# Learning with Matrix Factorizations

#### Nati Srebro

Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology

Adviser: Tommi Jaakkola (MIT)

Committee: Alan Willsky (MIT), Tali Tishby (HUJI), Josh Tenenbaum (MIT)

Joint work with Shie Mannor (McGill), Noga Alon (TAU) and Jason Rennie (MIT)

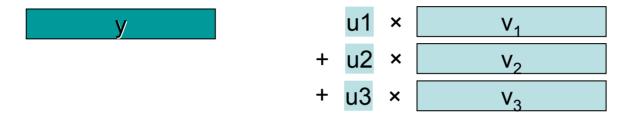
Lots of help from John Barnett, Karen Livescu, Adi Shraibman, Michael Collins, Erik Demaine, Michel Goemans, David Karger and Dmitry Panchenko

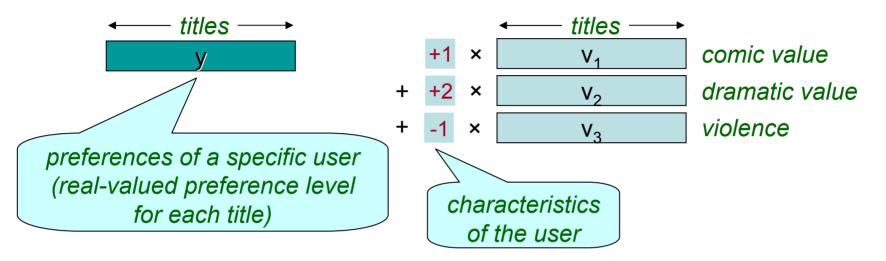
### **Dimensionality Reduction:**

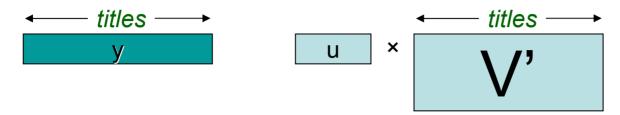
Low dimensional representation capturing important aspects of high dimensional data

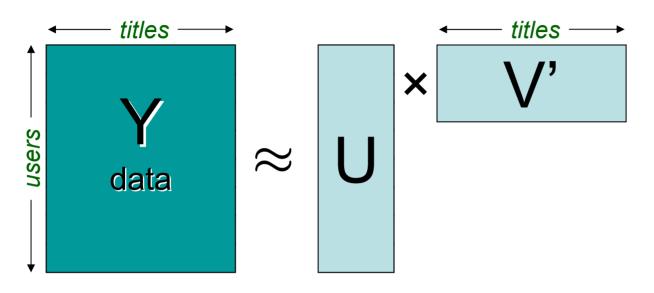


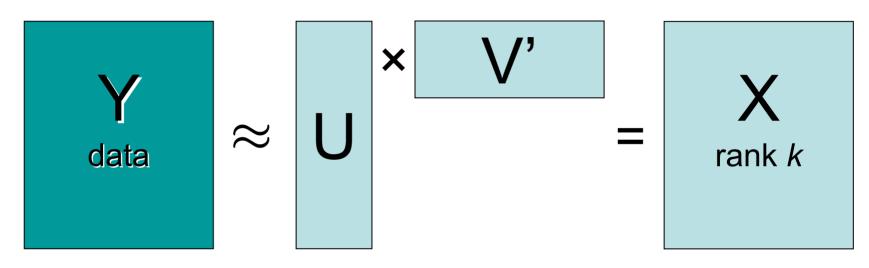
- Compression (mostly to reduce processing time)
- Reconstructing latent signal
  - biological processes through gene expression
- Capturing structure in a corpus
  - documents, images, etc
- Prediction: collaborative filtering



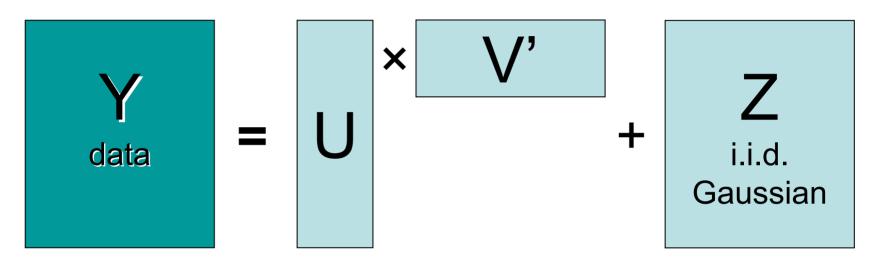








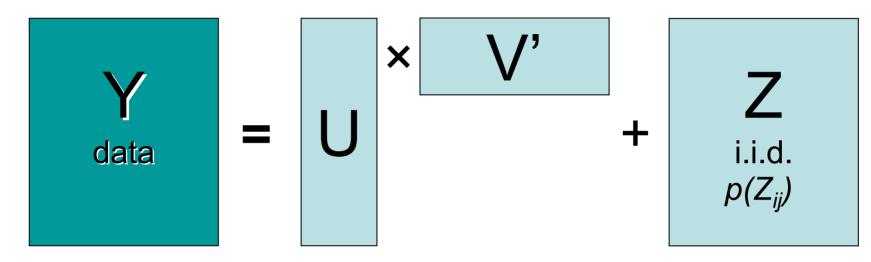
- Non-Negativity [LeeSeung99]
- Stochasticity (convexity) [LeeSeung97][Barnett04]
- Sparsity
  - Clustering as an extreme (when rows of U sparse)
- Unconstrained: Low Rank Approximation



Additive Gaussian noise

minimize |Y-UV'|<sub>Fro</sub>

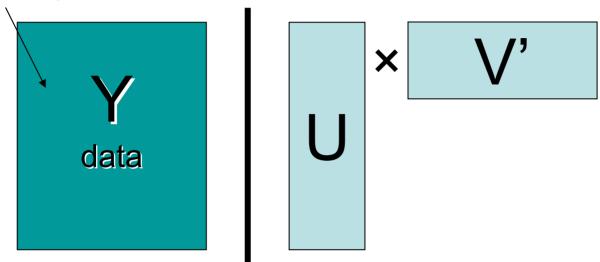
$$\log L(UV';Y) = \sum_{ij} \log P(Y_{ij} | UV'_{ij}) = \frac{-1}{2\sigma^2} \sum_{ij} (Y_{ij} - UV'_{ij})^2 + const$$



