

Probabilistic Graphical Models

parameter learning in undirected models

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Fall 2019

Learning objectives

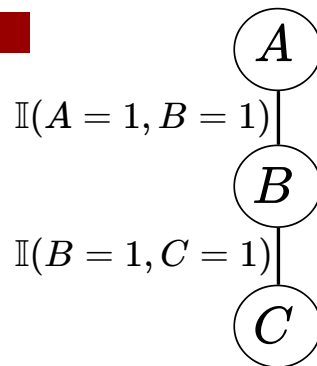
- the form of likelihood for undirected models
 - why is it difficult to optimize?
- conditional likelihood in undirected models
- different approximations for parameter learning
 - MAP inference and regularization
 - pseudo likelihood
 - pseudo moment-matching
 - contrastive learning

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

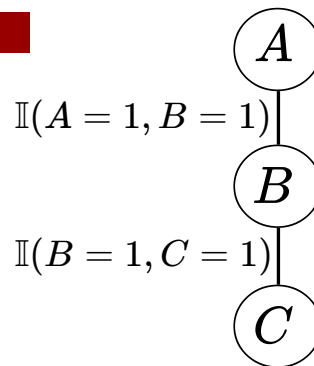
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observations $|\mathcal{D}| = 100$

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



Likelihood in MRFs

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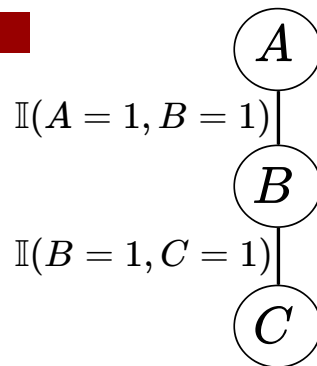
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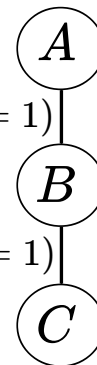
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log-likelihood: $\log p(\mathcal{D}; \theta) = \sum_{a,b,c \in \mathcal{D}} \theta_1 \mathbb{I}(a = 1, b = 1) + \theta_2 \mathbb{I}(b = 1, c = 1) - 100 \log Z(\theta)$
 $= 40\theta_1 + 40\theta_2 - 100 \log Z(\theta)$



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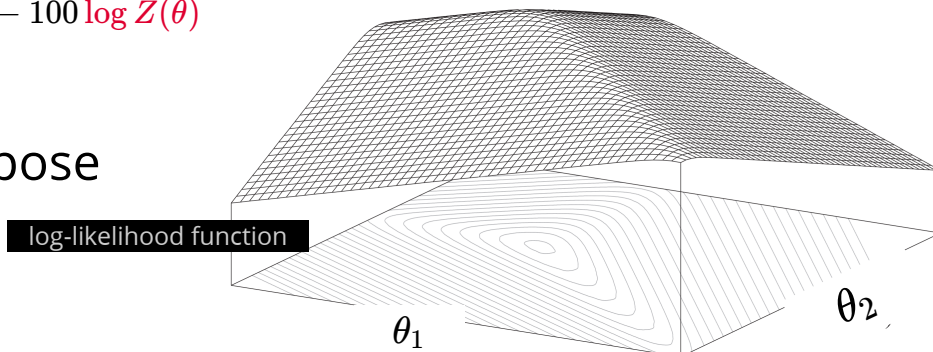
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 $= 40\theta_1 + 40\theta_2 - 100 \log Z(\theta)$

because of the partition function

the likelihood does not decompose



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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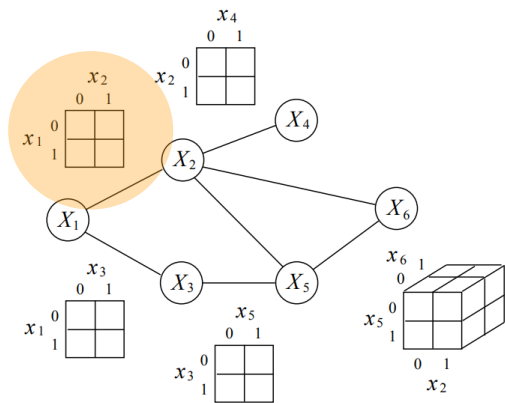


