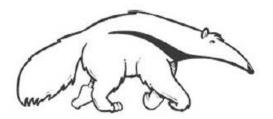
# Bottom-up Approaches to Approximate Inference and Learning

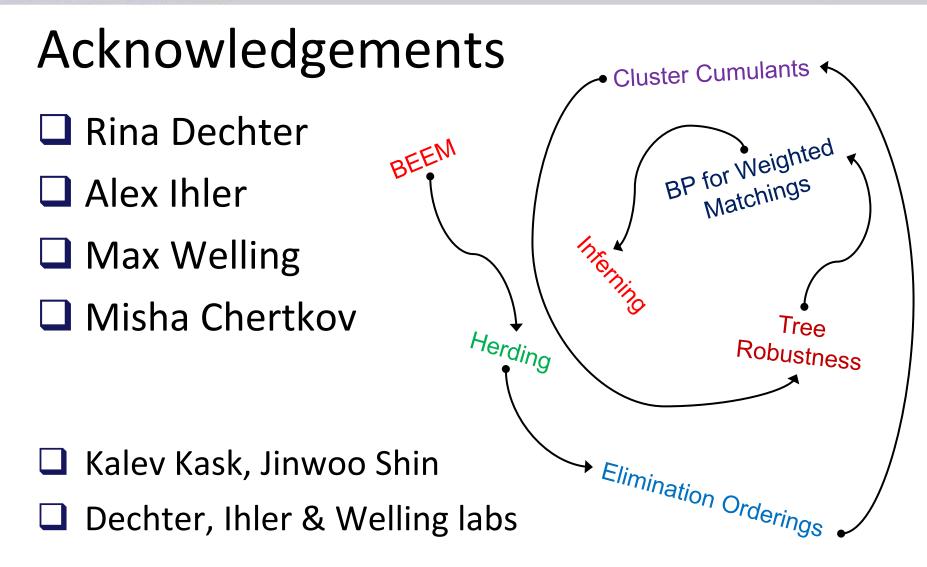
Andrew Gelfand Final Defense April 10, 2014









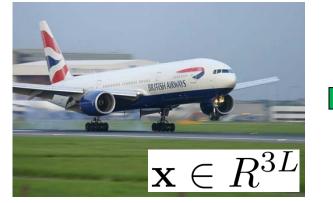




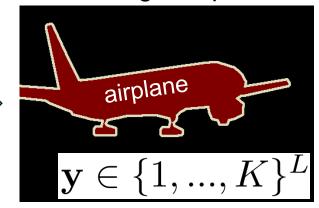


## **Statistical Modeling**

#### RGB image with *L* pixels



Labeling of *L* pixels



- 1. How do we represent  $p(\mathbf{y}, \mathbf{x})$ ?
- **2**. How do we learn  $p(\mathbf{y}, \mathbf{x})$  from data?
- **3.** How do we predict, *e.g.* compute  $p|\mathbf{y}|$







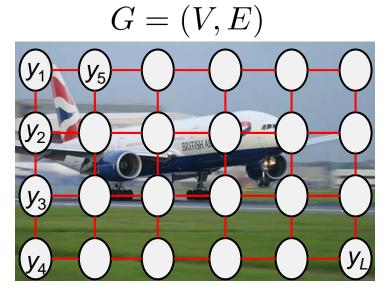
## **Graphical Models**

- Compact representation of large distributions
- Graph encodes probabilistic dependencies
- <u>Ex</u>: Pairwise model

$$p(\mathbf{y}|\mathbf{x}) \propto \prod_{i \in V} \psi_i(y_i, \mathbf{x}) \prod_{(i,j) \in E} \psi_{ij}(y_i, y_j, \mathbf{x})$$

$$y_i = \{\text{sky}, \text{plane}, ..., \text{car}\}$$

Only 
$$|V|K + |E|K^2$$
 parameters!

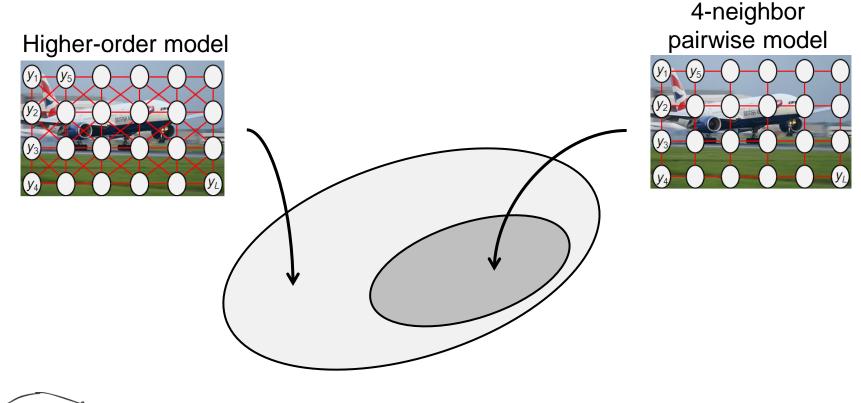






# Complexity of Graphical Models

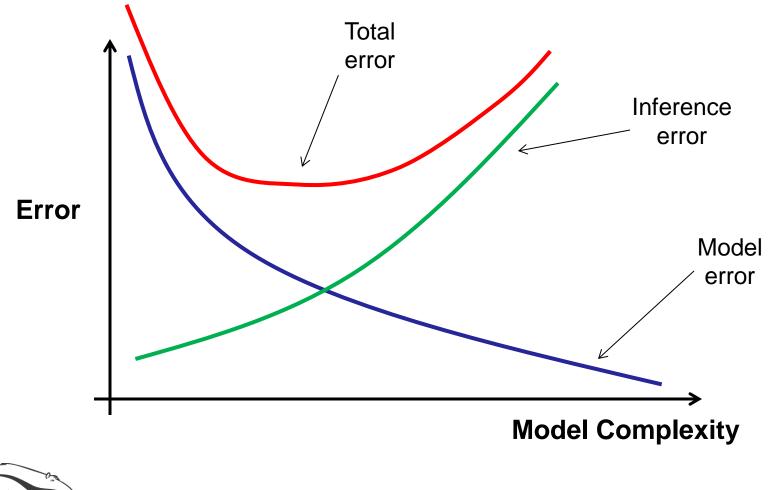
## A graphical model defines family of distributions







## Are richer models more accurate?





## **Thesis Statement**

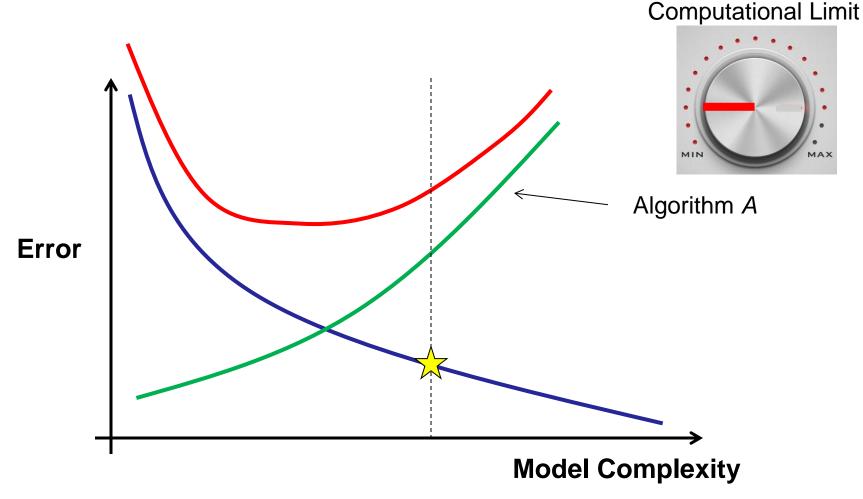
- Advocate a "bottom-up" approach to approximate inference & learning
  - Start with *simple*, cheap approximation
  - Improve through additional computation







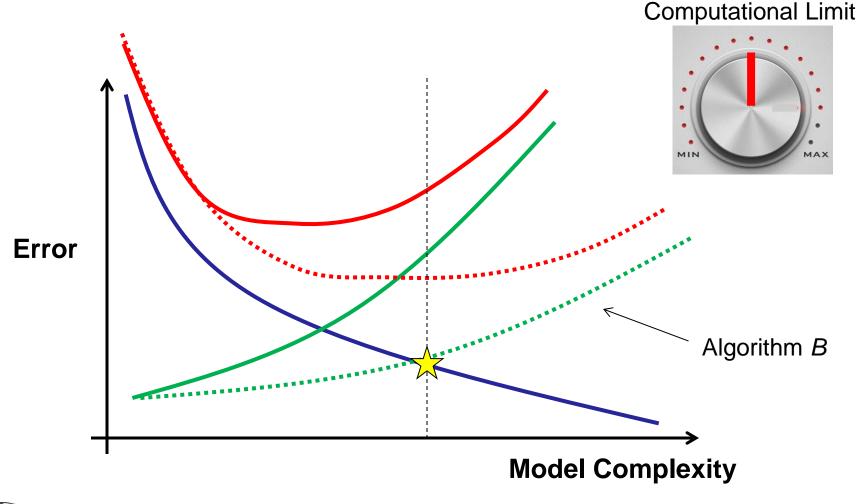
## The "Bottom-up" approach







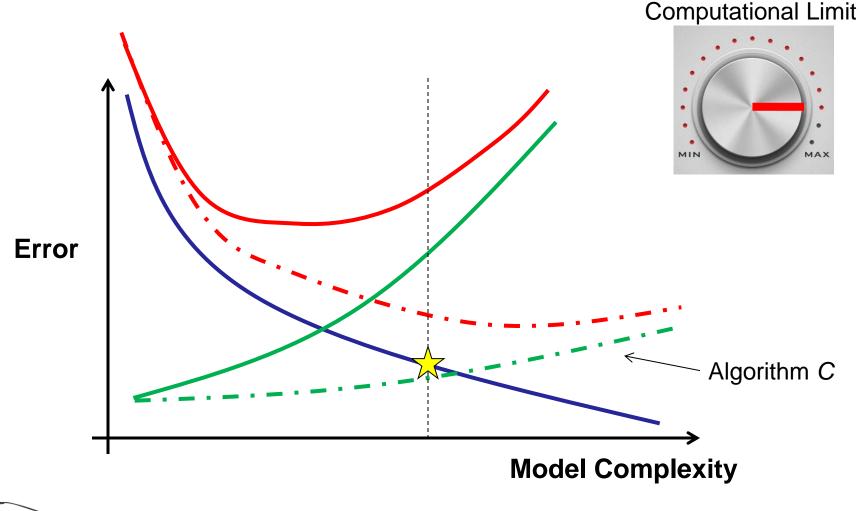
## The "Bottom-up" approach







## The "Bottom-up" approach







## **Overview of Thesis**

- 1. Max Likelihood Learning
  - Computation-limited, approximate learning
- 2. Computing Marginal Probabilities
  - Region choice for Generalized Belief Propagation
- 3. Most Probable (MAP) Configuration
  - Cutting-plane algorithm for weighted matchings







