Graphical models and variational methods: Message-passing, convex relaxations, and all that

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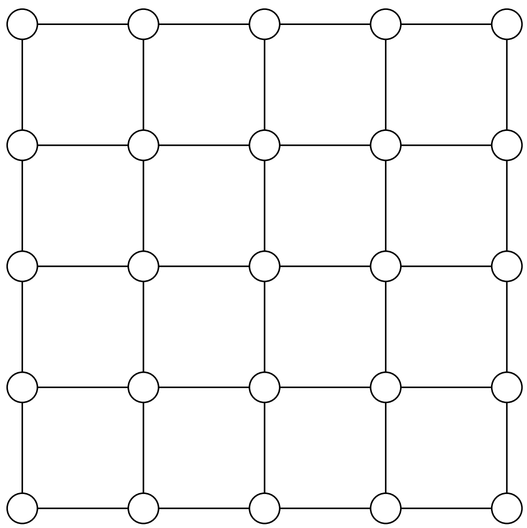
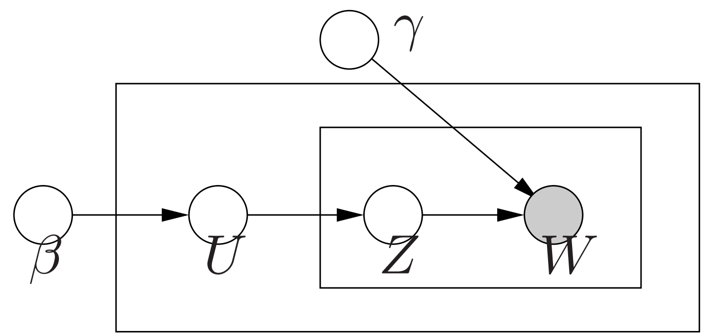
Introduction

- graphical model:
  - $*$ graph $G = (V, E)$ with N vertices
  - $*$ random vector: $(X_1, X_2, \ldots, X_N)$

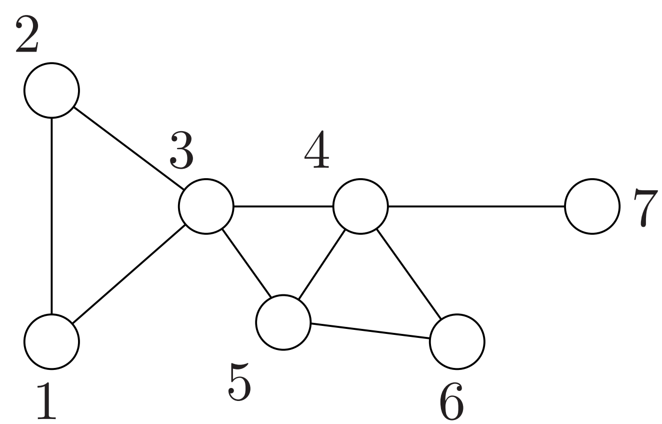




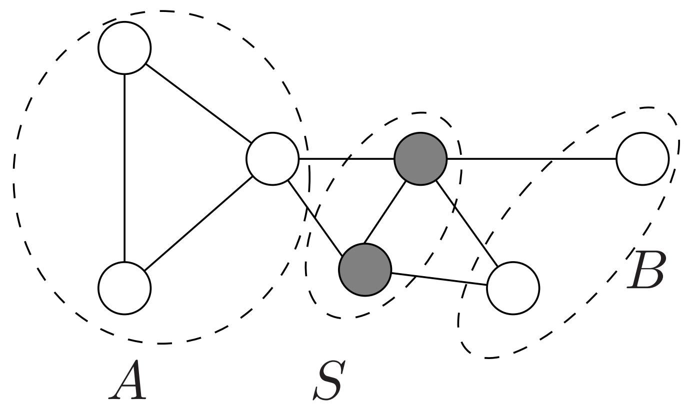
- useful in many statistical and computational fields:
  - machine learning, artificial intelligence
  - computational biology, bioinformatics
  - statistical signal/image processing, spatial statistics
  - statistical physics
  - communication and information theory

Graphs and random variables

- associate to each node $s \in V$ a random variable X_s
- for each subset $A \subseteq V$, random vector $X_A := \{X_s, s \in A\}$.



Maximal cliques $(123), (345), (456), (47)$



Vertex cutset S

- a *clique* $C \subseteq V$ is a subset of vertices all joined by edges
- a *vertex cutset* is a subset $S \subset V$ whose removal breaks the graph into two or more pieces

Factorization and Markov properties

The graph G can be used to impose constraints on the random vector $X = X_V$ (or on the distribution p) in different ways.

Markov property: X is *Markov w.r.t G* if X_A and X_B are conditionally indpt. given X_S whenever S separates A and B.

Factorization: The distribution p *factorizes according to G* if it can be expressed as a product over cliques:

$$p(\mathbf{x}) \quad = \quad \underbrace{\frac{1}{Z}}_{\text{Normalization}} \quad \prod_{C \in \mathcal{C}} \underbrace{\exp\left\{\theta_C(x_C)\right\}}_{\text{compatibility function on clique } C}$$

Hammersley-Clifford: For strictly positive $p(\cdot)$, the Markov property and the Factorization property are equivalent.

Core computational challenges

Given an undirected graphical model (Markov random field):

$$p(\mathbf{x}) \quad = \quad \frac{1}{Z} \quad \prod_{C \in \mathcal{C}} \exp\{\theta_C(x_C)\}$$

How to efficiently compute?

- the data likelihood or normalization constant

  Summation/integration $$Z \;=\; \sum_{x \in \mathcal{X}^N} \prod_{C \in \mathcal{C}} \exp\{\theta_C(x_C)\}$$

- marginal distributions at single sites, or subsets:

  Summation/integration $$p(X_s = x_s) = \sum_{x_t,\, t \neq s} \prod_{C \in \mathcal{C}} \exp\{\theta_C(x_C)\}.$$

- most probable configuration (MAP estimate):

  Maximization $$\widehat{\mathbf{x}} = \arg\max_{\mathbf{x} \in \mathcal{X}^N} p(\mathbf{x}) \;=\; \arg\max_{\mathbf{x} \in \mathcal{X}^N} \prod_{C \in \mathcal{C}} \exp\{\theta_C(x_C)\}.$$

Variational methods

- *"variational":* umbrella term for optimization-based formulations
- many modern algorithms are variational in nature:
  - dynamic programming, finite-element methods
  - max-product message-passing
  - sum-product message-passing: generalized belief propagation, convexified belief propagation, expectation-propagation
  - mean field algorithms

Classical example: Courant-Fischer for eigenvalues:

$$\lambda_{\max}(Q) = \max_{\|x\|_2=1} x^T Qx$$

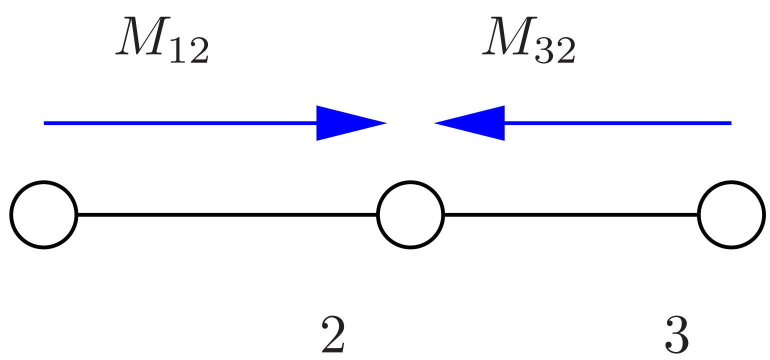
Variational principle: Representation of intersting quantity $\mathbf{u}^\star$ as the solution of an optimization problem.

1. $\mathbf{u}^\star$ can be analyzed/bounded through "lens" of the optimization
2. approximate $\mathbf{u}^\star$ by relaxing the variational principle

§1. Convex relaxations and message-passing for MAP

Goal: Compute most probable configuration (MAP estimate) on a tree:

$$\widehat{\mathbf{x}} \;=\; \arg\max_{\mathbf{x}\in\mathcal{X}^N} \left\{ \prod_{s\in V} \exp(\theta_s(x_s)) \prod_{(s,t)\in E} \exp(\theta_{st}(x_s, x_t)) \right\}.$$

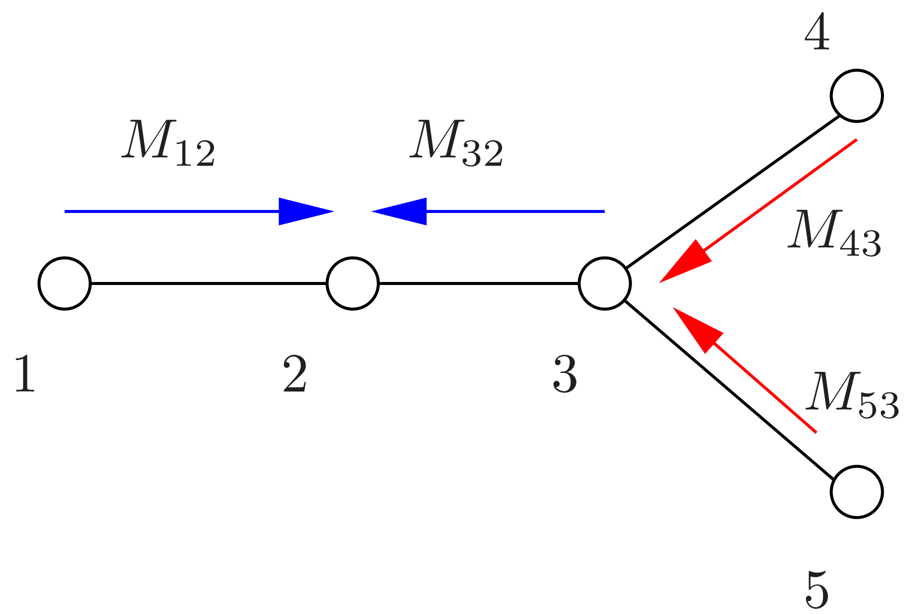


$$\max_{x_1,x_2,x_3} p(\mathbf{x}) \;=\; \max_{x_2} \left[\exp(\theta_1(x_1)) \prod_{t\in 1,3} \left\{ \max_{x_t} \exp[\theta_t(x_t) + \theta_{2t}(x_2, x_t)] \right\} \right]$$

Max-product strategy: "Divide and conquer": break global maximization into simpler sub-problems. (Lauritzen & Spiegelhalter, 1988)

Max-product on trees

Decompose: $\max_{x_1,x_2,x_3,x_4,x_5} p(\mathbf{x}) \;=\; \max_{x_2} \Big[\exp(\theta_1(x_1)) \prod_{t \in N(2)} M_{t2}(x_2)\Big].$



Update messages:

$$M_{32}(x_2) \;=\; \max_{x_3} \left[\exp(\theta_3(x_3) + \theta_{23}(x_2, x_3)) \prod_{v \in N(3) \backslash 2} M_{v3}(x_3)\right]$$

Variational view: Max-product and linear programming

- MAP as integer program: $f^* = \max_{\mathbf{x} \in \mathcal{X}^N} \Big\{ \sum_{s \in V} \theta_s(x_s) + \sum_{(s,t) \in E} \theta_{st}(x_s, x_t) \Big\}$

- define local marginal distributions (e.g., for $m = 3$ states):

$$\mu_s(x_s) \;=\; \begin{bmatrix} \mu_s(0) \\ \mu_s(1) \\ \mu_s(2) \end{bmatrix} \qquad \mu_{st}(x_s, x_t) \;=\; \begin{bmatrix} \mu_{st}(0,0) & \mu_{st}(0,1) & \mu_{st}(0,2) \\ \mu_{st}(1,0) & \mu_{st}(1,1) & \mu_{st}(1,2) \\ \mu_{st}(2,0) & \mu_{st}(2,1) & \mu_{st}(2,2) \end{bmatrix}$$

- alternative formulation of MAP as linear program?

$$g^* \;=\; \max_{(\mu_s, \mu_{st}) \in \mathbb{M}(G)} \Big\{ \sum_{s \in V} \mathbb{E}_{\mu_s}[\theta_s(x_s)] \;+\; \sum_{(s,t) \in E} \mathbb{E}_{\mu_{st}}[\theta_{st}(x_s, x_t)] \Big\}$$

Local expectations: $\qquad \mathbb{E}_{\mu_s}[\theta_s(x_s)] \;:=\; \sum_{x_s} \mu_s(x_s) \theta_s(x_s).$

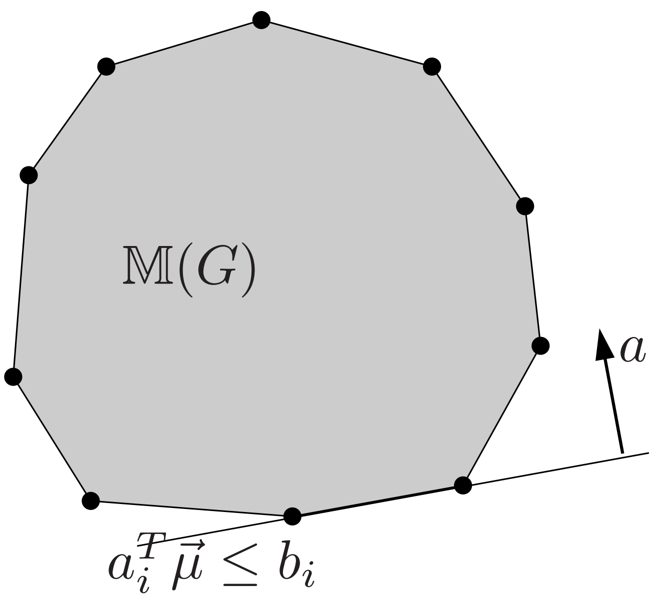
Key question: What constraints must local marginals $\{\mu_s, \mu_{st}\}$ satisfy?

