Caltech

Machine Learning & Data Mining

CS/CNS/EE 155

Lecture 10:

Latent Factor Models &

Non-Negative Matrix Factorization

CALTECH AI4SCIENCE 2ND WORKSHOP

February 14, 2019

https://sites.google.com/view/ai-for-science-workshop/home

RSVP:

https://www.eventbrite.com/e/caltech-ai4science-workshop-registration-55391262758

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Machine Learning for Chemistry

Azita Emami

Brain/Computer Interfaces

David Van Valen

Deep Learning for Cellular Biology

Brandon Rothrock

Making Planetary Images Searchable

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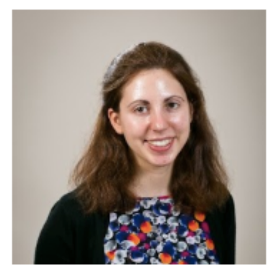
Active Learning using Gaussian Processes



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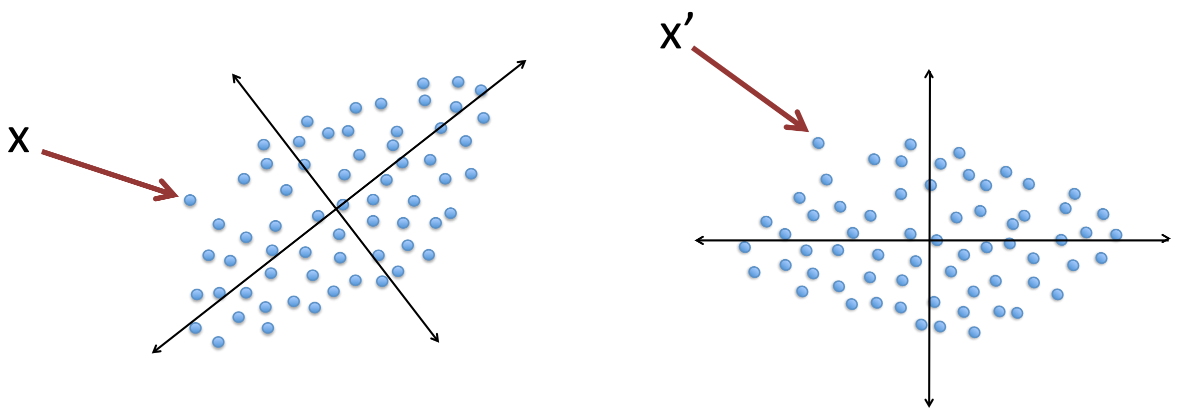
Active Learning for Nanophotonics

Today

- Some useful matrix properties
  - Useful for Homework 5
- Latent Factor Models
  - Low-rank models with missing values
- Non-negative matrix factorization

Recap: Orthogonal Matrix

- A matrix U is orthogonal if $UU^T = U^TU = I$
  - For any column u: $u^Tu = 1$
  - For any two columns u, u': $u^Tu' = 0$
  - U is a rotation matrix, and U^T is the inverse rotation
  - If $x' = U^Tx$, then $x = Ux'$



Recap: Orthogonal Matrix

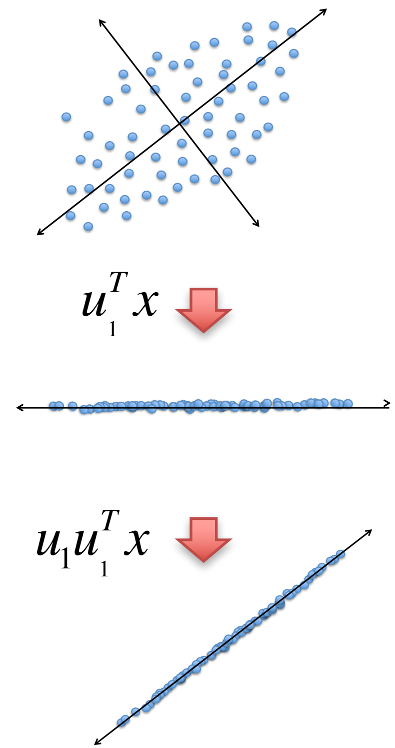
- Any subset of columns of U defines a subspace

$$x' = U_{1:K}^T x$$

Transform into new coordinates
Treat $U_{1:K}$ as new axes

$$proj_{U_{1:K}}(x) = U_{1:K} U_{1:K}^T x$$

Project x onto $U_{1:K}$ in original space
"Low Rank" Subspace



Recap: Singular Value Decomposition

$$X = \left[x_1, \ldots, x_N \right] \in \mathrm{Re}^{D \times N}$$

$$X = U \Sigma V^T$$

Orthogonal

Orthogonal Diagonal

SVD

$$\sum_{i=1}^{N} \left\| x_i - U_{1:K} U_{1:K}^T x_i \right\|^2$$

"Residual"

$U_{1:K}$ is the K-dim subspace with smallest residual

Recap: SVD & PCA

$$\underbrace{XX^T = U}_{\text{Orthogonal}}\underbrace{\Lambda}_{\text{Diagonal}} U^T$$

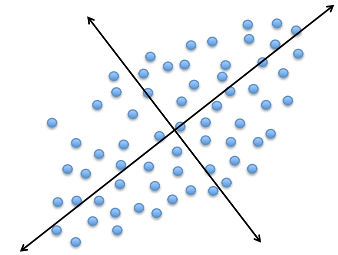
PCA

$$X = \underbrace{U}_{\text{Orthogonal}}\underbrace{\Sigma}_{\text{Diagonal}}\underbrace{V^T}_{\text{Orthogonal}}$$

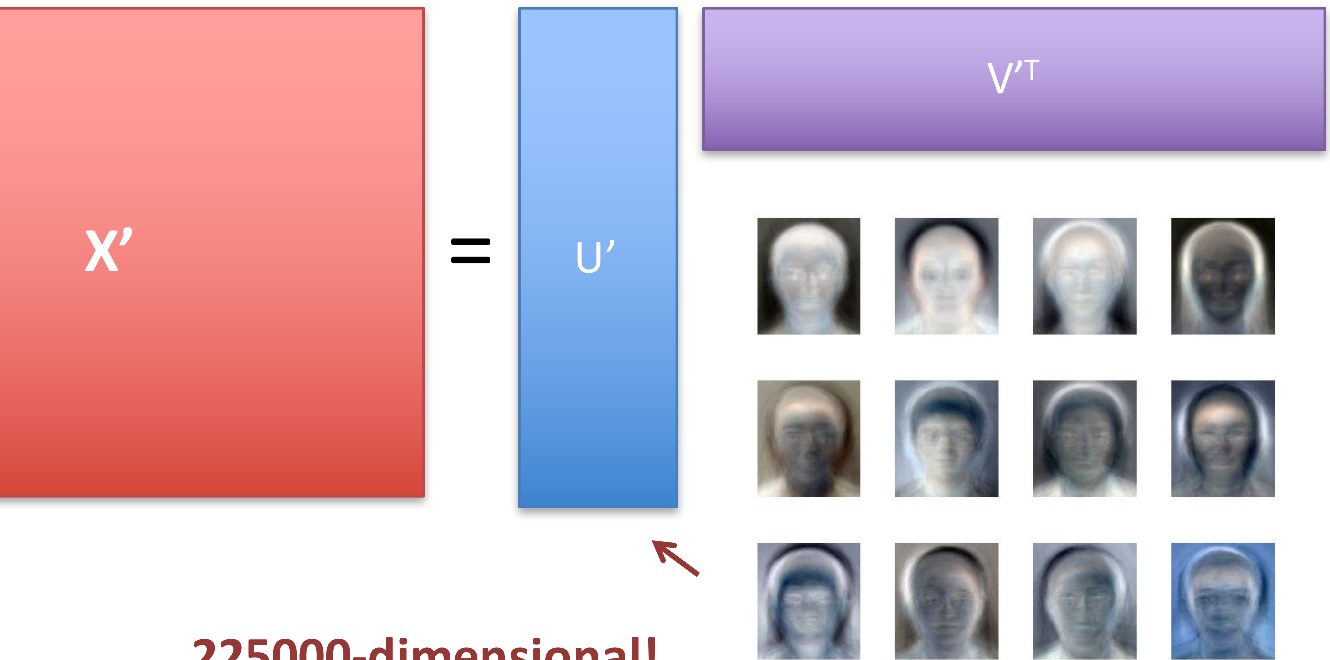
SVD

$$XX^T = \left(U\Sigma V^T\right)\left(U\Sigma V^T\right)^T = U\Sigma V^T V\Sigma U^T = U\Sigma^2 U^T$$

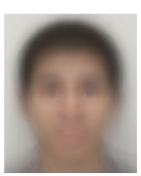
Recap: Eigenfaces



- Each col of U' is an "Eigenface"
- Each col of V'^T = coefficients of a student



Avg Face



225000-dimensional!

Matrix Norms

- Frobenius Norm

$$\|X\|_{Fro} = \sqrt{\sum_{ij} X_{ij}^2} = \sqrt{\sum_d \sigma_d^2}$$

- Trace Norm

$$\|X\|_* = \sum_d \sigma_d = \mathrm{trace}\left(\sqrt{X^T X}\right)$$

$$X = U \Sigma V^T$$

Each σ_d is guaranteed to be non-negative
By convention: $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_D \geq 0$

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_D \end{bmatrix}$$

Properties of Matrix Norms

$$\|X\|_{Fro}^2 = \mathrm{trace}\left(X^T X\right) = \mathrm{trace}\left(\left(U\Sigma V^T\right)^T U\Sigma V^T\right)$$

$$= \mathrm{trace}\left(V\Sigma^2 V^T\right) = \mathrm{trace}\left(\Sigma^2 V^T V\right)$$

$$= \mathrm{trace}\left(\Sigma^2\right) = \sum_d \sigma_d^2$$

$$X = U\Sigma V^T$$

Each σ_d is guaranteed to be non-negative
By convention: $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_D \geq 0$

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_D \end{bmatrix}$$

$$\mathrm{trace}(ABC) = \mathrm{trace}(BCA) = \mathrm{trace}(CAB)$$

Properties of Matrix Norms

$$\|X\|_* = \text{trace}\left(\sqrt{\left(U\Sigma V^T\right)^T U\Sigma V^T}\right) = \text{trace}\left(\sqrt{V\Sigma U^T U\Sigma V^T}\right)$$

$$= \text{trace}\left(\sqrt{V\Sigma\Sigma V^T}\right) = \text{trace}\left(\sqrt{V\Sigma^2 V^T}\right) = \text{trace}\left(V\Sigma V^T\right)$$

$$= \text{trace}\left(\Sigma V^T V\right) = \text{trace}\left(\Sigma\right) = \sum_d \sigma_d$$

$$X = U\Sigma V^T$$

Each σ_d is guaranteed to be non-negative
By convention: $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_D \geq 0$

