Roadmap

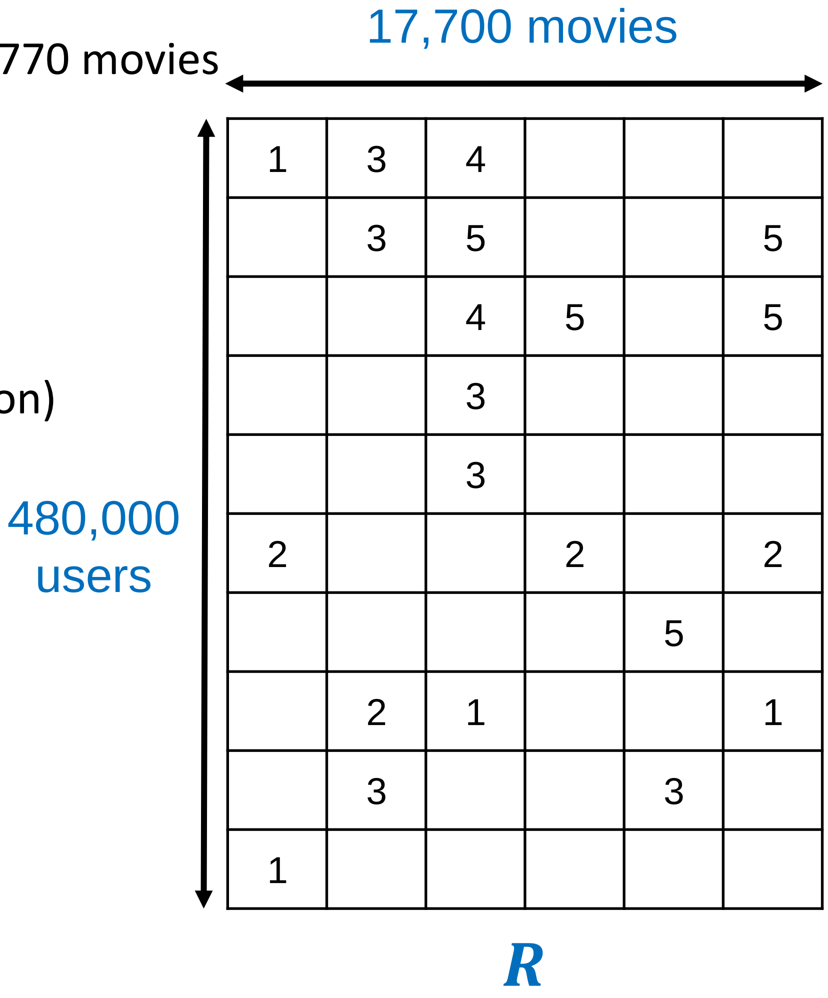
- Chapter: Dimensionality Reduction & Matrix Factorization
  1. Introduction
  2. Principal Component Analysis (PCA)
  3. Singular Value Decomposition (SVD)
  4. **Matrix Factorization**
     - **Motivation & Approach**
     - Regularization & Sparsity
     - Further Factorization Models
  5. Neighbor Graph Methods
  6. Autoencoders (Non-linear Dimensionality Reduction)

Motivation: The Netflix Prize

- Training data
  - 100 million ratings, 480,000 users, 17,770 movies
  - 6 years of data: 2000-2005
- Test data
  - Last few ratings of each user (2.8 million)
  - Root Mean Square Error (RMSE)
  - Netflix's system RMSE: 0.9514

trivial: 1.054

- Competition
  - 2,700+ teams
  - $1 million prize for 10% improvement



1	3	4			
	3	5			5
		4	5		5
		3			
		3			
2			2		2
				5	
	2	1			1
	3			3	
1					

Evaluating Recommender Systems

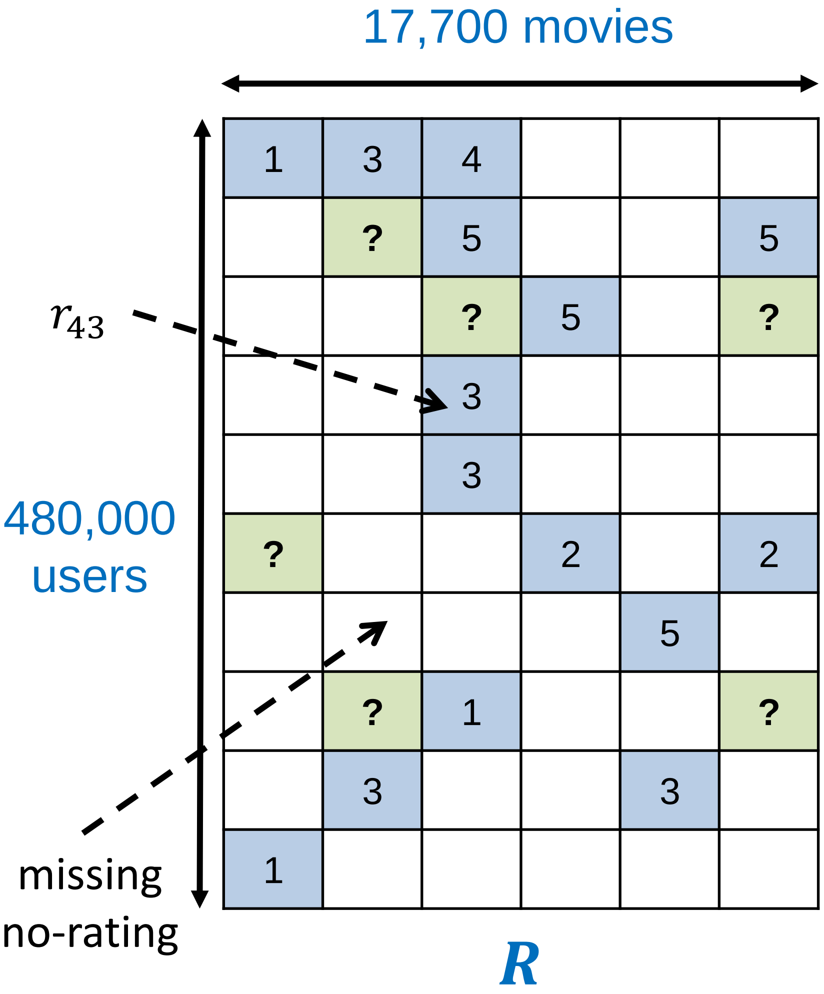
- S = set of tuples (u, i) of users u that have rated item i with a rating of r_{ui}

- RMSE $= \frac{1}{|S|}\sqrt{\sum_{(u,i)\in S}(r_{ui} - \hat{r}_{ui})^2}$

  true rating of user u for item i

  predicted rating

- Legend:
  - 🟦 Training and validation data
  - 🟩 Test data
  - ☐ Missing data

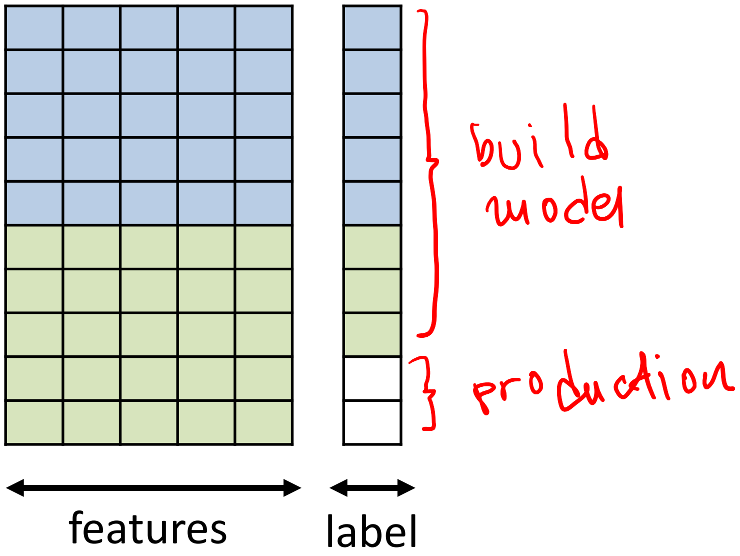


1	3	4			
	?	5			5
		?	5		?
		3			
		3			
?			2		2
				5	
	?	1			?
	3			3	
1					

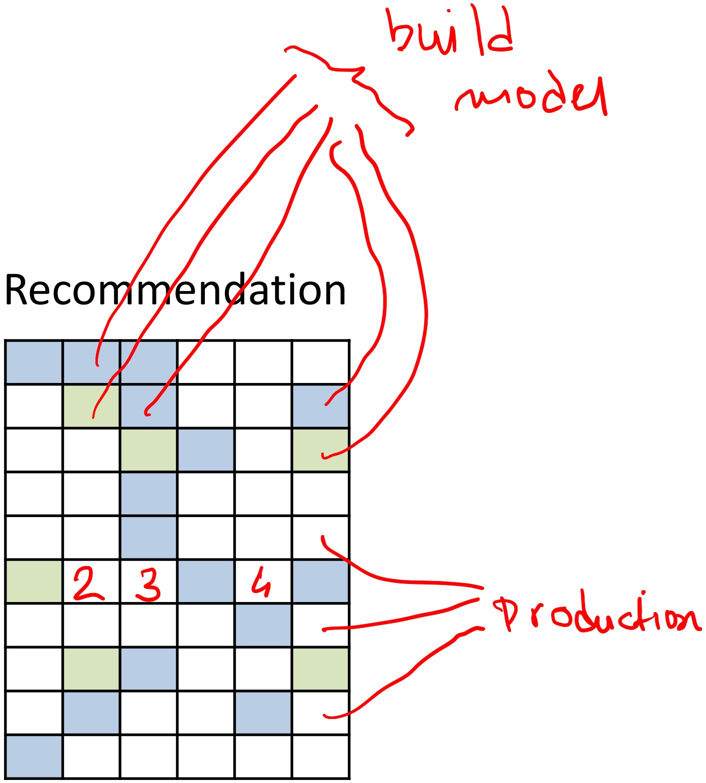
Regression vs. Recommendation

- Legend:
  - 🟦 Training and validation data
  - 🟩 Test data
  - ⬜ Missing data

Regression



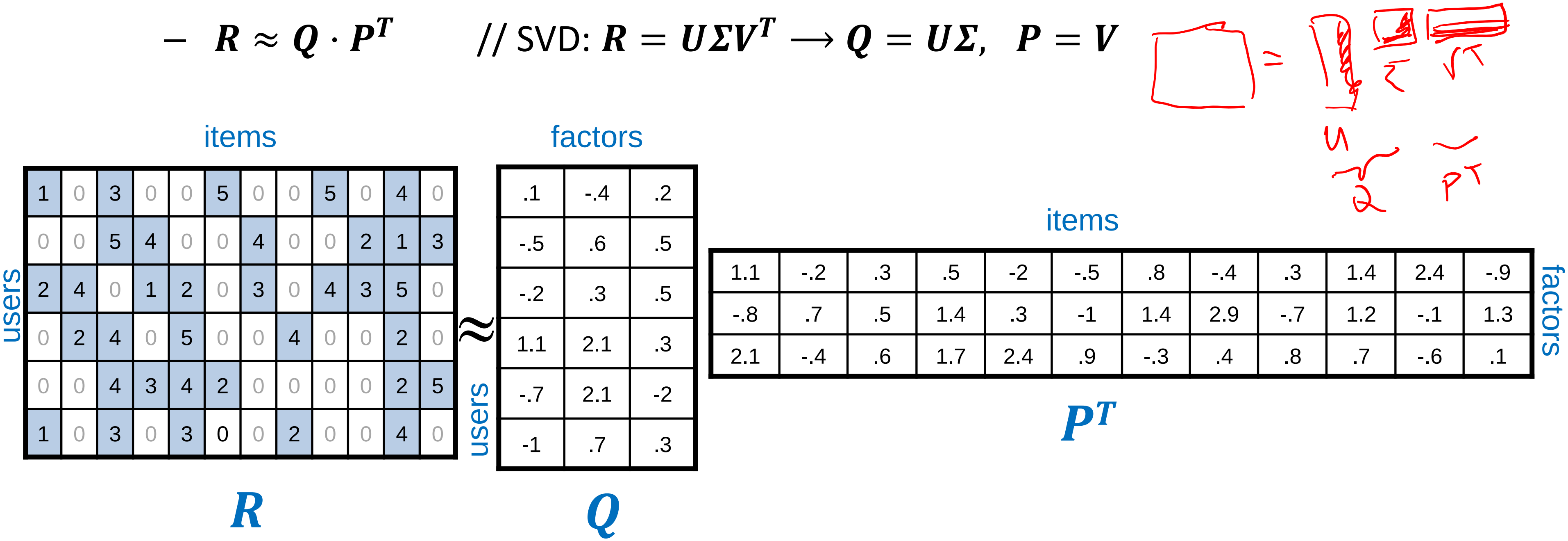
Recommendation



Matrix Completion

SVD on Rating Data

- Goal: Make good recommendations
  - Good performance on observed (user, item) ratings, i.e. low RMSE
  - Generalize to the unseen test data
- Can we use SVD to obtain the solution?
  - SVD on the rating matrix $\boldsymbol{R} \in \mathbb{R}^{n \times d}$ where we replace **missing** entries with **zeros**
  - $\boldsymbol{R} \approx \boldsymbol{Q} \cdot \boldsymbol{P}^{\boldsymbol{T}}$ // SVD: $\boldsymbol{R} = \boldsymbol{U\Sigma V^T} \longrightarrow \boldsymbol{Q} = \boldsymbol{U\Sigma}, \quad \boldsymbol{P} = \boldsymbol{V}$



