Exponential Family Graphical Models: Inference, Learning and Convexity

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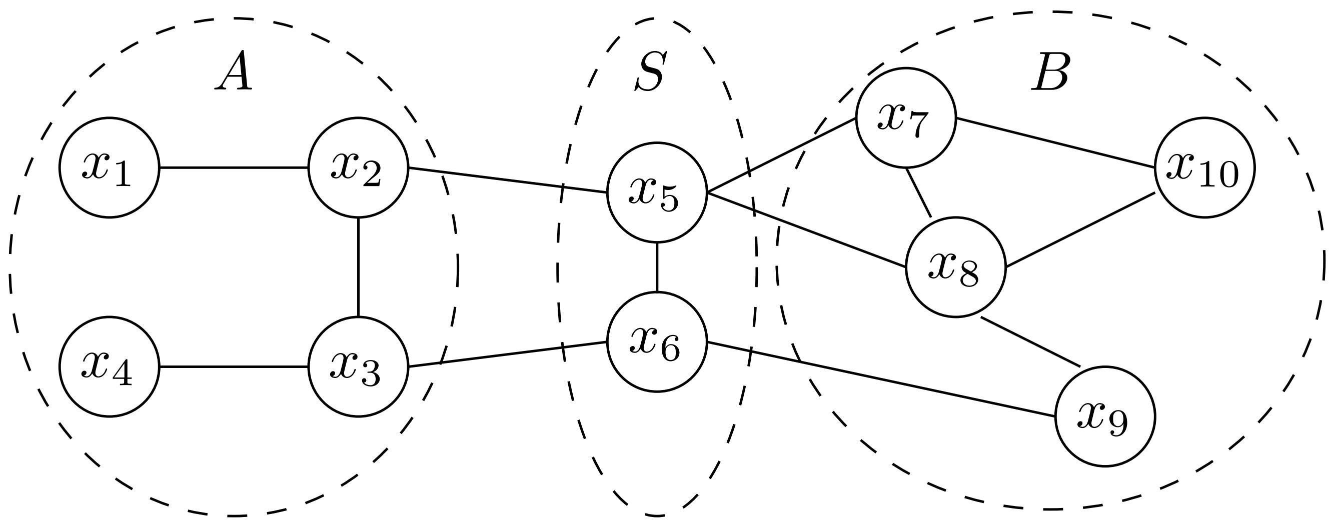
Outline

- Graphical Models and Recursive Inference (Pat)
  - Markovianity & Factorization
  - Exponential Families: Ising & Gaussian Models
  - Illustrative Example: 3×3 Ising Model
  - "Belief" Propagation: Sum/Max-Product & Gaussian Elim.
  - Exact inference gets hard! Many approximate methods...

- Model Identification in Exponential Families (Jason)
  - Convexity & Duality in Exponential Families
  - Variational Principles for Inference & Learning
  - Information Geometry & Iterative Projection Methods

Graphical Models: Markovianity

- Graph $G = (V, E)$ defines family of probability distributions
  - Node set V identifies random vector $x = (x_1, \ldots, x_{|V|})$
  - Edge set E indicates Markov properties with "separation"

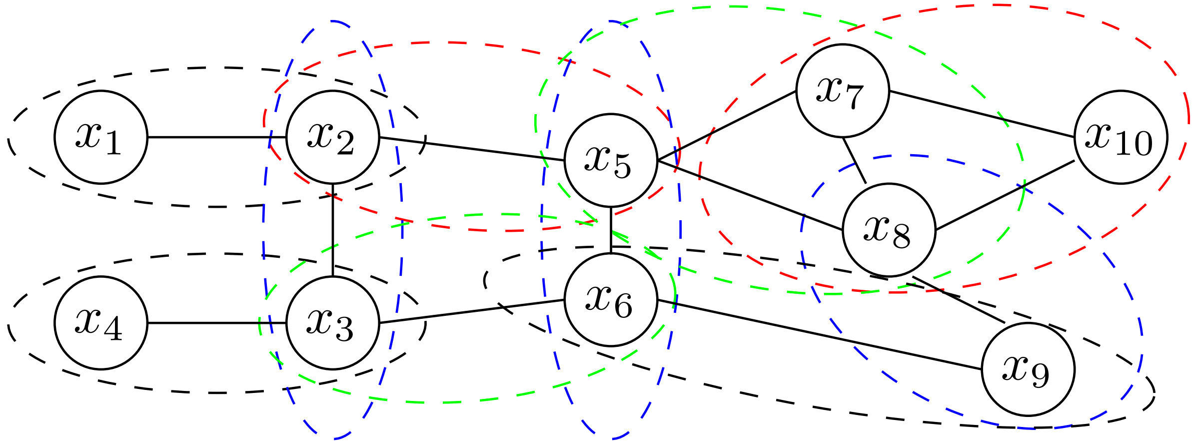


- **Definition:** Random vector x is *Markov on* G if and only if, for *every* triplet $A, S, B \subset V$ such that S separates A and B,

$$p\left(x_A, x_B | x_S\right) = p\left(x_A | x_S\right) p\left(x_B | x_S\right)$$

Graphical Models: Factorization

- Let edge set E define $p(x)$ as product of "local" functions
- But is there a notion of "local" applicable for general G?
  - Choose domains $C \subset V$ over *maximal cliques* of G



  - For each C, choose *potential function* $\psi_C : \mathcal{X}_C \to (0, \infty)$

- **Definition:** $p(x)$ *factors over* G if, for *at least one* collection $\{\psi_C\}$ of (maximal) clique potentials,

$$p(x) = \frac{1}{Z} \prod_C \psi_C(x_C) \quad (Z \in \mathbb{R} \text{ for normalization})$$

Graphical Models: Punchline & Asides

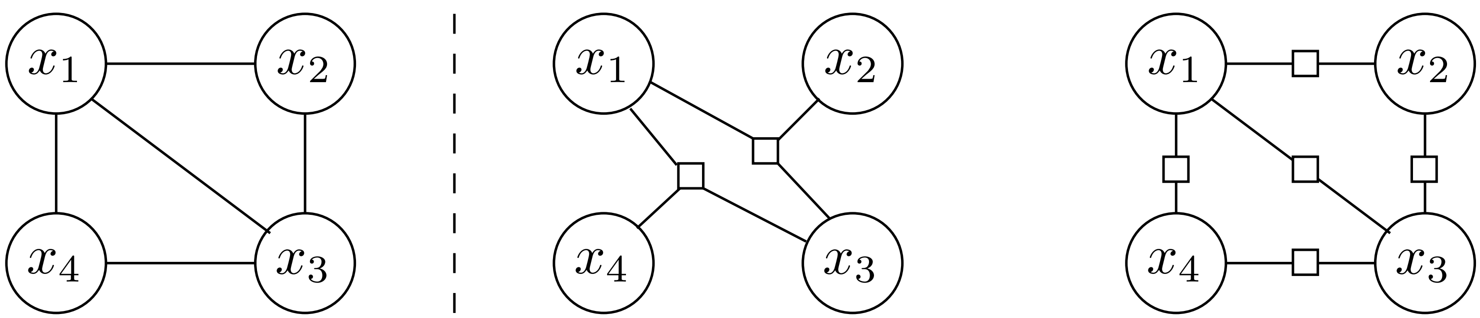
- **Theorem (Hammersley-Clifford):** "x Markov on G" and "p(x) factors over G" define equivalent families of distributions