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_D \end{bmatrix}$$

$$\text{trace}(ABC) = \text{trace}(BCA) = \text{trace}(CAB)$$

Frobenius Norm = Squared Norm

- Matrix version of L2 Norm:

$$\|X\|_{Fro}^2 = \sum_{ij} X_{ij}^2 = \sum_d \sigma_d^2$$

- Useful for regularizing matrix models

$$X = U \Sigma V^T \qquad \Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_D \end{bmatrix}$$

Recall: L1 & Sparsity

- w is sparse if mostly 0's:
  - Small L0 Norm

$$\|w\|_0 = \sum_d 1_{[w_d \neq 0]}$$

- Why not L0 Regularization?
  - **Not continuous!**

$$\underset{w}{\operatorname{argmin}} \, \lambda \|w\|_0 + \sum_{i=1}^{N} \left(y_i - w^T x_i\right)^2$$

- L1 induces sparsity
  - And is continuous!

$$\underset{w}{\operatorname{argmin}} \, \lambda |w| + \sum_{i=1}^{N} \left(y_i - w^T x_i\right)^2$$

Omitting b &
for simplicity

Trace Norm = L1 of Eigenvalues

- A matrix X is considered low rank if it has few non-zero singular values:

$$\|X\|_{Rank} = \sum_d 1_{[\sigma_d > 0]}$$

Not continuous!

$$\|X\|_* = \sum_d \sigma_d = \mathrm{trace}\left(\sqrt{X^T X}\right)$$

aka "spectral sparsity"

$$X = U \Sigma V^T$$

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_D \end{bmatrix}$$

Other Useful Properties

- Cauchy Schwarz:

$$\langle A,B\rangle^2 = \mathrm{trace}(A^T B)^2 \le \langle A,A\rangle\langle B,B\rangle = \mathrm{trace}(A^T A)\mathrm{trace}(B^T B) = \|A\|_F^2 \|B\|_F^2$$

- AM-GM Inequality:

$$\|A\|\|B\| = \sqrt{\|A\|^2 \|B\|^2} \le \frac{1}{2}\left(\|A\|^2 + \|B\|^2\right)$$

True for any norm

- Orthogonal Transformation Invariance of Norms:

$$\|UA\|_F = \|A\|_F \qquad \|UA\|_* = \|A\|_*$$

If U is a full-rank orthogonal matrix

- Trace Norm of Diagonals

$$\|A\|_* = \sum_i |A_{ii}|$$

If A is a square diagonal matrix

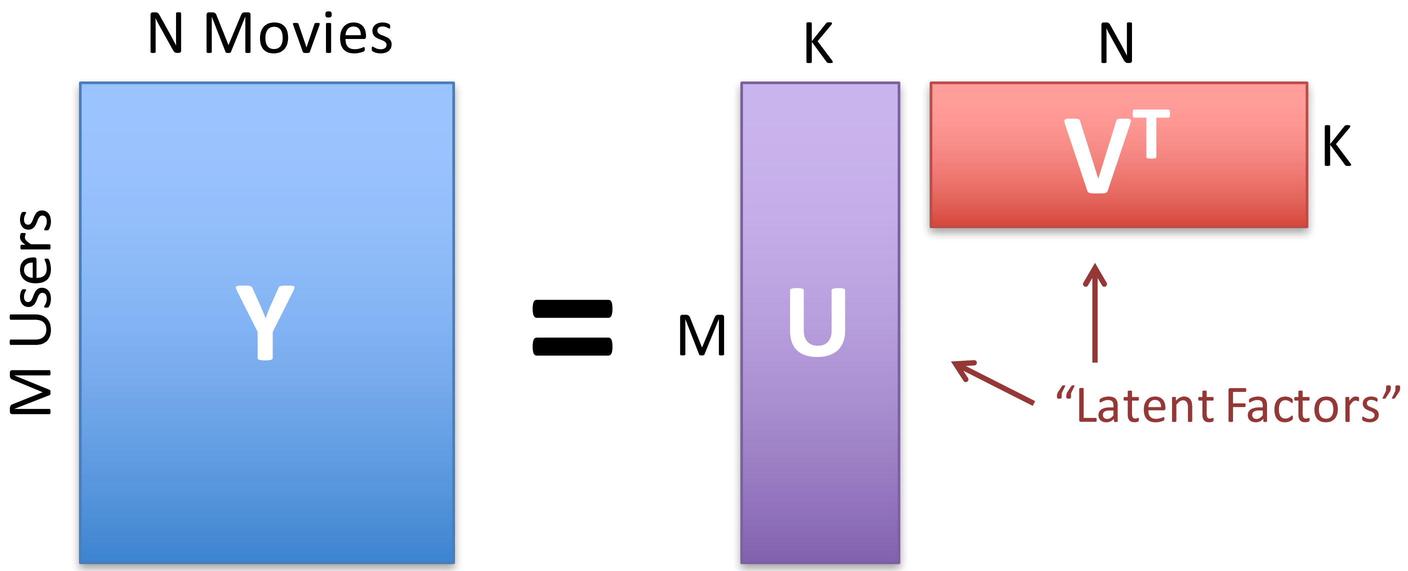
Recap: SVD & PCA

- SVD: $$X = U \Sigma V^T$$
- PCA: $$XX^T = U \Sigma^2 U^T$$
- The first K columns of U are the best rank-K subspace that minimizes the Frobenius norm residual:

$$\left\| X - U_{1:K} U_{1:K}^T X \right\|_{Fro}^2$$

Latent Factor Models

Netflix Problem

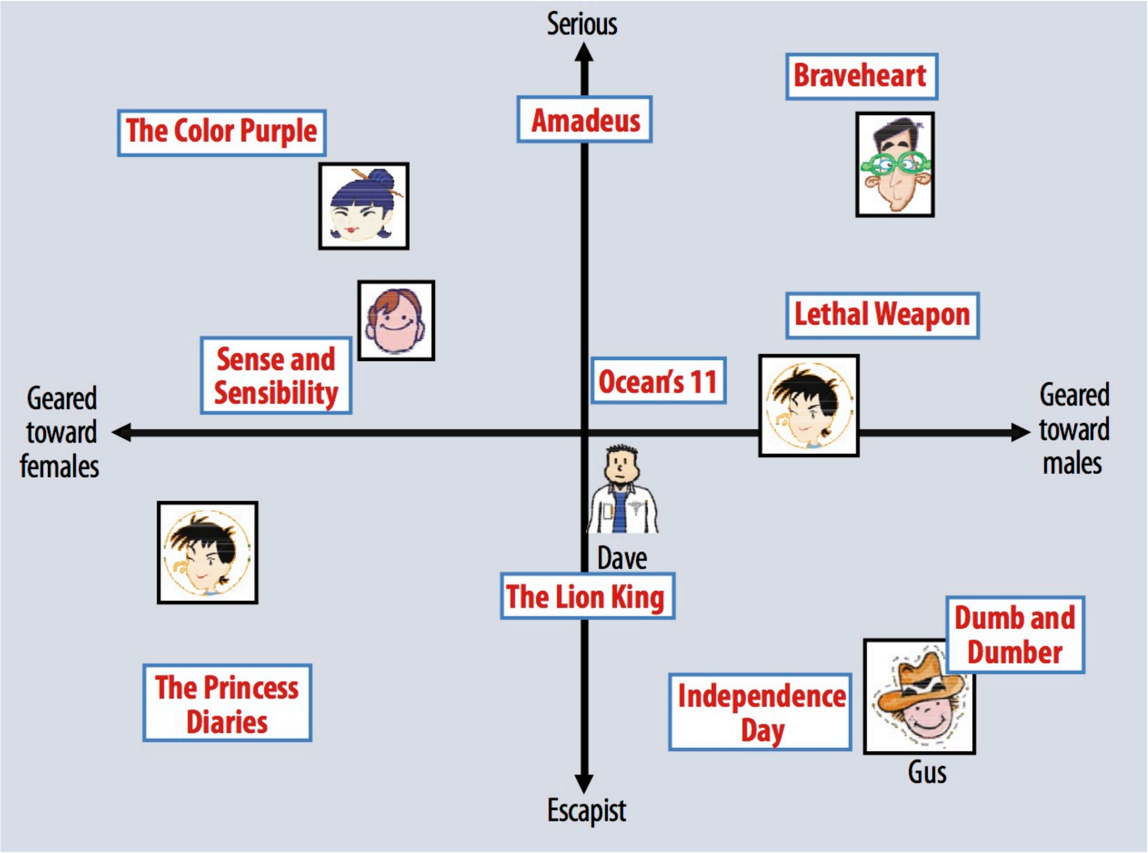


- Y_{ij} = rating user i gives to movie j

$$y_{ij} \approx u_i^T v_j$$

- Solve using SVD!

