Lecture 13: March 4, 2015 cs 573: Probabilistic Reasoning Professor Nevatia Spring 2015

#### Review

- Assignment # 4 due March 9
- Exam 1may be graded by March 11
- Last lecture:
  - Loopy Belief Propagation Algorithm
  - Very brief intro to Gaussian Distributions
- Today's objective
  - Inference in Gaussian Networks

### Multi-variate Gaussian Distribution

• Eq. 7.1

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} \exp\left[-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu})\right]$$

- Mean vector,  $\mu$ ;  $\mu = E(X)$ ;  $\mu_i$  is mean of  $X_i$
- $-\Sigma$  is n x n covariance matrix,
  - $\Sigma = E[X X^T] E[X] E[X^T]$
  - $\Sigma_{i,i}$  is the variance of  $X_{i,i}$
  - $\Sigma_{i,j} = \Sigma_{j,i}$  is the *covariance* between  $X_i$  and  $X_j$ -  $\mathbf{Cov}[X_i; X_j] = \mathbf{E}[X_i X_j] - \mathbf{E}[X_i] \mathbf{E}[X_j]$
- $\Sigma$  must be positive definite,  $\mathbf{x}^T\Sigma \mathbf{x} > 0$ ,  $\mathbf{x} \neq 0$ , for density to be well defined; Equivalent property: all eigenvalues are > 0
- Standard Multivariate Gaussian:  $\mu = 0$  (vector),  $\Sigma = I$  (identity matrix) (1s on diagonal, 0s elsewhere)

### Multi-variate Gaussian Distribution

• 2-D example

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \quad \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_x^2 & \rho \sigma_x \sigma_y \\ \rho \sigma_x \sigma_y & \sigma_y^2 \end{pmatrix}.$$

• 3-D example

$$\mu = \begin{pmatrix} 1 \\ -3 \\ 4 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$$

# Marginalize a Gaussian Distribution

• For multiple variables, best not to expand the terms

$$p(\boldsymbol{X},\boldsymbol{Y}) = \mathcal{N}\left(\left(\begin{array}{c} \boldsymbol{\mu}_{\boldsymbol{X}} \\ \boldsymbol{\mu}_{\boldsymbol{Y}} \end{array}\right); \left[\begin{array}{cc} \boldsymbol{\Sigma}_{\boldsymbol{X}\boldsymbol{X}} & \boldsymbol{\Sigma}_{\boldsymbol{X}\boldsymbol{Y}} \\ \boldsymbol{\Sigma}_{\boldsymbol{Y}\boldsymbol{X}} & \boldsymbol{\Sigma}_{\boldsymbol{Y}\boldsymbol{Y}} \end{array}\right]\right)$$

- 1st term in matrix above is n x n, 2nd is n x m, and 3rd is m x n,
   4th is n x n (X has n elements, Y has m elements)
- Can be shown that marginal over Y (sum out X) is Gaussian, given by  $N(\mu_{Y}, \Sigma_{YY})$ 
  - Derivation is straight-forward but requires some manipulation of matrix terms; for a derivation see <a href="http://fourier.eng.hmc.edu/e161/lectures/gaussianprocess/node7.html">http://fourier.eng.hmc.edu/e161/lectures/gaussianprocess/node7.html</a>

# Computing Conditional Distribution

- Say Y = y
- Substitute in the density formula; consider 2 variable case

$$f(x,y) = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho^2}} \exp\left(-\frac{1}{2(1-\rho^2)} \left[ \frac{(x-\mu_x)^2}{\sigma_x^2} + \frac{(y-\mu_y)^2}{\sigma_y^2} - \frac{2\rho(x-\mu_x)(y-\mu_y)}{\sigma_x\sigma_y} \right] \right),$$

- Result is p(X), y is treated as a constant (parameter)
- Equation represents a valid Gaussian
- For multi-variate case, expressions for the new  $\mu$  and  $\Sigma$  are complex and require some matrix inversions
  - See next slide

