MAP Estimation with Perfect Graphs

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In 1960, Claude Berge introduces perfect graphs and two conjectures:

- **Perfect iff every induced subgraph has clique \# = coloring \#**
  - Weak conjecture: G is perfect iff its complement is perfect
  - Strong conjecture: all perfect graphs are Berge graphs

- **Weak perfect graph theorem (Lovász 1972)**
- **Link between perfection and integral LPs (Lovász 1972)**
- **Strong perfect graph theorem (SPGT) open for 4+ decades**
Background on Perfect Graphs

- SPGT Proof (Chudnovsky, Robertson, Seymour, Thomas 2003)
- Berge passes away shortly after hearing of the proof
- Many NP-hard and hard to approximate problems are P for perfect graphs
  - Graph coloring
  - Maximum clique
  - Maximum independent set
- Recognizing perfect graphs is $O(n^9)$ (Chudnovsky et al. 2006)
Perfect graph theory for MAP and graphical models (J 2009)

Graphical model: a graph \( G = (V, E) \) representing a distribution \( p(X) \) where \( X = \{x_1, \ldots, x_n\} \) and \( x_i \in \mathbb{Z} \)

Distribution factorizes over graph cliques

\[
p(x_1, \ldots, x_n) = \frac{1}{Z} \prod_{c \in C} \psi_c(X_c)
\]

E.g. \( p(x_1, \ldots, x_6) = \psi(x_1, x_2)\psi(x_2, x_3)\psi(x_3, x_4, x_5)\psi(x_4, x_5, x_6) \)
Graphical Models

Canonical Problems for Graphical Models

- Given a factorized distribution
  \[ p(x_1, \ldots, x_n) = \frac{1}{Z} \prod_{c \in C} \psi_c(X_c) \]

- Inference: recover various marginals like \( p(x_i) \) or \( p(x_i, x_j) \)
  \[ p(x_i) = \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_n} p(x_1, \ldots, x_n) \]

- Estimation: find most likely configurations \( x_i^* \) or \( (x_1^*, \ldots, x_n^*) \)
  \[ x_i^* = \arg \max_{x_i} \max_{x_1} \cdots \max_{x_{i-1}} \max_{x_{i+1}} \cdots \max_{x_n} p(x_1, \ldots, x_n) \]

- In general both are NP-hard, but for chains and trees just P
Given a chain-factorized distribution

\[ p(x_1, \ldots, x_5) = \frac{1}{Z} \psi(x_1, x_2) \psi(x_2, x_3) \psi(x_3, x_4) \psi(x_4, x_5) \]

Inference: recover various marginals like \( p(x_i) \) or \( p(x_i, x_j) \)

\[ p(x_5) \propto \sum_{x_1} \sum_{x_2} \psi(x_1, x_2) \sum_{x_3} \psi(x_2, x_3) \sum_{x_4} \psi(x_3, x_4) \psi(x_4, x_5) \]

Estimation: find most likely configurations \( x_i^* \) or \( (x_1^*, \ldots, x_n^*) \)

\[ x_5^* = \arg \max_{x_5} \max_{x_1} \max_{x_2} \psi(x_1, x_2) \max_{x_3} \psi(x_2, x_3) \max_{x_4} \psi(x_3, x_4) \psi(x_4, x_5) \]

The work distributes and becomes efficient!
The idea of distributed computation extends nicely to trees.
On trees (which subsume chains) do a collect/distribute step.
Alternatively, can perform distributed updates asynchronously.
Each step is a sum-product or a max-product update.
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Alternatively, can perform distributed updates asynchronously.
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MAP Estimation

Let’s focus on finding most probable configurations efficiently

\[ X^* = \arg \max p(x_1, \ldots, x_n) \]

- Useful for image processing, protein folding, coding, etc.
- Brute force requires \( \prod_{i=1}^{n} |x_i| \)
- Efficient for trees and singly linked graphs (Pearl 1988)
- NP-hard for general graphs (Shimony 1994)

Approach A: relaxations and variational methods
- First order LP relaxations (Wainwright et al. 2002)
- TRW max-product (Kolmogorov & Wainwright 2006)
- Higher order LP relaxations (Sontag et al. 2008)
- Fractional and integral LP rounding (Ravikumar et al. 2008)
- Open problem: when are LPs tight?

