LECTURE 21 (LAST ONE!):

REVIEW

Kevin Murphy 1 December 2004

JORDAN CHAPTERS

Chap.	Handout	Title
2	n	Cond. Indep and factorization
3	n	The elimination algorithm
4	n	Prob. propagation and factor graphs
5	у	Statistical concepts
6	n	Linear regression and LMS
7	n	Linear classification
8	у	Exponential family and GLIMs
9	у	Completely observed GMs (IPF, etc)
10	у	Mixtures and conditional mixtures
11	у	The EM algorithm
12	у	HMMs
13	у	The multivariate Gaussian
14	у	Factor analysis
15	у	Kalman filtering and smoothing
16	n	Markov properties of graphs

Koller & Friedman Chapters

Trobbett & Tribbinit chin Teles						
Chap.	Handout	Title				
2	у	Foundations (math review)				
3	у	The BN representation (Bayes ball, I-maps)				
4	у	Local probabilistic models (CPDs, CSI)				
5	у	Undirected GMs (BN \leftrightarrow MN)				
6	у	Inference with GMs (overview)				
7	у	Variable elimination				
8	у	Clique trees				
9	у	Particle based approximations				
10	n	Inference as optimization (unfinished)				
11	n	Inference in hybrid networks				
12	у	Learning: introduction				
13	у	Parameter estimation (fully obs. BNs)				
14	у	Structure learning in BNs				
15	у	Partially observed data (EM for BNs)				

JORDAN CHAPTERS CONT'D

Chap.	Handout	Title
17	n	The junction tree algorithm
18	n	HMM and state space models revisited
19	у	Features, maxent and duality
20	у	Iterative scaling algorithms
21	n	Sampling methods
22	n	Decision graphs
23	n	Bio-informatics

What we covered 2

- 1 node models
 - Coins/dice (Dirichlet priors), Gaussians, exponential family
 - Bayesian vs frequentist (ML/MAP) estimation
 - Bayesian model selection (Occam's razor)
- 2 node BNs
 - Linear regression
 - Linear classification (logistic regression)
 - Generalized linear models (GLIMs)
 - Mixture models: MoG, K-means, EM
 - Latent variable models: PCA, FA
- 3 node BNs
 - Mixtures of FA
 - Mixtures of experts

What we covered 3

- General graphs: representation
 - Independence properties (Bayes Ball, I-maps)
 - Directed vs undirected graphs, chordal graphs
- General graphs: exact inference
 - Variable elimination
 - Junction tree
- General graphs: parameter learning
 - Bayesian param. est. for fully observed BNs
 - ML for latent BNs (EM)
 - ML for fully observed UGs (IPF)
 - ML for fully observed CRFs (conjugate gradient)

Chains

- HMMs, forwards-backwards algorithm, EM
- LDS, Kalman filter, EM
- EKF, UKF, particle filtering, RB PF
- Trees
 - Belief propagation
 - Structure learning (max spanning tree)

What we covered 4

- General BNs: structure learning
 - Search and score
 - Partial observability (structural EM, variational Bayes EM)
- General GMs: stochastic approximations
 - Likelihood weighting, Gibbs sampling, Metropolis Hastings
- General GMs: variational approximations
 - Mean field, structured, loopy belief propagation
- Applications
 - SLAM, tracking, image labeling (CRFs), language modeling (HMMs)

- Swendsen-Wang sampling, perfect sampling, details of MCMC
- Generalized BP, theory of BP, cluster variational methods
- Details of expectation propagation (EP)
- Forwards propagation/ backwards sampling
- Non-parametric Bayes (Dirichlet process, Gaussian process)
- Quickscore/ QMR-DT and other speedup tricks (e.g., lazy Jtree)
- Decision making (influence diagrams, LIMIDS, POMDPs etc)
- First order probabilistic inference (FOPI)
- Causality
- Frequentist hypothesis testing
- Conditional Gaussian models (mixed/ hybrid GMs)
- Applications to error correcting codes, biology, vision, speech

Coins (Bernoulli Trials)

