Introduction to Graphical Models

The 15th Winter School of Statistical Physics POSCO International Center & POSTECH, Pohang 2018. 1. 8-12 (Mon.-Fri.)

Yung-Kyun Noh

Seoul National University

https://github.com/nohyung/SPWS2018



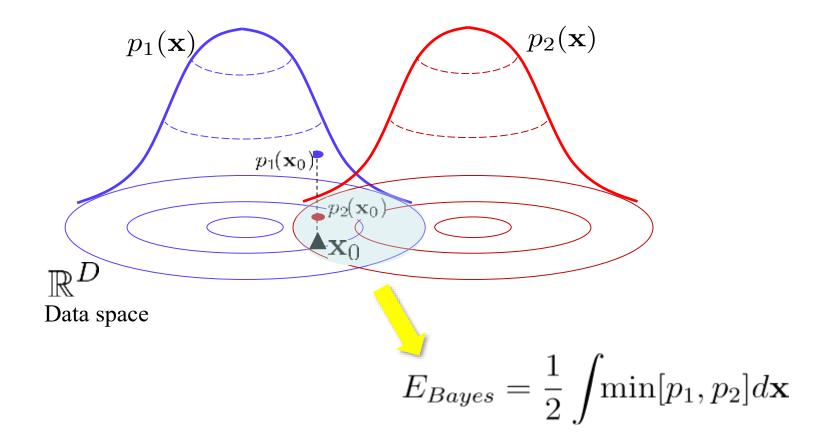


GENERALIZATION FOR PREDICTION



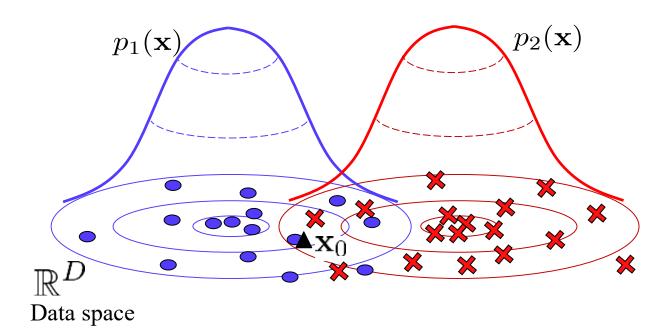
Probabilistic Assumption and Bayes Classification

Bayes Error





Probabilistic Assumption and Bayes Classification



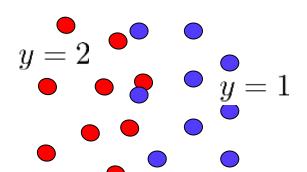
$$\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^N \sim p_1(\mathbf{x}), p_2(\mathbf{x})$$



Learning

• Data

(Regularity)
$$\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^N \sim P$$



Prediction

$$\mathbf{x} \in \mathbb{R}^D \xrightarrow{y = f(\mathbf{x})} y \in \{1, 2, \dots, C\}$$
$$y \in \mathbb{R}$$

- Learning
 - Learn prediction function $f(\mathbf{x}) \in \mathcal{H}$ from data \mathcal{D} (\mathcal{H} : Hypothesis set/Candidate set)



Quantify the Evaluation

Measure of quality: expected loss

$$L = \mathbb{E}_P[l(y, f(\mathbf{x}))]$$
 $l(y, y')$: loss function

Estimated error

$$\hat{L} = \sum_{n} l(y_n, f(\mathbf{x}_n)), \quad f(\mathbf{x}) \in \mathcal{H}$$

Examples

$$l(y, f(\mathbf{x})) = \mathbf{I}(y \neq f(\mathbf{x}))$$

$$l(y, f(\mathbf{x})) = ||y_n - f(\mathbf{x}_n)||^2$$



Consistent Learner

• ${\cal H}$ satisfies

$$\widehat{L}_{N
ightarrow\infty}L$$

$$P\{\sup_{f\in\mathcal{H}}(L(f)-\widehat{L}(f))>\epsilon\}\to 0\quad\text{for}\quad\epsilon>0$$

 Uniform convergence>

- Caution:
 - The definition of consistency is not

$$\widehat{L}(f) \to L(f)$$
 for $f \in \mathcal{H}$



Quiz 1

Consider a hypothesis set H which satisfies

$$\mathbb{E}_{P}\left[\left[L(f) - \widehat{L}(f, N)\right]^{2} \mid f(\mathbf{x}; \theta)\right] = \left(\frac{1}{N}\right)^{b}$$

$$\mathcal{H} = \left\{f(\mathbf{x}; \theta) \mid \theta > 0\right\}$$

Explain that learning with \mathcal{H} is not consistent though it satisfies $\widehat{L}(f) \to L(f)$.

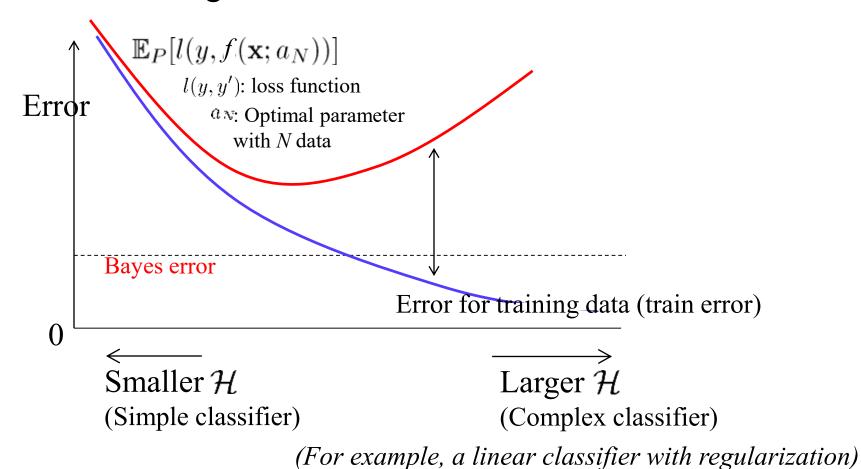
$$\mathbb{E}_{P}\left[[L(f) - \widehat{L}(f, N)]^{2} \mid f(\mathbf{x}; \theta)\right]$$

What is the possible problem in this case?



Consistency and Bayes Error

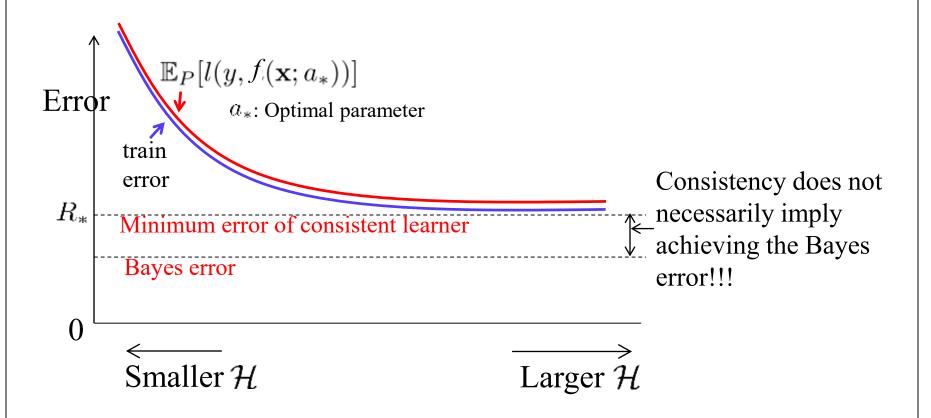
 Minimizing expected error (objective) vs. minimizing estimated error





Consistency and Bayes Error

Consistent learner with many data



(For example, a linear classifier with regularization)



Related Terms with Confining H

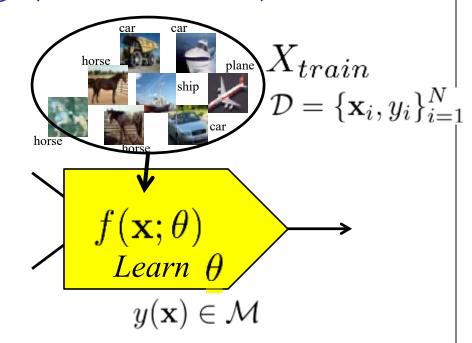
- Linear model

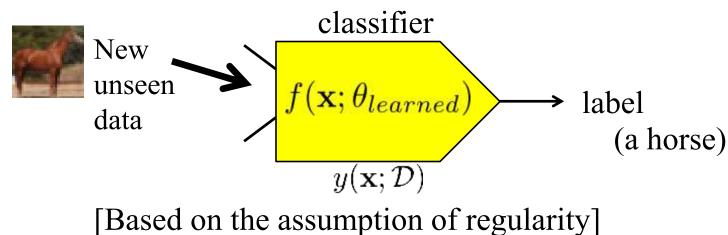
 VC-dim for classification = Dimensionality + 1
- Small number of parameters
- Large margin
- Regularization
- Bias-Variance trade-off
- Generalization ability, overfitting
 - → Many terms are theoretically connected



Supervised Learning (Prediction)

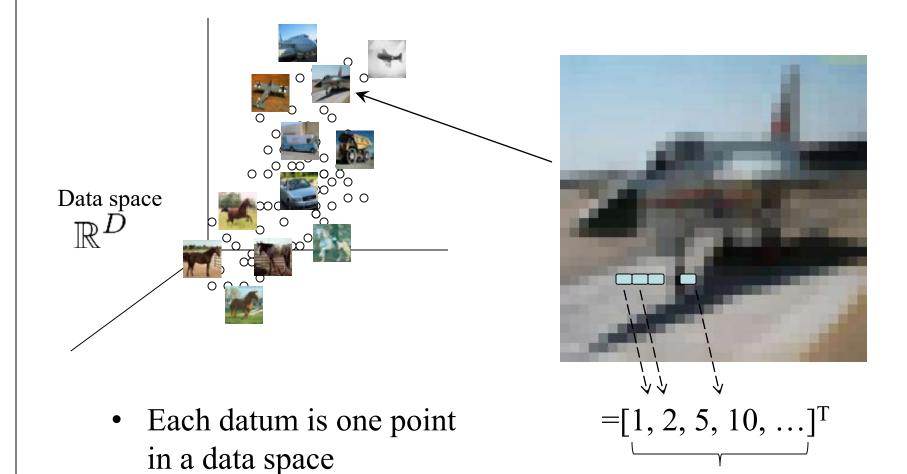
- Method:
 - Learning from
 examples and can
 classify an unseen
 data







Representation of Data





D elements

Classification \mathbb{R}^D





Bayes Optimal Classifier

Our ultimate goal is not a zero error.