  $\Rightarrow$ Graph structure tied to complexity of inference/learning $\Leftarrow$

- Connection to *Boltzmann distribution* in statistical physics

$$p(x) = \frac{1}{Z}\exp\left(-H(x)\right) \quad \left(\text{energy } H(x) = -\textstyle\sum_C \log\left[\psi_C(x_C)\right]\right)$$

- *Factor graphs* characterize more specific "local" structure



$\Downarrow$ $\quad$ $\Downarrow$ $\quad$ $\Downarrow$

$p(x) \propto \psi_{123}\psi_{134}$ $\quad$ $p(x) \propto \psi_{123}\psi_{134}$ $\quad$ $p(x) \propto \psi_{12}\psi_{23}\psi_{14}\psi_{34}$

Exponential Family Models

- All distributions on $\mathcal{X}$ that can be expressed in the form

$$p(x) = \exp\left[\theta' \phi(x) - \Psi(\theta)\right] \quad (\Psi : \mathbb{R}^d \to \mathbb{R} \text{ for normalization})$$

  with *parameters* $\theta \in \mathbb{R}^d$ and *features* $\phi : \mathcal{X} \to \mathbb{R}^d$

- Ising Models: if $x_i \in \{+1, -1\}$, then $d = |V| + |E|$ and

$$p(x) \propto \exp\left[\sum_{(i,j)\in E} \theta_{ij} x_i x_j + \sum_{i \in V} \theta_i x_i\right]$$

- Gaussian Models: if $x \sim N(J^{-1}h, J^{-1})$, let $\theta = (h, J)$ so

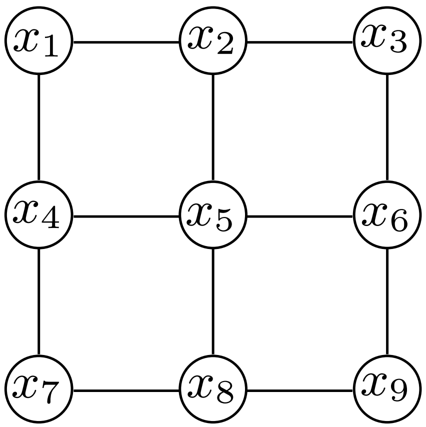
$$p(x) \propto \exp\left[-\frac{1}{2} x' J x + h' x\right]$$

