

#### **Probabilistic Graphical Models**

#### Spectral Learning for Graphical Models

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#### **Latent Variable Models**





#### **Mixed membership models**

## Latent Variable PCFG [Matsuzaki et al., 2005,

Petrov et al. 2006]



#### Latent Variable PCFG





Since latent variables are not observed in the data, we have to use Expectation Maximization (EM) to learn parameters

- Slow
- Local Minima

## **Spectral Learning**

- Different paradigm of learning in latent variable models based on linear algebra
- Theoretically,
  - Provably consistent
  - Can offer deeper insight into the identifiability
- Practically,
  - Local minima free
  - As if now, performs comparably to EM with 10-100x speed-up
  - Can also model non-Gaussian continuous data using kernels (usually performs much better than EM in this case)

#### **Related References**

#### • Relevant works

- Hsu et al. 2009 Spectral HMMs (also Bailly 2009)
- Siddiqi et al. 2009 Features in Spectral Learning
- Parikh et al. 2011/2012 Tensors to Generalize to Trees/Low Treewidth Graphs
- Cohen et al. 2012 / 2013 Spectral Learning of latent PCFGs
- Will present it from "matrix factorization" view:
  - Balle et al. 2012 Connection between Spectral Learning / Hankel Matrix Factorization
  - Song et al. 2013 Spectral Learning as Hierarchical Tensor Decomposition

#### **Focusing on Prediction**

- In many applications that use latent variable models, the end task is not to recover the latent states, but rather to use the model for prediction among observed variables.
- Dynamical Systems Predict future given past



# **Focusing on Prediction**



• We will only be concerned with quantities related to the observed variables:

$$\mathbb{P}[X_1, X_2, X_3, X_4, X_5]$$

• We do not care about the latent variables explicitly.



• Do we still need EM to learn the parameters?

# But if we don't care about the latent variables....

- Why don't we just integrate them out?
- Because integrating them out results in a clique ⊗





#### **Marginal Does Not Factorize**

$$\mathbb{P}[X_1, X_2, X_3, X_4, X_5] = \sum_{H_1, \dots, H_5} \mathbb{P}[H_1] \mathbb{P}[H_1] \prod_{i=2}^5 \mathbb{P}[H_i | H_{i-1}] \prod_{i=1}^5 \mathbb{P}[X_i | H_i]$$

Does not factorize due to the outer sum (Can somewhat distribute the sum, but doesn't solve problem)

# But isn't an HMM different from a clique?

- It depends on the number of latent states.
- Consider the following model.



#### If H has only one state.....

• Then the observed variables are independent!



## What if H has many states?



- Let us say the observed variables each have *m* states.
- Then if H has *m*<sup>3</sup> states then the latent model can be exactly equivalent to a clique (depending on how parameters are set).



• But what about all the other cases?

#### **The Question**



- Under existing methods, latent models all require EM to learn regardless of the number of hidden states.
- However, is there a formulation of latent variable models where the difficulty of learning is a function of the number of latent states?
- This is the question that the *spectral view* will answer.

### Sum Rule (Matrix Form)

• Sum Rule

$$\mathbb{P}[X] = \sum_{Y} \mathbb{P}[X|Y]\mathbb{P}[Y]$$

• Equivalent view using Matrix Algebra

$$\mathcal{P}[X] = \mathcal{P}[X|Y] \times \mathcal{P}[Y]$$

$$\begin{pmatrix} \mathbb{P}[X=0]\\ \mathbb{P}[X=1] \end{pmatrix} = \begin{pmatrix} \mathbb{P}[X=0|Y=0] & \mathbb{P}[X=0|Y=1]\\ \mathbb{P}[X=1|Y=0] & \mathbb{P}[X=1|Y=1] \end{pmatrix} \times \begin{pmatrix} \mathbb{P}[Y=0]\\ \mathbb{P}[Y=1] \end{pmatrix}$$