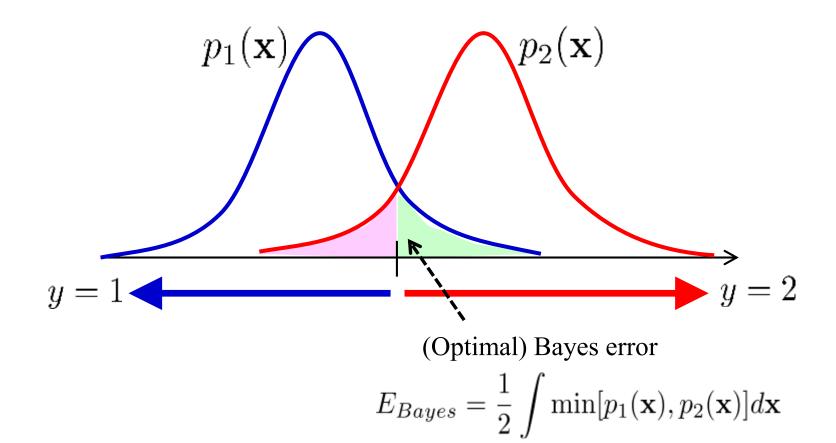


Figure credit: Masashi Sugiyama





FISHER DISCRIMINANT ANALYSIS



Gaussian Random Variable

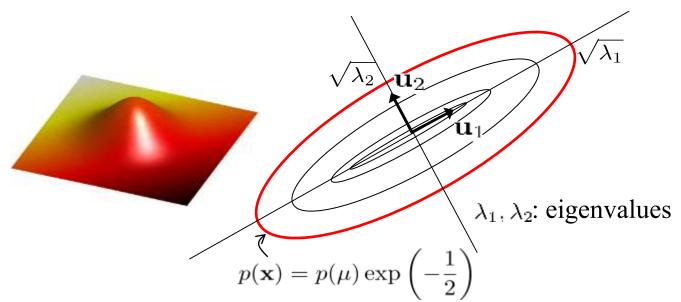
$$p(\mathbf{x}) = \frac{1}{\sqrt{2\pi^D} |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu)^{\top} \Sigma^{-1}(\mathbf{x} - \mu)\right)$$

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_D \end{pmatrix} \in \mathbb{R}^D$$

$$Principal \ axes \ are \ the \ eigenvector \ directions \ of \ \Sigma$$

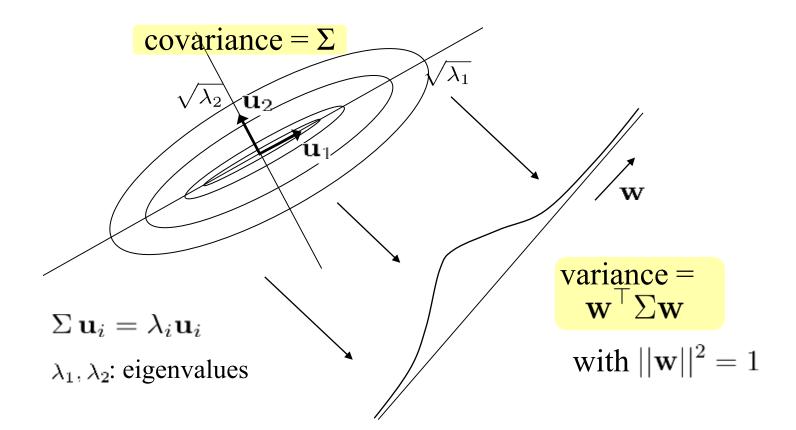
$$\Sigma \ \mathbf{u}_i = \lambda_i \mathbf{u}_i$$

$$\Sigma \mathbf{u}_i = \lambda_i \mathbf{u}_i$$





Covariance Matrix and Projection





Parameter Estimation

Maximum Likelihood Estimation

Data:
$$\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^D$$

Mean vector:
$$\widehat{\mu} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}_i \in \mathbb{R}^D$$

Covariance matrix:
$$\widehat{\Sigma} = \frac{1}{N} \sum_{i=1}^{N} (\mathbf{x}_i - \widehat{\mu}) (\mathbf{x}_i - \widehat{\mu})^{\top} \in \mathbb{R}^{D \times D}$$



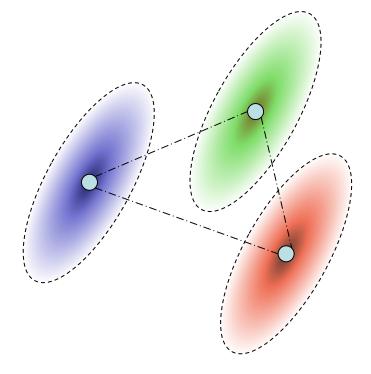
Fisher Discriminant Analysis - Consider Two Statistics

Between-class variance

$$var_B(\mathbf{w}) = \mathbf{w}^{\top} S_B \mathbf{w}$$

$$S_B = \sum_{c=1}^C \frac{N_c}{N} (\mathbf{m}_c - \mathbf{m}) (\mathbf{m}_c - \mathbf{m})^{\top}$$

$$\mathbf{m} = \sum_{i=1}^{N} \frac{1}{N} \mathbf{x}_{i} \qquad \mathbf{m}_{c} = \frac{1}{N_{c}} \sum_{i \in C_{c}} \mathbf{x}_{i}$$



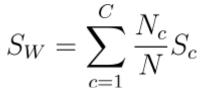


Fisher Discriminant Analysis - Consider Two Statistics

Within-class variance

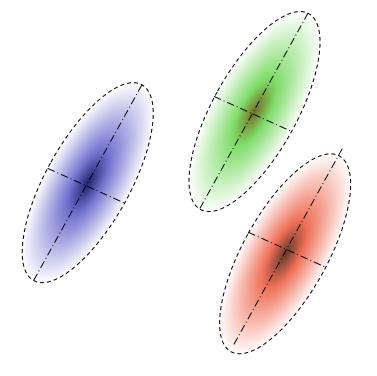
$$var_W(\mathbf{w}) = \mathbf{w}^{\top} S_W \mathbf{w}$$

$$S_W = \sum_{c=1}^C \frac{N_c}{N} S_c$$



 S_c : covariance matrix of each class

$$S_c = \frac{1}{N_c} \sum_{i \in C_c} (\mathbf{x}_i - \mathbf{m}_c) (\mathbf{x}_i - \mathbf{m}_c)^{\top} \qquad \mathbf{m}_c = \frac{1}{N_c} \sum_{i \in C_c} \mathbf{x}_i$$



Total Variance

Total covariance matrix:

$$S_T = \frac{1}{N} \sum_{i=1}^{N} (\mathbf{x}_i - \mathbf{m}) (\mathbf{x}_i - \mathbf{m})^{\mathsf{T}}$$
$$S_T = S_W + S_B$$

Total variance along w:

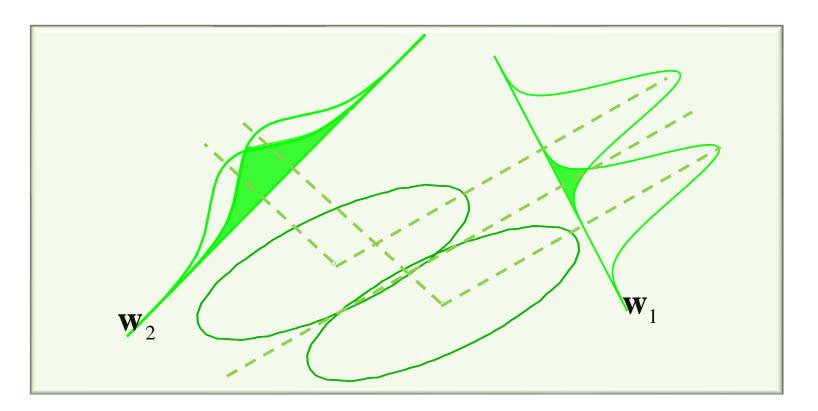
$$var(\mathbf{w}) = var_W(\mathbf{w}) + var_B(\mathbf{w})$$



Fisher Discriminant Analysis (FDA)

• Find w having maximal $var_B(\mathbf{w})$ for give $var_W(\mathbf{w})$.

$$\arg \max_{\mathbf{w}} J(\mathbf{w}) = \frac{\mathbf{w}^{\top} S_B \mathbf{w}}{\mathbf{w}^{\top} S_W \mathbf{w}} \underbrace{\qquad \qquad \underline{\text{Within class variance}}}_{\text{Within class variance}}$$





Take the Derivative

$$\mathbf{w} = \arg\max_{\mathbf{w}} \frac{var_B(\mathbf{w})}{var_W(\mathbf{w})} = \arg\max_{\mathbf{w}} \frac{\mathbf{w}^{\top} S_B \mathbf{w}}{\mathbf{v}^{\top} S_W \mathbf{w}}$$

Take the derivative

$$J(\mathbf{w}) = \frac{\mathbf{w}^{\top} S_B \mathbf{w}}{\mathbf{w}^{\top} S_W \mathbf{w}}$$

$$J'(\mathbf{w}) = \frac{1}{(\mathbf{w}^{\top} S_W \mathbf{w})^2} \left[2S_B \mathbf{w} (\mathbf{w}^{\top} S_W \mathbf{w}) - 2\mathbf{w}^{\top} S_W (\mathbf{w} S_B \mathbf{w}) \right] = 0$$

$$S_B \mathbf{w} = \left(\frac{\mathbf{w}^{\top} S_B \mathbf{w}}{\mathbf{w}^{\top} S_W \mathbf{w}}\right) S_W \mathbf{w} = \lambda S_W \mathbf{w}$$

→ Generalized eigenvector problem



Quiz 1: Closed Form Solution

- Problem: $S_B \mathbf{w} = \lambda S_W \mathbf{w}$
- For two class problem with $N_1 = N_2$:

$$S_B = \sum_{c=1}^{2} \frac{N_c}{N} (\mathbf{m}_c - \mathbf{m}) (\mathbf{m}_c - \mathbf{m})^{\top}$$
$$= \frac{1}{2} (\mathbf{m}_1 - \mathbf{m}_2) (\mathbf{m}_1 - \mathbf{m}_2)^{\top}$$

Assume S_W is a full-rank matrix.

Find the closed form solution:

$$\mathbf{w} = ?$$



Quiz 2: How to solve the generalized eigenvector problem?

• Problem: $S_B \mathbf{w} = \lambda S_W \mathbf{w}$

Are the solution eigenvalues real? (non-complex)?

If not, how are these eigenvalues are treated?



Quiz 3: Two different FDAs

Some papers consider the criterion

$$J_T(\mathbf{w}) = \frac{\mathbf{w}^\top S_B \mathbf{w}}{\mathbf{w}^\top S_T \mathbf{w}}$$

instead of
$$J(\mathbf{w}) = \frac{\mathbf{w}^{\top} S_B \mathbf{w}}{\mathbf{w}^{\top} S_W \mathbf{w}}$$

What is the difference?