$\boldsymbol{R}$

1	0	3	0	0	5	0	0	5	0	4	0
0	0	5	4	0	0	4	0	0	2	1	3
2	4	0	1	2	0	3	0	4	3	5	0
0	2	4	0	5	0	0	4	0	0	2	0
0	0	4	3	4	2	0	0	0	0	2	5
1	0	3	0	3	0	0	2	0	0	4	0

$\boldsymbol{Q}$

.1	-.4	.2
-.5	.6	.5
-.2	.3	.5
1.1	2.1	.3
-.7	2.1	-2
-1	.7	.3

$\boldsymbol{P}^{\boldsymbol{T}}$

1.1	-.2	.3	.5	-2	-.5	.8	-.4	.3	1.4	2.4	-.9
-.8	.7	.5	1.4	.3	-1	1.4	2.9	-.7	1.2	-.1	1.3
2.1	-.4	.6	1.7	2.4	.9	-.3	.4	.8	.7	-.6	.1

SVD on Rating Data

- SVD gives **minimum reconstruction error** (Sum of Squared Errors):

$$\min_{\boldsymbol{U},\boldsymbol{\Sigma},\boldsymbol{V}} \sum_{\substack{u=1\ldots n\\ i=1\ldots d}} \left(\underline{\boldsymbol{R}_{ui}} - \underbrace{[\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T]}_{B}{}_{ui}\right)^2$$

$$\min_{B} \|R-B\|_F^2$$

$$\text{rank}(B)=k$$

$$UU^T = \underline{I}$$

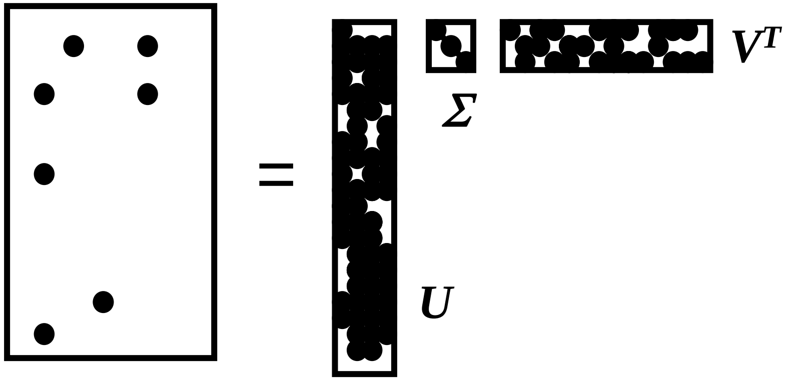
$$VV^T = \underline{I}$$

  - SSE and RMSE are monotonically related:
    - $\text{RMSE} = \frac{1}{\text{const.}}\sqrt{\text{SSE}}$
    - Great news: SVD is minimizing RMSE

- **Complication:**
  - The sum in the SVD error term is over **all** entries (no-rating = zero-rating)
  - But our $\boldsymbol{R}$ has **missing** entries!
  - (Classical) SVD isn't defined when entries are missing!
- Also: We actually don't care about orthogonality and normalization

Discussion: SVD/PCA

- Optimal low-rank approximation
  - In terms of Frobenius norm (and also in terms of the spectral norm)
- Missing elements (we have no information/not observed) are treated as 0 (a very low rating)
  - Critical for many applications (e.g. recommender systems)
  - General problem: two kinds of "zeros" (not observed/missing $\neq$ 0)
- Lack of Sparsity
  - Singular vectors are dense
  - Potential interpretability problem
- Orthogonality really required/useful?



Latent Factor Models

- Our goal: Find $\boldsymbol{Q} \in \mathbb{R}^{n \times k}$ and $\boldsymbol{P} \in \mathbb{R}^{d \times k}$ such that:

$$\min_{\boldsymbol{P},\boldsymbol{Q}} \sum_{(u,i) \in S} \left(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}}\right)^2$$

$q_u \quad 1 \times k$

$p_i \quad 1 \times k$

$q_u \cdot p_i^{T} \quad 1 \times k \, (1 \times k)^{T}$

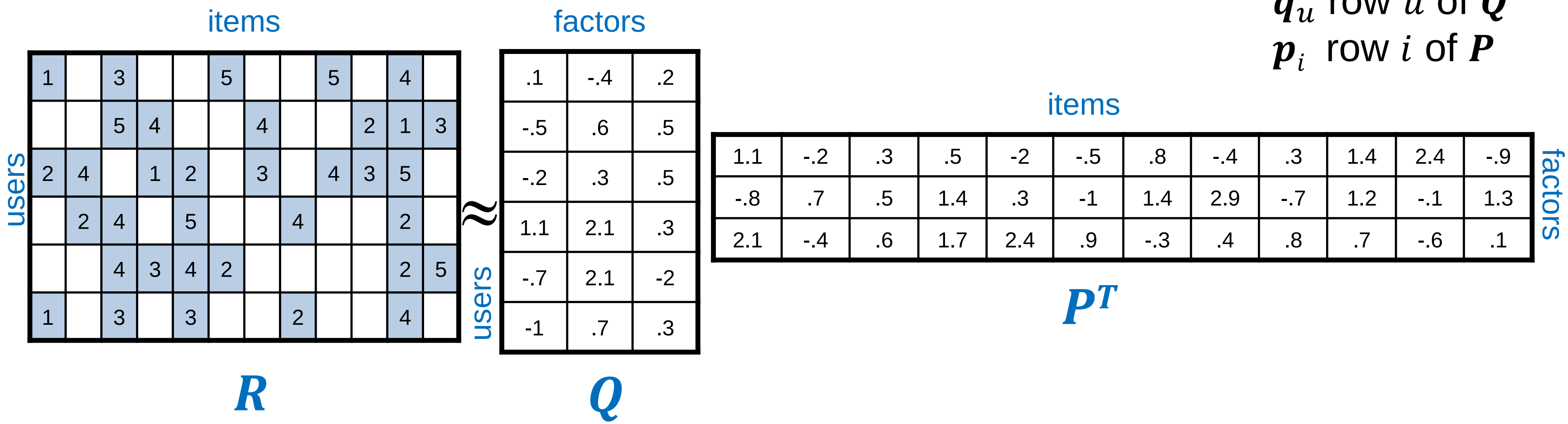
$= 1 \times 1$

  - We only sum over existing entries, i.e. the set $S = \{(u,i) \mid r_{ui} \neq \text{missing}\})$
  - We don't require columns of $\boldsymbol{P}, \boldsymbol{Q}$ to be orthogonal or unit length
- Use standard optimization techniques to solve this problem

$$\hat{r}_{ui} = \boldsymbol{q}_u \cdot \boldsymbol{p}_i^T$$

$\boldsymbol{q}_u$ row u of $\boldsymbol{Q}$

$\boldsymbol{p}_i$ row i of $\boldsymbol{P}$



$\boldsymbol{R}$

1		3			5			5		4	
		5	4			4			2	1	3
2	4		1	2		3		4	3	5	
	2	4		5			4			2	
		4	3	4	2					2	5
1		3		3			2			4	

≈

$\boldsymbol{Q}$

.1	-.4	.2
-.5	.6	.5
-.2	.3	.5
1.1	2.1	.3
-.7	2.1	-2
-1	.7	.3

$\boldsymbol{P}^T$

1.1	-.2	.3	.5	-2	-.5	.8	-.4	.3	1.4	2.4	-.9
-.8	.7	.5	1.4	.3	-1	1.4	2.9	-.7	1.2	-.1	1.3
2.1	-.4	.6	1.7	2.4	.9	-.3	.4	.8	.7	-.6	.1

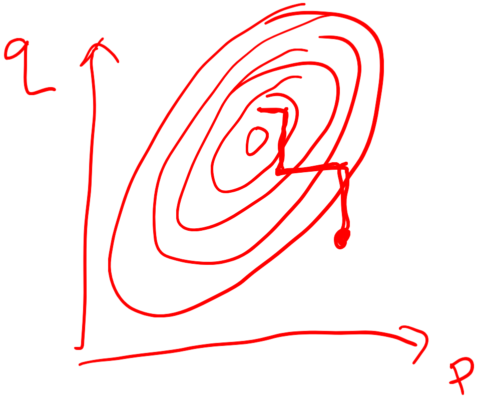
Finding the Latent Factors (I)

- Goal: $\min_{\boldsymbol{P},\boldsymbol{Q}} \sum_{(u,i)\in S} \left(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}}\right)^2 =: \min_{\boldsymbol{P},\boldsymbol{Q}} f(\boldsymbol{P},\boldsymbol{Q})$

- One approach: **Alternating Optimization** // a.k.a. block coordinate minimization
  - Pick initial values for $\boldsymbol{P}$ and $\boldsymbol{Q}$
  - Alternatingly keep one variable fix and optimize for the other
  - Repeat until convergence

- Pseudo-Code:

```
1. initialize $\boldsymbol{P}^{(0)}, \mathbf{Q}^{(0)}, t = 0$
2. $\boldsymbol{P}^{(t+1)} = \mathrm{argmin}_{\boldsymbol{P}}\ f(\boldsymbol{P}, \boldsymbol{Q}^{(t)})$
3. $\boldsymbol{Q}^{(t+1)} = \mathrm{argmin}_{\boldsymbol{Q}}\ f(\boldsymbol{P}^{(t+1)}, \boldsymbol{Q})$
4. $t = t + 1$
5. goto 2 until convergence
```



Finding the Latent Factors (II)

- Initialization of $\boldsymbol{P}$ and $\boldsymbol{Q}$:
  - Use, e.g., SVD where missing entries are replaced by 0 (or overall mean)

- How to solve $\boldsymbol{P}^{(t+1)} = \underset{\boldsymbol{P}}{\operatorname{argmin}} f(\boldsymbol{P}, \boldsymbol{Q}^{(t)}) = \underset{\boldsymbol{P}}{\operatorname{argmin}} \sum_{(\mathrm{u},i)\in S} \left(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^T\right)^2$
  - Observation 1: Since $\boldsymbol{Q}$ is fixed, the problem can be solved for **each** vector $\boldsymbol{p}_i$ **independently**

$$\sum_{(u,1)\in S} (r_{u1} - q_u p_1^T)^2 + \sum_{(u,2)\in S} (r_{u2} - q_u p_2^T)^2 + \dots$$

$$\min_{\boldsymbol{P}} \sum_{(u,i)\in S} \left(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}}\right)^2 = \sum_{i=1\dots d} \min_{\boldsymbol{p}_i} \sum_{\mathrm{u}\in S_{*,i}} \left(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}}\right)^2$$

where $S_{*,i} = \{u \mid (u,i) \in S\}$ // = only users u who have rated item i

  - Equivalently for vector $\boldsymbol{q}_u$ based on the set $S_{u,*} = \{i \mid (u,i) \in S\}$

Finding the Latent Factors (III)

- *Observation 2:* $\min_{\boldsymbol{p}_i} \sum_{u \in S_{*,i}} \left(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}}\right)^2$ is an **ordinary least squares regression** problem

$$X = \begin{bmatrix} — \\ — x_j^T — \\ — \end{bmatrix}$$

$$y = [y_1, y_2, \ldots]$$

  - $\min_{\mathbf{w}} \sum_{j=1}^{n} \left(y_j - \boldsymbol{w}^T \boldsymbol{x}_j\right)^2$ // y_j is scalar, $\boldsymbol{x}_j$ and $\boldsymbol{w}$ (column) vectors
  - Optimal solution in closed form: $\boldsymbol{w} = \Big(\underbrace{\frac{1}{n}\sum_{j=1}^{n} \boldsymbol{x}_j \boldsymbol{x}_j^T}_{D \times D}\Big)^{-1} \cdot \frac{1}{n}\sum_{j=1}^{n} \boldsymbol{x}_j y_j = (X^T X)^{-1} X^T y$

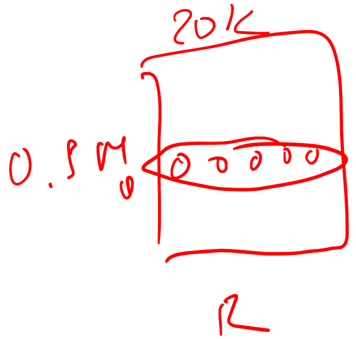
$$= (D \times 1)(1 \times D)$$

  - In our case: $\boldsymbol{p}_i^T = \left(\frac{1}{|S_{*,i}|}\sum_{u \in S_{*,i}} \boldsymbol{q}_u^T \boldsymbol{q}_u\right)^{-1} \cdot \frac{1}{|S_{*,i}|}\sum_{u \in S_{*,i}} \boldsymbol{q}_u^T r_{ui}$
  - Equivalently for $\boldsymbol{q}_u$

- Computation of $\operatorname{argmin}_{\boldsymbol{P}}(\boldsymbol{P}, \boldsymbol{Q}^{(t)})$ reduces to a standard problem

Alternating Optimization: Discussion

- May provide solution to difficult optimization problems
- Here: sequence of simple OLS problems
  - Overall algorithm can be implemented in a few lines in, e.g., Python
  - Quite efficient: since data is sparse, the sets $S_{*,i}$ (and $S_{u,*}$) are relatively small



- **Drawback** of Alternating Optimization:
  - Solution is only an approximation
  - No guarantee that close to the optimal solution
  - Highly depends on initial solution

SGD for Matrix Factorization

- Stochastic Gradient Descent as an alternative

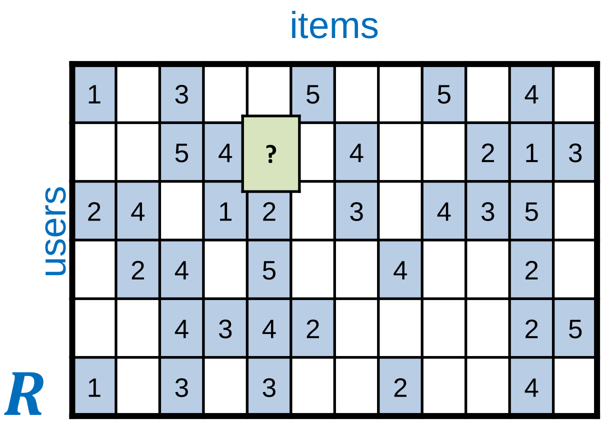
- SGD on the objective $\mathcal{L} := \sum_{(u,\,i) \in S} \left(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}} \right)^2$
  - Pick a random user u and a random item i with rating r_{ui} (batch size 1)
  - Compute the gradients w.r.t. the parameters $\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}_u}$ and $\frac{\partial \mathcal{L}}{\partial \boldsymbol{p}_i}$
  - Update the parameters $\boldsymbol{q}_u \leftarrow \boldsymbol{q}_u - \eta \frac{\partial \mathcal{L}}{\partial \boldsymbol{q}_u}$ $\boldsymbol{p}_i \leftarrow \boldsymbol{p}_i - \eta \frac{\partial \mathcal{L}}{\partial \boldsymbol{p}_i}$

learning rate

- In this case the gradient update step is rather simple
  - $e_{ui} \leftarrow r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}}$ \\ helper variable, the current error
  - $\boldsymbol{q}_u \leftarrow \boldsymbol{q}_u + 2\eta(e_{ui}\,\boldsymbol{p}_i)$
  - $\boldsymbol{p}_i \leftarrow \boldsymbol{p}_i + 2\eta(e_{ui}\,\boldsymbol{q}_u)$

Rating Prediction

- How to estimate the missing rating of user u for item i?