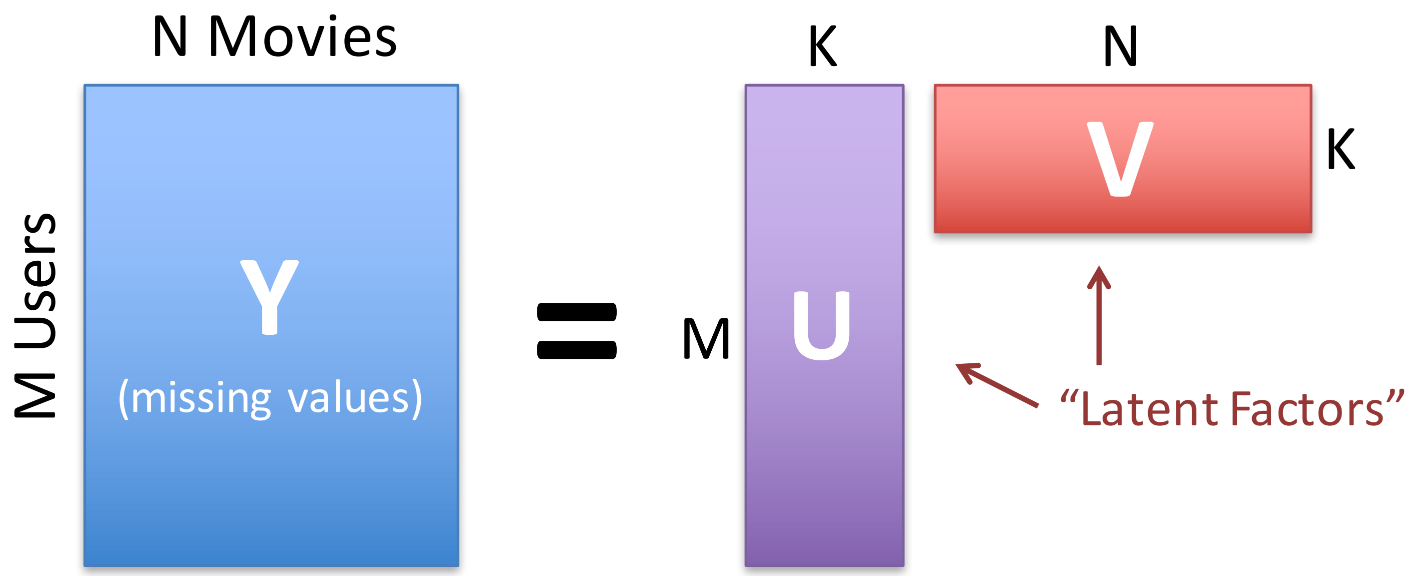
Example



$$y_{ij} \approx u_i^T v_j$$

http://www2.research.att.com/~volinsky/papers/ieeecomputer.pdf

Actual Netflix Problem



- Many missing values!

Collaborative Filtering

- M Users, N Items
- Small subset of user/item pairs have ratings
- Most are missing

- Applicable to any user/item rating problem
  - Amazon, Pandora, etc.

- **Goal:** Predict the missing values.

Latent Factor Formulation

- Only labels, no features

$$S = \{y_{ij}\}$$

- Learn a **latent** representation over users U and movies V such that:

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \sum_{ij}\left(y_{ij} - u_i^T v_j\right)^2$$

Connection to Trace Norm

- Suppose we consider all U,V that achieve perfect reconstruction: $Y=UV^T$

- Find U,V with lowest complexity:

$$\underset{Y=UV^T}{\operatorname{argmin}} \frac{1}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right)$$

- Complexity equivalent to trace norm:

$$\|Y\|_* = \min_{Y=UV^T} \frac{1}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right)$$

Proof (One Direction)

We will prove: $\|Y\|_* \geq \min_{Y=AB^T} \frac{1}{2}\left(\|A\|_{Fro}^2 + \|B\|_{Fro}^2\right)$

$$Y = U\Sigma V^T$$

SVD

Choose: $A = U\sqrt{\Sigma}, \qquad B = V\sqrt{\Sigma}$

Then:

$$\begin{aligned}
\min_{Y=AB^T} \frac{1}{2}\left(\|A\|_{Fro}^2 + \|B\|_{Fro}^2\right) &\leq \frac{1}{2}\left(\left\|U\sqrt{\Sigma}\right\|_{Fro}^2 + \left\|V\sqrt{\Sigma}\right\|_{Fro}^2\right) \\
&= \frac{1}{2}\left(\text{trace}\left(\left(U\sqrt{\Sigma}\right)^T\left(U\sqrt{\Sigma}\right)\right) + \text{trace}\left(\left(V\sqrt{\Sigma}\right)^T\left(V\sqrt{\Sigma}\right)\right)\right) \\
&= \frac{1}{2}\left(\text{trace}\left(\sqrt{\Sigma}U^TU\sqrt{\Sigma}\right) + \text{trace}\left(\sqrt{\Sigma}V^TV\sqrt{\Sigma}\right)\right) \\
&= \frac{1}{2}\left(\text{trace}\left(\sqrt{\Sigma}\sqrt{\Sigma}\right) + \text{trace}\left(\sqrt{\Sigma}\sqrt{\Sigma}\right)\right) \\
&= \frac{1}{2}\left(\text{trace}(\Sigma) + \text{trace}(\Sigma)\right) = \text{trace}(\Sigma) = \|Y\|_*
\end{aligned}$$

Interpreting Model

- Latent-Factor Model Objective

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \sum_{ij}\left(y_{ij} - u_i^T v_j\right)^2$$

- Related to:

$$\underset{W}{\operatorname{argmin}} \lambda \|W\|_* + \sum_{ij}\left(y_{ij} - w_{ij}\right)^2$$

Find the best low-rank approximation to Y!

$$\|W\|_* = \min_{W=UV^T} \frac{1}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right)$$

Equivalent when U,V = rank of W

User/Movie Symmetry

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \sum_{ij}\left(y_{ij} - u_i^T v_j\right)^2$$

- If we knew V, then linear regression to learn U
  - Treat V as features

- If we knew U, then linear regression to learn V
  - Treat U as features

Optimization

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \sum_{ij} \omega_{ij}\left(y_{ij} - u_i^T v_j\right)^2 \qquad \omega_{ij} \in \{0,1\}$$

- Only train over observed y_{ij}
- Two ways to Optimize
  - Gradient Descent
  - Alternating optimization
    - Closed Form (for each sub-problem)
  - Homework question

Gradient Calculation

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \frac{1}{2}\sum_{ij}\omega_{ij}\left(y_{ij} - u_i^T v_j\right)^2$$

$$\partial_{u_i} = \lambda u_i - \sum_j \omega_{ij} v_j \left(y_{ij} - u_i^T v_j\right)^T$$

Closed Form Solution (assuming V fixed):

$$u_i = \left(\lambda I_K + \sum_j \omega_{ij} v_j v_j^T\right)^{-1}\left(\sum_j \omega_{ij} y_{ij} v_j\right)$$

Gradient Descent Options

- Stochastic Gradient Descent
  - Update all model parameters for single data point

- Alternating SGD:
  - Update a single column of parameters at a time

$$u_i = u_i - \eta \partial_{u_i}$$

$$\partial_{u_i} = \lambda u_i - \sum_j \omega_{ij} v_j \left(y_{ij} - u_i^T v_j \right)$$

Alternating Optimization

- Initialize U & V randomly
- Loop
  - Choose next u_i or v_j
  - Solve optimally:

$$u_i = \left(\lambda I_K + \sum_j \omega_{ij} v_j v_j^T \right)^{-1} \left(\sum_j \omega_{ij} y_{ij} v_j \right)$$

    - (assuming all other variables fixed)

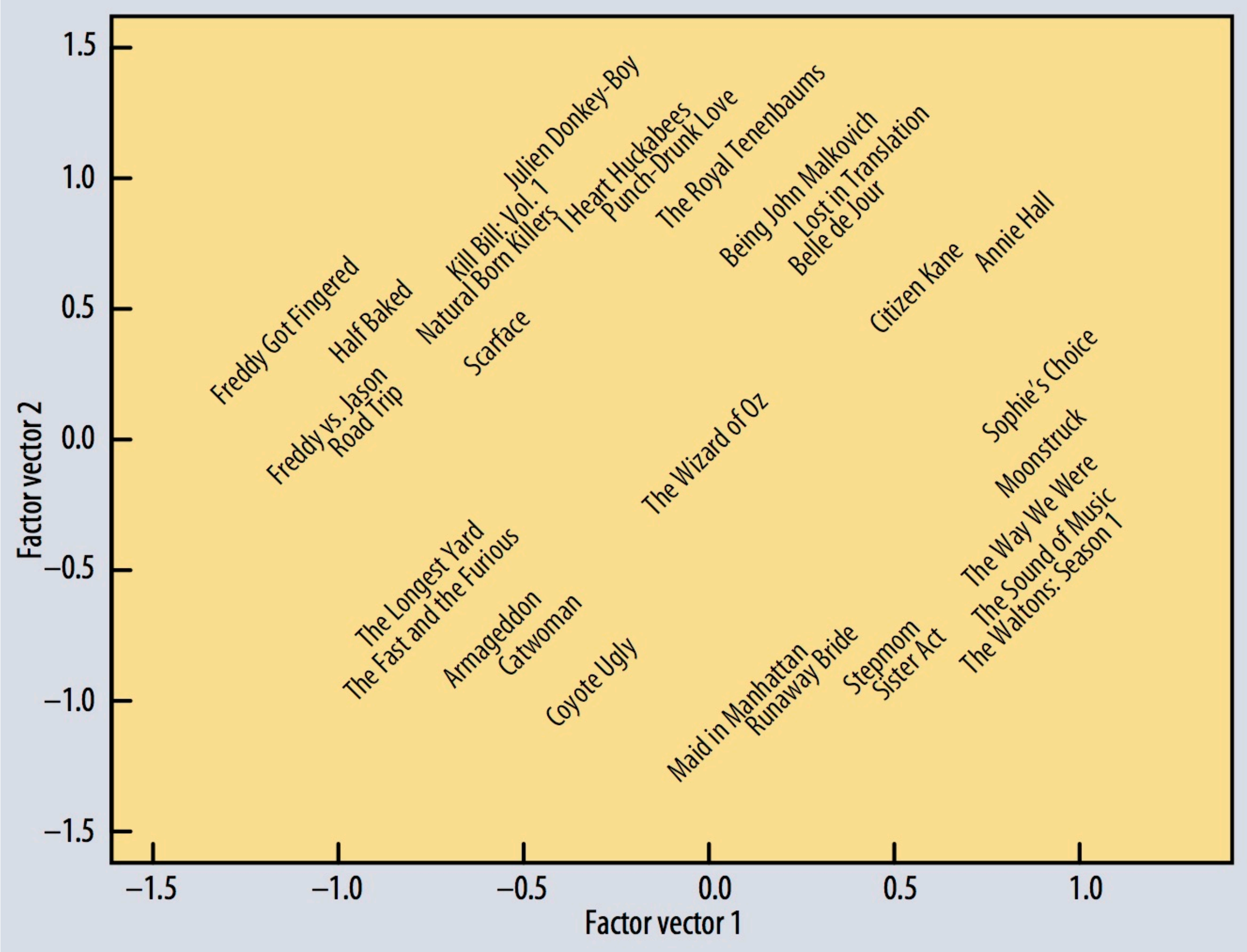
Tradeoffs

- Alternating optimization much faster in terms of #iterations
  - But requires inverting a matrix:

$$u_i = \left(\lambda I_K + \sum_j \omega_{ij} v_j v_j^T \right)^{-1} \left(\sum_j \omega_{ij} y_{ij} v_j \right)$$