#### **Important Notation**



- Calligraphic P to denotes that the probability is being treated as a matrix/vector/tensor
- Probabilities

$$\mathbb{P}[X,Y] = \mathbb{P}[X|Y]\mathbb{P}[Y]$$

• Probability Vectors/Matrices/Tensors

$$\mathcal{P}[X] = \mathcal{P}[X|Y]\mathcal{P}[Y]$$

#### Chain Rule (Matrix Form)



• Chain Rule

 $\mathbb{P}[X,Y] = \mathbb{P}[X|Y]\mathbb{P}[Y] = \mathbb{P}[Y|X]\mathbb{P}[Y]$ 

• Equivalent view using Matrix Algebra



$$\mathcal{P}[X,Y] = \mathcal{P}[X|Y]$$

 $\times \mathcal{P}[\oslash Y]$ 

 $\begin{pmatrix} \mathbb{P}[X=0,Y=0] & \mathbb{P}[X=0,Y=1] \\ \mathbb{P}[X=1,Y=0] & \mathbb{P}[X=1,Y=1] \end{pmatrix} = \\ \begin{pmatrix} \mathbb{P}[X=0|Y=0] & \mathbb{P}[X=0|Y=1] \\ \mathbb{P}[X=1|Y=0] & \mathbb{P}[X=1|Y=1] \end{pmatrix} & \swarrow \begin{pmatrix} \mathbb{P}[Y=0] & 0 \\ 0 & \mathbb{P}[Y=1] \end{pmatrix}$ 

 Note how diagonal is used to keep Y from being marginalized out.

### **Graphical Models: The Linear Algebra View**





A and B have m states each.

• In general, nothing we can say about the nature of this matrix.

### Independence: The Linear Algebra View



• What if we know A and B are independent?



 Joint probability matrix is rank one, since all rows are multiples of one another!!

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# Independence and Rank В А $\mathcal{P}[A,B]$ has rank m (at most) В Α ${oldsymbol{\mathcal{P}}}[A,B]$ has rank 1

• What about rank in between 1 and m?

#### Low Rank Structure

• **A** and **B** are not marginally independent (They are only conditionally independent given **X**).



- Assume X has k states (while A and B have m states).
- Then,  $rank(\mathcal{P}[A, B]) \leq k$
- Why?

#### Low Rank Structure





#### **The Spectral View**

- Latent variable models encode low rank dependencies among variables (both marginal and conditional)
- Use tools from linear algebra to exploit this structure.
  - Rank
  - Eigenvalues
  - SVD
  - Tensors



#### **A More Interesting Example**





#### Low Rank Matrices "Factorize"

# M = LR If M has rank k m by n m by k k by n

#### We already know one factorization!!!

$$\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}] = \mathcal{P}[X_{\{1,2\}} | H_2] \mathcal{P}[\oslash H_2] \mathcal{P}[X_{\{3,4\}} | H_2]^\top$$
  
Factor of 4 variables Factor of 3 variables Factor of 3 variables Factor of 1 variable

#### **Alternate Factorizations**



- The key insight is that this factorization is not unique.
- Consider Matrix Factorization. Can add any invertible transformation:

$$egin{aligned} M &= L R \ M &= L S S^{-1} R \end{aligned}$$

• The magic of spectral learning is that there exists an alternative factorization that only depends on observed variables!



#### **An Alternate Factorization**

• Let us say we only want to factorize this matrix of 4 variables

$$\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}]$$

such that it is product of matrices that contain at most three **observed** variables e.g.

 $\mathcal{P}[X_{\{1,2\}}, X_3]$  $\mathcal{P}[X_2, X_{\{3,4\}}]$ 



#### **An Alternate Factorization**

• Note that

$$\mathcal{P}[X_{\{1,2\}}, X_3] = \mathcal{P}[X_{\{1,2\}}|H_2]\mathcal{P}[\oslash H_2]\mathcal{P}[X_3|H_2]^\top$$
$$\mathcal{P}[X_2, X_{\{3,4\}}] = \mathcal{P}[X_2|H_2]\mathcal{P}[\oslash H_2]\mathcal{P}[X_{\{3,4\}}|H_2]^\top$$

- Product of green terms (in some order) is  $\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}]$
- Product of red terms (in some order) is  $\, {oldsymbol {\mathcal P}}[X_2,X_3] \,$



#### **An Alternate Factorization**

$$\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}] = \mathcal{P}[X_{\{1,2\}}, X_3] \mathcal{P}[X_2, X_3]^{-1} \mathcal{P}[X_2, X_{\{3,4\}}]$$

factor of 4 variables factor of 3 variables factor of 3 variables

Advantage: Factors are only functions of observed variables! Can be directly computed from data without EM!!!!

**Caveat:** some factors are no longer probability tables (do not have to be non-negative)

We will call this factorization the observable factorization.

