# Log-Linear Models, Logistic Regression and Conditional Random Fields

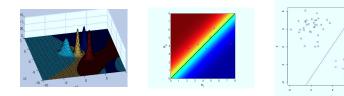
February 21, 2013

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## Generative, Conditional and Discriminative

- Given  $\mathcal{D} = (x_t, y_t)_{t=1}^T$  sampled *iid* from unknown P(x, y)
- Generative Learning (maximum likelihood Gaussians)
  - Choose family of functions  $p_{\theta}(x, y)$  parametrized by  $\theta$
  - Find  $\theta$  by maximizing likelihood:  $\prod_{t=1}^{T} p_{\theta}(x_i, y_i)$
  - Given x, output  $\hat{y} = \arg \max_{y} \frac{p_{\theta}(x,y)}{\sum_{y} p_{\theta}(x,y)}$
- Conditional Learning (logistic regression)
  - Choose family of functions  $p_{\theta}(y|x)$  parametrized by  $\theta$
  - Find  $\theta$  by maximizing conditional likelihood:  $\prod_{t=1}^{T} p_{\theta}(y_i|x_i)$
  - Given x, output  $\hat{y} = \arg \max_{y} p_{\theta}(y|x)$
- Discriminative Learning (support vector machines)
  - Choose family of functions  $y = f_{\theta}(x)$  parametrized by  $\theta$
  - Find  $\theta$  by minimizing classification error  $\sum_{t=1}^{T} \ell(y_i, f_{\theta}(x_i))$
  - Given x, output  $\hat{y} = f_{\theta}(x)$

## Generative, Conditional and Discriminative



Generative Conditional Discriminative

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#### Generative: Maximum Entropy

Maximum entropy (or generally) minimum relative entropy  $\mathcal{RE}(p||h) = \sum_{y} p(y) \ln \frac{p(y)}{h(y)}$  subject to linear constraints

$$\min_{p} \mathcal{RE}(p \| h) \text{ s.t.} \sum_{y} p(y) \mathbf{f}(y) = \mathbf{0}, \sum_{y} p(y) \mathbf{g}(y) \ge \mathbf{0}$$

Solution distribution looks like an exponential family model

$$p(y) = h(y) \exp \left( \boldsymbol{\theta}^{\top} \mathbf{f}(y) + \boldsymbol{\vartheta}^{\top} \mathbf{g}(y) \right) / Z(\boldsymbol{\theta}, \boldsymbol{\vartheta})$$

Maximize the dual (the negative log-partition) to get  $\theta$ ,  $\vartheta$ .

$$\max_{\theta,\vartheta \ge \mathbf{0}} -\ln Z(\theta,\vartheta) = \max_{\theta,\vartheta \ge \mathbf{0}} -\ln \sum_{y} h(y) \exp\left(\theta^{\top} \mathbf{f}(y) + \vartheta^{\top} \mathbf{g}(y)\right)$$

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## Generative: Exponential Family and Maximum Likelihood

All maximum entropy models give an exponential family form:

$$p(y) = h(y) \exp(\boldsymbol{\theta}^{\top} \mathbf{f}(y) - \boldsymbol{a}(\boldsymbol{\theta}))$$

This is also a *log-linear model* over discrete  $y \in \Omega$  where  $|\Omega| = n$ 

$$p(y|\theta) = \frac{1}{Z(\theta)}h(y)\exp\left(\theta^{\top}\mathbf{f}(y)\right)$$

- Parameters are vector  $oldsymbol{ heta} \in \mathbb{R}^d$
- Features are  $\mathbf{f}: \Omega \mapsto \mathbb{R}^d$  mapping each y to some vector
- Prior is  $h: \Omega \mapsto \mathbb{R}^+$  a fixed non-negative measure
- Partition function ensures that  $p(y|\theta)$  normalizes

$$Z(\theta) = \sum_{y} h(y) \exp(\theta^{\top} \mathbf{f}(y))$$

#### Generative: Exponential Family and Maximum Likelilhood

We are given some *iid* data  $y_1, \ldots, y_T$  where  $y \in \{0, 1\}$ . If we wanted to find the best parameters of an exponential family distribution known as the Bernouilli distribution:

$$p(y|\theta) = h(y) \exp(\theta^{\top} \mathbf{f}(y) - a(\theta))$$
$$= \theta^{y} (1 - \theta)^{1-y}$$

This is unsupervised generative learning We simply find the  $\theta$  that maximizes the likelihood

$$L(\boldsymbol{\theta}) = \prod_{t=1}^{T} p(y_t | \boldsymbol{\theta}) = \theta^{\sum_t y_t} (1-\theta)^{T-\sum_t y_t}$$

Taking log then derivatives and setting to zero gives  $\theta = \frac{1}{T} \sum_{t} y_t$ .