Marginal polytopes for general undirected models

- $\mathbb{M}(G) \equiv$ set of all *globally realizable* marginals $\{\mu_s, \mu_{st}\}$:

$$\left\{ \vec{\mu} \in \mathbb{R}^d \;\Big|\; \mu_s(x_s) \;=\; \sum_{x_t,\, t \neq s} p_\mu(\mathbf{x}), \text{ and } \mu_{st}(x_s, x_t) \;=\; \sum_{x_u,\, u \neq s,t} p_\mu(\mathbf{x}) \right\}$$

for some $p_\mu(\cdot)$ over $(X_1, \ldots, X_N) \in \{0, 1, \ldots, m-1\}^N$.



- polytope in $d = m|V| + m^2|E|$ dimensions (m per vertex, m^2 per edge)
- with m^N vertices
- number of facets?

Marginal polytope for trees

- $\mathbb{M}(T) \equiv$ special case of marginal polytope for tree T
- local marginal distributions on nodes/edges (e.g., $m = 3$)

$$\mu_s(x_s) \;=\; \begin{bmatrix} \mu_s(0) \\ \mu_s(1) \\ \mu_s(2) \end{bmatrix} \qquad \mu_{st}(x_s, x_t) \;=\; \begin{bmatrix} \mu_{st}(0,0) & \mu_{st}(0,1) & \mu_{st}(0,2) \\ \mu_{st}(1,0) & \mu_{st}(1,1) & \mu_{st}(1,2) \\ \mu_{st}(2,0) & \mu_{st}(2,1) & \mu_{st}(2,2) \end{bmatrix}$$

Deep fact about tree-structured models: If $\{\mu_s, \mu_{st}\}$ are non-negative and *locally consistent*:

$$\textbf{Normalization}: \qquad \sum_{x_s} \mu_s(x_s) \;=\; 1$$

$$\textbf{Marginalization}: \qquad \sum_{x'_t} \mu_{st}(x_s, x'_t) \;=\; \mu_s(x_s),$$

then on any tree-structured graph T, they are *globally consistent*.

Follows from junction tree theorem (Lauritzen & Spiegelhalter, 1988).

Max-product on trees: Linear program solver

- MAP problem as a simple linear program:

$$f(\widehat{\mathbf{x}}) \quad = \quad \arg \max_{\vec{\mu} \in \mathbb{M}(T)} \left\{ \sum_{s \in V} \mathbb{E}_{\mu_s}[\theta_s(x_s)] + \sum_{(s,t) \in E} \mathbb{E}_{\mu_{st}}[\theta_{st}(x_s, x_t)] \right\}$$

subject to $\vec{\mu}$ in tree marginal polytope:

$$\mathbb{M}(T) \;=\; \left\{ \vec{\mu} \geq 0, \quad \sum_{x_s} \mu_s(x_s) \;=\; 1, \qquad \sum_{x'_t} \mu_{st}(x_s, x'_t) \;=\; \mu_s(x_s) \right\}.$$

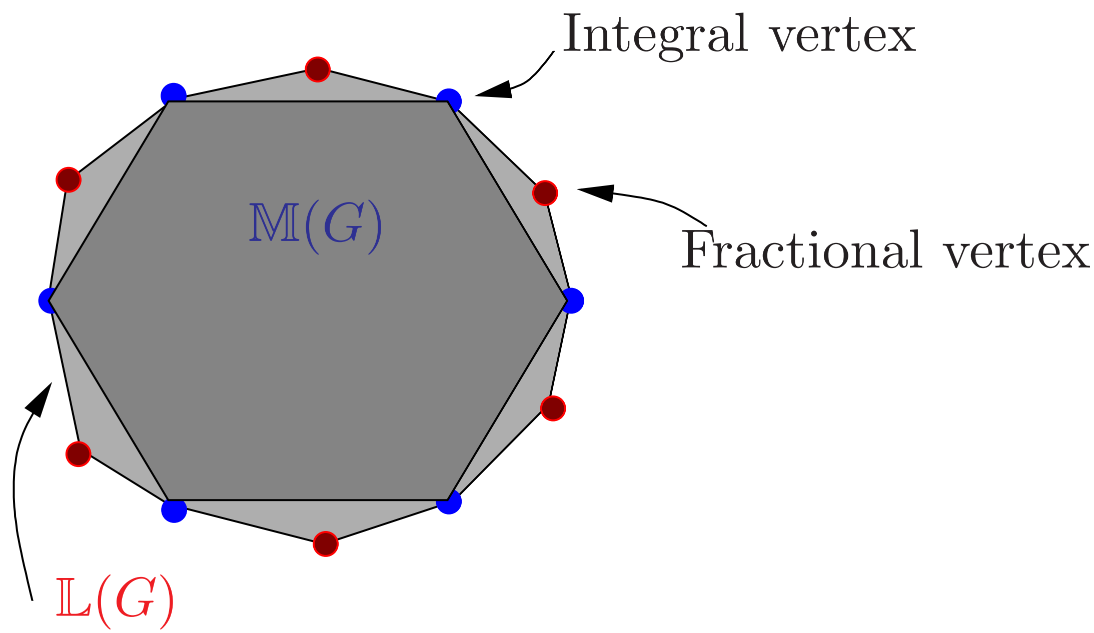
Max-product and LP solving:

- on tree-structured graphs, max-product is a dual algorithm for solving the tree LP. (Wai. & Jordan, 2003)
- max-product message $M_{ts}(x_s) \equiv$ Lagrange multiplier for enforcing the constraint $\sum_{x'_t} \mu_{st}(x_s, x'_t) \;=\; \mu_s(x_s)$.

Tree-based relaxation for graphs with cycles

Set of *locally consistent pseudomarginals* for general graph G:

$$\mathbb{L}(G) = \left\{ \vec{\tau} \in \mathbb{R}^d \mid \vec{\tau} \geq 0, \; \sum_{x_s} \tau_s(x_s) = 1, \quad \sum_{x_t} \tau_{st}(x_s, x'_t) = \tau_s(x_s) \right\}.$$



Key: For a general graph, $\mathbb{L}(G)$ is an outer bound on $\mathbb{M}(G)$, and yields a *linear-programming relaxation* of the MAP problem:

$$f(\widehat{\mathbf{x}}) = \max_{\vec{\mu} \in \mathbb{M}(G)} \theta^T \vec{\mu} \leq \max_{\vec{\tau} \in \mathbb{L}(G)} \theta^T \vec{\tau}.$$

Max-product and graphs with cycles

Early and on-going work:

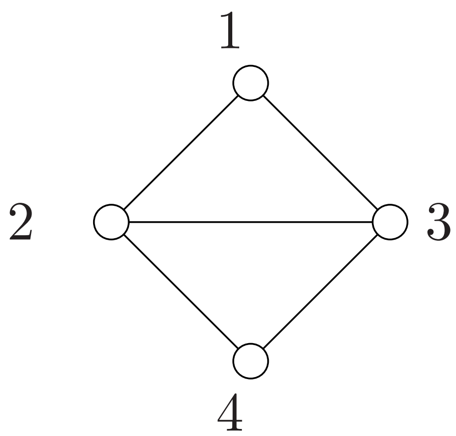
- single-cycle graphs and Gaussian models
  (Aji & McEliece, 1998; Horn, 1999; Weiss, 1998, Weiss & Freeman, 2001)
- local optimality guarantees:
  - "tree-plus-loop" neighborhoods (Weiss & Freeman, 2001)
  - optimality on more general sub-graphs (Wainwright et al., 2003)
- exactness for matching problems (Bayati et al., 2005, 2008, Jebara & Huang, 2007, Sanghavi, 2008)

A natural "variational" conjecture:

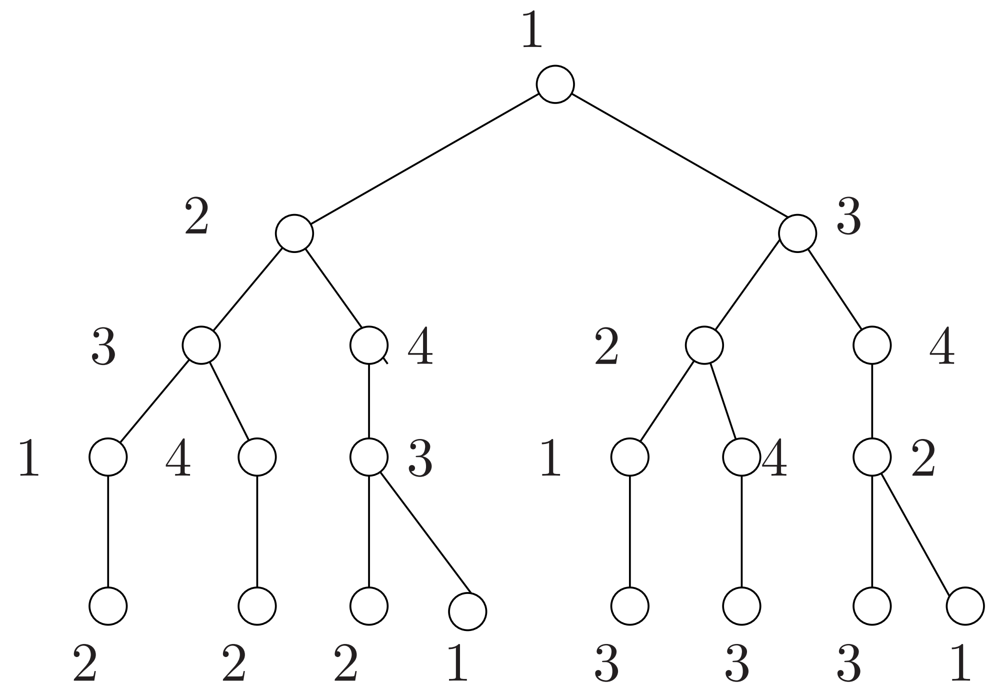
- max-product on trees is a method for solving a linear program
- is max-product solving the first-order LP relaxation on graphs with cycles?

Standard analysis via computation tree

- standard tool: computation tree of message-passing updates
  (Gallager, 1963; Weiss, 2001; Richardson & Urbanke, 2001)



(a) Original graph



(b) Computation tree (4 iterations)

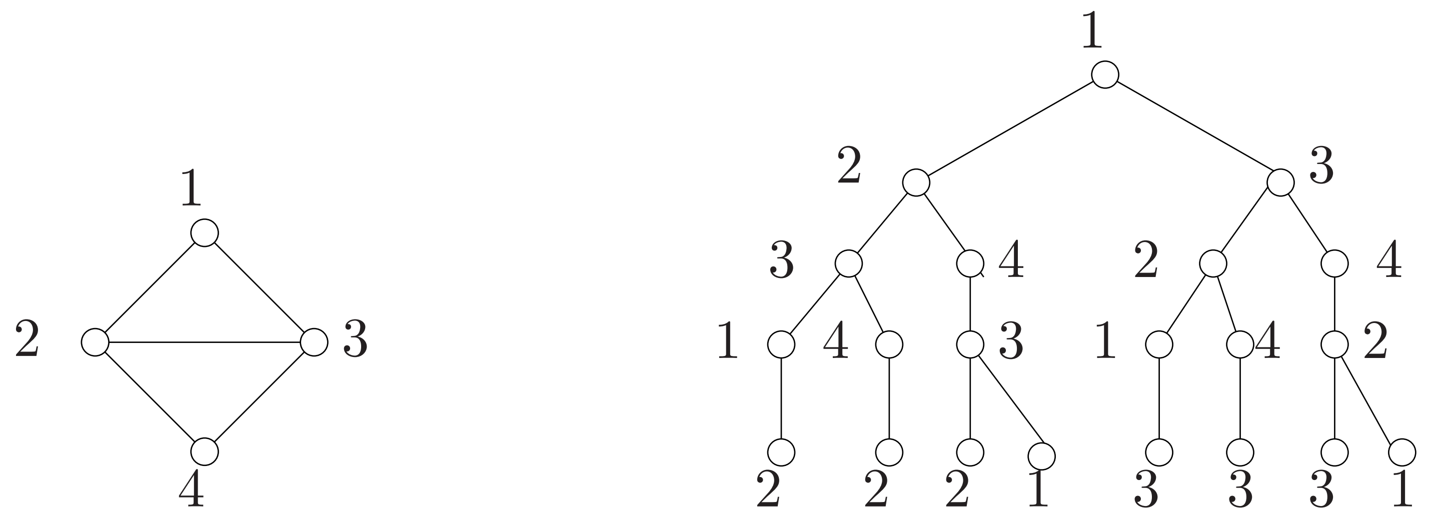
- level t of tree: all nodes whose messages reach the root (node 1) after t iterations of message-passing

Example: Standard max-product does not solve LP

(Wainwright et al., 2005)

Intuition:

- max-product solves (exactly) a modified problem on computation tree
- nodes *not equally weighted* in computation tree $\Rightarrow$ max-product can output an incorrect configuration