- We observe M iid coin flips: $\mathcal{D}=H,H,T,H,\ldots$
- Model: $p(H) = \theta$ $p(T) = (1 \theta)$
- \bullet We want to estimate θ from D.
- Frequentist (maximum likelihood) approach (point estimate):

$$\hat{\theta}_{ML} = \operatorname{argmax}_{\theta} \ell(\theta; \mathcal{D})$$

where

$$\ell(\theta; D) = \log p(D|\theta) = \sum_{m} \log p(x^{m}|\theta)$$

Bayesian approach

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})}$$

or

$$posterior = \frac{likelihood \times prior}{marginal \ likelihood}$$

- Jordan ch 5, 8, 13; Mackay ch 3, 23, 37
- Coins/dice, Gaussians, exponential family
- Bayesian vs frequentist (ML/MAP) estimation
- Bayesian vs classical hypothesis testing

MLE FOR BERNOULLI TRIALS (L10)

• Likelihood:

$$\ell(\theta; \mathcal{D}) = \log p(\mathcal{D}|\theta) = \log \prod_{m} \theta^{\mathbf{x}^{m}} (1 - \theta)^{1 - \mathbf{x}^{m}}$$
$$= \log \theta \sum_{m} \mathbf{x}^{m} + \log(1 - \theta) \sum_{m} (1 - \mathbf{x}^{m})$$
$$= \log \theta N_{H} + \log(1 - \theta) N_{T}$$

• Take derivatives and set to zero:

$$\frac{\partial \ell}{\partial \theta} = \frac{N_{\rm H}}{\theta} - \frac{N_{\rm T}}{1 - \theta}$$
$$\Rightarrow \theta_{\rm ML}^* = \frac{N_{\rm H}}{N_{\rm H} + N_{\rm T}}$$

• The counts $N_H = \sum_m x^m$ and $N_T = \sum_m (1-x^m)$ are sufficient statistics of the data D.

Likelihood

$$P(D|\theta) = \theta^{N_H} (1-\theta)^{N_T}$$

Conjugate Beta Prior

$$P(\theta|\alpha) = \mathcal{B}(\theta; \alpha_h, \alpha_t) \stackrel{\text{def}}{=} \frac{1}{Z(\alpha_h, \alpha_t)} \theta^{\alpha_h - 1} (1 - \theta)^{\alpha_t - 1}$$

Posterior

$$P(\theta|D,\alpha) = \frac{P(\theta|\alpha)P(D|\theta)}{P(D|\alpha)}$$

$$= \frac{1}{Z(\alpha_h, \alpha_t)P(D|\alpha)} \theta^{\alpha_h - 1} \theta^{N_h} (1 - \theta)^{\alpha_t - 1} (1 - \theta)^{N_t}$$

$$= \mathcal{B}(\theta; \alpha_h + N_h, \alpha_t + N_t)$$

ullet Posterior mean $E heta = rac{lpha_h}{lpha_h + lpha_t}.$

BAYESIAN HYPOTHESIS TESTING

• We want to compute the posterior ratio of the 2 hypotheses:

$$\frac{P(H_1|D)}{P(H_0|D)} = \frac{P(D|H_1)P(H_1)}{P(D|H_0)P(H_0)}$$

- Let us assume a uniform prior $P(H_0) = P(H_1) = 0.5$.
- Then we just focus on the ratio of the marginal likelihoods:

$$P(D|H_1) = \int_0^1 d\theta \ P(D|\theta, H_1) P(\theta|H_1)$$

ullet For H_0 , there is no free parameter, so

$$P(D|H_0) = 0.5^N$$

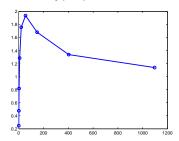
where N is the number of coin tosses in D.

Example of classical hypothesis testing (L15)

- ullet When spun on edge N=250 times, a Belgian one-euro coin came up heads Y=140 times and tails 110.
- We would like to distinguish two models, or hypotheses: H_0 means the coin is unbiased (so p=0.5); H_1 means the coin is biased (has probability of heads $p \neq 0.5$).
- p-value is "less than 7%": $p = P(Y \ge 140) + P(Y \le 110) = 0.066$: n=250; p = 0.5; y = 140; p = (1-binocdf(y-1,n,p)) + binocdf(n-y,n,p)
- ullet If Y=141, we get p=0.0497, so we can reject the null hypothesis at significance level 0.05.
- But is the coin really biased?