#### Conditional: Logistic Regression

Given input-output *iid* data  $(x_1, y_1), \ldots, (x_T, y_T)$  where  $y \in \{0, 1\}$ . Binary logistic regression computes a probability for y = 1 by

$$p(y = 1|x, \vartheta) = rac{1}{1 + \exp(-artheta^ op \phi(x))}.$$

And the probability for  $p(y = 0|x, \theta) = 1 - p(y = 1|x, \theta)$ . This is supervised conditional learning. We find the  $\theta$  that maximizes the *conditional* likelihood

$$L(\vartheta) = \prod_{t=1}^{T} p(y_t|x_t, \vartheta)$$

We can maximize this by doing gradient ascent. Logistic regression is an example of a *log-linear model*.

## Conditional: Log-linear Models

Like an exponential family, but allow Z, h and f also depend on x

$$p(y|x, \theta) = \frac{1}{Z(x, \theta)} h(x, y) \exp \left( \theta^{\top} \mathbf{f}(x, y) \right)$$

- Parameters are just one long vector  $oldsymbol{ heta} \in \mathbb{R}^d$
- Functions  $\mathbf{f}:\Omega_x imes\Omega_y\mapsto\mathbb{R}^d$  map x,y to a vector
- Prior is  $h: \Omega_x \times \Omega_y \mapsto \mathbb{R}^+$  a fixed non-negative measure
- Partition function ensures that  $p(y|x, \theta)$  normalizes

To make a prediction, we simply output

$$\hat{y} = \arg \max_{y} p(y|x, \theta).$$

Let's mimic (multi-class) logistic regression with this form.

#### Conditional: Log-linear Models

In multi-class logistic regression, we have  $y \in \{1, \ldots, n\}$ .

$$p(y|x, \theta) = \frac{1}{Z(x, \theta)} h(x, y) \exp \left( \theta^{\top} \mathbf{f}(x, y) \right)$$

If  $\phi(x) \in \mathbb{R}^k$ , then  $\mathbf{f}(x, y) \in \mathbb{R}^{kn}$ . Choose the following for the feature function

$$\mathbf{f}(x,y) = \left[\delta[y=1]\phi(x)^{\top} \ \delta[y=2]\phi(x)^{\top} \dots \delta[y=n]\phi(x)^{\top}\right]^{\top}$$

If n = 2 and h(x, y) = 1, get traditional binary logistic regression!

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#### Conditional: Log-linear Models

Rewrite binary logistic regression  $p(y = 1|x, \vartheta) = \frac{1}{1 + \exp(-\vartheta^{\top}\phi(x))}$  as a log-linear model with n = 2, h(x, y) = 1 and  $\mathbf{f}(x, y)$  as before

$$p(y|x,\theta) = \frac{h(x,y)\exp\left(\theta^{\top}\mathbf{f}(x,y)\right)}{Z(x,\theta)}$$
  
= 
$$\frac{\exp\left(\mathbf{f}(x,y)^{\top}\theta\right)}{\sum_{y=0}^{1}\exp\left(\mathbf{f}(x,y)^{\top}\theta\right)}$$
$$p(y=1|x,\theta) = \frac{\exp\left(\left[\mathbf{0} \ \phi(x)^{\top} \ \mathbf{0}\right]\theta\right)}{\exp\left(\left[\phi(x)^{\top} \ \mathbf{0}\right]\theta\right) + \exp\left(\left[\mathbf{0} \ \phi(x)^{\top}\right]\theta\right)}$$
  
= 
$$\frac{1}{1 + \exp\left(\left[\phi(x)^{\top} \ \mathbf{0}\right]\theta - \left[\mathbf{0} \ \phi(x)^{\top}\right]\theta\right)}$$

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Can you see how to write  $\vartheta$  in terms of  $\theta$ ?

