# INTRODUCTION TO DATA SCIENCE

This lecture is based on course by E. Fox and C. Guestrin, Univ of Washington

WFAiS UJ, Informatyka Stosowana I stopień studiów

#### Dimensionality reduction

- Input data may have thousands or millions of dimensions!
  - e.g., text data
- Dimensionality reduction: represent data with fewer dimensions
  - easier learning fewer parameters
  - visualization hard to visualize more than 3D or 4D
  - discover "intrinsic dimensionality" of data
    - high dimensional data that is truly lower dimensional

 Rather than picking a subset of the features, we can create new features that are combinations of existing features

ithobs 
$$= 2.5 \times i \times 17 + 3 \times i \times 27 + 7 \times i \times 137 + \cdots$$

$$= 2i \times 27 = 2.5 \times i \times 17 + 3 \times i \times 127 + 7 \times i \times 137 + \cdots$$

$$= 2i \times 27 = 2.5 \times i \times 17 + 3 \times i \times 127 + 7 \times i \times 137 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + 7 \times i \times 137 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + 7 \times i \times 137 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + 7 \times i \times 137 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + 7 \times i \times 137 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + 7 \times i \times 137 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + 7 \times i \times 127 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + 7 \times i \times 127 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + 7 \times i \times 127 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + 3 \times i \times 127 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times i \times 17 + \cdots$$

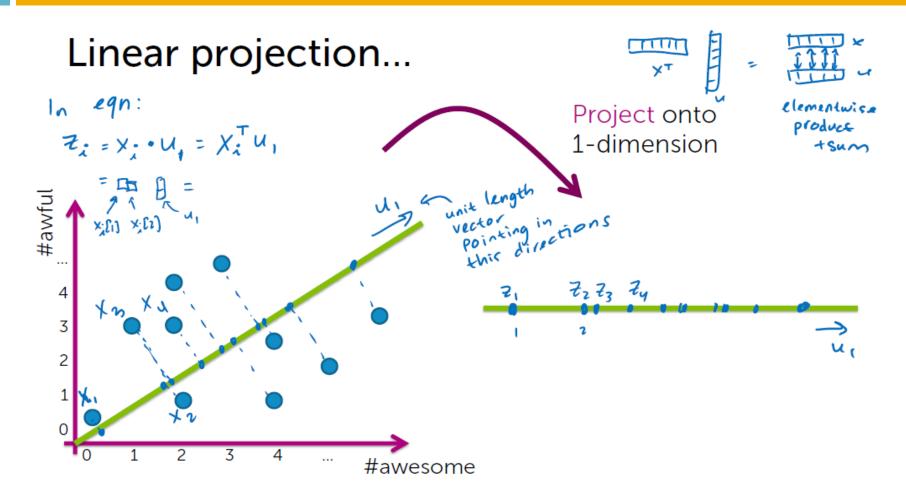
$$= 2i \times 17 = 2.5 \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times 17 + \cdots$$

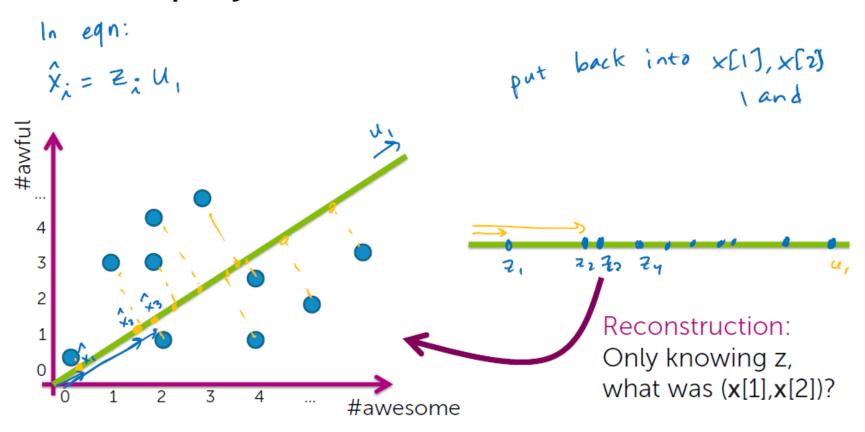
$$= 2i \times 17 = 2.5 \times 17 + \cdots$$

$$= 2i \times 17 = 2.5 \times 17 +$$

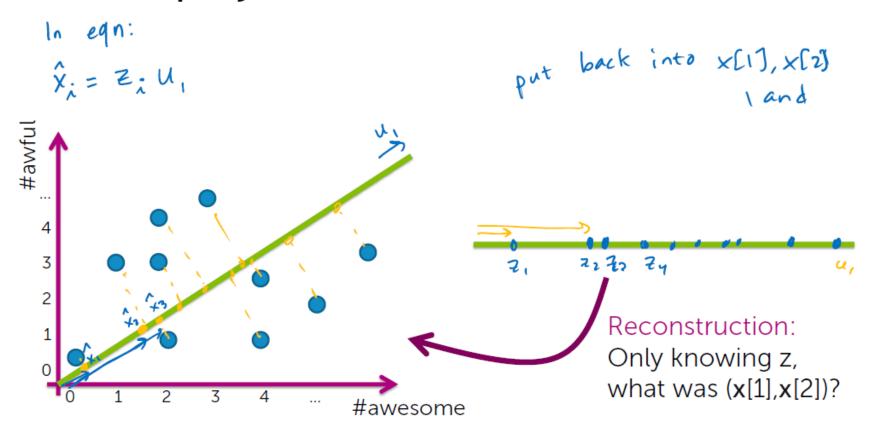
- Let's see this in the unsupervised setting
  - just x, but no y