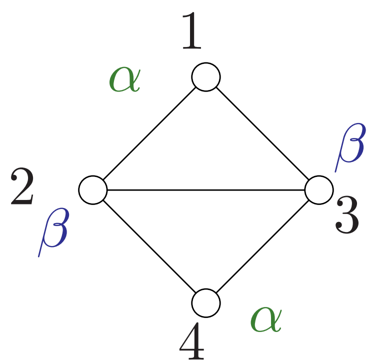


(a) Diamond graph G_{dia} (b) Computation tree (4 iterations)

- for example: asymptotic node fractions ω in this computation tree:

$$\begin{bmatrix}\omega(1) & \omega(2) & \omega(3) & \omega(4)\end{bmatrix} = \begin{bmatrix}0.2393 & 0.2607 & 0.2607 & 0.2393\end{bmatrix}$$

A whole family of non-exact examples



$$\theta_s(x_s) \quad \begin{cases} \alpha x_s & \text{if } s = 1 \text{ or } s = 4 \\ \beta x_s & \text{if } s = 2 \text{ or } s = 3 \end{cases}$$

$$\theta_{st}(x_s, x_t) \quad = \quad \begin{cases} -\gamma & \text{if } x_s \neq x_t \\ 0 & \text{otherwise} \end{cases}$$

- for γ sufficiently large, optimal solution is always either $1^4 = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}$ or $(-1)^4 = \begin{bmatrix} (-1) & (-1) & (-1) & (-1) \end{bmatrix}$
- first-order LP relaxation always exact for this problem
- max-product and LP relaxation give *different* decision boundaries:

<u>Optimal/LP boundary:</u> $\quad \widehat{\mathbf{x}} = \begin{cases} 1^4 & \text{if } 0.25\alpha + 0.25\beta \geq 0 \\ (-1)^4 & \text{otherwise} \end{cases}$

<u>Max-product boundary:</u> $\quad \widehat{\mathbf{x}} = \begin{cases} 1^4 & \text{if } 0.2393\alpha + 0.2607\beta \geq 0 \\ (-1)^4 & \text{otherwise} \end{cases}$

Tree-reweighted max-product algorithm

(Wainwright, Jaakkola & Willsky, 2002)

Message update from node t to node s:

$$M_{ts}(x_s) \quad \leftarrow \quad \kappa \max_{x'_t \in \mathcal{X}_t} \Bigg\{ \exp\Big[\underbrace{\frac{\theta_{st}(x_s, x'_t)}{\rho_{st}}}_{\text{reweighted edge}} + \theta_t(x'_t) \Big] \frac{\prod_{v \in \Gamma(t) \backslash s} \overbrace{\big[M_{vt}(x_t)\big]^{\rho_{vt}}}^{\text{reweighted messages}}}{\underbrace{\big[M_{st}(x_t)\big]^{(1-\rho_{ts})}}_{\text{opposite message}}} \Bigg\}.$$

Properties:

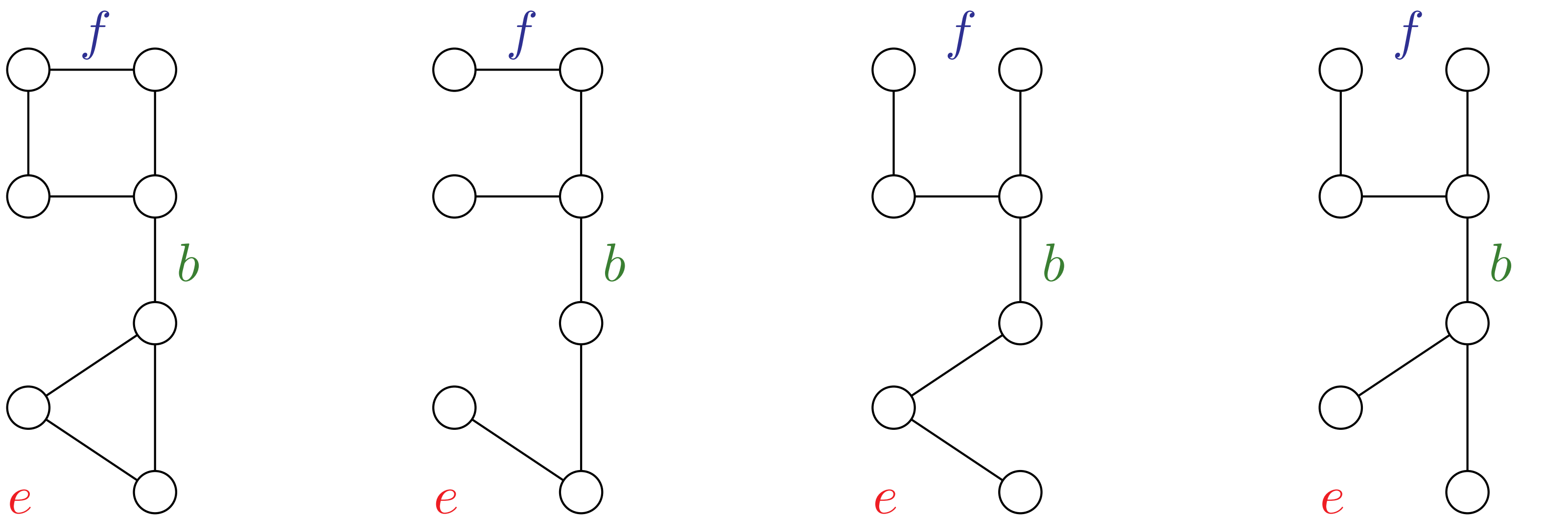
1. Modified updates remain *distributed* and *purely local* over the graph.

2. Key differences:
   - Messages are reweighted with $\rho_{st} \in [0, 1]$.
   - Potential on edge (s, t) is rescaled by $\rho_{st} \in [0, 1]$.
   - Update involves the reverse direction edge.

3. The choice $\rho_{st} = 1$ for all edges (s, t) recovers standard update.

Edge appearance probabilities

Experiment: What is the probability ρ_e that a given edge $e \in E$ belongs to a tree T drawn randomly under $\boldsymbol{\rho}$?



(a) Original (b) $\rho(T^1) = \frac{1}{3}$ (c) $\rho(T^2) = \frac{1}{3}$ (d) $\rho(T^3) = \frac{1}{3}$

In this example: $\rho_b = 1$; $\rho_e = \frac{2}{3}$; $\rho_f = \frac{1}{3}$.

The vector $\boldsymbol{\rho_e} = \{ \rho_e \mid e \in E \}$ must belong to the *spanning tree polytope.* (Edmonds, 1971)

TRW max-product and LP relaxation

First-order (tree-based) LP relaxation:

$$f(\widehat{\mathbf{x}}) \;\leq\; \max_{\vec{\tau} \in \mathbb{L}(G)} \left\{ \sum_{s \in V} \mathbb{E}_{\tau_s}[\theta_s(x_s)] + \sum_{(s,t) \in E} \mathbb{E}_{\tau_{st}}[\theta_{st}(x_s, x_t)] \right\}$$

Results: (Wainwright et al., 2003; Kolmogorov & Wainwright, 2005):

(a) **Strong tree agreement** Any TRW fixed-point that satisfies the strong tree agreement condition specifies an optimal LP solution.

(b) **LP solving:** For any binary pairwise problem, TRW max-product solves the first-order LP relaxation.

(c) **Persistence for binary problems:** Let $S \subseteq V$ be the subset of vertices for which there exists a single point $x_s^* \in \arg\max_{x_s} \nu_s^*(x_s)$. Then for *any optimal solution*, it holds that $y_s = x_s^*$.

On-going work: Distributed methods for solving LPs

- tree-reweighted max-product solves first-order LP for any binary pairwise problem (Kolmogorov & Wainwright, 2005)
- convergent dual ascent scheme; LP-optimal for binary pairwise problems (Globerson & Jaakkola, 2007)
- convex free energies and zero-temperature limits (Wainwright et al., 2005, Weiss et al., 2006; Johnson et al., 2007)
- coding problems: adaptive cutting-plane methods (Taghavi & Siegel, 2006; Dimakis et al., 2006)
- arbitrary problems: proximal minimization and rounding schemes with correctness guarantees (Ravikumar et al., ICML 2008)

Hierarchies of conic programming relaxations

- tree-based LP relaxation using $\mathbb{L}(G)$: first in a hierarchy of hypertree-based relaxations (Wainwright & Jordan, 2004)
- hierarchies of SDP relaxations for polynomial programming (Lasserre, 2001; Parrilo, 2002)
- intermediate between LP and SDP: second-order cone programming (SOCP) relaxations (Ravikumar & Lafferty, 2006; Pawan et al., 2008)
- all relaxations: particular outer bounds on the marginal polyope

Key questions:

- when are particular relaxations tight?
- when does more computation (e.g., LP $\rightarrow$ SDP) yield performance gains?

Variational principles for marginalization/summation

Undirected graphical model:

$$p(\mathbf{x}) \quad = \quad \frac{1}{Z} \prod_{C \in \mathbf{C}} \exp\{\theta_C(x_C)\}.$$

<u>Core computational challenges</u>

(a) computing most probable configurations $\widehat{\mathbf{x}} \in \arg\max_{\mathbf{x} \in \mathcal{X}^N} p(\mathbf{x})$

(b) computing normalization constant Z

(c) computing local marginal distributions (e.g., $p(x_s) = \sum_{x_t, t \neq s} p(\mathbf{x})$)

Variational formulation of problems (b) and (c): not immediately obvious!

Approach: Develop variational representations using exponential families, and convex duality.

Maximum entropy formulation of graphical models

- suppose that we have measurements $\widehat{\mu}$ of the average values of some (local) functions $\phi_\alpha : \mathcal{X}^n \to \mathbb{R}$
- in general, will be many distributions p that satisfy the measurement constraints $\mathbb{E}_p[\phi_\alpha(\mathbf{x})] = \widehat{\mu}$
- will consider finding the p with maximum "uncertainty" subject to the observations, with uncertainty measured by entropy

$$H(p) = -\sum_{\mathbf{x}} p(\mathbf{x}) \log p(\mathbf{x}).$$

Constrained maximum entropy problem: Find $\widehat{p}$ to solve

$$\max_{p \in \mathcal{P}} H(p) \qquad \text{such that} \qquad \mathbb{E}_p[\phi_\alpha(\mathbf{x})] = \widehat{\mu}$$

- elementary argument with Lagrange multipliers shows that solution belongs to exponential family

$$\widehat{p}(\mathbf{x};\theta) \;\propto\; \exp\Big\{\sum_{\alpha \in \mathcal{I}} \theta_\alpha \phi_\alpha(\mathbf{x})\Big\}.$$

Examples: Scalar exponential families

Family	$\mathcal{X}$	$\boldsymbol{\nu}$	$\log p(\mathbf{x};\theta)$	$A(\theta)$
Bernoulli	$\{0,1\}$	Counting	$\theta x - A(\theta)$	$\log[1+\exp(\theta)]$
Gaussian	$\mathbb{R}$	Lebesgue	$\theta_1 x + \theta_2 x^2 - A(\theta)$	$\frac{1}{2}[\theta_1 + \log \frac{2\pi e}{-\theta_2}]$
Exponential	$(0,+\infty)$	Lebesgue	$\theta\,(-x) - A(\theta)$	$-\log\theta$
Poisson	$\{0,1,2\ldots\}$	Counting $h(x) = 1/x!$	$\theta x - A(\theta)$	$\exp(\theta)$

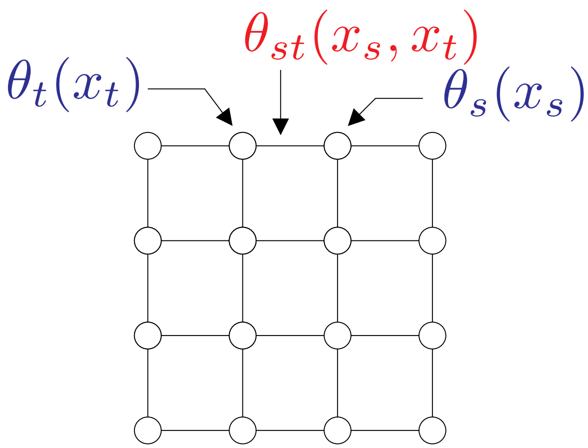
- parameterized family of densities (w.r.t. some base measure)

$$p(\mathbf{x};\theta) \quad = \quad \exp\Big\{\sum_{\alpha} \theta_\alpha \phi_\alpha(\mathbf{x}) \; - \; A(\theta)\Big\}$$

- cumulant generating function (log normalization constant):

$$A(\theta) = \log\Big(\int \exp\{\langle\theta,\, \boldsymbol{\phi}(\mathbf{x})\rangle\}\boldsymbol{\nu}(d\mathbf{x})\Big)$$

Example: Discrete Markov random field



Indicators: $\mathbb{I}_j(x_s) = \begin{cases} 1 & \text{if } x_s = j \\ 0 & \text{otherwise} \end{cases}$

Parameters: $\theta_s = \{\theta_{s;j}, j \in \mathcal{X}_s\}$

$\theta_{st} = \{\theta_{st;jk}, (j,k) \in \mathcal{X}_s \times \mathcal{X}_t\}$

Compact form: $\theta_s(x_s) := \sum_j \theta_{s;j} \mathbb{I}_j(x_s)$

$\theta_{st}(x_s, x_t) := \sum_{j,k} \theta_{st;jk} \mathbb{I}_j(x_s) \mathbb{I}_k(x_t)$

Probability mass function of form:

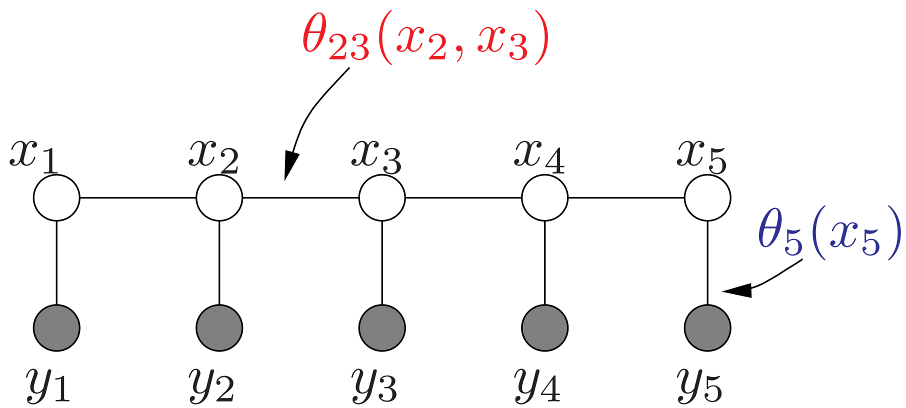
$$p(\mathbf{x};\theta) \quad \propto \quad \exp\Big\{\sum_{s \in V} \theta_s(x_s) + \sum_{(s,t)\in E} \theta_{st}(x_s, x_t)\Big\}$$

Cumulant generating function (log normalization constant):

$$A(\theta) \quad = \quad \log \sum_{\mathbf{x} \in \mathcal{X}^n} \exp\Big\{\sum_{s \in V} \theta_s(x_s) + \sum_{(s,t)\in E} \theta_{st}(x_s, x_t)\Big\}$$

Special case: Hidden Markov model

- Markov chain $\{X_1, X_2, \ldots\}$ evolving in time, with noisy observation Y_t at each time t



- an HMM is a particular type of discrete MRF, representing the conditional $p(\mathbf{x} \,|\, \mathbf{y}; \theta)$
- exponential parameters have a concrete interpretation

$$\begin{aligned} \theta_{23}(x_2, x_3) &= \log p(x_3 \,| x_2) \\ \theta_5(x_5) &= \log p(y_5 \,| x_5) \end{aligned}$$

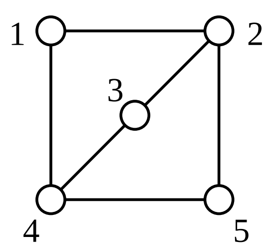
- the cumulant generating function $A(\theta)$ is equal to the log likelihood $\log p(\mathbf{y}; \theta)$

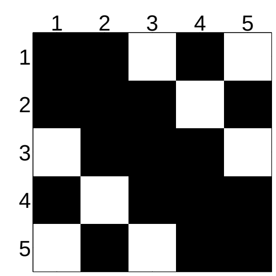
Example: Multivariate Gaussian

$U(\theta)$: Matrix of natural parameters $\phi(\mathbf{x})$: Matrix of sufficient statistics

$$\begin{bmatrix} 0 & \theta_1 & \theta_2 & \ldots & \theta_n \\ \theta_1 & \theta_{11} & \theta_{12} & \ldots & \theta_{1n} \\ \theta_2 & \theta_{21} & \theta_{22} & \ldots & \theta_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \theta_n & \theta_{n1} & \theta_{n2} & \ldots & \theta_{nn} \end{bmatrix} \qquad \begin{bmatrix} 1 & x_1 & x_2 & \ldots & x_n \\ x_1 & (x_1)^2 & x_1 x_2 & \ldots & x_1 x_n \\ x_2 & x_2 x_1 & (x_2)^2 & \ldots & x_2 x_n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n & x_n x_1 & x_n x_2 & \ldots & (x_n)^2 \end{bmatrix}$$

Edgewise natural parameters $\theta_{st} = \theta_{ts}$ must respect graph structure:

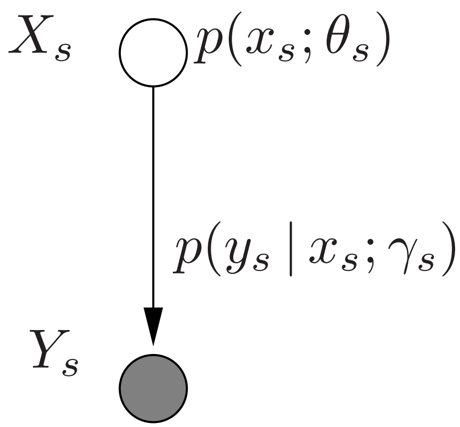




(a) Graph structure   (b) Structure of $[Z(\theta)]_{st} = \theta_{st}$.

Example: Mixture of Gaussians

- can form *mixture models* by combining different types of random variables
- let Y_s be conditionally Gaussian given the discrete variable X_s with parameters $\gamma_{s;j} = (\mu_{s;j}, \sigma^2_{s;j})$:



$$\begin{aligned} X_s &\equiv \text{mixture indicator} \\ Y_s &\equiv \text{mixture of Gaussian} \end{aligned}$$

- couple the mixture indicators $\mathbf{X} = \{X_s, s \in V\}$ using a discrete MRF
- overall model has the exponential form

$$p(\mathbf{y}, \mathbf{x}; \theta, \gamma) \;\propto\; \prod_{s \in V} p(y_s \,|\, x_s; \gamma_s)\; \exp\Big\{ \sum_{s \in V} \theta_s(x_s) + \sum_{(s,t) \in E} \theta_{st}(x_s, x_t)\Big]\Big\}.$$

Conjugate dual functions

- conjugate duality is a fertile source of variational representations
- any function f can be used to define another function f^* as follows:

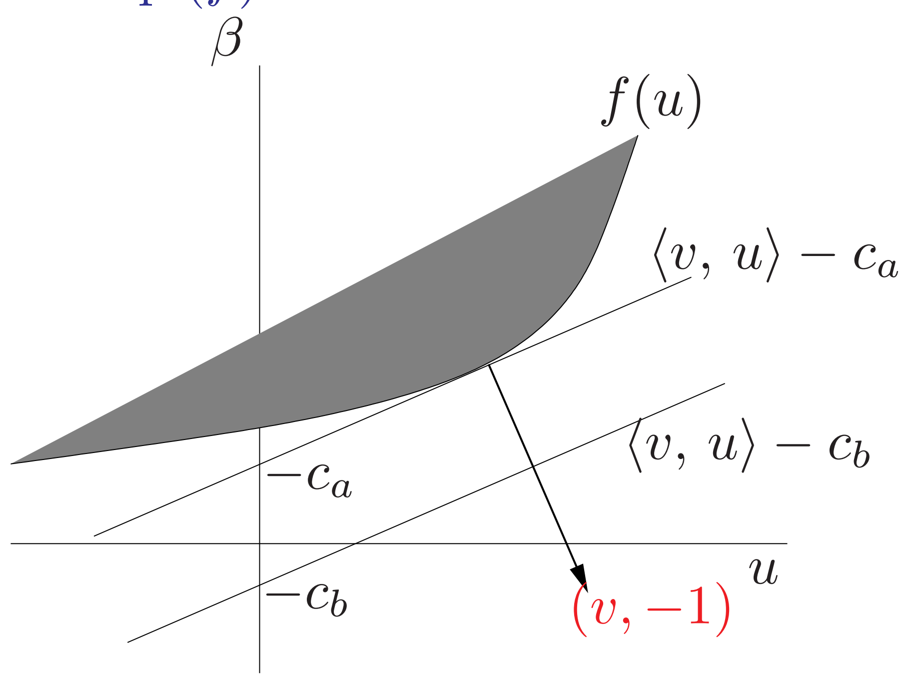
$$f^*(v) \quad := \quad \sup_{u \in \mathbb{R}^n} \big\{ \langle v,\, u \rangle - f(u) \big\}.$$

- easy to show that f^* is always a convex function
- how about taking the "dual of the dual"? I.e., what is $(f^*)^*$?
- when f is well-behaved (convex and lower semi-continuous), we have $(f^*)^* = f$, or alternatively stated:

$$f(u) \quad = \quad \sup_{v \in \mathbb{R}^n} \big\{ \langle u,\, v \rangle - f^*(v) \big\}$$

Geometric view: Supporting hyperplanes

Question: Given all hyperplanes in $\mathbb{R}^n \times \mathbb{R}$ with normal $(v, -1)$, what is the intercept of the one that supports $\mathrm{epi}(f)$?



Epigraph of f:

$\mathrm{epi}(f) := \{(u, \beta) \in \mathbb{R}^{n+1} \mid f(u) \leq \beta\}$.

Analytically, we require the smallest $c \in \mathbb{R}$ such that:

$$\langle v,\, u\rangle - c \quad \leq \quad f(u) \quad \text{for all} \quad u \in \mathbb{R}^n$$

By re-arranging, we find that this optimal c^* is the dual value:

$$c^* \quad = \quad \sup_{u \in \mathbb{R}^n} \big\{\langle v,\, u\rangle - f(u)\big\}.$$

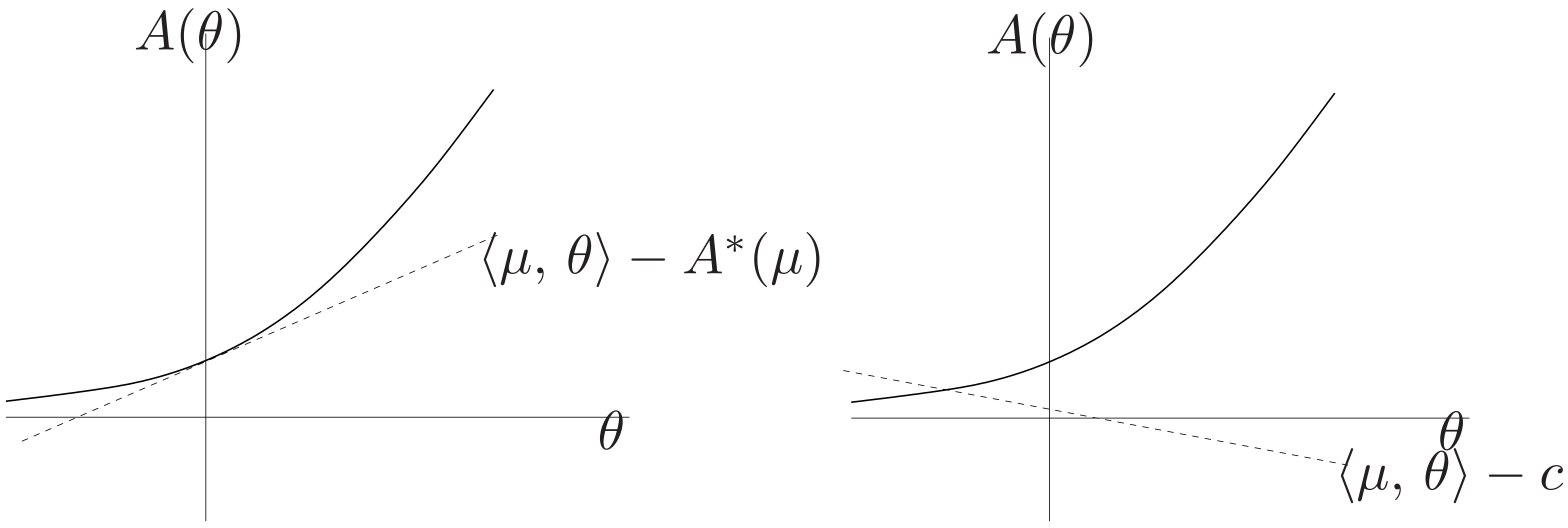
Example: Single Bernoulli

Random variable $X \in \{0, 1\}$ yields exponential family of the form:

$$p(x; \theta) \propto \exp\left\{\theta\, x\right\} \quad \text{with} \quad A(\theta) = \log\left[1 + \exp(\theta)\right].$$

Let's compute the dual $A^*(\mu) := \sup_{\theta \in \mathbb{R}} \left\{\mu\theta - \log[1 + \exp(\theta)]\right\}$.

(Possible) stationary point: $\mu = \exp(\theta)/[1 + \exp(\theta)]$.



(a) Epigraph supported (b) Epigraph *cannot* be supported

We find that: $$A^*(\mu) = \begin{cases} \mu \log \mu + (1 - \mu) \log(1 - \mu) & \text{if } \mu \in [0, 1] \\ +\infty & \text{otherwise.} \end{cases}.$$

Leads to the variational representation: $A(\theta) = \max_{\mu \in [0,1]} \left\{\mu \cdot \theta - A^*(\mu)\right\}$.