#### **Graphical Relationship**







#### **Another Factorization**



 $\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}] = \mathcal{P}[X_{\{1,2\}}, X_4] \mathcal{P}[X_1, X_4]^{-1} \mathcal{P}[X_1, X_{\{3,4\}}]$ 



• Seems we would do better empirically if you could "combine" both factorizations. Will come back to this later.

### Relationship to Original Factorization



• What is the relationship between the original factorization and the new factorization?

$$\frac{\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}]}{M} = \frac{\mathcal{P}[X_{\{1,2\}}|H_2]\mathcal{P}[\oslash H_2]\mathcal{P}[X_{\{3,4\}}|H_2]^{\top}}{L}$$

$$M = LR$$
  
 $M = LSS^{-1}R$   
Can I choose S to get the observable factorization?

### Relationship to Original Factorization



• Let

$$\boldsymbol{S} := \boldsymbol{\mathcal{P}}[X_3 | H_2]$$

$$\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}] = \frac{\mathcal{P}[X_{\{1,2\}}, X_3]\mathcal{P}[X_2, X_3]^{-1}\mathcal{P}[X_2, X_{\{3,4\}}]}{= LS} = S^{-1}R$$

#### **Our Alternate Factorization**



$$\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}] = \mathcal{P}[X_{\{1,2\}}, X_3] \mathcal{P}[X_2, X_3]^{-1} \mathcal{P}[X_2, X_{\{3,4\}}]$$

factor of 4 variables

factor of 3 variables

factor of 3 variables

- It may not seem very amazing at the moment (we have only reduced the size of the factor by 1)
- What is cool is that every latent tree of **V** variables has such a factorization where:
  - All factors are of size 3
  - All factors are only functions of observed variables

# Training / Testing with Spectral Learning

• We have that

$$\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}] = \mathcal{P}[X_{\{1,2\}}, X_3] \mathcal{P}[X_2, X_3]^{-1} \mathcal{P}[X_2, X_{\{3,4\}}]$$

• In training, we compute estimates:

 $\mathcal{P}_{MLE}[X_{\{1,2\}}, X_3] \quad \mathcal{P}_{MLE}[X_2, X_3]^{-1} \quad \mathcal{P}_{MLE}[X_2, X_{\{3,4\}}]$ 

• In test time, we can compute probability estimates (let lowercase letters denote fixed evidence values):

$$\widehat{\mathbb{P}}_{spec}[x_1, x_2, x_3, x_4] = \mathcal{P}_{MLE}[x_{\{1,2\}}, X_3] \mathcal{P}_{MLE}[X_2, X_3]^{-1} \mathcal{P}_{MLE}[X_2, x_{\{3,4\}}]^{\top}$$



#### **Generalizing To More Variables**

• Consider HMM with 5 observations. Using similar arguments as before we will get that:

$$\mathcal{P}[X_{\{1,2\}}, X_{\{3,4,5\}}] = \mathcal{P}[X_{\{1,2\}}, X_3] \mathcal{P}[X_2, X_3]^{-1} \mathcal{P}[X_2, X_{\{3,4,5\}}]$$

reshape and decompose recursively

$$\mathcal{P}[X_{\{2,3\}}, X_{\{4,5\}}] = \mathcal{P}[X_{\{2,3\}}, X_4] \mathcal{P}[X_3, X_4]^{-1} \mathcal{P}[X_3, X_{\{4,5\}}]$$
$\mathcal{P}_{MLE}[X_1, X_2; X_3, X_4] \rightarrow \mathcal{P}[X_1, X_2; X_3, X_4]$ 

• While this is consistent, it is not very statistically efficient

## Consistency

- A trivial consistent estimator is to simply attempt to estimate the "big" probability table from the data without making any conditional independence assumptions

as number of samples

increases



### Consistency

• A better estimate is to get compute likelihood estimates of the factorization:

$$\mathcal{P}_{MLE}[X_{\{1,2\}}|H_2]\mathcal{P}_{MLE}[\oslash H_2]\mathcal{P}_{MLE}[X_{\{3,4\}}|H_2]^\top \rightarrow \mathcal{P}[X_1, X_2; X_3, X_4]$$

• But this requires running EM, which will get stuck in local optima and is not guaranteed to obtain the MLE of the factorized model



### Consistency

• In spectral learning, we estimate the alternate factorization from the data

$$\mathcal{P}_{MLE}[X_{\{1,2\}}, X_3] \mathcal{P}_{MLE}[X_2, X_3]^{-1} \mathcal{P}_{MLE}[X_2, X_{\{3,4\}}] \\ \to \mathcal{P}[X_1, X_2; X_3, X_4]$$

• This is consistent and computationally tractable (at some loss of statistical efficiency due to the dependence on the inverse)

### Where's the Catch?



- Before we said that if the number of latent states was very large then the model was equivalent to a clique.
- Where does that scenario enter in our factorization?

$$\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}] = \mathcal{P}[X_{\{1,2\}}, X_3] \mathcal{P}[X_2, X_3]^{-1} \mathcal{P}[X_2, X_{\{3,4\}}]$$
  
When does this inverse exist?