## Outline of this Talk

## 1. Max Likelihood Learning

- Sources of error in likelihood-based learning
- Computation-accuracy trade-offs in approximate learning

## 2. Computing Marginal Probabilities

- Review of Belief Propagation (BP) & Generalized BP
- Choosing Regions via Cycle Bases

### 3. Summary







## Outline of this Talk

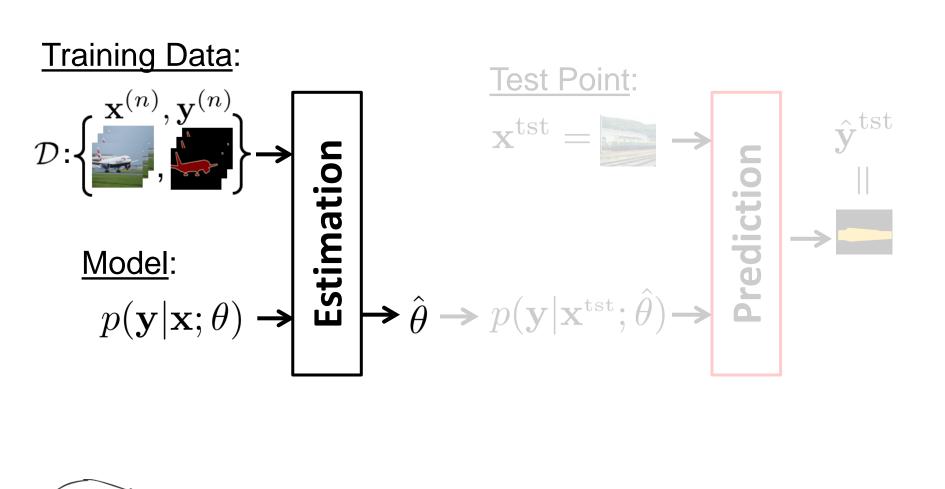
- 1. Max Likelihood Learning
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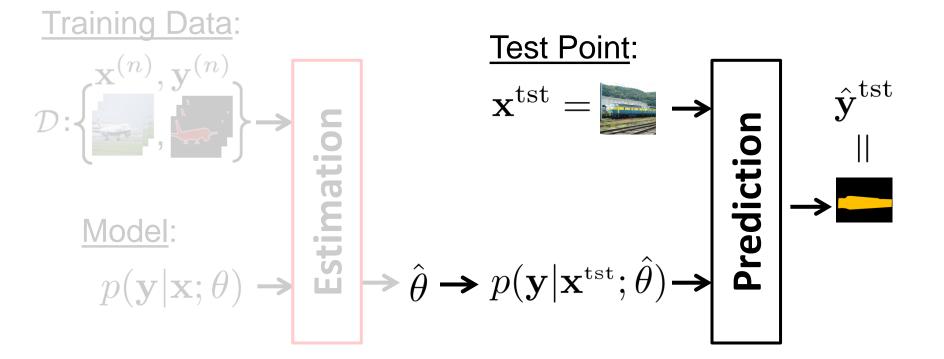
## **Parameter Estimation & Prediction**







## **Parameter Estimation & Prediction**









## Max Likelihood Estimation

Given a model, 
$$p(\boldsymbol{y}; \boldsymbol{\theta}) = \exp\left(\sum_{c \in C} \theta_c(\boldsymbol{y}_c) - \log Z(\boldsymbol{\theta})\right)$$
,

$$\hat{oldsymbol{ heta}} = rg\max_{oldsymbol{ heta} \in \mathbb{R}^D} \ell_N(oldsymbol{ heta})$$

where,

find

$$\ell_N(\boldsymbol{\theta}) = \frac{1}{N} \sum_{n=1}^N \log p(\boldsymbol{y}^{(n)}; \boldsymbol{\theta}) = \bar{\boldsymbol{\mu}}_N \cdot \boldsymbol{\theta} - \log Z(\boldsymbol{\theta})$$

$$\swarrow$$
vector of empirical marginals:  $\bar{\mu}(\boldsymbol{y}_c) = \frac{1}{N} \sum_n I[\boldsymbol{Y}_c^{(n)} = \boldsymbol{y}_c]$ 



# Surrogate Likelihood [Wainwright '06]

 $\Box$  Approximate  $\log Z(\theta)$  with  $\log \tilde{Z}(\theta)$ ,

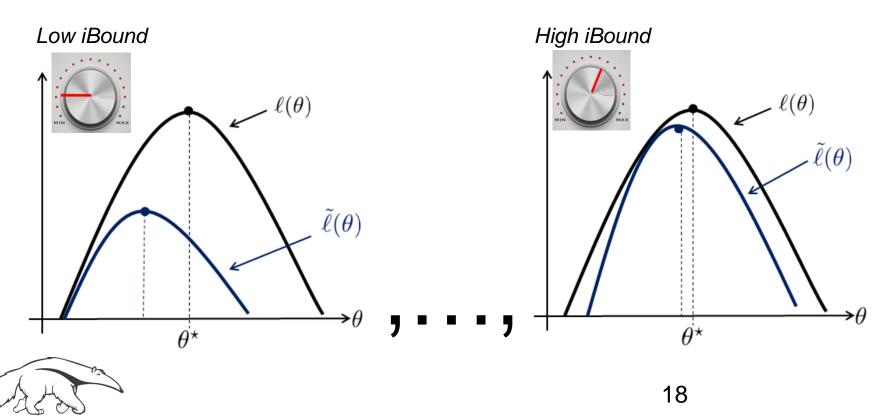
$$\ell_N(\boldsymbol{\theta}) \approx \tilde{\ell}_N(\boldsymbol{\theta}) = \bar{\boldsymbol{\mu}}_N \cdot \boldsymbol{\theta} - \log \tilde{Z}(\boldsymbol{\theta})$$





# Surrogate Likelihood [Wainwright '06] Approximate $\log Z(\theta)$ with $\log \tilde{Z}(\theta)$ ,

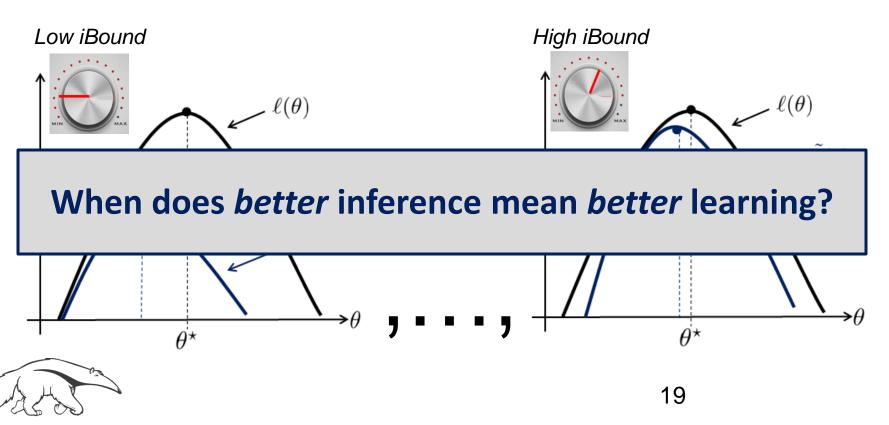
$$\ell_N(\boldsymbol{\theta}) \approx \tilde{\ell}_N(\boldsymbol{\theta}) = \bar{\boldsymbol{\mu}}_N \cdot \boldsymbol{\theta} - \log \tilde{Z}(\boldsymbol{\theta})$$





# Surrogate Likelihood [Wainwright '06] Approximate $\log Z(\theta)$ with $\log \tilde{Z}(\theta)$ ,

$$\ell_N(\boldsymbol{\theta}) \approx \tilde{\ell}_N(\boldsymbol{\theta}) = \bar{\boldsymbol{\mu}}_N \cdot \boldsymbol{\theta} - \log \tilde{Z}(\boldsymbol{\theta})$$





#### 1. Model Error

Error in approximation to true (unknown) distribution

#### 2. Estimation Error

Error due to use of finite sample

#### 3. Optimization Error

• *Gap* between true and surrogate likelihood functions

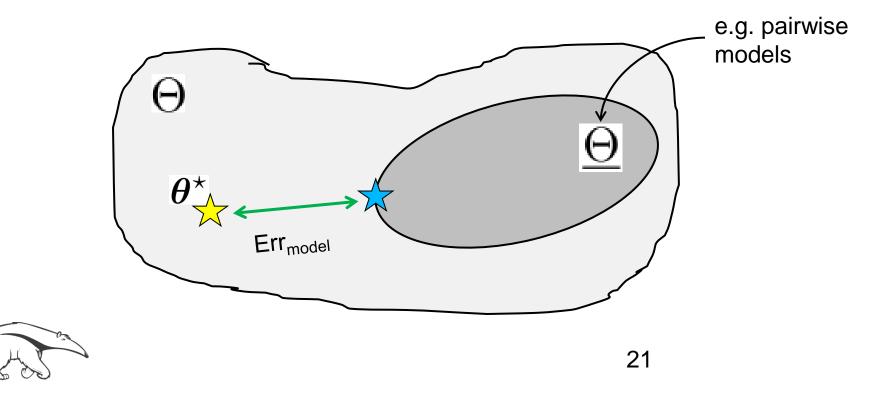






#### 1. Model Error

- data sampled as  $\boldsymbol{y}^{(n)} \stackrel{\text{\tiny iid}}{\sim} p(\boldsymbol{y}; \boldsymbol{\theta}^{\star})$ , where  $\boldsymbol{\theta}^{\star} \in \Theta$
- fit model with  $\theta \in \Theta$

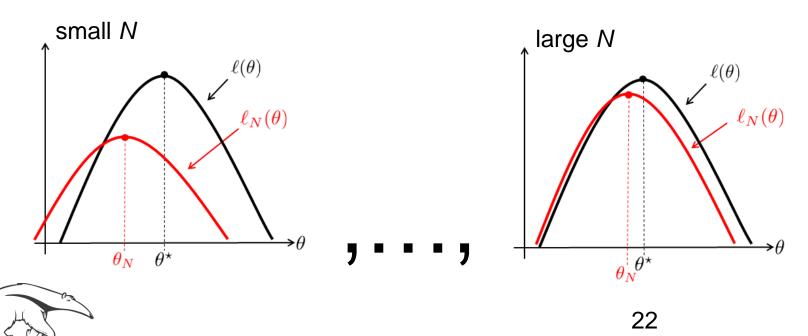




#### 2. Estimation Error

optimize empirical (not expected) risk

 $\ell_N(\boldsymbol{\theta}) = \frac{1}{N} \sum_{n=1}^N \log p(\boldsymbol{y}^{(n)}; \boldsymbol{\theta}) \stackrel{a.s.}{\to} \mathbb{E}_{\boldsymbol{\theta}^{\star}} \left[ \log p(\boldsymbol{y}; \boldsymbol{\theta}) \right] = \sum_{\boldsymbol{y}} p(\boldsymbol{y}; \boldsymbol{\theta}^{\star}) \log p(\boldsymbol{y}; \boldsymbol{\theta})$ 