- Additive Gaussian noise
- General additive noise

minimize  $|Y-UV'|_{Fro}$ minimize  $\sum -\log p(Y_{ij}-UV'_{ij})$ 

 $p(Y_{ij}|UV'_{ij})$ 

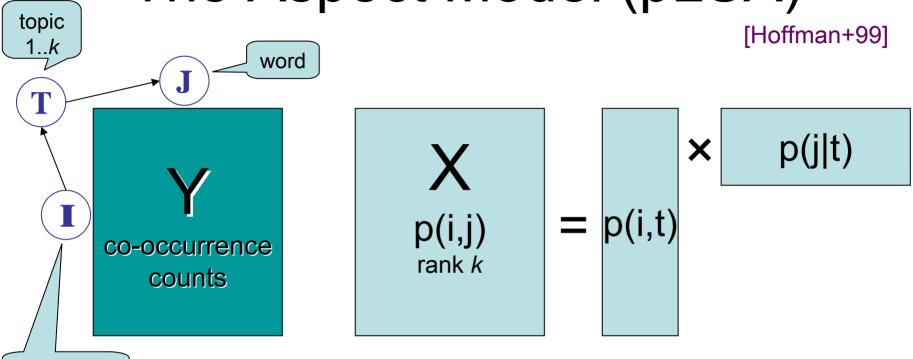


- Additive Gaussian noise
- General additive noise
- General conditional models
  - Multiplicative noise
  - Binary observations: Logistic LRA
  - Exponential PCA [Collins+01]
  - Multinomial (pLSA [Hofman01])
- Other loss functions [Gordon02]

minimize  $|Y-UV'|_{Fro}$ minimize  $\sum -\log p(Y_{ij}-UV'_{ij})$ minimize  $\sum -\log p(Y_{ii}|UV'_{ii})$ 

minimize ∑loss(UV';;Y;)

## The Aspect Model (pLSA)



 $Y|X \sim Multinomial(N,X)$ 

document

$$Y_{ij}|X_{ij} \sim Binomial(N,X_{ij})$$

# Low-Rank Models for Matrices of Counts, Occurrences or Frequencies

	Multinomial	Independent Binomials	Independent Bernoulli
Mean parameterization	Aspect Model (pLSA) [Hoffman+99]	$Y_{ij} X_{ij}\sim Bin(N,X_{ij})$	$P(Y_{ij}=1)=X_{ij}$
$0 \le X_{ij} \le 1$ $E[Y_{ij} X_{ij}]=X_{ij}$	■ NMF if $\sum X_{ij} = 1$	≈ NMF [Lee+01]	
Natural parameterization unconstrained X <sub>ij</sub>	Sufficient Dimensionality Reduction [Globerson+02]	Y <sub>ij</sub>  X <sub>ij</sub> ~Bin(N,g(X <sub>ij</sub> ))  Exponential PCA:	Logistic Low Rank Approximation [Schein+03] los
		$p(Y_{ij} X_{ij}) \propto exp(Y_{ij})$	$X_{ij}+F(Y_{ij})$

 $g(x)=1/(1+e^{x})$ 

### Outline

- Finding Low Rank Approximations
  - Weight Low Rank Approx: minimize  $\sum_{ij} \mathbf{W}_{ij} (\mathbf{Y}_{ij} \mathbf{X}_{ij})^2$
  - Use WLRA Basis for other losses / conditional models
- Consistency of Low Rank Approximation
   When more data is available, do we converge to correct solution? Not always...
- Matrix Factorization for Collaborative Filtering
  - Maximum Margin Matrix Factorization
  - Generalization Error Bounds (Low Rank & MMMF)

### Finding Low Rank Approximation

Find rank- $k \times minimizing \sum loss(X_{ij}; Y_{ij}) (=log p(Y|X))$ 

- Non-convex:
  - "X is rank-k" is a non-convex constraint
  - ∑loss((UV)<sub>ii</sub>;Y<sub>ii</sub>) not convex in U,V
- rank- $k \times minimizing \sum (Y_{ij}-X_{ij})^2$ :
  - non-convex, but no (non-global) local minima
  - solution: leading components of SVD
- For other loss functions, or with missing data: cannot use SVD, local minima, difficult problem
- Weighted Low Rank Approximation:

minimize 
$$\sum W_{ij}(Y_{ij}-X_{ij})^2$$

Arbitrarily specified weights (part of input)

## WLRA: Optimization

$$J(UV') = \sum_{ij} W_{ij} (Y - UV')_{ij}^2$$

For fixed *V*, find optimal *U* For fixed *U*, find optimal *V* 

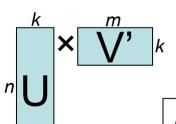
$$J^*(V) = \min_{U} J(UV')$$
$$\frac{\partial}{\partial V} J^*(V') = 2U^*((U^*V' - Y) \otimes W)$$

Conjugate gradient descent on  $J^*$ Optimize km parameters instead of k(n+m)

EM approach:

elementwise product

 $X \leftarrow \text{LowRankApprox}(W \otimes Y + (1-W) \otimes X)$ 

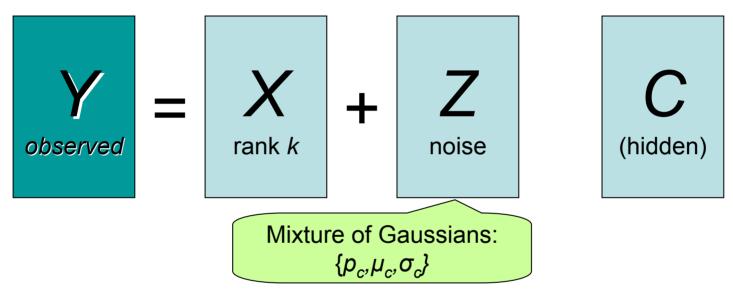


# Newton Optimization for Non-Quadratic Loss Functions

minimize 
$$\sum_{ij} loss(X_{ij}; Y_{ij})$$
  
 $loss(X_{ij}; Y_{ij})$  convex in  $X_{ij}$ 

- Iteratively optimize quadratic approximations of objective
- Each such quadratic optimization is a weighted low rank approximation

# Maximum Likelihood Estimation with Gaussian Mixture Noise



E step: calculate posteriors of C

M step: WLRA with

$$W_{ij} = \sum_{c} \frac{\Pr(C_{ij} = c)}{\sigma_{C}^{2}} \qquad A_{ij} = Y_{ij} + \sum_{c} \frac{\Pr(C_{ij} = c)\mu_{C}}{\sigma_{C}^{2}} / W_{ij}$$

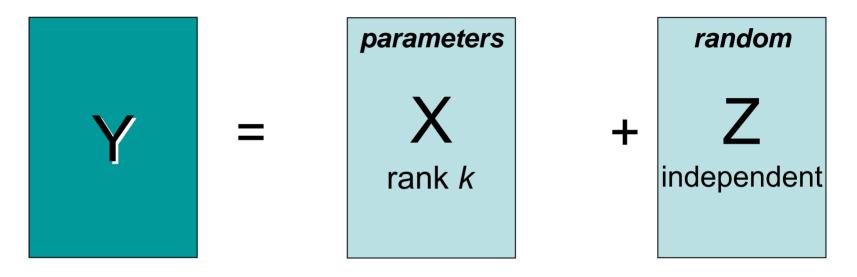
### Outline

- Finding Low Rank Approximations
  - Weight Low Rank Approx: minimize ∑<sub>ii</sub>W<sub>ii</sub>(Y<sub>ii</sub>-X<sub>ii</sub>)<sup>2</sup>
  - Use WLRA Basis for other losses / conditional models
- Consistency of Low Rank Approximation

When more data is available, do we converge to correct solution? Not always...