1		3			5			5		4	
		5	4	?		4			2	1	3
2	4		1	2		3		4	3	5	
	2	4		5			4			2	
		4	3	4	2					2	5
1		3		3			2			4	

$$\approx$$

$$\hat{r}_{ui} = \boldsymbol{q}_u \cdot \boldsymbol{p}_i^T = \sum_k q_{uk} \cdot p_{ik}$$

$\boldsymbol{q}_u$ row u of $\boldsymbol{Q}$
$\boldsymbol{p}_i$ row i of $\boldsymbol{P}$

factors

users

$\boldsymbol{Q}$

.1	-.4	.2
-.5	.6	.5
-.2	.3	.5
1.1	2.1	.3
-.7	2.1	-2
-1	.7	.3

•

items

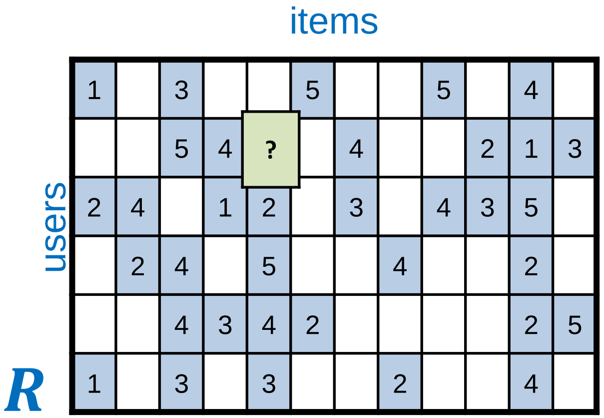
factors

1.1	-.2	.3	.5	-2	-.5	.8	-.4	.3	1.4	2.4	-.9
-.8	.7	.5	1.4	.3	-1	1.4	2.9	-.7	1.2	-.1	1.3
2.1	-.4	.6	1.7	2.4	.9	-.3	.4	.8	.7	-.6	.1

$\boldsymbol{P}^T$

Rating Prediction

- How to estimate the missing rating of user u for item i?



1		3			5			5		4	
		5	4	?		4			2	1	3
2	4		1	2		3		4	3	5	
	2	4		5			4			2	
		4	3	4	2					2	5
1		3		3			2			4	

$\approx$

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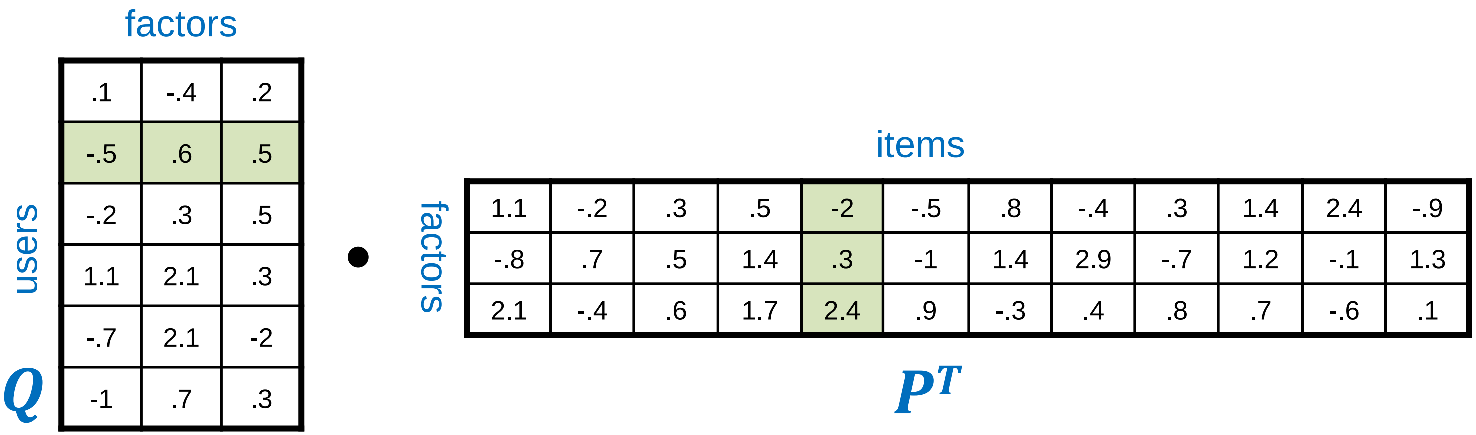

.1	-.4	.2
-.5	.6	.5
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1.1	2.1	.3
-.7	2.1	-2
-1	.7	.3

•

1.1	-.2	.3	.5	-2	-.5	.8	-.4	.3	1.4	2.4	-.9
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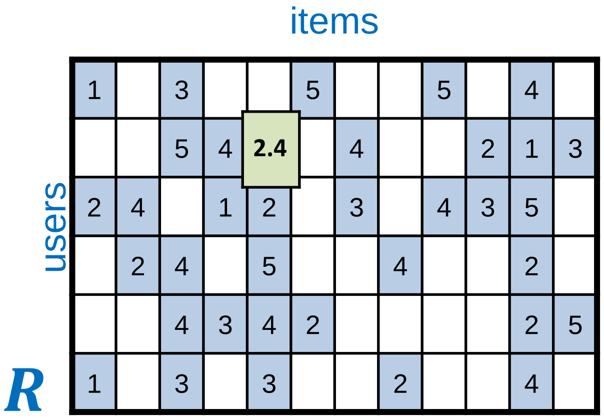
Rating Prediction

- How to estimate the missing rating of user u for item i?



1		3			5			5		4	
		5	4	**2.4**		4			2	1	3
2	4		1	2		3		4	3	5	
	2	4		5			4			2	
		4	3	4	2					2	5
1		3		3			2			4	

$\approx$

$$\hat{r}_{ui} = \boldsymbol{q}_u \cdot \boldsymbol{p}_i^T = \sum_k q_{uk} \cdot p_{ik}$$

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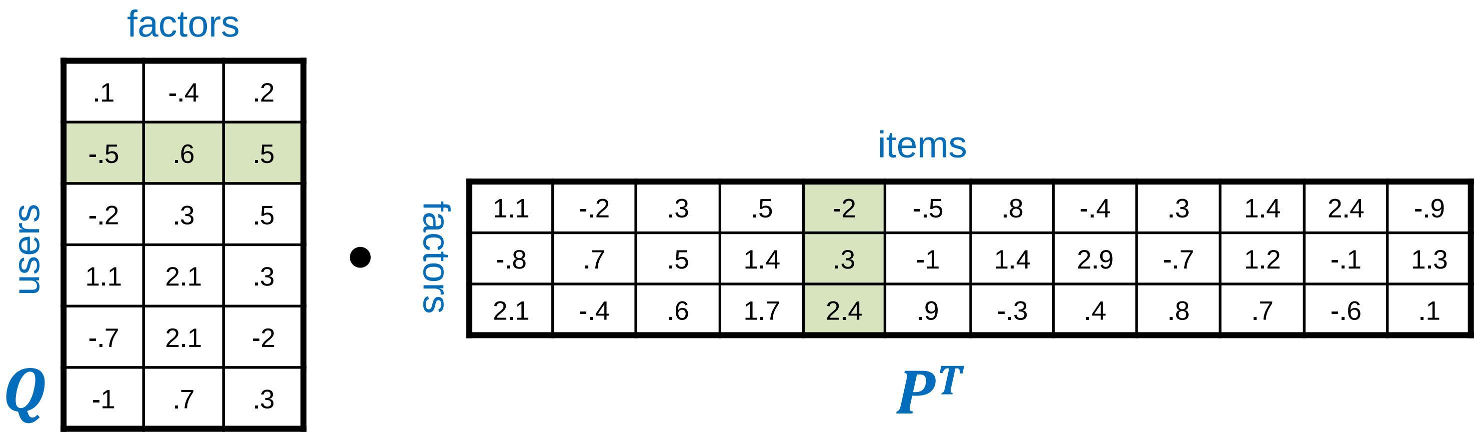

.1	-.4	.2
-.5	.6	.5
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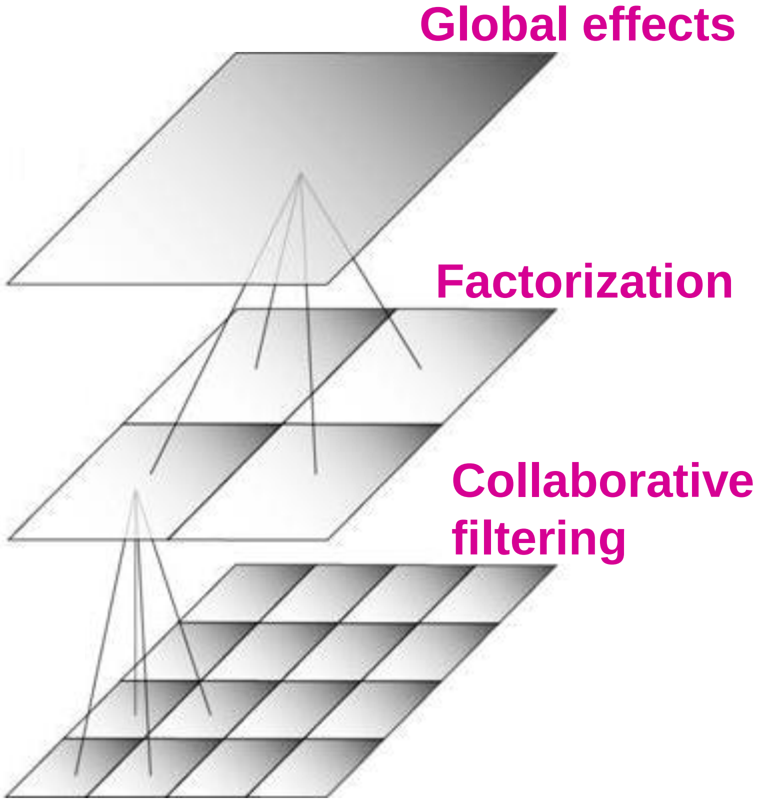
$\bullet$

1.1	-.2	.3	.5	-2	-.5	.8	-.4	.3	1.4	2.4	-.9
-.8	.7	.5	1.4	.3	-1	1.4	2.9	-.7	1.2	-.1	1.3
2.1	-.4	.6	1.7	2.4	.9	-.3	.4	.8	.7	-.6	.1

Side-note: BellKor Recommender System

- The winner of the Netflix Challenge uses matrix factorization as **one** building block
  - The overall model is a combination of multiple ideas

- Multi-scale modeling of the data: Combine top level, "regional" modeling of the data, with a refined, local view:
  - **Global**:
    - Overall deviations of users/movies
  - **Factorization**:
    - Addressing "regional" effects
  - **Collaborative filtering**:
    - Extract local patterns



User and Item Biases

- Certain users might give overly optimistic or pessimistic rating
- Certain movies tend to always have low ratings

- We introduce additional bias terms to capture these effects
  - Each user u can have a bias term b_u
  - Each u~~s~~er item i can have a bias term b_i
  - Additional global bias term b shared by everyone

- The resulting optimization problem can be easily solved with SGD

$$\min_{\substack{\boldsymbol{P},\boldsymbol{Q}\\ b_u, b_i, b}} \sum_{(u,i)\in S} \left(r_{ui} - (\boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}} + b_u + b_i + b)\right)^2$$

- The **cold start** problem is another important issue

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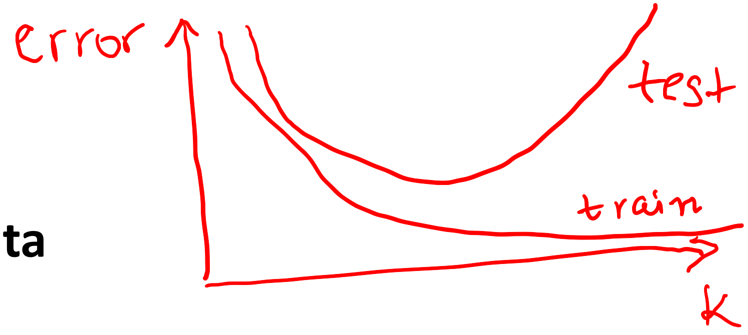
Challenge: Overfitting



- Final Goal: Minimize SSE for **unseen test data**
- Proxy: Minimize SSE on **training data**
  - Want large k (number of factors) to capture all the signals
  - But, SSE on **test data** begins to rise for larger k
  - Why?