- Gradient descent faster for high-dim problems
  - Also allows for streaming data

$$u_i = u_i - \eta \partial_{u_i}$$



http://www2.research.att.com/~volinsky/papers/ieeecomputer.pdf

Recap: Collaborative Filtering

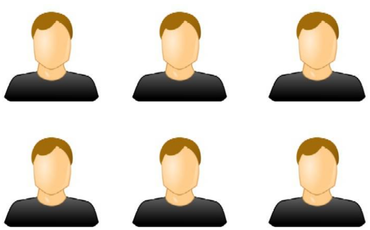
- **Goal:** predict every user/item rating
- **Challenge:** only a small subset observed
- **Assumption:** there exists a low-rank subspace that captures all the variability in describing different users and items

Aside: Multitask Learning

- M Tasks: $S^m = \left\{(x_i, y_i^m)\right\}_{i=1}^{N}$

$$\underset{W}{\operatorname{argmin}} \frac{\lambda}{2} \underbrace{R(W)}_{\text{Regularizer}} + \frac{1}{2}\sum_{m}\sum_{i}\left(y_i - w_m^T x_i\right)^2$$

- Example: personalized recommender system
  - One task per user:



How to Regularize?

$$\underset{W}{\operatorname{argmin}} \frac{\lambda}{2} R(W) + \frac{1}{2} \sum_m \sum_i \left(y_i - w_m^T x_i \right)^2 \qquad S^m = \left\{ (x_i, y_i^m) \right\}_{i=1}^N$$

- Standard L2 Norm:

$$\underset{W}{\operatorname{argmin}} \frac{\lambda}{2} \|W\|^2 + \sum_m \sum_i \left(y_i - w_m^T x_i \right)^2 = \sum_m \left[\frac{\lambda}{2} \|w_m\|^2 + \sum_i \left(y_i - w_m^T x_i \right)^2 \right]$$

- Decomposes to independent tasks
  - For each task, learn D parameters

How to Regularize?

$$\underset{W}{\operatorname{argmin}} \frac{\lambda}{2} R(W) + \frac{1}{2} \sum_m \sum_i \left(y_i - w_m^T x_i \right)^2 \qquad S^m = \left\{ (x_i, y_i^m) \right\}_{i=1}^N$$

- Trace Norm:

$$\underset{W}{\operatorname{argmin}} \frac{\lambda}{2} \|W\|_* + \sum_m \sum_i \left(y_i - w_m^T x_i \right)^2$$

- Induces W to have low rank across all task

Recall: Trace Norm & Latent Factor Models

- Suppose we consider all U,V that achieve perfect reconstruction: $W=UV^T$

- Find U,V with lowest complexity:

$$\underset{W=UV^T}{\operatorname{argmin}} \frac{1}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right)$$

- Complexity equivalent to trace norm:

$$\|W\|_* = \min_{W=UV^T} \frac{1}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right)$$

How to Regularize?

$$\underset{W}{\operatorname{argmin}} \frac{\lambda}{2} R(W) + \frac{1}{2} \sum_m \sum_i \left(y_i - w_m^T x_i \right)^2 \qquad S^m = \left\{ (x_i, y_i^m) \right\}_{i=1}^N$$

- Latent Factor Approach

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2} \left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2 \right) + \frac{1}{2} \sum_m \sum_i \left(y_i - u_m^T V x_i \right)^2$$

- Learns a feature projection x' = Vx
- Learns a K dimensional model per task

Tradeoff

- D*N parameters:

$$\underset{W}{\operatorname{argmin}} \sum_m \left[\frac{\lambda}{2} \|w_m\|^2 + \frac{1}{2} \sum_i \left(y_i - w_m^T x_i \right)^2 \right]$$

- D*K + N*K parameters:

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2} \left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2 \right) + \frac{1}{2} \sum_m \sum_i \left(y_i - u_m^T V x_i \right)^2$$

  - Statistically more efficient
  - Great if low-rank assumption is a good one

Multitask Learning

- M Tasks: $S^m = \left\{(x_i, y_i^m)\right\}_{i=1}^{N}$

$$\operatorname*{argmin}_{U,V} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \frac{1}{2}\sum_m \sum_i \left(y_i^m - u_m^T V x_i\right)^2$$

- Example: personalized recommender system
  - One task per user:
  - If x is topic feature representation
    - V is subspace of correlated topics
    - Projects multiple topics together

Reduction to Collaborative Filtering

$$\operatorname*{argmin}_{U,V} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \frac{1}{2}\sum_m \sum_i \left(y_i^m - u_m^T V x_i\right)^2 \qquad S^m = \left\{(x_i, y_i^m)\right\}_{i=1}^N$$

$$x_i = \begin{bmatrix} \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}$$

- Suppose each x_i is single indicator $x_i = e_i$
- Then: $Vx_i = v_i$
- Exactly Collaborative Filtering!

$$\operatorname*{argmin}_{U,V} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \frac{1}{2}\sum_m \sum_i \left(y_i^m - u_m^T v_i\right)^2$$

Latent Factor Multitask Learning vs Collaborative Filtering

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \frac{1}{2}\sum_m \sum_i \left(y_i^m - u_m^T V x_i\right)^2$$

- Projects x into low-dimensional subspace Vx
- Learns low-dimensional model per task

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \frac{1}{2}\sum_m \sum_i \left(y_i^m - u_m^T v_i\right)^2$$

- Creates low dimensional feature for each movie
- Learns low-dimensional model per user

General Bilinear Models

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \sum_i \left(y_i - z_i^T U^T V x_i\right)^2 \qquad S = \{(x_i, z_i, y_i)\}$$

- Users described by features z
- Items described by features x

- Learn a projection of z and x into common low-dimensional space
  - Linear model in low dimensional space

Why are Bilinear Models Useful?

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \frac{1}{2}\sum_m \sum_i \left(y_i - u_m^T v_i\right)^2$$

U: MxK
V: NxK

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \frac{1}{2}\sum_m \sum_i \left(y_i - u_m^T V x_i\right)^2$$

U: MxK
V: DxK

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \frac{1}{2}\sum_i \left(y_i - z_i^T U^T V x_i\right)^2$$

$$S = \{(x_i, z_i, y_i)\}$$

U: FxK
V: DxK

Story So Far: Latent Factor Models

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \frac{1}{2}\sum_i \left(y_i - z_i^T U^T V x_i\right)^2 \quad S = \{(x_i, z_i, y_i)\}$$

- **Simplest Case:** reduces to SVD of matrix Y
  - No missing values
  - (z,x) indicator features
- **General Case:** projects high-dimensional feature representation into low-dimensional linear model

Aside: Non-Linear "Projections"

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \frac{1}{2}\sum_i \left(y_i - z_i^T U^T V x_i\right)^2 \quad S = \{(x_i, z_i, y_i)\}$$

- Vx is a linear mapping
  - From x to low-dimensional space

- Can also learn non-linear mapping
  - E.g., the hidden layer activations of a neural net