  with matrix J *sparse* in correspondence with edge set E

Illustrative Example: 3×3 Ising Model

Graphical Model

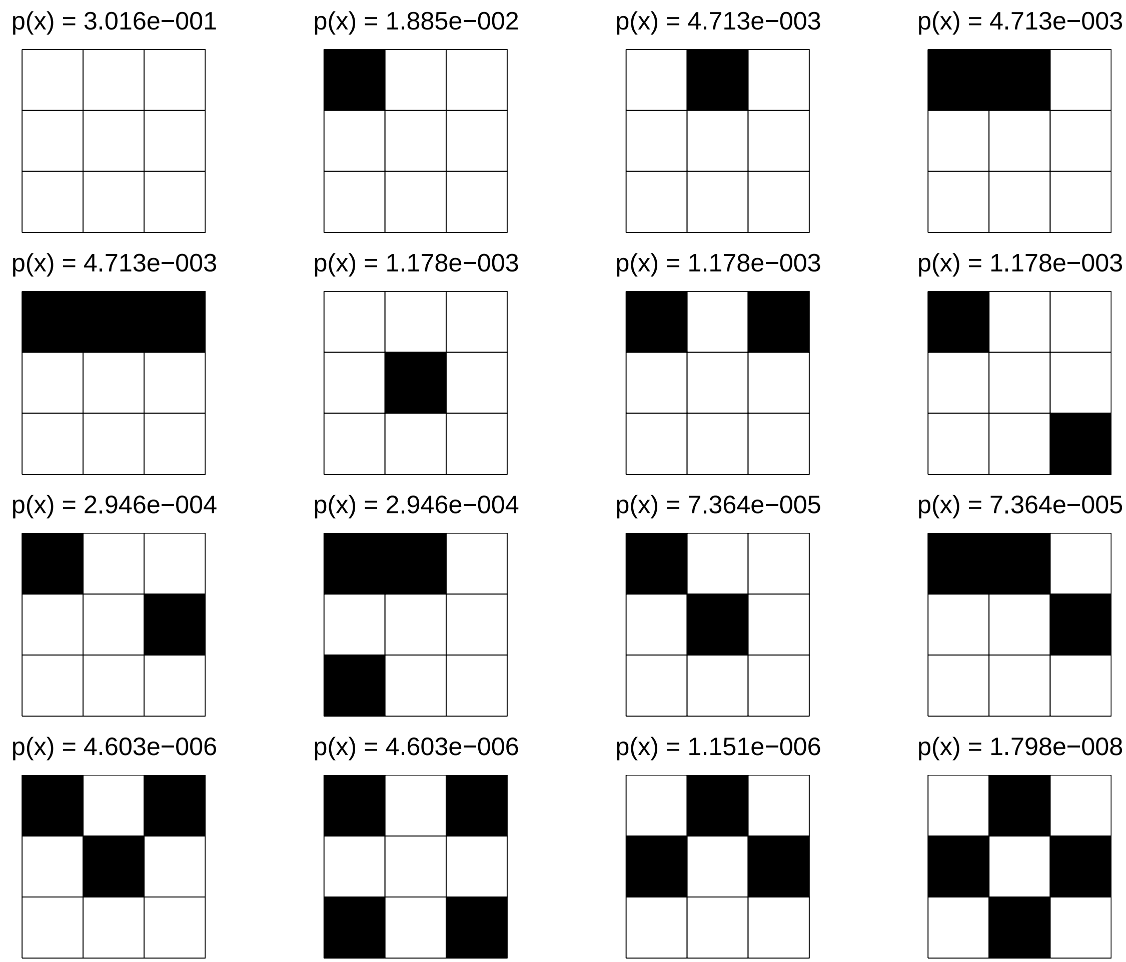
$$x_i \in \{-1, +1\}$$



$$\underbrace{\theta_i = 0,\ \ i \in V}_{\text{“uniform”}}$$

$$\underbrace{\theta_{ij} = 0.7,\ \ (i,j) \in E}_{\text{“attractive”}}$$

Samples



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Graphical Model

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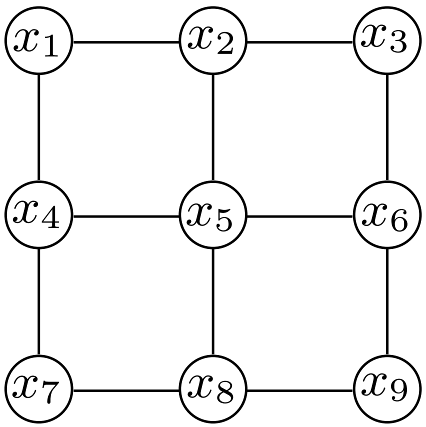

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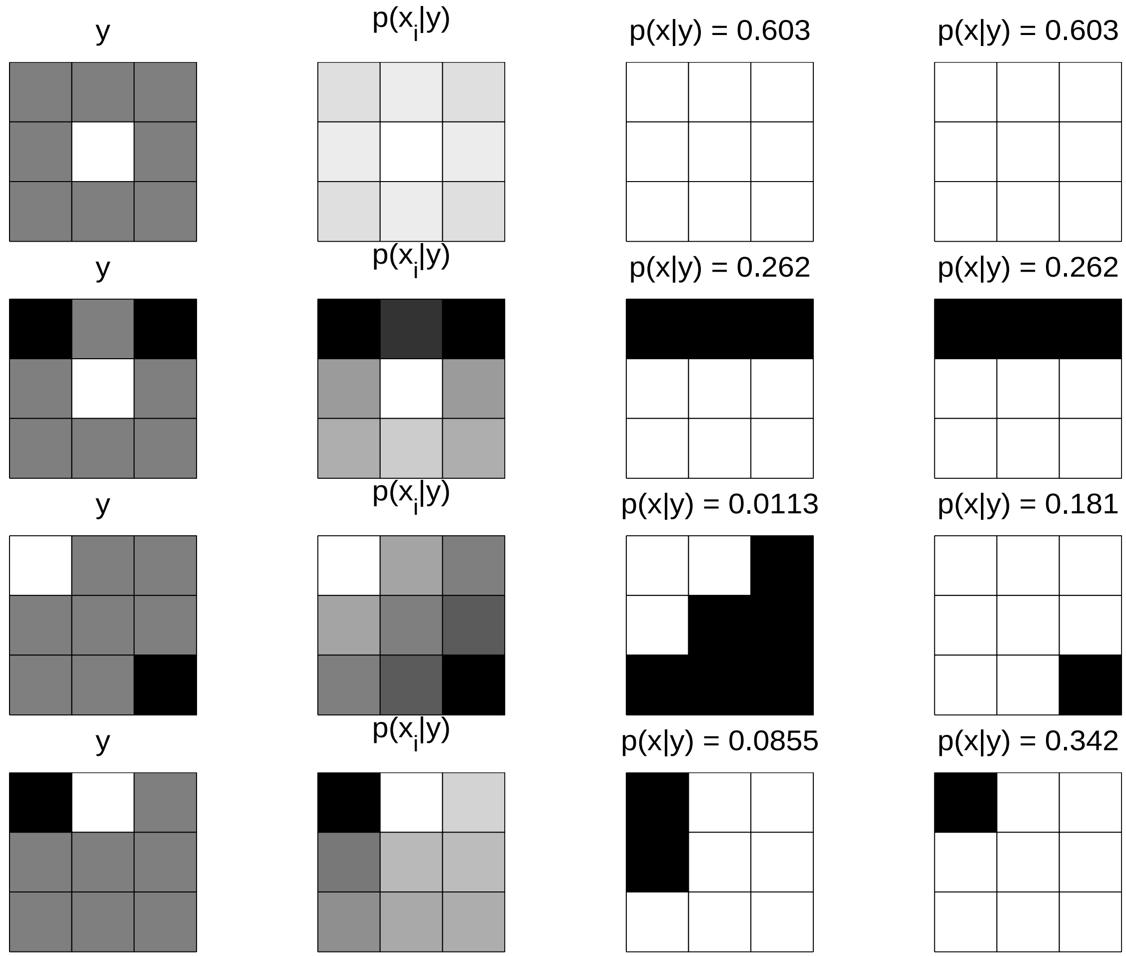
Inference



Inference Problems & Variable Elimination

- *Marginalization:* compute $p(x_A) = \sum_{x_{V \setminus A}} p(x)$