## Conditional Random Fields (CRFs)

- Conditional random fields generalize maximum entropy
- Trained on *iid* data  $\{(x_1, y_1), \dots, (x_t, y_t)\}$
- A CRF is just a log-linear model with big n

$$p(y|x_j, \theta) = \frac{1}{Z(x_j, \theta)} h(x_j, y) \exp(\theta^{\top} \mathbf{f}(x_j, y))$$

Maximum conditional log-likelihood objective function is

$$J(\boldsymbol{\theta}) = \sum_{j=1}^{t} \ln \frac{h(x_j, y_j)}{Z(x_j, \boldsymbol{\theta})} + \boldsymbol{\theta}^{\top} \mathbf{f}(x_j, y_j)$$
(1)

Regularized conditional maximum likelihood is

$$J(\boldsymbol{\theta}) = \sum_{j=1}^{t} \ln \frac{h(x_j, y_j)}{Z(x_j, \boldsymbol{\theta})} + \boldsymbol{\theta}^{\top} \mathbf{f}(x_j, y_j) - \frac{t\lambda}{2} \|\boldsymbol{\theta}\|^2$$
(2)

# Conditional Random Fields (CRFs)

- To train a CRF, we maximize (regularized) conditional likelihood
- Traditionally, maximum entropy, log-linear models and CRFs were trained using *majorization* (the EM algorithm is a majorization method)
- The algorithms were called *improved iterative scaling (IIS)* or *generalized iterative scaling (GIS)*

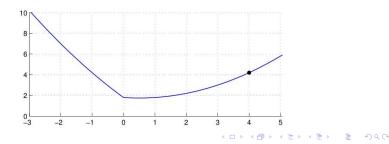
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- Maximum entropy [Jaynes '57]
- Conditional random fields [Lafferty, et al. '01]
- Log-linear models [Darroch & Ratcliff '72]

If cost function  $\theta^* = \arg \min_{\theta} C(\theta)$  has no closed form solution Majorization uses with a surrogate Q with closed form update to monotonically minimize the cost from an initial  $\theta_0$ 

- Find bound  $Q(\theta, \theta_i) \ge C(\theta)$  where  $Q(\theta_i, \theta_i) = C(\theta_i)$
- Update  $\theta_{i+1} = \arg \min_{\theta} Q(\theta, \theta_i)$

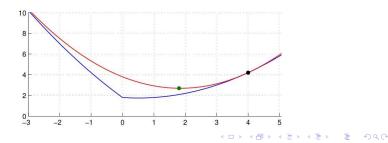
Repeat until converged



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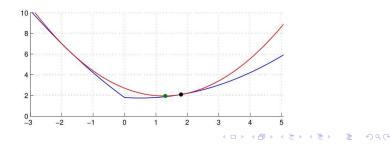
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- Update  $\theta_{i+1} = \arg \min_{\theta} Q(\theta, \theta_i)$

Repeat until converged



IIS and GIS were preferred until [Wallach '03, Andrew & Gao '07]

Method	Iterations	LL Evaluations	Time (s)
IIS	$\geq 150$	$\geq 150$	$\geq 188.65$
Conjugate gradient (FR)	19	99	124.67
Conjugate gradient (PRP)	27	140	176.55
L-BFGS	22	22	29.72

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Gradient descent appears to be faster But newer majorization methods are faster still

#### Gradient Ascent for CRFs

We have the following model

$$p(y|x, \theta) = \frac{1}{Z(x, \theta)} h(x, y) \exp \left( \theta^{\top} \mathbf{f}(x, y) \right)$$

We want to maximize the conditional (log) likelihood:

$$\log L(\theta) = \sum_{t=1}^{T} \log p(y_t | x_t, \theta)$$
  
= 
$$\sum_{t=1}^{T} -\log Z(x_t, \theta) + \log(h(x_t, y_t)) + \theta^{\top} \mathbf{f}(x_t, y_t)$$
  
= 
$$const - \sum_{t=1}^{T} \log Z(x_t, \theta) + \theta^{\top} \sum_{t=1}^{T} \mathbf{f}(x_t, y_t)$$