### Conditional Distribution Formulas

#### From Wikipedia

If  $\mu$  and  $\Sigma$  are partitioned as follows

$$oldsymbol{\mu} = egin{bmatrix} oldsymbol{\mu}_1 \ oldsymbol{\mu}_2 \end{bmatrix} ext{with sizes} egin{bmatrix} q imes 1 \ (N-q) imes 1 \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \text{ with sizes } \begin{bmatrix} q \times q & q \times (N-q) \\ (N-q) \times q & (N-q) \times (N-q) \end{bmatrix}$$

then, the distribution of  $\mathbf{x}_1$  conditional on  $\mathbf{x}_2 = a$  is multivariate normal  $(\mathbf{x}_1 | \mathbf{x}_2 = \mathbf{a}) \sim \mathcal{N}(\overline{\mu}, \overline{\Sigma})$  where

$$\bar{\boldsymbol{\mu}} = \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \left( \mathbf{a} - \boldsymbol{\mu}_2 \right)$$

and covariance matrix

$$\overline{oldsymbol{\Sigma}} = oldsymbol{\Sigma}_{11} - oldsymbol{\Sigma}_{12} oldsymbol{\Sigma}_{22}^{-1} oldsymbol{\Sigma}_{21}.^{[8]}$$

### **Information Form**

Information matrix, J, (also called precision matrix)

$$J = \Sigma^{-1}$$

$$-1/2 (x-\mu)^{T} \Sigma^{-1} (x-\mu) = -1/2 (x-\mu)^{T} J (x-\mu)$$

$$= -1/2 [x^{T}Jx - 2x^{T}J\mu + \mu^{T}J \mu]$$

$$p(\boldsymbol{x}) \propto \exp\left[-\frac{1}{2}\boldsymbol{x}^T J \boldsymbol{x} + (J \boldsymbol{\mu})^T \boldsymbol{x}\right]$$

- $\mathbf{h} = J\mathbf{\mu}$  is called the potential vector
- J must be positive definite (also symmetric)
- Conditioning:
  - Info form has terms such as  $(1/2)*J_{ii}x_i^2 J_{ii}x_ix_i + h_ix_i +$ constant
  - If  $X_i$  is in evidence (conditioning set), linear term and square terms (containing only  $x_i$ ) become constants, product term becomes linear
- $\underset{\text{USC CS573: Prob Reasoning, Spring 2015}}{- \text{Resulting form is same as original information form}}$

#### Canonical Form

- Similar to information form
- Expand the Gaussian density expression as:

$$\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1}(\boldsymbol{x} - \boldsymbol{\mu})\right) 
= \exp\left(-\frac{1}{2}\boldsymbol{x}^T \Sigma^{-1} \boldsymbol{x} + \boldsymbol{\mu}^T \Sigma^{-1} \boldsymbol{x} - \frac{1}{2}\boldsymbol{\mu}^T \Sigma^{-1} \boldsymbol{\mu} - \log\left((2\pi)^{n/2}|\Sigma|^{1/2}\right)\right)$$

• Let:

$$K = \Sigma^{-1}$$

$$h = \Sigma^{-1} \mu$$

$$g = -\frac{1}{2} \mu^T \Sigma^{-1} \mu - \log \left( (2\pi)^{n/2} |\Sigma|^{1/2} \right)$$

$$C(\mathbf{X}; K, \mathbf{h}, g) = \exp\left(-\frac{1}{2}\mathbf{X}^T K \mathbf{X} + \mathbf{h}^T \mathbf{X} + g\right)$$
 Eq 14.1