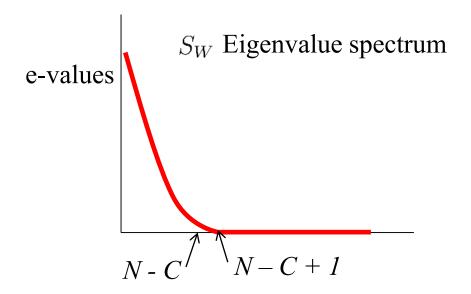
In High Dimensional Space (1/2)

$$D>N$$

$$rank(S_T=S_W+S_B)=N-1$$

$$rank(S_W)=N-C \longrightarrow S_W \text{: not a full rank matrix}$$

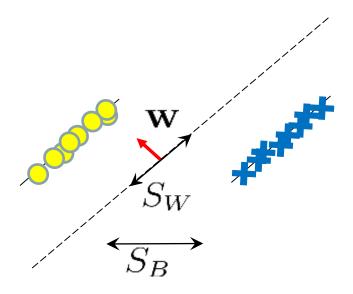
$$rank(S_B)=C-1$$





In High Dimensional Space (2/2)

• FDA will trivially pick up the null space of S_W as solution.



$$J(\mathbf{w}) = \infty$$

More seriously, the nullspace varies by sampling

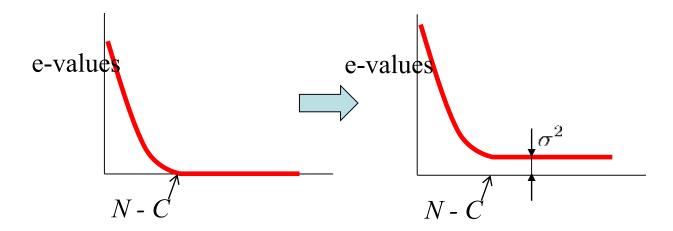
→ Ill-posed problem



Regularization in FDA

Regularize

$$S_W \to S_W + \sigma^2 I$$

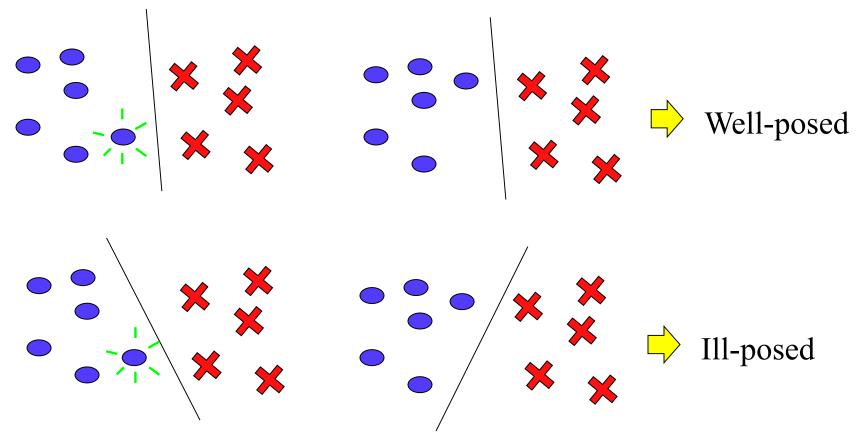


The problem becomes well-posed.

New solution:
$$\mathbf{w} = (S_W + \sigma^2 I)^{-1} (\mathbf{m}_1 - \mathbf{m}_2)$$
 for two classes



Well-posed Problem vs. Ill-Posed Problem



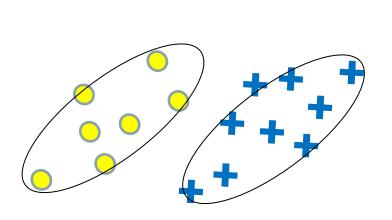
The variation of configuration may come from the sampling variation.

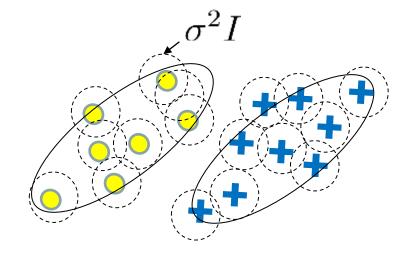




Quiz 4: New Sw with Infinite Data

If infinite number of data are generated around each datum with isotropic Gaussian





$$S_W = \frac{1}{N} \sum_{c=1}^C \sum_{i \in C_c} (\mathbf{x}_i - \mathbf{m}_c) (\mathbf{x}_i - \mathbf{m}_c)^{\mathsf{T}} \qquad S_W \to S_W + \sigma^2 I$$

$$S_W \to S_W + \sigma^2 I$$

GRAPHICAL MODELS

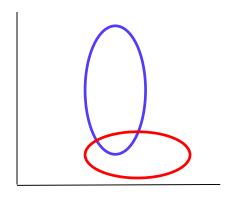


Naïve Bayes As An Extreme Case

Naïve Bayes

$$p(\mathbf{x}) = \prod_{d=1}^{D} p_d(x_d)$$

= $p_1(x_1)p_2(x_2) \dots p_D(x_D)$



- Simply ignore every correlation and dependencies between variables
- True decomposition:

$$p(\mathbf{x}) = \sum_{p(x_1)p(x_2|x_1)p(x_3|x_1, x_2) \dots p(x_D|x_1, \dots, x_{D-1})}$$





Number of Parameters

• D = 1000

- Number of parameters of a Gaussian:

$$1000 + 1001*(1000)/2 = 501,500$$

$$\mu = \left(\begin{array}{c} \\ \\ \\ \\ \end{array} \right) \in \mathbb{R}^D \times D$$



<u>Independence</u>

•
$$p(\mathbf{x}) = p_1(\mathbf{x}_1)p_2(\mathbf{x}_2)$$

 $\mathbf{x} \in \mathbb{R}^D, \mathbf{x}_1 \in \mathbb{R}^{D_1}, \mathbf{x}_2 \in \mathbb{R}^{D_2}$ $D = D_1 + D_2$

- $D_1 = 500$, $D_2 = 500$
 - Number of parameters

$$500 + 501*(500)/2 + 500 + 501*(500)/2$$

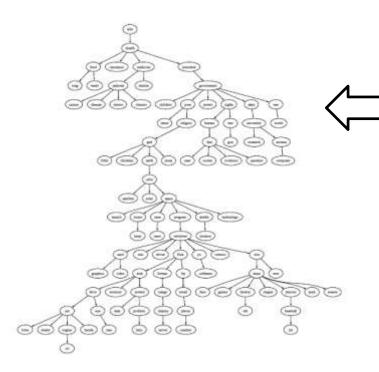
= 251,500

 Incorporating one independence can reduce the number of parameters into half.



Graphical Models

 We utilize probabilities that are represented by the graph structure. (directed & undirected)

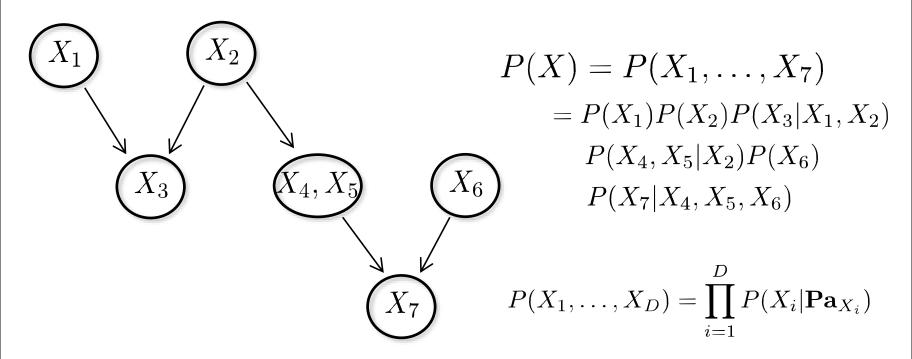


Use probabilistic *independencies* and *conditional independencies* that can be captured by graph structure



Directed Graphical Models

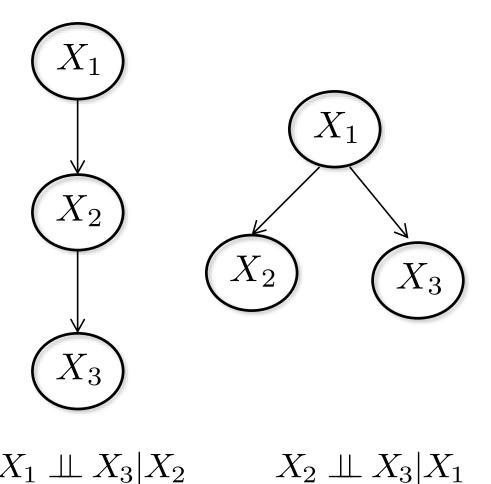
Factorization of a (large) joint pdf



 For given data, make a model for each decomposed probability, then estimate parameters separately.