So, is the coin biased or not?

• We plot the Bayes factor vs hyperparameter α :



- \bullet For a uniform prior, $\frac{P(H_1|D)}{P(H_0|D)}=0.48$ (weakly) favoring the fair coin hypothesis $H_0!$
- \bullet At best, for $\alpha=50,$ we can make the biased hypothesis twice as likely.
- Not as dramatic as saying "we reject the null hypothesis (fair coin) with significance 6.6%".

$$P(D|\vec{\theta}) = \prod_{i} \theta_i^{N_i}$$

Prior: beta → Dirichlet

$$P(\vec{\theta}|\vec{\alpha}) = \frac{1}{Z(\vec{\alpha})} \prod_{i} \theta_i^{\alpha_i - 1}$$

where

$$Z(\vec{\alpha}) = \frac{\prod_{i} \Gamma(\alpha_i)}{\Gamma(\sum_{i} \alpha_i)}$$

ullet Posterior: beta o Dirichlet

$$P(\vec{\theta}|D) = Dir(\vec{\alpha} + \vec{N})$$

• Evidence (marginal likelihood)

$$P(D|\vec{\alpha}) = \frac{Z(\vec{\alpha} + \vec{N})}{Z(\vec{\alpha})} = \frac{\prod_{i} \Gamma(\alpha_{i} + N_{i})}{\prod_{i} \Gamma(\alpha_{i})} \frac{\Gamma(\sum_{i} \alpha_{i})}{\Gamma(\sum_{i} \alpha_{i} + N_{i})}$$

FUN WITH GAUSSIANS

- Bayesian estimation of 1D Gaussian (homework 5)
- MLE for multivariate Gaussian (Jordan ch 13)
- Bayesian estimation for multivariate Gaussian (Minka TR)
- Inference with multivariate Gaussians (Jordan ch 13)
- Moment vs canonical parameters (Jordan ch 13)

MLE FOR UNIVARIATE NORMAL (L10)

- We observe M iid real samples: $\mathcal{D}=1.18,-.25,.78,...$
- Model: $p(x) = (2\pi\sigma^2)^{-1/2} \exp\{-(x-\mu)^2/2\sigma^2\}$
- Log likelihood:

$$\ell(\theta; \mathcal{D}) = \log p(\mathcal{D}|\theta)$$

$$= -\frac{M}{2} \log(2\pi\sigma^2) - \frac{1}{2} \sum_{m} \frac{(x^m - \mu)^2}{\sigma^2}$$

• Take derivatives and set to zero:

$$\begin{split} \frac{\partial \ell}{\partial \mu} &= (1/\sigma^2) \sum_m (x_m - \mu) \\ \frac{\partial \ell}{\partial \sigma^2} &= -\frac{M}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_m (x_m - \mu)^2 \\ \Rightarrow \mu_{\rm ML} &= (1/M) \sum_m x_m \\ \sigma_{\rm ML}^2 &= (1/M) \sum_m (x_m - \mu_{\rm ML})^2 \end{split}$$

EXPONENTIAL FAMILY (L4, L10)

ullet For a numeric random variable ${f x}$

$$p(\mathbf{x}|\eta) = h(\mathbf{x}) \exp\{\eta^{\top} T(\mathbf{x}) - A(\eta)\}$$
$$= \frac{1}{Z(\eta)} h(\mathbf{x}) \exp\{\eta^{\top} T(\mathbf{x})\}$$

is an exponential family distribution with natural (canonical) parameter η .