  - Elimination of nodes $V \setminus A$ by summation/integration
  - Basic operation to compute conditionals and likelihoods

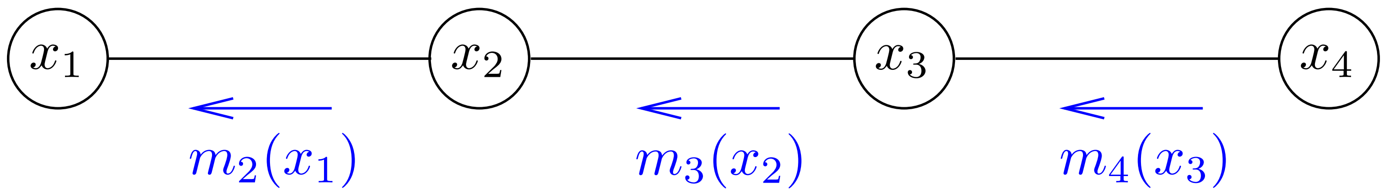
- Example: let $p(x) \propto \psi_{12}\psi_{13}\psi_{24}\psi_{35}\psi_{256}$ with $|\mathcal{X}_i| = r$ for $i \in V$
  - Direct computation of $p(x_1) = \sum_{x_2,\ldots,x_6} p(x)$ scales as r^6
  - Exploiting factorization in computation of $p(x_1)$ scales as r^3

$$p(x_1) = \frac{1}{Z} \sum_{x_2} \psi_{12} \sum_{x_3} \psi_{13} \sum_{x_4} \psi_{24} \sum_{x_5} \psi_{35} \sum_{x_6} \psi_{256}$$

- *Max-Marginalization:* compute $\nu(x_A) = \max_{x_{V \setminus A}} p(x)$
  - Elimination of nodes $V \setminus A$ by maximization
  - Basic operation to compute a mode of $p(x)$ (with caveat!)