http://www.cs.cornell.edu/~andreas/iccv15.pdf

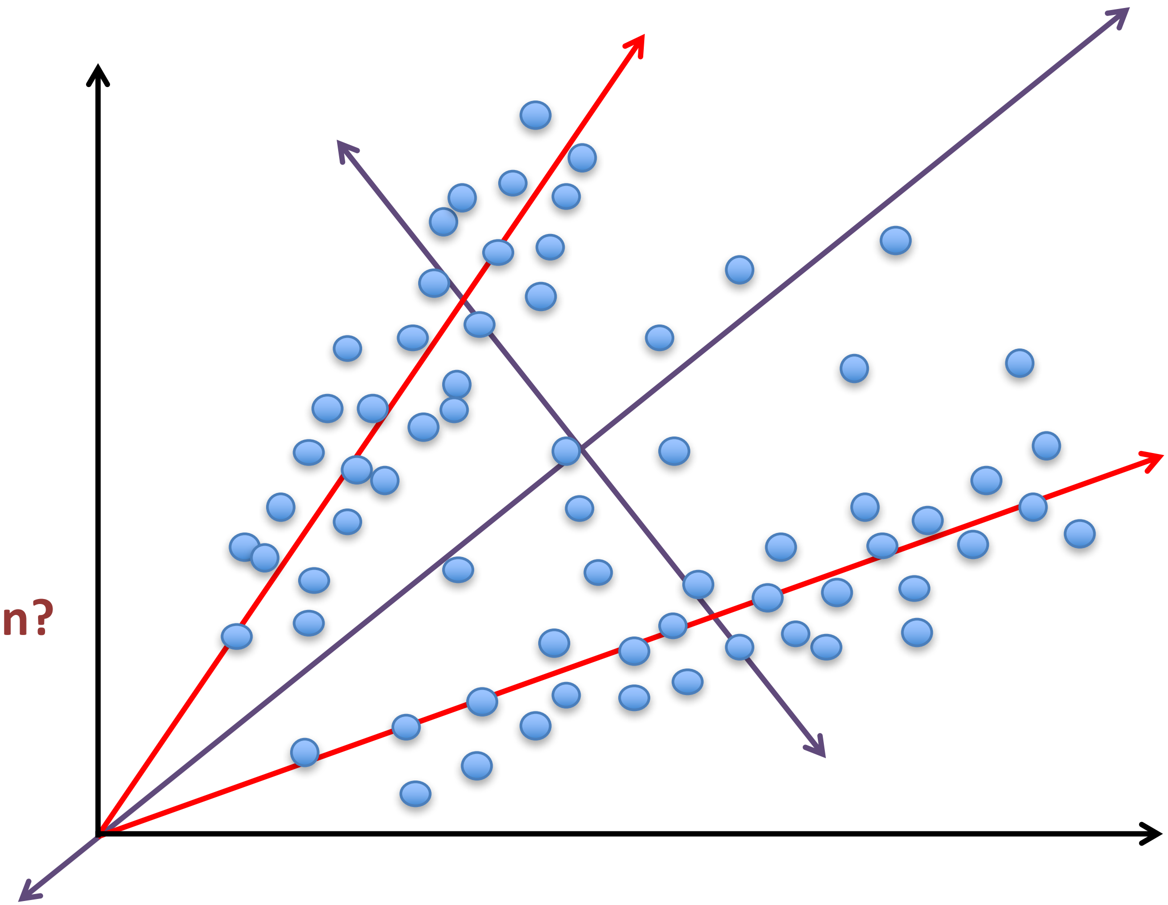
Non-Negative Matrix Factorization

Limitations of PCA & SVD

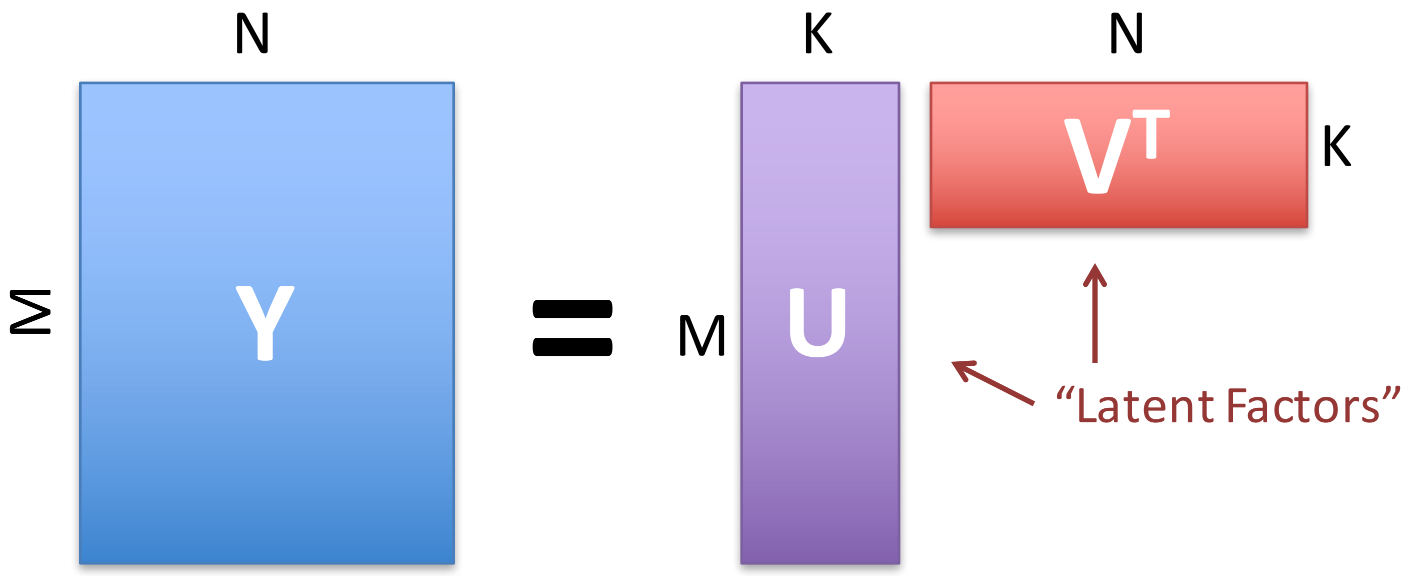
All features non-negative

PCA/SVD Solution

Better Solution?

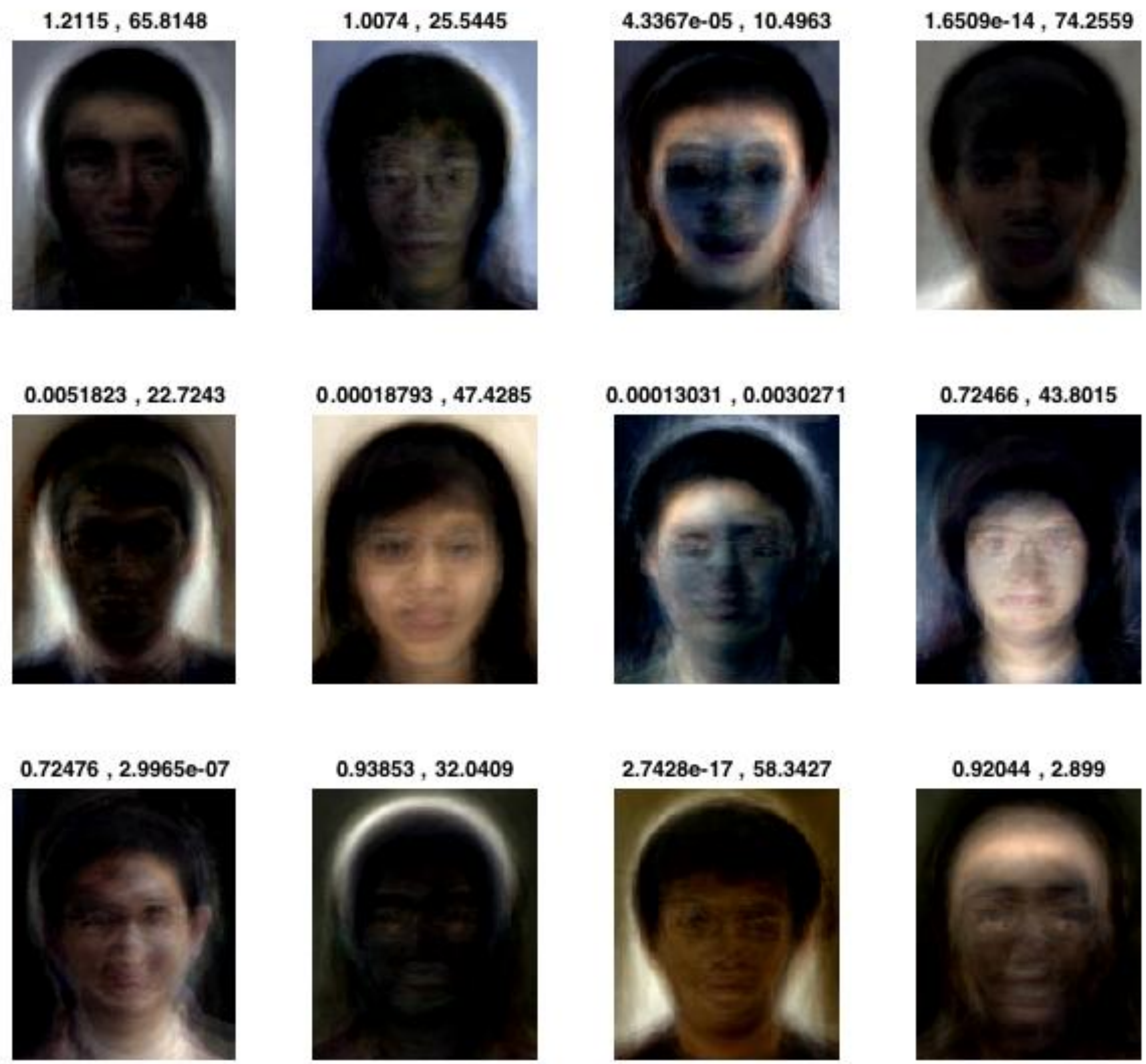


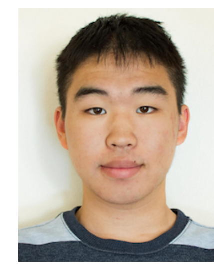
Non-Negative Matrix Factorization



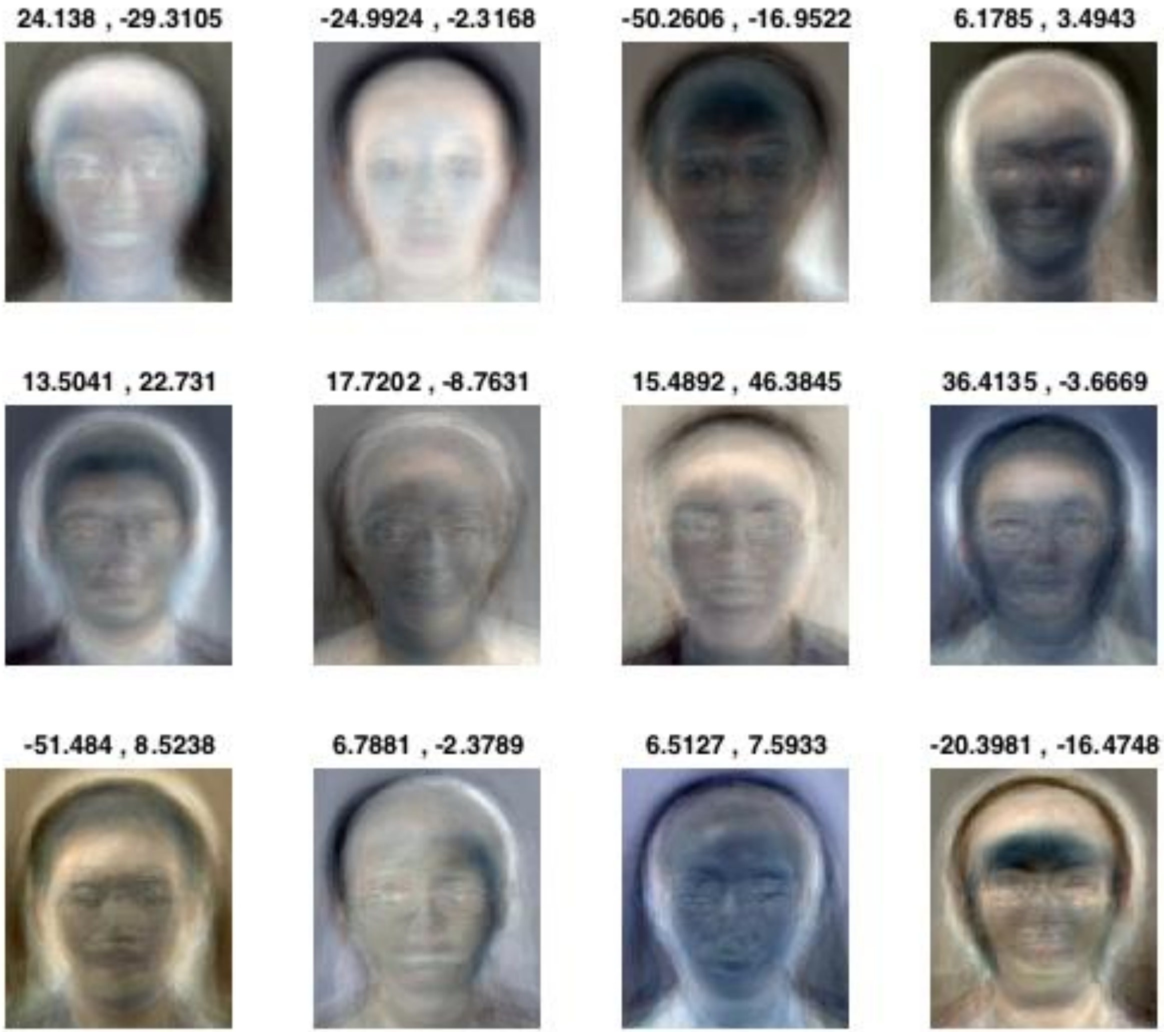
- Assume Y is non-negative
- Find non-negative U & V