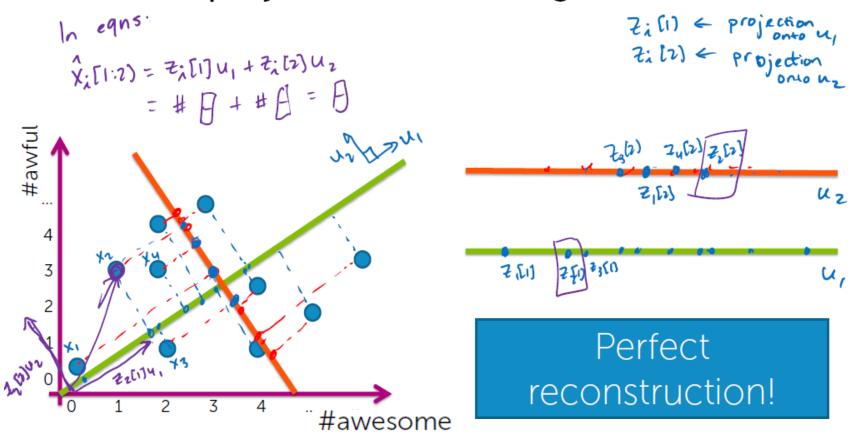
#### Linear projection and reconstruction



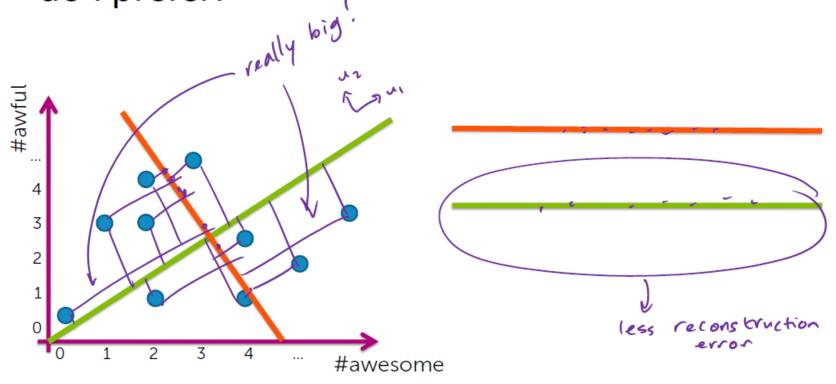
#### Linear projection and reconstruction



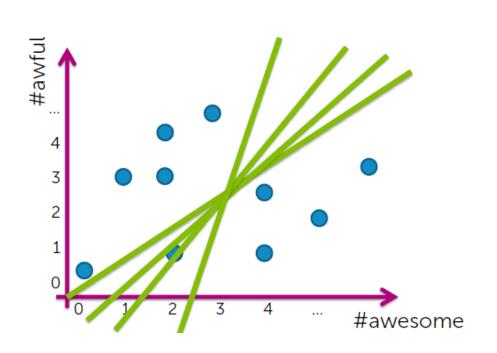
#### What if we project onto d orthogonal vectors?



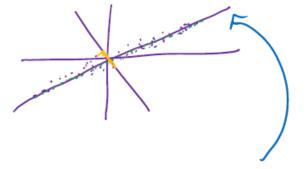
If I had to choose one of these vectors, which do I prefer?



#### What about over all single vectors?



Consider extreme data example:



Choose direction of greatest variations

#### Basic idea

- Project d-dimensional data into k-dimensional space while preserving as much information as possible:
  - e.g., project space of 10000 words into 3-dimensions
  - e.g., project 3-d into 2-d
- Choose projection with minimum reconstruction error

#### Basic PCA algorithm



- Form data matrix X
  - Each row is a different data point...like our typical data tables





$$\Sigma_{\text{ts}} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}_{c,i}[t] \mathbf{x}_{c,i}[s]$$



- Find basis:
  - Compute eigendecomposition of  $\Sigma$
  - Select (u[0,...,u[0)) to be eigenvectors with largest eigenvalues