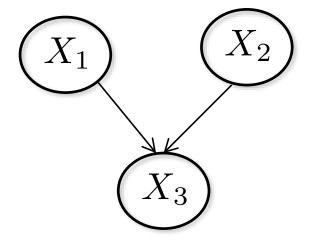


D-Separations



 $X_1 \perp \!\!\! \perp X_3 | X_2$ Causal path

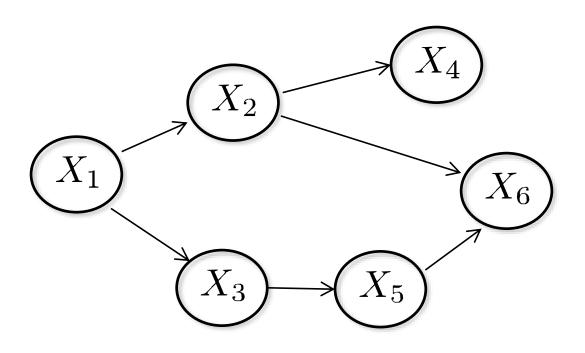
Common cause



 $X_1 \perp \!\!\! \perp X_2$ $X_1 \perp \!\!\! \perp X_2 | X_3$ Common effect



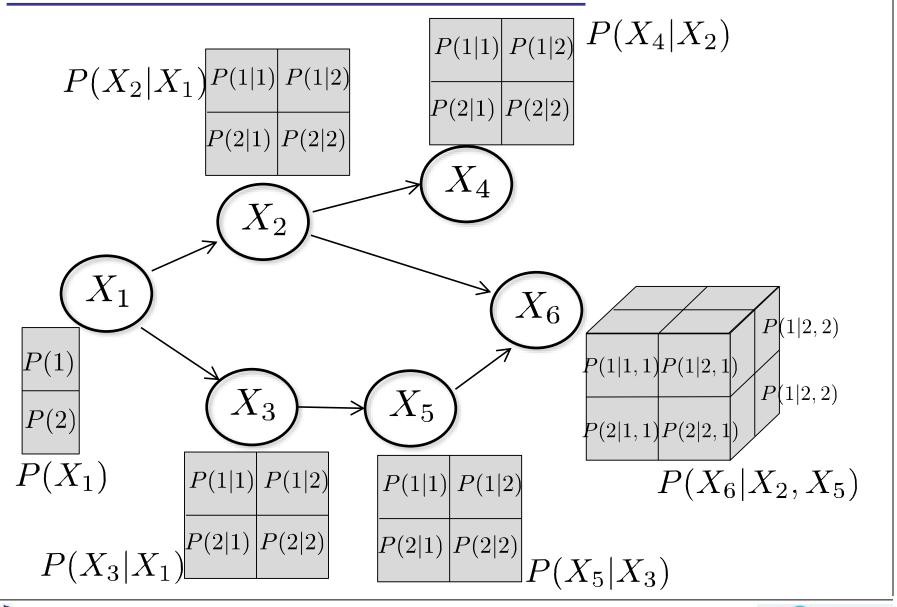
Discrete Random Variables



$$P(X_1, \dots, X_6) = P(X_1)P(X_2|X_1)P(X_3|X_1)P(X_4|X_2)$$
$$P(X_5|X_3)P(X_6|X_2, X_5)$$

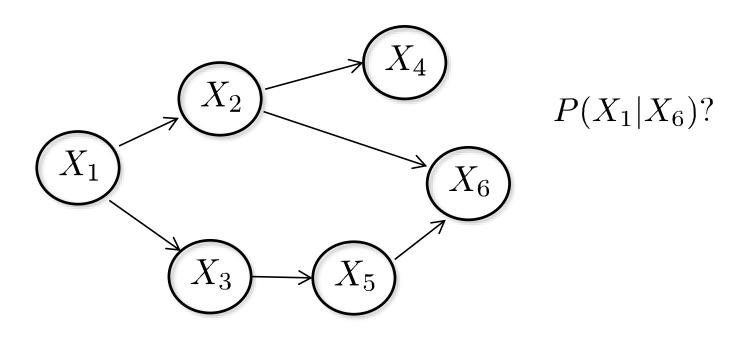


Discrete Random Variables









$$P(X_1, X_6) = \sum_{X_2, X_3, X_4, X_5} P(X_1, \dots, X_6)$$

$$= \sum_{X_2, \dots, X_5} P(X_1) P(X_2 | X_1) P(X_3 | X_1) P(X_4 | X_2)$$

$$P(X_5 | X_3) P(X_6 | X_2, X_5)$$

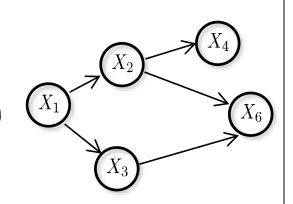


$$\sum_{X_2,...,X_5} P(X_1)P(X_2|X_1)P(X_3|X_1)P(X_4|X_2)P(X_5|X_3)P(X_6|X_2,X_5)$$

$$= \sum_{X_2, X_3, X_4} P(X_1)P(X_2|X_1)P(X_3|X_1)P(X_4|X_2) \sum_{X_5} P(X_5|X_3)P(X_6|X_2, X_5)$$

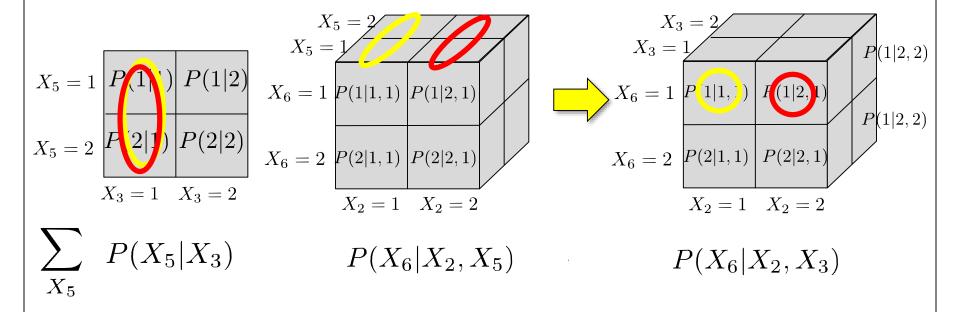
Marginalize X₅

$$\sum_{X_5} P(X_5|X_3)P(X_6|X_2,X_5) \to \sum_{X_5} P(X_5,X_6|X_2,X_3)$$
$$= P(X_6|X_2,X_3)$$



Marginalize X₅

$$P(X_6|X_2,X_3) = \sum_{X_5} P(X_5|X_3)P(X_6|X_2,X_5)$$





$$\sum_{X_2, X_3, X_4} P(X_1)P(X_2|X_1)P(X_3|X_1)P(X_4|X_2) \sum_{X_5} P(X_5|X_3)P(X_6|X_2, X_5)$$

$$= \sum_{X_2, X_3, X_4} P(X_1)P(X_2|X_1)P(X_3|X_1)P(X_4|X_2)P(X_6|X_2, X_3)$$

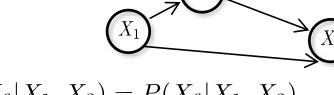
$$= \sum_{X_2, X_3} P(X_1)P(X_2|X_1)P(X_3|X_1)P(X_6|X_2, X_3) \sum_{X_4} P(X_4|X_2)$$

$$= \sum_{X_2,X_3} P(X_1)P(X_2|X_1)P(X_3|X_1)P(X_6|X_2,X_3)$$

$$= \sum_{X_2} P(X_1)P(X_2|X_1) \sum_{X_3} P(X_3|X_1)P(X_6|X_2,X_3)$$

Marginalize X₃

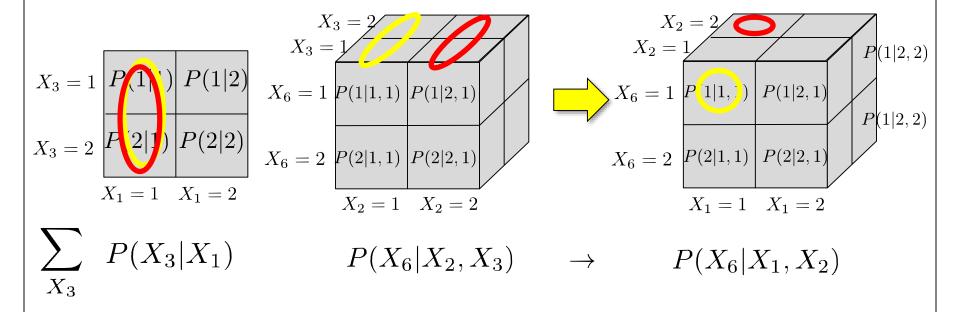
$$\sum_{X_3} P(X_3|X_1)P(X_6|X_2,X_3) \to \sum_{X_3} P(X_3,X_6|X_1,X_2) = P(X_6|X_1,X_2)$$





Marginalize X₃

$$P(X_6|X_1, X_2) = \sum_{X_3} P(X_3|X_1)P(X_6|X_2, X_3)$$





$$\sum_{X_2} P(X_1)P(X_2|X_1) \sum_{X_3} P(X_3|X_1)P(X_6|X_2, X_3)$$

$$= \sum_{X_2} P(X_1)P(X_2|X_1)P(X_6|X_1, X_2)$$

$$= P(X_1) \sum_{X_2} P(X_2|X_1)P(X_6|X_1, X_2)$$

Marginalize X₂

$$P(X_6|X_1) = \sum_{X_2} P(X_2|X_1) P(X_6|X_1, X_2)$$



$$P(X_1) \sum_{X_2} P(X_2|X_1) P(X_6|X_1, X_2)$$

$$\to P(X_1) \sum_{X_2} P(X_2, X_6|X_1) = P(X_1) P(X_6|X_1)$$

$$= P(X_1, X_6)$$

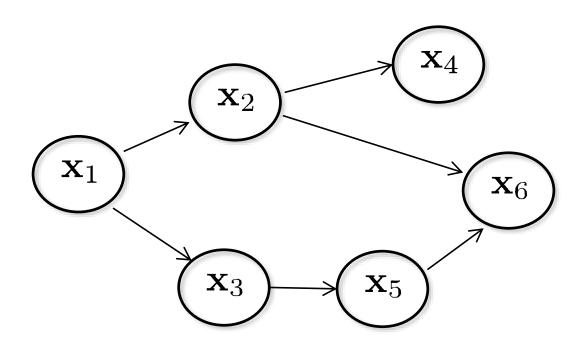
From the joint distribution,

$$P(X_6) = \sum_{X_1} P(X_1, X_6)$$

$$P(X_1|X_6) = \frac{P(X_1, X_6)}{P(X_6)}$$



Continuous Random Variables



$$p(\mathbf{x}_1, \dots, \mathbf{x}_6) = p(\mathbf{x}_1)p(\mathbf{x}_2|\mathbf{x}_1)p(\mathbf{x}_3|\mathbf{x}_1)p(\mathbf{x}_4|\mathbf{x}_2)$$
$$p(\mathbf{x}_5|\mathbf{x}_3)p(\mathbf{x}_6|\mathbf{x}_2, \mathbf{x}_5)$$

Each probability density is a Gaussian



Continuous Random Variables

$$p(\mathbf{x}_1, \dots, \mathbf{x}_6) = p(\mathbf{x}_1)p(\mathbf{x}_2|\mathbf{x}_1)p(\mathbf{x}_3|\mathbf{x}_1)p(\mathbf{x}_4|\mathbf{x}_2)$$
$$p(\mathbf{x}_5|\mathbf{x}_3)p(\mathbf{x}_6|\mathbf{x}_2, \mathbf{x}_5)$$

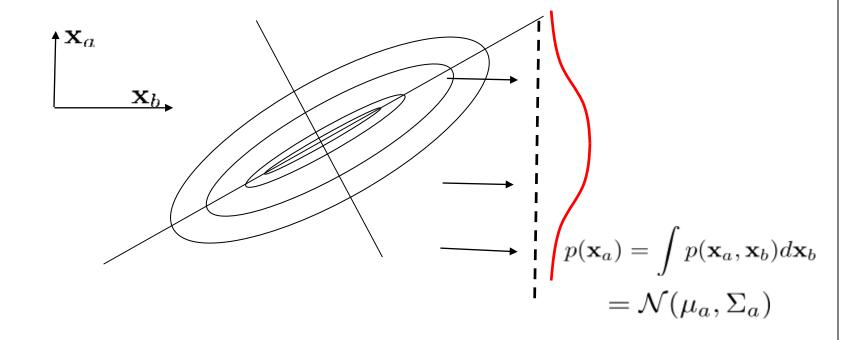
- Jointly Gaussian with 6 variables
 - Need 6 + 6*7/2 = 27 parameters
- Using graphical model:
 - Need to obtain the parameters of $p(\mathbf{x}_1, \mathbf{x}_2), p(\mathbf{x}_1, \mathbf{x}_3), p(\mathbf{x}_2, \mathbf{x}_4), p(\mathbf{x}_3, \mathbf{x}_5), p(\mathbf{x}_2, \mathbf{x}_5, \mathbf{x}_6)$
 - We need to estimate only the following 19 parameters

$$\mu_1, \ldots, \mu_6, \sigma_1^2, \ldots, \sigma_6^2, \sigma_{12}, \sigma_{13}, \sigma_{24}, \sigma_{35}, \sigma_{25}, \sigma_{26}, \sigma_{56}$$



Gaussian Random Variable - Marginal

$$p(\mathbf{x}) = \frac{1}{\sqrt{2\pi^D} |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu)^{\top} \Sigma^{-1}(\mathbf{x} - \mu)\right)$$
$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix} \quad \mathbf{x}_a \in \mathbb{R}^{D_a} \quad \mu = \begin{pmatrix} \mu_a \\ \mu_b \end{pmatrix} \quad \Sigma = \begin{pmatrix} \Sigma_a & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_b \end{pmatrix}$$