More general computation of the dual A^*

- consider the definition of the dual function:

$$A^*(\mu) \quad = \quad \sup_{\theta \in \mathbb{R}^d} \big\{ \langle \mu,\, \theta \rangle - A(\theta) \big\}.$$

- taking derivatives w.r.t θ to find a stationary point yields:

$$\mu - \nabla A(\theta) \quad = \quad 0.$$

- <u>Useful fact:</u> Derivatives of A yield *mean parameters:*

$$\frac{\partial A}{\partial \theta_\alpha}(\theta) \quad = \quad \mathbb{E}_\theta[\phi_\alpha(\mathbf{X})] \;:=\; \int \phi_\alpha(\mathbf{x}) p(\mathbf{x};\theta) \boldsymbol{\nu}(\mathbf{x}).$$

Thus, stationary points satisfy the equation:

$$\mu \quad = \quad \mathbb{E}_\theta[\boldsymbol{\phi}(\mathbf{X})] \tag{1}$$

Computation of dual (continued)

- assume solution $\theta(\mu)$ to equation $\mu = \mathbb{E}_\theta[\boldsymbol{\phi}(\mathbf{X})]$ $\qquad (*)$
- strict concavity of objective guarantees that $\theta(\mu)$ attains global maximum with value

$$\begin{aligned} A^*(\mu) &= \langle \mu,\, \theta(\mu)\rangle - A(\theta(\mu)) \\ &= \mathbb{E}_{\theta(\mu)}\Big[\langle \theta(\mu),\, \boldsymbol{\phi}(\mathbf{X})\rangle - A(\theta(\mu))\Big] \\ &= \mathbb{E}_{\theta(\mu)}[\log p(\mathbf{X}; \theta(\mu))] \end{aligned}$$

- recall the definition of *entropy*:

$$H(p(\mathbf{x})) \quad := \quad -\int \big[\log p(\mathbf{x})\big] p(\mathbf{x}) \boldsymbol{\nu}(d\mathbf{x})$$

- thus, we recognize that $A^*(\mu) = -H(p(\mathbf{x}; \theta(\mu)))$ when equation $(*)$ has a solution

Question: For which $\mu \in \mathbb{R}^d$ does equation $(*)$ have a solution $\theta(\mu)$?

Sets of realizable mean parameters

- for any distribution $p(\cdot)$, define a vector $\mu \in \mathbb{R}^d$ of *mean parameters*:

$$\mu_\alpha \quad := \quad \int \phi_\alpha(\mathbf{x}) p(\mathbf{x}) \boldsymbol{\nu}(d\mathbf{x})$$

- now consider the set $\mathbb{M}(G; \boldsymbol{\phi})$ of all realizable mean parameters:

$$\mathbb{M}(G; \boldsymbol{\phi}) = \left\{ \mu \in \mathbb{R}^d \;\middle|\; \mu_\alpha = \int \phi_\alpha(\mathbf{x}) p(\mathbf{x}) \boldsymbol{\nu}(d\mathbf{x}) \quad \text{for } \textit{some } p(\cdot) \right\}$$

- for discrete families, we refer to this set as a *marginal polytope* (as discussed previously)

Examples of $\mathbb{M}$: Gaussian MRF

$\boldsymbol{\phi}(\mathbf{x})$ Matrix of sufficient statistics

$$\begin{bmatrix} 1 & x_1 & x_2 & \dots & x_n \\ x_1 & (x_1)^2 & x_1 x_2 & \dots & x_1 x_n \\ x_2 & x_2 x_1 & (x_2)^2 & \dots & x_2 x_n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n & x_n x_1 & x_n x_2 & \dots & (x_n)^2 \end{bmatrix}$$

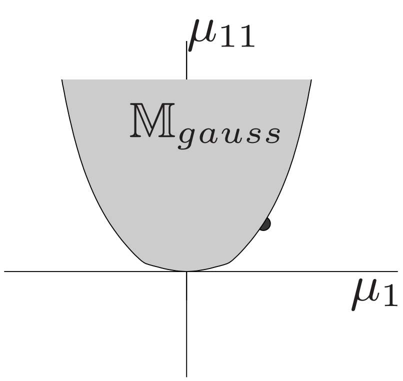
$U(\mu)$ Matrix of mean parameters

$$\begin{bmatrix} 1 & \mu_1 & \mu_2 & \dots & \mu_n \\ \mu_1 & \mu_{11} & \mu_{12} & \dots & \mu_{1n} \\ \mu_2 & \mu_{21} & \mu_{22} & \dots & \mu_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mu_n & \mu_{n1} & \mu_{n2} & \dots & \mu_{nn} \end{bmatrix}$$

- Gaussian mean parameters are specified by a single semidefinite constraint as $\mathbb{M}_{Gauss} = \{\mu \in \mathbb{R}^{n+\binom{n}{2}} \mid U(\mu) \succeq 0\}$.

Scalar case:

$$U(\mu) = \begin{bmatrix} 1 & \mu_1 \\ \mu_1 & \mu_{11} \end{bmatrix}$$

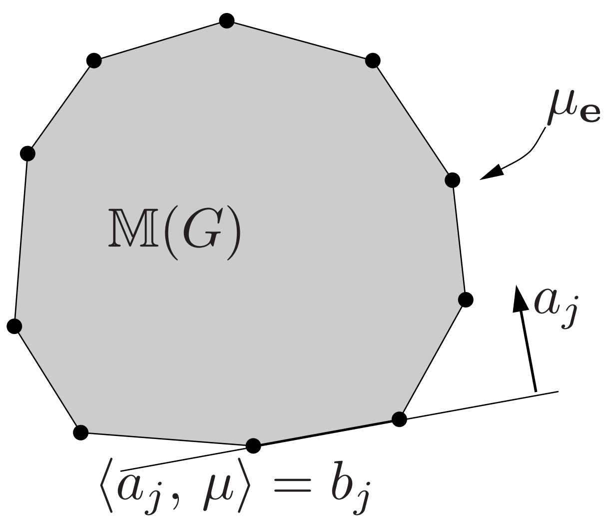


Examples of $\mathbb{M}$: Discrete MRF

- sufficient statistics:
$$\begin{array}{ll} \mathbb{I}_j(x_s) & \text{for } s = 1, \ldots n, \quad j \in \mathcal{X}_s \\ \mathbb{I}_{jk}(x_s, x_t) & \text{for} (s,t) \in E, \quad (j,k) \in \mathcal{X}_s \times \mathcal{X}_t \end{array}$$

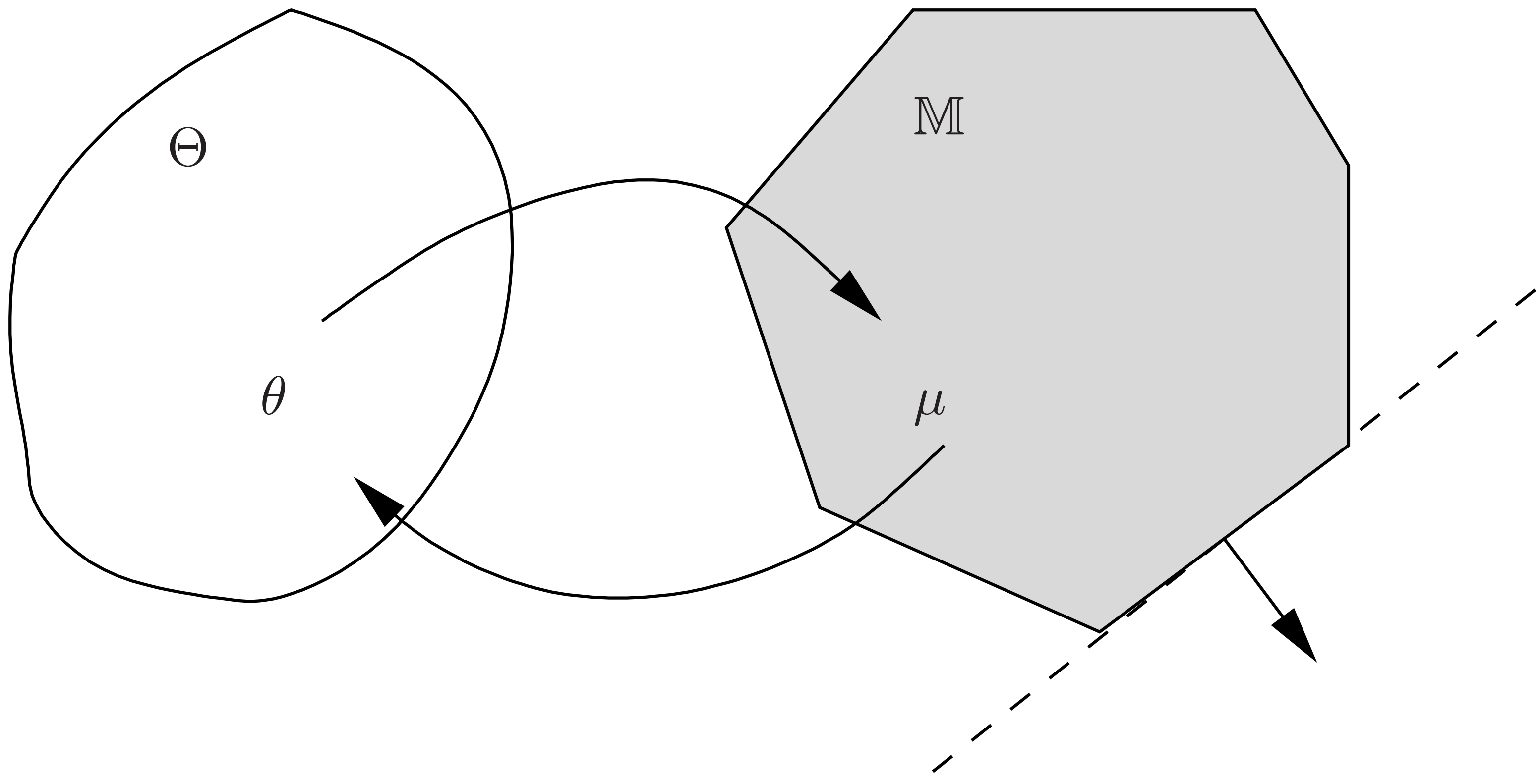
- mean parameters are simply marginal probabilities, represented as:

$$\mu_s(x_s) \;:=\; \sum_{j \in \mathcal{X}_s} \mu_{s;j} \mathbb{I}_j(x_s), \qquad \mu_{st}(x_s, x_t) \;:=\; \sum_{(j,k) \in \mathcal{X}_s \times \mathcal{X}_t} \mu_{st;jk} \mathbb{I}_{jk}(x_s, x_t)$$



- denote the set of realizable μ_s and μ_{st} by $\mathbb{M}(G)$
- refer to it as the *marginal polytope*
- extremely difficult to characterize for general graphs

Geometry and moment mapping



For suitable classes of graphical models in exponential form, the gradient map ∇A is a bijection between Θ and the interior of $\mathbb{M}$.

(e.g., Brown, 1986; Efron, 1978)

Variational principle in terms of mean parameters

- The conjugate dual of A takes the form:

$$A^*(\mu) \quad = \quad \begin{cases} -H(p(\mathbf{x}; \theta(\mu))) & \text{if } \mu \in \operatorname{int} \mathbb{M}(G; \boldsymbol{\phi}) \\ +\infty & \text{if } \mu \notin \operatorname{cl} \mathbb{M}(G; \boldsymbol{\phi}). \end{cases}$$

  Interpretation:

  – $A^*(\mu)$ is finite (and equal to a certain negative entropy) for any μ that is globally realizable

  – if $\mu \notin \operatorname{cl} \mathbb{M}(G; \boldsymbol{\phi})$, then the max. entropy problem is *infeasible*

- The cumulant generating function A has the representation:

$$\underbrace{A(\theta)}_{\text{cumulant generating func.}} \quad = \quad \underbrace{\sup_{\mu \in \mathbb{M}(G;\boldsymbol{\phi})} \{\langle \theta, \, \mu \rangle \; - \; A^*(\mu)\},}_{\text{max. ent. problem over } \mathbb{M}}$$

- in contrast to the "free energy" approach, solving this problem provides both the value $A(\theta)$ and the exact mean parameters $\widehat{\mu}_\alpha = \mathbb{E}_\theta[\phi_\alpha(\mathbf{x})]$

Alternative view: Kullback-Leibler divergence

- Kullback-Leibler divergence defines "distance" between probability distributions:

$$D(p \,||\, q) \quad := \quad \int \Big[\log \frac{p(\mathbf{x})}{q(\mathbf{x})}\Big] p(\mathbf{x}) \boldsymbol{\nu}(d\mathbf{x})$$

- for two exponential family members $p(\mathbf{x};\theta^1)$ and $p(\mathbf{x};\theta^2)$, we have

$$D(p(\mathbf{x};\theta^1) \,||\, p(\mathbf{x};\theta^2)) \quad = \quad A(\theta^2) - A(\theta^1) - \langle \mu^1, \, \theta^2 - \theta^1 \rangle$$

- substituting $A(\theta^1) = \langle \theta^1, \, \mu^1 \rangle - A^*(\mu^1)$ yields a *mixed form*:

$$D(p(\mathbf{x};\theta^1) \,||\, p(\mathbf{x};\theta^2)) \quad \equiv \quad D(\mu^1 \,||\, \theta^2) \; = \; A(\theta^2) + A^*(\mu^1) - \langle \mu^1, \, \theta^2 \rangle$$

Hence, the following two assertions are equivalent:

$$A(\theta^2) \quad = \quad \sup_{\mu^1 \in \mathbb{M}(G;\boldsymbol{\phi})} \quad \{\langle \theta^2, \, \mu^1 \rangle \; - \; A^*(\mu^1)\}$$

$$0 \quad = \quad \inf_{\mu^1 \in \mathbb{M}(G;\boldsymbol{\phi})} D(\mu^1 \,||\, \theta^2)$$

Challenges

1. In general, mean parameter spaces $\mathbb{M}$ can be very difficult to characterize (e.g., multidimensional moment problems).