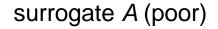




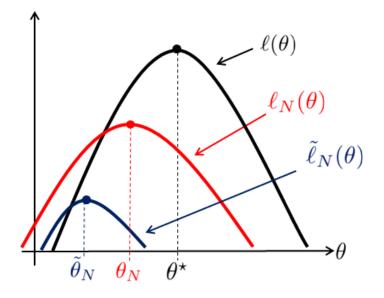


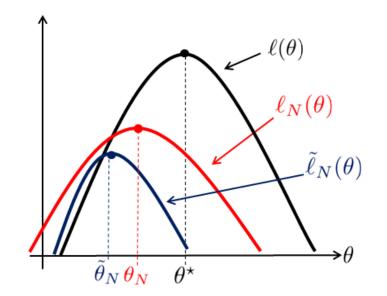
#### 3. Optimization Error

• optimize a surrogate likelihood  $\tilde{\ell}_N(\boldsymbol{\theta}) \approx \ell_N(\boldsymbol{\theta})$ 











## Empirical Study (I) – Estimation

$$\underline{\text{Data:}} \ \mathcal{D}: \left\{ \begin{array}{l} (\boldsymbol{x}^{(n)}, \boldsymbol{y}^{(n)}) \\ \hline \boldsymbol{\omega}^{(n)}, \boldsymbol{\omega}^{(n)} \\ \hline \boldsymbol{\omega}^{(n)}, \boldsymbol{\omega}^{(n)} \\ \hline \boldsymbol{\omega}^{(n)}, \boldsymbol{y}^{(n)} \\ \hline \boldsymbol{\omega}^{(n)}, \boldsymbol{\omega}^{(n)} \\ \hline \boldsymbol{\omega}^{(n)} \\ \hline \boldsymbol{\omega}^{(n)}, \boldsymbol{\omega}^{(n)} \\ \hline \boldsymbol$$

Study estimation error (MSE) as we vary:

- Optimization Error: inference procedures
- Estimation Error: data set size
- Model Error: mismatch between  $\Theta$  and  $\Theta$





## **Experimental Setup**

## Create *L* statistically identifiable models

• Sample  $\theta_i(y_i) \sim \mathcal{N}(0, \sigma_i^2)$  and  $\theta_{ij}(y_i, y_j) \sim \mathcal{N}(0, \sigma_{ij}^2)$  for

$$p(\boldsymbol{y};\boldsymbol{\theta}) = \exp\left(\sum_{i \in V} \theta_i(y_i) + \sum_{(i,j) \in E} \theta_{ij}(y_i, y_j) - \log Z(\boldsymbol{\theta})\right)$$

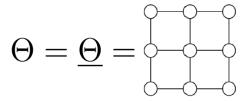
- □ Sample data sets of size *N* = {100,...,10000}
- $\Box \operatorname{\mathsf{Find}} \tilde{\theta}_N = \operatorname{arg\,max}_{\boldsymbol{\theta}} \tilde{\ell}_N(\boldsymbol{\theta})$ 
  - Using different approximate inference algorithms

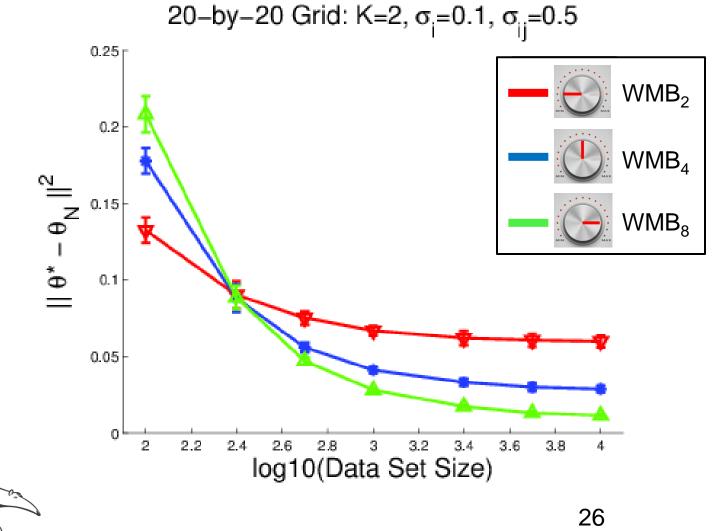






## **Grid Experiments**

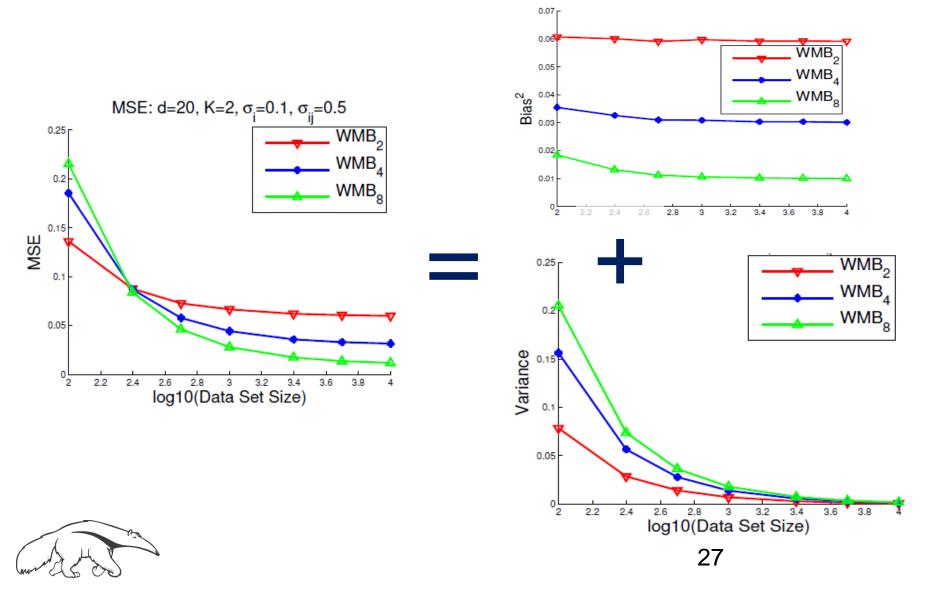








## **Bias–Variance Trade-off**







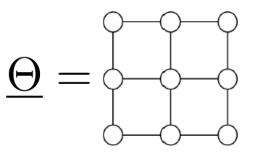
## **Model Error Experiments**

# $\Theta = \bigcup_{i=1}^{i}$

 $m{y}^{(n)} \stackrel{\mathrm{iid}}{\sim} p(m{y}; m{ heta}^{\star})$  where  $m{ heta}^{\star} \in \Theta$ 

 $\theta_{ik}(y_i, y_k) \sim \mathcal{N}(0, \sigma_{ik}^2)$ 



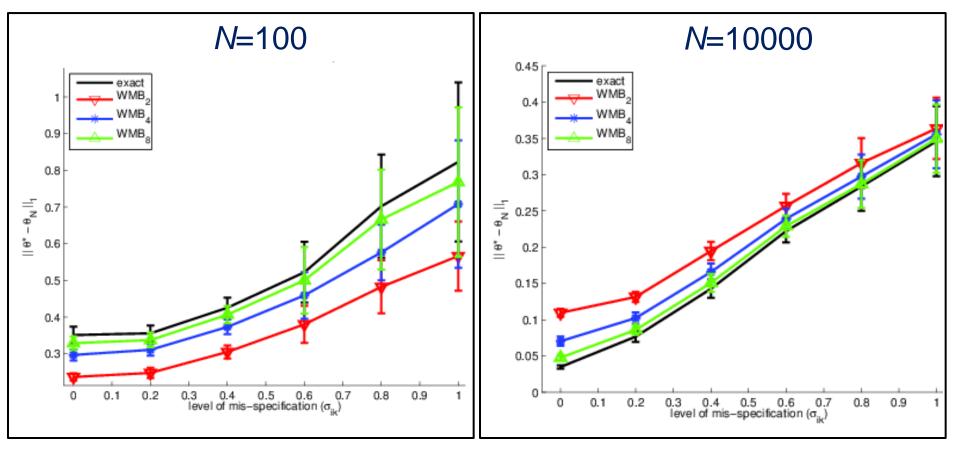


 $p(oldsymbol{y};oldsymbol{ heta})$  where  $oldsymbol{ heta}\in\underline{\Theta}$ 





## **Model Error Experiments**

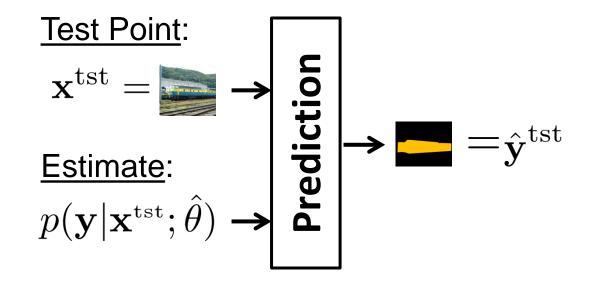


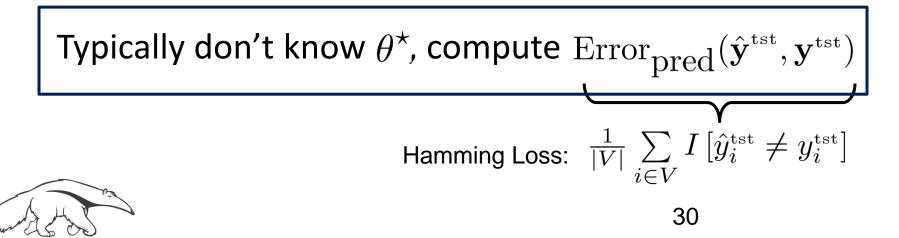
Increasing amount of mis-specification





## Empirical Study (II) – Prediction





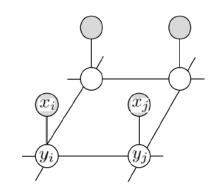


# MRF De-Noising Experiments

USPS digits data (1100, 16x16 pixel grayscale images)

- Convert to binary and flip pixels with probability p
- Assume a 4-neighbor model:

$$p(\boldsymbol{y}, \boldsymbol{x}; \boldsymbol{\theta}) \propto \exp\left(\sum_{i} \theta_{i} y_{i} + \sum_{ij} \theta_{ij} y_{i} y_{j} + \sum_{i} \theta_{ii} y_{i} x_{i}\right)$$