• Project data: Project each data point onto each vector

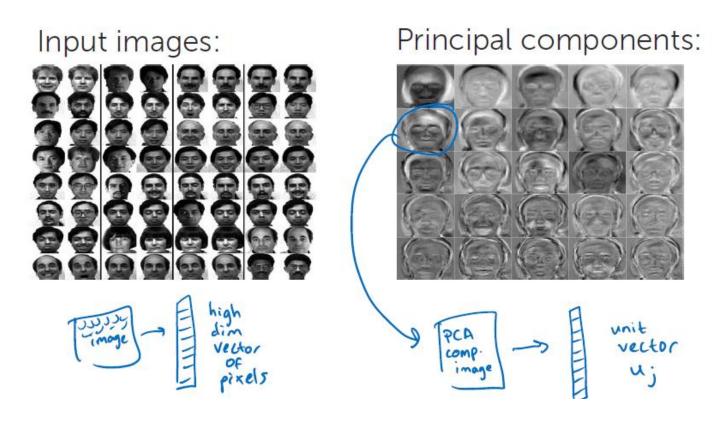


#### Reconstruction

Using our principal components, reconstruct observation

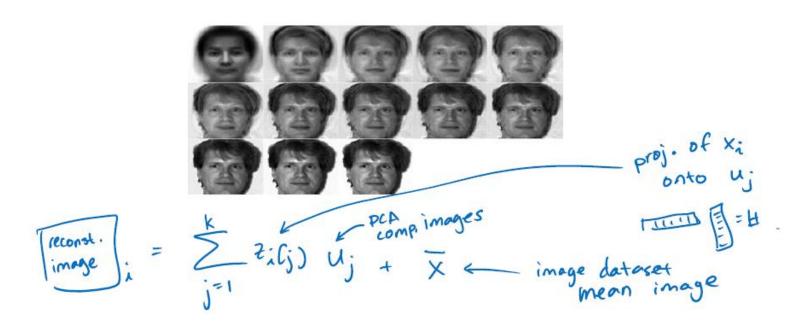
in original domain:

#### Eigenfaces [Turk, Pentland '91]



#### Eigenfaces reconstruction

Each image corresponds to adding 8 principal components:



#### Scaling up

- Covariance matrix can be really big!
  - $-\Sigma$  is d by d
  - Say, only 10000 features
  - finding eigenvectors is very slow...
- Use singular value decomposition (SVD)
  - finds up to k eigenvectors
  - great implementations available

# Recommender system: films

Machine learning: recommender system

Personalizacja



Information overload



Browsing is "history"

 Need new ways to discover content

Personalization: Connects users & items

viewers

videos

# Recomender system: films



Connect users with movies they may want to watch

# Recomender system: music



Recommendations form coherent & diverse sequence

# Recomender system: friends

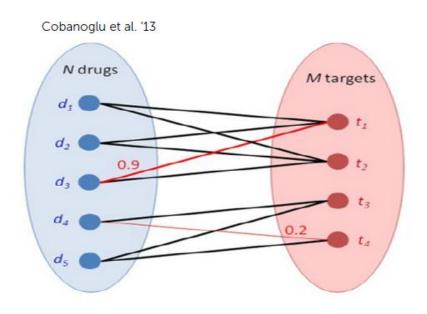
#### Friend recommendations



Users and "items" are of the same "type"

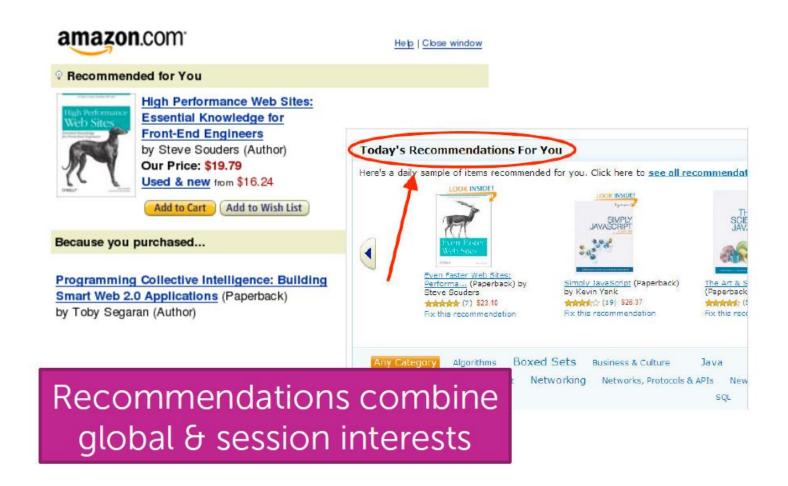
### Recomender system: medicine

#### Drug-target interactions



What drug should we "repurpose" for some disease?

### Recomender system:

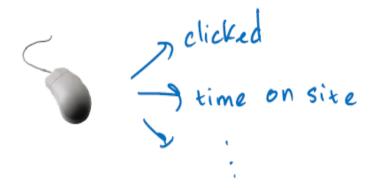


# Challenges: Type of feedback

Explicit – user tells us what she likes



Implicit – we try to infer what she likes from usage data



### Challenges: what is the goal?

#### Top K versus diverse outputs

- Top K recommendations may be very redundant
  - People who liked Rocky 1 also enjoyed Rocky 2, Rocky 3, Rocky 4, Rocky 5,...
- Diverse recommendations
  - Users are multi-facetted & want to hedge our bets
  - Rocky 2, It's Always Sunny in Philadelphia, Gandhi

### Challenges: Cold-start problem

#### A new movies walks into a bar...







Cold-start problem: recommendations for new users or new movies

- Need side information about user/movie
  - A.K.A. features!

action, actors, sequel, ..

Could also play 20-questions game...