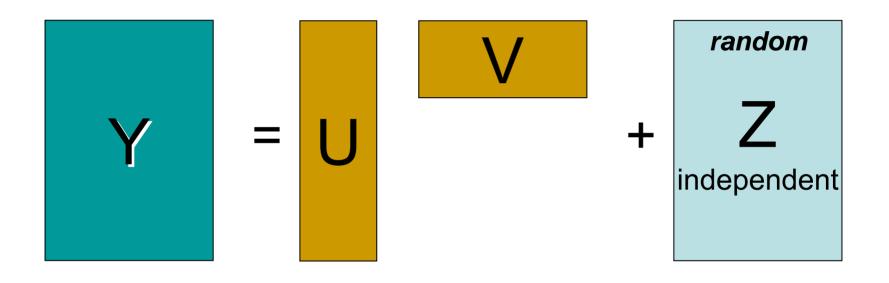
- Matrix Factorization for Collaborative Filtering
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## Asymptotic Behavior of Low Rank Approximation

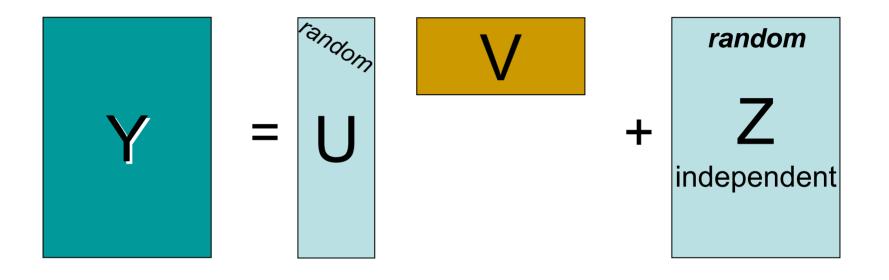


Single observation, Number of parameters is linear in number of observables

Can never approach correct estimation of parameters

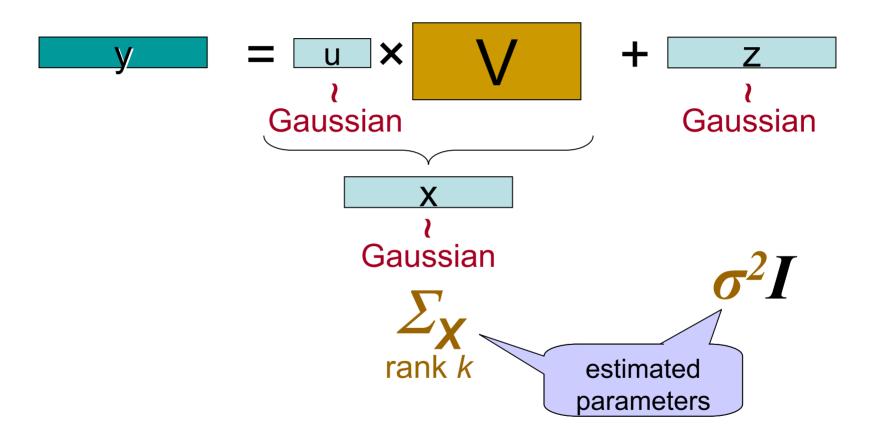


Number of parameters is linear in number of observables



Multiple samples of random variable y

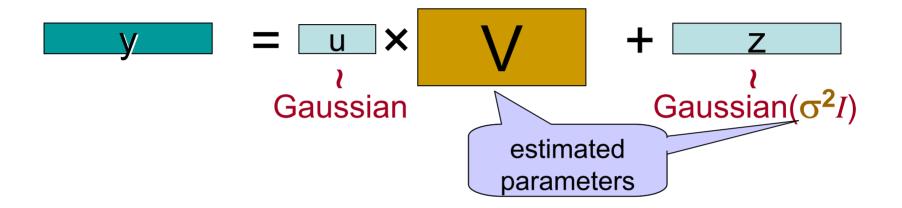
#### Probabilistic PCA



Maximum likelihood ≡ PCA

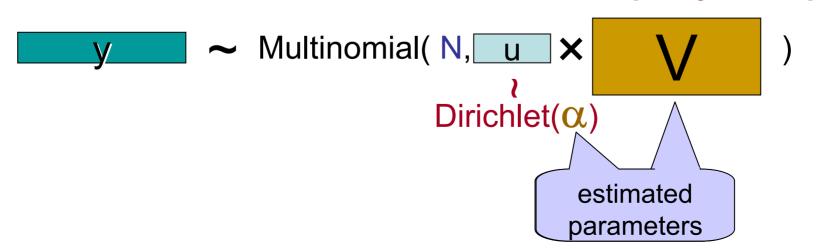
#### Probabilistic PCA

[Tipping Bishop 97]

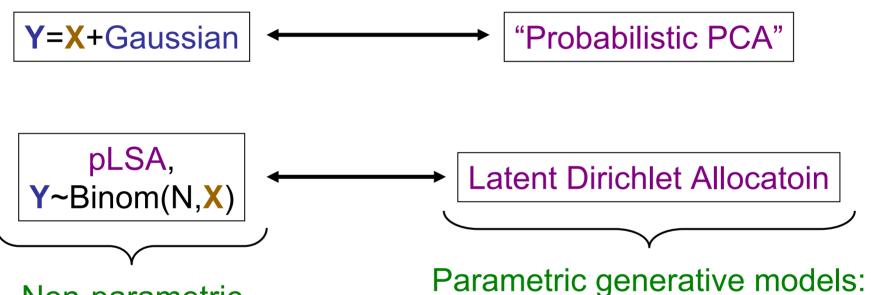


#### Latent Dirichlet Allocation

[Blei Ng Jordan 03]