- Compute both Err<sub>est</sub> and Err<sub>pred</sub>
  - $\operatorname{Err}_{\operatorname{est}}$  computed wrt  $\ell_N(\boldsymbol{\theta})$  (using exact inference)

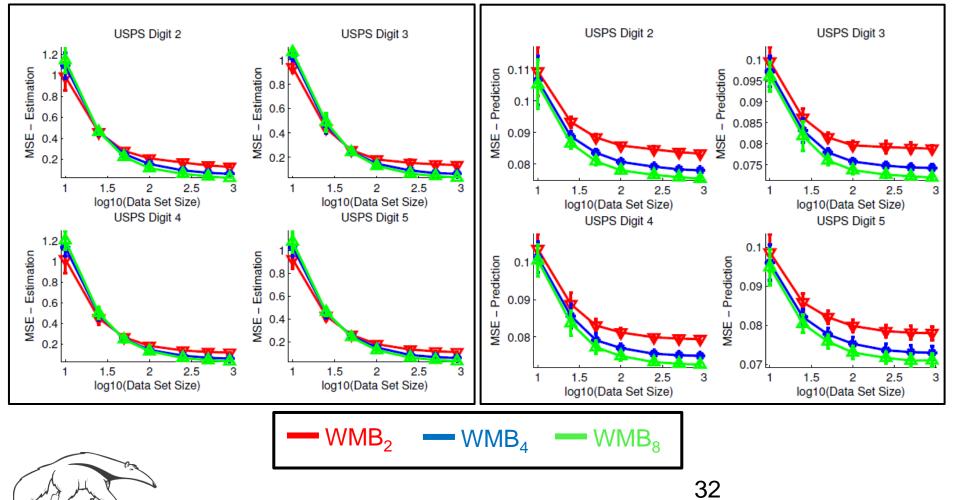




## **MRF De-Noising Experiments**

#### Estimation Error

#### **Prediction Error**



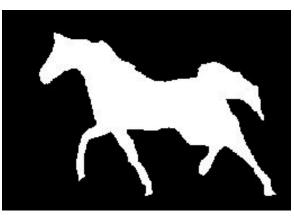


## Foreground/Background Segmentation

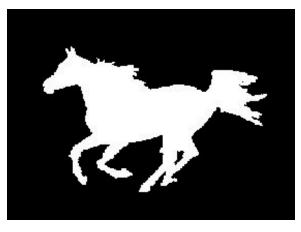
#### Input, x



#### Output, y







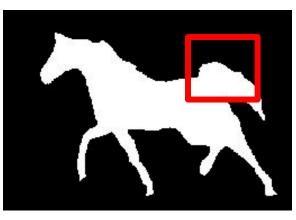


## Foreground/Background Segmentation

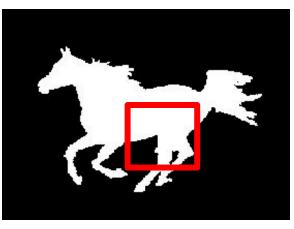
#### Input, x



#### Output, y





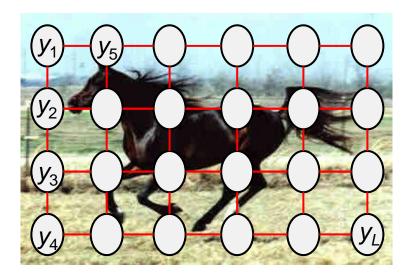






## **Conditional Random Field Model**

$$p(\mathbf{y}|\mathbf{x};\theta) \propto \exp\left(\sum_{i \in V} \sum_{u} \theta_{u} f_{u}(y_{i},\mathbf{x}) + \sum_{(i,j) \in E} \sum_{p} \theta_{p} f_{p}(y_{i},y_{j},\mathbf{x})\right)$$



#### **Unary Features:**

$$f_u(y_i, x_i) = \begin{cases} \operatorname{color}(x_i), & \text{if } y_i = \text{'horse'.} \\ 0, & \text{otherwise.} \end{cases}$$

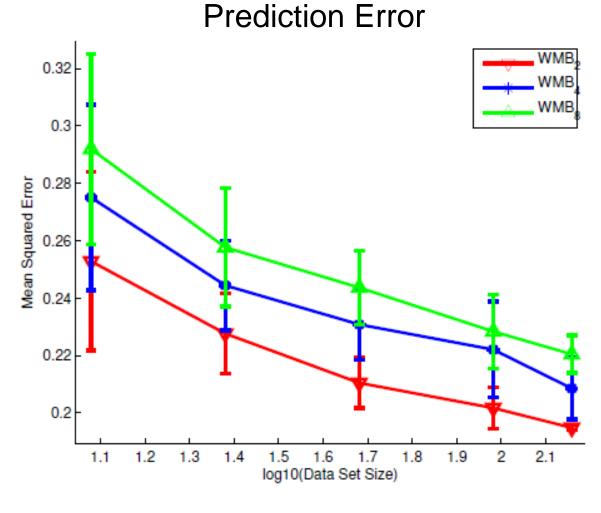
#### Pairwise Features:

$$f_p(y_i, y_j, \mathbf{x}) = \begin{cases} 1, & \text{if } y_i = y_j \ , ||x_i - x_j|| < \epsilon \\ 0, & \text{otherwise.} \end{cases}$$



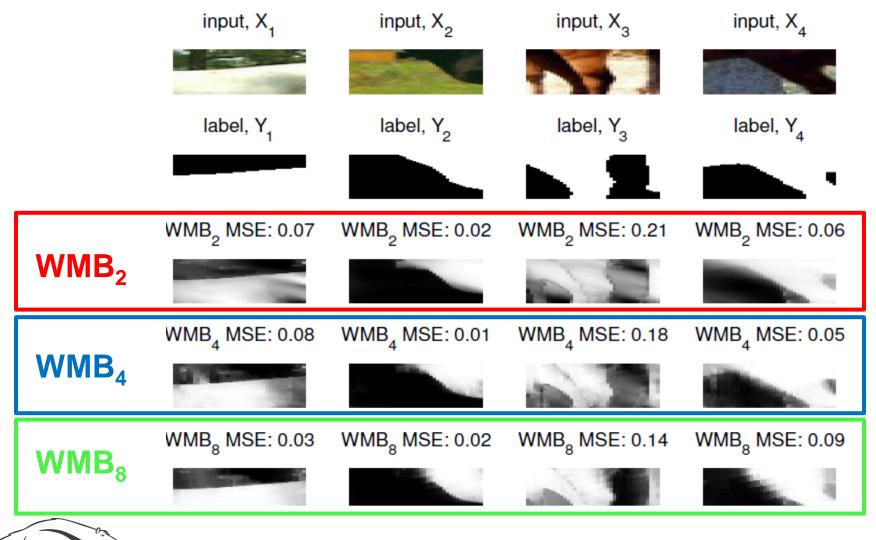


## **Quantitative Results**





### **Qualitative Results**

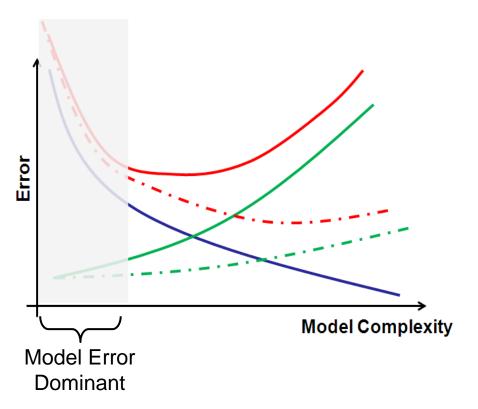




# Summary of Experimental Study

- □ If data set is small use a lower *iBound* method
  - Trade smaller variance for increased bias

Higher *iBound* does not yield better predictions if model error is dominant

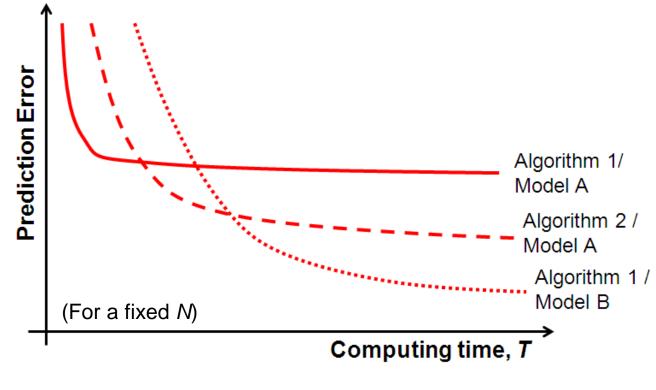






# The Dream Scenario...

Given data set N and time budget T, choose the model and algorithm that minimize test error









# Outline of this Talk

#### 1. Max Likelihood Learning

- Sources of error in likelihood-based learning
- Computation-accuracy trade-offs in approximate learning

#### 2. Computing Marginal Probabilities

- Review of Belief Propagation (BP) & Generalized BP
- Choosing Regions via Cycle Bases

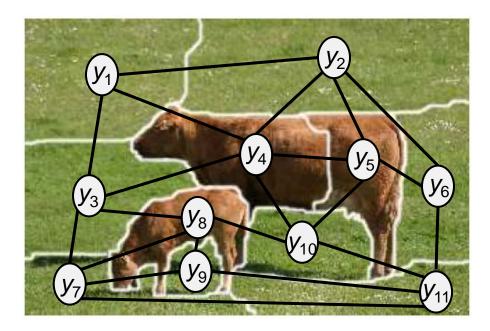
#### 3. Summary





# **Computing Marginals**

### After learning $p(\mathbf{y}) \propto \psi_{12}(y_1, y_2)\psi_{13}(y_1, y_3)\cdots$



...want to compute:  $p(y_2 = 'grass')$ ?  $p(y_5 = 'cow')$ ?