Recursive Inference: “Message-Passing”

- Discrete-variable chain with $|V| = 4 \;\Rightarrow\; p(x) \propto \psi_{12}\psi_{23}\psi_{34}$

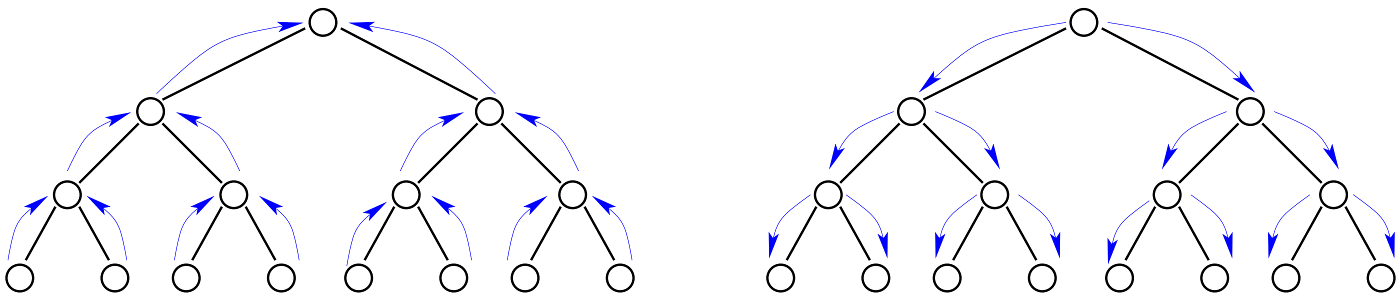


$$p(x_1) = \frac{1}{Z}\underbrace{\sum_{x_2}\psi_{12}(x_1,x_2)\underbrace{\sum_{x_3}\psi_{23}(x_2,x_3)\underbrace{\sum_{x_4}\psi_{34}(x_3,x_4)}_{m_4(x_3)}}_{m_3(x_2)}}_{m_2(x_1)}$$

- Key idea: apply most efficient elimination ordering
  - Marginalization at all nodes share intermediate terms m_i
  - “Message” interpretation useful for distributed settings

"Belief" Propagation on Trees

- Markov tree: $p(x) \propto \prod_{i \in V} \psi(x_i) \prod_{(i,j) \in E} \psi(x_i, x_j)$



- *Sum-Product* algorithm efficiently finds all marginals $p(x_i)$

$$m_{j \to i}(x_i) \;=\; \sum_{x_j} \psi(x_i, x_j) \left(\psi(x_j) \prod_{k \in N(j) \setminus i} m_{k \to j}(x_j) \right)$$

$$p(x_v) \;\propto\; \psi(x_v) \prod_{i \in N(v)} m_{i \to v}(x_v)$$

- *Max-Product* algorithm efficiently finds all max-marginals $\nu(x_i)$

Gaussian Elimination (GE) is a form of BP!

- Consider solution of $Jx = h$ by *Gaussian elimination*. Partition $V = A \cup B$ and eliminate variables B from equations A we obtain $\hat{J}_A x_A = \hat{h}_A$ where:

$$\begin{aligned} \hat{J}_A &= J_A - J_{A,B} J_B^{-1} J_{B,A} \\ \hat{h}_A &= h_A - J_{A,B} J_B^{-1} h_B \end{aligned}$$

  This is the *Schur complement* form of Gaussian elimination.

- Let $K(x; h, J) = \exp\{-\frac{1}{2} x' J x + h' x\}$. Then,

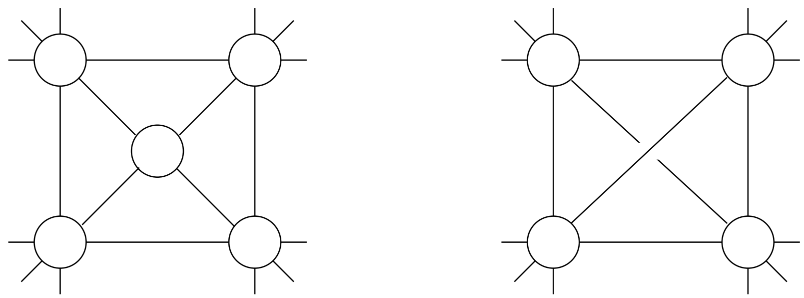
  1. *Integration*: $\int_{x_B} K(x_A, x_B; h, J) dx_B \propto K(x_A; \hat{h}_A, \hat{J}_A)$
  2. *Maximization*: $\max_{x_B} K(x_A, x_B; h, J) = K(x_A; \hat{h}_A, \hat{J}_A)$

  Consequently, Gaussian BP involves identical steps as in GE.

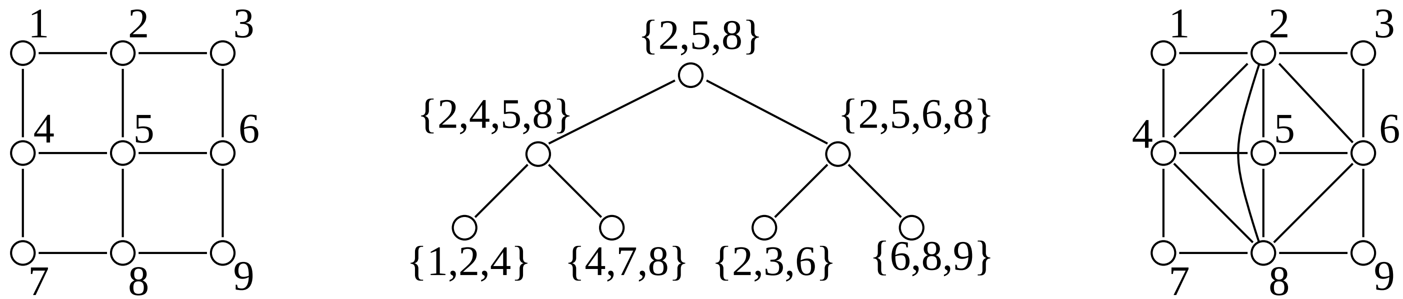
- The *Kalman filter* is also a form of BP on a Gauss-Markov chain but is based on a directed (causal) factorization.