### Challenges: evolving with time

#### That's so last year...

- Interests change over time...
  - Is it 1967?
  - Or 1977?
  - Or 1988?
  - Or 1998?
  - Or 2011?
- Models need flexibility to adapt to users
  - Macro scale
  - Micro scale intention now
- And keep checking that system still accurate



macys.com

# Challenges: Scalability

For N users and M movies, some approaches take  $O(N^3+M^3)$ 

Not so good for billions of users...

#### Big focus has been on:

- Efficient implementations
- Fast exact & approximate methods as needed

#### Building a recomender system

Solution 0: Popularity

Solution 1: Classification model

Solution 2: People who bought this also bought...

Solution 3: Discovering hidden structure by matrix factorization

### Recommender system: popularity?

#### Simplest approach: Popularity

What are people viewing now?

Rank by global popularity

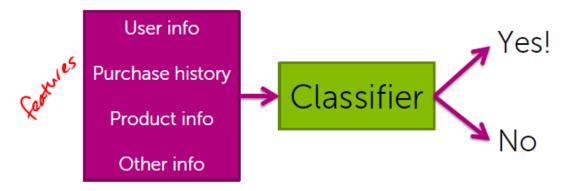
#### Limitation:

No personalization



# Recommender system: classification

#### What's the probability I'll buy this product?



#### Pros:



Considers user info & purchase history



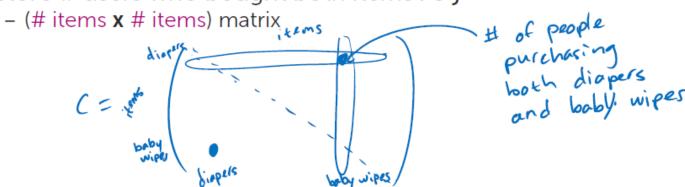
- Features can capture context: Time of the day, what I just saw,...
- Even handles limited user history:
   Age of user, ...

#### Cons:

- 🛶 Features may not be available
  - Often doesn't perform as well as collaborative filtering methods (next)

#### Co-occurrence matrix

- People who bought diapers also bought baby wipes
- Matrix C: store # users who bought both items i & j



- Symmetric: # purchasing  $i \delta j$  same as # for  $j \delta i$  ( $C_{ij} = C_{ji}$ )

# Making recommendations using co-occurences



1. Look at *diapers* row of matrix



- 2. Recommend other items with largest counts
  - baby wipes, milk, baby food,...

#### Recommender system: correlations

# Co-occurrence matrix must be normalized

What if there are very popular items?

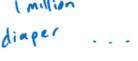
Popular baby item:
 Pampers Swaddlers diapers



– For any baby item (e.g., i=Sophie giraffeh) large count  $C_{ij}$  for j=Pampers Swaddlers

Result:





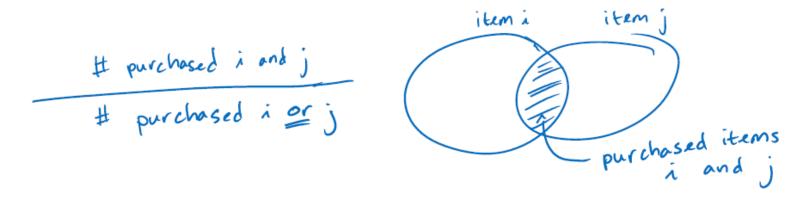


- Drowns out other effects
- Recommend based on popularity

# Normalize co-occurrences: Similarity matrix

Jaccard similarity: normalizes by popularity

- Who purchased *i* and *j* divided by who purchased *i* or *j* 



Many other similarity metrics possible. e.a.. cosine similarity

#### Limitations

- Only current page matters, no history
  - Recommend similar items to the one you bought
- What if you purchased many items?
  - Want recommendations based on purchase history

#### (Weighted) Average of purchased items

User bought items {diapers, milk}

- Compute user-specific score for each item *j* in inventory by

combining similarities: should we recommend this?

Score( $\sqrt{s}$ , baby wipes) =  $\frac{1}{2}$  ( $S_{baby\ wipes,\ diapers} + S_{baby\ wipes,\ milk}$ )

Could also weight recent purchases more

Sort  $Score(\begin{cases} \begin{cases} \be$ 

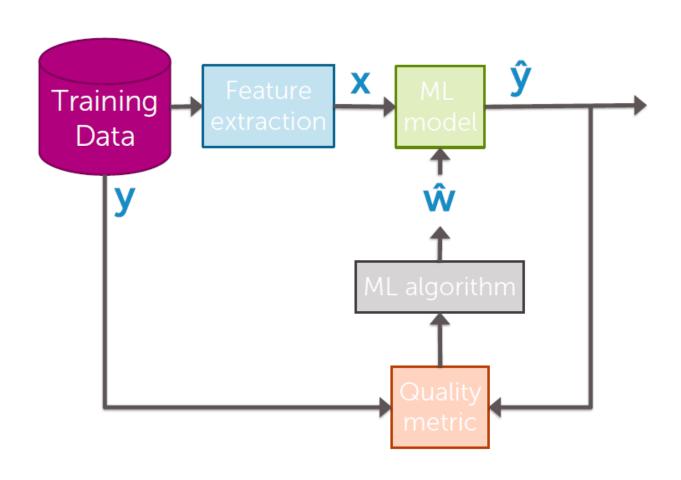
#### Limitations

- Does not utilize:
  - context (e.g., time of day)
  - user features (e.g., age)
  - product features (e.g., baby vs. electronics)
- Scalability similarity matrix M<sup>2</sup> size
- Cold start problem
  - What if a new user or product arrives?