2. Entropy $A^*(\mu)$ as a function of *only* the mean parameters μ typically lacks an explicit form.

Remarks:

1. Variational representation clarifies why certain models are tractable.

2. For intractable cases, one strategy is to solve an approximate form of the optimization problem.

Example: Multivariate Gaussian (fixed covariance)

Consider the set of all Gaussians with fixed *inverse* covariance $Q \succ 0$.

- potentials $\boldsymbol{\phi}(\mathbf{x}) = \{x_1, \ldots, x_n\}$ and natural parameter $\theta \in \Theta = \mathbb{R}^n$.
- cumulant generating function:

$$A(\theta) \quad = \quad \log \int_{\mathbb{R}^n} \overbrace{\exp\Big\{\sum_{s=1}^{n} \theta_s x_s\Big\}}^{\text{density}} \quad \underbrace{\exp\Big\{-\frac{1}{2}\mathbf{x}^T Q \mathbf{x}\Big\} d\mathbf{x}}_{\text{base measure}}$$

- completing the square yields $A(\theta) = \frac{1}{2}\theta^T Q^{-1}\theta + \text{constant}$
- straightforward computation leads to the dual
$$A^*(\mu) = \tfrac{1}{2}\mu^T Q \mu - \text{constant}$$
- putting the pieces back together yields the variational principle

$$A(\theta) \quad = \quad \sup_{\mu \in \mathbb{R}^n} \Big\{\theta^T \mu - \frac{1}{2}\mu^T Q \mu\Big\} + \text{constant}$$

- optimum is uniquely obtained at the familiar Gaussian mean $\widehat{\mu} = Q^{-1}\theta$.

Example: Multivariate Gaussian (arbitrary cov.)

- matrices of sufficient statistics, natural parameters, and mean parameters:

$$\phi(\mathbf{X}) = \begin{bmatrix} 1 \\ \mathbf{X} \end{bmatrix} \begin{bmatrix} 1 & \mathbf{X} \end{bmatrix}, \quad U(\theta) := \begin{bmatrix} 0 & [\theta_s] \\ [\theta_s] & [\theta_{st}] \end{bmatrix} \quad U(\mu) := \mathbb{E}\left\{ \begin{bmatrix} 1 \\ \mathbf{X} \end{bmatrix} \begin{bmatrix} 1 & \mathbf{X} \end{bmatrix} \right\}$$

- cumulant generating function:

$$A(\theta) \quad = \quad \log \int \exp\Big\{ \operatorname{trace}(U(\theta)\, \phi(\mathbf{x})) \Big\} d\mathbf{x}$$

- computing the dual function:

$$A^*(\mu) \quad = \quad -\frac{1}{2} \log\det U(\mu) - \frac{n}{2} \log 2\pi e,$$

- exact variational principle is a *log-determinant problem*:

$$A(\theta) \quad = \quad \sup_{U(\mu) \succ 0,\ \ [U(\mu)]_{11} = 1} \Big\{ \operatorname{trace}(U(\theta)\, U(\mu)) + \frac{1}{2} \log\det U(\mu) \} + C \Big\}.$$

- solution yields the *normal equations* for Gaussian mean and covariance.

Example: Belief propagation and Bethe principle

Problem set-up

- discrete variables $X_s \in \{0, 1, \ldots, m_s - 1\}$ on graph $G = (V, E)$
- sufficient statistics: indicator functions for each node and edge

$$\begin{aligned} \mathbb{I}_j(x_s) \quad & \text{for} \quad s = 1, \ldots n, \quad j \in \mathcal{X}_s \\ \mathbb{I}_{jk}(x_s, x_t) \quad & \text{for} \quad (s,t) \in E, \quad (j,k) \in \mathcal{X}_s \times \mathcal{X}_t. \end{aligned}$$

- exponential representation of distribution:

$$p(\mathbf{x}; \theta) \quad \propto \quad \exp\Big\{ \sum_{s \in V} \theta_s(x_s) + \sum_{(s,t) \in E} \theta_{st}(x_s, x_t) \Big\}$$

where $\theta_s(x_s) := \sum_{j \in \mathcal{X}_s} \theta_{s;j} \mathbb{I}_j(x_s)$ (and similarly for $\theta_{st}(x_s, x_t)$)

Two main ingredients:

1. Exact entropy $-A^*(\mu)$ is intractable, so let's approximate it.
2. The *marginal polytope* $\mathbb{M}(G)$ is also difficult to characterize, so let's use the tree-based outer bound $\mathbb{L}(G)$.

Bethe entropy approximation

- mean parameters are simply marginal probabilities, represented as:

$$\mu_s(x_s) \;:=\; \sum_{j \in \mathcal{X}_s} \mu_{s;j} \mathbb{I}_j(x_s), \qquad \mu_{st}(x_s, x_t) \;:=\; \sum_{(j,k) \in \mathcal{X}_s \times \mathcal{X}_t} \mu_{st;jk} \mathbb{I}_{jk}(x_s, x_t)$$

- Bethe entropy approximation

$$-A^*_{Bethe}(\mu) \;=\; \sum_{s \in V} H_s(\mu_s) - \sum_{(s,t) \in E} I_{st}(\mu_{st}),$$

where

Single node entropy: $H_s(\mu_s) := -\sum_{x_s} \mu_s(x_s) \log \mu_s(x_s)$

Mutual information: $I_{st}(\mu_{st}) := \sum_{x_s, x_t} \mu_{st}(x_s, x_t) \log \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s)\mu_t(x_t)}$.

- exact for trees, using the factorization:

$$p(\mathbf{x}; \theta) \;=\; \prod_{s \in V} \mu_s(x_s) \prod_{(s,t) \in E} \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s)\mu_t(x_t)}$$

Bethe variational principle

- Bethe entropy approximation, and outer bound $\mathbb{L}(G)$:

$$\mathbb{L}(G) \quad = \quad \left\{ \vec{\tau} \mid \sum_{x_s} \tau_s(x_s) = 1, \quad \sum_{x'_t} \tau_{st}(x_s, x'_t) = \tau_s(x_s) \right\}.$$

- combining these ingredients leads to the *Bethe variational prorblem* (BVP):

$$\max_{\tau \in \mathbb{L}(G)} \left\{ \langle \theta, \tau \rangle + \sum_{s \in V} H_s(\mu_s) - \sum_{(s,t) \in E} I_{st}(\tau_{st}) \right\}$$

Key fact: Belief propagation can be derived as an iterative method for solving a Lagrangian formulation of the BVP (Yedidia et al., 2002)

Lagrangian derivation of belief propagation

- let's try to solve this problem by a (partial) Lagrangian formulation
- assign a Lagrange multiplier $\lambda_{ts}(x_s)$ for each constraint $C_{ts}(x_s) := \tau_s(x_s) - \sum_{x_t} \tau_{st}(x_s, x_t) = 0$
- will enforce the normalization ($\sum_{x_s} \tau_s(x_s) = 1$) and non-negativity constraints explicitly
- the Lagrangian takes the form:

$$\mathcal{L}(\tau; \lambda) = \langle \theta, \tau \rangle + \sum_{s \in V} H_s(\tau_s) - \sum_{(s,t) \in E(G)} I_{st}(\tau_{st}) + \sum_{(s,t) \in E} \Big[\sum_{x_t} \lambda_{st}(x_t) C_{st}(x_t) + \sum_{x_s} \lambda_{ts}(x_s) C_{ts}(x_s) \Big]$$

Lagrangian derivation (part II)

- taking derivatives of the Lagrangian w.r.t τ_s and τ_{st} yields

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \tau_s(x_s)} &= \theta_s(x_s) - \log \tau_s(x_s) + \sum_{t \in \mathcal{N}(s)} \lambda_{ts}(x_s) + C \\
\frac{\partial \mathcal{L}}{\partial \tau_{st}(x_s, x_t)} &= \theta_{st}(x_s, x_t) - \log \frac{\tau_{st}(x_s, x_t)}{\tau_s(x_s)\tau_t(x_t)} - \lambda_{ts}(x_s) - \lambda_{st}(x_t) + C'
\end{aligned}$$

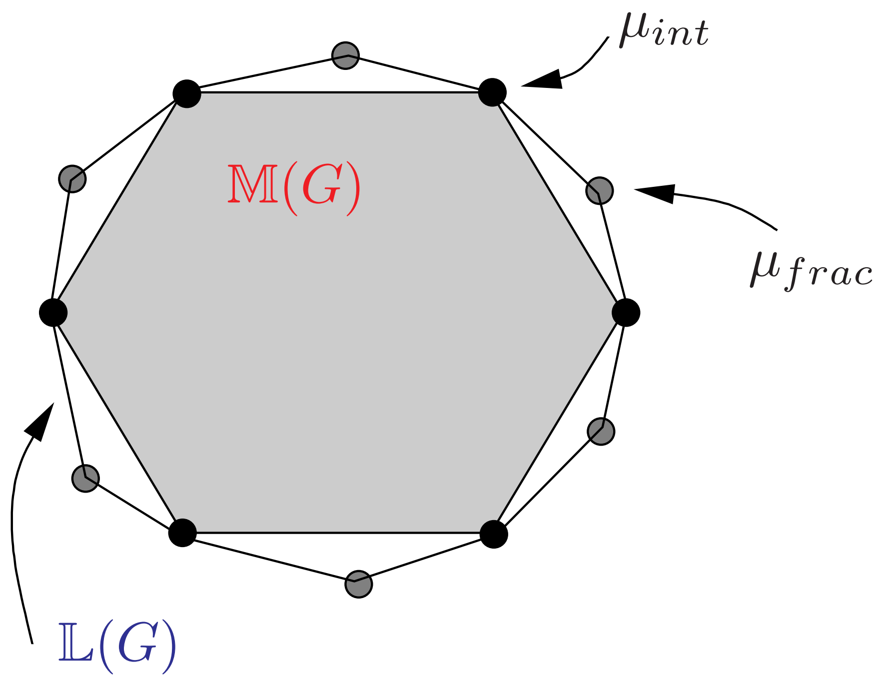
- setting these partial derivatives to zero and simplifying:

$$\begin{aligned}
\tau_s(x_s) &\propto \exp\{\theta_s(x_s)\} \prod_{t \in \mathcal{N}(s)} \exp\{\lambda_{ts}(x_s)\} \\
\tau_s(x_s, x_t) &\propto \exp\{\theta_s(x_s) + \theta_t(x_t) + \theta_{st}(x_s, x_t)\} \times \\
&\qquad \prod_{u \in \mathcal{N}(s) \backslash t} \exp\{\lambda_{us}(x_s)\} \prod_{v \in \mathcal{N}(t) \backslash s} \exp\{\lambda_{vt}(x_t)\}
\end{aligned}$$

- enforcing the constraint $C_{ts}(x_s) = 0$ on these representations yields the familiar update rule for the *messages* $M_{ts}(x_s) = \exp(\lambda_{ts}(x_s))$:

$$M_{ts}(x_s) \leftarrow \sum_{x_t} \exp\{\theta_t(x_t) + \theta_{st}(x_s, x_t)\} \prod_{u \in \mathcal{N}(t) \backslash s} M_{ut}(x_t)$$

Geometry of Bethe variational problem



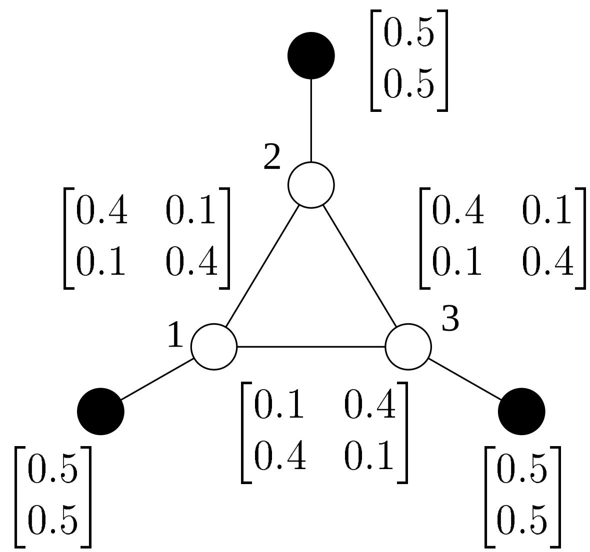
- belief propagation uses a *polyhedral outer approximation* to $\mathbb{M}(G)$:
  - for any graph, $\mathbb{L}(G) \supseteq \mathbb{M}(G)$.
  - equality holds $\iff$ G is a tree.

Natural question: Do BP fixed points ever fall outside of the marginal polytope $\mathbb{M}(G)$?

Illustration: Globally inconsistent BP fixed points

Consider the following assignment of pseudomarginals τ_s, τ_{st}:

Locally consistent (pseudo)marginals



- can verify that $\tau \in \mathbb{L}(G)$, and that τ is a fixed point of belief propagation (with all constant messages)
- however, τ is globally inconsistent

Note: More generally: for any τ in the interior of $\mathbb{L}(G)$, can construct a distribution with τ as a BP fixed point.