- Function $T(\mathbf{x})$ is a sufficient statistic.
- Function $A(\eta) = \log Z(\eta)$ is the log normalizer.
- Examples: Bernoulli, multinomial, Gaussian, Poisson, gamma,...
- ullet A distribution p(x) has finite sufficient statistics (independent of number of data cases) iff it is in the exponential family.
- See Jordan ch 8

- Linear regression (Jordan ch 6)
- Linear classification (logistic regression; Jordan ch 7)
- Generalized linear models (GLIMs; Jordan ch 8)
- Mixture models: MoG, K-means, EM (Jordan ch 10)
- Latent variable models: PCA, FA (Jordan ch 14)

MLE FOR LINEAR REGRESSION

• For vector outputs,

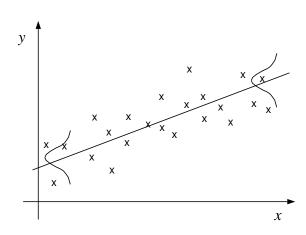
$$A = S_{YX'} S_{XX'}^{-1}$$

where $S_{YX'} = \sum_m y_m x_m^T$ and $S_{XX'} = \sum_m x_m x_m^T$.

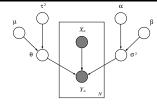
ullet In the special case of scalar outputs, let $A=\theta^T$, and the design matrix $X=[x_m^T]$ stacked as rows and $Y=[y_m]$ a column vector. Then we get the normal equations

$$\theta = (X^T X)^{-1} X^T Y$$





BAYESIAN 1D LINEAR REGRESSION



• For scalar (1D) output

$$p(y_n|x_n, \theta, \sigma^2)p(\theta|\mu, \tau^2)p(\sigma^2|\alpha, \beta)$$

Gaussian × Gaussian × Gamma

• For vector output

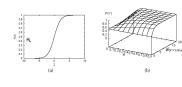
$$p(y_n|x_n,A,\Sigma)p(A|\mu,\tau^2)p(\Sigma|\alpha,\beta)$$

Gaussian × matrix-Gaussian × Wishart

• See Tom Minka tutorial

$$P(Y = 1|X_1, \dots, X_n) = \sigma(w_0 + \sum_{i=1}^n w_i X_i)$$

P(Y=1) vs number of X's that are on vs w



- a: 1D sigmoid
- b: $w_0 = 0$
- c: $w_0 = -5$
- multiplied by 10
- ullet d: w and w_0 are

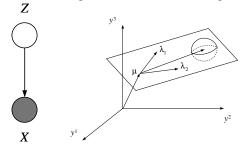
FACTOR ANALYSIS (L17)

• Unsupervised linear regression is called factor analysis.

$$p(x) = \mathcal{N}(x; 0, I)$$

$$p(y|x) = \mathcal{N}(y; \mu + \Lambda x, \Psi)$$

where Λ is the factor loading matrix and Ψ is diagonal.



- To generate data, first generate a point within the manifold then add noise. Coordinates of point are components of latent variable.
- PCA (Karhunen-Loeve Transform) is zero noise limit of FA.

anon	icai CPL	is for $\Lambda \to 1$	(L4)
	X	Y	p(Y X)
•	\mathbb{R}^n	\mathbb{R}^m	$Gauss(Y; WX + \mu, \Sigma)$
	\mathbb{R}^n	$\{0, 1\}$	$Bernoulli(Y; p = \frac{1}{1 + e_1^{-\theta T} x})$
	$\{0,1\}^n$	$\{0, 1\}$	$Bernoulli(Y; p = \frac{1 + e^{-\theta^T x}}{1 + e^{-\theta^T x}})$
	\mathbb{R}^n	$\{1,\ldots,K\}$	$Multinomial(Y; p_i = softmax(x, \theta))$

GENERALIZED LINEAR MODELS

Learn using IRLS or conjugate gradient (L11)

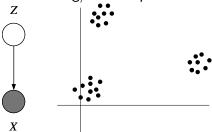
MIXTURES OF GAUSSIANS (L12)

• Mixture of Gaussians:

$$P(Z = i) = \theta_i$$

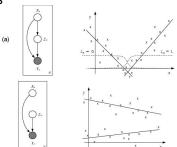
$$p(X = x | Z = i) = \mathcal{N}(x; \mu_i, \Sigma_i)$$

• This can be used for classification (supervised) and clustering/vector quantization (unsupervised).