## Recommender system: matrix factorization

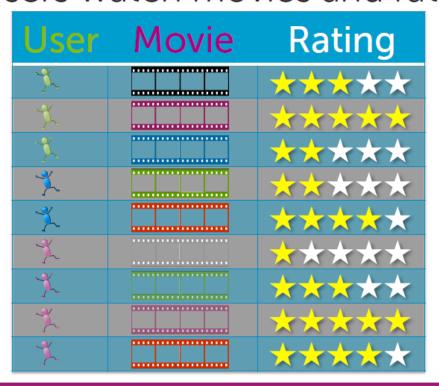
# Discovering hidden structure by matrix factorization

## Flow chart



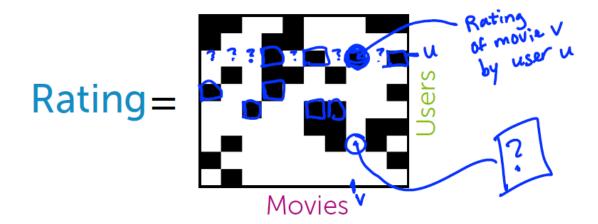
## Training Data

Users watch movies and rate them



Each user only watches a few of the available movies

## Training Data: matrix completion



Data: Users score some movies

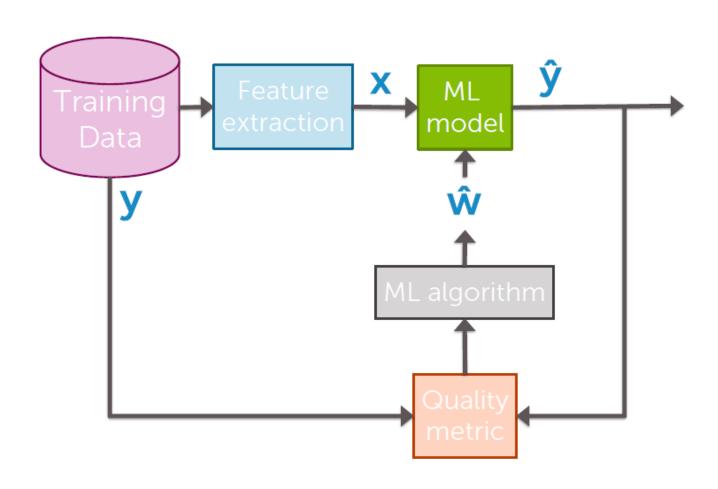
Rating(u,v) known for black cells Rating(u,v) unknown for white cells

• Goal: Filling missing data?





## Flow chart



## ML model

### Suppose we had d topics for each user & movie

- Describe movie v with topics  $R_v$ 
  - How much is it action, romance, drama,...

- Describe user u with topics  $L_u$

- How much she likes action, romance, drama,...

$$Lu = \{2.5, 0, 0.8, \dots \}$$

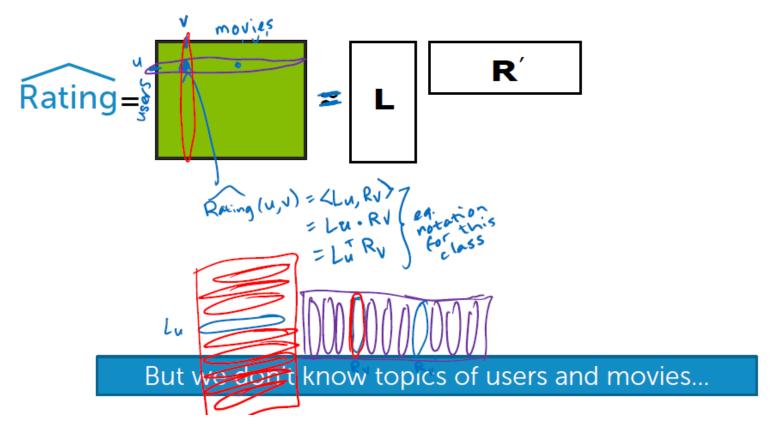
Rating(u,v) is the product of the two vectors

$$R_{\nu} = \{0.3 \text{ 0.01 } 1.5 \dots \} \longrightarrow 0.3*2.5*0*1.5*0.8*\dots = 1.2$$
 $Lu = \{0.3 \text{ 0.01 } 1.5 \dots \} \longrightarrow 0.4*1.5*0.8*\dots = 0.8$ 
 $Lu' = \{0.3 \text{ 0.01 } \dots \} \longrightarrow 0.4*1.5*0.01*\dots = 0.8$ 

Recommendations: sort movies user hasn't watched by Rating(u,v)