- Classical example of overfitting:
  - With too many degrees freedom (too many free parameters) the model starts fitting noise
  - The model fits too well the training data but does not generalize well to unseen test data

Challenge: Overfitting

- Problem can easily be seen in our scenario:
  - In each step of the alternating optimization we solve an OLS regression
    - Number of regression parameters = k = number of latent factors
    - Number of data points used for regression = cardinality of $S_{*,i}$ / $S_{u,*}$
  - Lots of parameters but not enough data points → regression can overfit
  - If k is large this might even lead to an **underdetermined** system of equations
  - Problem is ill-posed

- Solution: **Regularization**
  - Interpretation for underdetermined systems: "In the absence of any other information, the parameter vector should be small (i.e. only small effect of features)“
  - Equivalently: We put a prior on the weights

Regularization

- To solve overfitting we introduce regularization:
  - Allow rich model where we have sufficient data
  - Shrink aggressively where data are scarce

$$\min_{\boldsymbol{P},\boldsymbol{Q}} \underbrace{\sum_{(u,i)\in S} \left(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}}\right)^2}_{\text{“error”}} + \underbrace{\left[\lambda_1 \sum_u \|\boldsymbol{q}_u\|^2 + \lambda_2 \sum_i \|\boldsymbol{p}_i\|^2\right]}_{\text{“length”}}$$

  - λ_1 and λ_2 are user-defined regularization parameters

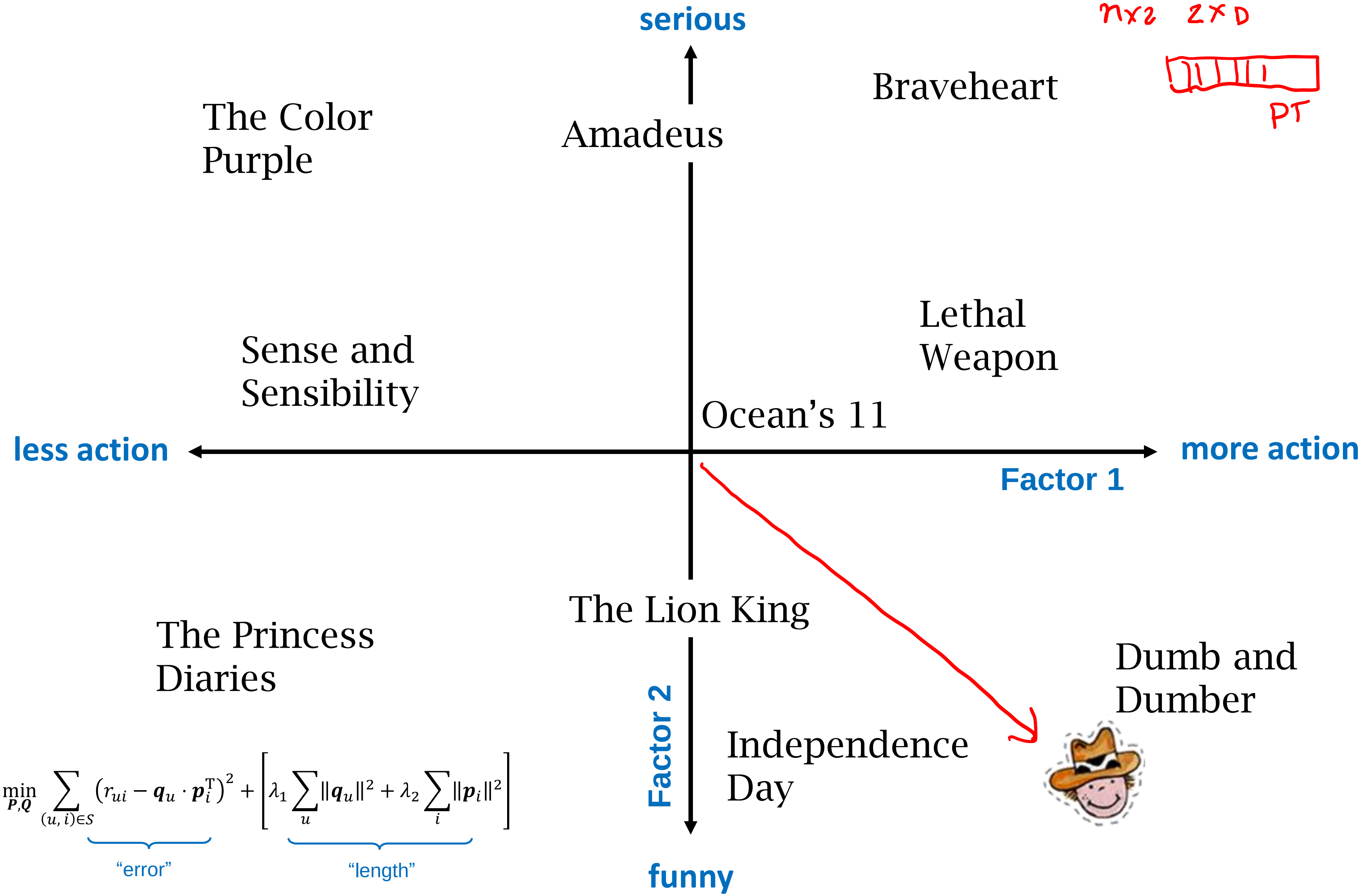
- Note: We do not care about the actual value of the objective function, but we care about the $\boldsymbol{P}, \boldsymbol{Q}$ that achieve the minimum of the objective

The Effect of Regularization

$R \approx Q \cdot P^T$

$n \times 2 \quad 2 \times D$

P^T



serious

The Color Purple

Amadeus

Braveheart

Sense and Sensibility

Lethal Weapon

Ocean's 11

less action

more action

Factor 1

The Princess Diaries

The Lion King

Dumb and Dumber

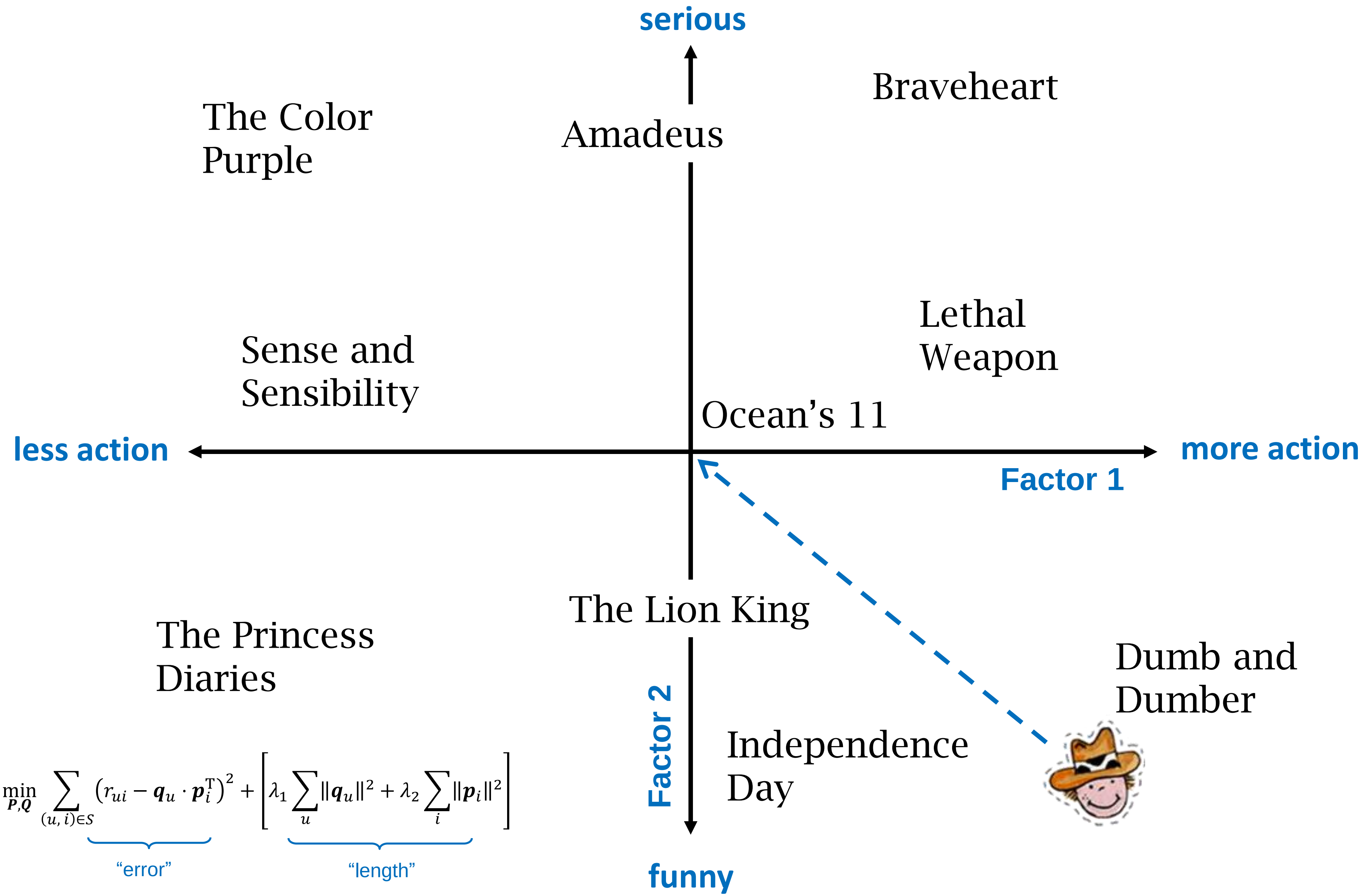
Independence Day

Factor 2

funny

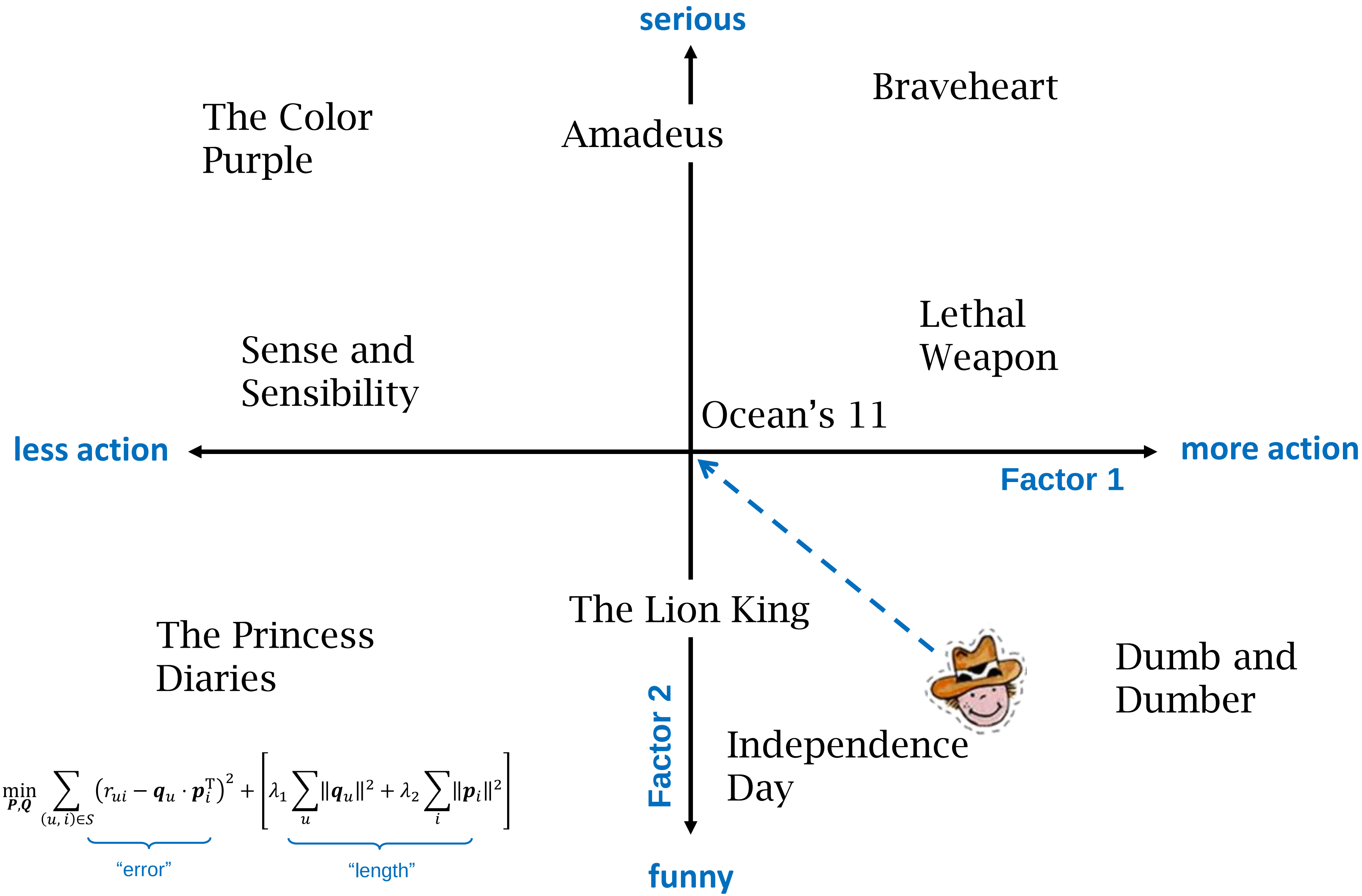
$$\min_{\boldsymbol{P},\boldsymbol{Q}} \underbrace{\sum_{(u,i)\in S} (r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}})^2}_{\text{“error”}} + \underbrace{\left[\lambda_1 \sum_u \|\boldsymbol{q}_u\|^2 + \lambda_2 \sum_i \|\boldsymbol{p}_i\|^2\right]}_{\text{“length”}}$$