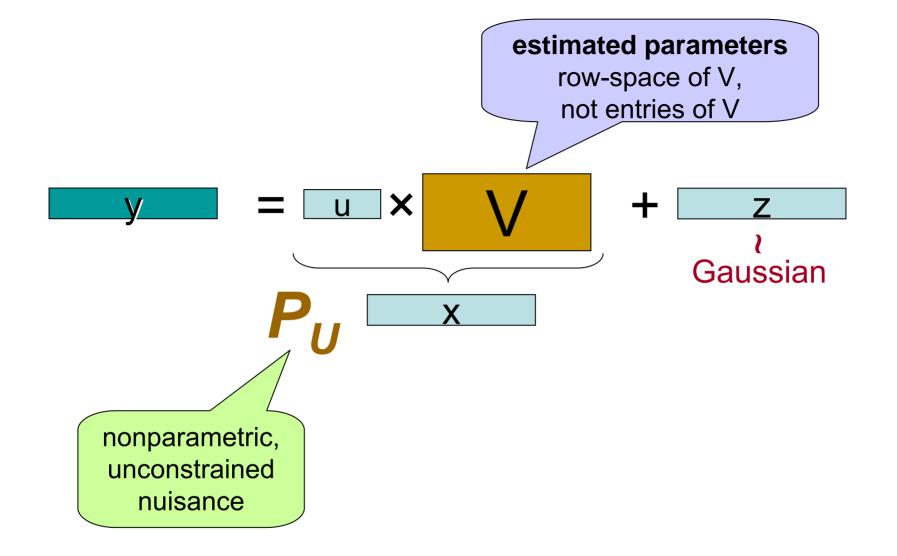


### Generative and Non-Generative Low Rank Models

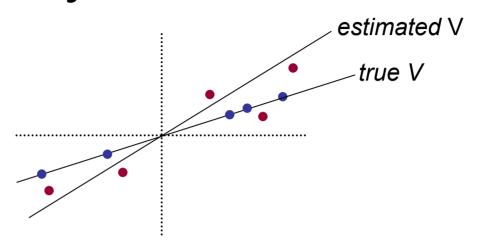


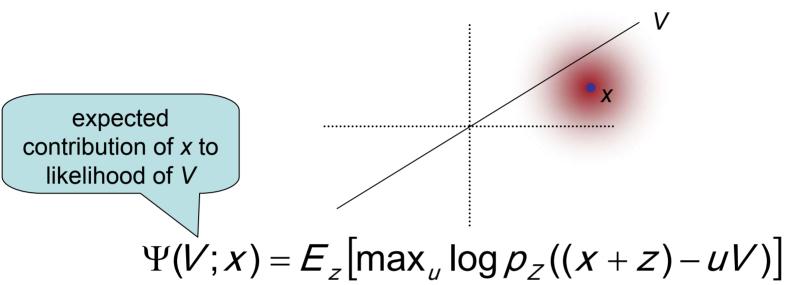
Non-parametric generative models

Consistency of Maximum Likelihood estimation guaranteed if model assumptions hold (both on Y|X and on U)



Non-parametric model, estimation of a parametric part of the model Maximum Likelihood ≡ "Single Observed Y"





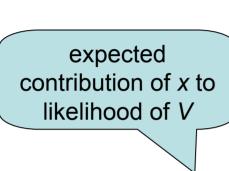
ML estimator is consistent for any  $P_{ij}$ 

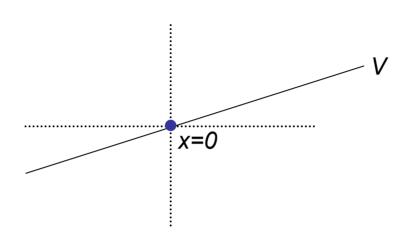


for all x,  $\bigvee$  V maximizes  $\Psi(V;x)$ iff V spans x

When Z~Gaussian,  $\Psi(V; X) = \mathbf{E}[L_2]$  distance of x+z from V

For iid Gaussian noise, ML estimation (PCA) of the low-rank sub-space is consistent





$$\Psi(\dot{V};x) = E_z[\max_u \log p_z((x+z)-uV)]$$

ML estimator is consistent for any  $P_u$ 

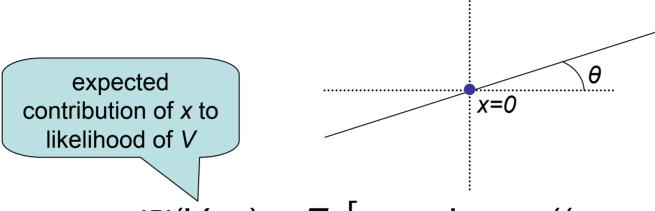


for all x, V maximizes  $\Psi(V;x)$ iff V spans x

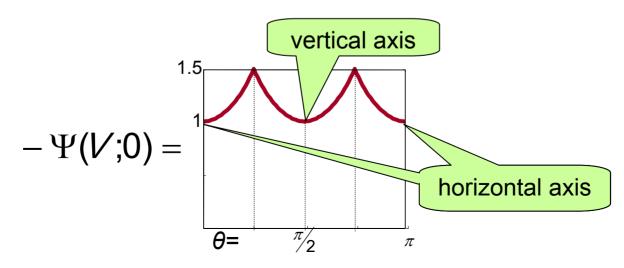
ML estimator is consistent for any  $P_u$ 



 $\Psi(V;0)$  is constant for all V



$$\Psi(V; x) = E_z[\max_u \log p_Z((x+z)-uV)]$$
  
Laplace:  $p_Z(Z[i]) = \frac{1}{2}e^{-|z[i]|}$ 



General conditional model for Y|X

expected contribution of *x* to likelihood of *V* 

$$\Psi(V; x) = E_{Y|X} \left[ \max_{u} \log p_{Y|X} (Y \mid uV) \mid x \right]$$

ML estimator is consistent for any  $P_u$ 

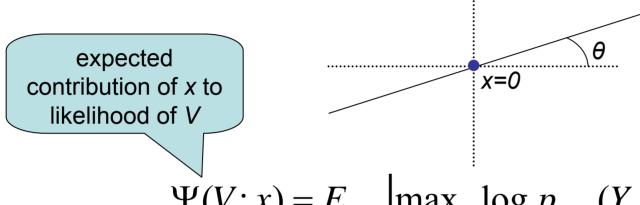


for all x, V maximizes  $\Psi(V; x)$ iff V spans x

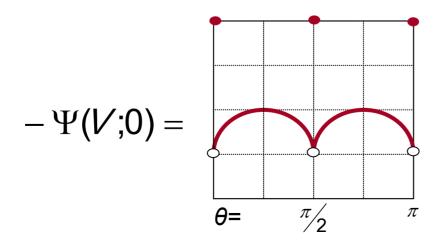
ML estimator is consistent for any  $P_u$ 



 $\Psi(V;0)$  is constant for all V



$$\Psi(V; x) = E_{Y|X} \left[ \max_{u} \log p_{Y|X} (Y | uV) | x \right]$$
Logistic:  $p_{Y|X} (Y[i] = 1 | x[i]) = \frac{1}{1 - e^{-x[i]}}$ 



Additive i.i.d. noise Y=X+Z:

Maximum Likelihood generally not consistent PCA is consistent (for any noise distribution)

Span of 
$$k$$
 leading  $\Sigma_Y \longrightarrow \Sigma_X + \sigma^2 I$  eigenvectors of  $\Sigma_Y \longrightarrow \Sigma_X + \sigma^2 I$ 

Additive i.i.d. noise Y=X+Z:

Maximum Likelihood generally not consistent

PCA is consistent (for any noise distribution)

$$\hat{\Sigma}_{Y} \to \Sigma_{Y} = \Sigma_{X} + \Sigma_{Z} = \Sigma_{X} + \sigma^{2}I$$

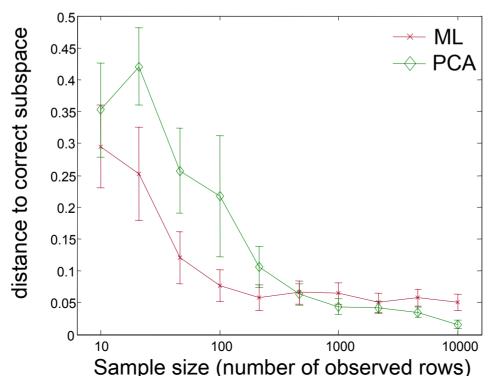
$$s_{1}, s_{2}, ..., s_{k}, 0, 0, ..., 0$$

$$s_{2} = \Sigma_{X} + \sigma^{2}I$$

Additive i.i.d. noise Y=X+Z:

Maximum Likelihood generally not consistent

PCA is consistent (for any noise distribution)



Noise: 0.99 *N*(0,1) + 0.01 *N*(0,100)

- Additive i.i.d. noise Y=X+Z:
   Maximum Likelihood generally not consistent
   PCA is consistent (for any noise distribution)
- Unbiased noise E[Y|X]=X:
   Maximum Likelihood generally not consistent
   PCA not consistent
  - -- Can correct by ignoring diagonal of covariance
- Exponential PCA (X are natural parameters)
   Maximum Likelihood generally not consistent
   Covariance methods not consistent
   ???