# Variational Perspective [Wainwright & Jordan '08]

#### Convert from a summation task...

$$\log Z = \log \sum_{\mathbf{y} \in \mathbf{Y}} \prod_{i \in V} \psi_i(y_i) \prod_{(i,j) \in E} \psi_{ij}(y_i, y_j)$$

#### ...to an optimization task

$$\log Z = \max_{\substack{b \in \mathbb{P} \\ \neg}} \left[ E_b \left[ \log \psi(\mathbf{y}) \right] + H(\mathbf{y}; b) \right]$$

Set of valid probability distributions

Entropy of distribution *b*(*y*)







# Variational Approximations

#### GBP introduces *two* approximations

$$\log Z = \max_{\substack{b \in \mathbb{L}}} \left[ E_b \left[ \log \psi(\mathbf{y}) \right] + \tilde{H}(\mathbf{y}; b) \right]$$

1) Locally consistent beliefs

2) Approximate Entropy

$$\tilde{H}_{\text{GBP}}(\mathbf{y}; b) = -\sum_{R \in \mathcal{R}} c_R H(\mathbf{y}_R; b) = -\sum_{R \in \mathcal{R}} c_R \sum_{\mathbf{y}_R} b_R(\mathbf{y}_R) \log b_R(\mathbf{y}_R)$$

Marginal Entropy on Region *R*, where  $\mathbf{y}_R \subset \mathbf{y}$ 



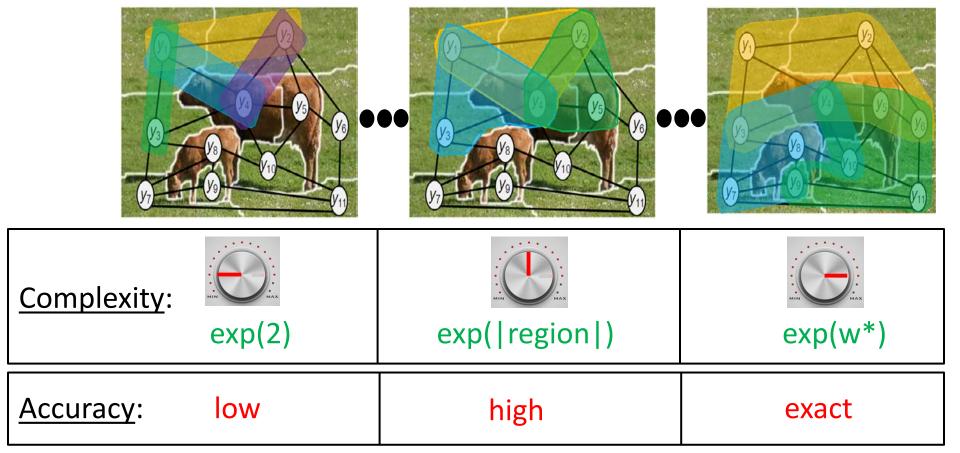


# Which Regions do we choose?

Bethe / BP

Kikuchi / GBP

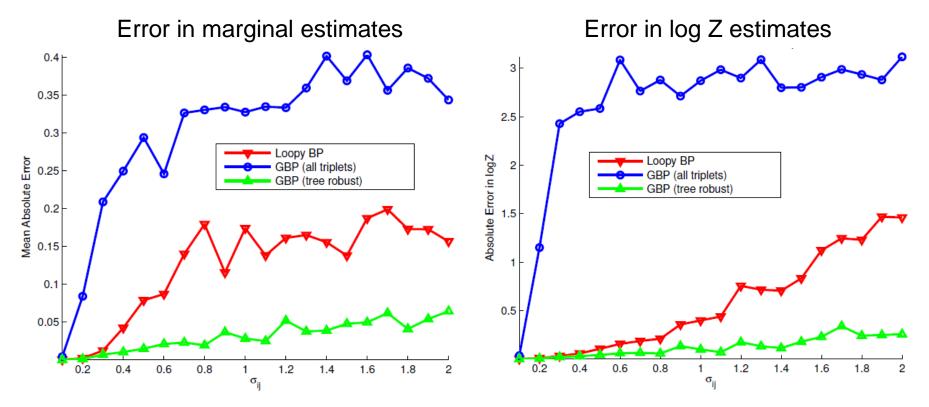
Exact







## Region choice is important!



Same complexity; very different accuracies!





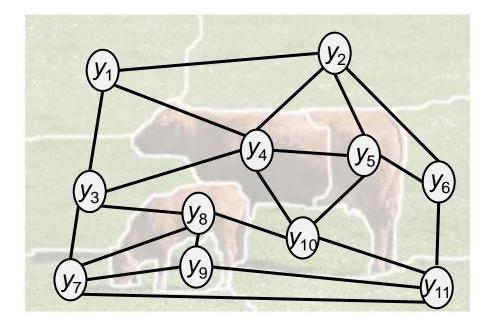
# Existing Guidance on Region Choice Choose Regions so that:

- $\tilde{H}_{\text{GBP}}(\mathbf{y}; b)$  exact when  $p(\mathbf{y})$  nearly uniform [Yedidia, Freeman, Weiss '02] [Pakzad & Anantharam '05]
- $\label{eq:gbp} \tilde{H}_{\rm GBP}({\bf y};b) \mbox{ exact when } p({\bf y}) \mbox{ nearly deterministic [Yedidia, Freeman, Weiss '02]}$
- All fixed points are uniform when p(y) is uniform [Welling, Minka, Teh '05]





# **Tree-Robustness** [Gelfand & Welling '12] **Consider a pairwise model** $p(\mathbf{y}) \propto \prod_{(i,j)\in E} \psi_{ij}(y_i, y_j)$

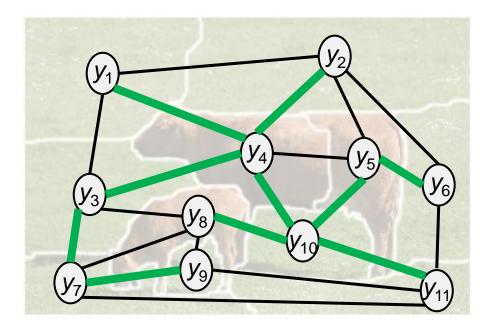






#### Tree-Robustness [Gelfand & Welling '12]

□ Consider a pairwise model  $p(\mathbf{y}) \propto \prod_{(i,j)\in E} \psi_{ij}(y_i, y_j)$ □ Let  $T \subset E$  be a tree in G

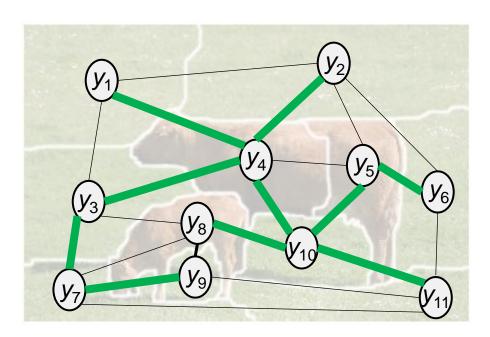






### Tree-Robustness [Gelfand & Welling '12]

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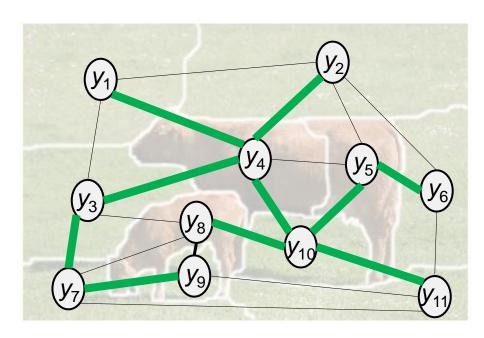
Assume uniform off-tree factors:  $\psi_{ij}(y_i, y_j) = \mathbf{1}$ 





### Tree-Robustness [Gelfand & Welling '12]

□ Consider a pairwise model  $p(\mathbf{y}) \propto \prod_{(i,j)\in E} \psi_{ij}(y_i, y_j)$ □ Let  $T \subseteq E$  be a tree in G



Assume uniform off-tree factors:  $\psi_{ij}(y_i, y_j) = \mathbf{1}$ 

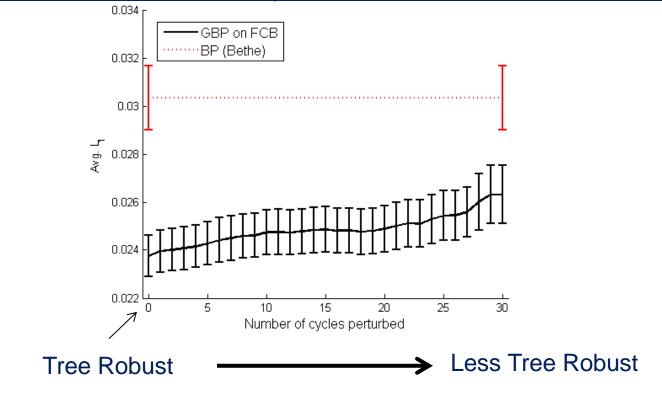
$$\label{eq:HGBP} \begin{split} \begin{gathered} \tilde{H}_{\rm GBP}(\mathbf{y};b) \, \text{is exact} \\ & \text{on } p_T(\mathbf{y}) \, \text{and all} \\ & \text{such trees in } G! \end{split}$$





### Is Tree Robustness Desirable?

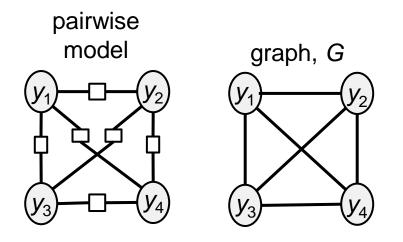
Accuracy degrades as Regions becomes less Tree Robust!







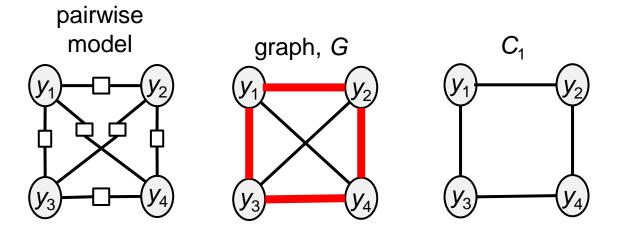








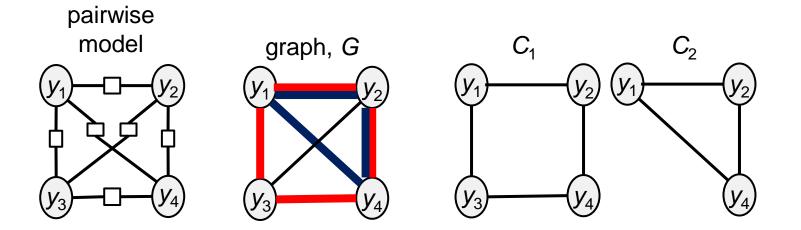








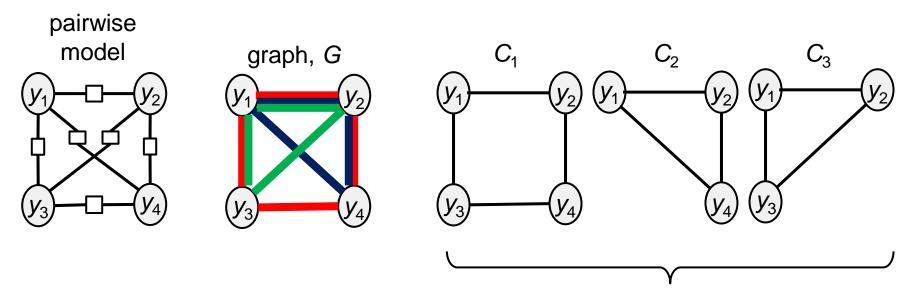












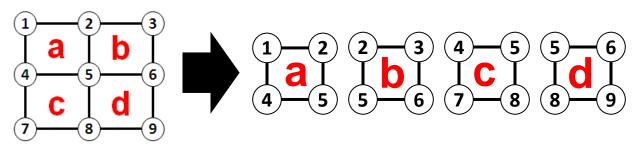
Collection of outer regions





# Identifying Tree-Robust Regions

- □ Selecting TR Regions = Finding TR Cycle Basis
  - Faces of a planar graph:



'Star' Construction

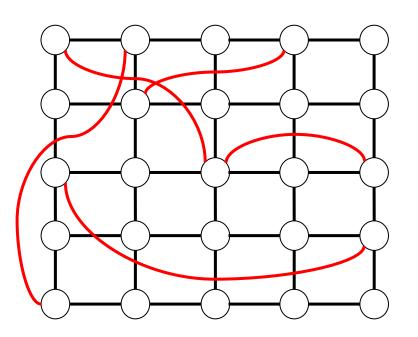
$$1 \\ 2 \\ 3 \\ 4$$





# **Experimental Results**

Grids with long range interactions



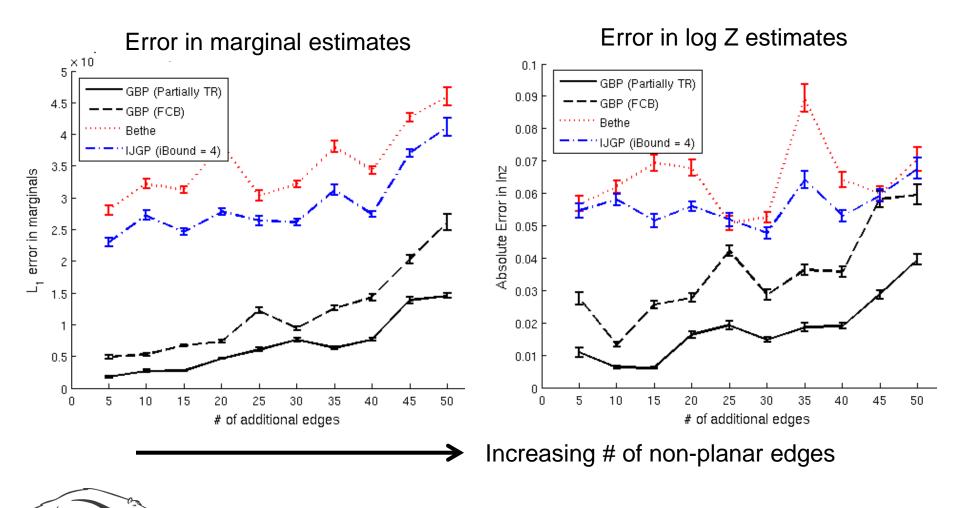
#### <u>Algorithms</u>

- 1. GBP with Tree-Robust Core
- 2. GBP with 'ear' construction
- 3. Loopy BP
- 4. Iterative Join Graph Prop.(IJGP) w/ *iBound* = 4





### **Experimental Results**







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#### 3. Summary





# Summary

Continued need for *better* inference methods

- Advocate a "bottom-up" approach to inference
- Computation-Accuracy Trade-offs in Learning
  - Small N => Low computation inference
  - Better inference does not mean better predictions
- Proposed tree-robustness for choosing regions
   Connected finding regions to finding cycle bases



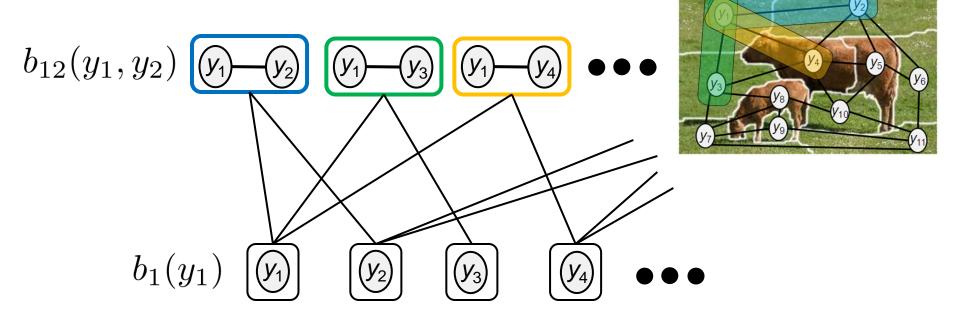








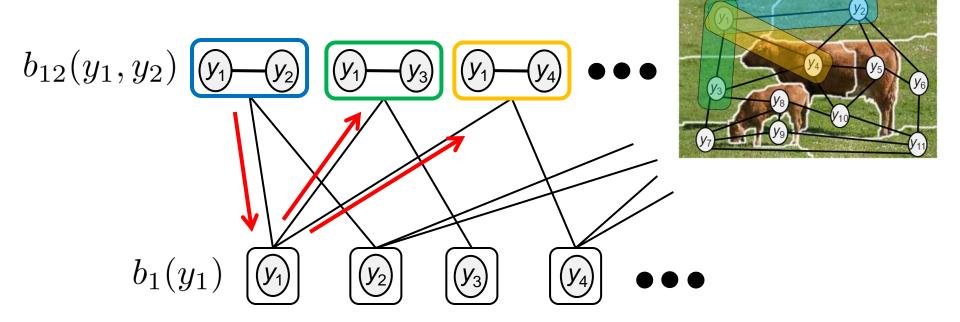
# Belief Propagation (BP) [Pearl '88]







# Belief Propagation (BP) [Pearl '88]

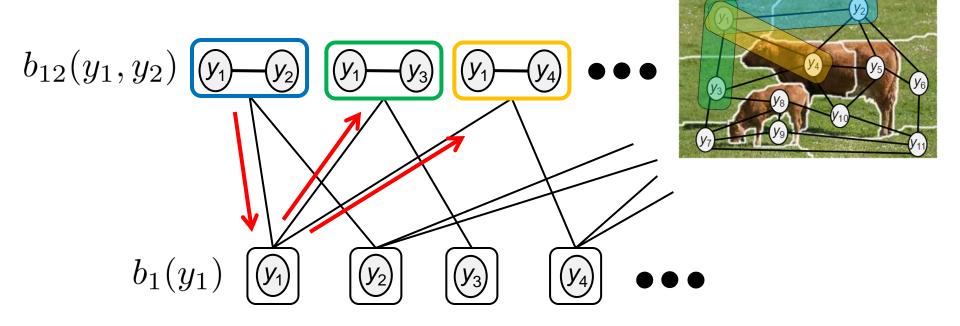


$$m_{12\to1}(y_1) = \frac{\sum_{y_2} b_{12}(y_1, y_2)}{b_1(y_1)}$$
$$= m_{1\to13}(y_1)$$
$$= m_{1\to14}(y_1)$$

$$b_1(y_1) \leftarrow b_1(y_1) \underbrace{m_{12 \to 1}(y_1)}_{}$$



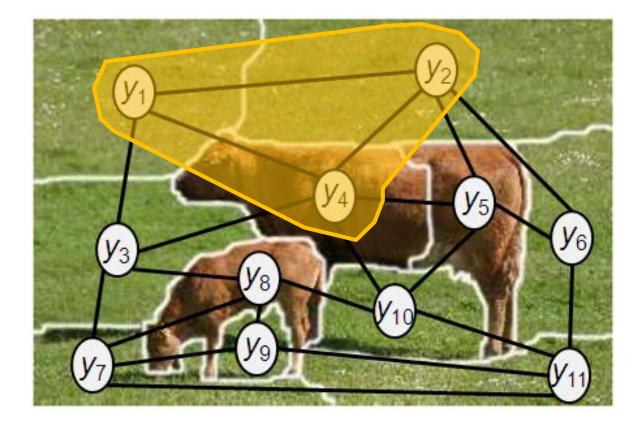
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#### Iterate until beliefs are *consistent* !

