

Graphical Models

parameter learning in undirected models

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Winter 2018

Learning objectives

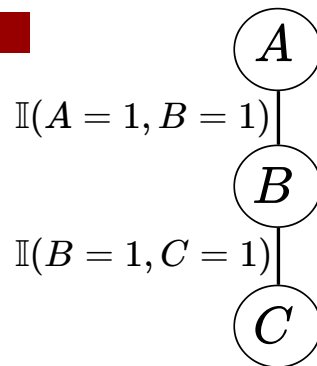
- the form of likelihood for undirected models
 - why is it difficult to optimize?
- **conditional** likelihood in undirected models
- different approximations for parameter learning

Likelihood in MRFs

example

probability dist.

$$p(A, B, C; \theta) = \frac{1}{Z} \exp(\theta_1 \mathbb{I}(A = 1, B = 1) + \theta_2 \mathbb{I}(B = 1, C = 1))$$



Likelihood in MRFs

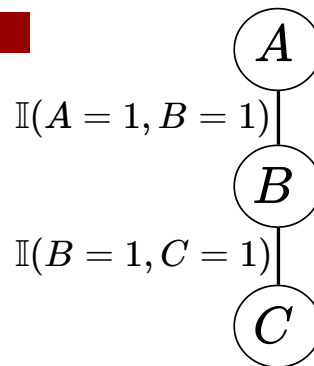
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observations $|\mathcal{D}| = 100$

- $\mathbb{E}_{\mathcal{D}}[\mathbb{I}(A = 1, B = 1)] = .4, \mathbb{E}_{\mathcal{D}}[\mathbb{I}(B = 1, C = 1)] = .4$



Likelihood in MRFs

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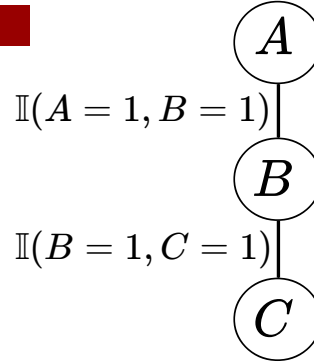
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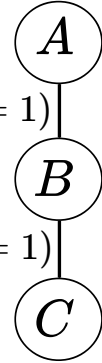
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log-likelihood: $\log p(\mathcal{D}; \theta) = \sum_{a,b,c \in \mathcal{D}} \theta_1 \mathbb{I}(a = 1, b = 1) + \theta_2 \mathbb{I}(b = 1, c = 1) - 100 \log Z(\theta)$
 $= 40\theta_1 + 40\theta_2 - 100 \log Z(\theta)$



Likelihood in MRFs

example



$$\mathbb{I}(A = 1, B = 1)$$

$$\mathbb{I}(B = 1, C = 1)$$

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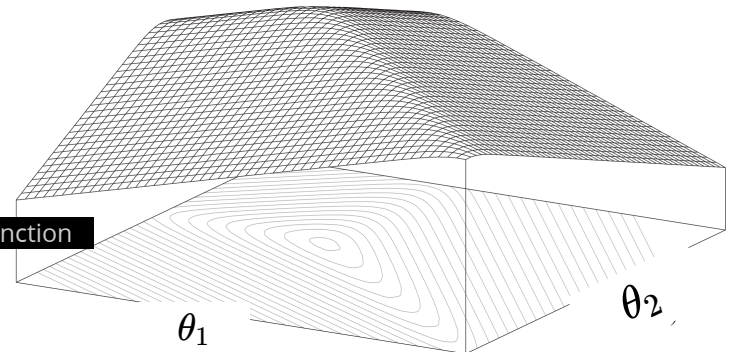
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because of the partition function

the likelihood does not decompose

log-likelihood function



Likelihood in **linear exponential family** (log-linear models)

probability distribution $p(x; \theta) = \frac{1}{Z(\theta)} \exp(\langle \theta, \phi(x) \rangle)$
sufficient statistics