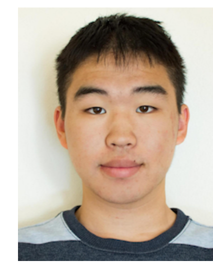
CS 155 Non-Negative Face Basis





CS 155 Eigenfaces





Aside: Non-Orthogonal Projections

- If columns of A are not orthogonal, $A^TA \neq I$
  - How to reverse transformation $x' = A^Tx$?
  - **Solution: Pseudoinverse!**

$$A = U\Sigma V^T$$

SVD

$$A^+ = V\Sigma^+ U^T$$

Pseudoinverse

$$\Sigma^+ = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \sigma_D \end{bmatrix} \qquad \sigma^+ = \begin{cases} 1/\sigma & \text{if } \sigma > 0 \\ 0 & \text{otherwise} \end{cases}$$

Intuition: use the rank-K orthogonal basis that spans A.

$$A^{+T} A^T x = U\Sigma^+ V^T V \Sigma U^T x$$

$$= U_{1:K} U_{1:K}^T x$$

Objective Function

$$\operatorname*{argmin}_{U \geq 0, V \geq 0} \sum_{ij} \ell(y_{ij}, u_i^T v_j)$$

- Squared Loss:
  - Penalizes squared distance

$$\ell(a,b) = (a-b)^2$$

- Generalized Relative Entropy
  - Aka, unnormalized KL divergence
  - Penalizes ratio

$$\ell(a,b) = a \log \frac{a}{b} - a + b$$

- Train using gradient descent

http://hebb.mit.edu/people/seung/papers/nmfconverge.pdf

SVD/PCA vs NNMF

- **SVD/PCA:**
  - Finds the best orthogonal basis faces
    - Basis faces can be neg.
  - Coeffs can be negative
  - Often trickier to visualize
  - Better reconstructions with fewer basis faces
    - Basis faces capture the most variations

- **NNMF:**
  - Finds best set of non-negative basis faces
  - Non-negative coeffs
    - Often non-overlapping
  - Easier to visualize
  - Requires more basis faces for good reconstructions

Non-Negative Latent Factor Models

$$\underset{U,V}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2\right) + \sum_i \ell\left(y_i, z_i^T U^T V x_i\right) \qquad S = \{(x_i, z_i, y_i)\}$$

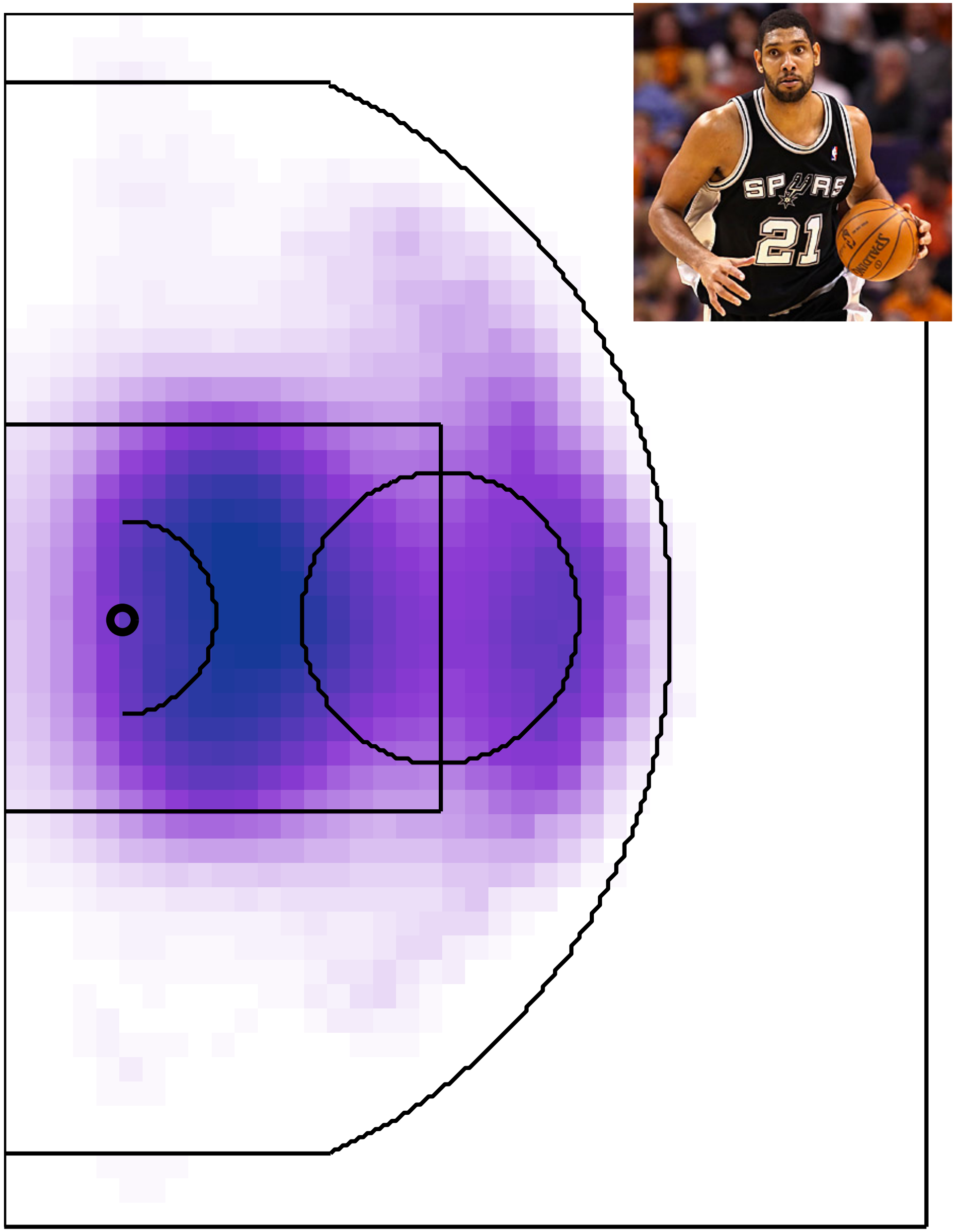
- **Simplest Case:** reduces to NNMF of matrix Y
  - No missing values
  - (z,x) indicator features
- **General Case:** projects high-dimensional non-negative features into low-dimensional non-negative linear model

Modeling NBA Gameplay Using Non-Negative Spatial Latent Factor Models

Fine-Grained Spatial Models

- Discretize court
  - 1x1 foot cells
  - 2000 cells
- 1 weight per cell
  - 2000 weights

$$F_s(\mathbf{x}):$$



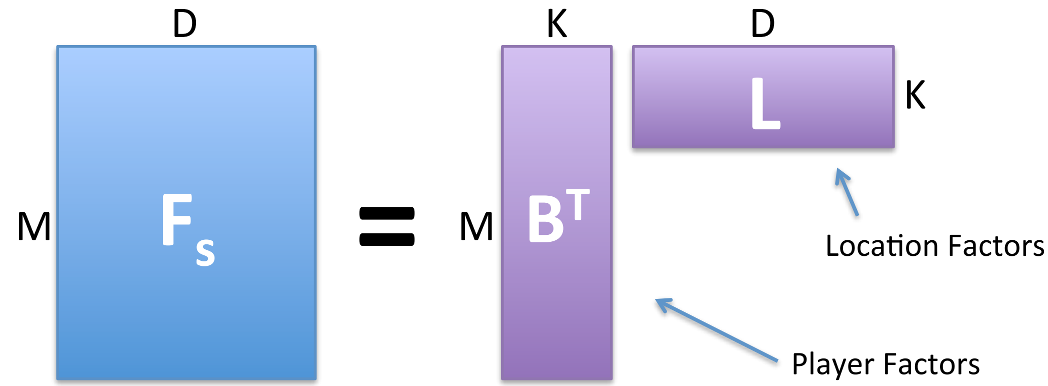
40 feet

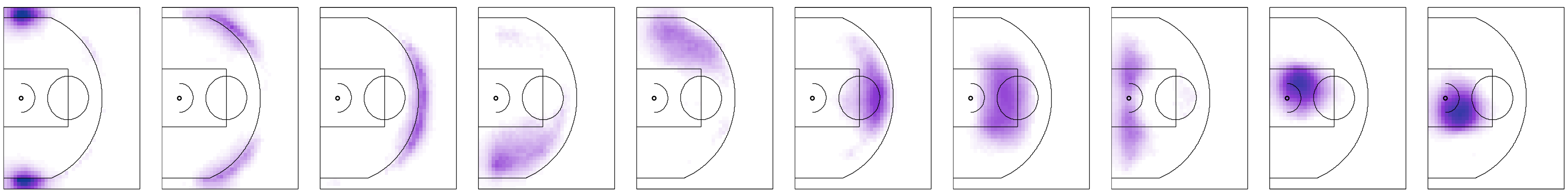
Fine-Grained Spatial Models

- Discretize court
  - 1x1 foot cells
  - 2000
- 1 weig
  - 2000 weights

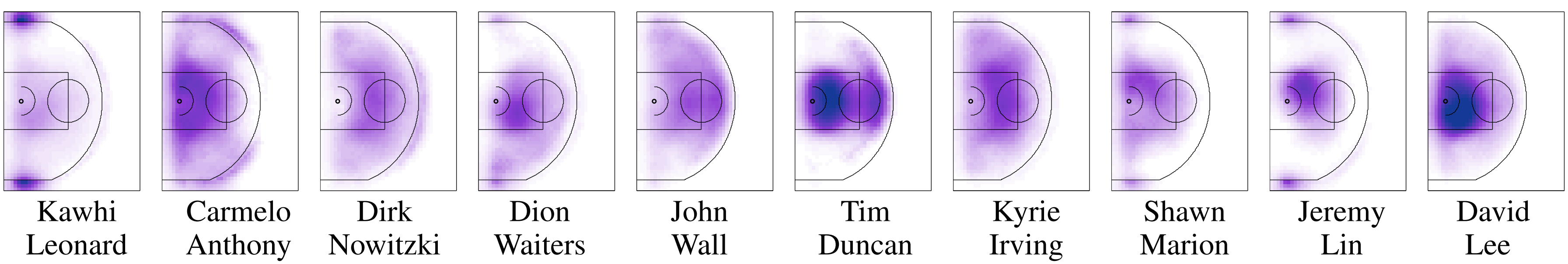
But most players haven't played that much!