Approach B: loopy max product and message passing
Max Product Message Passing

1. For each $x_i$ to each $X_c$:  
   $$m_{i \rightarrow c}^{t+1} = \prod_{d \in \text{Ne}(i) \setminus c} m_{d \rightarrow i}^t$$
2. For each $X_c$ to each $x_i$:  
   $$m_{c \rightarrow i}^{t+1} = \max_{X_c \setminus x_i} \psi_c(X_c) \prod_{j \in c \setminus i} m_{j \rightarrow c}^t$$
3. Set $t = t + 1$ and goto 1 until convergence
4. Output $x_i^* = \arg \max_{x_i} \prod_{d \in \text{Ne}(i)} m_d^{t \rightarrow i}$

- Simple and fast algorithm for MAP
- Exact for trees (Pearl 1988)
- Exact for single-loop graphs (Weiss & Freeman 2001)
- Local optimality guarantees (Wainwright et al. 2003)
- Performs well in practice for images, turbo codes, etc.
- Similar to first order LP relaxation
- Recent progress
  - Exact for matchings (Bayati et al. 2005)
  - Exact for generalized $b$ matchings (Huang and J 2007)
Bipartite Matching

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→ \( C = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \)

- Given \( W \), \( \max_{C \in \mathbb{B}^{n \times n}} \sum_{ij} W_{ij} C_{ij} \) such that \( \sum_i C_{ij} = \sum_j C_{ij} = 1 \)
- Classical Hungarian marriage problem \( O(n^3) \)
- Creates a very loopy graphical model
- Max product takes \( O(n^3) \) for exact MAP (Bayati et al. 2005)
Bipartite Generalized Matching

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\[ C = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \]

- Given \( W \), \( \max_{C \in \mathbb{B}^{n \times n}} \sum_{ij} W_{ij} C_{ij} \) such that \( \sum_i C_{ij} = \sum_j C_{ij} = b \)
- Combinatorial \( b \)-matching problem \( O(bn^3) \), (Google Adwords)
- Creates a very loopy graphical model
- Max product takes \( O(bn^3) \) for exact MAP (Huang & J 2007)
Graph $G = (U, V, E)$ with $U = \{u_1, \ldots, u_n\}$ and $V = \{v_1, \ldots, v_n\}$ and $M(.)$, a set of neighbors of node $u_i$ or $v_j$

Define $x_i \in X$ and $y_i \in Y$ where $x_i = M(u_i)$ and $y_i = M(v_j)$

Then $p(X, Y) = \frac{1}{Z} \prod_i \prod_j \psi(x_i, y_j) \prod_k \phi(x_k) \phi(y_k)$ where

$\phi(y_j) = \exp(\sum_{u_i \in y_j} W_{ij})$ and $\psi(x_i, y_j) = - (v_j \in x_i \oplus u_i \in y_j)$
Bipartite Generalized Matching

**Theorem (Huang & J 2007)**

\[ \text{Max product on } G \text{ converges in } O(bn^3) \text{ time.} \]

**Proof.**

Form unwrapped tree \( T \) of depth \( \Omega(n) \), maximizing belief at root of \( T \) is equivalent to maximizing belief at corresponding node in \( G \).
Bipartite Generalized Matching

Generalized Matching

Applications:
unipartite matching
clustering (J & S 2006)
classification (H & J 2007)
collaborative filtering (H & J 2008)
semisupervised (J et al. 2009)
visualization (S & J 2009)

Max product is $O(n^2)$ on dense graphs (Salez & Shah 2009)
Much faster than other solvers
Above is $k$-nearest neighbors with $k = 2$
Above is unipartite $b$-matching with $b = 2$
Left is $k$-nearest neighbors, right is unipartite $b$-matching.
Unipartite Generalized Matching

\[
\begin{array}{c|cccc}
 & p_1 & p_2 & p_3 & p_4 \\
 p_1 & 0 & 2 & 1 & 2 \\
p_2 & 2 & 0 & 2 & 1 \\
p_3 & 1 & 2 & 0 & 2 \\
p_4 & 2 & 1 & 2 & 0 \\
\end{array}
\rightarrow C = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}
\]