Same as minimizing the sum of log partition functions plus linear

#### Gradient Ascent for CRFs

$$\frac{\partial \log L}{\partial \theta} = \frac{\partial}{\partial \theta} \left( \theta^{\top} \sum_{t=1}^{T} \mathbf{f}(x_t, y_t) - \sum_{t=1}^{T} \log Z(x_t, \theta) \right)$$

$$= \sum_{t=1}^{T} \mathbf{f}(x_t, y_t) - \sum_{t=1}^{T} \frac{1}{Z(x_t, \theta)} \sum_{y} h(x_t, y) \frac{\partial}{\partial \theta} \exp\left(\theta^{\top} \mathbf{f}(x_t, y)\right)$$

$$= \sum_{t=1}^{T} \mathbf{f}(x_t, y_t) - \sum_{t=1}^{T} \sum_{y} \frac{h(x_t, y)}{Z(x_t, \theta)} \exp\left(\theta^{\top} \mathbf{f}(x_t, y)\right) \mathbf{f}(x_t, y)$$

$$= \sum_{t=1}^{T} \mathbf{f}(x_t, y_t) - \sum_{t=1}^{T} \sum_{y} \mathbf{f}(x_t, y) \rho(y|x_t, \theta)$$

The gradient is the difference between the feature vectors at the true labels minus the expected feature vectors under the current distribution. To update,  $\theta \leftarrow \theta + \eta \frac{\partial \log L}{\partial \theta}$ .

#### Stochastic Gradient Ascent for CRFs

Given current heta, update by taking a small step along the gradient

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \eta \frac{\partial \log \boldsymbol{L}}{\partial \boldsymbol{\theta}}.$$

We can use the full derivative:

$$\frac{\partial \log L}{\partial \theta} = \sum_{t=1}^{T} \mathbf{f}(x_t, y_t) - \sum_{t=1}^{T} \sum_{y} \mathbf{f}(x_t, y) p(y|x_t, \theta)$$

Or do stochastic gradient with only a single random datapoint t:

$$\frac{\partial \log L}{\partial \theta} = \mathbf{f}(x_t, y_t) - \sum_{y} \mathbf{f}(x_t, y) p(y|x_t, \theta)$$

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Recall log-linear model over discrete  $y \in \Omega$  where  $|\Omega| = n$ 

$$p(y|\theta) = \frac{1}{Z(\theta)}h(y)\exp\left(\theta^{\top}\mathbf{f}(y)\right)$$

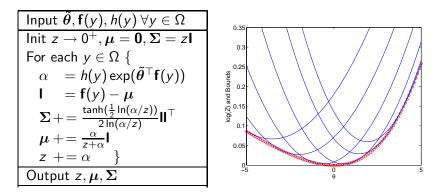
- Parameters are vector  $oldsymbol{ heta} \in \mathbb{R}^d$
- Features are  $\mathbf{f}: \Omega \mapsto \mathbb{R}^d$  mapping each y to some vector
- Prior is  $h: \Omega \mapsto \mathbb{R}^+$  a fixed non-negative measure
- Partition function ensures that  $p(y|\theta)$  normalizes

$$Z(\theta) = \sum_{y} h(y) \exp(\theta^{\top} \mathbf{f}(y))$$

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Problem: it's ugly to minimize (unlike a quadratic function)

The bound  $\ln Z(\theta) \leq \ln z + \frac{1}{2}(\theta - \tilde{\theta})^{\top} \Sigma(\theta - \tilde{\theta}) + (\theta - \tilde{\theta})^{\top} \mu$ is tight at  $\tilde{\theta}$  and holds for parameters given by



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#### Bound Proof.

1) Start with bound  $\log(e^{ heta}+e^{- heta})\leq c heta^2$  [Jaakkola & Jordan '99]

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- 2) Prove scalar bound via Fenchel dual using  $heta=\sqrt{artheta}$
- 3) Make bound multivariate  $\log(e^{\theta^{\top}\mathbf{1}} + e^{-\theta^{\top}\mathbf{1}})$
- 4) Handle scaling of exponentials  $\log(h_1 e^{\theta^{\top} \mathbf{f}_1} + h_2 e^{-\theta^{\top} \mathbf{f}_2})$
- 5) Add one term  $\log(h_1 e^{\theta^{\top} \mathbf{f}_1} + h_2 e^{-\theta^{\top} \mathbf{f}_2} + h_3 e^{-\theta^{\top} \mathbf{f}_3})$
- 6) Repeat extension for *n* terms