Gaussian Random Variable - Marginal

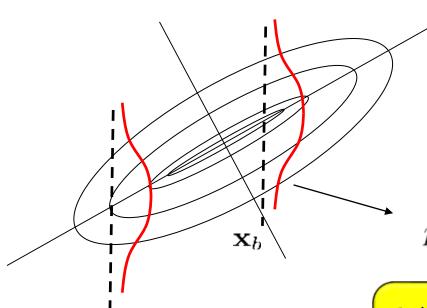
$$p(\mathbf{x}_{a}, \mathbf{x}_{b}) = \frac{1}{\sqrt{2\pi^{D}} \left| \begin{pmatrix} \Sigma_{a} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{b} \end{pmatrix} \right|^{\frac{1}{2}}} \exp \left(-\frac{1}{2} \begin{pmatrix} \mathbf{x}_{a} - \mu_{a} \\ \mathbf{x}_{b} - \mu_{b} \end{pmatrix}^{\top} \begin{pmatrix} \Sigma_{a} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{b} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{x}_{a} - \mu_{a} \\ \mathbf{x}_{b} - \mu_{b} \end{pmatrix} \right)$$

$$\int p(\mathbf{x}_a, \mathbf{x}_b) d\mathbf{x}_b = \frac{1}{\sqrt{2\pi^D} |\Sigma_a|^{\frac{1}{2}}} \exp\left(-\frac{1}{2} (\mathbf{x}_a - \mu_a)^\top \Sigma_a^{-1} (\mathbf{x}_a - \mu_a)\right)$$
$$= \mathcal{N}(\mu_a, \Sigma_a)$$



Gaussian Random Variable - Conditional

$$p(\mathbf{x}) = \frac{1}{\sqrt{2\pi^D} |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu)^{\top} \Sigma^{-1}(\mathbf{x} - \mu)\right)$$



$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix} \quad \mathbf{x}_a \in \mathbb{R}^{D_a}$$
$$\mathbf{x}_b \in \mathbb{R}^{D_b}$$
$$\mu = \begin{pmatrix} \mu_a \\ \mu_b \end{pmatrix} \quad \Sigma = \begin{pmatrix} \Sigma_a & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_b \end{pmatrix}$$

$$p(\mathbf{x}_a|\mathbf{x}_b) = \mathcal{N}(\mu_{a|b}, \Sigma_{a|b})$$

$$\begin{cases} \mu_{a|b} = \mu_a + \Sigma_{ab} \Sigma_b^{-1} (\mathbf{x}_b - \mu_b) \\ \Sigma_{a|b} = \Sigma_a - \Sigma_{ab} \Sigma_b^{-1} \Sigma_{ba} \end{cases}$$

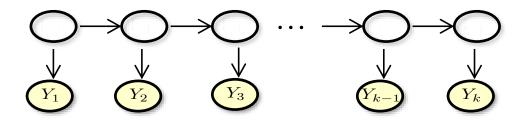


KALMAN FILTER



Filtering

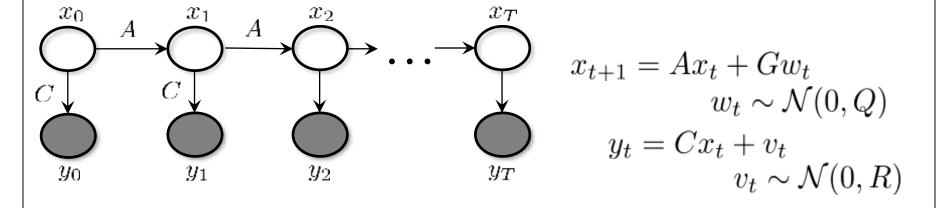
 Linear Dynamical Systems (LDS) with Gaussian noise

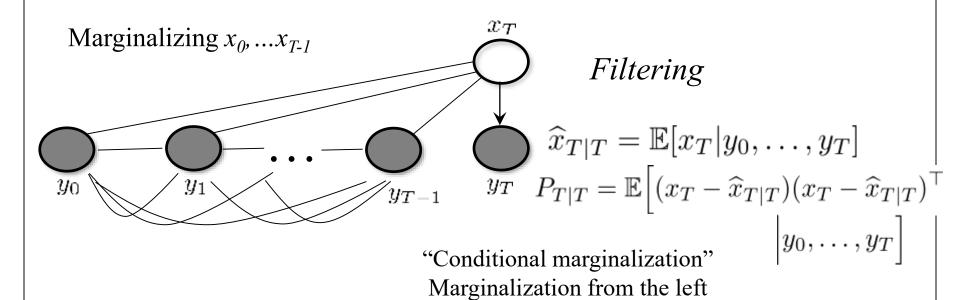


$$p(y_1, \dots, y_K, x_1, \dots, x_K) = p(x_1)p(y_1|x_1) \prod_{t=1}^{M-1} p(x_{t+1}|x_t)p(y_t|x_t)$$

$$x_{t+1} = Ax_t + Gw_t \quad w_t \sim \mathcal{N}(0, Q)$$
$$y_t = Cx_t + v_t \quad v_t \sim \mathcal{N}(0, R)$$

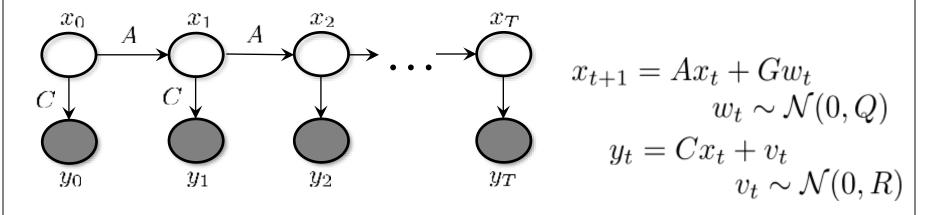






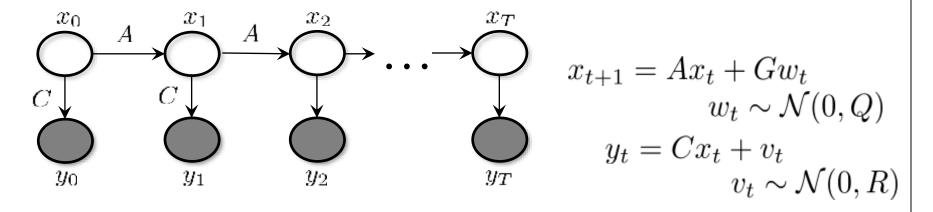






Unconstrained distribution

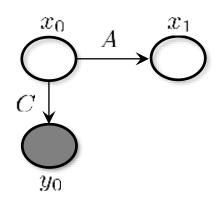




Unconstrained distribution

$$\begin{array}{l}
\overset{x_t}{\bigcirc} & \mu_{y_t} = 0 \\
\Sigma_{y_t} = \mathbb{E}[y_t y_t^\top] & y_t = Cx_t + v_t \\
= \mathbb{E}[(Cx_t + v_t)(Cx_t + v_t)^\top] \\
= C\mathbb{E}[x_t x_t^\top] C^\top + \mathbb{E}[v_t v_t^\top]^\top \\
= C\Sigma_t C^\top + R
\end{array}$$





$$\left(\begin{array}{c} \mu_0 \\ \mu_1 \\ \mu_{y_0} \end{array}\right)$$

$$\begin{pmatrix} \Sigma_0 & \Sigma_{01} & \Sigma_{0y_0} \\ \Sigma_{10} & \Sigma_1 & \Sigma_{1y_0} \\ \Sigma_{y_00} & \Sigma_{y_01} & \Sigma_{y_0} \end{pmatrix} \qquad \Sigma_{y_0}$$

Constrained distribution

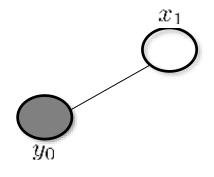
$$\mu_{1|0} = \mu_{x_1|y_0}$$

$$= \mu_1 + \sum_{1y_0} \sum_{y_0}^{-1} (y_0 - \mu_{y_0})$$

$$\sum_{1|0} = \sum_{x_1|y_0} \sum_{y_0}^{-1} \sum_{y_0} \sum$$

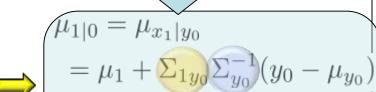
Same

Marginalizing x_0



$$\left(\begin{array}{c} \mu_1 \\ \mu_{y_0} \end{array}\right)$$

$$\left(\begin{array}{ccc} \Sigma_1 & \Sigma_{1y_0} \\ \Sigma_{y_0 1} & \Sigma_{y_0} \end{array}\right)$$

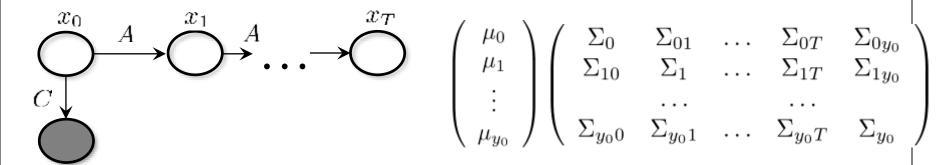


$$\Sigma_{1|0} = \Sigma_{x_1|y_0}$$

$$= \Sigma_1 - \Sigma_{1y_0} \Sigma_{y_0}^{-1} \Sigma_{y_0 1}$$

 Σ_{y_0} and Σ_1 are from unconstrained distribution. What matters is Σ_{1y_0} .





Marginalizing
$$x_{l},...x_{T-l}$$

$$\begin{pmatrix} \mu_{T} \\ \mu_{y_{0}} \end{pmatrix}$$

$$\begin{pmatrix} \Sigma_{T} & \Sigma_{Ty_{0}} \\ \Sigma_{y_{0}T} & \Sigma_{y_{0}} \end{pmatrix}$$

$$\mu_{T|0} = \mu_T + \sum_{Ty_0} \sum_{y_0}^{-1} (y_0 - \mu_{y_0})$$

$$\sum_{T|0} = \sum_T - \sum_{Ty_0} \sum_{y_0}^{-1} \sum_{y_0} T$$

What matters is how we can find the covariance of joint density function!!



 y_0



Filtering

$$\widehat{x}_{t|t} = \mathbb{E}[x_t|y_0, \dots, y_t]$$

$$P_{t|t} = \mathbb{E}[(x_t - \hat{x}_{t|t})(x_t - \hat{x}_{t|t})^{\top} | y_0, \dots, y_t]$$

"Conditional marginalization" Marginalization from the left

$$\widehat{x}_{t|t} \& P_{t|t} \longrightarrow \widehat{x}_{t+1|t+1} \& P_{t+1|t+1}$$

Why filtering? Once we know $\hat{x}_{t|t} \& P_{t|t}$, we don't have to know (or keep) y_0, \ldots, y_t .