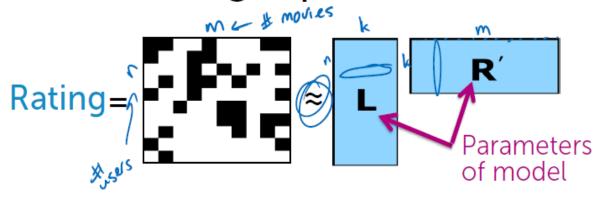
## ML model

### Predictions in matrix form



## Matrix factorisation model

# Matrix factorization model: Discovering topics from data



# params for model w/ k topics:

nk + k.m < n.m

learn this predict this using only black squares 1

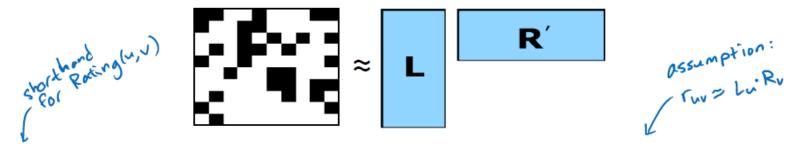
- Only use observed values to estimate "topic" vectors  $\widehat{\mathcal{I}}_u$  and  $\widehat{\mathcal{R}}_v$
- Use estimated  $\hat{\mathcal{L}}_u$  and  $\hat{\mathcal{R}}_v$  for recommendations

Many efficient algorithms for factorization

## Matrix factorisation model

### Is the problem well posed?

Can we uniquely identify the latent factors?



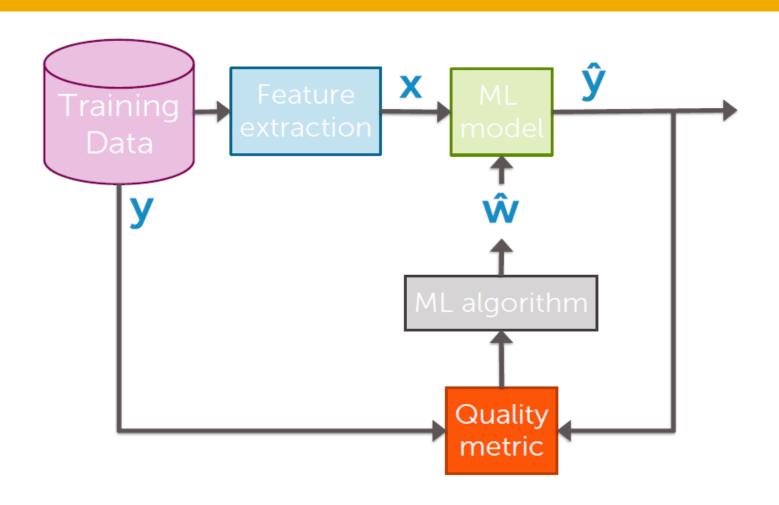
If  $r_{uv}$  is described by  $L_u$ ,  $R_v$  what happens if we redefine the "topics" as

Then,

Then,  $\tilde{L}_{u}\cdot\tilde{R}_{v}=cL_{u}\cdot\frac{1}{c}R_{v}=c\frac{1}{c}(L_{u}\cdot R_{v})=L_{u}\cdot R_{v}=r_{uv}$ Other (orthonormal) transformations can have the same effect.

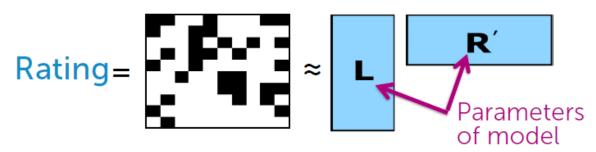
(an't uniquely identify  $L_{u}$ ,  $R_{v}=r_{uv}$ 

## Flow chart



## Matrix factorisation model

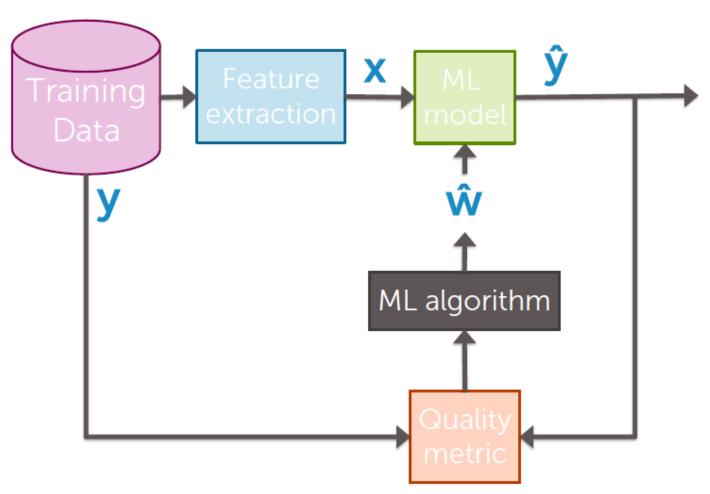
### Matrix factorization objective



- Minimize mean squared error:
  - (Other loss functions are possible)

· Non-convex objective convergence to local mode

## Flow chart



### Coordinate descent

Goal: Minimize some function g

Often, hard to find minimum for all coordinates, but easy for each coordinate

Coordinate descent:

Initialize  $\hat{\mathbf{w}} = 0$  (or smartly...)

while not converged pick a coordinate just min over aligned steps

### Coordinate descent for matrix factorization

$$\min_{L,R} \sum_{(u,v):r_{uv}\neq ?} (L_u \cdot R_v - r_{uv})^2$$

- Fix movie factors  $R_v$ , optimize for user factors  $L_u$
- First key insight:

min 
$$\sum (Lu \cdot P_v - ruv)^2$$
 $V_u \stackrel{b}{=} set of movies user u has rated user u has rated user u has rated user u has rated for each user

 $V_u \stackrel{b}{=} set of movies user u has rated u has rated user u has rated u has rate$$ 

### Comments on coordinate descent

How do we pick next coordinate?