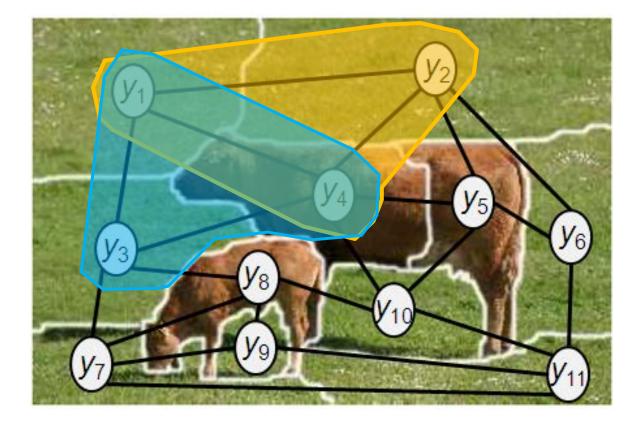






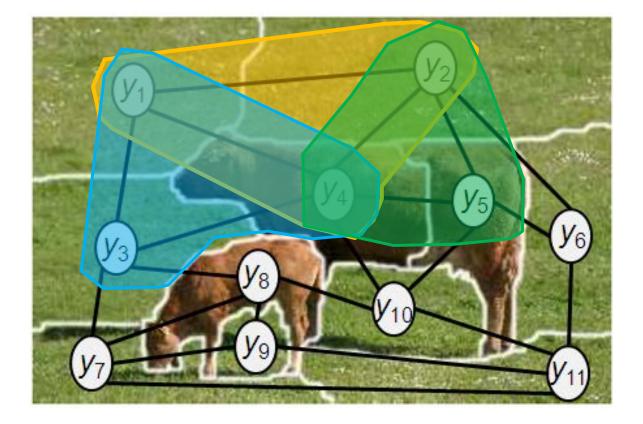






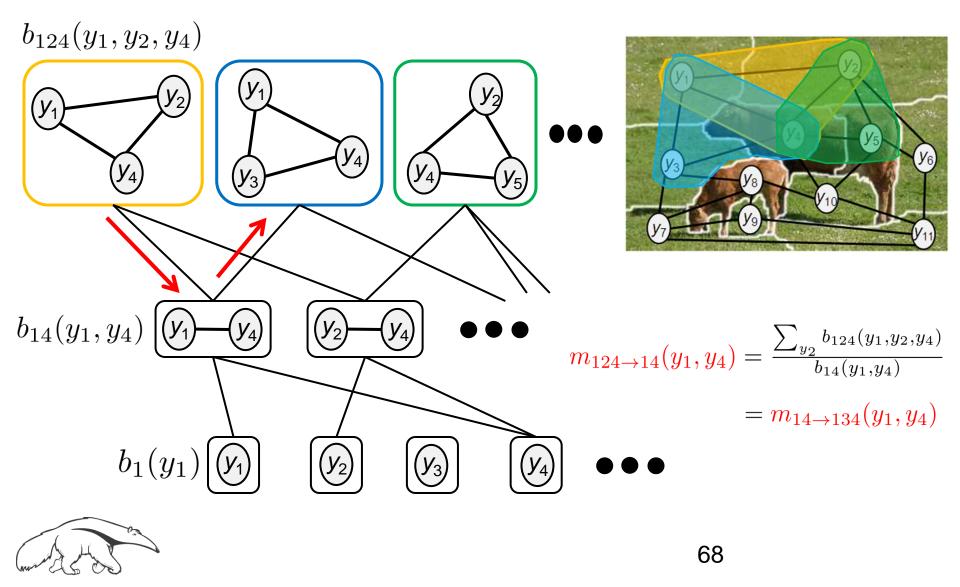






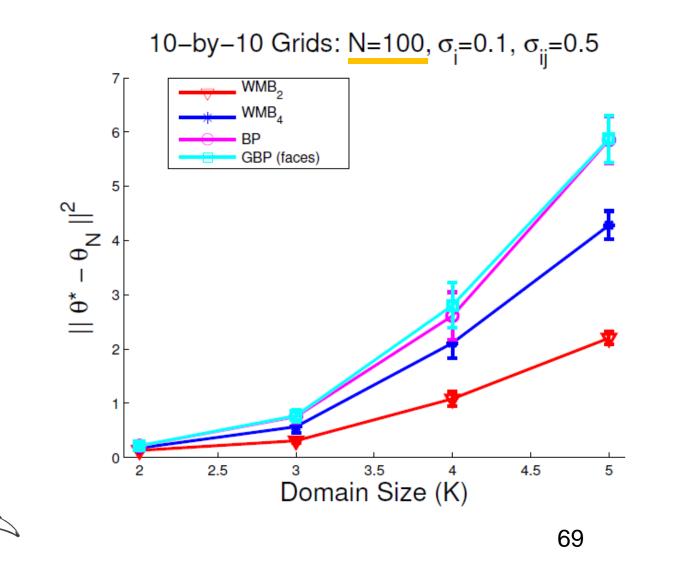






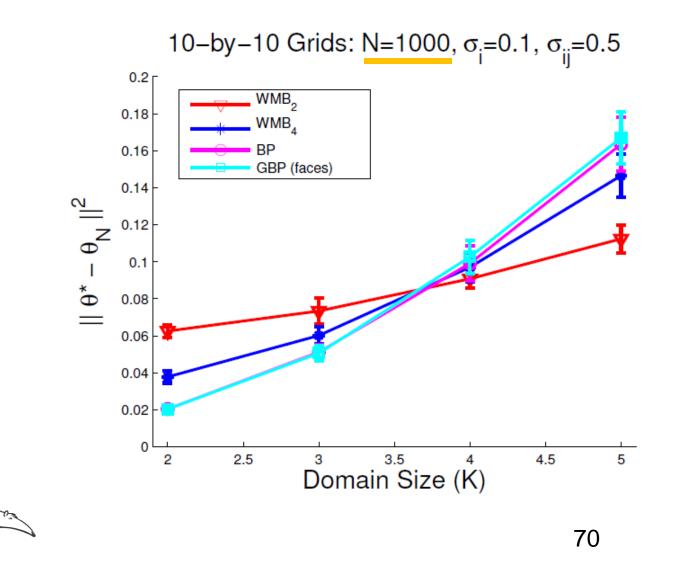


### **Domain Size Experiments**



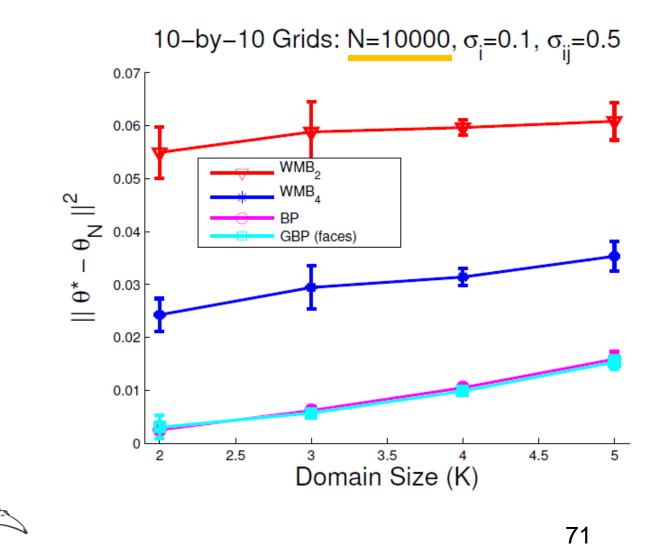


### **Domain Size Experiments**





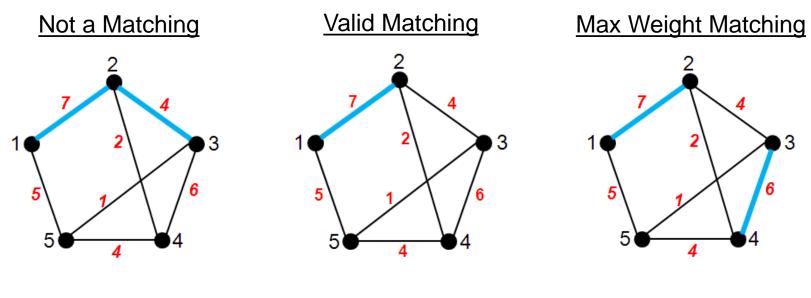
### **Domain Size Experiments**





# Weighted Matching Problem

- Given graph G=(V,E) with edge weights  $\{w_e\}_{e\in E}$ 
  - find a *matching* of total maximum weight
  - Matching: subset of E, such that no 2 edges share a vertex







## Solving Weighted Matching Problems

#### Many efficient algorithms exist

Edmonds	1965	$O( V ^2  E )$
Lawler	1973	<i>O</i> (  <i>V</i>   <sup>3</sup> )
Gabow	1974	<i>O</i> (  <i>V</i>   <sup>3</sup> )
Galil, Micali, Gabow	1986	$O( V  E \log V )$
Gabow	1990	$O( V ( E + V \log V ))$

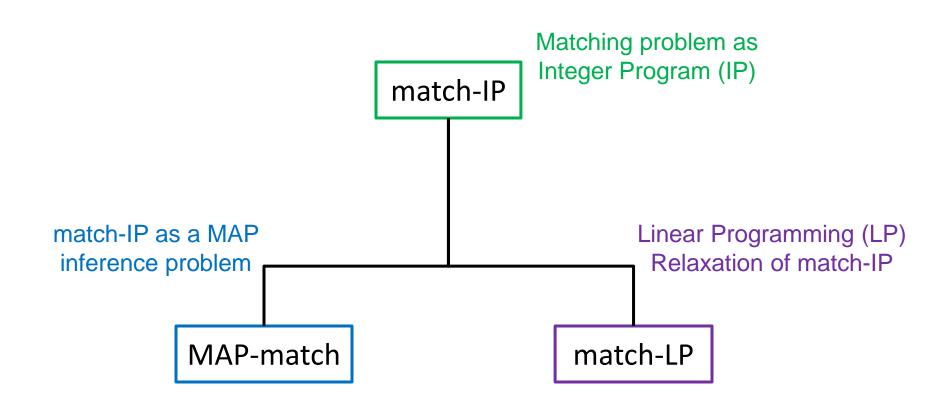
#### Recent results using Belief Propagation

Bayati, Shah, Sharma [bipartite graphs]		<i>O</i> (c   <i>V</i>   <sup>3</sup> )
Sanghavi, Malioutov, Willsky [general graphs]		$O(c \ w^{\max}  V ^3)$





## Solving Weighted Matching Problems

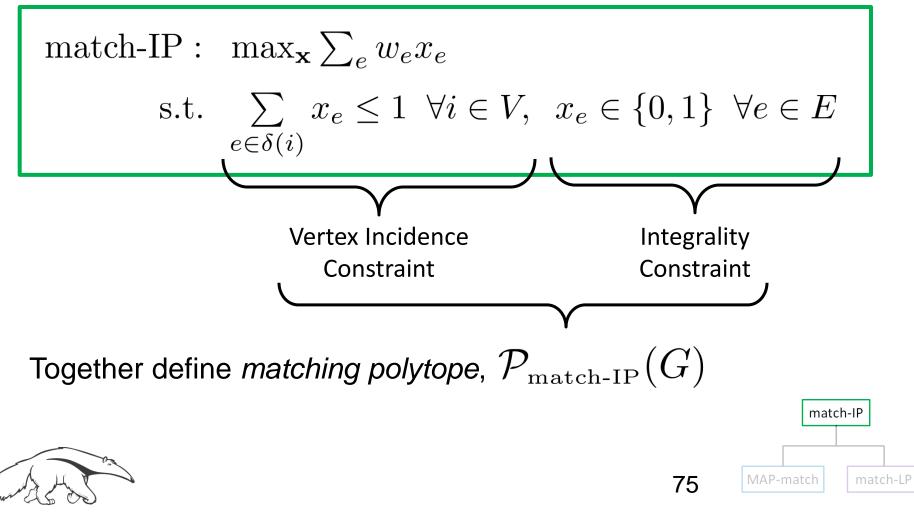






# Matching as an Integer Program (IP)

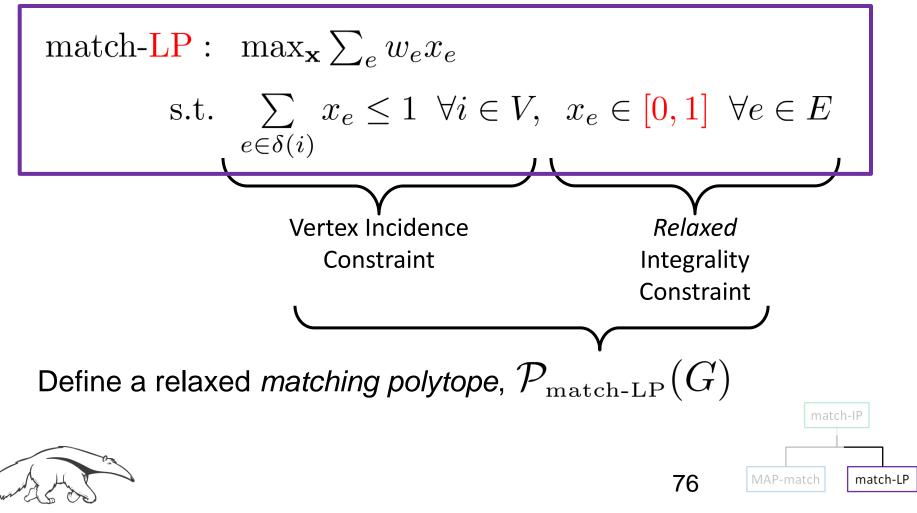
Given graph G=(V,E) with edge weights  $\{w_e\}_{e\in E}$ 