High-level perspective: A broad class of methods

- message-passing algorithms (e.g., mean field, belief propagation) are solving approximate versions of exact variational principle in exponential families
- there are two *distinct* components to approximations:
  (a) can use either inner or outer bounds to $\mathbb{M}$
  (b) various approximations to entropy function $-A^*(\mu)$

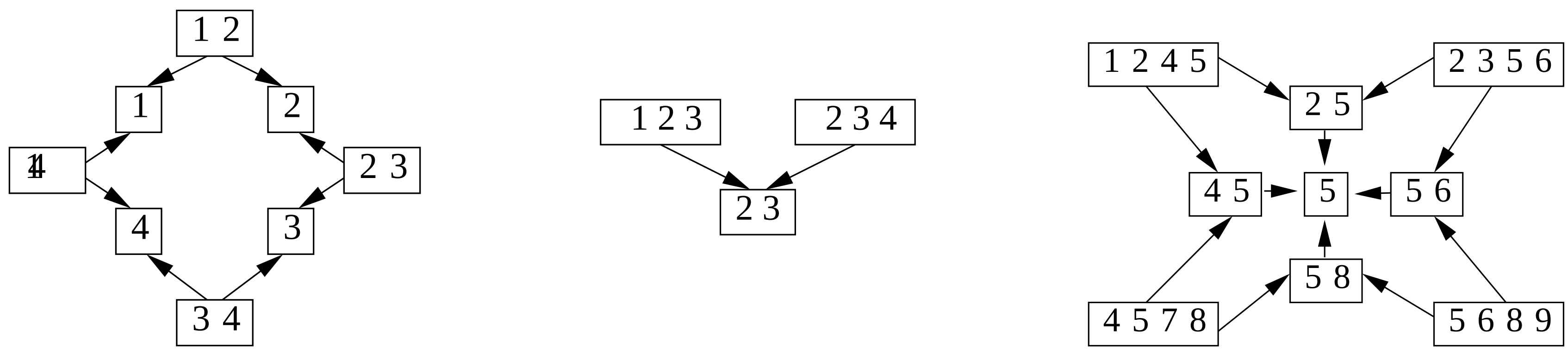
Refining one or both components yields better approximations:

- BP: polyhedral outer bound and non-convex Bethe approximation
- Kikuchi and variants: tighter polyhedral outer bounds and better entropy approximations (e.g.,Yedidia et al., 2002)
- Expectation-propagation: better outer bounds and Bethe-like entropy approximations (Minka, 2002)

Generalized belief propagation on hypergraphs

(Yedidia et al., 2002)

- a *hypergraph* is a natural generalization of a graph
- it consists of a set of vertices V and a set E of hyperedges, where each *hyperedge* is a subset of V



(a) Ordinary graph (b) Hypertree (width 2) (c) Hypergraph

- ancestor/descendant relationships:
  - $g \subset h$ if g is contained within hyperedge h
  - $g \supset h$ for opposite relationship

Hypertree factorization

- for each hyperedge: $\log \varphi_h(x_h) := \sum_{g \subseteq h} (-1)^{|h \backslash g|} \; [\log \tau_g(x_g)]$.

- any hypertree-structured distribution is guaranteed to factor as:

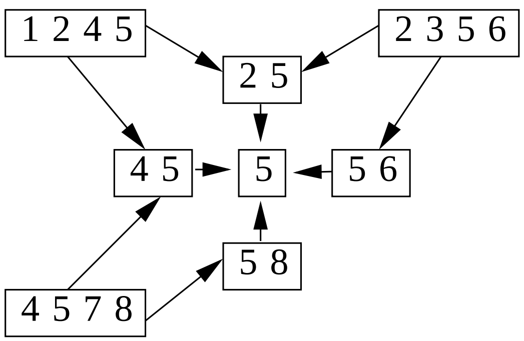
$$p(\mathbf{x}) \;=\; \prod_{h \in E} \varphi_h(x_h).$$

- **Ordinary tree:**

$$\varphi_s(x_s) \;=\; \mu_s(x_s) \qquad \text{for any vertex } s$$

$$\varphi_{st}(x_s, x_t) \;=\; \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s)\;\mu_t(x_t)} \qquad \text{for edge } (s,t).$$

- **Hypertree:**



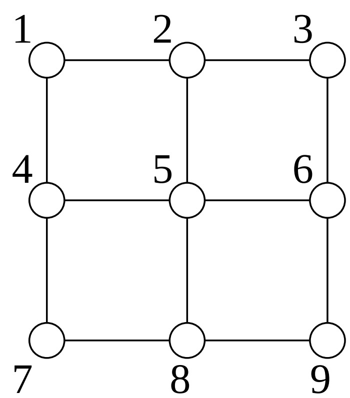
$$\varphi_{1245} \;=\; \frac{\mu_{1245}}{\frac{\mu_{25}}{\mu_5}\,\frac{\mu_{45}}{\mu_5}\,\mu_5}$$

$$\varphi_{45} \;=\; \frac{\mu_{45}}{\mu_5}$$

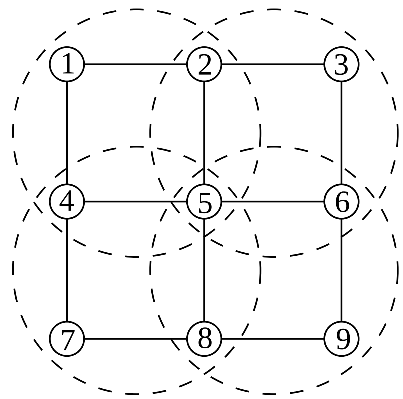
$$\varphi_5 \;=\; \mu_5$$

Building augmented hypergraphs

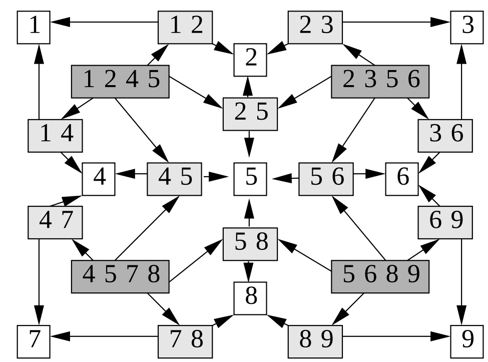
Better entropy approximations via augmented hypergraphs.



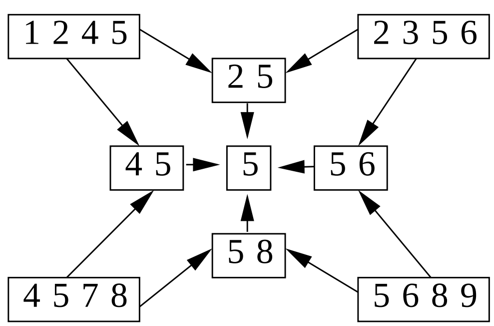
(a) Original



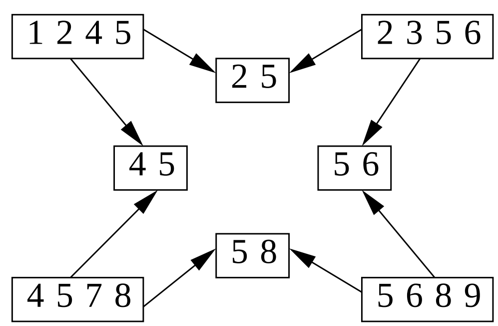
(b) Clustering



(c) Full covering



(d) Kikuchi



(e) Fails single counting

Expectation-propagation (EP)

- originally derived in terms of assumed density filtering (Minka, 2002)
- another instance of a relaxed variational principle:
  - "Bethe-like" (termwise) approximation to entropy
  - local consistency constraints on marginals
- distribution with tractable/intractable decomposition:

$$f(\mathbf{x}, \gamma, \Gamma) \quad \propto \quad \underbrace{\exp(\langle \gamma,\, \phi(\mathbf{x}) \rangle)}_{\text{Tractable}} \; \underbrace{\prod_{i=1}^{k} T_i(\mathbf{x})}_{\text{Intractable}}$$

- auxiliary parameters θ, and term-by-term entropy approx.:

$$H(f) \quad \approx \quad \underbrace{H(q_{base}(\mathbf{x}; \theta, \gamma))}_{\text{Base entropy}} + \underbrace{\sum_{i=1}^{k} \Big[H(q^{i}_{aug}(\mathbf{x}; \theta, \gamma, T_i)) - H(q_{base}(\mathbf{x}; \theta, \gamma)) \Big]}_{\text{Term approximations}}$$

EP updates for Gaussian mixtures

- distribution formed by tractable/intractable combination:

$$f(\mathbf{x}, \Sigma) \quad \propto \quad \exp\left(-\frac{1}{2}\mathbf{x}^T \Sigma^{-1} \mathbf{x}\right) \prod_{i=1}^{n} f(\mathbf{y}^i \mid \mathbf{X} = \mathbf{x})$$

- Gaussian mixture likelihoods

$$f(y^i \mid \mathbf{X} = \mathbf{x}) \quad = \quad \alpha \mathcal{N}(\mathbf{y}^i; 0, \sigma_0^2) + (1-\alpha)\mathcal{N}(\mathbf{y}^i; \mathbf{x}, \sigma_1^2)$$

- base/augmented distributions take form:

Base: $q_{base}(\mathbf{x}; \Sigma, \theta, \Theta) \quad \propto \quad \exp\left(\langle \gamma,\, x\rangle - \frac{1}{2}\operatorname{trace}(\Theta + \Sigma^{-1}\, \mathbf{x}\mathbf{x}^T)\right)$

Augmented: $q^i_{aug}(\mathbf{x}; \Sigma, \theta, \Theta, T_i) \quad \propto \quad q(\mathbf{x}; \Sigma, \theta, \Theta)\; T_i(\mathbf{x}).$

- variational problem: maximize term-by-term entropy approximation, subject to marginalization constraints:

$$\mathbb{E}_{q_{base}}[\mathbf{X}] = \mathbb{E}_{q^i_{aug}}[\mathbf{X}]$$
$$\mathbb{E}_{q_{base}}[\mathbf{X}\mathbf{X}^{\mathbf{T}}] = \mathbb{E}_{q^i_{aug}}[\mathbf{X}\mathbf{X}^{\mathbf{T}}].$$

Convex relaxations and upper bounds

Possible concerns with Bethe/Kikuchi, expectation-propagation etc.?

(a) lack of convexity $\Rightarrow$ multiple local optima, and algorithmic complications

(b) failure to bound the log partition function

Goal: Techniques for approximate computation of marginals and parameter estimation based on:

(a) convex variational problems $\Rightarrow$ unique global optimum

(b) relaxations of exact problem $\Rightarrow$ upper bounds on $A(\theta)$

Usefulness of bounds:

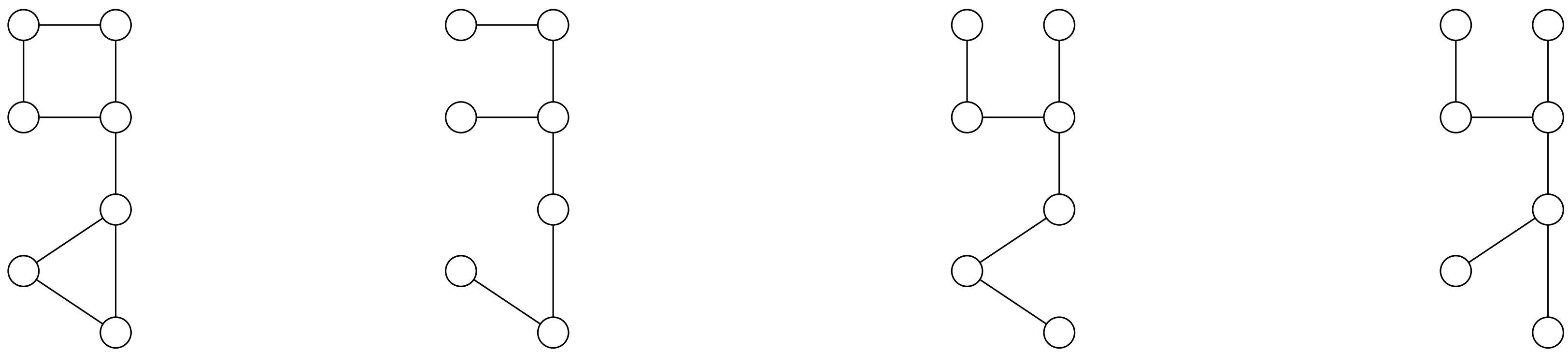
(a) interval estimates for marginals

(b) approximate parameter estimation

(c) large deviations (prob. of rare events)

Bounds from “convexified” Bethe/Kikuchi problems

Idea: Upper bound $-A^*(\mu)$ by convex combination of tree-structured entropies.



$$-A^*(\mu) \quad \leq \quad -\rho(T^1)A^*(\mu(T^1)) \quad - \quad \rho(T^2)A^*(\mu(T^2)) \quad - \quad \rho(T^3)A^*(\mu(T^3))$$

- given any spanning tree T, define the moment-matched tree distribution:

$$p(\mathbf{x};\mu(T)) \quad := \quad \prod_{s \in V} \mu_s(x_s) \prod_{(s,t) \in E} \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s)\ \mu_t(x_t)}$$

- use $-A^*(\mu(T))$ to denote the associated tree entropy
- let $\boldsymbol{\rho} = \{\rho(T)\}$ be a probability distribution over spanning trees

Optimal bounds by tree-reweighted message-passing

Recall the constraint set of locally consistent marginal distributions:

$$\mathbb{L}(G) \quad = \quad \{\, \tau \geq 0 \mid \underbrace{\sum_{x_s} \tau_s(x_s) = 1,}_{\text{normalization}} \; \underbrace{\sum_{x_s} \tau_{st}(x_s, x_t) = \tau_t(x_t)}_{\text{marginalization}} \,\}.$$

Theorem: (Wainwright et al., UAI-02)

(a) For any given edge weights $\boldsymbol{\rho_e} = \{\rho_e\}$ in the spanning tree polytope, the optimal upper bound over *all* tree parameters is given by:

$$A(\theta) \;\leq\; \max_{\tau \in \mathbb{L}(G)} \Big\{ \langle \theta,\, \tau \rangle + \sum_{s \in V} H_s(\tau_s) - \sum_{(s,t) \in E} \rho_{st} I_{st}(\tau_{st}) \,\Big\}.$$

(b) This optimization problem is strictly convex, and its unique optimum is specified by the fixed point of $\boldsymbol{\rho_e}$-reweighted sum-product:

$$M^*_{ts}(x_s) = \kappa \sum_{x'_t \in \mathcal{X}_t} \left\{ \exp\left[\frac{\theta_{st}(x_s, x'_t)}{\rho_{st}} + \theta_t(x'_t) \right] \frac{\prod_{v \in \Gamma(t) \backslash s} \big[M^*_{vt}(x_t) \big]^{\rho_{vt}}}{\big[M^*_{st}(x_t) \big]^{(1 - \rho_{ts})}} \right\}.$$

Semidefinite constraints in convex relaxations

Fact: Belief propagation and its hypergraph-based generalizations all involve polyhedral (i.e., *linear*) outer bounds on the marginal polytope.