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## Collaborative Filtering

Based on preferences so far, and preferences of others:

⇒ Predict further preferences

		11104163										
users		2 5		1			4				5	
		5		4						1		3
			3		5			2				
	4						5		3			
			4		1	3				5		
				2				1				4
		1					5		5		4	
			2			5				4		
		3		က		1		5		<u>4</u>		1
		3 4				Υ_			23		က	
		4			5	Υ_			က			
			3				3				5	
	2			1		1						
			5			2			4		4	
		1		3		1	5		4		<u>4</u>	
	1		2			4				5		

movies

Implicit or explicit preferences?

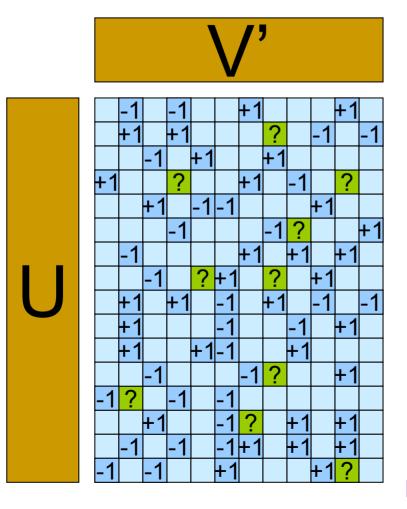
Type of queries.

## **Matrix Completion**

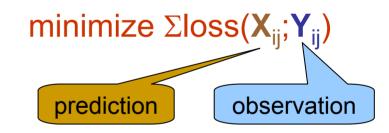
Based on partially observed matrix:

 $\Rightarrow$  Predict unobserved entries "Will user *i* like movie *j*?"

#### Matrix Completion with Matrix Factorization

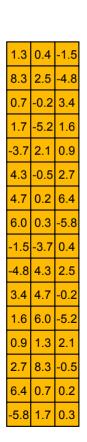


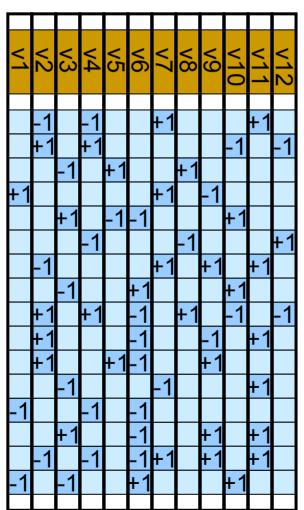
Fit factorizable (low-rank) matrix **X=UV**' to observed entries.



Use matrix X to predict unobserved entries.

#### Matrix Completion with Matrix Factorization





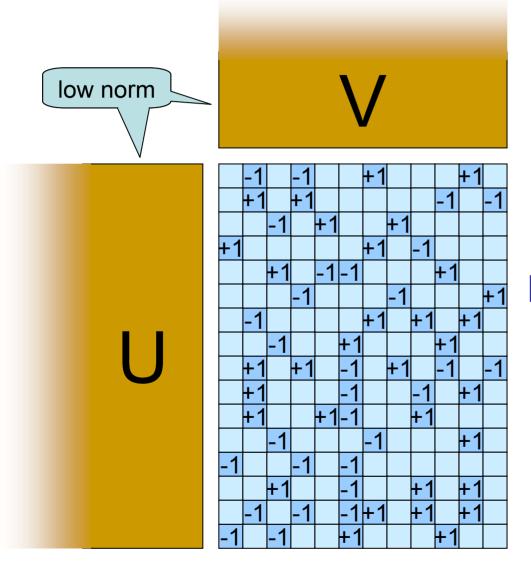
When U is fixed, each row is a linear classification problem:

- rows of U are feature vectors
- columns of V are linear classifiers

Fitting U and V:

Learning features that work well across all classification problems.

## Max-Margin Matrix Factorization



Instead of bounding dimensionality of U,V, bound norms of U,V

For observed  $Y_{ij} \in \pm 1$ :

$$Y_{ij} X_{ij} \ge Margin$$

## Max-Margin Matrix Factorization





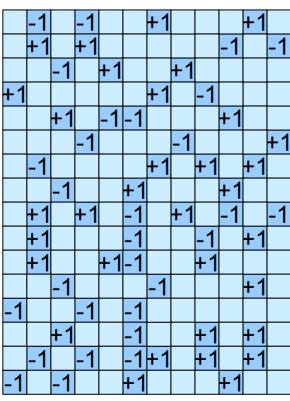
bound norms on average:

$$\left(\sum_{i} |U_{i}|^{2}\right) \left(\sum_{j} |V_{j}|^{2}\right) \leq 1$$

bound norms uniformly:

$$(\max_i |U_i|^2) (\max_i |V_i|^2) \le 1$$

U

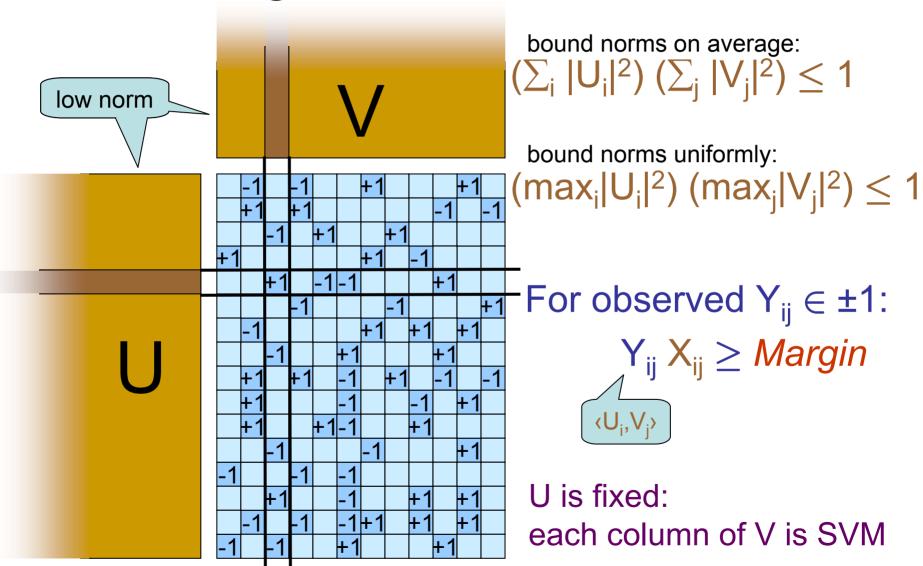


For observed  $Y_{ij} \in \pm 1$ :