- \[\max_{C \in \mathbb{B}^{n \times n}, C_{ii}=0} \sum_{ij} W_{ij} C_{ij} \text{ such that } \sum_i C_{ij} = b, \ C_{ij} = C_{ji}\]
- Combinatorial unipartite matching is efficient (Edmonds 1965)
- Makes an LP with exponentially many blossom inequalities
- Max product exact if LP is integral (Sanghavi et al. 2008)

\[p(X) = \prod_{i \in V} \delta \left( \sum_{j \in \text{Ne}(i)} x_{ij} \leq 1 \right) \prod_{ij \in E} \exp(W_{ij} x_{ij})\]
Back to Perfect Graphs

- Max product and exact MAP depend on the LP’s integrality
- Matchings have special integral LPs (Edmonds 1965)
- How to generalize beyond matchings?
- Perfect graphs imply LP integrality (Lovász 1972)

**Lemma (Lovász 1972)**

For every non-negative vector \( \vec{f} \in \mathbb{R}^N \), the linear program

\[
\beta = \max_{\vec{x} \in \mathbb{R}^N} \vec{f}^T \vec{x} \quad \text{subject to} \quad \vec{x} \geq 0 \text{ and } A\vec{x} \leq \vec{1}
\]

recovers a vector \( \vec{x} \) which is integral if and only if the (undominated) rows of \( A \) form the vertex versus maximal cliques incidence matrix of some perfect graph.
Lemma (Lovász 1972)

\[ \beta = \max_{\bar{x} \in \mathbb{R}^N} \bar{f}^\top \bar{x} \text{ subject to } \bar{x} \geq 0 \text{ and } A\bar{x} \leq \bar{1} \]

\[ A = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix} \]
Lovász's lemma is not solving $\max p(X)$ on $G$

We have $p(x_1, \ldots, x_n) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \psi_c(X_c)$

How to apply the lemma to any model $G$ and space $X$?

Without loss of generality assume $\psi_c(X_c) \leftarrow \frac{\psi_c(X_c)}{\min_{X_c} \psi_c(X_c)} + \epsilon$

Consider procedure to convert $G$ to $\mathcal{G}$ in NMRF form

NMRF is a nand Markov random field over space $X$

- all variables are binary $X = \{x_1, \ldots, x_N\}$
- all potential functions are pairwise nand gates
  $\psi_{ij}(x_i, x_j) = \Phi(x_i, x_j) = \delta(x_i + x_j \leq 1)$
nand Markov Random Fields

**Figure:** Binary graphical model $G$ (left) and nand MRF $\mathcal{G}$ (right).

**Algorithm:**

1. Initialize $\mathcal{G}$ as the empty graph.
2. For each clique $c$ in graph $G$ do:
   - For each configuration $k \in X_c$ do:
     - Add a corresponding binary node $x_{c,k}$ to $\mathcal{G}$.
     - For each $x_{d,l} \in \mathcal{G}$ which is incompatible with $x_{c,k}$:
       - Connect $x_{c,k}$ and $x_{d,l}$ with an edge.
Obtain the following distribution from $\mathcal{G}$

$$\rho(X) = \prod_{c \in C} \prod_{k} |X_c| e^{f_{c,k} x_{c,k}} \prod_{d \in C} \prod_{l=1}^{X_d} \Phi(x_{c,k}, x_{d,l}) E(x_{c,k}, x_{d,l})$$

where $f_{c,k} = \log \psi_c(k)$.

Cardinality of $\mathcal{G}$ is $|X| = \sum_{c \in C} \left( \prod_{i \in c} |x_i| \right) = N$

If node $x_{c,k} = 1$ then clique $c$ is in configuration $k \in X_c$.

Clearly surjective, more configurations $X$ than $X$.