The Effect of Regularization



$$\min_{\boldsymbol{P},\boldsymbol{Q}} \sum_{(u,i)\in S} \underbrace{\left(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}}\right)^2}_{\text{“error”}} + \underbrace{\left[\lambda_1 \sum_u \|\boldsymbol{q}_u\|^2 + \lambda_2 \sum_i \|\boldsymbol{p}_i\|^2\right]}_{\text{“length”}}$$

The Effect of Regularization



serious

Braveheart

The Color Purple

Amadeus

Lethal Weapon

Sense and Sensibility

Ocean’s 11

less action

more action

Factor 1

The Lion King

The Princess Diaries

Dumb and Dumber

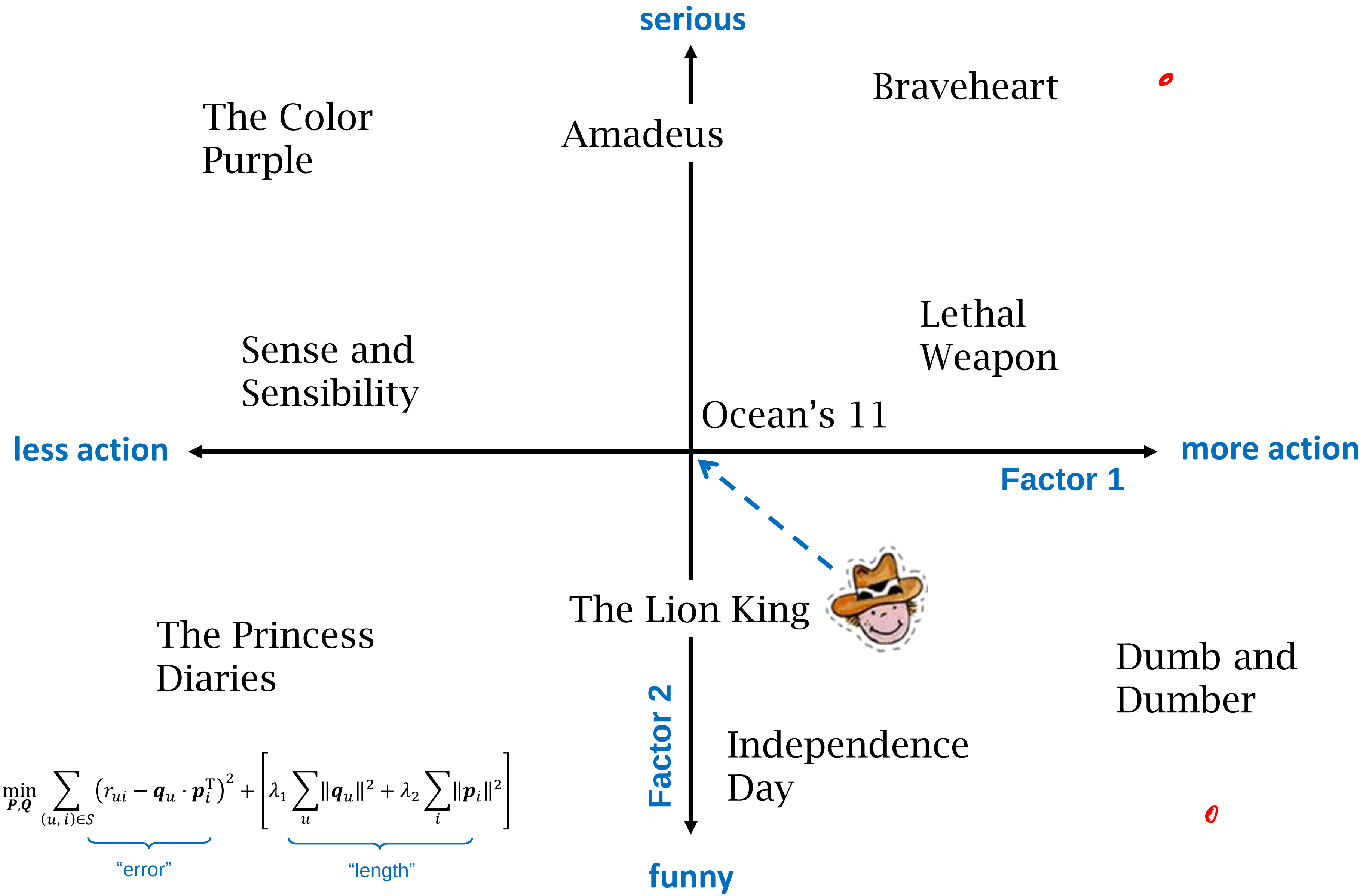
Factor 2

Independence Day

funny

$$\min_{\boldsymbol{P},\boldsymbol{Q}} \sum_{(u,i)\in S} \underbrace{(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}})^2}_{\text{“error”}} + \left[\underbrace{\lambda_1 \sum_u \|\boldsymbol{q}_u\|^2 + \lambda_2 \sum_i \|\boldsymbol{p}_i\|^2}_{\text{“length”}}\right]$$

The Effect of Regularization



$$\min_{\boldsymbol{P},\boldsymbol{Q}} \sum_{(u,i)\in S} \underbrace{(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}})^2}_{\text{“error”}} + \left[\underbrace{\lambda_1 \sum_u \|\boldsymbol{q}_u\|^2 + \lambda_2 \sum_i \|\boldsymbol{p}_i\|^2}_{\text{“length”}} \right]$$

Regularization in Our Use Case

- Regularized Problem: $\min_{\boldsymbol{P},\boldsymbol{Q}} \sum_{(u,\,i)\in S} \left(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}}\right)^2 + \left[\lambda_1 \sum_u \|\boldsymbol{q}_u\|^2 + \lambda_2 \sum_i \|\boldsymbol{p}_i\|^2\right]$
- Recap of unregularized problem: In each iteration of the alternating optimization we solved an OLS regression problem
- For the regularized version this becomes **ridge regression**
  - $\min_{\boldsymbol{p}_i} \sum_{i\in S_{*,i}} \left(r_{ui} - \boldsymbol{q}_u \cdot \boldsymbol{p}_i^T\right)^2 + \lambda_2 \|\boldsymbol{p}_i\|^2$
  - Effect: parameter values are forced to become smaller
  - Large values that only capture noise are avoided

- You know how to solve this!
  - Closed form solution (see linear regression slides)
  - Gradient decent

$(X^T X + \lambda I)^{-1} X^T y$

SGD for MF with Regularization and Biases

- SGD on the objective

$$\mathcal{L} := \min_{\substack{\boldsymbol{P},\boldsymbol{Q}\\ b_u, b_i, b}} \sum_{(u,\,i)\in S} \left(r_{ui} - (\boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}} + b_u + b_i + b)\right)^2 + \left[\lambda_1 \sum_u \|\boldsymbol{q}_u\|^2 + \lambda_2 \sum_i \|\boldsymbol{p}_i\|^2\right]$$

- Pick a random user u and a random item i with rating r_{ui} (batch size 1)
- The gradient update step is very similar to before
  - $e_{ui} \leftarrow r_{ui} - (\boldsymbol{q}_u \cdot \boldsymbol{p}_i^{\mathrm{T}} + b_u + b_i + b)$ \\ helper variable, the current error
  - $\boldsymbol{q}_u \leftarrow \boldsymbol{q}_u + 2\eta(e_{ui}\, \boldsymbol{p}_i - \lambda_1 \boldsymbol{q}_u)$
  - $\boldsymbol{p}_i \leftarrow \boldsymbol{p}_i + 2\eta(e_{ui}\, \boldsymbol{q}_u - \lambda_2 \boldsymbol{p}_i)$

$\|\cdot\|_2$ $\|\cdot\|_1$

  - $b_u \leftarrow b_u + \eta e_{ui}$
  - $b_i \leftarrow b_i + \eta e_{ui}$
  - Usually directly set b to the global mean $b = \frac{1}{|S|}\sum_{(u,\,i)\in S} r_{ui}$

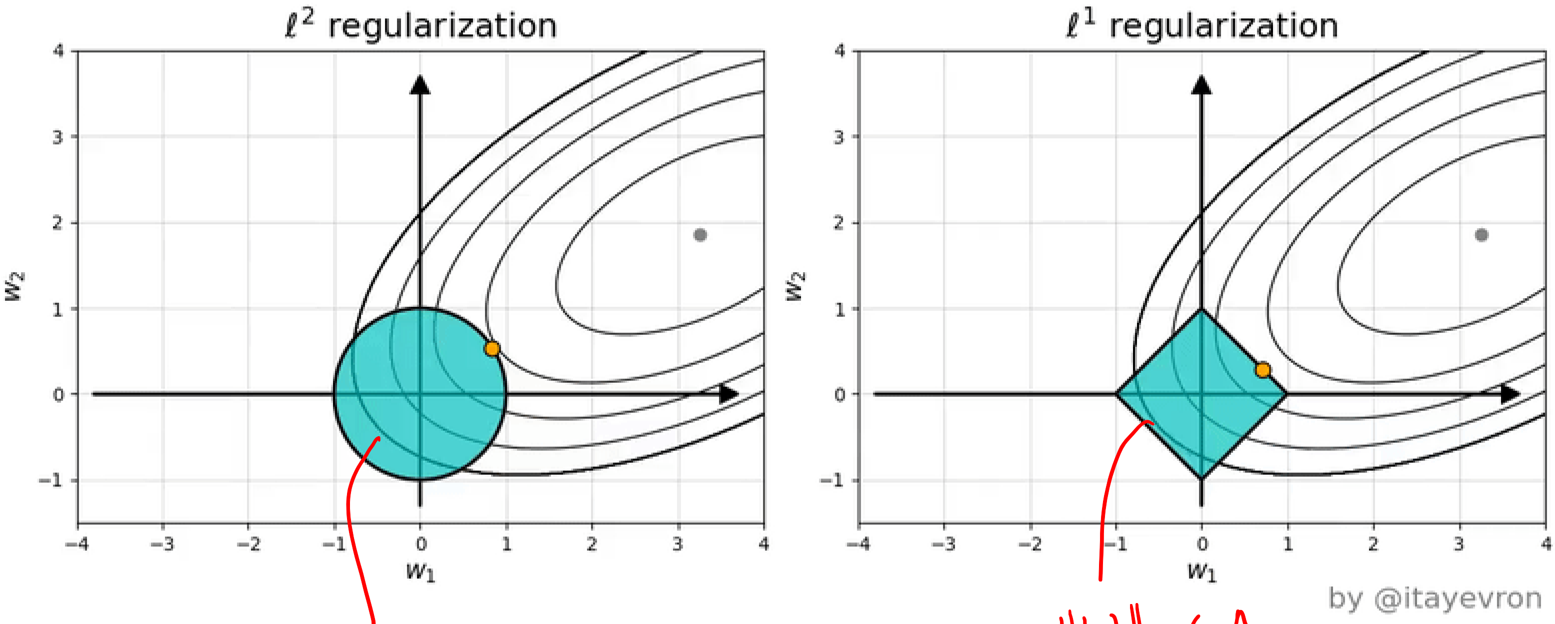
L2 vs. L1 Regularization

- Comparison: L2 vs. L1 regularization
  - L2 tries to "shrink" the parameter vector $\boldsymbol{w}$ **equally**
    - Large values are highly penalized due to the square in the L2 norm
    - Unlikely that any component will be **exactly 0**
  - L1 allows large values in individual components of $\boldsymbol{w}$ by shrinking other components to 0
  - L1 is suited to enforce **sparsity** of the parameter vector

- Why sparsity?
  - Better interpretation
    - Only few values contribute to result
    - Unintuitive that **sparse input data** is generated based on **dense signal**
  - Less storage, faster processing

L2 vs. L1 Intuition

- An L1 constraint promotes sparsity



by @itayevron

$\|w\|_2 \le 1$

$\|w\|_1 \le 1$

$$\min_{w} f(w) \quad \xrightarrow{\underline{\text{dual}}} \quad f(w) + \lambda(\|w\|-1)$$

$\|w\| \le 1$

Roadmap

- Chapter: Dimensionality Reduction & Matrix Factorization

  1. Introduction
  2. Principal Component Analysis (PCA)
  3. Singular Value Decomposition (SVD)
  4. **Matrix Factorization**
     - Motivation & Approach
     - Regularization & Sparsity
     - **Further Factorization Models**
  5. Neighbor Graph Methods
  6. Autoencoders (Non-linear Dimensionality Reduction)

Further Factorization Models

- Matrix factorization is extremely powerful
  - Dimensionality reduction, data analysis/data understanding, prediction of missing values, …

- Various extensions have been proposed
  - Enforcing different constraints or operating on different data types
  - Important goal: better interpretation of result

- Non-Negative Matrix Factorization (next slides)
- Boolean Matrix Factorization
  - Factorize Boolean $\boldsymbol{A}$ in Boolean $\boldsymbol{Q}$ and $\boldsymbol{P}$

Non-Negative Matrix Factorization

- Often data is given in form of non-negative values
  - Rating values between 1 to 5; income, age, … of persons; number of words in a document; grayscale images; etc.