- We can find MLE/MAP estimates of the parameters using EM.
- K-means is a deterministic approximation (vector quantization).

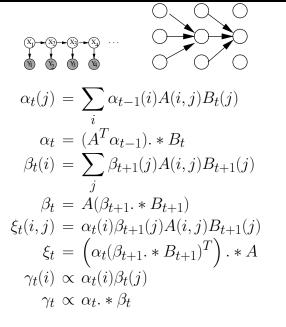
• Mixtures of experts



• Mixtures of factor analysers



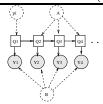
FORWARDS-BACKWARDS ALGORITHM (L8)



• HMMs (Jordan ch 12, Rabiner tutorial)

- LDS (Jordan ch 15, handouts on web)
- Nonlinear state space models (my DBN tutorial)

LEARNING AN HMM (L10, L12)



- Consider a time-invariant hidden Markov model (HMM)
 - -State transition matrix $A(i,j) \stackrel{\text{def}}{=} P(X_t = j | X_{t-1} = i)$,
 - Discrete observation matrix $B(i,j) \stackrel{\mathrm{def}}{=} P(Y_t = j | X_t = i)$
 - -State prior $\pi(i) \stackrel{\text{def}}{=} P(X_1 = i)$.
- If all nodes are observed, we can find the globally optimal MLE.
- Otherwise using EM (aka Baum Welch).

- LDS model: $x_t = Ax_{t-1} + v_t$, $y_t = Cx_t + w_t$
- Time update (prediction step):

$$x_{t|t-1} = Ax_{t-1|t-1}, P_{t|t-1} = AP_{t-1|t-1}A^T + Q, y_{t|t-1} = Cx_{t|t-1}$$

• Measurement update (correction step):

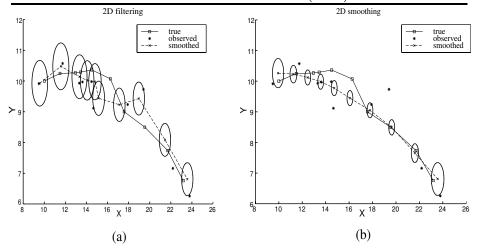
$$ilde{y}_t = y_t - \hat{y}_{t|t-1}$$
 (error/ innovation)
$$P_{\tilde{y}_t} = CP_{t|t-1}C^T + R \text{ (covariance of error)}$$

$$P_{x_ty_t} = P_{t|t-1}C^T \text{ (cross covariance)}$$

$$K_t = P_{x_t y_t} P_{\tilde{y}_t}^{-1} \text{ (Kalman gain matrix)}$$

$$x_{t|t} = x_{t|t-1} + K_t (y_t - y_{t|t-1})$$

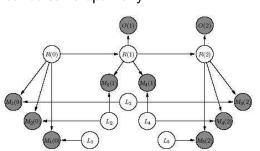
$$P_{t|t} = P_{t|t-1} - K_t P_{x_t y_t}^T$$



KF FOR SLAM (L18)

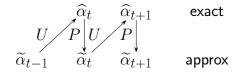
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- \bullet State is location of robot and landmarks $X_t = (R_t, L_t^{1:N})$
- Measure location of subset of landmarks at each time step.
- Assume everything is linear Gaussian.
- Use Kalman filter to solve optimally.



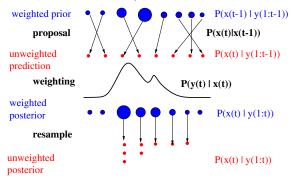
Approximate determinsitic filtering (L18)

- Extended Kalman filter (EKF)
- Unscented Kalman filter (UKF)
- Assumed density filter (ADF)



Particle filtering (sequential Monte Carlo) (L19)

- PF is sequential importance sampling with resampling (SISR).
- ullet Goal is to estimate $P(x_{1:t}|y_{1:t})$ recursively (online) for a state-space model for which Kalman filter/ HMM filter is inapplicable.