# Better Majorization for CRFs (Bound also Finds Gradient)

Init 
$$z \to 0^+$$
,  $\mu = \mathbf{0}$ ,  $\Sigma = z\mathbf{I}$   
For each  $y \in \Omega$  {  
 $\alpha = h(y) \exp(\tilde{\theta}^\top \mathbf{f}(y))$   
 $\mathbf{I} = \mathbf{f}(y) - \mu$   
 $\Sigma + = \frac{\tanh(\frac{1}{2}\ln(\alpha/z))}{2\ln(\alpha/z)} \mathbf{I}^\top$   
 $\mu + = \frac{\alpha}{z + \alpha} \mathbf{I}$   
 $z + = \alpha$  }  
Output  $z, \mu, \Sigma$ 

Recall gradient 
$$\frac{\partial \log L}{\partial \theta} = \sum_{t=1}^{T} \mathbf{f}(x_t, y_t) - \sum_{t=1}^{T} \sum_{y} \mathbf{f}(x_t, y) \mathbf{p}(y|x_t, \theta)$$

The bound's  $\mu$  give part of gradient (can skip  $\Sigma$  updates).

$$\mu = \sum_{y} \mathbf{f}(x_t, y) p(y | x_t, \theta)$$

Input  $x_j, y_j$  and functions  $h_{x_j}, \mathbf{f}_{x_j}$  for j = 1, ..., tInput regularizer  $\lambda \in \mathbb{R}^+$ Initialize  $\theta_0$  anywhere and set  $\tilde{\theta} = \theta_0$ While not converged For j = 1 to t compute bound for  $\mu_j, \Sigma_j$  from  $h_{x_j}, \mathbf{f}_{x_j}, \tilde{\theta}$ Set  $\tilde{\theta} = \arg \min_{\theta} \sum_j \frac{1}{2} (\theta - \tilde{\theta})^\top (\Sigma_j + \lambda \mathbf{I}) (\theta - \tilde{\theta})$   $+ \sum_j \theta^\top (\mu_j - \mathbf{f}_{x_j}(y_j) + \lambda \tilde{\theta})$ Output  $\hat{\theta} = \tilde{\theta}$ 

#### Theorem

$$\begin{split} & If \, \|\mathbf{f}(x_j, y)\| \leq r \, get \, J(\hat{\boldsymbol{\theta}}) - J(\boldsymbol{\theta}_0) \geq (1 - \epsilon) \max_{\boldsymbol{\theta}} (J(\boldsymbol{\theta}) - J(\boldsymbol{\theta}_0)) \\ & within \, \left\lceil \ln\left(1/\epsilon\right) / \ln\left(1 + \frac{\lambda \log n}{2r^2 n}\right) \right\rceil \, steps \end{split}$$

## **Convergence** Proof

#### Proof.

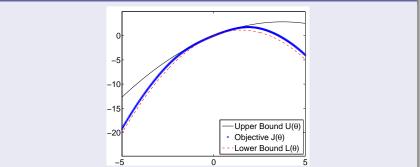


Figure: Quadratic bounding sandwich. Compare upper and lower bound curvatures to bound maximum # of iterations.

## Experiments - Multi-Class Classification & Linear Chains

Data-set	SRB	СТ	Tumor	s	Tex	t	SecSt	r	CoNLL	-	PennTre	e
Size	<i>n</i> = 4		<i>n</i> = 26 <i>n</i> = 2		<i>n</i> = 2		<i>m</i> = 9		<i>m</i> = 45			
	t =	83	<i>t</i> = 30	8	t = 15	500	t = 836	579	t = 100	0	t = 100	0
	d = 9	9236	d = 3902	260	d = 23	922	d = 63	32	<i>d</i> = 336	15	d = 141	75
	$\lambda =$	$10^{1}$	$\lambda = 10$	1	$\lambda = 1$	.0 <sup>2</sup>	$\lambda = 10$	$D^1$	$\lambda = 10$	1	$\lambda = 10^{-10}$	1
Algorithm	time	iter	time	iter	time	iter	time	iter	time	iter	time	iter
LBFGS	6.10	42	3246.83	8	15.54	7	881.31	47	25661.54	17	62848.08	7
Grad	7.27	43	18749.15	53	153.10	69	1490.51	79	93821.72	12	156319.31	12
Congrad	40.61	100	14840.66	42	57.30	23	667.67	36	88973.93	23	76332.39	18
Bound	3.67	8	1639.93	4	6.18	3	27.97	9	16445.93	4	27073.42	2

Table: Time in seconds and iterations to match LBFGS solution for multi-class logistic regression (on SRBCT, Tumors, Text and SecStr data-sets where *n* is the number of classes) and Markov CRFs (on CoNLL and PennTree data-sets, where *m* is the number of classes). Here, *t* is the number of samples, *d* is the dimensionality of the feature vector and  $\lambda$  is the cross-validated regularization setting.