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expected sufficient statistics $\mu_{\mathcal{D}}$

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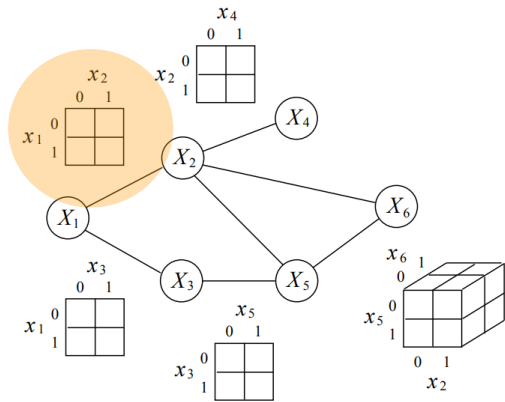


image: Michael Jordan's draft

expected sufficient statistics

$$\mathbb{E}_{\mathcal{D}}[\mathbb{I}(X_1 = 0, X_2 = 0)] = P(X_1 = 0, X_2 = 0)$$

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params.

$$\theta_{1,2,0,0}$$

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$\log Z(\theta)$ has interesting **properties**

$$\frac{\partial}{\partial \theta_i} \log Z(\theta) = \frac{\frac{\partial}{\partial \theta_i} \sum_x \exp(\langle \theta, \phi(x) \rangle)}{Z(\theta)} = \frac{1}{Z(\theta)} \sum_x \phi_i(x) \exp(\langle \theta, \phi(x) \rangle) = \mathbb{E}_p[\phi_i(x)] \quad \text{SO} \quad \nabla_{\theta} \log Z(\theta) = \mathbb{E}_{\theta}[\phi(x)]$$

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$$\frac{\partial^2}{\partial \theta_i \partial \theta_j} \log Z(\theta) = \mathbb{E}[\phi_i(x) \phi_j(x)] - \mathbb{E}[\phi_i(x)] \mathbb{E}[\phi_j(x)] = \text{Cov}(\phi_i, \phi_j)$$

so the Hessian matrix is positive definite $\rightarrow \log Z(\theta)$ is **convex**

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concave



Likelihood in **linear exponential family** (log-linear models)

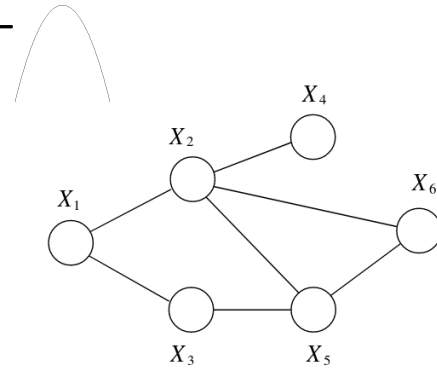
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should be easy to maximize (?) **NO!**

- estimating $Z(\theta)$ is a **difficult inference problem**
- how about just using the **gradient** info?
 - involves inference as well $\nabla_{\theta} \log Z(\theta) = \mathbb{E}_{\theta}[\phi(x)]$



○ any combination of inference-gradient based optimization for learning undirected models

Moment matching for linear exponential family

probability distribution $p(x; \theta) = \frac{1}{Z(\theta)} \exp(\langle \theta, \phi(x) \rangle)$

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set its derivative to zero $\nabla_{\theta} \ell(\theta, \mathcal{D}) = |\mathcal{D}| (\mathbb{E}_{\mathcal{D}}[\phi(x)] - \mathbb{E}_{p_{\theta}}[\phi(x)]) = 0$
 $\Rightarrow \mathbb{E}_{p_{\theta}}[\phi(x)] = \mathbb{E}_{\mathcal{D}}[\phi(x)]$

find the parameter θ

that results in the same expected sufficient statistics as the data

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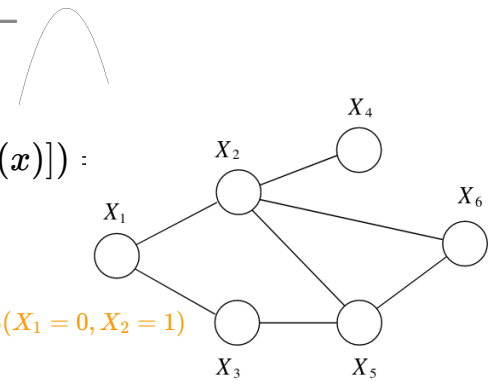
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$$p(X_1 = 0, X_2 = 1; \theta) = p_{\mathcal{D}}(X_1 = 0, X_2 = 1)$$