Time update

$$p(x_t|y_0,\ldots,y_t) \to p(x_{t+1}|y_0,\ldots,y_t)$$

Measurement update

$$p(x_{t+1}|y_0,\ldots,y_t)\to p(x_{t+1}|y_0,\ldots,y_t,y_{t+1})$$

Time update

$$\widehat{x}_{t+1|t} = A\widehat{x}_{t|t} P_{t+1|t} = \mathbb{E}[(x_{t+1} - \widehat{x}_{t+1|t})(x_{t+1} - \widehat{x}_{t+1|t})^{\top} | y_0, \dots, y_t] = \mathbb{E}[(Ax_t + Gw_t - A\widehat{x}_{t|t})(Ax_t + Gw_t - A\widehat{x}_{t|t})^{\top} | y_0, \dots, y_t] = AP_{t|t}A^{\top} + GQG^{\top}$$

Similar to the unconstrained distribution calculation!





$$\mathbb{E}[y_{t+1}|y_0,\dots,y_t] = \mathbb{E}[Cx_{t+1} + v_{t+1}|y_0,\dots,y_t] = C\widehat{x}_{t+1|t}$$

$$\mathbb{E}[(y_{t+1} - \widehat{y}_{t+1|t})(y_{t+1} - \widehat{y}_{t+1|t})^{\top}|y_0, \dots, y_t]$$

$$= \mathbb{E}[(Cx_{t+1} + v_{t+1} - C\widehat{x}_{t+1|t})(Cx_{t+1} + v_{t+1} - C\widehat{x}_{t+1|t})^{\top}|y_0, \dots, y_t]$$

$$= CP_{t+1|t}C^T + R$$

Also,

$$\mathbb{E}[(y_{t+1} - \widehat{y}_{t+1|t})(x_{t+1} - \widehat{x}_{t+1|t})^{\top} | y_0, \dots, y_t]$$

$$= \mathbb{E}[(Cx_{t+1} + v_{t+1} - C\widehat{x}_{t+1|t})(x_{t+1} - \widehat{x}_{t+1|t})^{\top} | y_0, \dots, y_t]$$

$$= CP_{t+1|t}$$

Joint:

$$p(x_{t+1}, y_{t+1}|y_0, \dots, y_t) = \mathcal{N}\left(\begin{pmatrix} \hat{x}_{t+1|t} \\ C\hat{x}_{t+1|t} \end{pmatrix}, \begin{pmatrix} P_{t+1|t} & P_{t+1|t}C^{\top} \\ CP_{t+1|t} & CP_{t+1|t}C^{\top} + R \end{pmatrix}\right)$$





Measurement update (Conditional density)

$$p(x_{t+1}|y_0,\ldots,y_{t+1}) = \mathcal{N}(\widehat{x}_{t+1|t+1},P_{t+1|t+1})$$

$$\begin{cases}
\widehat{x}_{t+1|t+1} = \widehat{x}_{t+1|t} + P_{t+1|t}C^{\top}(CP_{t+1|t}C^{\top} + R)^{-1}(y_{t+1} - C\widehat{x}_{t+1|t}) \\
P_{t+1|t+1} = P_{t+1|t} - P_{t+1|t}C^{\top}(CP_{t+1|t}C^{\top} + R)^{-1}CP_{t+1|t}
\end{cases}$$

Sum - ups

$$\widehat{x}_{t+1|t} = A\widehat{x}_{t|t}$$

$$P_{t+1|t} = AP_{t|t}A^{\top} + GQG^{\top}$$

$$\widehat{x}_{t+1|t+1} = \widehat{x}_{t+1|t} + P_{t+1|t}C^{\top}(CP_{t+1|t}C^{\top} + R)^{-1}(y_{t+1} - C\widehat{x}_{t+1|t})$$

$$P_{t+1|t+1} = P_{t+1|t} - P_{t+1|t}C^{\top}(CP_{t+1|t}C^{\top} + R)^{-1}CP_{t+1|t}$$



With different notation,

$$K_{t+1} \equiv P_{t+1|t} C^{\top} (C P_{t+1|t} C^{\top} + R)^{-1}$$
$$\widehat{x}_{t+1|t+1} = \widehat{x}_{t+1|t} + K_{t+1} (y_{t+1} - C \widehat{x}_{t+1|t})$$

Alternative form of K_{t+1}

$$K_{t+1} = P_{t+1|t}C^{\top}(CP_{t+1|t}C^{\top} + R)^{-1}$$

$$= (P_{t+1|t}^{-1} + C^{\top}RC)^{-1}C^{\top}R^{-1}$$

$$= (P_{t+1|t} + P_{t+1|t}C^{\top}(CP_{t+1|t}C^{\top} + R)^{-1}CP_{t+1|t})C^{\top}R^{-1}$$

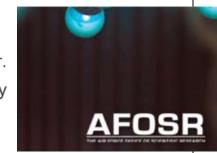
$$= P_{t+1|t+1}C^{\top}R^{-1}$$



The Kalman Filter? A Tool We Use Everyday

Posted on April 3, 2012 by ekrayer

Almost all modern control systems, both military and commercial, use the Kalman filter. It guided the Apollo 11 lunar module to the moon's surface and is used in phased-array radars to track missiles, inertial guidance systems in aircraft, submarines, missile autopilots, the Global Positioning System, the Space Shuttle and rockets.



AFOSR initiated support for Dr. Rudolph E. Kalman and Dr. Richard Bucy in 1958 to investigate the use of modern mathematical statistical methods in estimation. At the time, AFOSR program managers saw an opportunity in science for the creation of new mathematical techniques that could alter control applications. With AFOSR support, Kalman and Bucy wrote several papers that revolutionized the area of estimation.

This research ultimately led to the development of what is now known as the Kalman filter, which revolutionized the field of estimation, and had an enormous impact on the design and development of precise navigation systems. The Kalman and Bucy technique of combining and filtering information from multiple sensor sources achieved accuracies that clearly constituted a major breakthrough in guidance technology.

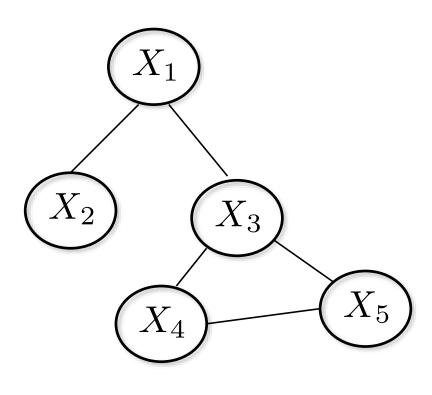
http://afrl.dodlive.mil/2012/04/03/the-kalman-filter-a-tool-we-use-everyday/http://www.wpafb.af.mil/News/Article-Display/Article/401306/computer-mouse-kalman-filter-trace-origins-to-air-force-basic-research-funding/





Markov Random Field

Undirected Graph



If there is a direct edge between X_i and X_j :

$$X_i \not\perp \!\!\! \perp X_j | X_{\setminus i,j}$$

If there is no direct edge between X_i and X_i :

$$X_i \perp \!\!\! \perp X_j | X_{\setminus i,j}$$

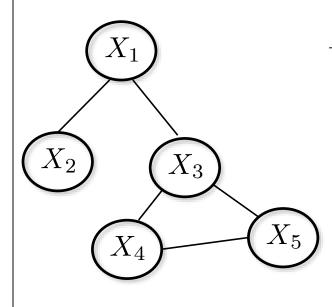
$$X_1 \perp \!\!\! \perp X_3 | X_2, X_4, X_5$$

 $X_1 \perp \!\!\! \perp X_5 | X_3$



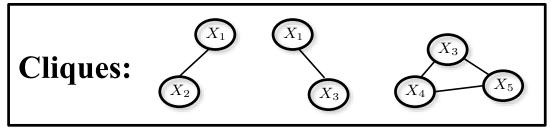
Joint Distribution

Product of functions on cliques



$$P(X_{1}, X_{2}, X_{3}, X_{4}, X_{5}) = \frac{1}{Z} \psi_{1,2}(X_{1}, X_{2}) \psi_{1,3}(X_{1}, X_{3}) \psi_{3,4,5}(X_{3}, X_{4}, X_{5})$$

$$\left(Z = \sum_{X_{1}, X_{2}, X_{3}, X_{4}, X_{5}} \psi_{1,2}(X_{1}, X_{2}) \psi_{1,3}(X_{1}, X_{3}) \psi_{3,4,5}(X_{3}, X_{4}, X_{5})\right)$$



The set of distributions satisfying MRF conditions (Markov random field)

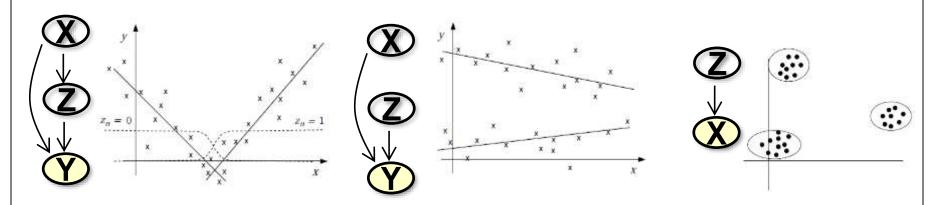
= The set of distributions decomposed by cliques (Gibbs random field)

(Hammersley-Clifford Theorem)

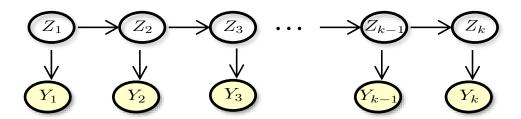


More Fancy Models

Latent Variable Model

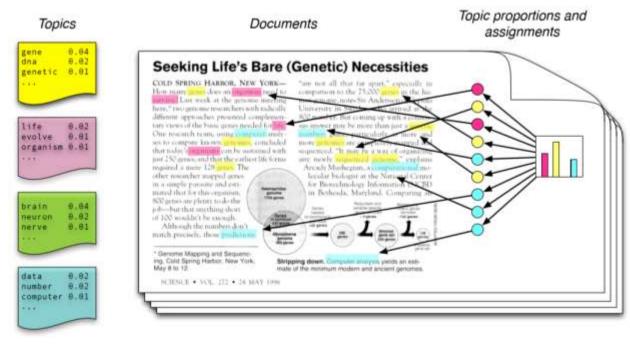


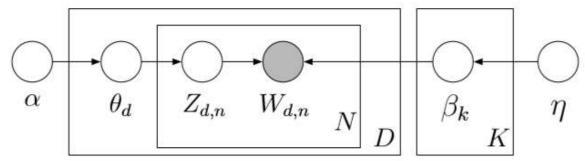
Filtering





Topic Models





$$p(\beta_{1:K}, \theta_{1:D}, z_{1:D}, w_{1:D}) = \prod_{i=1}^{K} p(\beta_i) \prod_{d=1}^{D} p(\theta_d) \left(\prod_{n=1}^{N} p(z_{d,n} | \theta_d) p(w_{d,n} | \beta_{1:K}, z_{d,n}) \right)$$





 $Topic\ Models \ {\tiny \frac{http://machinelearning.snu.ac.kr/NIPS2015/NIPS2015_Accepted/nipsnice.htm.}{ {\tiny \frac{http://cs.stanford.edu/people/karpathy/nipspreview/}}}$

NIPS 2012 papers

(in nicer format than this) maintained by @karpathy source code on github

> Below every paper are TOP 100 most-occurring words in that paper and their color is based on LDA topic model with k = 7. (It looks like 0 = theory, 1 = reinforcement learning, 2 = graphical models, 3 = deep learning/vision, 4 = optimization, 5 = neuroscience, 6 = embeddings etc.)

