

# Probabilistic Graphical Models

Gaussian Network Models

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# Learning objectives

- multivariate Gaussian density:
  - different parametrizations
  - marginalization and conditioning
  - expression as Markov & Bayesian networks

# Univariate Gaussian density

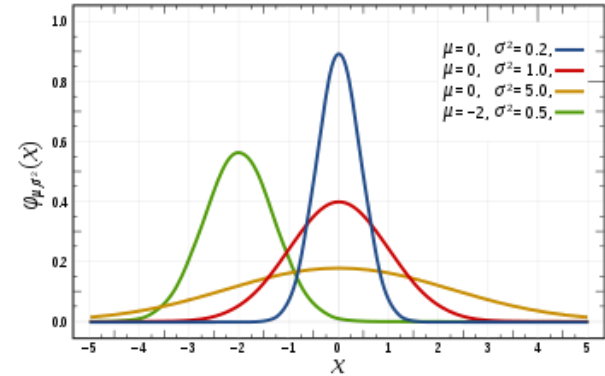
$$p(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- motivated by central limit theorem
- max-entropy dist. with a fixed variance

$$\mu \in \mathfrak{R}, \sigma^2 > 0$$

$$\mathbb{E}[X] = \mu,$$


$$\mathbb{E}[X^2] - \mathbb{E}[X]^2 = \sigma^2$$



# Multivariate Gaussian

$\mathbf{x} \in \mathfrak{R}^n$  is a column vector (*convention*)

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


$$(2\pi)^{-\frac{n}{2}} |\Sigma|^{-\frac{1}{2}}$$

compre to  $p(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

# Multivariate Gaussian: **sufficient statistics**

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

$$\mu = \mathbb{E}[\mathbf{X}]$$

$$\Sigma = \underbrace{\mathbb{E}[\mathbf{X}\mathbf{X}^T]}_{n \times n} - \underbrace{\mathbb{E}[\mathbf{X}]\mathbb{E}[\mathbf{X}^T]}_{n \times n} \quad \text{the covariance matrix} \quad \left| \begin{array}{l} \Sigma_{i,i} = \text{Var}(X_i) \\ \Sigma_{i,j} = \text{Cov}(X_i, X_j) \end{array} \right.$$

only captures these two statistics

# Multivariate Gaussian: **covariance matrix**

since  $\mathbf{y}^T \Sigma \mathbf{y} = (\mathbf{y}^T \mathbb{E}[(\mathbf{X} - \mathbb{E}[\mathbf{X}])(\mathbf{X} - \mathbb{E}[\mathbf{X}])^T] \mathbf{y}) = a^2 > 0$

↑  
move this expectation out

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- $\Sigma \succ 0$
- is **symmetric positive definite** (PD)  $\mathbf{y}^T \Sigma \mathbf{y} > 0 \quad \forall \mathbf{y}; \|\mathbf{y}\| > 0$
  - the inverse of a PD matrix is PD
    - the **precision matrix**  $\Lambda = \Sigma^{-1} \succ 0$
  - is diagonalized by orthonormal matrices

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$$\Sigma = \mathbf{Q} \mathbf{D} \mathbf{Q}^T$$

↓     ↓  
      diagonal

- orthogonal rows & columns of unit norm  $\mathbf{Q} \mathbf{Q}^T = \mathbf{Q}^T \mathbf{Q} = \mathbf{I}$
- rotation and reflection



# Multivariate Gaussian: covariance matrix

$$\Sigma = Q D Q^T$$

↓ diagonal (scaling)

- orthogonal rows & columns of unit norm  $Q Q^T = Q^T Q = I$
- rotation and reflection