Learning needs inference in an inner loop

maximizing the likelihood: $\arg \max_{\theta} \log p(\mathcal{D}|\theta)$

- gradient $\propto \mathbb{E}_{\mathcal{D}}[\phi(x)] - \mathbb{E}_{p_{\theta}}[\phi(x)]$

- optimality condition $\mathbb{E}_{\mathcal{D}}[\phi(x)] = \mathbb{E}_{p_{\theta}}[\phi(x)]$

easy to calculate

inference in the graphical model

example: in discrete pairwise MRF $p_{\mathcal{D}}(x_i, x_j) = p(x_i, x_j; \theta) \quad \forall i, j \in \mathcal{E}$

empirical marginals

marginals in our current model

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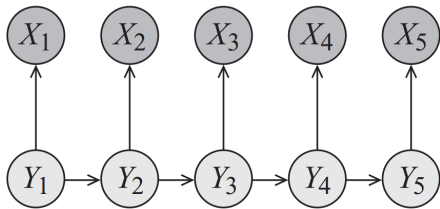
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what if exact inference is infeasible?

- learning with approx. inference often \equiv exact optimization of approx. objective
 - use sampling, variational inference ...

Conditional training

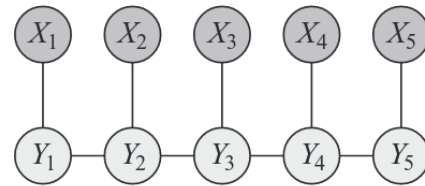
Recall generative vs. discriminative training



Hidden Markov Model (HMM) trained generatively

$$\ell(\mathcal{D}, \theta) = \sum_{(x,y) \in \mathcal{D}} \log p(x, y)$$

- easy to train the Bayes-net
- the likelihood decomposes



Conditional random fields (CRF)

- trained discriminatively
- maximizing conditional log-likelihood

$$\ell_{Y|X}(\mathcal{D}, \theta) = \sum_{(x,y) \in \mathcal{D}} \log p(y|x)$$

- how to maximize this?

Conditional training

objective: $\arg \max_{\theta} \ell_{Y|X}(\mathcal{D}, \theta) = \arg \max_{\theta} \sum_{(x,y) \in \mathcal{D}} \log p(y|x)$

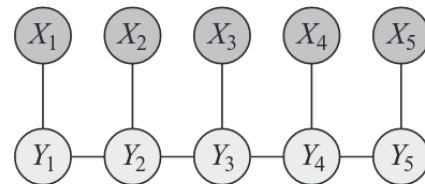
again consider the gradient

$$\nabla_{\theta} \ell_{Y|X}(\mathcal{D}, \theta) = \sum_{(x',y') \in \mathcal{D}} \phi(x', y') - \mathbb{E}_{p(\cdot|x;\theta)}[\phi(x', y)]$$

- conditional expectation of sufficient statistics
- it's conditioned on the observed x'

to obtain the gradient:

- for each instance $(x, y) \in \mathcal{D}$
 - run inference conditioned on x



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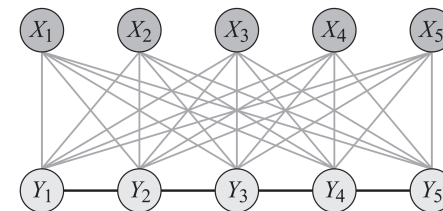
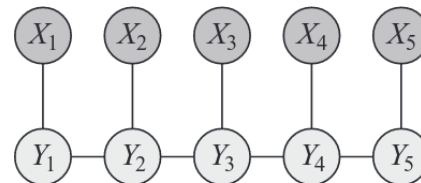
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to obtain the gradient:

- for each instance $(x, y) \in \mathcal{D}$
 - run inference conditioned on x
- compared to generative training in undirected models
 - pro:** conditioning could simplify inference
 - con:** have to run inference for each datapoint



inference on the reduced MRF
is easy in this case

Local priors & regularization

max-likelihood can lead to over-fitting

Bayesian approach:

- in Bayes-nets: decomposed prior $p(\theta)$ \rightarrow decomposed posterior $p(\theta | \mathcal{D})$
- in Markov nets: posterior does not decompose (because of the likelihood)

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alternative to a full-Bayesian approach

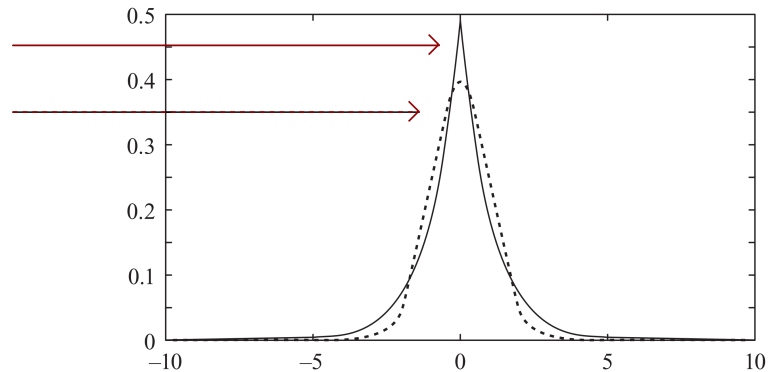
MAP inference: find the maximum of the posterior $\arg \max_{\theta} \log p(\mathcal{D}|\theta) + \log p(\theta)$

- does not model uncertainty
- sensitive to parametrization
- serves as a regularization
- does not have to be conjugate

Gaussian & Laplacian priors

MAP inference: find the maximum of the posterior $\arg \max_{\theta} \log p(\mathcal{D}|\theta) + \log p(\theta)$

- $p(\theta)$
- the product of univariate Laplacian (L1 reg.)
 - the product of univariate Gaussian (L2 reg.)



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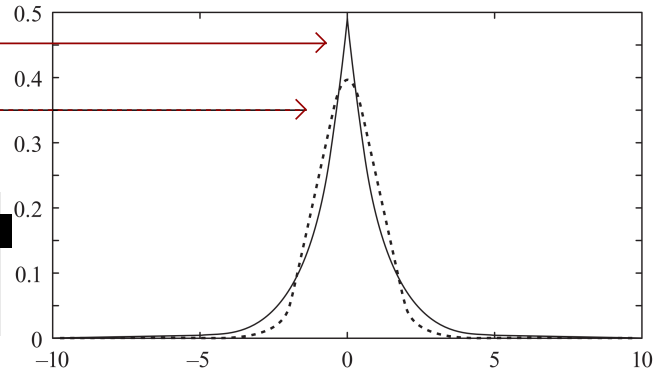
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$$p(\theta | \sigma) \propto \prod_i \exp\left(-\frac{\theta_i^2}{2\sigma^2}\right) \Rightarrow$$

