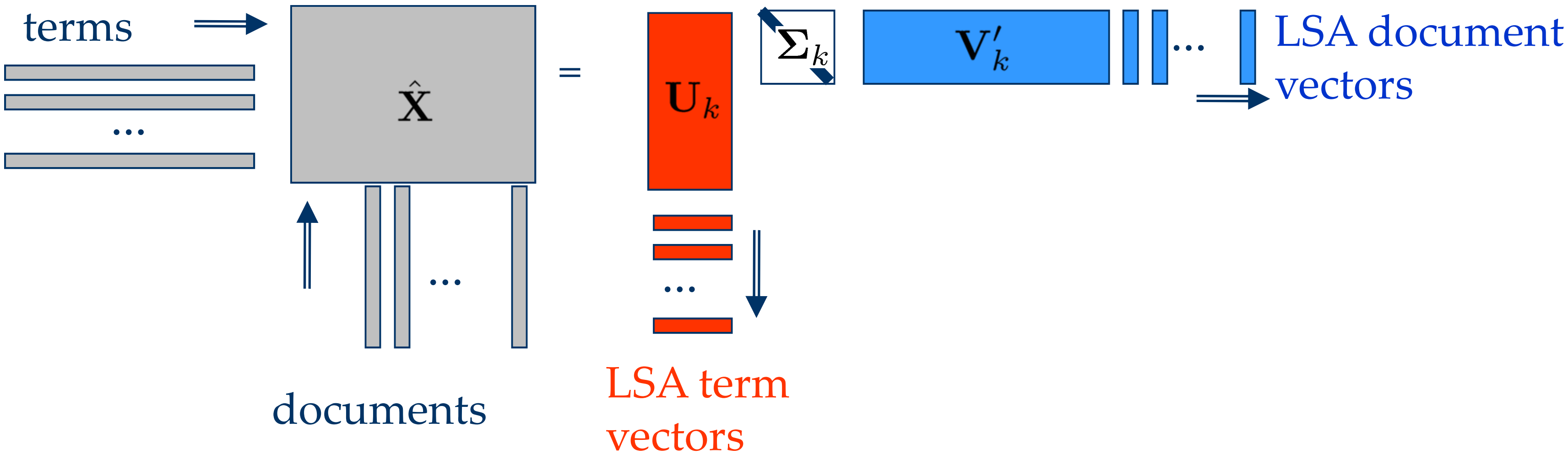
- Given an SVD of X, the following two relations hold:

$$X^T X = V\Sigma^T U^T U\Sigma \mathrm{V}^{\mathrm{T}} = \mathrm{V}\left(\Sigma^T\Sigma\right)\mathrm{V}^{\mathrm{T}}$$

$$XX^T = U\Sigma V^T V\Sigma^T U^T = U\left(\Sigma\Sigma^T\right)U^T$$

# Latent Semantic Analysis (Indexing)

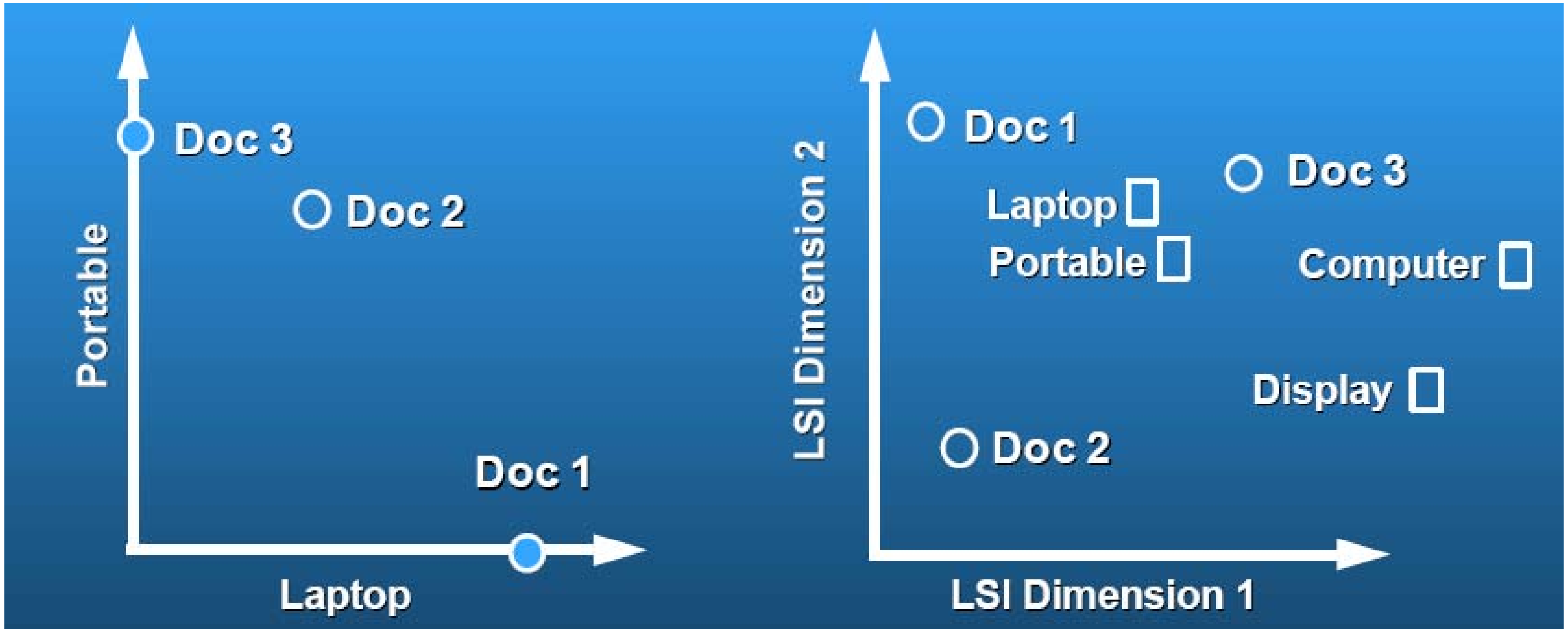
- The Latent Semantic Analysis via SVD can be summarized as follows:




- Document **similarity** 
- $\langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle = \langle \Sigma_k \boldsymbol{v}_i, \Sigma_k \boldsymbol{v}_j \rangle$

# Latent Semantic Analysis

- **Latent semantic space**: illustrating example



# Relation to Topic Modeling

$$P(w|d) = \frac{n(d,w)}{\sum_{w'} n(d,w')}$$

$$\hat{\boldsymbol{P}}(\boldsymbol{w}|\boldsymbol{d}) = \sum_{\boldsymbol{z}} \boldsymbol{P}(\boldsymbol{w}|\boldsymbol{z})\boldsymbol{P}(\boldsymbol{z}|\boldsymbol{d})$$

$$X = \begin{bmatrix} P(w_1|d_1) & \cdots & P(w_1|d_n) \\ \vdots & \ddots & \vdots \\ P(w_m|d_1) & \cdots & P(w_m|d_n) \end{bmatrix}$$

$$U = \begin{bmatrix} \hat{P}(w_1|z_1) & \cdots & \hat{P}(w_1|z_k) \\ \vdots & \ddots & \vdots \\ \hat{P}(w_m|z_1) & \cdots & \hat{P}(w_m|z_k) \end{bmatrix}$$

$$\hat{X} = \begin{bmatrix} \hat{P}(w_1|d_1) & \cdots & \hat{P}(w_1|d_n) \\ \vdots & \ddots & \vdots \\ \hat{P}(w_m|d_1) & \cdots & \hat{P}(w_m|d_n) \end{bmatrix}$$

$$V = \begin{bmatrix} \hat{P}(z_1|d_1) & \cdots & \hat{P}(z_k|d_1) \\ \vdots & \ddots & \vdots \\ \hat{P}(z_1|d_n) & \cdots & \hat{P}(z_k|d_n) \end{bmatrix}$$

$$X \approx \hat{X} = UV^T$$

# Nonnegative Matrix Factorization

$$X \in \mathcal{R}^{m \times n}$$

$$U \in \mathcal{R}^{m \times k}, \qquad V \in \mathcal{R}^{k \times n}$$

$$UV = \tilde{X} \approx X$$

$$u_{ij} \geq 0, v_{ij} \geq 0$$

- Low rank assumption ($k$ hidden factors)
- Nonnegative assumption

# Non-negative Matrix Factorization

$$X \cong \hat{X} = UV^T, u_{ij} \geq 0, v_{ij} \geq 0$$

- Two cost functions
  - Euclidean distance

$$||A - B||^2 = \Sigma_{ij}(A_{ij} - B_{ij})^2$$

  - Divergence

$$D(A||B) = \Sigma_{ij}(A_{ij} \log \frac{A_{ij}}{B_{ij}} - A_{ij} + B_{ij})$$

# Optimization Problems

- Minimize $\left\|X - UV^T\right\|^2$ with respect to $U$ and $V$, subject to the constraints $U, V \geq 0$.

- Minimize $D(X||UV^T)$ with respect to $U$ and $V$, subject to the constraints $U, V \geq 0$.