Toggle LDA topics to sort by: TOPIC0 TOPIC1





OPIC5

Discriminatively Trained Sparse Code Gradients for Contour Detection

Ren Xiaofeng, Liefeng Bo

[pdf] [bibtex] [supplementary] [rank by tf-idf similarity to this] [abstract]

[set, algorithm, including] [average, approach, benchmark, evaluation] [comparing, normal, hierarchical] [contour, gpb, local, detection, depth, scg. color, image, oriented, matching, contrast, object, grayscale, precision, recognition, transform, work, learned, pooling, pixel, representation, double, global, learn, accuracy, scale, level, segmentation, figure, feature, nyu, globalization, scene, training, rich, single, automatically, apply, discriminative, codewords, ieee, half, directly, unsupervised, higher, chromaticity] [sparse, dictionary, gradient, pursuit, size, spectral, analysis, edge, step, sparsity] [power, coding, surface, natural] [code, learning, linear, data, orthogonal, dataset, svm, large, better, table, well, datasets)

Deep Learning of Invariant Features via Simulated Fixations in Video

Will Zou, Andrew Ng, Shenghuo Zhu, Kai Yu











[pdf] [bibtex] [supplementary]

[rank by tf-idf similarity to this]





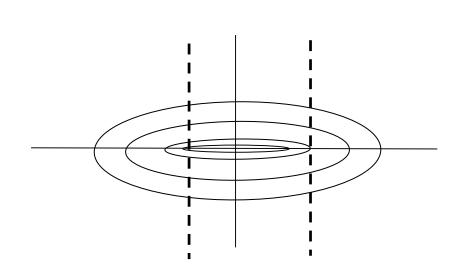
[abstract]

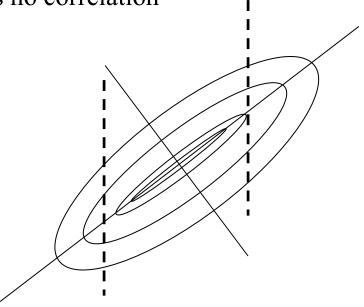
Independency

Correlation and Independency

$$p(\mathbf{x}_a, \mathbf{x}_b) = p(\mathbf{x}_a)p(\mathbf{x}_b)$$

Independency in Gaussian means no correlation



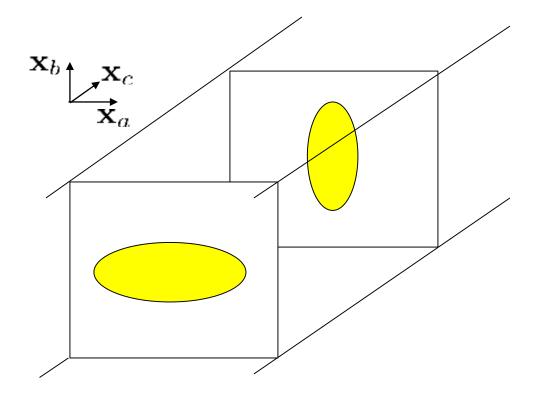


Naïve Bayes?
Mixture of Gaussian?



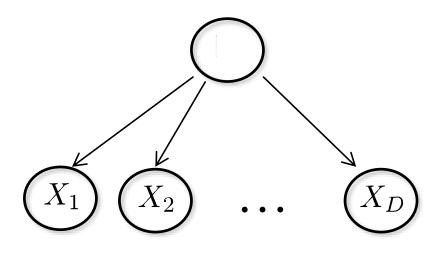
Conditional Independency

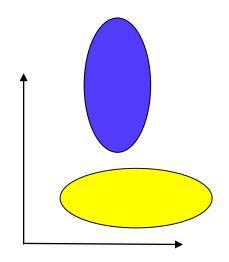
$$p(\mathbf{x}_a, \mathbf{x}_b) = p(\mathbf{x}_a)p(\mathbf{x}_b)$$
vs.
$$p(\mathbf{x}_a, \mathbf{x}_b | \mathbf{x}_c) = p(\mathbf{x}_a | \mathbf{x}_c)p(\mathbf{x}_b | \mathbf{x}_c)$$





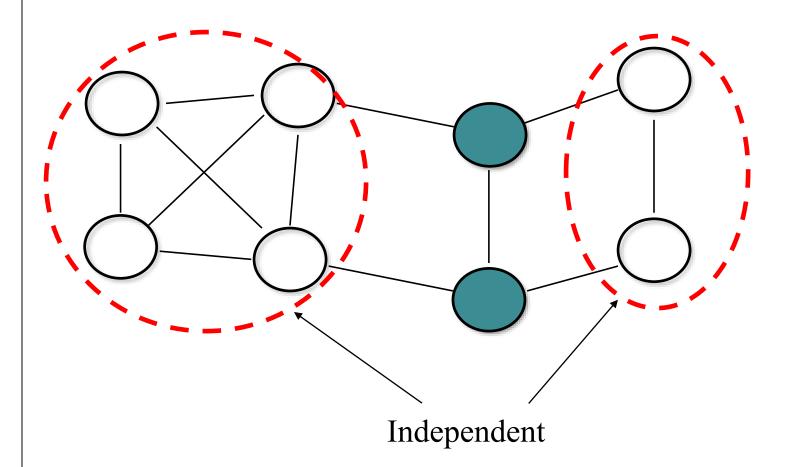
Naïve Bayes for Classification





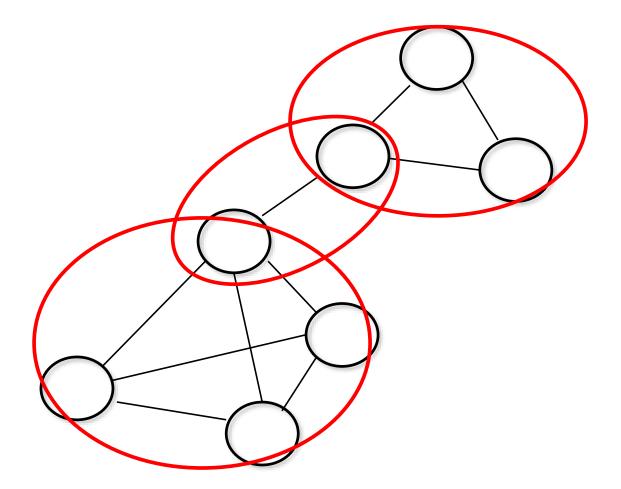
$$P(X,Y) = P(Y)P(X_1|Y) \dots P(X_D|Y)$$







Find all maximal cliques:





Potential functions on cliques

$$\Psi_1(X_1), \Psi_2(X_2), \dots$$
 $(X_1, X_2, \dots : \text{maximal cliques})$

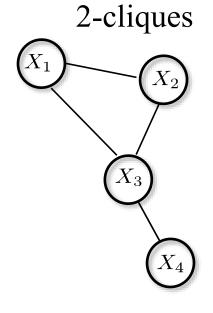
$$P(X) = \frac{1}{Z}\Psi_1(X_1)\Psi_2(X_2)\cdots\Psi_C(X_C)$$

$$Z = \sum_{X_1, X_2, \cdots, X_D} \Psi_1(X_1) \cdots \Psi_C(X_C) \quad \text{Discrete}$$

$$Z = \int_{X_1, X_2, \cdots, X_D} \Psi_1(X_1) \cdots \Psi_C(X_C) dX_1 \cdots X_C$$

$$Continuous$$
Partition function





$$Z = \sum_{X_1, X_2, X_3, X_4} \Psi_{X_1, X_2, X_3}(X_1, X_2, X_3) \Phi_{X_3, X_4}(X_3, X_4)$$

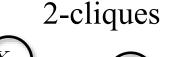
$$= \Psi_{X_1, X_2, X_3}(1, 1, 1) \Phi_{X_3, X_4}(1, 1) + \Psi_{X_1, X_2, X_3}(1, 1, 1) \Phi_{X_3, X_4}(1, 0) + \dots$$

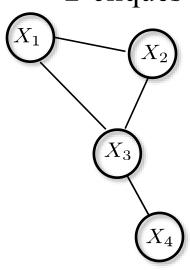
$$= 2 \cdot 1 + 2 \cdot 0 + \dots = 2 + 3 + 2 + 3 = 10$$

$$\text{Ex.} \quad P(1, 0, 0, 0) = \frac{1}{Z} \Psi_{X_1, X_2, X_3}(1, 0, 0) \Phi_{X_3, X_4}(0, 0) = \frac{1}{10} \cdot 1 \cdot 3 = \frac{3}{10}$$



Estimating Parameters





$$X_3 X_4$$

$$1 \quad 1 = \Phi_{1,1}$$

$$1 \quad 0 = \Phi_{1,0}$$

$$0 \quad 1 \quad \vdots$$

$$0 \quad 0 \quad \bullet$$

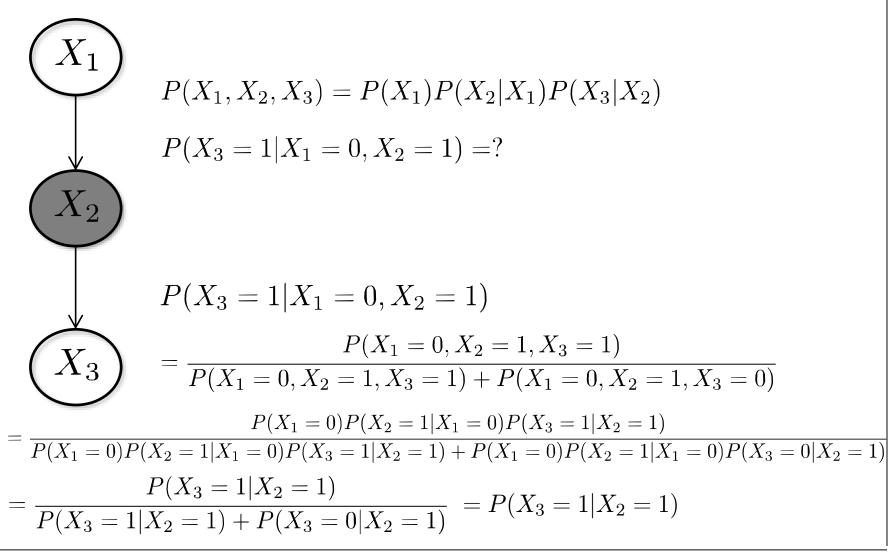
12 parameters

$$\Psi_{X_1,X_2,X_3}$$
: 8 Φ_{X_3,X_4} : 4

Without graphical model: <u>15 parameters</u> $(2^4 - 1)$

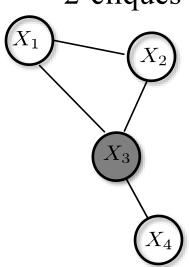
$$X_1 X_2 X_3 X_4$$
 $1 1 1 1 = P(1, 1, 1, 1)$
 $1 1 1 0 = P(1, 1, 1, 0)$
 $1 1 0 1$