- However: SVD (and the other approaches presented before) might lead to factors containing **negative values**
  - Difficult to interpret: non-negative data is "generated" based on negative factors; what do these negative factors mean?
  - Predicted values might also become negative

- Solution: Non-Negative Matrix Factorization

Non-Negative Matrix Factorization

- Task: Factorize non-negative $\boldsymbol{A}$ in non-negative $\boldsymbol{Q}$ and $\boldsymbol{P}$, i.e. $\mathbf{A} \approx \boldsymbol{Q} \cdot \boldsymbol{P}^{\boldsymbol{T}}$

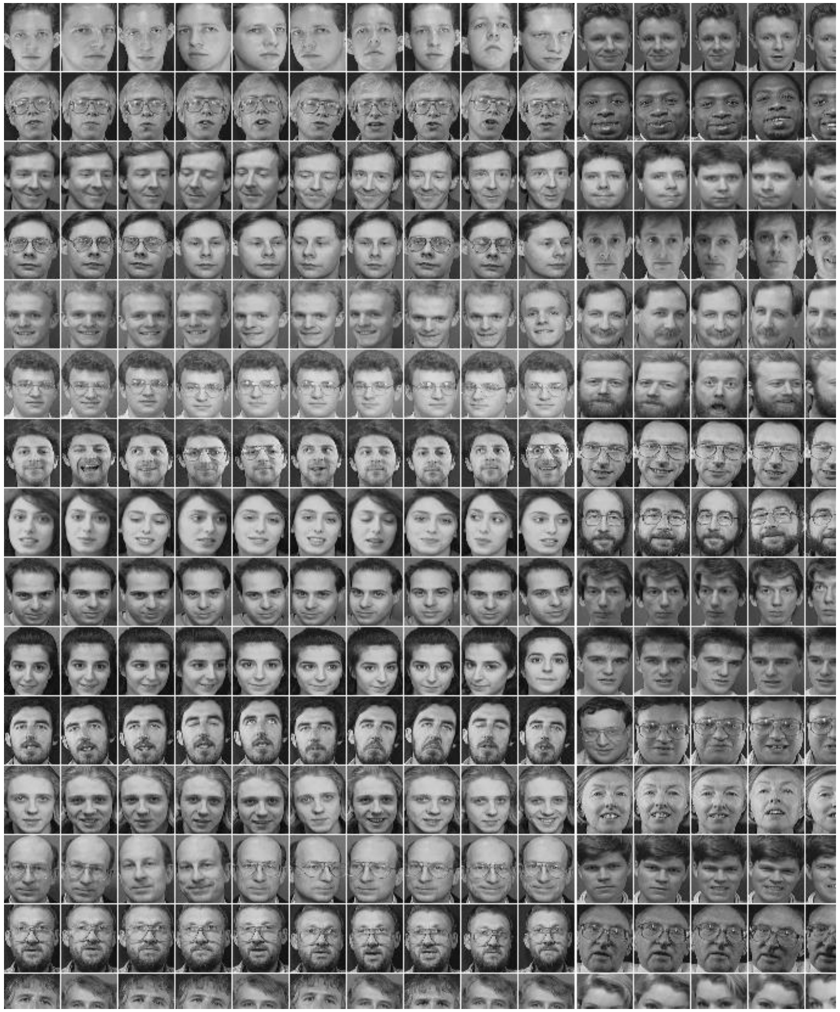
- Formally:
  - Given $\boldsymbol{A} \in \mathbb{R}^{n \times d}$ with $\boldsymbol{A}_{ij} \geq 0$ and integer k, find $\overset{Q}{\cancel{\boldsymbol{P}}} \in \mathbb{R}^{n \times k}, \overset{P}{\cancel{\boldsymbol{Q}}} \in \mathbb{R}^{\overset{d \times k}{\cancel{k \times d}}}$ such that $\left\| \boldsymbol{A} - \boldsymbol{Q} \cdot \boldsymbol{P}^{\boldsymbol{T}} \right\|_F$ is minimized subject to $\boldsymbol{Q} \geq 0$ and $\boldsymbol{P} \geq 0$

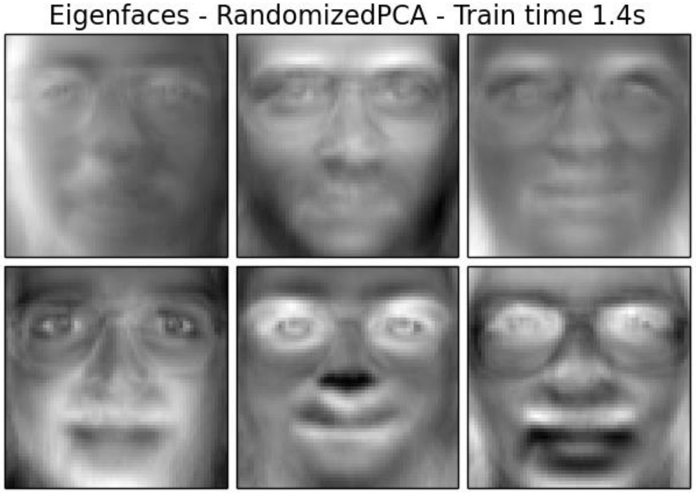
$$\min_{\boldsymbol{P} \geq 0, \boldsymbol{Q} \geq 0} \left\| \boldsymbol{A} - \boldsymbol{Q} \cdot \boldsymbol{P}^{\boldsymbol{T}} \right\|_F$$

  - Constrained optimization

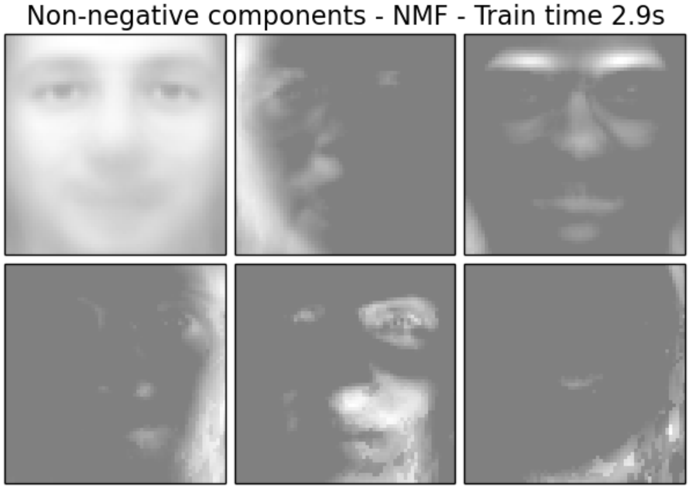
NNMF Example: Olivetti Faces Data

$X =$





Eigenfaces - RandomizedPCA - Train time 1.4s



Non-negative components - NMF - Train time 2.9s

results according to scikit-learn

Roadmap

- Chapter: Dimensionality Reduction & Matrix Factorization
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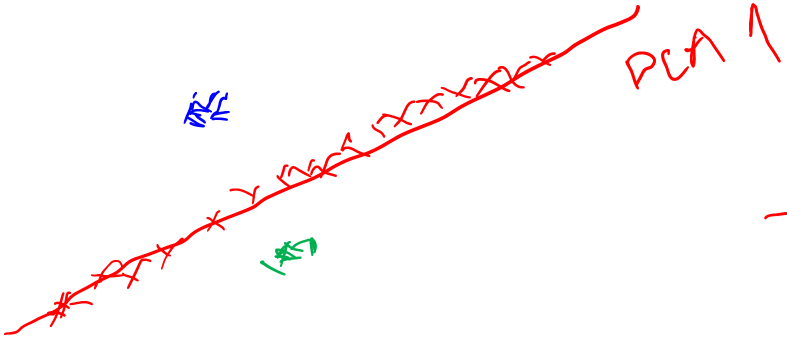
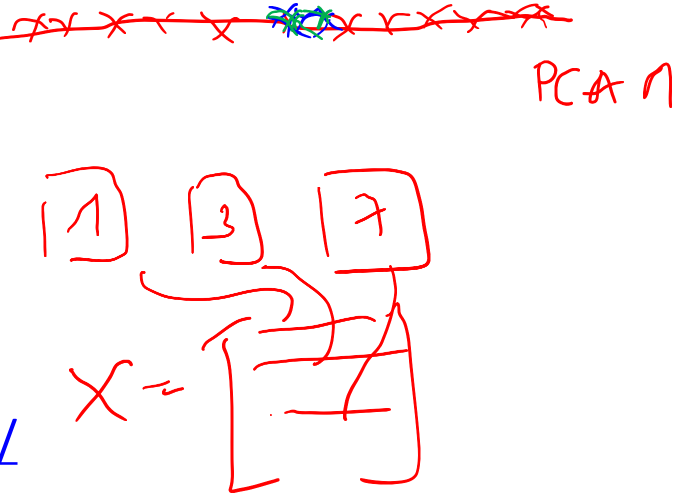
  3. Singular Value Decomposition (SVD)
  4. Matrix Factorization
  5. **Neighbor Graph Methods**
  6. Autoencoders (Non-linear Dimensionality Reduction)

Preserving global vs. preserving local similarity

- PCA tries to find a global structure
  - Can lead to local inconsistencies
  - Far away point can become nearest neighbors
- Illustration (during lecture):



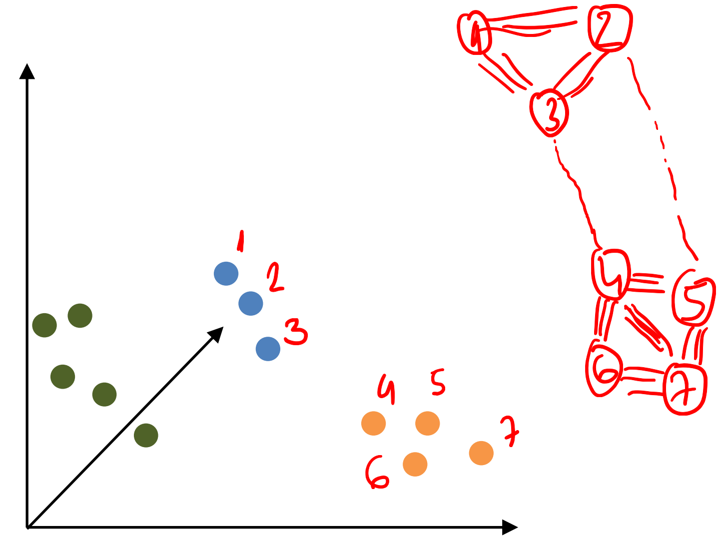


- Idea: Preserve local structure instead
- Example: https://projector.tensorflow.org/

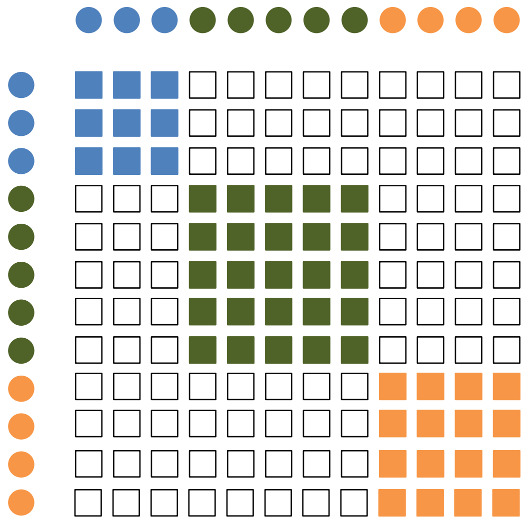
Neighbor Graph Methods

- All methods we have seen so far are based on **matrix factorizations**
- An alternative class of methods based on **neighbor graphs**

Highdimensional data:



Neighbor / similarity graph:



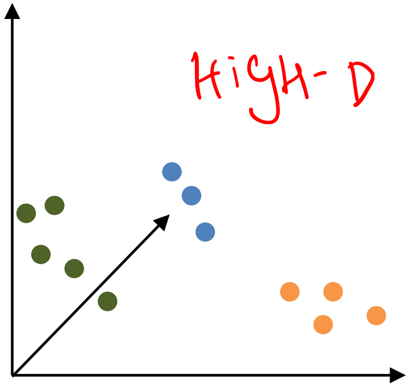
- Idea: Low dimensional neighborhood similar to the original neighborhood

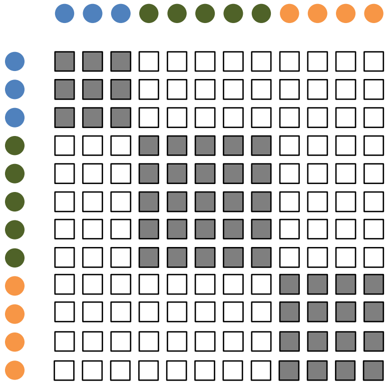
Neighbor Graph Methods

■ - High similarity

□ - low similarity

1. Construct neighbor graph of high-dimensional data
2. Initialize points in low-dimensional space
3. Optimize coordinates in low-dimensional space s.t. similarities align