$$\log p(\theta | \sigma) = -\frac{1}{2\sigma^2} \sum_i \theta_i^2 + c$$

Gaussian prior

L2 regularization penalty term



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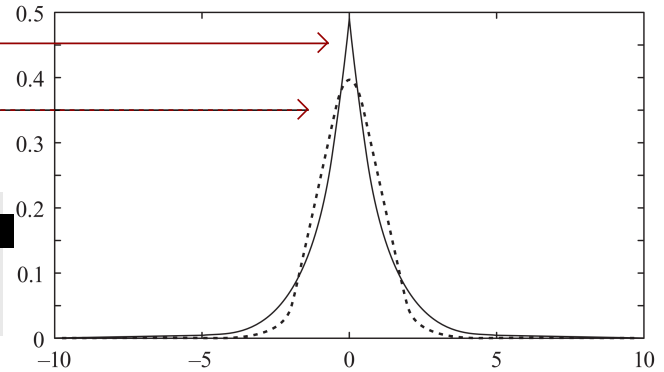
$$\log p(\theta | \sigma) = -\frac{1}{2\sigma^2} \sum_i \theta_i^2 + c \quad \text{L2 regularization penalty term}$$

$$p(\theta | \beta) = \prod_i \frac{1}{2\beta} \exp\left(-\frac{|\theta_i|}{\beta}\right) \Rightarrow$$

Laplacian prior

sparsity-inducing

$$\log p(\theta | \beta) = -\frac{1}{\beta} \sum_i |\theta_i| \quad \text{L1 regularization penalty term}$$



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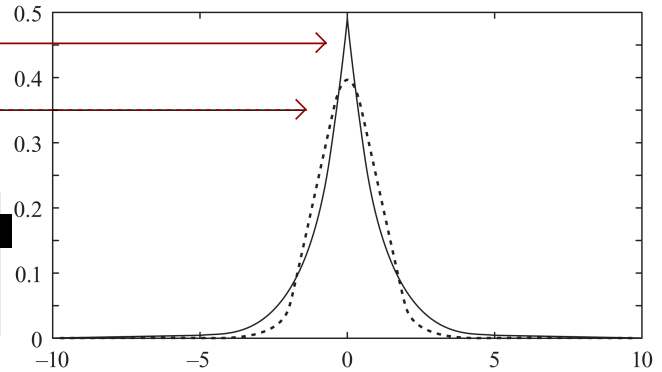
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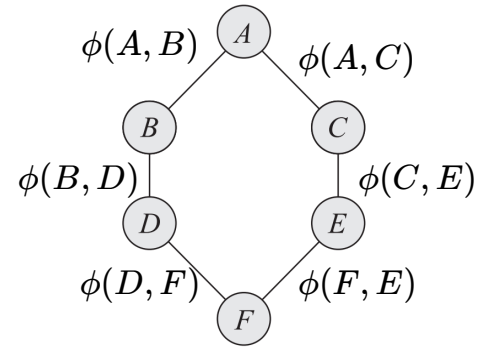
- both of these bias the posterior towards **smaller parameters**
 - why is this a good idea?

Pseudo-moment matching

we want to set the parameters θ such that
if/when loopy BP converges:

$$p_{\mathcal{D}}(A, B) = \hat{p}(A, B; \theta), p_{\mathcal{D}}(B, D) = \hat{p}(B, D; \theta) \dots$$

empirical marginals marginals using BP



Pseudo-moment matching

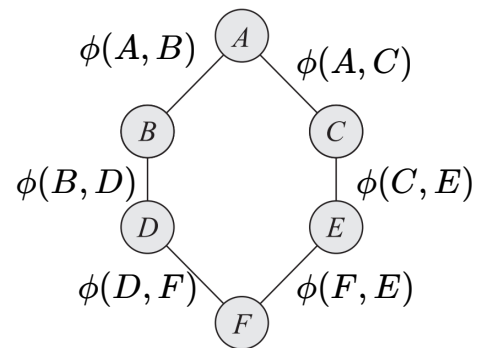
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empirical marginals
marginals using BP

idea: use the reparametrization in BP

$$\bullet \bullet \bullet p(A, B, C, D, E, F) \propto \frac{\hat{p}(A, B) \dots \hat{p}(C, A)}{\hat{p}(A) \dots \hat{p}(F)}$$