Scaling along axes in some rotated/reflected coordinate system

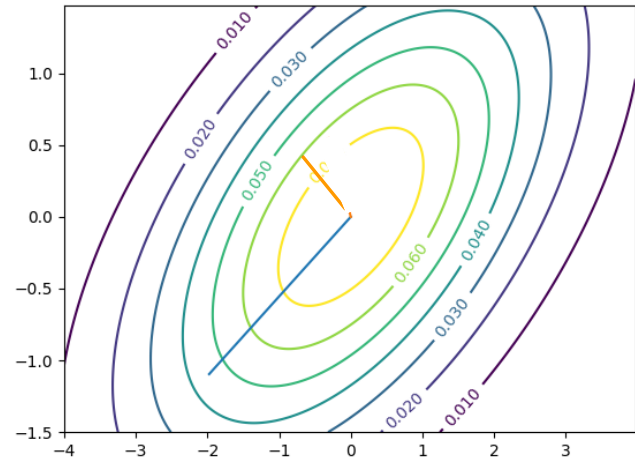
# Multivariate Gaussian: **example**

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

$$\Sigma = \begin{bmatrix} 4, & 2 \\ 2, & \frac{1}{2} \end{bmatrix} \approx \begin{bmatrix} -.87, & -.48 \\ -.48, & .87 \end{bmatrix} \begin{bmatrix} 5.1, & 0 \\ 0, & .39 \end{bmatrix} \begin{bmatrix} -.87, & -.48 \\ -.48, & .87 \end{bmatrix}^T$$

$\downarrow$   $Q$                        $D$                        $Q^T$

columns of  $Q$  are the new bases



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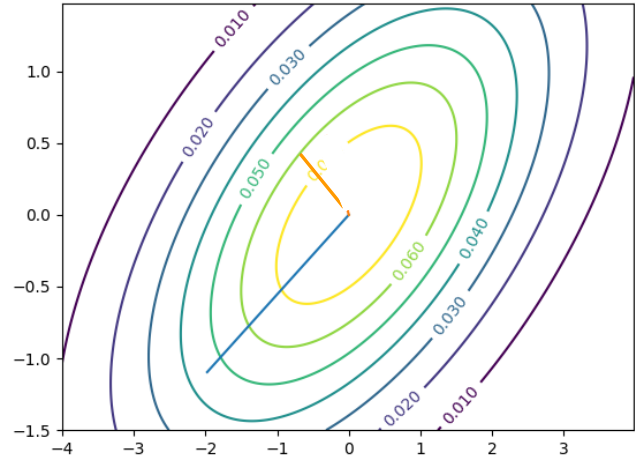
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**Alternatively**

approximately  $\begin{bmatrix} \cos(208^\circ), \sin(208^\circ) \\ \sin(208^\circ), -\cos(208^\circ) \end{bmatrix}$

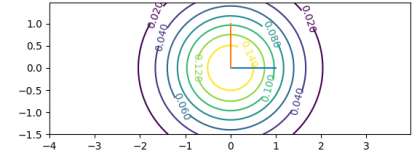
reflection of coordinates by the line making an angle  $\theta/2 = 104^\circ$



# Multivariate Gaussian: **from univariates**

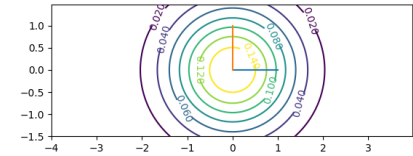
given n univariate Gaussians

$$\mathbf{X} \sim \mathcal{N}(0, I)$$

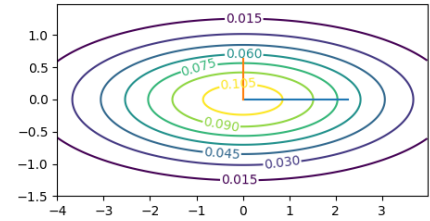


# Multivariate Gaussian: **from univariates**

given  $n$  univariate Gaussians  $\mathbf{X} \sim \mathcal{N}(0, I)$



**scale** them by  $\sqrt{D_{ii}}$   $D^{\frac{1}{2}} \mathbf{X} \sim \mathcal{N}(0, D)$



# Multivariate Gaussian: **from univariates**

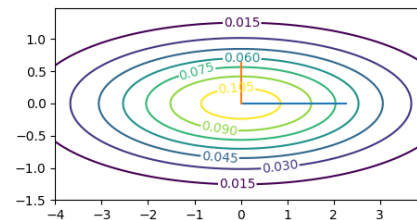
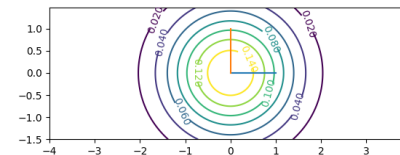
given n univariate Gaussians  $\mathbf{X} \sim \mathcal{N}(0, I)$