# NMF Optimization (Euclidean Distance)

$$\min \left\|X - UV^T\right\|^2, s.t. u_{ij} \geq 0, v_{ij} \geq 0$$

$$J = \left\|X - UV^T\right\|^2 = \mathrm{tr}\left(\left(X - UV^T\right)^T\left(X - UV^T\right)\right)$$
$$= \mathrm{tr}\left(X^TX - X^TUV^T - VU^TX + VU^TUV^T\right)$$

$\Gamma$, same size as $U$

$\Phi$, same size as $V$

$$\mathcal{L} = \mathrm{tr}\left(X^TX\right) - 2\mathrm{tr}\left(X^TUV^T\right) + \mathrm{tr}\left(VU^TUV^T\right) + \mathrm{tr}\left(\Gamma U^T\right) + \mathrm{tr}\left(\Phi V^T\right)$$

$$\frac{\partial \mathcal{L}}{\partial U} = -2XV + 2UV^TV + \Gamma \qquad \left(UV^TV\right)_{ik}u_{ik} - (XV)_{ik}u_{ik} = 0$$

$$\boxed{u_{ik} \leftarrow \frac{(XV)_{ik}}{(UV^TV)_{ik}} u_{ik}}$$

$$\frac{\partial \mathcal{L}}{\partial V} = -2X^TU + 2VU^TU + \Phi \qquad \left(VU^TU\right)_{jk}v_{jk} - \left(X^TU\right)_{jk}v_{jk} = 0$$

$$\boxed{v_{jk} \leftarrow \frac{\left(X^TU\right)_{jk}}{(VU^TU)_{jk}} v_{jk}}$$

# Multiplicative Update Rules

- *The Euclidean distance* $\left\|X - UV^T\right\|^2$ *is nonincreasing under the update rules*

$$u_{ik} \leftarrow \frac{(XV)_{ik}}{(UV^TV)_{ik}} u_{ik} \qquad v_{jk} \leftarrow \frac{\left(X^TU\right)_{jk}}{(VU^TU)_{jk}} v_{jk}$$

*The Euclidean distance is invariant under these updates if and only if U and V are at a stationary point of the distance.*

# NMF vs PLSA

$X \cong \hat{X} = UV^T, u_{ij} \geq 0, v_{ij} \geq 0$

$D(A||B) = \sum_{ij}\left(A_{ij}\log\frac{A_{ij}}{B_{ij}} - A_{ij} + B_{ij}\right) \qquad = \sum_{ij}(A_{ij}\log A_{ij} - A_{ij} - A_{ij}\log B_{ij} + B_{ij})$

$$\max \sum_{ij}(A_{ij}\log B_{ij} - B_{ij})$$

$$X = [n(d_i, w_j)] \times diag\left(\frac{1}{l(d_i)}\right) \qquad U = [p(w_j|z_k)] \qquad V^T = [p(z_k|d_i)]$$

$$\max \sum_i \frac{1}{l(d_i)} \sum_j n(d_i, w_j) \log \sum_k p(w_j|z_k) p(z_k|d_i) - n$$

$$l(\theta, \pi; \mathbf{N}) = \sum_{d,w} n(d,w)\log\left(\sum_z P(w|z;\theta)P(z|d;\pi)\right)$$

# Sparse Coding

$$X \approx \hat{X} = UV^T$$

$$\begin{bmatrix} \\ \boldsymbol{x}_i \\ \\ \end{bmatrix} = v_{i1} \begin{bmatrix} \\ \boldsymbol{u}_1 \\ \\ \end{bmatrix} + v_{i2} \begin{bmatrix} \\ \boldsymbol{u}_2 \\ \\ \end{bmatrix} + \cdots + v_{ik} \begin{bmatrix} \\ \boldsymbol{u}_k \\ \\ \end{bmatrix}$$

$$\text{minimize}_{U,V} \quad \left\|X - UV^T\right\|_F^2 + \lambda f(V)$$

$$\text{subject to} \quad \Sigma_i u_{i,k}^2 \leq c, \forall k = 1, \ldots, K.$$

- Represent input vectors approximately as a weighted linear combination of a small number of "basis vectors."

# Matrix Factorization: Summary

$$X \in \mathcal{R}^{m \times n}$$

$$U \in \mathcal{R}^{m \times k}, \qquad V \in \mathcal{R}^{k \times n}$$

$$UV = \tilde{X} \approx X$$

- Low rank assumption ($k$ hidden factors)
  - SVD
- Nonnegative assumption
  - NMF
- Sparseness assumption
  - Sparse Coding