Idea: *Semidefinite* constraints to generate more global outer bounds.

Example: For the Ising model, relevant mean parameters are $\mu_s = p(X_s = 1)$ and $\mu_{st} = p(X_s = 1, X_t = 1)$.

Define $\mathbf{Y} = [1 \;\; \mathbf{X}]^T$, and consider the second-order moment matrix:

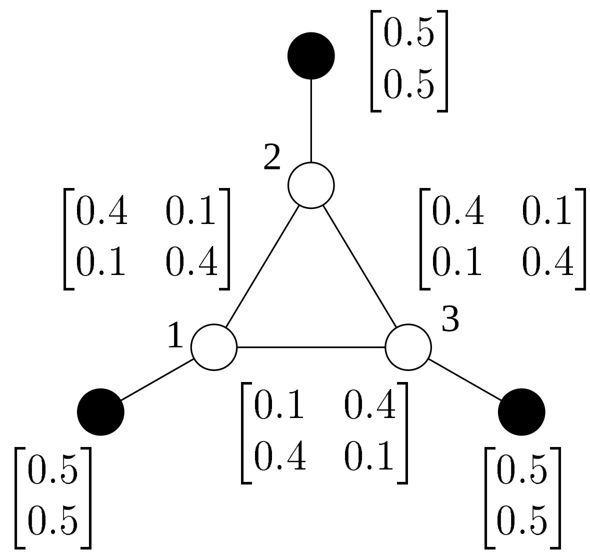
$$\mathbb{E}[\mathbf{Y}\mathbf{Y}^T] \; = \begin{bmatrix} 1 & \mu_1 & \mu_2 & \cdots & \mu_n \\ \mu_1 & \mu_1 & \mu_{12} & \cdots & \mu_{1n} \\ \mu_2 & \mu_{12} & \mu_2 & \cdots & \mu_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mu_n & \mu_{n1} & \mu_{n2} & \cdots & \mu_n \end{bmatrix} \; = \; M_1[\mu].$$

- since it must be positive semidefinite, this (an infinite number of) linear constraints on μ_s, μ_{st}.
- defines the *first-order semidefinite relaxation of* $\mathbb{M}(G)$:

$$\mathbb{S}(G) \quad = \quad \left\{ \mu \in \mathbb{R}^d \mid M_1[\mu] \succeq 0 \right\}.$$

Illustrative example

Locally consistent (pseudo)marginals



Second-order moment matrix

$$\begin{bmatrix}\mu_1 & \mu_{12} & \mu_{13}\\ \mu_{21} & \mu_2 & \mu_{23}\\ \mu_{31} & \mu_{32} & \mu_3\end{bmatrix} = \begin{bmatrix}0.5 & 0.4 & 0.1\\ 0.4 & 0.5 & 0.4\\ 0.1 & 0.4 & 0.5\end{bmatrix}$$

Not positive-semidefinite!

Log-determinant relaxation

- based on optimizing over covariance matrices $M_1(\mu) \in \mathbb{S}_1(K_n)$

Theorem: Consider an outer bound $\mathbb{O}(K_n)$ that satisfies:

$$\mathbb{M}(K_n) \quad \subseteq \quad \mathbb{O}(K_n) \;\subseteq\; \mathbb{S}_1(K_n)$$

For any such outer bound, $A(\theta)$ is upper bounded by:

$$\max_{\mu \in \mathbb{O}(K_n)} \left\{ \langle \theta,\, \mu \rangle + \frac{1}{2} \log\det \left[M_1(\mu) + \frac{1}{3} \operatorname{blkdiag}[0, I_n] \right] \right\} + \frac{n}{2} \log(\frac{\pi e}{2})$$

Remarks:

1. Log-det. problem can be solved efficiently by interior point methods.
2. Relevance for applications (e.g., Banerjee et al., 2008)
   (a) Upper bound on $A(\theta)$.
   (b) Method for computing approximate marginals.

(Wainwright & Jordan, 2003)

Mean field theory

Recap: All variational methods discussed until now are based on:

- *outer bounding* the set of valid mean parameters.
- approximating the entropy (negative dual function $-A^*(\mu)$)

Different idea: Restrict μ to a *subset* of distributions for which $-A^*(\mu)$ has a tractable form.

Examples:

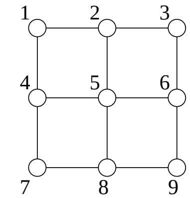
(a) For product distributions $p(\mathbf{x}) = \prod_{s \in V} \mu_s(x_s)$, entropy decomposes as $-A^*(\mu) = \sum_{s \in V} H_s(x_s)$.

(b) Similarly, for trees (more generally, decomposable graphs), the junction tree theorem yields an explicit form for $-A^*(\mu)$.

Definition: A subgraph H of G is *tractable* if the entropy has an explicit form for any distribution that respects H.

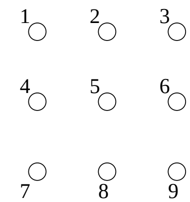
Geometry of mean field

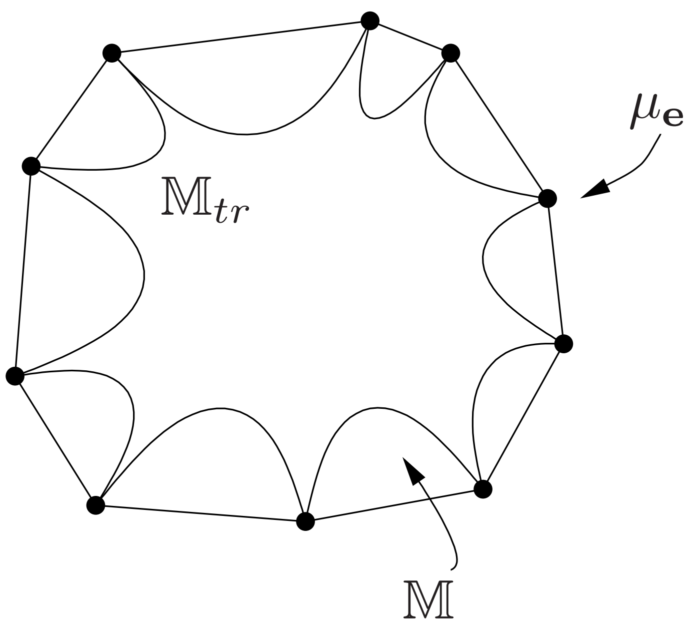
- let H represent a *tractable subgraph* (i.e., for which A^* has explicit form)



- let $\mathbb{M}_{tr}(G; H)$ represent tractable mean parameters:

$$\mathbb{M}_{tr}(G; H) := \{\mu \mid \mu = \mathbb{E}_\theta[\boldsymbol{\phi}(\mathbf{x})] \;\; \text{s. t. } \theta \;\text{ respects }\; H\}.$$





- under mild conditions, $\mathbb{M}_{tr}$ is a non-convex *inner approximation* to $\mathbb{M}$
- optimizing over $\mathbb{M}_{tr}$ (as opposed to $\mathbb{M}$) yields *lower bound*:

$$A(\theta) \;\geq\; \sup_{\widetilde{\mu} \in \mathbb{M}_{tr}} \big\{\langle \theta,\, \widetilde{\mu}\rangle - A^*(\widetilde{\mu})\big\}.$$

Alternative view: Minimizing KL divergence

- recall the *mixed form* of the KL divergence between $p(\mathbf{x};\theta)$ and $p(\mathbf{x};\widetilde{\theta})$:

$$D(\widetilde{\mu}\,||\,\theta) \quad = \quad A(\theta) + A^*(\widetilde{\mu}) - \langle \widetilde{\mu},\, \theta \rangle$$

- try to find the "best" approximation to $p(\mathbf{x};\theta)$ in the sense of KL divergence

- in analytical terms, the problem of interest is

$$\inf_{\widetilde{\mu} \in \mathbb{M}_{tr}} D(\widetilde{\mu}\,||\,\theta) \quad = \quad A(\theta) + \inf_{\widetilde{\mu} \in \mathbb{M}_{tr}} \Big\{ A^*(\widetilde{\mu}) - \langle \widetilde{\mu},\, \theta \rangle \Big\}$$

- hence, finding the tightest lower bound on $A(\theta)$ is equivalent to finding the best approximation to $p(\mathbf{x};\theta)$ from distributions with $\widetilde{\mu} \in \mathbb{M}_{tr}$

Example: Naive mean field algorithm for Ising model

- consider completely disconnected subgraph $H = (V, \emptyset)$
- permissible exponential parameters belong to subspace

$$\mathcal{E}(H) = \{\theta \in \mathbb{R}^d \mid \theta_{st} = 0 \;\; \forall \;\; (s,t) \in E\}$$

- allowed distributions take product form $p(\mathbf{x}; \theta) = \prod_{s \in V} p(x_s; \theta_s)$, and generate

$$\mathbb{M}_{tr}(G; H) = \{\mu \mid \mu_{st} = \mu_s \mu_t, \;\; \mu_s \in [0,1]\;\}.$$

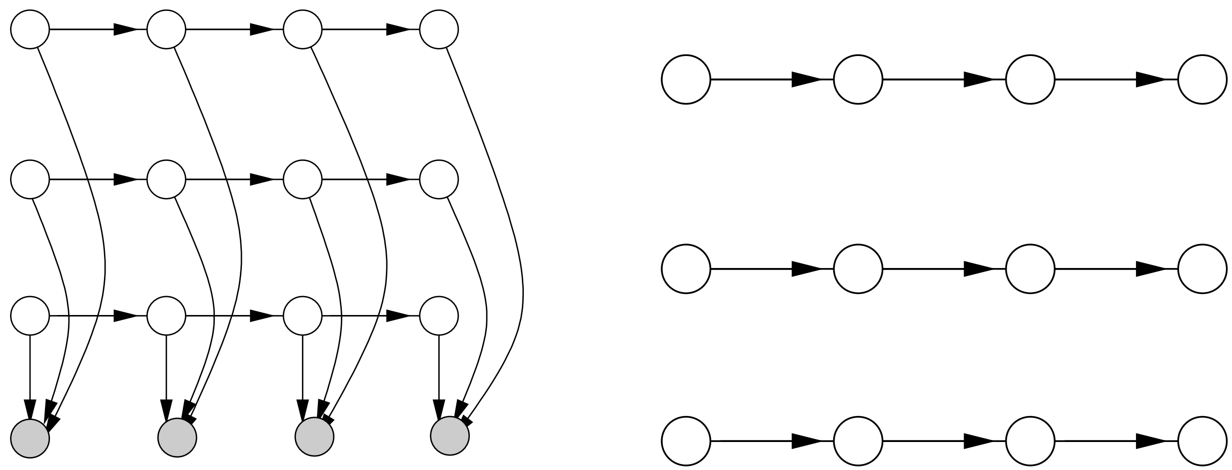
- approximate variational principle:

$$\max_{\mu_s \in [0,1]} \Big\{ \sum_{s \in V} \theta_s \mu_s + \sum_{(s,t) \in E} \theta_{st} \mu_s \mu_t - \big[\sum_{s \in V} \mu_s \log \mu_s + (1-\mu_s) \log(1-\mu_s) \big] \Big\}.$$

- **Co-ordinate ascent:** with all $\{\mu_t, t \neq s\}$ fixed, problem is strictly concave in μ_s and optimum is attained at

$$\mu_s \quad \longleftarrow \quad \big\{1 + \exp[-(\theta_s + \sum_{t \in \mathcal{N}(s)} \theta_{st} \mu_t)]\big\}^{-1}$$

Example: Structured mean field for coupled HMM



(a) (b)

- entropy of distribution that respects H decouples into sum: one term for each chain.
- *structured mean field updates* are an iterative method for finding the tightest approximation (either in terms of KL or lower bound)

Summary and future directions

- variational methods: statistical/computational tasks converted to optimization problems:
  (a) complementary to sampling-based methods (e.g., MCMC)
  (b) require entropy approximations, and characterization of marginal polytopes (sets of valid mean parameters)
  (c) a variety of new "relaxations" remain to be explored

- many open questions:
  (a) strong performance guarantees? (only for special cases thus far...)
  (b) extension to non-parametric settings?
  (c) hybrid techniques (variational and MCMC)
  (d) variational methods in parameter estimation
  (e) fast techniques for solving large-scale relaxations (e.g., SDPs, other convex programs)