$$F_s(\mathbf{x}):$$





Visualizing location factors L



Visualizing players B_bL

http://www.yisongyue.com/publications/icdm2014_bball_predict.pdf

Training Data

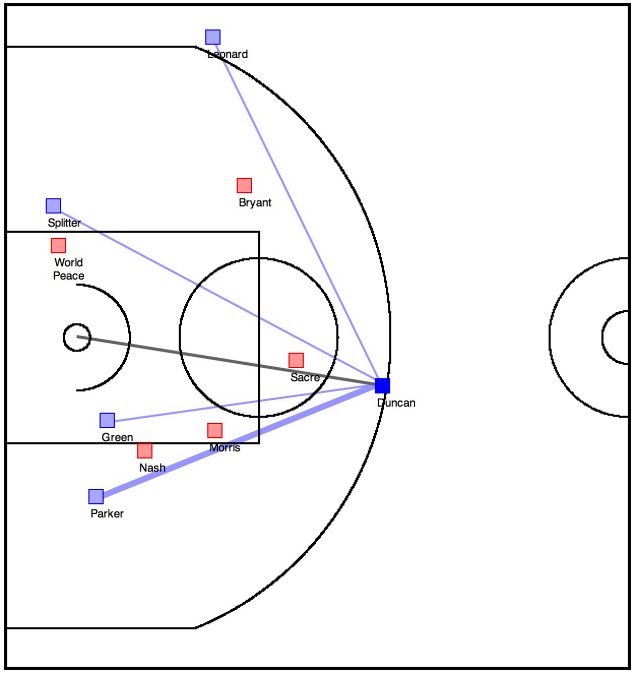
STATS SportsVU

2012/2013 Season, 630 Games,

80K Possessions, 380 frames per possession

Prediction

- Game state: **x**
  - Coordinates of all players
  - Who is the ball handler
- Event: y
  - Ball handler will shoot
  - Ball handler will pass (to whom?)
  - Ball handler will hold onto the ball
  - 6 possibilities
- **Goal:** Learn P(y|**x**)



http://www.yisongyue.com/publications/icdm2014_bball_predict.pdf

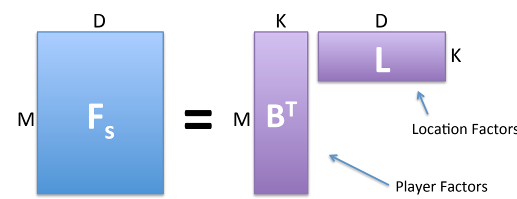
Logistic Regression

(Simple Version: Just for Shooting)

$$P(y \mid \mathbf{x}) = \frac{\exp\left\{F(y \mid \mathbf{x})\right\}}{Z(\mathbf{x} \mid F)} \qquad Z(\mathbf{x} \mid F) = \sum_{y' \in \{s, \perp\}} \exp\left\{F(y' \mid \mathbf{x})\right\}$$

$$F(y' \mid \mathbf{x}) = \begin{cases} F_s(\mathbf{x}) & y' = s \quad \text{Shot} \\ F_\perp & y' = \perp \quad \text{Hold on to ball} \end{cases}$$

Offset or bias



$$P(y = s \mid \mathbf{x}) = \frac{1}{1 + \exp\left\{-F_s(\boldsymbol{x}) + F_\perp\right\}}$$

Learning the Model

- Given training data: $S = \{(\boldsymbol{x}, y)\}$

Player Configuration

What Happened Next

- Learn parameters of model:

$$\underset{F_s, F_\perp}{\operatorname{argmin}} \frac{\lambda}{2} \|F_s\|^2 + \sum_{(\boldsymbol{x},y)\in S} \underbrace{\ell\left(y, F_s(x) - F_\perp\right)}_{\text{Log Loss}}$$

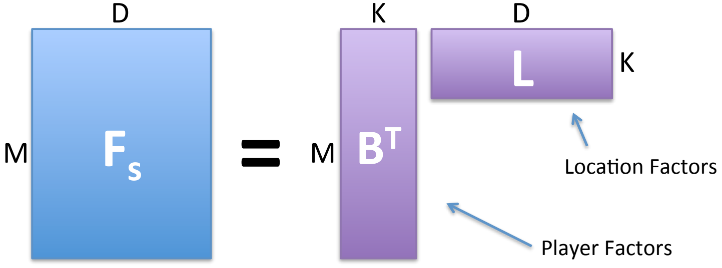
$$P(y = s \mid \mathbf{x}) = \frac{1}{1 + \exp\left\{-F_s(\boldsymbol{x}) + F_\perp\right\}}$$

Optimization via Gradient Descent

$$\underset{B\geq 0, L\geq 0, F_\perp}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|B\|^2 + \|L\|^2\right) + \sum_{(\boldsymbol{x},y)} \ell\left(y, B_{b(\boldsymbol{x})}^T L_{l(\boldsymbol{x})} - F_\perp\right)$$

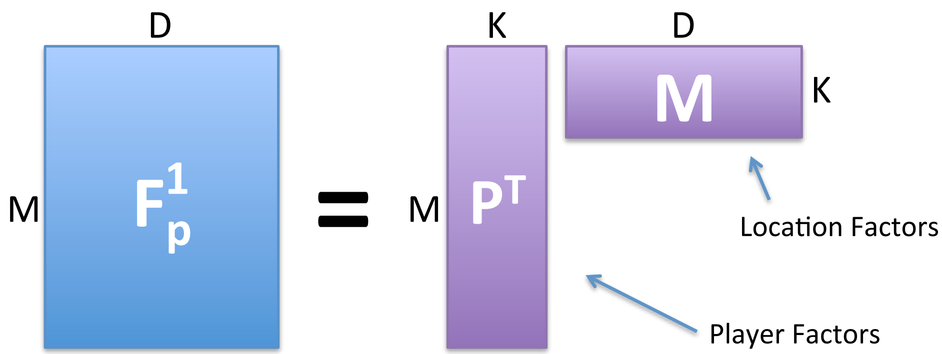
$$\partial_{L_i} = \lambda_1 L_i - \sum_{(\boldsymbol{x},y)} \frac{\partial \log P(y \mid \boldsymbol{x})}{\partial L_i}$$

$$\frac{\partial \log P(y \mid \boldsymbol{x})}{\partial L_i} = \left(1_{[y=s]} - P(s \mid \boldsymbol{x})\right) B_{b(\boldsymbol{x})}$$

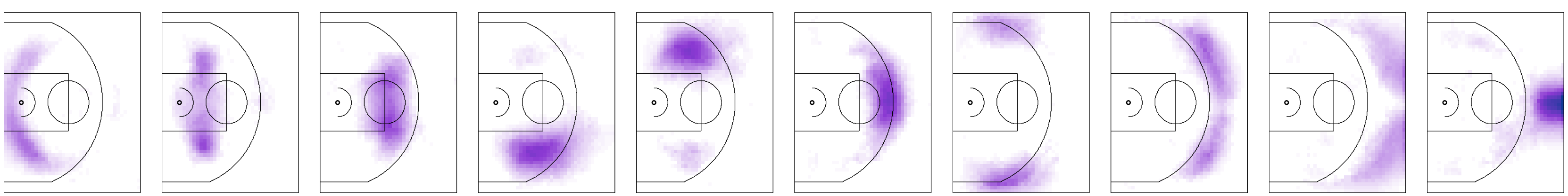


http://www.yisongyue.com/publications/icdm2014_bball_predict.pdf

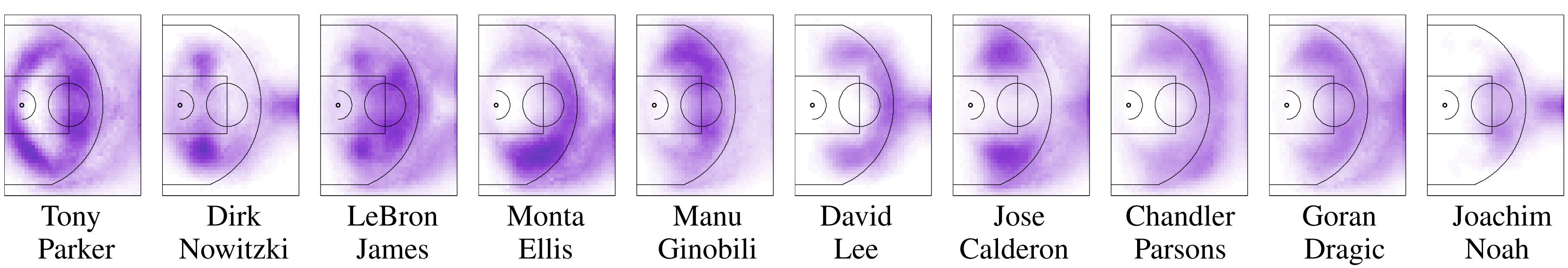
Where are Players Likely to Receive Passes?



