LECTURE 21 (LAST ONE!):

REVIEW

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Koller & Friedman Chapters

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

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

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

- 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
 - $-\operatorname{Mixtures}$ of FA
 - Mixtures of experts

• Chains

- -HMMs, forwards-backwards algorithm, EM
- -LDS, Kalman filter, EM
- -EKF, UKF, particle filtering, RB PF

• Trees

- Belief propagation
- Structure learning (max spanning tree)

- 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)

- General BNs: structure learning
 - $-\operatorname{Search}$ 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

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

- We observe M iid coin flips: $\mathcal{D}=H,H,T,H,\ldots$
- Model: $p(H) = \theta$ $p(T) = (1 \theta)$
- 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

$$\mathsf{posterior} = rac{\mathsf{likelihood} imes \mathsf{prior}}{\mathsf{marginal} \ \mathsf{likelihood}}$$

• Likelihood:

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

• 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.

BAYESIAN ESTIMATION FOR BERNOULLI TRIALS (L11)

• 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

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

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

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

• Posterior mean $E\theta = \frac{\alpha_h}{\alpha_h + \alpha_t}$.

- 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)

- 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?

• 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:

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

• 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.

• We plot the Bayes factor vs hyperparameter α :



- 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%".

• Likelihood: binomial \rightarrow multinomial $P(D|\vec{\theta}) = \prod_{i} \theta_{i}^{N_{i}}$

• Prior: beta \rightarrow Dirichlet

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

where

$$Z(\vec{\alpha}) = \frac{\prod_i \Gamma(\alpha_i)}{\Gamma(\sum_i \alpha_i)}$$

• Posterior: beta \rightarrow Dirichlet

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

• Evidence (marginal likelihood)

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

- We observe M iid real samples: $\mathcal{D}=1.18,-.25,.78,\ldots$
- 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:

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

- 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)

 \bullet For a numeric random variable ${\bf x}$

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

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,...
- 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)



• For vector outputs,

$$A = S_{YX'}S_{XX'}^{-1}$$
 where $S_{YX'} = \sum_m y_m x_m^T$ and $S_{XX'} = \sum_m x_m x_m^T$.

• 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

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

 ${\cal P}(Y=1)$ vs number of $X{\rm 's}$ that are on vs w





- a: 1D sigmoid
- b: $w_0 = 0$

• c:
$$w_0 = -5$$

• d: w and w_0 are multiplied by 10

GENERALIZED LINEAR MODELS

Canor	nical CPE	Os for $X \to Y$	Y (L4)
	X	Y	p(Y X)
	\mathbb{R}^n	\mathbb{R}^m	$Gauss(Y;WX+\mu,\Sigma)$
	\mathbb{R}^{n}	$\{0, 1\}$	$Bernoulli(Y; p = \frac{1}{1 + e^{-\theta T_x}})$
	$\{0,1\}^n$	$\{0, 1\}$	$Bernoulli(Y; p = \frac{1+e^{-1}}{1+e^{-\theta Tx}})$
	\mathbb{R}^{n}	$\{1,\ldots,K\}$	$Multinomial(Y; p_i = softmax(x, \theta))$

Learn using IRLS or conjugate gradient (L11)

• 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.

• 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



- HMMs (Jordan ch 12, Rabiner tutorial)
- LDS (Jordan ch 15, handouts on web)
- Nonlinear state space models (my DBN tutorial)





$$\alpha_{t}(j) = \sum_{i} \alpha_{t-1}(i)A(i,j)B_{t}(j)$$

$$\alpha_{t} = (A^{T}\alpha_{t-1}) \cdot *B_{t}$$

$$\beta_{t}(i) = \sum_{j} \beta_{t+1}(j)A(i,j)B_{t+1}(j)$$

$$\beta_{t} = A(\beta_{t+1} \cdot *B_{t+1})$$

$$\xi_{t}(i,j) = \alpha_{t}(i)\beta_{t+1}(j)A(i,j)B_{t+1}(j)$$

$$\xi_{t} = \left(\alpha_{t}(\beta_{t+1} \cdot *B_{t+1})^{T}\right) \cdot *A$$

$$\gamma_{t}(i) \propto \alpha_{t}(i)\beta_{t}(j)$$

$$\gamma_{t} \propto \alpha_{t} \cdot *\beta_{t}$$

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 $B(i, j) \stackrel{\text{def}}{=} P(Y_t = j | X_t = i)$ - 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):

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

• Measurement update (correction step):

$$\begin{split} \tilde{y}_t &= y_t - \hat{y}_{t|t-1} \text{ (error/ innovation)} \\ P_{\tilde{y}_t} &= CP_{t|t-1}C^T + R \text{ (covariance of error)} \\ P_{x_ty_t} &= P_{t|t-1}C^T \text{ (cross covariance)} \\ K_t &= P_{x_ty_t}P_{\tilde{y}_t}^{-1} \text{ (Kalman gain matrix)} \\ x_{t|t} &= x_{t|t-1} + K_t(y_t - y_{t|t-1}) \\ P_{t|t} &= P_{t|t-1} - K_tP_{x_ty_t}^T \end{split}$$

KF for 2D tracking (L17)



KF for SLAM (L18)

- 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)

$$\begin{array}{ccc} & \widehat{\alpha}_t & \widehat{\alpha}_{t+1} & \text{exact} \\ & & & & \\ U & P & & \\ & & & & \\ & & & & \\ & \widetilde{\alpha}_{t-1} & \widetilde{\alpha}_t & \widetilde{\alpha}_{t+1} & \text{approx} \end{array}$$

Particle filtering (sequential Monte Carlo) (L19)

- PF is sequential importance sampling with resampling (SISR).
- 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.



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



- 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



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

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



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.



- Defn: the global Markov properties of a UG H are $I(H) = \{(X \perp Y | Z) : sep_H(X; Y | Z)\}$
- 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).





Converting Bayes nets to Markov nets (L3)

- 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 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.



VARIABLE ELIMINATION ALGORITHM (L7)



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

$$P(J) = \sum_{L} \sum_{S} \sum_{G} \sum_{H} \sum_{I} \sum_{D} \sum_{C} P(C, D, I, G, S, L, J, H)$$

$$= \sum_{L} \sum_{S} \sum_{G} \sum_{H} \sum_{I} \sum_{D} \sum_{C} P(C)P(D|C)P(I)P(G|I, D)P(S|I)P(L|G)P(J|L, S)P(H|G, J)$$

$$= \sum_{L} \sum_{S} \sum_{G} \sum_{H} \sum_{I} \sum_{D} \sum_{C} \phi_{C}(C)\phi_{D}(D, C)\phi_{I}(I)\phi_{G}(G, I, D)\phi_{S}(S, I)\phi_{L}(L, G)\phi_{J}(J, L, S)\phi_{H}(H, G, J)$$

$$= \sum_{L} \sum_{S} \phi_{J}(J, L, S) \sum_{G} \phi_{L}(L, G) \sum_{H} \phi_{H}(H, G, J) \sum_{I} \phi_{S}(S, I)\phi_{I}(I) \sum_{D} \phi_{C}(G, I, D) \sum_{C} \phi_{C}(C)\phi_{D}(D, C)$$



• 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:

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



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

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

Х3

X4

X4

Х3

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

- 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 PARTIALLY OBSERVED BNs (L12)

- Use (conjugate) gradient or EM
- \bullet 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)





LEARNING STRUCTURE OF PARTIALLY OBSERVED BNS (L16)

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





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



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



A Generative Model for Generative Models