Note K is same as J in information form

### Conditional Distribution in Canonical Form

• In canonical form, marginalize over Y (eq 14.6)

$$K = \begin{bmatrix} K_{XX} & K_{XY} \\ K_{YX} & K_{YY} \end{bmatrix} \quad ; \quad h = \begin{pmatrix} h_{X} \\ h_{Y} \end{pmatrix}$$

$$K' = K_{XX}$$

$$h' = h_X - K_{XY}y$$

$$g' = g + h_Y^T y - \frac{1}{2}y^T K_{YY}y$$

# Independencies

- $X_i$  and  $X_j$  = are independent iff  $\Sigma_{i,j} = 0$  (no edge in directed graph)
- $J_{i,j} = 0 iff(X_i \perp X_j | X \{X_i, X_j\})$ 
  - Information matrix directly defines a minimal I-map
  - If  $J_{i,i} \neq 0$ , edge between *i* and *j* nodes (in undirected graph)
- Ex 7.2

$$J = \begin{pmatrix} 0.3125 & -0.125 & 0 \\ -0.125 & 0.5833 & 0.3333 \\ 0 & 0.3333 & 0.3333 \end{pmatrix}$$

$$\mu = \begin{pmatrix} 1 \\ -3 \\ 4 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$$

# Gaussian Bayesian Networks (GBN)

• In a GBN, all variables are continuous; all CPDs are linear Gaussian

Let Y be a continuous variable with continuous parents  $X_1, \ldots, X_k$ . We say that Y has a linear Gaussian model if there are parameters  $\beta_0, \ldots, \beta_k$  and  $\sigma^2$  such that

$$p(Y \mid x_1,\ldots,x_k) = \mathcal{N}\left(\beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k; \sigma^2\right).$$

In vector notation,

$$p(Y \mid \boldsymbol{x}) = \mathcal{N}\left(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x}; \sigma^2\right).$$

- Thm 7.3

Given:  $p(Y|x) = \mathcal{N}(\beta_0 + \beta^T x; \sigma^2)$ ;  $X_1,..., X_k$  distributed as  $N(\mu, \Sigma)$ 

We can show that: Y is a normal distribution  $N(\mu_Y; \sigma_Y^2)$ 

$$\mu_Y = \beta_0 + \boldsymbol{\beta}^T \boldsymbol{\mu}$$

$$\sigma_Y^2 = \sigma^2 + \boldsymbol{\beta}^T \boldsymbol{\Sigma} \boldsymbol{\beta}$$

Also that  $\{X,Y\}$  is a normal distribution where

$$\operatorname{Cov}[X_i;Y] = \sum_{j=1}^k \beta_j \Sigma_{i,j}$$

#### Distribution to GBN

- Previous slide shows how given a GBN (network parameters), we can get joint distribution parameters.
- Reverse: given the joint distribution, recover the linear model (thm 7.4)

Given:  $p(X, Y) = \mathcal{N}\left(\begin{pmatrix} \mu_X \\ \mu_Y \end{pmatrix}; \begin{bmatrix} \Sigma_{XX} & \Sigma_{XY} \\ \Sigma_{YX} & \Sigma_{YY} \end{bmatrix}\right)$ 

Derive: 
$$p(Y \mid X) = \mathcal{N}\left(\beta_0 + \boldsymbol{\beta}^T X; \sigma^2\right)$$

$$\beta_0 = \mu_Y - \Sigma_{YX} \Sigma_{XX}^{-1} \mu_X$$

$$\beta = \Sigma_{XX}^{-1} \Sigma_{YX}$$

$$\sigma^2 = \Sigma_{YY} - \Sigma_{YX} \Sigma_{XX}^{-1} \Sigma_{XY}$$

#### Distribution to GBN

- Given a distribution over *n* variables, we can construct a GBN (BN with linear Gaussian Models) that is an I-map of the distribution
- A key difference with discrete case: number of parameters in GBN is not necessarily smaller than in the joint distribution itself as the joint distribution is compact by itself.
- We can also go from distributions to Markov networks
  - Jij help define pairwise (log) potentials
  - However, additional complexity in case of MN; not every set of potentials induces a valid Gaussian distributions
    - Sufficient but not necessary condition is that each edge potential be normalizable (corresponding information matrix is positive definite)
  - We skip other details of Gaussian Markov Random Fields (sec
     7.3)