- At random ("random" or "stochastic" coordinate descent), round robin, ...

No stepsize to choose!

Super useful approach for many problems

- Converges to optimum in some cases (e.g., "strongly convex")

### Coordinate descent for matrix factorization

$$\min_{L,R} \sum_{(u,v):r_{uv}\neq ?} (L_u \cdot R_v - r_{uv})^2$$

- Fix movie factors  $R_v$ , optimize for user factors  $L_u$
- · First key insight:

min 
$$\geq (Lu \cdot Rv - ruv)^2$$
 $l_{1,...,Ln} (u_iv): ruvt?$ 
 $= min \qquad \geq (Lu \cdot Rv - ruv)^2$ 
 $= l_{1,...,Ln} \qquad u \qquad veVu$ 
 $= u \qquad veVu$ 

### Minimize objective separately for each user

• For each user u:  $\min_{L_u} \sum_{v \in V_u} \int_{\eta} (L_u \cdot R_v - r_{uv})^2$ • Second key insight: Looks like linear regression!  $\min_{u \in V} \sum_{i=1}^{N} (\omega \cdot h(x_i) - y_i)^2$   $\sup_{v \in V_u} \int_{\eta} (\omega \cdot h(x_i) - y_i)^2$   $\sup_{v \in V_u} \int_{\eta} (\omega \cdot h(x_i) - y_i)^2$ 

### Overall coordinate descent algorithm

$$\min_{L,R} \sum_{(u,v):r_{uv}\neq ?} (L_u \cdot R_v - r_{uv})^2$$

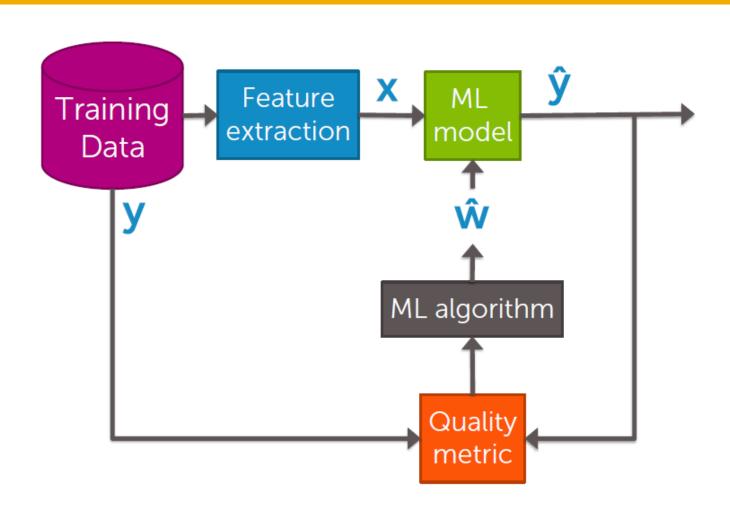
- Fix movie factors optimize for user factors
  - Independent least-squares over users

$$\min_{L_u} \sum_{v \in V_u} (L_u \cdot R_v - r_{uv})^2 \quad + \quad \lambda_{\mathbf{u}}$$

- Fix user factors, optimize for movie factors
  - Independent least-squares over movies

- System may be underdetermined: use regularization
- · Converges to local optima
- Choices of regularizers and impact on algorithm: L: \( \bar{\mathbb{L}} \| \lambda \| \l

## Flow chart



## Recommendation

## Using the results of matrix factorization

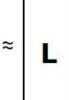
- Discover "topics"  $R_v$  for each movie  $v \longrightarrow R_v$
- Discover "topics"  $L_u$  for each user  $u \longrightarrow L_u$
- Score(u,v) is the product of the two vectors →
   Predict how much a user will like a movie

Recommendations: sort movies user hasn't watched by Score(u,v)

### Example topics discovered from Wikipedia

#### Application to text data:





R

#### partylaw government election court president elected

council general minister political national members committee united office federal massachusetts president member house parliament vote named jersey born boston ......

#### sondied married family king daughter john

death william father born wife royal ireland irish henry house lord charles sir prince brother children england queen duke thomas years marriage george earl edward english ......

#### school students

university high college schools Appartition of large long colorings all some offices are coloring appared to the coloring colorings are colorings are coloring colorings are colorings are coloring colorings are colorings are coloring colorings are colorings are colorings are colorings are coloring colorings are colorings are

#### vorkcounty american united city washington john texas served virginia

pennsylvania war moved ohio chicago william carolina north florida illinois george james died army centuries dynasty over

#### seasonteam

#### game league games species family played coach football

record teams baseball field year birds small long large animals second career play basketball bird plants genus and return hockey three yards won .....