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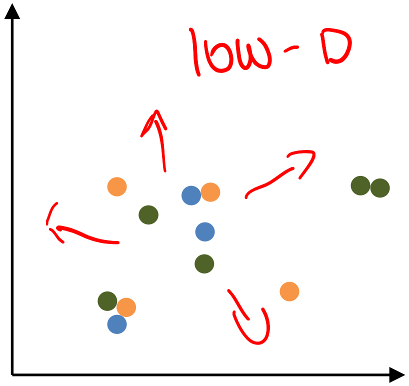
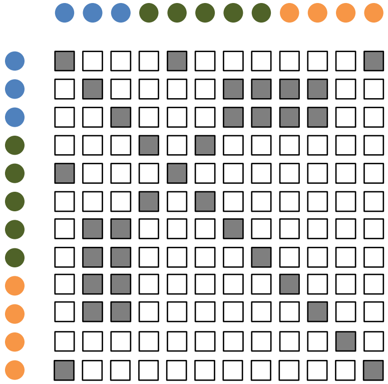
adjacency matrix of the graph /

pairwise similarity matrix /

pairwise distance matrix





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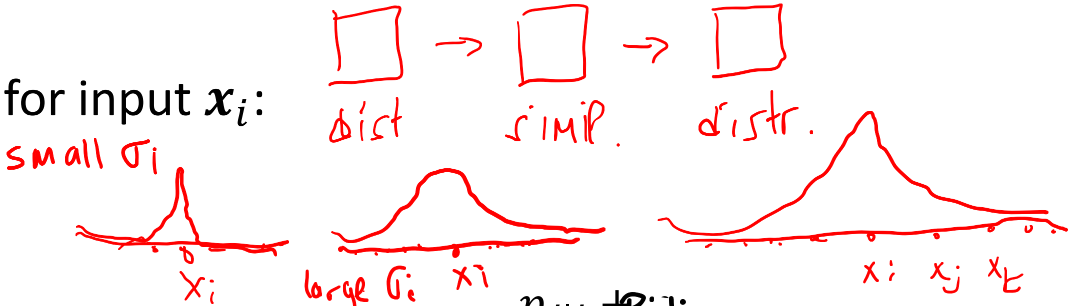
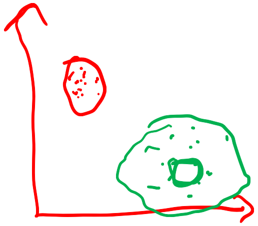
t-SNE: t-Distributed Stochastic Neighbor Embedding

- High-dimensional similarities for input $\boldsymbol{x}_i$:



$$p_{j|i} = \frac{\exp\left(-\frac{\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2}{2\sigma_i^2}\right)}{\sum_{k\neq i} \exp\left(-\frac{\|\boldsymbol{x}_i - \boldsymbol{x}_k\|^2}{2\sigma_i^2}\right)} \qquad p_{ii} = 0 \qquad p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$$



  - σ_i chosen to achieve fixed perplexity (effective number of neighbors)

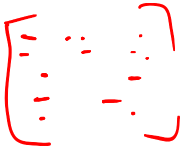
$x_i = [0\ 0.1\ 2\ 3\ 4\ 5\ ]$

$x_j = [\ .\ \ .\ \ .\ \ .\ \ .\ \ .\ \ .\ ]$

- Low-dimensional similarities for (to be optimized) parameters $\boldsymbol{y}_i$:

variables to be optimized

$$q_{ij} = \frac{\left(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2\right)^{-1}}{\sum_k \sum_{l\neq k} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}} \qquad q_{ii} = 0$$



- Minimize the KL divergence: $\min\limits_{\boldsymbol{y}_i} KL(P||Q) = \sum\limits_i \sum\limits_{j\neq i} p_{ij} \log \frac{p_{ij}}{q_{ij}}$

Note on the KL Divergence

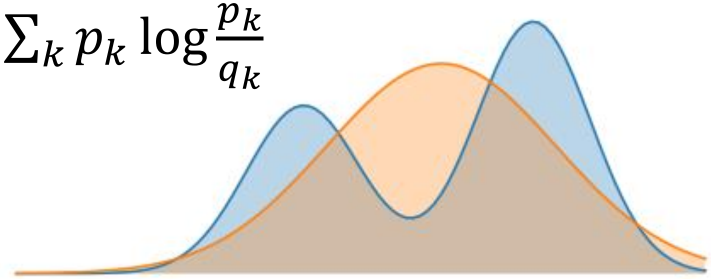
$P = [p_1\ p_2 \ldots p_K]$

$p(\theta) = q = [q_1\ q_2 \cdots q_K]$

- $KL(P||Q) \geq 0$ for any P and Q, $KL(P||Q) = 0$ iff $P = Q$
- The KL Divergence is asymmetric $KL(P||Q) \neq KL(\mathrm{Q}||\mathrm{P})$
  - Example: Given P we are optimizing over Q

$\int$

- $KL(P||Q) = \sum_k p_k \log \frac{p_k}{q_k}$

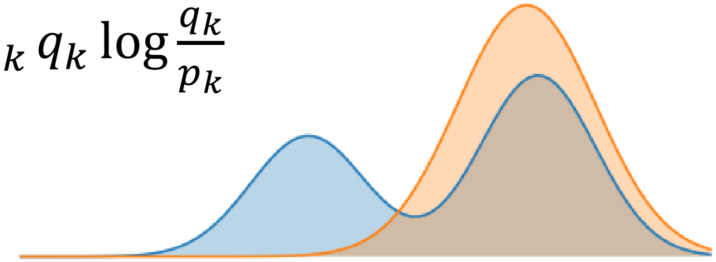


Forward KL is Mean-Seeking

$KL(P||Q)$

$\int$

- $KL(\mathrm{Q}||\mathrm{P}) = \sum_k q_k \log \frac{q_k}{p_k}$

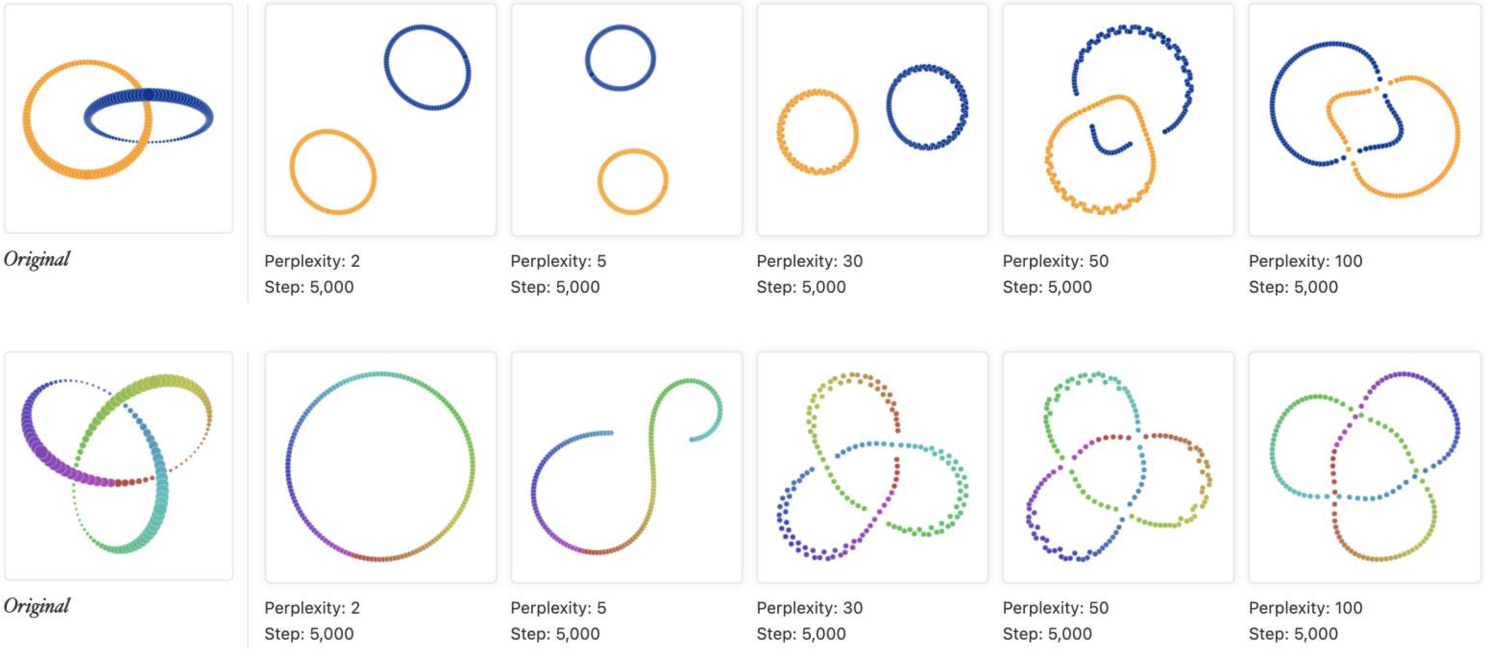


Reverse KL is Mode-Seeking

$KL(\mathrm{Q}||\mathrm{P})$

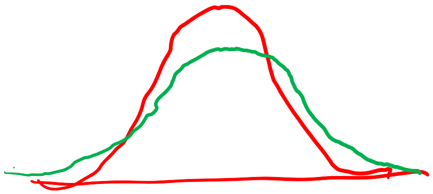
Figures adapted from Dibya Ghosh.

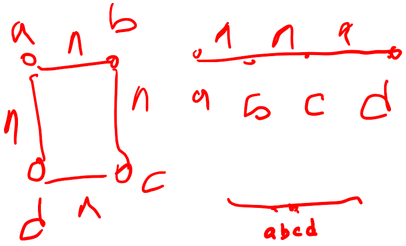
Interactive t-SNE



Source of illustration, for more details and interactive widgets.

The Advantages and Disadvantages of t-SNE



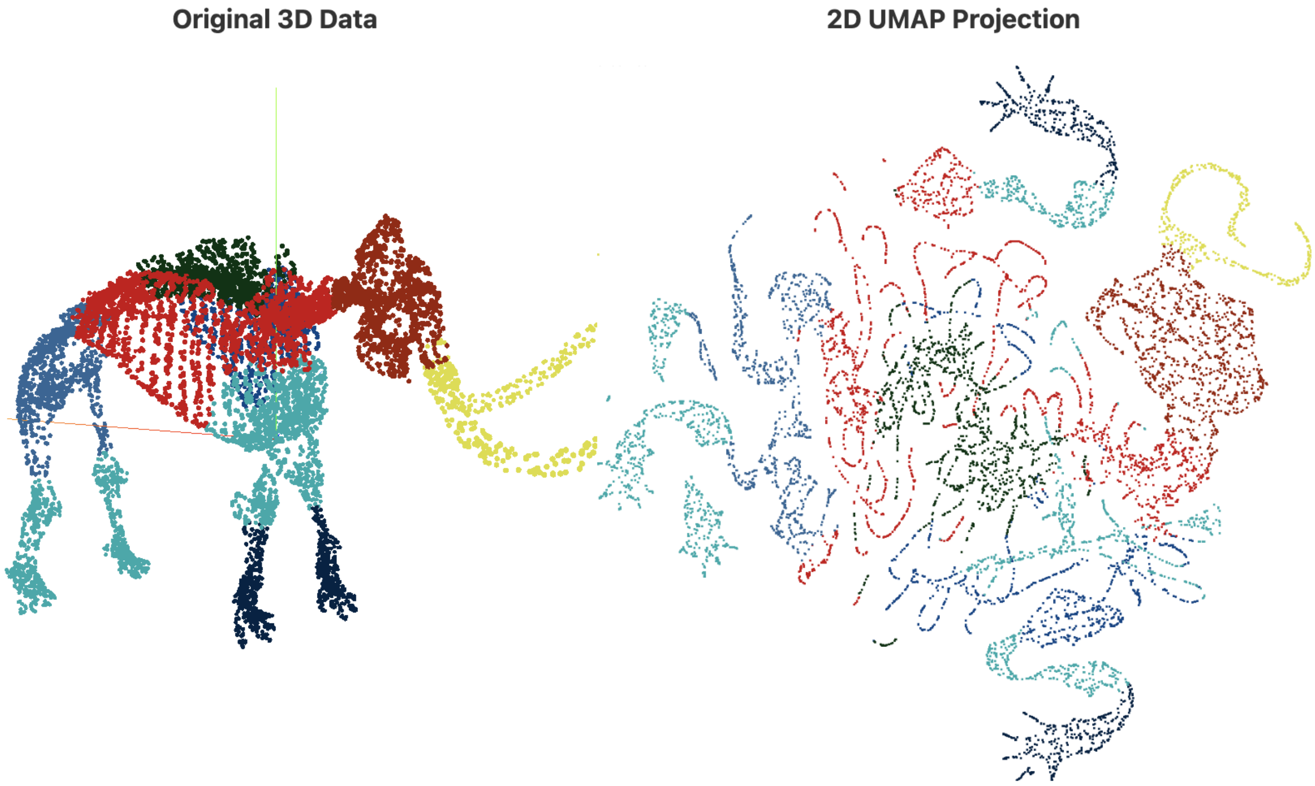


- The current standard for visualizing high-dimensional data
- Helps understand ”black-box” algorithms like DNN
- Reduced ”crowding problem” with heavy tailed distribution

- t-SNE plots can sometimes be mysterious or misleading
  - Be careful with cluster sizes and cluster distances
- Can be sensitive to hyperparameters
  - Random noise does not always look random
- No easy way to compute the embedding of new data
- Not great for more than 3 dimensions

Uniform Manifold Approximation and Projection

- Principled approach relying on toplogical spaces, category theory, …



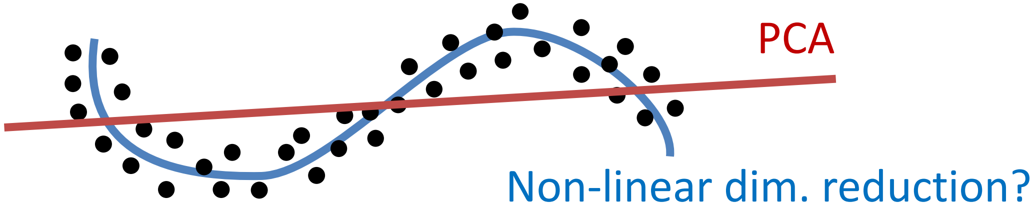
Link for details, widgets, a comparison to T-SNE, …