### Inference in Networks with Continuous Variables

- Essentially, all the algorithms for discrete case apply
- Sum-Product algorithm
  - Steps consist of multiplying factors (product) and marginalizing over some variables (sum) and passing messages to other nodes
  - Iterate until convergence (two passes suffice for trees)
  - We already know how to marginalize Gaussians
  - Now consider product and division

### Marginalize in Canonical Form

• More complex then in covariance form (eq 14.5)

$$K = \begin{bmatrix} K_{XX} & K_{XY} \\ K_{YX} & K_{YY} \end{bmatrix} ; h = \begin{pmatrix} h_{X} \\ h_{Y} \end{pmatrix}$$

$$K' = K_{XX} - K_{XY}K_{YY}^{-1}K_{YX}$$

$$h' = h_X - K_{XY}K_{YY}^{-1}h_Y$$

$$g' = g + \frac{1}{2} \left( \log|2\pi K_{YY}^{-1}| + h_Y^T K_{YY}^{-1}h_Y \right)$$

- We can switch between the covariance and canonical forms, depending on the desired computation
  - However, switching requires inverting K or  $\Sigma$  matrices as well.

# Operations on Canonical Forms

- Product of two canonical forms over the same set of variables:
- $C(\mathbf{X}, K_1, \mathbf{h}_1, g_1)$ .  $C(\mathbf{X}, K_2, \mathbf{h}_2, g_2) = C(\mathbf{X}, K_1 + K_2, \mathbf{h}_1 + \mathbf{h}_2, g_1 + g_2)$ 
  - Formula follows from the definition of the canonical form; we are just multiplying two Gaussians over X
  - If scopes of two factors are different, expand each by including zeros entries in K and h for entries corresponding to absent variables
- Example 14.1

$$\phi_1(X,Y) = \mathcal{C}\left(X,Y; \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \begin{pmatrix} 1 \\ -1 \end{pmatrix}, -3 \right)$$

$$\phi_2(Y,Z) = \mathcal{C}\left(Y,Z; \begin{bmatrix} 3 & -2 \\ -2 & 4 \end{bmatrix}, \begin{pmatrix} 5 \\ -1 \end{pmatrix}, 1 \right).$$

$$\phi_1(X,Y,Z) = \mathcal{C}\left(X,Y,Z; \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, -3 \right)$$

### Example 14.2

After multiplication

$$C\left(X, Y, Z; \begin{bmatrix} 1 & -1 & 0 \\ -1 & 4 & -2 \\ 0 & -2 & 4 \end{bmatrix}, \begin{pmatrix} 1 \\ 4 \\ -1 \end{pmatrix}, -2 \right)$$

Division

$$\frac{C(K_1, \mathbf{h}_1, g_1)}{C(K_2, \mathbf{h}_2, g_2)} = C(K_1 - K_2, \mathbf{h}_1 - \mathbf{h}_2, g_1 - g_2)$$

- Vacuous Canonical Form
  - K = 0, and h = 0, g = 0
  - Similar to factor with all 1 in discrete case
  - Multiplying by it has no effect, but can be used to initialize potentials and make them "ready" for passing messages

# SP and BP Algorithms

- Sum-Product algorithm
  - As before; need to show that resulting factors maintain K
     matrices to be positive definite so integration is not infinite
  - Shown in Proposition 14.1
- Gaussian Belief Propagation
  - Similar steps as in discrete case but the observation that the potentials are quadratic simplifies the equations (eqs 14.7 to 14.9)
  - Interesting property: If BP converges, resulting beliefs encode the correct means but estimated variances are underestimates (overconfident estimates)
  - Also convergence guaranteed if pairwise normalizability condition holds.
- We skip other details

### Next Class

• Read section 11.5.1 of the KF book