image: Michael Jordan's draft

expected sufficient statistics	params.
$\mathbb{E}_{\mathcal{D}}[\mathbb{I}(X_1 = 0, X_2 = 0)] = P(X_1 = 0, X_2 = 0)$	$\theta_{1,2,0,0}$
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$$\frac{\partial}{\partial \theta_i} \log Z(\theta) = \frac{\frac{\partial}{\partial \theta_i} \sum_x \exp(\langle \theta, \phi(x) \rangle)}{Z(\theta)} = \frac{1}{Z(\theta)} \sum_x \phi_i(x) \exp(\langle \theta, \phi(x) \rangle) = \mathbb{E}_p[\phi_i(x)] \quad \text{SO} \quad \nabla_{\theta} \log Z(\theta) = \mathbb{E}_{\theta}[\phi(x)]$$

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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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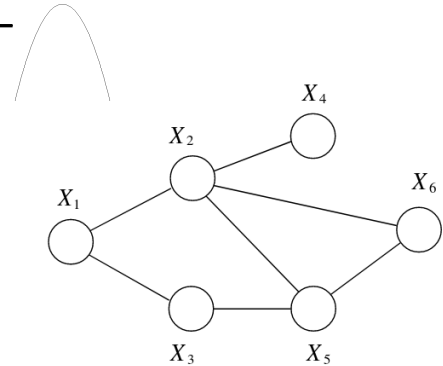
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- estimating $Z(\theta)$ is **a difficult inference problem**



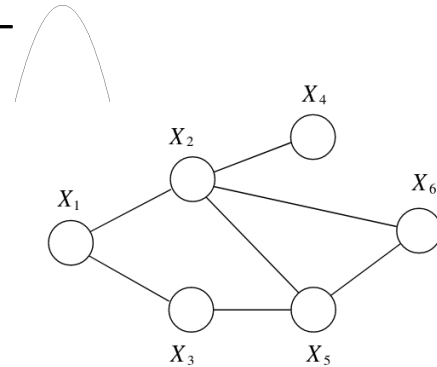
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should be easy to maximize (?) **NO!**


- 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

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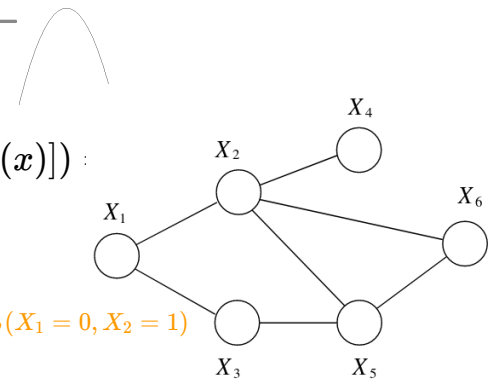
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$$p(X_1 = 0, X_2 = 1; \theta) = p_{\mathcal{D}}(X_1 = 0, X_2 = 1)$$

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

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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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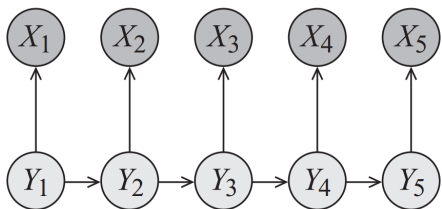
what if exact inference is infeasible?

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

Conditional training

Recall

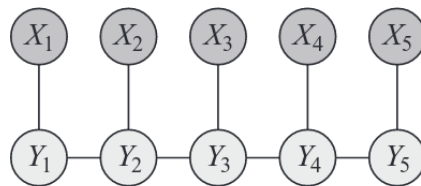
generative vs. discriminative training



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 (assuming full observation)
- the likelihood decomposes



Conditional random fields (CRF)

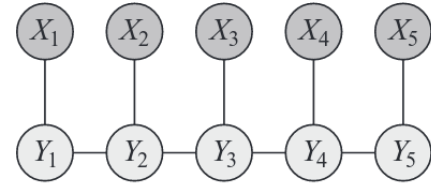
- trained discriminatively
- maximizing conditional log-likelihood

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

- how to maximize this?