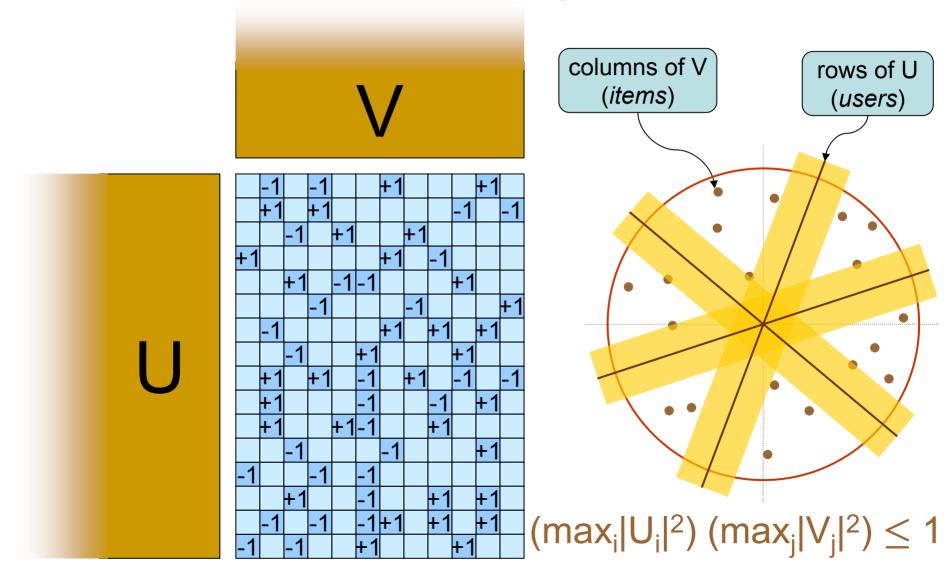
$$Y_{ij} X_{ij} \ge Margin$$

U is fixed: each column of V is SVM

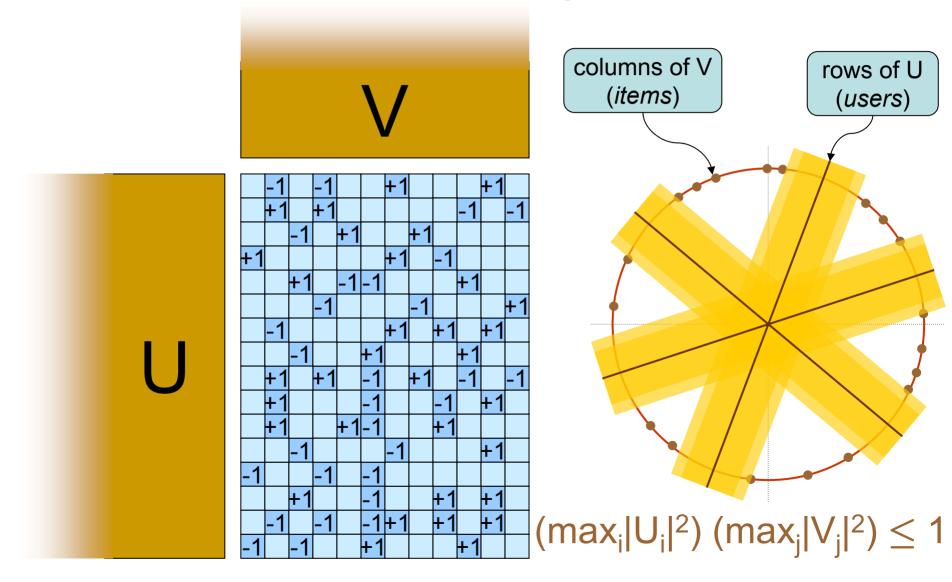
## Max-Margin Matrix Factorization



## Geometric Interpretation



## Geometric Interpretation

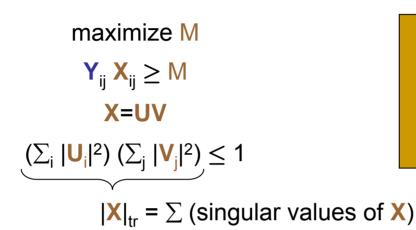


#### Finding Max-Margin Matrix Factorizations

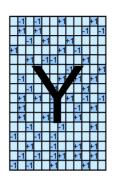
$$\begin{array}{ll} \text{maximize M} & \text{maximize M} \\ \mathbf{Y}_{ij} \ \mathbf{X}_{ij} \geq \mathbf{M} & \mathbf{Y}_{ij} \ \mathbf{X}_{ij} \geq \mathbf{M} \\ \mathbf{X} = \mathbf{UV} & \mathbf{X} = \mathbf{UV} \\ (\sum_{i} |\mathbf{U}_{i}|^{2}) \ (\sum_{j} |\mathbf{V}_{j}|^{2}) \leq 1 & (\text{max}_{i} |\mathbf{U}_{i}|^{2}) \ (\text{max}_{j} |\mathbf{V}_{j}|^{2}) \leq 1 \end{array}$$

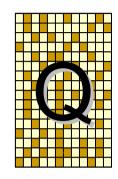
Unlike rank(X)  $\leq k$ , these are convex constraints!

#### Finding Max-Margin Matrix Factorizations









 $\begin{aligned} & \text{minimize tr}(\mathbf{A}) \text{+tr}(\mathbf{B}) \text{+ c } \sum & \xi_{ij} \\ & \mathbf{Y}_{ij} \ \mathbf{X}_{ij} \geq 1 \text{- } \xi_{ij} \\ & \mathbf{A} \ \mathbf{X} \\ & \mathbf{X}' \ \mathbf{B} \end{aligned} \text{ p.s.d.}$ 

Dual variable  $Q_{ij}$  for each observed (i,j)

maximize 
$$\sum \mathbf{Q}_{ij}$$
  
 $0 \leq \mathbf{Q}_{ij} \leq \mathbf{c}$   
 $||\mathbf{Q} \otimes \mathbf{Y}||_2 \leq 1$ 

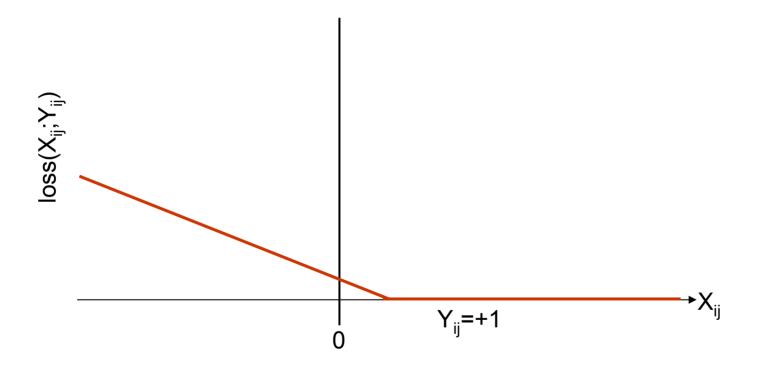
sparse elementwise product (zero for unobserved entries)