Nand relationship prevents inconsistent settings $\sum_k x_{c,k} \leq 1$

**Theorem**

*For $f_{c,k} > 0$, MAP estimate $X^*$ of $\rho(X)$ yields $\sum_k x_{c,k}^* = 1$ for all cliques $c \in C$.***
Packing Linear Programs

**Lemma**

The MAP estimate for $\rho(X)$ on $G$ recovers MAP for $p(X)$

- Relaxation of MAP on $\rho(X) \equiv$ set packing linear program
- If graph $G$ is perfect, LP efficiently solves MAP

**Lemma**

For every non-negative vector $\vec{f} \in \mathbb{R}^N$, the linear program

$$\beta = \max_{\vec{x} \in \mathbb{R}^N} \vec{f}^T \vec{x} \text{ subject to } \vec{x} \geq 0 \text{ and } A\vec{x} \leq \vec{1}$$

recovers a vector $\vec{x}$ which is integral if and only if the (undominated) rows of $A$ form the vertex versus maximal cliques incidence matrix of some perfect graph.
For general graph $G$, MAP is NP-hard (Shimony 1994)

- Convert $G$ to $\mathcal{G}$ (polynomial time)
- If graph $\mathcal{G}$ is perfect
  - Find maximal cliques (polynomial time)
  - Solve MAP via packing linear program (polynomial time)

**Theorem**

MAP estimation of any graphical model $G$ with cliques $c \in C$ over variables $\{x_1, \ldots, x_n\}$ producing a nand Markov random with a perfect graph $\mathcal{G}$ is in $P$ and requires no more than

$$O \left( \left( \sum_{c \in C} \left( \prod_{i \in c} |x_i| \right) \right)^3 \right).$$
For general graph $G$, MAP is NP-hard (Shimony 1994)

- Convert $G$ to $\mathcal{G}$ (polynomial time)
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For general graph $G$, MAP is NP-hard (Shimony 1994)

- Convert $G$ to $\mathcal{G}$ (polynomial time)
- If graph $\mathcal{G}$ is perfect (polynomial time!!)
  - Find maximal cliques (polynomial time)
  - Solve MAP via packing linear program (polynomial time)

**Theorem**

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$$O \left( \left( \sum_{c \in \mathcal{C}} \left( \prod_{i \in c} |x_i| \right) \right)^3 \right).$$
Perfect Graphs

- To determine if $G$ is perfect
  - Run algorithm on $G$ in $O(N^9)$ (Chudnovsky et al. 2005)
  - or use tools from perfect graph theory to prove perfection
- Clique number of a graph $\omega(G)$: size of its maximum clique
- Chromatic number of a graph $\chi(G)$: minimum number of colors such that no two adjacent vertices have the same color
- A perfect graph $G$ is a graph where every induced subgraph $\mathcal{H} \subseteq G$ has $\omega(\mathcal{H}) = \chi(\mathcal{H})$
Recognizing Perfect Graphs

**Strong Perfect Graph Theorem**

- A graph is perfect iff it is Berge (Chudnovsky et al. 2003)
- Berge graph: a graph that contains no odd hole and whose complement also contains no odd hole
- Hole: an induced subgraph of \( G \) which is a chordless cycle of length at least 5. An odd hole has odd cycle length.
- Complement: a graph \( \overline{G} \) with the same vertex set \( V(G) \) as \( G \), where distinct vertices \( u, v \in V(G) \) are adjacent in \( \overline{G} \) just when they are not adjacent in \( G \)
Recognizing Perfect Graphs

Recognition using Perfect Graphs Algorithm

- Could use slow $O(N^9)$ algorithm (Chudnovsky et al. 2005)
- Runs on $\mathcal{G}$ and then on complement $\overline{\mathcal{G}}$
  - Detect if the graph contains a pyramid structure by computing shortest paths between all nonuples of vertices. This is $O(N^9)$
  - Detect if the graph contains a jewel structure or other easily-detectable configuration
  - Perform a cleaning procedure. A vertex in the graph is $C$-major if its set of neighbors in $C$ is not a subset of the vertex set of any 3-vertex path of $C$. $C$ is clean if there are no $C$-major vertices in the graph
  - Search for the shortest odd hole in the graph by computing the shortest paths between all triples of vertices
- Faster methods find all holes (Nikolopolous & Palios 2004)
- Less conclusive than Chudnovsky but can run on $N \geq 300$
Recognizing Perfect Graphs