Conditional training

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



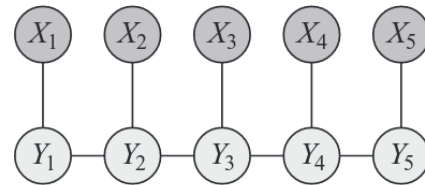
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again consider the gradient

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

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

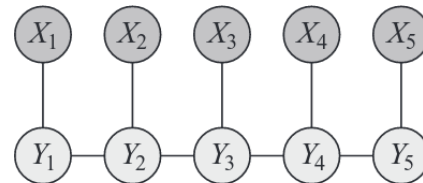


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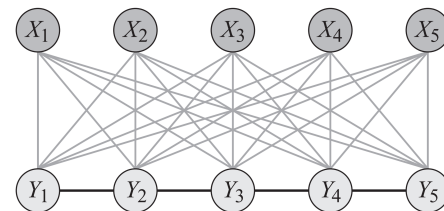
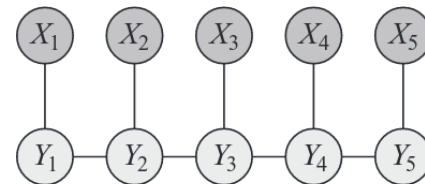
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compared to generative training in undirected models

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 the likelihood doesn't decomposed due to the partition function.)

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alternative to a full-Bayesian approach

MAP inference: maximize the log-posterior

- does not model uncertainty
- sensitive to parametrization

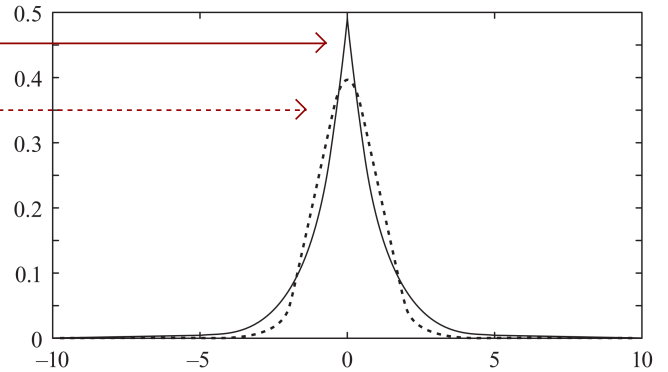
$$\arg \max_{\theta} \log p(\mathcal{D}|\theta) + \underline{\log p(\theta)}$$

- serves as a regularization
- does not have to be conjugate

Gaussian & Laplace 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.)
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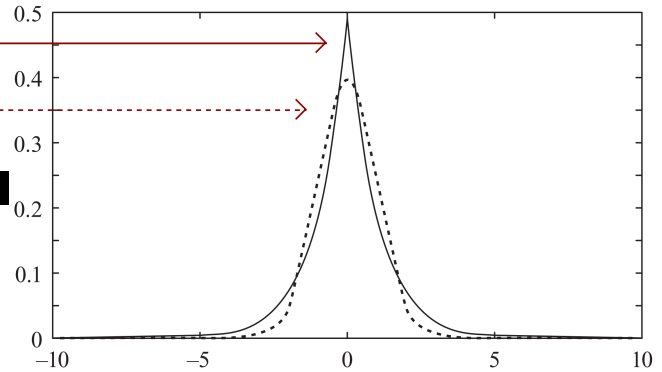
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$$p(\theta; \sigma) \propto \prod_i \exp\left(-\frac{\theta_i^2}{2\sigma^2}\right) \Rightarrow$$

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

L2 regularization penalty term

Gaussian prior



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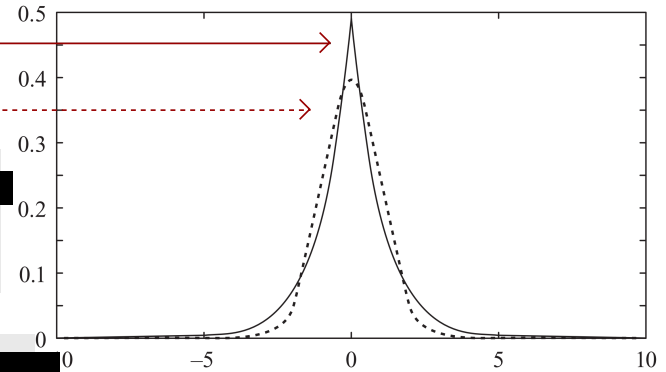
L2 regularization penalty term