#### Finding Max-Margin Matrix Factorizations

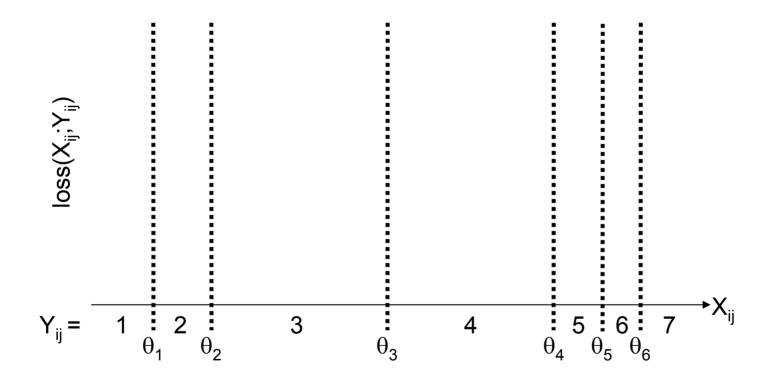
- Semi-definite program with sparse dual: Limited by number of observations, not size (for both average-norm and max-norm)
- Current implementation: use CSDP (off-the-shelf solver), up to 30k observations (e.g. 1000x1000, 3% observed)
- For large-scale problems: updates on dual alone?

$$\begin{aligned} & \text{minimize tr}(\mathbf{A}) \text{+tr}(\mathbf{B}) \text{+ c } \sum & \xi_{ij} \\ & \mathbf{Y}_{ij} \ \mathbf{X}_{ij} \geq 1 \text{- } \xi_{ij} \\ & \mathbf{A} \ \mathbf{X} \\ & \mathbf{X}' \ \mathbf{B} \end{aligned} \text{ p.s.d.}$$

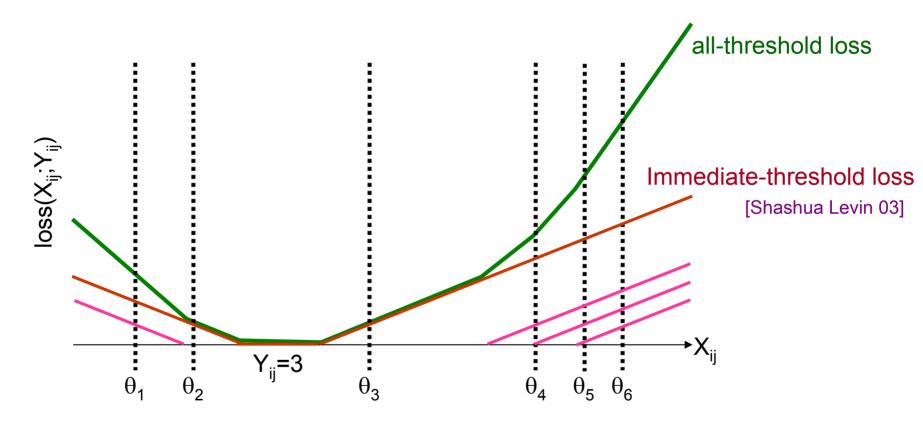
# Loss Functions for Rankings



# Loss Functions for Rankings



## Loss Functions for Rankings



- All-threshold loss is a bound on the absolute rank-difference
- For both loss functions: learn per-user  $\theta$ 's

# Experimental Results on MovieLens Subset

	all threshold MMMF	immediate threshold MMMF	K-medians K=2	Rank-1	Rank-2
Rank Difference	0.670	0.715	0.674	0.698	0.714
Zero One Error	0.553	0.542	0.558	0.559	0.553

100 users × 100 movies subset of MovieLens, 3515 training ratings, 3515 test ratings

#### Outline

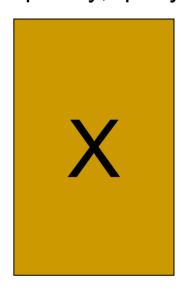
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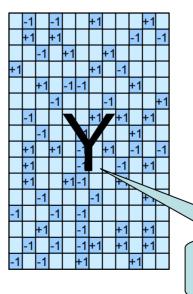
#### Generalization Error Bounds

$$D(X;Y) = \sum_{ij} loss(X_{ij};Y_{ij})$$
generalization error

Assuming a low-rank structure (eigengap):

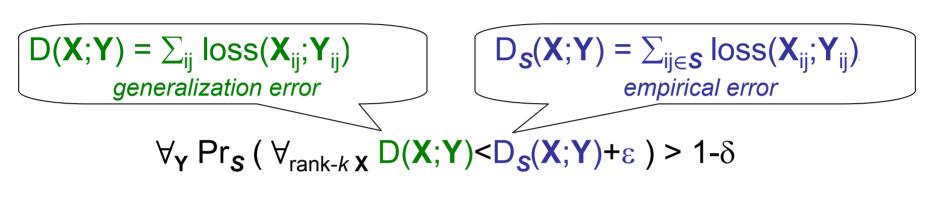
Asymptotic behavior [Azar+01]
Sample complexity, query strategy [Drineas+02]

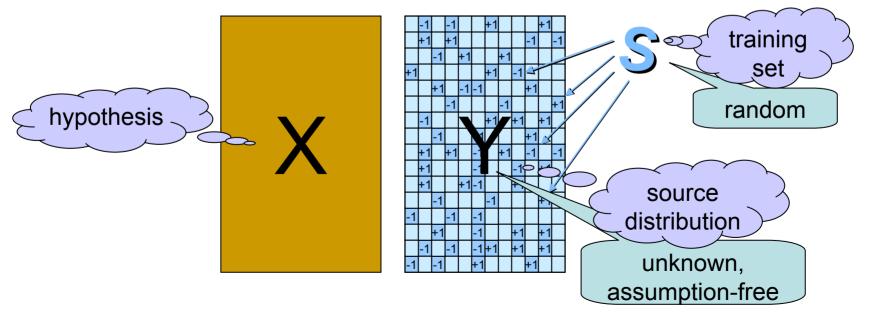




unknown, assumption-free

#### Generalization Error Bounds





#### Generalization Error Bounds

0/1 loss: loss( $X_{ii}$ ; $Y_{ii}$ ) = 1 when sign( $X_{ii}$ ) $\neq Y_{ii}$ 

$$D(\mathbf{X};\mathbf{Y}) = \sum_{ij} loss(\mathbf{X}_{ij};\mathbf{Y}_{ij})/nm$$
generalization error

$$D(\mathbf{X};\mathbf{Y}) = \sum_{ij} loss(\mathbf{X}_{ij};\mathbf{Y}_{ij})/nm \qquad D_{\mathbf{S}}(\mathbf{X},\mathbf{Y}) = \sum_{ij \in \mathbf{S}} loss(\mathbf{X}_{ij};\mathbf{Y}_{ij})/|\mathbf{S}|$$

$$empirical\ error$$

 $loss(X_{ij};Y_{ij}) \sim Bernoulli(D(X;Y))$ For particular **X**,**Y**:

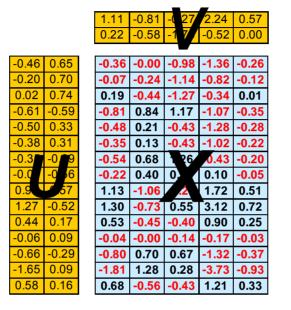
random 
$$Pr(D_s(X;Y) < D(X;Y)-\varepsilon) < e^{-2|S|\varepsilon^2}$$