### When Does the Inverse Exist



 $\boldsymbol{\mathcal{P}}[X_2, X_3] = \boldsymbol{\mathcal{P}}[X_2|H_2]\boldsymbol{\mathcal{P}}[\oslash H_2]\boldsymbol{\mathcal{P}}[X_3|H_2]^{\top}$ 

• All the matrices on the right hand side must have full rank. (This is in general a requirement of spectral learning, although it can be somewhat relaxed)

### When m > k

• The inverse cannot exist, but this situation is easily fixable (project onto lower dimensional space)

$$\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}] = \mathcal{P}[X_{\{1,2\}}, X_3] \mathbf{V} (\mathbf{U}^{\top} \mathcal{P}[X_2, X_3] \mathbf{V})^{-1} \mathbf{U}^{\top} \mathcal{P}[X_2, X_{\{3,4\}}]$$

• Where **U**, **V** are the top left/right **k** singular vectors of  $\mathcal{P}[X_2, X_3]$ 



### When k > m

• The inverse does exist. But it no longer satisfies the following property, which we used to derive the factorization

$$\boldsymbol{\mathcal{P}}[X_2, X_3]^{-1} = (\boldsymbol{\mathcal{P}}[X_3 | H_2]^{\top})^{-1} \boldsymbol{\mathcal{P}}[\oslash H_2]^{-1} \boldsymbol{\mathcal{P}}[X_2 | H_2]^{-1}$$

 This is much more difficult to fix, and intuitively corresponds to how the problem becomes intractable if k >> m.

### What does k>m mean?



- Intuitively, large *k*, small *m* means long range dependencies
- Consider following generative process:
  - (1) With probability 0.5, let S = X, and with probability 0.5 let S = Y.
  - (2) Print **A** *n* times.
  - (3) Print **S**
  - (4) Go back to step (2)

With *n=1* we either generate: AXAXAXA..... or AYAYAYA.....

With *n=2* we either generate: AAXAAXAA..... or AAYAAYAA......

# How many hidden states does HMM need?



- HMM needs **2n** states.
- Needs to remember count as well as whether we picked S=X or S=Y
- However, number of observed states *m* does not change, so our previous spectral algorithm will break for *n* > 2.
- How to deal with this in spectral framework?

### Making Spectral Learning Work In Practice



- We are only using marginals of pairs/triples of variables to construct the full marginal among the observed variables.
- Only works when *k < m*.



• However, in real problems we need to capture longer range dependencies.

### **Recall our factorization**







### Key Idea: Use Long-Range Features





Construct feature vector of left side

 ${oldsymbol{\phi}}_L$ 

Construct feature vector of right side





### **Spectral Learning With Features**

$$oldsymbol{\mathcal{P}}[X_2,X_3] = \mathbb{E}[oldsymbol{\delta}_2 \otimes oldsymbol{\delta}_3] := \mathbb{E}[oldsymbol{\delta}_2 oldsymbol{\delta}_3^ op]$$
  
Use more complex feature instead:  
 $\mathbb{E}[oldsymbol{\phi}_L \otimes oldsymbol{\phi}_R]$ 

 $\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}] = \mathbb{E}[\boldsymbol{\delta}_{1\otimes 2}, \boldsymbol{\delta}_{3\otimes 4}]$ =  $\mathbb{E}[\boldsymbol{\delta}_{1\otimes 2}, \boldsymbol{\phi}_R] \boldsymbol{V} (\boldsymbol{U}^{\top} \mathbb{E}[\boldsymbol{\phi}_L \otimes \boldsymbol{\phi}_R] \boldsymbol{V})^{-1} \boldsymbol{U}^{\top} \mathcal{P}[\boldsymbol{\phi}_L, X_{\{3,4\}}]$ 

## Experimentally,



- Has been shown by many authors that (with some work) spectral methods achieve comparable results to EM but are 10-50x faster
  - Parikh et al. 2011 / 2012
  - Balle et al. 2012
  - Cohen et al. 2012 / 2013

• The following are some synthetic and real data results demonstrating the comparison between EM and spectral methods.