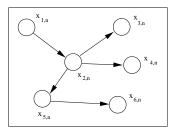


GENERAL GRAPHS

- Representation: Markov properties, CPDs, log linear models
- Exact inference: var elim, Jtree
- Fully observed param learning
- Fully observed structure learning
- Partially observed param learning
- Approximate inference

Trees

- Inference (belief propagation): L9, Yedidia tutorial
- Structure learning (max weight spanning tree): L16
- Application: KF trees for multiscale image analysis (skipped)



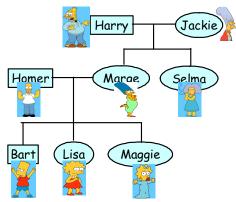
EXAMPLE BN: WATER SPRINKLER (L1)

$$P(X_{1:N}) = \prod_{i=1}^{N} P(X_i | \mathsf{Pa}(X_i))$$
 Cloudy Rain WetGrass

$$P(C, S, R, W) = P(C)P(S|C)P(R|C)P(W|S, R)$$

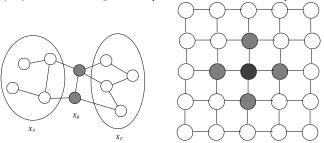
Bayes net for genetic pedigree analysis (L1)

- $G_i \in \{a, b, o\} \times \{a, b, o\} = \text{genotype (allele) of person } i$
- ullet $B_i \in \{a,b,o,ab\} = {\sf phenotype}$ (blood type) of person i



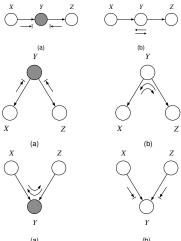
Markov properties for UGs (L3)

- \bullet Defn: the global Markov properties of a UG H are $I(H) = \{(X \perp Y|Z) : sep_H(X;Y|Z)\}$
- ullet Defn: The local markov independencies are $I_l(H) = \{(X \perp V \setminus \{X\} \setminus N_H(X) | N_H(X)) : X \in V\}$ where $N_H(X)$ are the neighbors (Markov blanket).



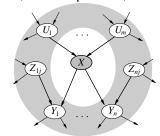
GLOBAL MARKOV PROPERTIES FOR DGS: BAYES-BALL (L2)

A is d-separated from B given C if we cannot send a ball from any node in A to any node in B according to the rules below, where shaded nodes are in C.



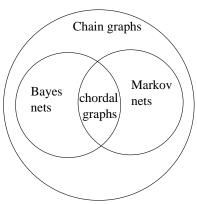
Converting Bayes nets to Markov nets (L3)

- ullet Defn: A Markov net H is an I-map for a Bayes net G if $I(H)\subseteq I(G).$
- We can construct a minimal I-map for a BN by finding the minimal Markov blanket for each node.
- We need to block all active paths coming into node
 X, from parents, children, and co-parents; so connect them all to X.

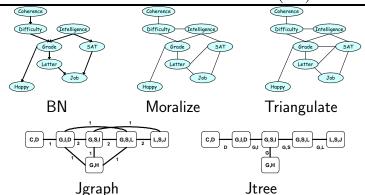


CHORDAL GRAPHS (L4)

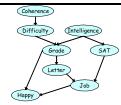
- Chordal graphs encode independencies that can be exactly represented by either directed or undirected graphs.
- Chain graphs combine directed and undirected graphs and represent a larger set of distributions.



FROM BAYES NET TO JTREE (L8)



Variable elimination algorithm (L7)

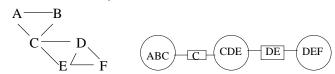


- Key idea 1: push sum inside products.
- Key idea 2: use (non-serial) dynamic programming to cache shared subexpressions.