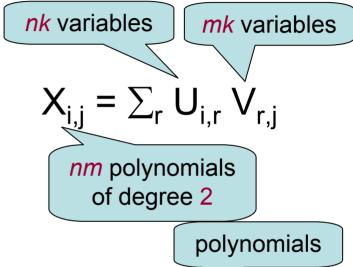
Union bound over all possible Xs:

$$\forall_{\mathbf{Y}} \operatorname{Pr}_{\mathbf{S}} (\forall_{\mathbf{X}} \operatorname{D}(\mathbf{X}, \mathbf{Y}) < \mathbf{D}_{\mathbf{S}}(\mathbf{X}, \mathbf{Y}) + \varepsilon) > 1 - \delta$$

$$\varepsilon = \sqrt{\frac{\log(\text{\# of possible Xs}) + \log \frac{1}{\delta}}{2|S|}}$$

#### Number of Sign Configurations of Rank-k Matrices





8

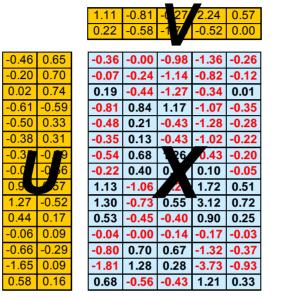
 $P_3(x_1,x_2)=0$ 

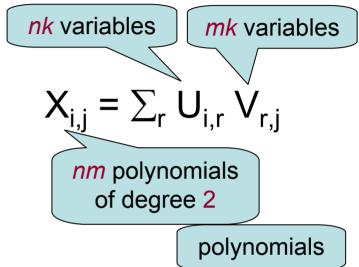
Warren (1968): The number of connected components of  $\{ \underline{x} \mid \forall_i P_i(\underline{x}) \neq 0 \}$ 

 $P_1(x_1,x_2)=0$ 

Based on [Alon95]

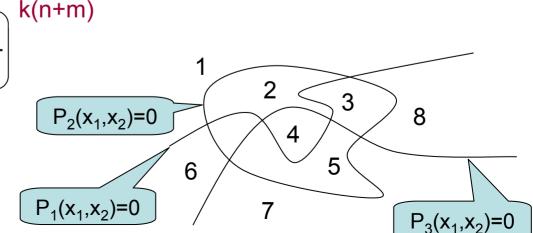
#### Number of Sign Configurations of Rank-k Matrices





Warren (1968): The number of connected components of  $\{ \underline{x} \mid \forall_i P_i(\underline{x}) \neq 0 \}$ 

is at most  $\frac{4 e \quad 2 \quad nm}{k(n+m)}$ Based on [Alon95]



#### Generalization Error Bounds: Low Rank Matrix Factorization

$$D(\mathbf{X};\mathbf{Y}) = \sum_{ij} loss(\mathbf{X}_{ij};\mathbf{Y}_{ij})/nm$$
generalization error

$$D_{S}(X,Y) = \sum_{ij \in S} loss(X_{ij};Y_{ij})/|S|$$
empirical error

$$\forall_{\mathbf{Y}} \operatorname{Pr}_{\mathbf{S}} (\forall_{\mathbf{X} \text{ of rank-}k} \operatorname{D}(\mathbf{X},\mathbf{Y}) < \operatorname{D}_{\mathbf{S}}(\mathbf{X},\mathbf{Y}) + \varepsilon) > 1 - \delta$$

$$0/1 loss: loss(X_{ij}; Y_{ij}) = sign(X_{ij}Y_{ij})$$

$$\varepsilon = \sqrt{\frac{k(n+m)\log\frac{8em}{k} + \log\frac{1}{\delta}}{2|S|}}$$

$$loss(X_{ij};Y_{ij}) \le 1$$
: (by bounding the psudodimension)

$$\varepsilon = 6\sqrt{\frac{k(n+m)\log\frac{8em}{k}\log\frac{|S|}{k(n+m)} + \log\frac{1}{\delta}}{|S|}}$$

# Generalization Error Bounds: Large Margin Matrix Factorization

$$D(\mathbf{X};\mathbf{Y}) = \sum_{ij} loss(\mathbf{X}_{ij};\mathbf{Y}_{ij})/nm$$

$$generalization\ error$$

$$loss(\mathbf{X}_{ij};\mathbf{Y}_{ij}) = sign(\mathbf{X}_{ij};\mathbf{Y}_{ij})$$

$$\begin{split} D_{\mathcal{S}}(\mathbf{X};\mathbf{Y}) &= \sum_{ij \in \mathcal{S}} loss^{1}(\mathbf{X}_{ij};\mathbf{Y}_{ij})/|\mathbf{S}| \\ & empirical\ error \\ loss^{1}(\mathbf{X}_{ij};\mathbf{Y}_{ij}) = sign(\mathbf{X}_{ij}\mathbf{Y}_{ij}-1) \end{split}$$

$$\forall_{\mathbf{Y}} \operatorname{Pr}_{\mathbf{S}} (\forall_{\mathbf{X}} \operatorname{D}(\mathbf{X}, \mathbf{Y}) < \operatorname{D}_{\mathbf{S}}(\mathbf{X}, \mathbf{Y}) + \varepsilon) > 1 - \delta$$

$$(\sum |U_i|^2/n)(\sum |V_i|^2/m) \le R^2$$
:

$$\varepsilon = K^{4} \sqrt{\ln m} \sqrt{\frac{R^{2}(n+m)\log n + \log \frac{1}{\delta}}{|S|}}$$

universal constant from [Seginer00] bound on spectral norm of random matrix

$$(\max |U_i|^2)(\max |V_i|^2) \le R^2$$
:

$$\varepsilon = 12\sqrt{\frac{R^2(n+m) + \log \frac{1}{\delta}}{|S|}}$$

# Maximum Margin Matrix Factorization as a Convex Combination of Classifiers

```
 \begin{array}{c} \text{conv}(\left\{ \text{ uv'} \mid \text{u} \in \pm 1^{\text{n}}, \, \text{v} \in \pm 1^{\text{m}} \right\}) \\ \quad \subset \left\{ \begin{array}{c} \text{UV} \mid (\text{max} \mid \text{U}_{i}\mid^{2})(\text{max} \mid \text{V}_{j}\mid^{2}) \leq 1 \right. \\ \quad \subset \left. 2 \text{ conv}(\left\{ \text{ uv'} \mid \text{u} \in \pm 1^{\text{n}}, \, \text{v} \in \pm 1^{\text{m}} \right\}) \right. \\ \\ \quad & \\ \text{Grothendiek's Inequality} \end{array}
```

## Summary

- Finding Low Rank Approximations
  - Weighted Low Rank Approximations
  - Basis for other loss function: Newton, Gaussian mixtures
- Consistency of Low Rank Approximation
  - ML for popular low-rank models is not consistent!
  - PCA consistent for additive noise; diagonal ignoring for unbiased
  - Efficient estimators?
  - Consistent estimators for Exponential-PCA?
- Maximum Margin Matrix Factorization
  - Correspondence with large margin linear classification
  - Sparse SDPs for both avarage-norm and max-norm formulations
  - Direct optimization of dual would enable large-scale applications
- Generalization Error Bounds for Collaborative Prediction
  - First "assumption free" bounds for matrix completion
  - Both for Low-Rank and for Max-Margin
  - Observation process?

# Average February Temperature

(centigrade)