### Synthetic Data [Parikh et al. 2012]



• Synthetic 3<sup>rd</sup> order HMM Example (Spectral/EM/Online EM):



### Empirical Results for Latent PCFGs [Cohen et al. 2013]



	sect	ion 22	section 23		
	EM	spectral	EM	spectral	
m = 8	86.87	85.60			
m = 16	88.32	87.77			
m = 24	88.35	88.53			
m = 32	88.56	88.82	87.76	88.05	

### Timing Results on Latent PCFGS[Cohen et al. 2013]



	single	EM	spectral algorithm						
	EM iter.	best model	total	feature	transfer + scaling	SVD	$a \rightarrow b \ c$	$a \rightarrow x$	
m = 8	6m	3h	3h32m	Ĩ		36m	1h34m	10m	
m = 16	52m	26h6m	5h19m	22m	49m	34m	3h13m	19m	
m = 24	3h7m	93h36m	7h15m			36m	4h54m	28m	
m = 32	9h21m	187h12m	9h52m	226		35m	7h16m	41m	

### Dealing with Nonparametric, Continuous Variables



• It is difficult to run EM if the conditional/marginal distributions are continuous and do not easily fit into a parametric family.



• However, we will see that Hilbert Space Embeddings can easily be combined with spectral methods for learning nonparametric latent models.

### **Connection to Hilbert Space Embeddings**



• Recall that we could substitute features for variables

$$\mathcal{P}[X_2, X_3] = \mathbb{E}[\boldsymbol{\delta}_2 \otimes \boldsymbol{\delta}_3] := \mathbb{E}[\boldsymbol{\delta}_2 \boldsymbol{\delta}_3^\top]$$

Use more complex feature instead:

 $\mathbb{E}[oldsymbol{\phi}_L \otimes oldsymbol{\phi}_R]$ 

### Can Also Use Infinite Dimensional Features



• Replace

$$\mathcal{P}[X_2, X_3] = \mathbb{E}[\boldsymbol{\delta}_2 \otimes \boldsymbol{\delta}_3] := \mathbb{E}[\boldsymbol{\delta}_2 \boldsymbol{\delta}_3^{\top}]$$

• with

$$\mathcal{C}[X_2, X_3] = \mathbb{E}[\phi_{X_2} \otimes \phi_{X_3}] \qquad \text{covariance} \\ \text{operator}$$

### **Connection to Hilbert Space Embeddings**

Discrete case:

$$\mathcal{P}[X_{\{1,2\}}, X_{\{3,4\}}] = \mathcal{P}[X_{\{1,2\}}, X_3] \mathbf{V} (\mathbf{U}^{\top} \mathcal{P}[X_2, X_3] \mathbf{V})^{-1} \mathbf{U}^{\top} \mathcal{P}[X_2, X_{\{3,4\}}]$$

Continuous case:

$$\mathcal{C}[X_{\{1,2\}}; X_{\{3,4\}}] = \mathcal{C}[X_{\{1,2\}}; X_3] \mathbf{V} (\mathbf{U}^{\top} \mathcal{C}[X_2, X_3] \mathbf{V})^{-1} \mathbf{U}^{\top} \mathcal{C}[X_2; X_{\{3,4\}}]$$



### Summary - EM & Spectral (Part I)

### EM

- Aims to Find MLE so more "statistically" efficient
- Can get stuck in local-optima
- Lack of theoretical guarantees
- Slow
- Easy to derive for new models

### **Spectral**

- Does not aim to find MLE so less statistically efficient.
- Local-optima-free
- Provably consistent
- Very fast
- Challenging to derive for new models (Unknown whether it can generalize to arbitrary loopy models)



### Summary - EM & Spectral (Part II)

### EM

• No issues with negative numbers

- Allows for easy modelling with conditional distributions
- Difficult to incorporate long-range features (since it increases treewidth).
- Generalizes poorly to non-Gaussian continuous variables.

### **Spectral**

- Problems with negative numbers. Requires explicit normalization to compute likelihood.
- Allows for easy modelling with marginal distributions
- Easy to incorporate long-range features.
- Easy to generalize to non-Gaussian continuous variables via Hilbert Space Embeddings