## Experiments - Linear Chains

Model	Error	oov Error
		45.59%
Maximum Entropy Markov Model	6.37%	54.61%
Conditional Random Field	5.55%	48.05%

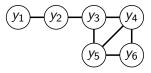
Table: Accuracy on Penn tree-bank data-set for parts-of-speech tagging with training on half of the 1.1 million word corpus. Note, the oov rate is the error rate on out-of-vocabulary words.

Parts of speech data-set where there are 45 labels per word, e.g.

$$p(y|\mathbf{x},\boldsymbol{\theta}) = \frac{1}{Z}\psi(y_1,y_2)\psi(y_2,y_3)\psi(y_3,y_4)\psi(y_4,y_5)\psi(y_5,y_6)\psi(y_6,y_7)$$

How big is y? Recall graphical models for large spaces.  $a = -2 \circ a \circ a$ 

## Bounding Graphical Models with Large n

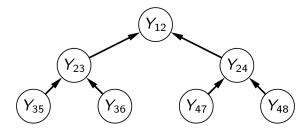


- Each iteration is O(tn), but what if *n* is large?
- Graphical model: an undirected graph G representing a distribution p(Y) where  $Y = \{y_1, \dots, y_n\}$  and  $y_i \in \mathbb{Z}$
- *p*(*Y*) factorizes as product of {*ψ*<sub>1</sub>,...,*ψ*<sub>C</sub>} functions over {*Y*<sub>1</sub>,...,*Y*<sub>C</sub>} subsets of variables over the maximal cliques of *G*

$$p(y_1,\ldots,y_n) = \frac{1}{Z}\prod_{c\in C}\psi_c(Y_c)$$

• E.g.  $p(y_1, \ldots, y_6) = \psi(y_1, y_2)\psi(y_2, y_3)\psi(y_3, y_4, y_5)\psi(y_4, y_5, y_6)$ 

## Bounding Graphical Models with Large n



- Instead of enumerating over all n, exploit graphical model
- Build junction tree and run a Collect algorithm
- Useful for computing  $Z(\theta)$ ,  $\frac{\partial \log Z(\theta)}{\partial \theta}$  and  $\Sigma$  efficiently
- Bound needs  $\mathcal{O}(t \sum_{c} |Y_{c}|)$  rather than  $\mathcal{O}(tn)$
- For an HMM, this is  $\mathcal{O}(TM^2)$  instead of  $\mathcal{O}(M^T)$

## Bounding Graphical Models with Large n

for 
$$c = 1, ..., m$$
 {  
 $Y_{both} = Y_c \cap Y_{pa(c)}; Y_{solo} = Y_c \setminus Y_{pa(c)}$   
for each  $u \in Y_{both}$  {  
initialize  $z_{c|x} \leftarrow 0^+$ ,  $\mu_{c|x} = \mathbf{0}, \Sigma_{c|x} = z_{c|x}\mathbf{I}$   
for each  $v \in Y_{solo}$  {  
 $w = u \otimes v; \quad \alpha_w = h_c(w)e^{\tilde{\theta}^\top \mathbf{f}_c(w)} \prod_{b \in ch(c)} z_{b|w}$   
 $\mathbf{I}_w = \mathbf{f}_c(w) - \mu_{c|u} + \sum_{b \in ch(c)} \mu_{b|w}$   
 $\Sigma_{c|u} + = \sum_{b \in ch(c)} \Sigma_{b|w} + \frac{\tanh(\frac{1}{2}\ln(\frac{\alpha_w}{z_{c|u}}))}{2\ln(\frac{\alpha_w}{z_{c|u}})} \mathbf{I}_w \mathbf{I}_w^\top$   
 $\mu_{c|u} + = \frac{\alpha_w}{z_{c|u} + \alpha_w} \mathbf{I}_w; \quad z_{c|u} + = \alpha_w$  }}

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