Inference on Graphs with Cycles

- Still variable elimination...but complicated by "entanglement"



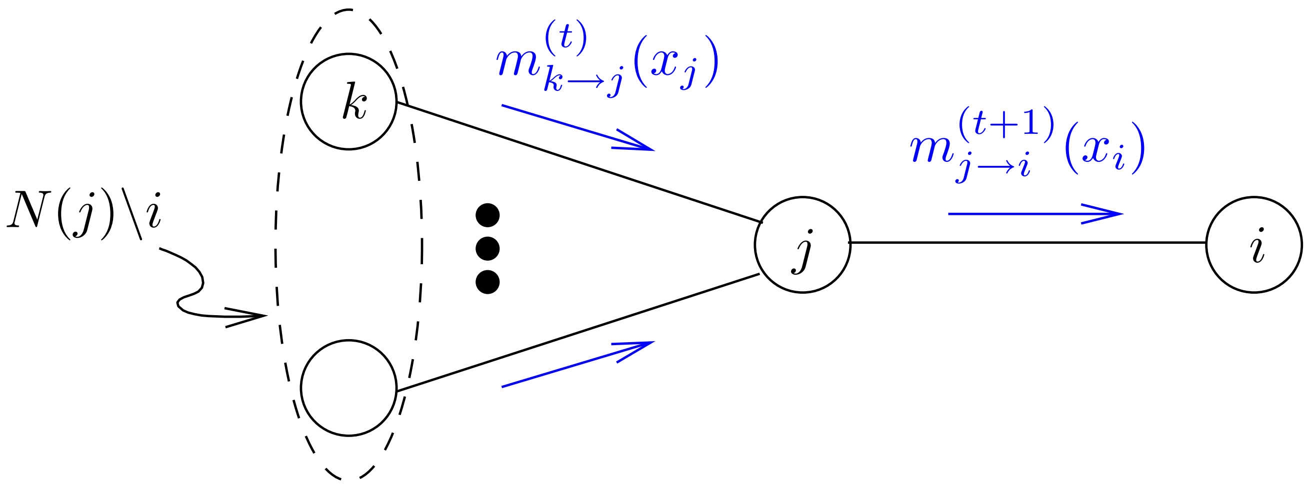
- *Junction Tree* algorithm performs exact computation
  - Key idea: aggregate nodes to equivalent tree



  - Tractable if aggregates are low-order (i.e., low "treewidth")

"Loopy Belief" Propagation

- Iterate BP equations at each node, ignorant of cycles



$$m^{(t+1)}_{j\to i}(x_i) = \sum_{x_j} \psi(x_i, x_j) \left(\psi(x_j) \prod_{k \in N(j)\backslash i} m^{(t)}_{k\to j}(x_j) \right)$$

- Need not converge: approximation if it does converge
  - Connection to coding: LDPC codes and "turbo codes"
  - Connection to physics: minimizing Bethe free energy

More about Exponential Families[a]...

- The *cumulant-generating function* plays a central role:

$$\Psi(\theta) = \log \int \exp\{\theta \cdot \phi(x)\} dx$$

e.g., $\Psi(\theta) = -\frac{1}{2} \log \det J(\theta) + \text{const}$ (Gaussian).

- Moment-generating property:

$$\nabla \Psi(\theta) = \mathbb{E}_\theta\{\phi(x)\} \equiv \eta(\theta)$$

where η are the *moments* $\equiv$ marginal probabilities (discrete), means, variances and edge-covariances (Gaussian).

- The curvature of $\Psi(\theta)$ is the *Fisher information matrix*:

$$\nabla^2 \Psi(\theta) = \mathbb{E}_\theta\{(\phi(x) - \eta(\theta))'(\phi(x) - \eta(\theta))\}$$

This is a spd covariance matrix, hence $\Psi(\theta)$ is convex.

[a]Barndorff-Nielsen '78.

Variational Principles

Fenchel duality [Fenchel '49; Rockafellar '74] The *convex conjugate* of Ψ equals the *negative entropy* as a function of the moments.

$$\Psi^*(\eta) \equiv \sup_\theta \{\eta \cdot \theta - \Psi(\theta)\} = -h(\eta)$$

Due to convexity of Ψ it holds that $(\Psi^*)^* = \Psi$.

Learning Given a desired set of moments η^* the corresponding parameters θ^* minimize the convex function:

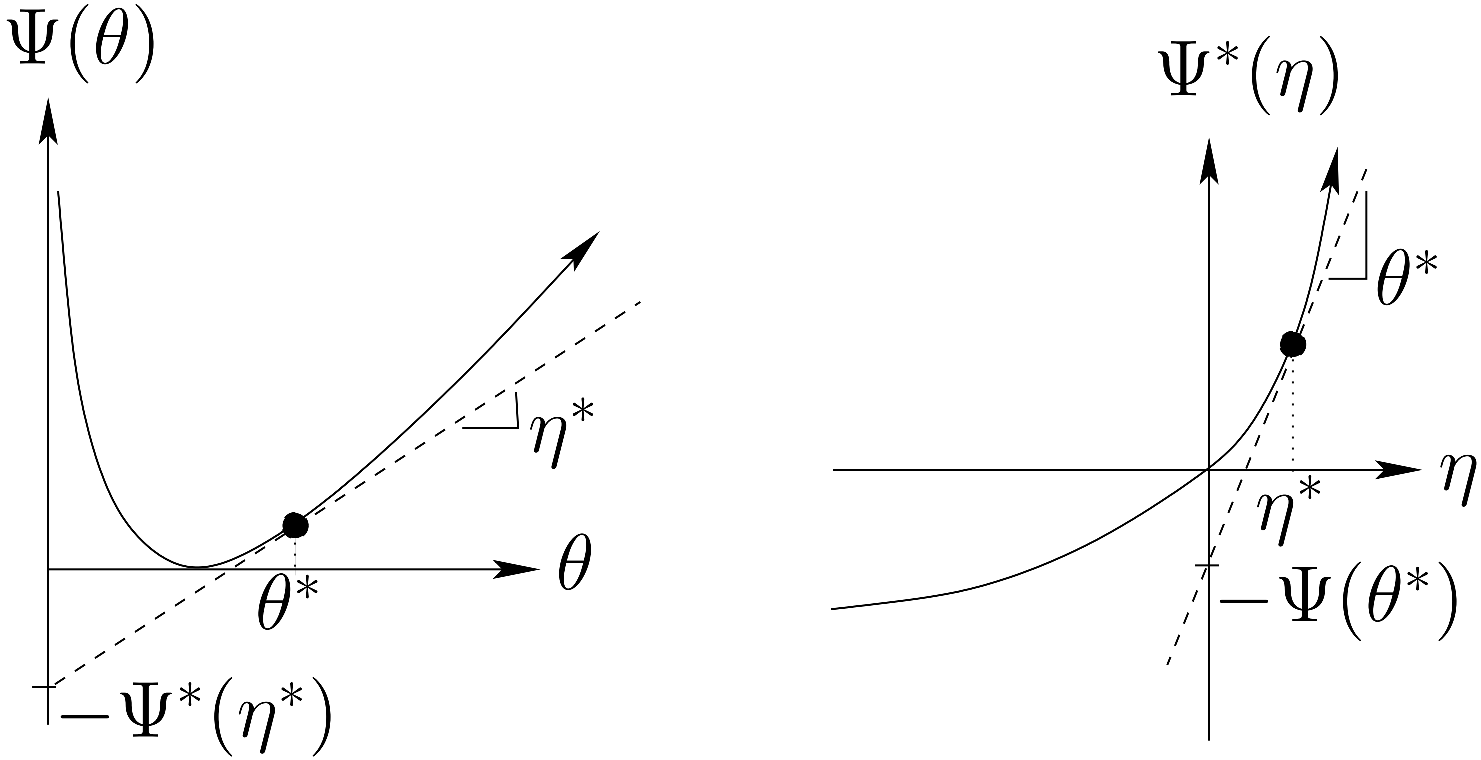
$$f(\theta) = \Psi(\theta) - \eta^* \cdot \theta$$