Recognition using Strong Perfect Graph Theorem

- SPGT implies that a Berge graph is one of these primitives
  - bipartite graphs
  - complements of bipartite graphs
  - line graphs of bipartite graphs
  - complements of line graphs of bipartite graphs
  - double split graphs
- or decomposes structurally (into graph primitives)
  - via a 2-join
  - via a 2-join in the complement
  - via an M-join
  - via a balanced skew partition
- Line graph: $L(G)$ a graph which contains a vertex for each edge of $G$ and where two vertices of $L(G)$ are adjacent iff they correspond to two edges of $G$ with a common end vertex
Recognizing Perfect Graphs

Recognition using Strong Perfect Graph Theorem

- SPGT and theory give tools to analyze graph
- Decompose using replication, 2-join, $M$-joins, skew partition...
- May help diagnose perfection when algorithm is too slow

**Lemma (Replication, Lovász 1972)**

Let $G$ be a perfect graph and let $v \in V(G)$. Define a graph $G'$ by adding a new vertex $v'$ and joining it to $v$ and all the neighbors of $v$. Then $G'$ is perfect.
Recognizing Perfect Graphs

Recognition using Strong Perfect Graph Theorem

- SPGT and theory give tools to analyze graph
- Decompose using replication, 2-join, $M$-joins, skew partition...
- May help diagnose perfection when algorithm is too slow

**Lemma (Gluing on Cliques, Skew Partition, Berge & Chvátal 1984)**

Let $G$ be a perfect graph and let $G'$ be a perfect graph. If $G \cap G'$ is a clique (clique cutset), then $G \cup G'$ is a perfect graph.
### Proving Exact MAP for Tree Graphs

**Theorem (J 2009)**

*Let $G$ be a tree, the NMRF $G'$ obtained from $G$ is a perfect graph.*

**Proof.**

First prove perfection for a star graph with internal node $v$ with $|v|$ configurations. First obtain $G$ for the star graph by only creating one configuration for non internal nodes. The resulting graph is a complete $|v|$-partite graph which is perfect. Introduce additional configurations for non-internal nodes one at a time using the replication lemma. The resulting $G'_{star}$ is perfect. Obtain a tree by induction. Add two stars $G'_{star}$ and $G'_{star'}$. The intersection is a fully connected clique (clique cutset) so by (Berge & Chvátal 1984), the resulting graph is perfect. Continue gluing stars until full tree $G$ is formed.
Theorem (J 2009)

The maximum weight bipartite matching graphical model

\[ p(X) = \prod_{i=1}^{n} \delta \left( \sum_{j=1}^{n} x_{ij} \leq 1 \right) \delta \left( \sum_{j=1}^{n} x_{ji} \leq 1 \right) \prod_{k=1}^{n} e^{f_{ik}x_{ik}} \]

with \( f_{ij} \geq 0 \) has integral LP and yields exact MAP estimates.

Proof.

The graphical model is in NMRF form so \( G \) and \( \mathcal{G} \) are equivalent. \( \mathcal{G} \) is the line graph of a (complete) bipartite graph (Rook’s graph). Therefore, \( \mathcal{G} \) is perfect, the LP is integral and recovers MAP.
The unipartite matching graphical model $G = (V, E)$ with $f_{ij} \geq 0$

$$p(X) = \prod_{i \in V} \delta \left( \sum_{j \in Ne(i)} x_{ij} \leq 1 \right) \prod_{ij \in E} e^{f_{ij}x_{ij}}$$

has integral LP and produces the exact MAP estimate if $G$ is a perfect graph.

Proof.