Conditional Independency



Conditional Independency





$$X_1 X_2 X_3$$
 $1 1 1 = \Psi_{1,1}$
 $1 0 1 = \Psi_{1,0}$
 $0 1 1 = \Psi_{0,1}$
 $0 0 1 = \Psi_{0,0}$
 $X_3 X_4$
 $1 1 = \Phi_1$

$$egin{array}{cccc} X_3 \ X_4 \ & 1 & 1 & = \Phi_1 \ & 1 & 0 & = \Phi_0 \end{array}$$

$$egin{array}{llll} X_1 \ X_2 \ X_3 \ & X_1 \ X_2 \ X_3 \ X_4 \ & 1 \ 1 \ 1 \ 1 \ = \Psi_{1,1} \Phi_1 \ & 1 \ 1 \ 1 \ 0 \ = \Psi_{1,1} \Phi_0 \ & 1 \ 1 \ 1 \ 0 \ = \Psi_{1,1} \Phi_0 \ & 1 \ 0 \ 1 \ 1 \ = \Psi_{1,0} \Phi_1 \ & 1 \ 0 \ 1 \ 0 \ = \Psi_{1,0} \Phi_0 \ & 0 \ 1 \ 1 \ = \Psi_{0,1} \Phi_1 \ & 0 \ 1 \ 1 \ = \Psi_{0,1} \Phi_1 \ & 0 \ \end{array}$$

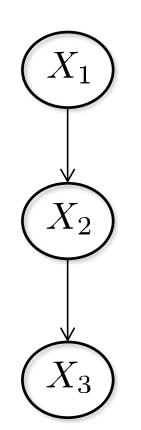
 $0 \ 1 \ 1 \ 0 = \Psi_{0,1}\Phi_0$

$$P(X_4 = 1 | X_1 = 0, X_2 = 1) = ?$$
 $P(X_4 = 1 | X_1 = 0, X_2 = 0) = ?$
 $P(X_4 = 1) = ?$

All answers are the same: $\frac{1}{\Phi_1 + \Phi_0}$

$$\frac{\Phi_1}{\Phi_1 + \Phi_0}$$

Marginalization

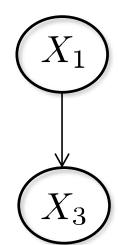


$$P(X_1, X_2, X_3) = P(X_1)P(X_2|X_1)P(X_3|X_2)$$

$$P(X_1, X_3) = \int P(X_1, X_2, X_3) dX_2$$

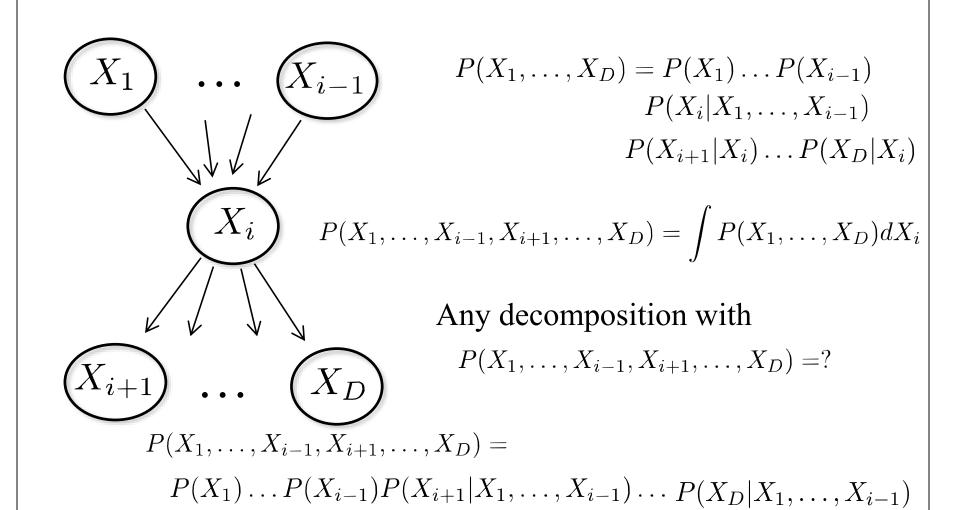
Any good property like

$$P(X_1, X_3) = P(X_1)P(X_3)$$
?



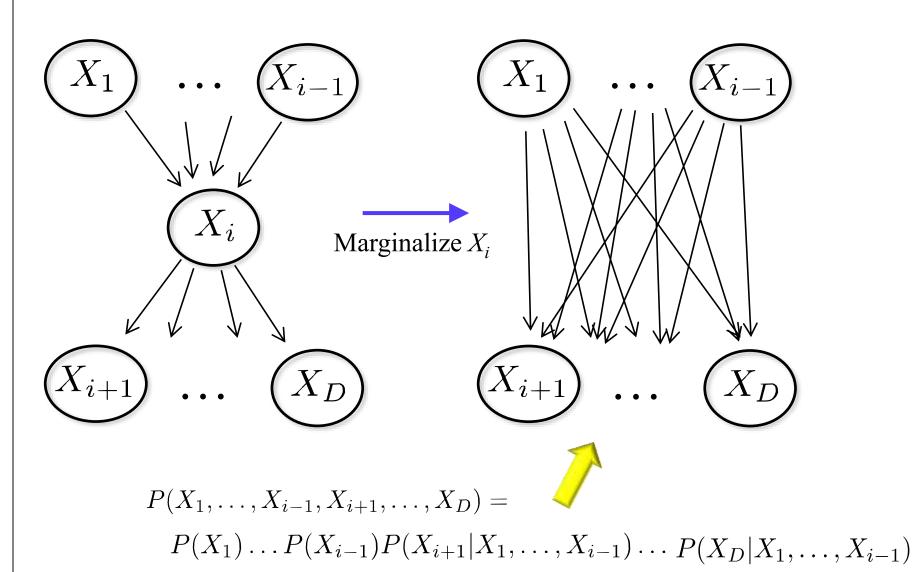


Marginalization



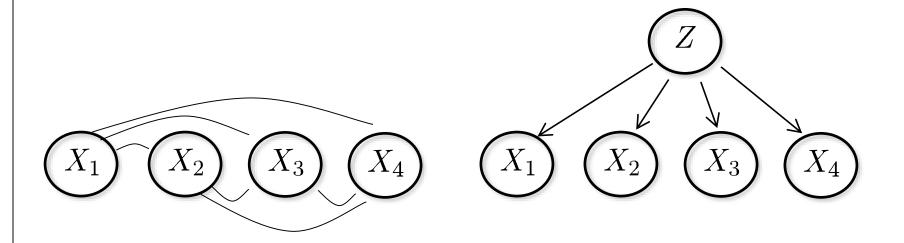


Marginalization





Introducing Latent Variables



 Issue: how can a model be simplified as much as possible, while the flexibility is kept enough to incorporate the true dependency.



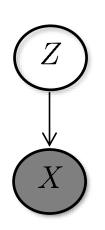
Expectation-Maximization Algorithm

- Parameter estimation with latent variables
 - We don't have data for latent variables
- E-step:
 - Data for latent variables are obtained from expectation with current parameter values.
- M-step:
 - With expected latent variables, parameters are obtained by maximizing the likelihood.
- E-step and M-step are repeated back and forth until the likelihood converges.



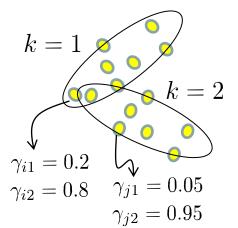
Expectation-Maximization Algorithm

Gaussian mixture model



Parameters:
$$\pi_k, \mu_k, \Sigma_k$$
 for $k = 1, \dots, K$
Unknown variables: $z_i = \begin{pmatrix} z_{i1} \\ \vdots \\ z_{iK} \end{pmatrix}$ for $i = 1, \dots, N$

We are given \mathbf{x}_i for $i = 1, \dots, N$



E-step: Distribution of \mathbf{z}_i (Responsibilities)

$$\gamma(z_{ik}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_i | \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}_i | \mu_j, \Sigma_j)}$$

using current parameters π_k, μ_k, Σ_k

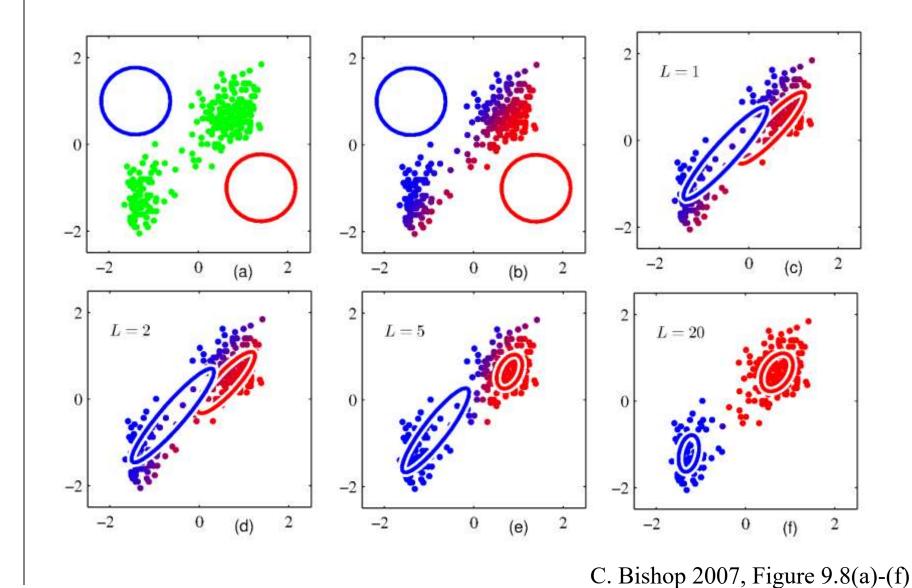
Expectation-Maximization Algorithm

M-step: Estimate parameters.

$$\begin{cases} \mu_k = \frac{1}{N_k} \sum_{i=1}^N \gamma(z_{ik}) \ \mathbf{x}_i \\ \Sigma_k = \frac{1}{N_k} \sum_{i=1}^N \gamma(z_{ik}) (\mathbf{x}_i - \mu_k) (\mathbf{x}_i - \mu_k)^\top \\ \pi_k = \frac{N_k}{N} \\ \text{for } N_k = \sum_{i=1}^N \gamma(z_{ik}) \end{cases}$$
 Iterate until $\ln p(X|\pi, \mu, \Sigma) = \sum_{i=1}^N \ln \left(\sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x}_i|\mu_k, \Sigma_k) \right)$ converges.



Gaussian Mixture Model With EM





ANY QUESTIONS?



THANK YOU

Yung-Kyun Noh nohyung@snu.ac.kr