In ML parameter estimation, η^* are the empirical moments.

Inference Given θ^* the corresponding moments η^* minimize the convex function:

$$g(\eta) = \Psi^*(\eta) - \theta^* \cdot \eta$$

Leads to approximate inference [Wainwright & Jordan '03].


$\Psi(\theta)$
η^*
θ
θ^*
$-\Psi^*(\eta^*)$
$\Psi^*(\eta)$
θ^*
η
η^*
$-\Psi(\theta^*)$

Information Geometry[a]

- The *Bregman distance*[b] induced by $\Psi(\theta)$ equals the *Kullback-Leibler divergence.*

$$D(\theta^* \| \theta) = \Psi(\theta) - \{\Psi(\theta^*) + \nabla \Psi(\theta^*) \cdot (\theta - \theta^*)\}$$

  Similar relation holds between $\Psi^*(\eta)$ and $D(\eta \| \eta^*)$.

- *Information Projection:* let $p \in \mathcal{F}$ and let $\mathcal{E} \subset \mathcal{F}$ is affine in θ.

$$p_{\mathcal{E}} \equiv \arg\min_{q \in \mathcal{E}} D(p \| q)$$

  Optimality condition: $(\eta(q) - \eta(p)) \perp (\theta(\mathcal{E}) - \theta(p_{\mathcal{E}}))$.

- *Pythagorean Relation:* $p_{\mathcal{E}}$ is unique member of $\mathcal{E}$ satisfying

$$D(p \| q) = D(p \| p_{\mathcal{E}}) + D(p_{\mathcal{E}} \| q)$$

  for all $q \in \mathcal{E}$.

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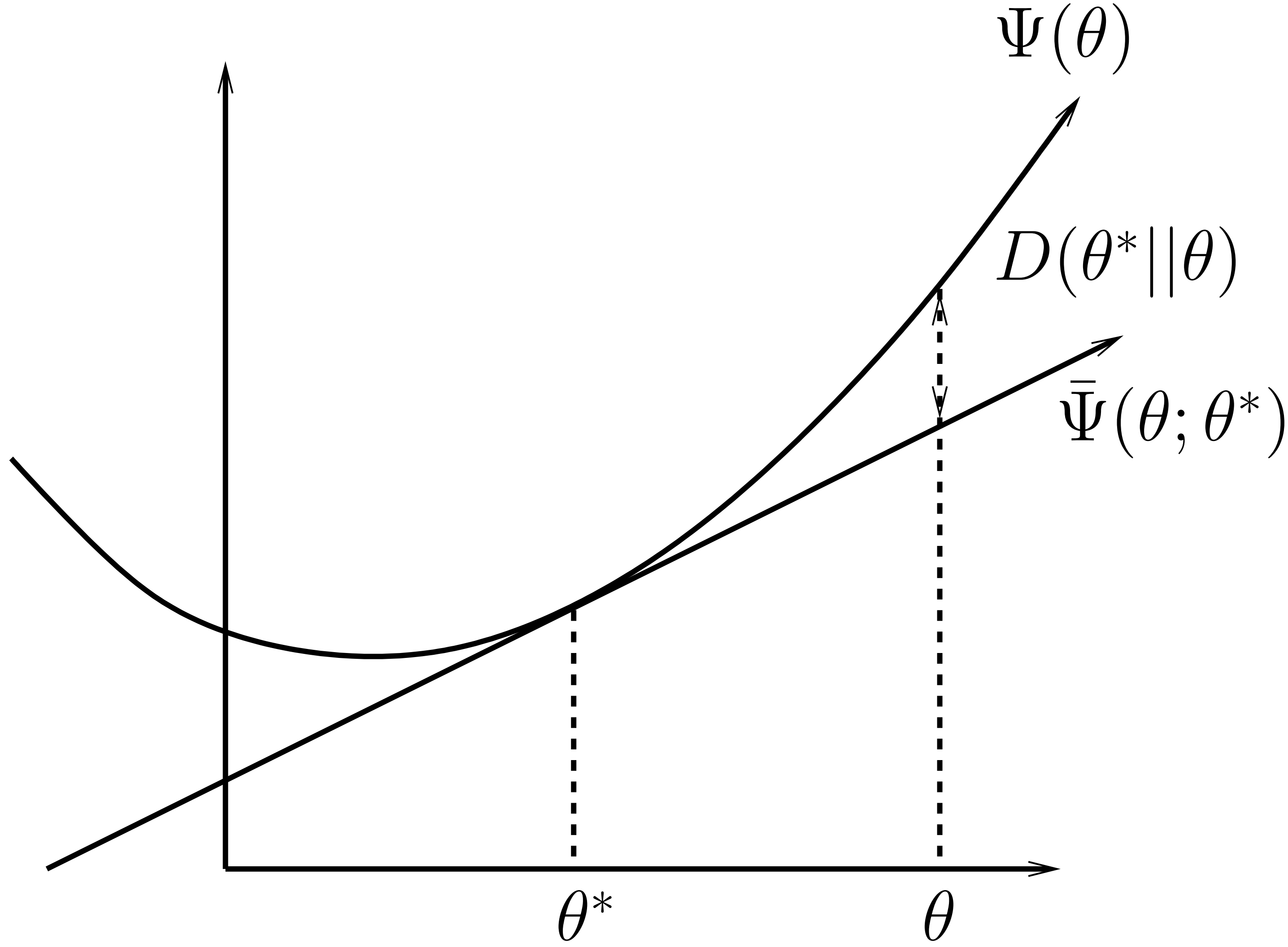
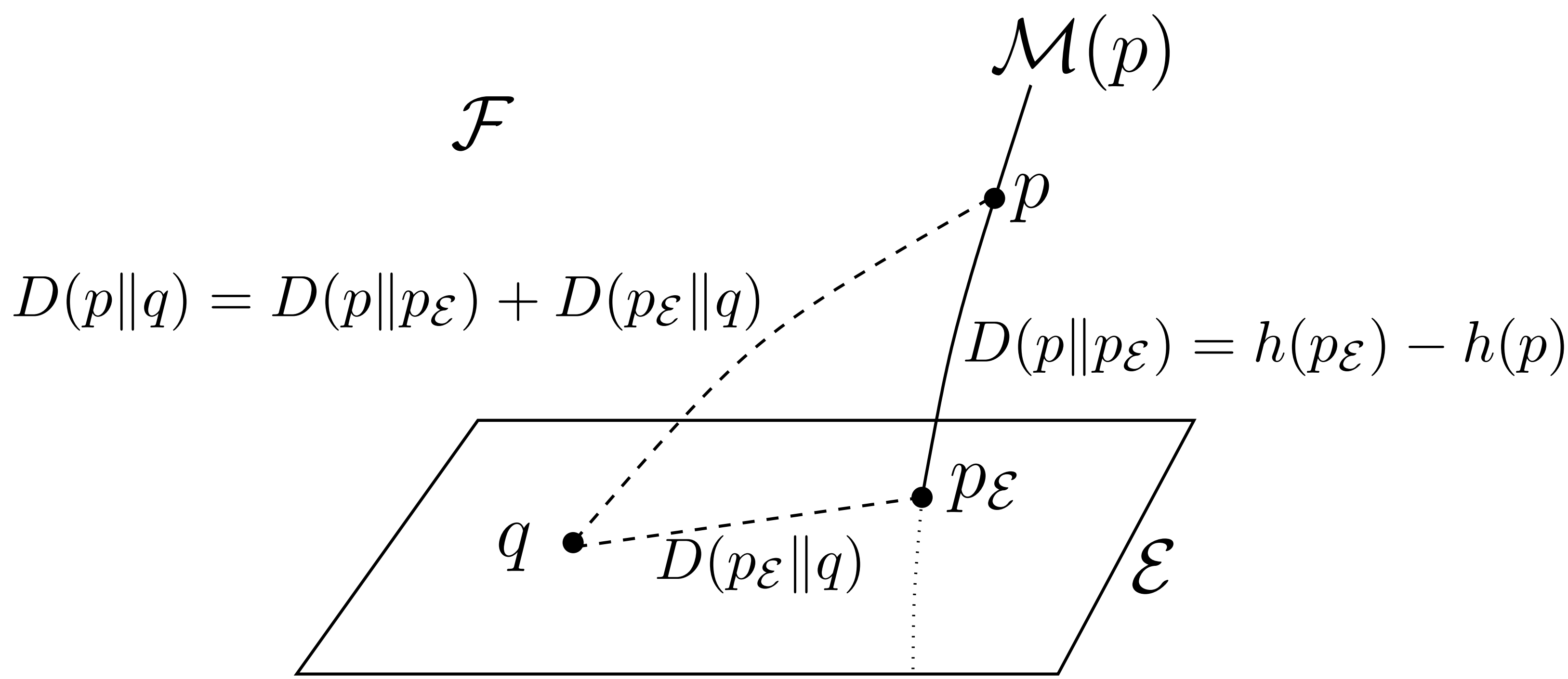
[a] Chentsov '72; Efron '78; Amari '01.