# Linear Programming (LP) Relaxation

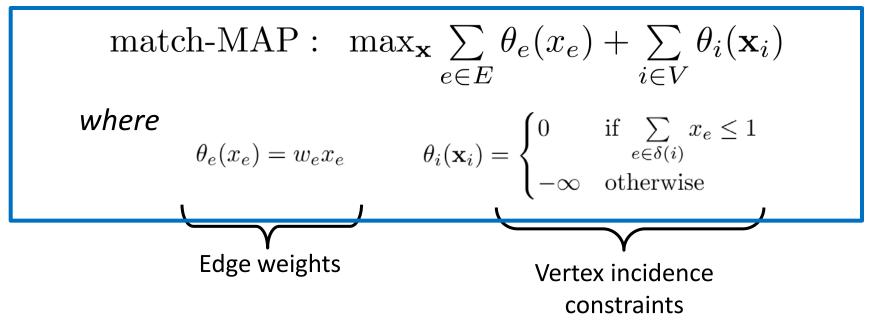
Given graph G=(V,E) with edge weights  $\{w_e\}_{e\in E}$ 

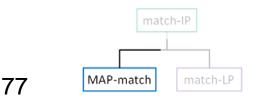




## Matching as MAP Inference

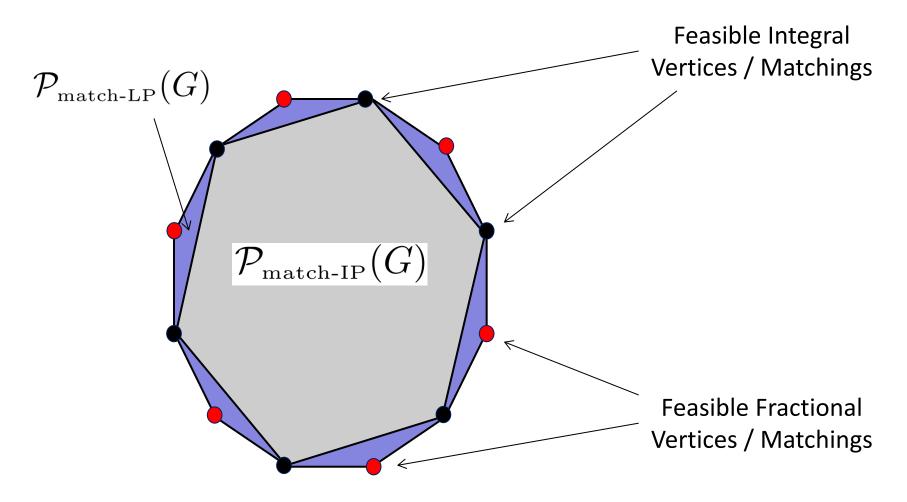
 $\Box$  Associate a variable with each edge  $\mathbf{x} = \{x_e\}_{e \in E}$ 







#### Relationship between polytopes





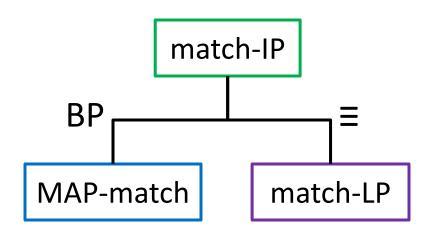


## Relationship between polytopes

 $\mathcal{P}_{\text{match-LP}}(G)$  $\mathcal{P}_{ ext{match-IP}}(G)$ 

If integral solution to match-LP, then max-product BP on MAPmatch is provably exact

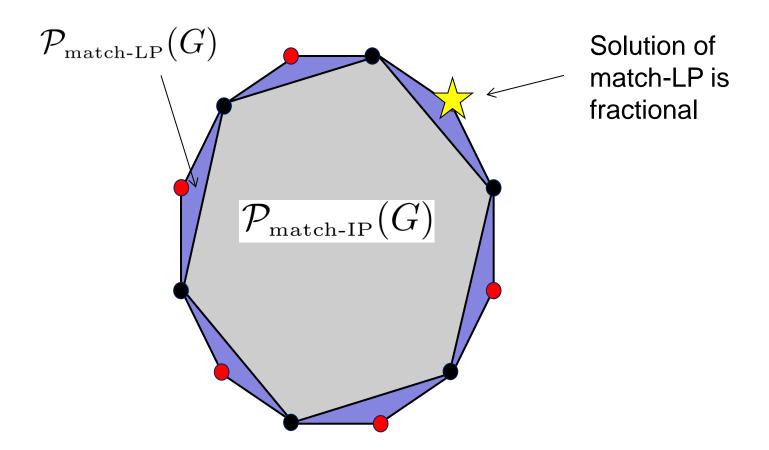
bipartite graphs [Bayati, Shah, Sharma '05] general graphs [Sanghavi, Malioutov, Willsky '07]







#### What if match-LP is loose?

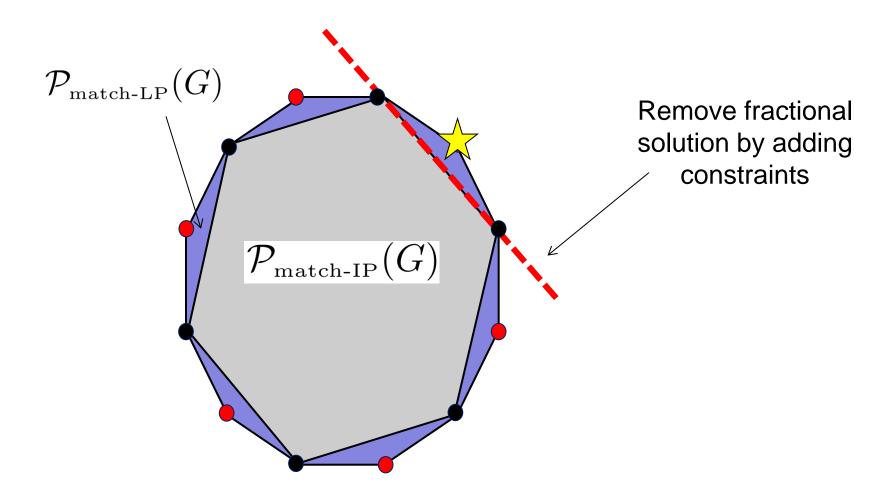








#### What if match-LP is loose?

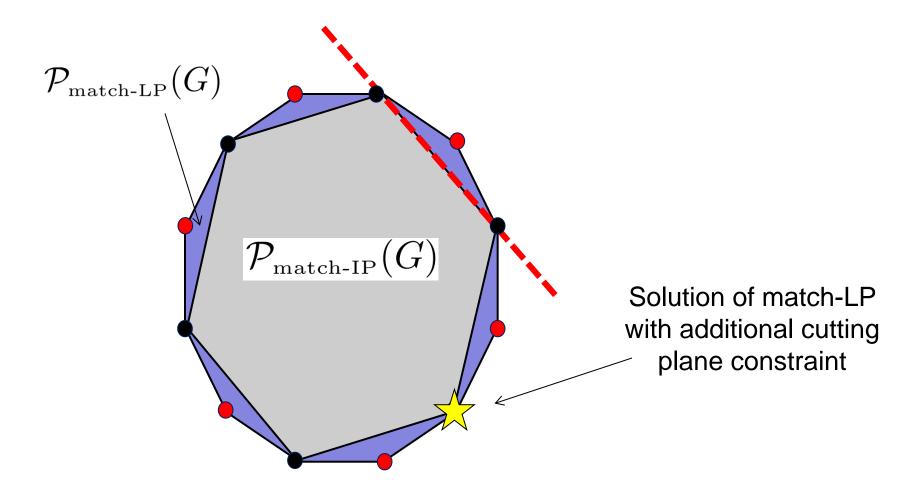








#### What if match-LP is loose?







# Edmonds and Blossom Constraints

□ Matching polytope is also given by [Edmonds 65]:

$$\mathcal{P}_{\text{match-IP}}(G) = \mathcal{P}_{\text{match-blossom-LP}}(G)$$

 $\mathcal{P}_{\text{match-blossom-LP}}(G) = \left\{ \mathbf{x} \in [0,1]^{|E|} \mid \mathbf{x}(\delta(i)) \le 1, \ \forall i \in V, \\ \sum_{e \in E(S)} x_e \le \frac{|S|-1}{2}, \ \forall S \in S \right\}$ 

Edges w/ both ends in S  $E(S) = \{(i, j) \in E \mid i, j \in S\}$  All odd-sized subsets of *V* 



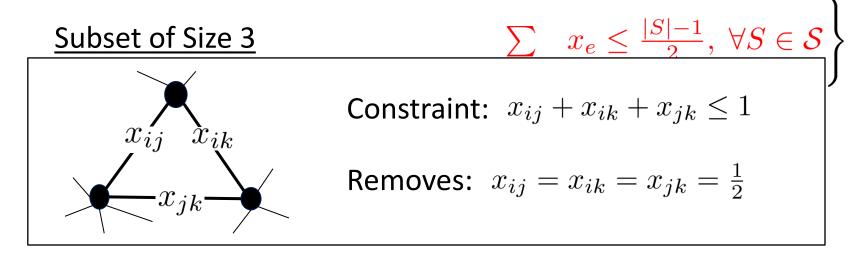


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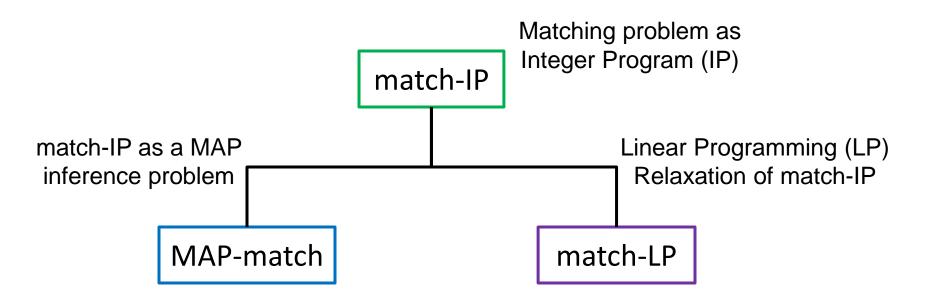
$$\mathcal{P}_{\text{match-blossom-LP}}(G) = \left\{ \mathbf{x} \in [0,1]^{|E|} \mid \mathbf{x}(\delta(i)) \le 1, \forall i \in V, \right\}$$







## Solving Weighted Matching Problems



Bayati, Shah, Sharma [bipartite graphs]	2005	<i>O</i> (c   <i>V</i>   <sup>3</sup> )
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## **Overview of Results**