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

Laplace prior

$$\log p(\theta; \beta) = -\frac{1}{\beta} \sum_i |\theta_i|$$

L1 regularization penalty term



sparsity-inducing

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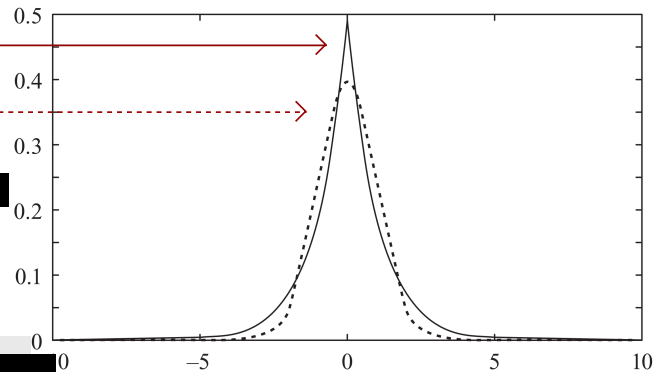
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sparsity-inducing



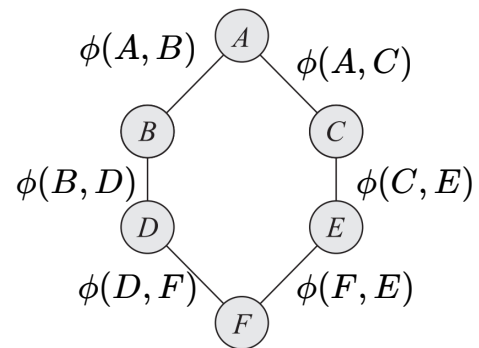
- both of these penalize large parameter values
 - both reduce fluctuations in the density

$$\log \frac{p(x;\theta)}{p(x';\theta)} = \theta^T (\phi(x) - \phi(x'))$$

Pseudo-moment matching

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

$$\underbrace{p_{\mathcal{D}}(A, B)}_{\text{empirical marginals}} = \underbrace{\hat{p}(A, B; \theta)}_{\text{marginals using BP}}, p_{\mathcal{D}}(B, D) = \hat{p}(B, D; \theta) \dots$$



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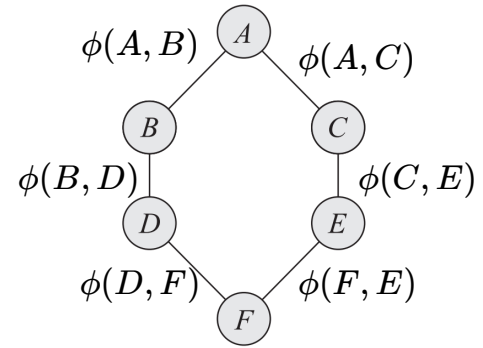
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empirical marginals marginals using BP

idea: use the reparametrization in BP

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

product of clique marginals
cancel the double-counts



Pseudo-moment matching

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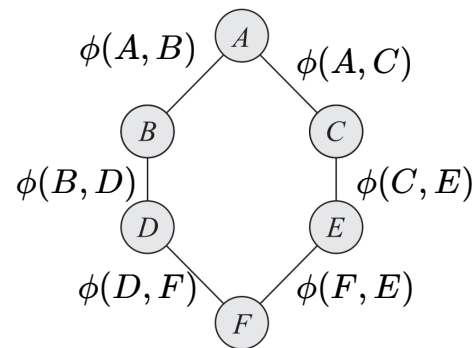
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empirical marginals
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\longrightarrow product of clique marginals
 \longrightarrow cancel the double-counts



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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it 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...
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at the limit of large data (assuming we have the right model), this is exact!

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, $\langle \theta, \phi(x) \rangle$



keep the total sum of unnormalized probabilities small $\log \sum_x \tilde{p}(x; \theta)$

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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

Structure Learning

Conditional independence test $X - Y \Rightarrow X \perp Y \mid MB(Y) \vee X \perp Y \mid MB(X)$

- similar to finding the *undirected skeleton* of a Bayes Net
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Maximizing a score:

- **likelihood score**
- **Bayesian score** (approx. BIC)
- these scores do not decompose
 - learn models with low-tree width
- **MAP score (L1 regularized log-likelihood)**
 - convex problem
 - introduce features 1-by-1 until convergence

Summary

- parameter learning in MRFs is difficult
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 - Bayesian inference is also difficult
- (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*