[b] Bregman '67; Bauschke & Bowein '97.



$\Psi(\theta)$
$D(\theta^*||\theta)$
$\bar{\Psi}(\theta;\theta^*)$
θ^*
θ


$\mathcal{M}(p)$
$\mathcal{F}$
p
$D(p\|q) = D(p\|p_{\mathcal{E}}) + D(p_{\mathcal{E}}\|q)$
$D(p\|p_{\mathcal{E}}) = h(p_{\mathcal{E}}) - h(p)$
$p_{\mathcal{E}}$
q
$D(p_{\mathcal{E}}\|q)$
$\mathcal{E}$

IPF as Projection onto Convex Sets

Iterate over cliques $\{C_k\}$ of graph $\mathcal{G}$, update potentials to enforce marginal constraints...

- *Iterative Proportional Fitting:*[a] marginal pmfs $p(x_{C_k})$

$$q^{(k+1)}(x) = q^{(k)}(x) \times \frac{p(x_{C_k})}{q^{(k)}(x_{C_k})}$$

- *Covariance Selection:*[b] marginal covariances P_{C_k}

$$J_{C_k}^{(k+1)} = J_{C_k}^{(k)} + (P_{C_k}^{-1} - (P_{C_k}^{(k)})^{-1})$$

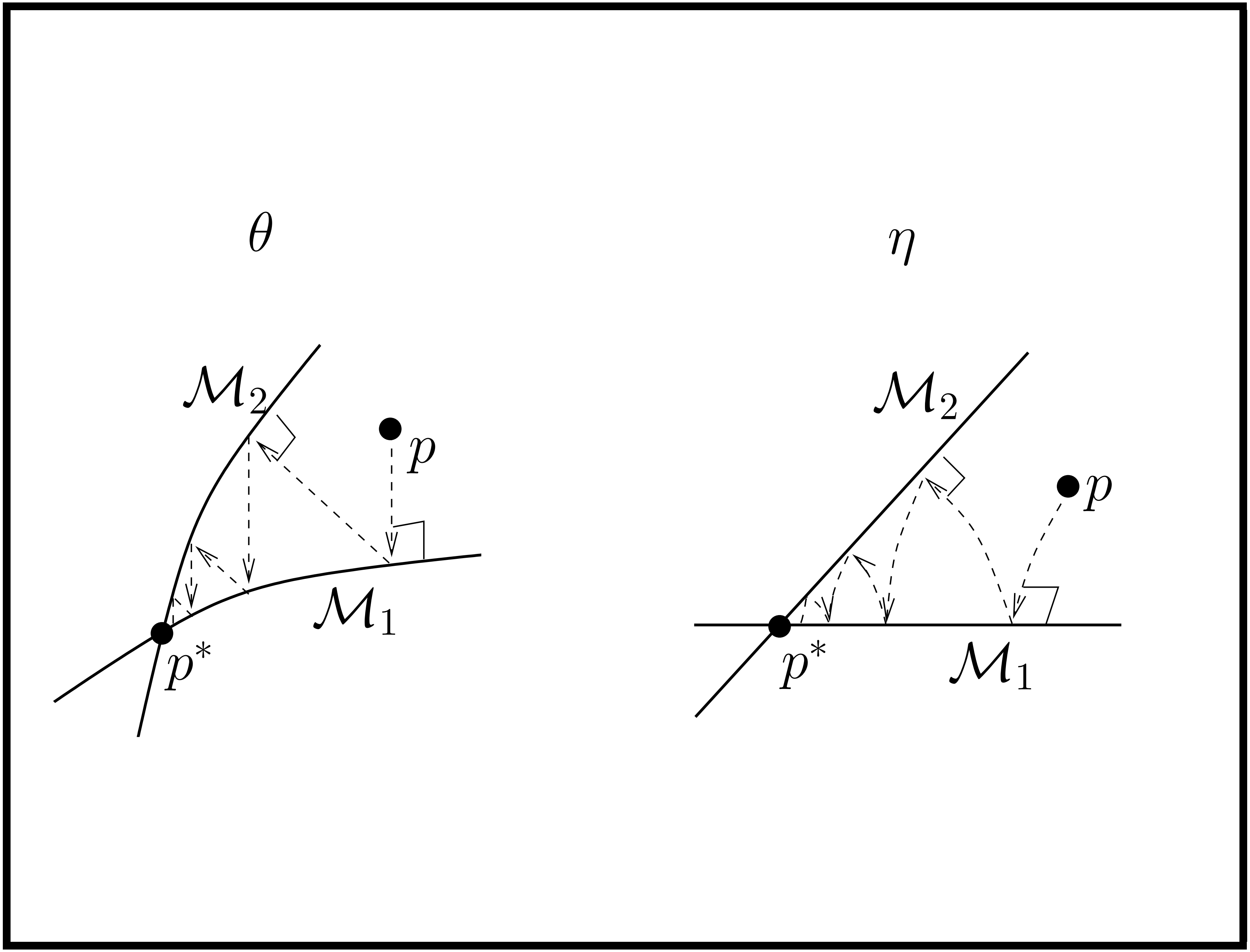
- *Projection Interpretation:*[c] $\mathcal{M}_k \subset \mathcal{F}$ affine in η imposes marginal moment constraints on clique C_k.

$$q^{(k+1)} = \arg \min_{p \in \mathcal{M}_k} D(p \| q^{(k)})$$

[a] Kullback '68.

[b] Dempster '77; Speed & Kiiveri '86.

[c] Csiszar '75.



θ
$\mathcal{M}_2$
p
$\mathcal{M}_1$
p^*
η
$\mathcal{M}_2$
p
p^*
$\mathcal{M}_1$

Expectation-Maximization as Alternating Projections

- Let $\mathcal{F} = \{p_\theta(x, y)\}$ be an exponential family, given observations $y_1, \ldots, y_n$, select θ to maximize the (marginal) log-likelihood:

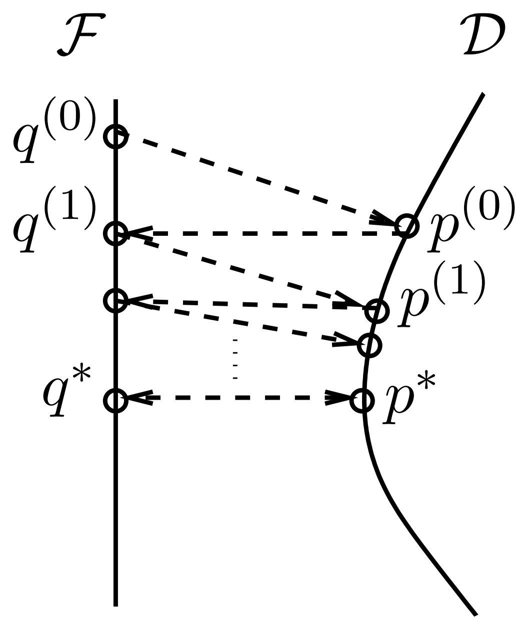
$$f(\theta) \equiv \sum_i \log \int p_\theta(x, y_i) dx$$

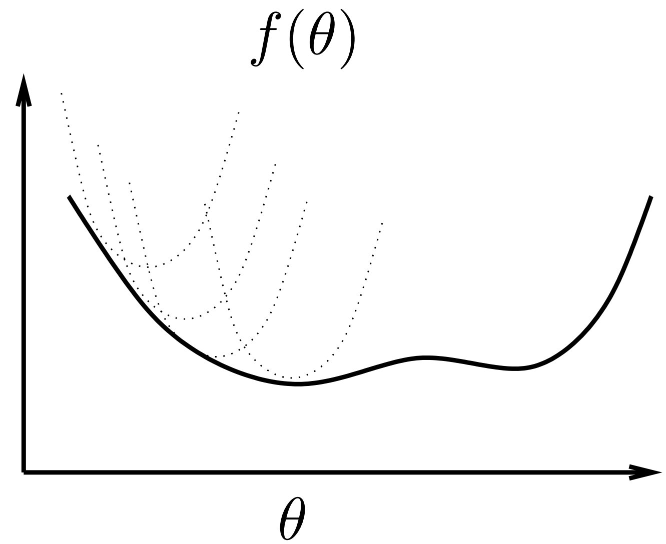
  Typically non-convex, possibly many local minima!

- Expectation-Maximization[a] (Alternating Projections): Let $q^{(0)} \in \mathcal{F}$ and $\mathcal{D} = \{p(x, y) | \int p(x, y) dy = p^*(y)\}$
  1. (E-step) $p^{(k+1)} = \arg\min_{p \in \mathcal{D}} D(p \| q^{(k)})$ (inference)
  2. (M-step) $q^{(k+1)} = \arg\min_{q \in \mathcal{F}} D(p^{(k+1)} \| q)$ (IPF)

  $\Rightarrow$ local minima of $f(\theta)$.

[a] Dempster, Laird & Rubin '77.


$\mathcal{F}$
$\mathcal{D}$
$q^{(0)}$
$q^{(1)}$
q^*
$p^{(0)}$
$p^{(1)}$
p^*


$f(\theta)$
θ

Summary: Exponential Family Graphical Models

- Graphical models combine graph theory and probability theory
- Exponential family representation links to convex analysis
- Lead to principled approximations for large-scale problems
  - Inference: compute marginals/modes of a given $p(x)$
  - Learning: design parameterized $p(x)$ given sample data
- Active research topics
  - Approximate Inference
  - Model Selection