#### albumband radiostation news television song released

channel broadcast music songs andle record

recorded rock bands release live tour video record albums broadcasting time format local people families older town size amaiory ampoor played partir label group recording getter beck

#### roman empire greek design model cars forces battle force british bc ancient emperor ii production built engines command general navy ship

centuryking engine car

kingdom period battle city vehicle class models time great war ad early reign kings it son rule power greece produced power front system version type series motor rear standard gun company introduced range ford sold tool

#### art museum work

works artists collection design arts painting artist gallery paintings exhibition style re-

#### wararmy military

division ships troops corps speed vehicles designed service naval regiment commander infantry attack men officer and entire or to others

#### whitered blackbluecalled

color will head green gold side small hand long arms top flag horse wear silver common light dog wood body type large

yellow to make dops oil popular left og gentrally traditional half forst rooms arrape

#### age 18 population music musical opera income average years

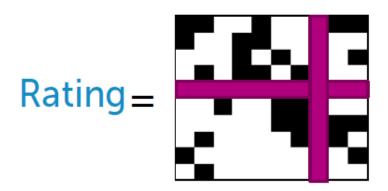
median living 65 males stations network media ty females households 100 family performance works come program bbc programming live city household miles density

program ooc programming into
microsity, and huge seaste to an urbal SIMPOCKSR strength pilet area microly
self-incedit coverage missi pro sociole
self-incedit coverage
self-incedit c

festival orchestra dance performed jazz plano theatre

### Limitations of matrix factorisation

- Cold-start problem
  - This model still cannot handle a new user or movie

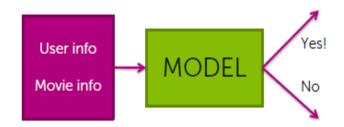


## Cold-start problem more formally

 $\min_{L,R} \frac{1}{2} \sum_{\text{(up)}^{T}uv} (L_u \cdot B_v - r_{uv})^2 + \frac{\lambda_u}{2} ||L||_F^2 + \frac{\lambda_v}{2} ||R||_F^2$  factor: Consider a new user u' and predicting that user's ratings  $\longrightarrow L_{u'}$  No previous observations - Objective considered so far: Optimal user factor: Lu' = 0 only penalty term present Predicted user ratings: always predict: run = 0 yv ... problem!

## Combining features and topics

- Features capture context
  - Time of day, what I just saw, user info, past purchases,...



- Discovered topics from matrix factorization capture groups of users who behave similarly
  - Women from Seattle who teach and have a baby
- Combine to mitigate cold-start problem
  - Ratings for a new user from features only
  - As more information about user is discovered, matrix factorization topics become more relevant

## Colaborative filtering

• Create feature vector for each movie (often have this even for new movies):

Define weights on these features for how much <u>all users</u> like each feature

Fit linear model:

• Minimize:

## Building in personalization

- Of course, users do not have identical preferences
- Include a user-specific deviation from the global set of user weights:

If we don't have any observations about a user, use wisdom of the crowd

As we gain more information about the user, forget the crowd

Can add in user-specific features, and cross-features, too

# Featurized matrix factorization: combined approach

### Feature-based approach:

- Feature representation of user and movies fixed
- Can address cold-start problem

### Matrix factorization approach:

- Suffers from cold-start problem
- User & movie features are learned from data

## Blending models

- Squeezing last bit of accuracy by blending models
- Netflix Prize 2006-2009
  - 100M ratings
  - 17,770 movies
  - 480,189 users
  - Predict 3 million ratings to highest accuracy



Winning team blended over 100 models

## The world of all baby products



### User likes subset of items



## Why not use classification accuracy?

- Classification accuracy = fraction of items correctly classified (liked vs. not liked)
- Here, not interested in what a person does not like
- Rather, how quickly can we discover the relatively few liked items?
  - (Partially) an imbalanced class problem

How many liked items were recommended?

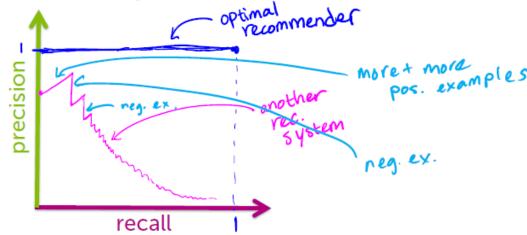


How many recommended items were liked?



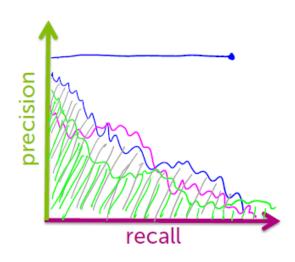
### Precision-recall curve

- Input: A specific recommender system
- Output: Algorithm-specific precision-recall curve
- To draw curve, vary threshold on # items recommended
  - For each setting, calculate the precision and recall



## Which Algorithm is Best?

- For a given precision, want recall as large as possible (or vice versa)
- One metric: largest area under the curve (AUC)
- Another: set desired recall and maximize precision (precision at k)



## Recommender system

### Models

- Collaborative filtering
- Matrix factorization
- PCA

### Algorithms

- Coordinate descent
- Eigen decomposition
- SVD

### Concepts

 Matrix completion, eigenvalues, random projections, cold-start problem, diversity, scaling up