Roadmap

- Chapter: Dimensionality Reduction & Matrix Factorization
  1. Introduction
  2. Principal Component Analysis (PCA)
  3. Singular Value Decomposition (SVD)
  4. Matrix Factorization
  5. Neighbor Graph Methods
  6. **Autoencoders (Non-linear Dimensionality Reduction)**

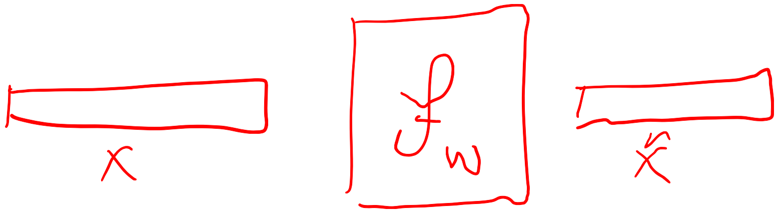
Motivation

- PCA / SVD can only capture linear structure (linear variations in the data)
  - Recall: transformed data is $\boldsymbol{Y} = \widetilde{\mathbf{X}} \cdot \boldsymbol{\Gamma}$
  - Linear projection by the eigenvectors $\boldsymbol{\Gamma}$
- However, data often lies on a non-linear low-dimensional manifold



- Idea: find a non-linear projection of the data

Autoencoders



- An **autoencoder** is a neural network that:
  - finds a compact representation of the data
  - by learning to reconstruct its input

$$f(\boldsymbol{x}, \boldsymbol{W}) \coloneqq \hat{\boldsymbol{x}} \approx \boldsymbol{x}$$

- Goal: minimize the reconstruction error between $\hat{\boldsymbol{x}}$ and $\boldsymbol{x}$

$$\min_{\boldsymbol{W}} \frac{1}{N} \sum_{i=1}^{N} \| f(\underset{\uparrow\,\text{noisy}}{\boldsymbol{x}_i}, \boldsymbol{W}) - \underset{\uparrow\,\text{clean}}{\boldsymbol{x}_i} \|^2$$

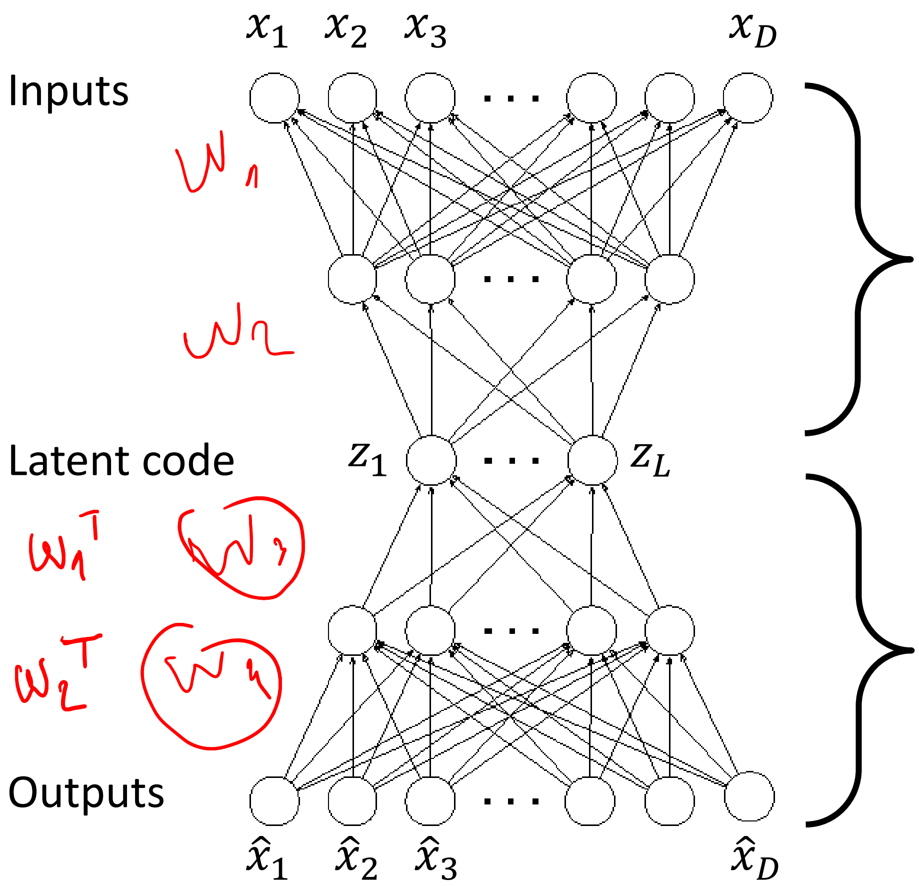
- Alternative view: find a **latent representation** $\boldsymbol{z} \in \mathbb{R}^L$ which is a compact code for $\boldsymbol{x} \in \mathbb{R}^D$ since $L \ll D$
  - $f_{enc}(\boldsymbol{x}) = \mathbf{z}$ # encoder: project the data to a lower dimension
  - $f_{dec}(\boldsymbol{z}) \approx \boldsymbol{x}$ # decoder: reconstruct the data from the latent code

$$f_{dec}\left(f_{enc}(\boldsymbol{x})\right) \approx \boldsymbol{x}$$

Autoencoders

- f_{enc} and f_{dec} are non-linear functions implemented by a neural network

$\sigma(\sigma(xw_1)w_2)$

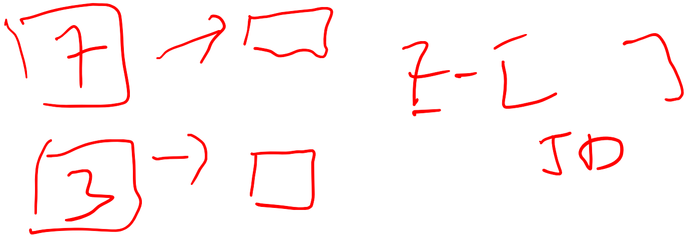


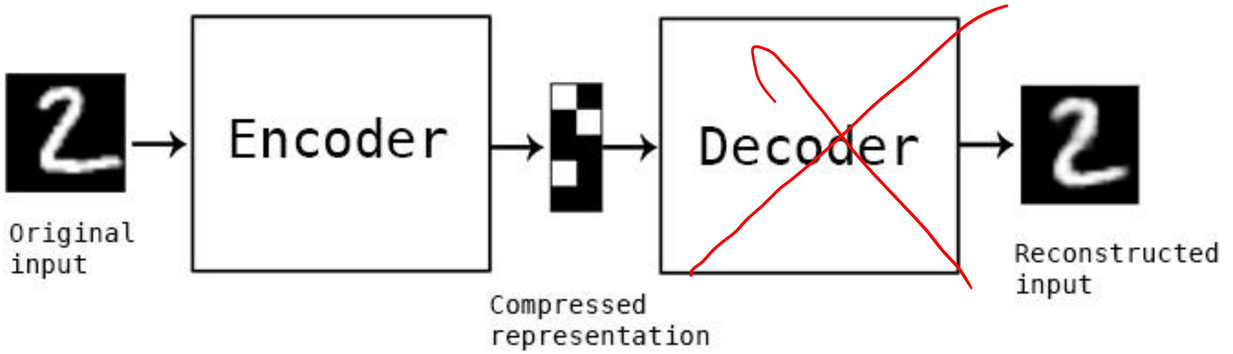
Encoder

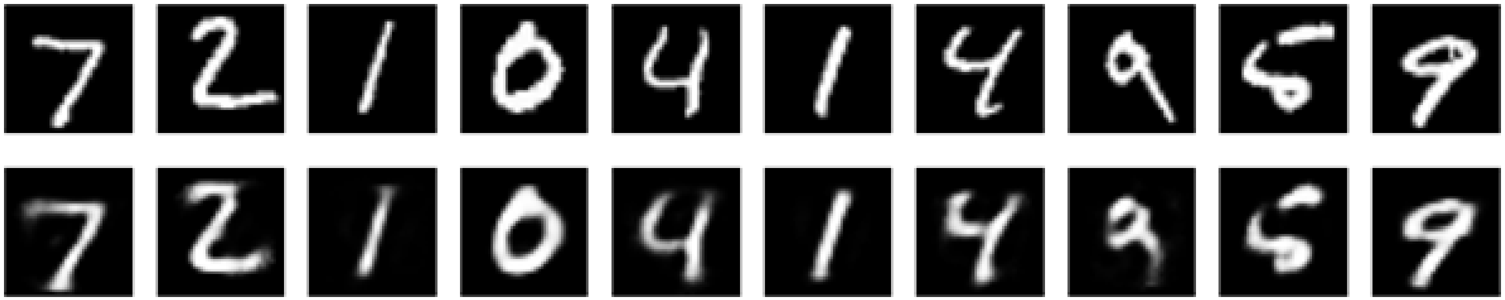
Bottleneck ($L \ll D$):
middle layer has fewer neurons

Decoder

Autoencoders: Example







Original image:

Reconstruction:

Autoencoders

- An autoencoder whose code dimension is less than the input dimension ($L \ll D$) is called **undercomplete**
  - Forces the autoencoder to capture the most salient features of the data
  - $L \geq D$ (**overcomplete**) the autoencoder can simply learn the identity function

- Training autoencoders in practice:
  - Add a regularization term to the SSE loss to prevent overfitting
  - Weight tying: f_{enc} and f_{dec} share the same weights

- Other extensions:
  - Denoising autoencoders (DAEs): receive a corrupted (noisy) training data point as input and predict the "clean" uncorrupted data point as output
  - Variational autoencoders (covered in our MLGS lecture)

(Linear) Autoencoders & PCA: Comparison

- What if f_{enc} and f_{dec} are linear functions?
  - $f_{enc}(\boldsymbol{x}, \boldsymbol{W}_1) = \boldsymbol{x}\boldsymbol{W}_1$ # $\boldsymbol{W}_1 \in \mathbb{R}^{D \times L}$
  - $f_{dec}(\boldsymbol{z}, \boldsymbol{W}_2) = \boldsymbol{z}\boldsymbol{W}_2$ # $\boldsymbol{W}_2 \in \mathbb{R}^{L \times D}$

$$\underset{D \times D}{W} := \underset{D \times L}{W_1} \, \underset{L \times D}{W_2}$$

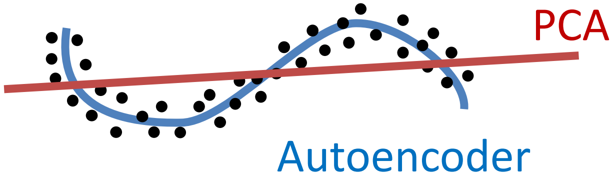
- We have: $f_{dec}\big(f_{enc}(\boldsymbol{x})\big) = \boldsymbol{x}\boldsymbol{W}_1\boldsymbol{W}_2$ and

$$\min_{\boldsymbol{W}_1\boldsymbol{W}_2} \frac{1}{N}\sum_{i=1}^{N} \|f(\boldsymbol{x}_i, \boldsymbol{W}) - \boldsymbol{x}_i\|^2 = \min_{\boldsymbol{W}_1\boldsymbol{W}_2} \frac{1}{N}\sum_{i=1}^{N} \|\boldsymbol{x}_i\boldsymbol{W}_1\boldsymbol{W}_2 - \boldsymbol{x}_i\|^2 = \underbrace{\min_{\boldsymbol{W}} \frac{1}{N}\sum_{i=1}^{N} \|\boldsymbol{x}_i\boldsymbol{W} - \boldsymbol{x}_i\|^2}_{\text{Equivalent: } \boldsymbol{W}_1\boldsymbol{W}_2 = \boldsymbol{W} \text{ s.t. rank of } \boldsymbol{W} \text{ is L}}$$

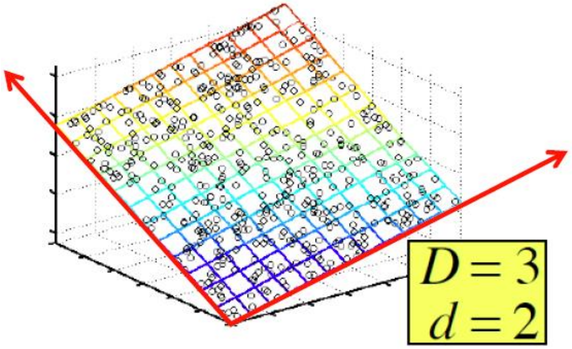
- Optimal solution (assuming normalization):
  - PCA: $\boldsymbol{W}^* = \boldsymbol{\Gamma}$ where $\boldsymbol{\Gamma}$ are the (top-L) eigenvectors of $\boldsymbol{X}^T\boldsymbol{X}$

Summary

- Dimensionality Reduction and Matrix Factorization are highly related
  - And can be used for various purposes
- PCA, SVD (and linear Autoencoders) are equivalent
  - Optimal low-rank approximation



- Matrix factorization for rating prediction
  - Very general formulation: allows to handle, e.g., missing entries
- Autoencoders and t-SNE perform non-linear dimensionality reduction
- Why are these techniques useful?
  - Less storage required
  - More efficient processing of the data
  - Remove redundant and noisy features
  - Discover hidden correlations/topics/concepts
  - Interpretation and visualization



Reading material

Reading material

- Bishop, chapters: 12.1, 12.2.1
- Leskovec, Rajaraman, Ullman - Mining of Massive Datasets: chapter 11
- Goodfellow - Deep Learning: chapter 14
- t-SNE
- Understanding UMAP