The graphical model is in NMRF form and graphs $G$ and $\mathcal{G}$ are equivalent. The set packing LP relaxation is integral and recovers the MAP estimate if $G$ is a perfect graph.
Possible to prune $G$ in search of perfection and efficiency

- **Two optional procedures:** **Disconnect** and **Merge**
  
  **Disconnect:** For each $c \in C$, denote the minimal configurations of $c$ as the set of nodes $\{x_{c,k}\}$ such that $f_{c,k} = \min_{\kappa} f_{c,\kappa} = \log(1 + \epsilon)$. **Disconnect** removes the edges between these nodes and all other nodes in the clique $X_c$.
  
  **Merge:** For any pair of unconnected nodes $x_{c,k}$ and $x_{d,l}$ in $G$ where $\text{Ne}(x_{c,k}) = \text{Ne}(x_{d,l})$, combine them into a single equivalent variable $x_{c,k}$ with the same connectivity and updates its corresponding weight as $f_{c,k} \leftarrow f_{c,k} + f_{d,l}$.
  
- Easy to get MAP for $G$ from $\text{Merge}(\text{Disconnect}(G))$
Convergent Message Passing

Instead of LP solver, use convergent message passing (Globerson & Jaakkola 2007) get faster solution

Input: Graph $G = (\mathcal{V}, \mathcal{E})$ and $\theta_{ij}$ for $ij \in \mathcal{E}$.
1. Initialize all messages to any value.
2. For each $ij \in \mathcal{E}$, simultaneously update
   \[
   \lambda_{ji}(x_i) \leftarrow -\frac{1}{2} \sum_{k \in \text{Ne}(i) \setminus j} \lambda_{ki}(x_i) + \frac{1}{2} \max_{x_j} \left[ \sum_{k \in \text{Ne}(j) \setminus i} \lambda_{kj}(x_j) + \theta_{ij}(x_i, x_j) \right]
   \]
   \[
   \lambda_{ij}(x_j) \leftarrow -\frac{1}{2} \sum_{k \in \text{Ne}(j) \setminus i} \lambda_{kj}(x_j) + \frac{1}{2} \max_{x_i} \left[ \sum_{k \in \text{Ne}(i) \setminus j} \lambda_{ki}(x_i) + \theta_{ij}(x_i, x_j) \right]
   \]
3. Repeat 2 until convergence.
4. Find $b(x_i) = \sum_{j \in \text{Ne}(i)} \lambda_{ji}(x_i)$ for all $i \in \mathcal{V}$.
5. Output $\hat{x}_i = \arg \max_{x_i} b(x_i)$ for all $i \in \mathcal{V}$. 
Theorem (Globerson & Jaakkola 2007)

*With binary variables* $x_i$, *fixed points of convergent message passing* recover the optimum of the LP.

**Corollary**

*Convergent message passing on an NMRF with a perfect graph finds the MAP estimate.*
MAP Experiments

- Investigate LP and message passing for unipartite matching
- Exact MAP estimate possible via Edmonds’ blossom algorithm
- Consider graphical model $G = (V, E)$ with $f_{ij} \geq 0$

$$p(X) = \prod_{i \in V} \delta \left( \sum_{j \in \text{Ne}(i)} x_{ij} \leq 1 \right) \prod_{ij \in E} e^{f_{ij}x_{ij}}$$

- Compare solution found by message passing on the NMRF
- Try various topologies for graph $G$, perfect or otherwise
Figure: Scores for the exact MAP estimate (horizontal axis) and message passing estimate (vertical axis) for random graphs and weights. Figure (a) shows scores for four types of basic Berge graphs while (b) shows scores for arbitrary graphs. Minor score discrepancies on Berge graphs arose due to numerical issues and early stopping.
Conclusions

- Perfect graph theory is fascinating
- It is a crucial tool for exploring LP integrality
- Many recent theoretical and algorithmic breakthroughs
- Integrality of LP is also crucial for exact MAP estimation
- MAP for any graphical model is exact if $G$ is perfect
- Efficient tests for perfection, maximum clique and LP
- Can use max product or message passing instead of LP
- Perfect graphs extend previous results on MAP for
  - Trees and singly-linked graphs
  - Single loop graphs
  - Matchings
  - Generalized matchings


Thanks to Maria Chudnovsky, Delbert Dueck and Bert Huang.