Enforce Non-Negativity
(Accuracy Worse)
(More Interpretable)

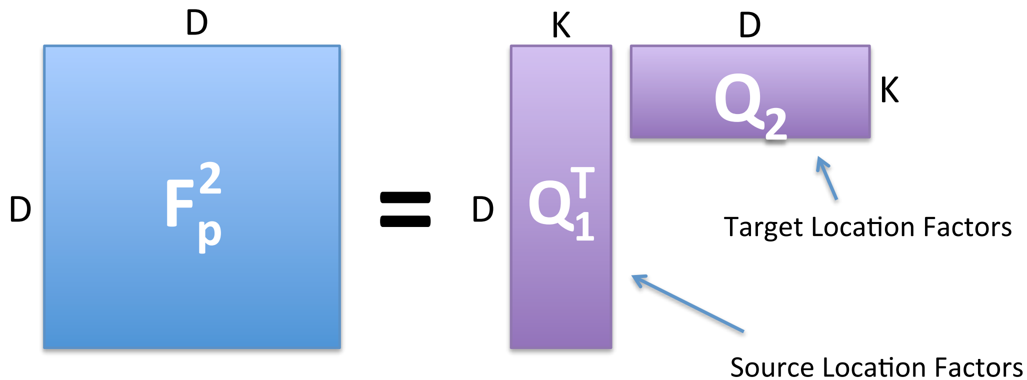


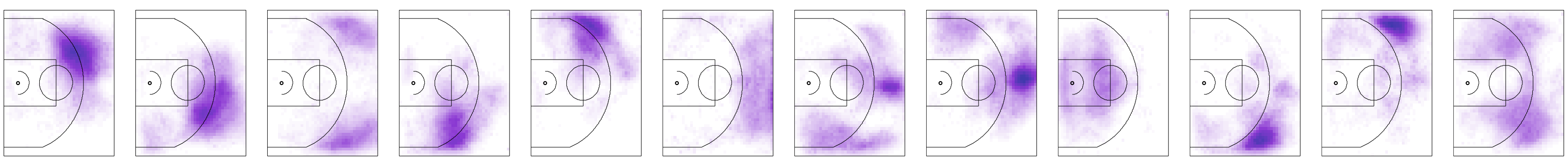
Visualizing Location Factors M



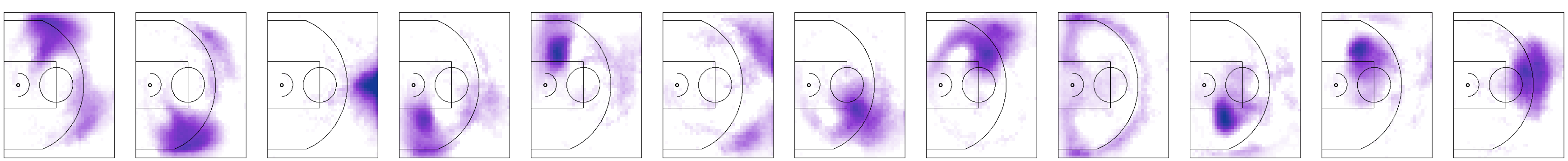
http://www.yisongyue.com/publications/icdm2014_bball_predict.pdf

How do passes tend to flow?





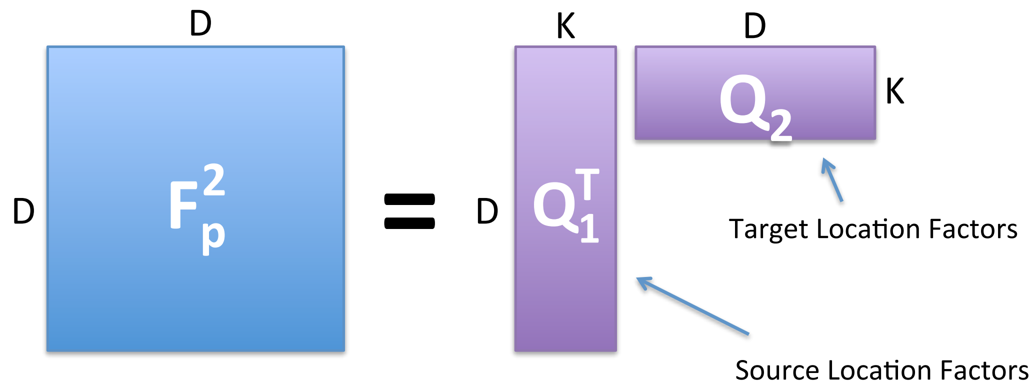
Q_1

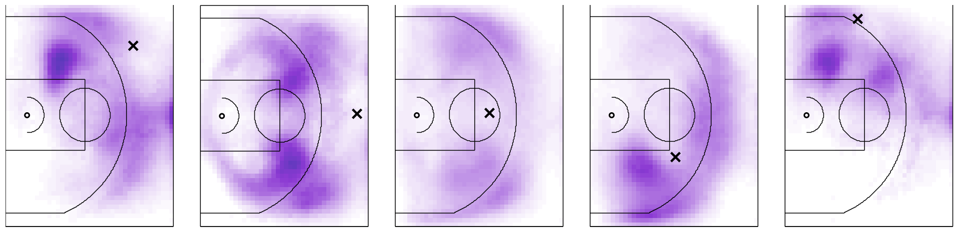


Q_2

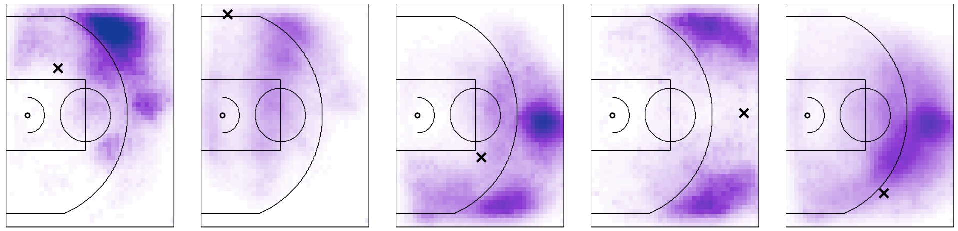
http://www.yisongyue.com/publications/icdm2014_bball_predict.pdf

How do passes tend to flow?





Passing From "X"

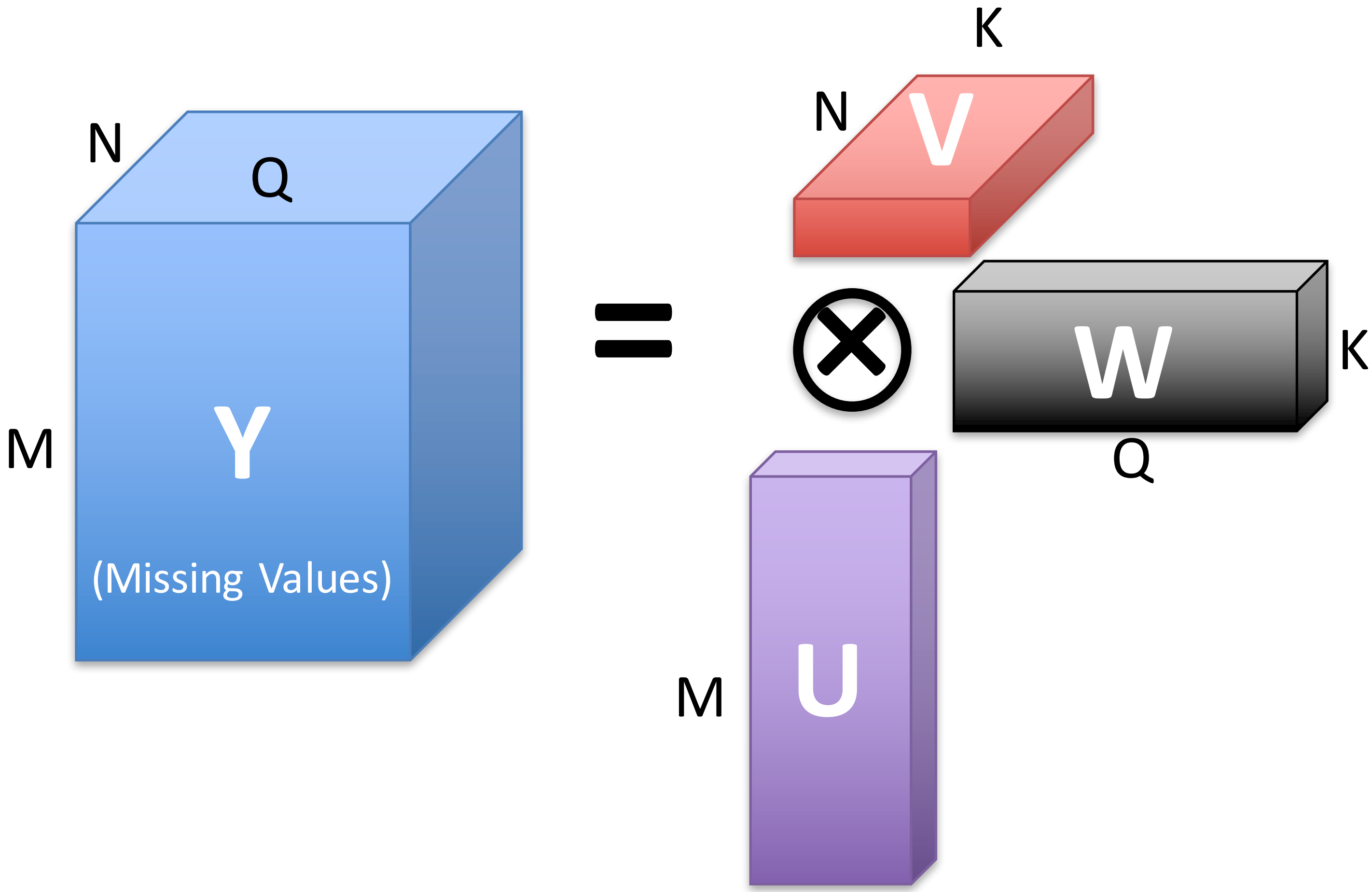


Passing To "X"

http://www.yisongyue.com/publications/icdm2014_bball_predict.pdf

Tensor Latent Factor Models

Tensor Factorization



Tri-Linear Model

$$\underset{U,V,W}{\operatorname{argmin}} \frac{\lambda}{2}\left(\|U\|_{Fro}^2 + \|V\|_{Fro}^2 + \|W\|_{Fro}^2\right) + \sum_i \ell\left(y_i, \left\langle U^T z_i, V^T x_i, W^T q_i \right\rangle\right)$$

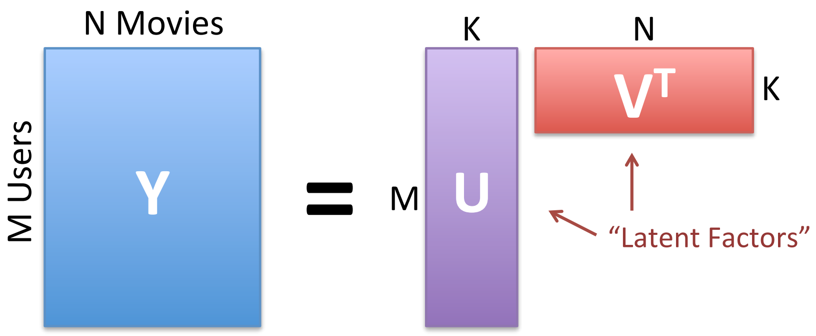
- Prediction via 3-way dot product: $\langle a,b,c\rangle = \sum_k a_k b_k c_k$
  - Related to Hadamard Product

- **Example:** online advertising
  - User profile z
  - Item description x
  - Query q

Solve using Gradient Descent

Summary: Latent Factor Models

- Learns a low-rank model of a matrix of observations Y
  - Dimensions of Y can have various semantics
- Can tolerate missing values in Y
- Can also use features
- Widely used in industry



Next Lecture

- Embeddings

- Word2Vec