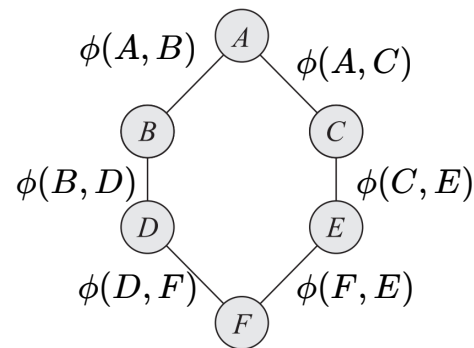
*product of clique marginals
cancel the double-counts*

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empirical marginals
marginals using BP



idea: use the **reparametrization** in BP

$$\bullet \bullet \bullet p(A, B, C, D, E, F) \propto \frac{\hat{p}(A, B) \dots \hat{p}(C, A)}{\hat{p}(A) \dots \hat{p}(F)}$$

\longrightarrow product of clique marginals
 \longrightarrow cancel the double-counts

set the factors using empirical marginals

- e.g., $\phi(A, B) \leftarrow p_{\mathcal{D}}(A, B) / p_{\mathcal{D}}(A)$
- each term in the numerator & denominator of $\bullet \bullet \bullet$ should be used exactly once
- if we run BP on the resulting model we will have $p_{\mathcal{D}}(A, B) = \hat{p}(A, B; \theta), p_{\mathcal{D}}(B, D) = \hat{p}(B, D; \theta) \dots$

Pseudo-likelihood

log-likelihood: $\log p(\mathcal{D}; \theta) = \sum_{x \in \mathcal{D}} \sum_i \log p(x_i | x_1, \dots, x_{i-1}; \theta)$ using the **chain rule**

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pseudo log-likelihood is an approximation

$$\log p(\mathcal{D}; \theta) \approx \sum_{x \in \mathcal{D}} \sum_i \log p(x_i | \overset{[x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n]}{x_{-i}}; \theta)$$

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$$\frac{p(x; \theta)}{\sum_{x_i} p(x; \theta)} = \frac{\tilde{p}(x; \theta)}{\sum_{x_i} \tilde{p}(x; \theta)} \quad \text{eliminated the normalization constant}$$

Pseudo-likelihood

log-likelihood: $\log p(\mathcal{D}; \theta) = \sum_{x \in \mathcal{D}} \sum_i \log p(x_i | x_1, \dots, x_{i-1}; \theta)$ using the **chain rule**

pseudo log-likelihood is an approximation

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this assumption simplifies the gradient:

- instead of calculating $\sum_{x \in \mathcal{D}} \phi_k(x) - |\mathcal{D}| \mathbb{E}_{p_\theta}[\phi_k(x)]$ **expensive!**
- use $\sum_{x \in \mathcal{D}} \phi_k(x) - \sum_i \mathbb{E}_{p(\cdot | x_{-i})}[\phi_k(x'_i, x_{-i})]$ can be further simplified using Markov blanket for each node...
- **upshot:** only conditional expectations are used (tractable!)

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a combination of

- pseudo likelihood
- +
• Laplacian prior

one of the most efficient methods for **structure learning**

Contrastive methods

log-likelihood: $\log p(\mathcal{D}; \theta) = \sum_{x \in \mathcal{D}} \log \tilde{p}(x; \theta) - \log Z(\theta)$



increase the unnormalize prob. of the data

- it's easy to evaluate: e.g, $\langle \theta, \phi(x) \rangle$



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contrastive methods: replace $\log Z(\theta)$ with a tractable alternative

- **contrastive divergence minimization:** only look at a small neighborhood of the data
- **margin-based training:** consider $\log \max_{x' \neq x} \tilde{p}(x'; \theta)$
 - only for conditional training

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- (conditional) log-likelihood is convex
 - **gradient** steps: need **inference** on the current model
 - global optima satisfies **moment-matching condition**
 - combine **inference methods + gradient descent** for learning
- alternative approaches:
 - *pseudo moment matching, pseudo likelihood, contrastive divergence, margin-based training*