$$\begin{split} P(J) &= \sum_{L} \sum_{S} \sum_{G} \sum_{H} \sum_{I} \sum_{D} \sum_{C} P(C,D,I,G,S,L,J,H) \\ &= \sum_{L} \sum_{S} \sum_{G} \sum_{H} \sum_{I} \sum_{D} \sum_{C} P(C)P(D|C)P(I)P(G|I,D)P(S|I)P(L|G)P(J|L,S)P(H|G,J) \\ &= \sum_{L} \sum_{S} \sum_{G} \sum_{H} \sum_{I} \sum_{D} \sum_{C} \phi_{C}(C)\phi_{D}(D,C)\phi_{I}(I)\phi_{G}(G,I,D)\phi_{S}(S,I)\phi_{L}(L,G)\phi_{J}(J,L,S)\phi_{H}(H,G,J) \\ &= \sum_{L} \sum_{S} \phi_{J}(J,L,S) \sum_{G} \phi_{L}(L,G) \sum_{H} \phi_{H}(H,G,J) \sum_{I} \phi_{S}(S,I)\phi_{I}(I) \sum_{D} \phi_{G}(I,D) \sum_{C} \phi_{C}(C)\phi_{D}(D,C) \end{split}$$

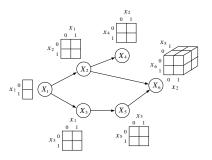
Message passing on Jtrees (L8, L9)

• Hugin vs Shafer Shenoy



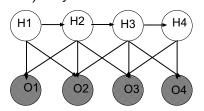
• If we assume the parameters for each CPD are globally independent, then the log-likelihood function decomposes into a sum of local terms, one per node:

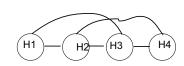
$$\log p(\mathcal{D}|\theta) = \log \prod_{m} \prod_{i} p(\mathbf{x}_{i}^{m}|x_{\pi_{i}}, \theta_{i}) = \sum_{i} \sum_{m} \log p(\mathbf{x}_{i}^{m}|x_{\pi_{i}}, \theta_{i})$$



LEARNING CRFs (L14)

- Conditional random fields are discriminative models.
- Assuming fully observed training data, learning can be done using conjugate gradient descent, just as in a regular MRF with non-maximal cliques.
- Gradient requires computing the partition function, which is (in general) only tractable for low treewidth models (eg chains).





MLE FOR FULLY OBSERVED UGM (L13)

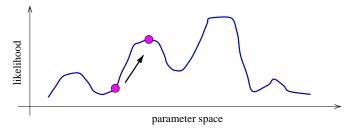
- Is the graph decomposable (triangulated)?
- Are all the clique potentials defined on maximal cliques (not subcliques)? e.g., ψ_{123} , ψ_{234} not ψ_{12} , ψ_{23} ,

• Are the clique potentials full tables (or Gaussians), or parameterized more compactly, e.g., $\psi_c(x_c)=exp(\sum_k w_k f_k(x_c))$?

Decomposable?	Max. Cliques	Tabular	Method
Yes	Yes	Yes	Direct
-	_	Yes	IPF
-	_	_	Gradient ascent
-	_	_	Iterative scaling

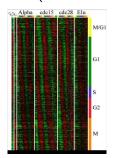
MLE for partially observed BNs (L12)

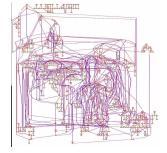
- Use (conjugate) gradient or EM
- M-step is what we did for the 1 node/2 node BNs



LEARNING STRUCTURE OF FULLY OBSERVED BNs (L15, L16)

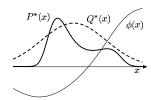
• Search + score (local search + Occam's razor)

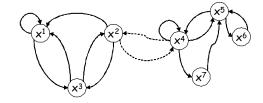




Monte Carlo Methods (L19)

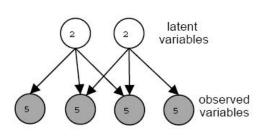
- Importance sampling
- Particle filtering
- RBPF
- MCMC: Gibbs sampling and Metropolis Hastings

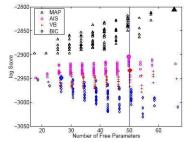




LEARNING STRUCTURE OF PARTIALLY OBSERVED BNs (L16)

- Search = local search
- Score = expected BIC (structural EM)
- Score = variational Bayes (VB-EM)





VARIATIONAL METHODS (L20)

- Iterative Conditional Modes (ICM)
- Mean field
- Structured variational methods
- Loopy belief propagation

D(q, p)



D(p, q)



A Generative Model for Generative Models