**scale** them by  $\sqrt{D_{ii}}$   $D^{\frac{1}{2}} \mathbf{X} \sim \mathcal{N}(0, D)$

**rotate/reflect** using  $Q$   $QD^{\frac{1}{2}} \mathbf{X} \sim \mathcal{N}(0, QDQ^T) = \mathcal{N}(0, \Sigma)$

**more generally**

$$\mathbf{X} \sim \mathcal{N}(\mu, \Sigma) \Rightarrow A\mathbf{X} + b \sim \mathcal{N}(A\mu + b, A\Sigma A^T)$$



# parametrization

**moment form** (*mean parametrization*)

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

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↓  
 $\eta = \Sigma^{-1} \mu$  : local potential  
 $\Lambda = \Sigma^{-1}$  : precision matrix



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**information form** (*cannonical parametrization*)


$$p(\mathbf{x}; \eta, \Lambda) = \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \exp\left(-\frac{1}{2}\mathbf{x}^T \Lambda \mathbf{x} + \eta^T \mathbf{x} - \frac{1}{2}\eta^T \Lambda \eta\right)$$

# parametrization

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$$\begin{aligned} \eta &= \Sigma^{-1} \mu : \text{local potential} \\ \Lambda &= \Sigma^{-1} : \text{precision matrix} \end{aligned}$$


$$\begin{aligned} \mu &= \Lambda^{-1} \eta \\ \Sigma &= \Lambda^{-1} \end{aligned}$$

**information form** (*cannonical parametrization*)

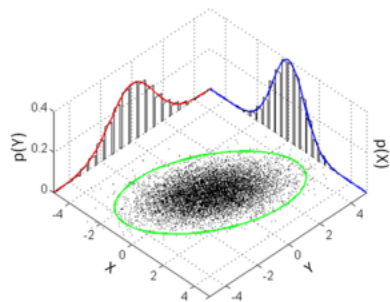
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the relationship between the two types goes beyond Gaussians

# Marginalization

moment form  $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

is useful for marginalization:



$$\mathbf{X} = [\mathbf{X}_A, \mathbf{X}_B]^T$$

$$\mathbf{X}_A \sim \mathcal{N}(\boldsymbol{\mu}_m, \boldsymbol{\Sigma}_m)$$

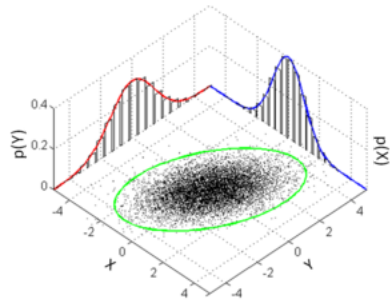
$$\boldsymbol{\mu} = [\boldsymbol{\mu}_A, \boldsymbol{\mu}_B]^T$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{AA} & \boldsymbol{\Sigma}_{AB} \\ \boldsymbol{\Sigma}_{BA} & \boldsymbol{\Sigma}_{BB} \end{bmatrix}$$

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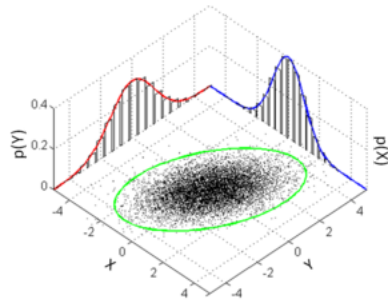
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marginalization as a **linear transformation**:  $A = [I_{AA}, \mathbf{0}]$

$$\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \Rightarrow A\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}_A, \boldsymbol{\Sigma}_{AA})$$

# Marginal independencies: moment form

**covariance** means dependence & vice versa

$$X_i \perp X_j \mid \emptyset \Leftrightarrow \Sigma_{i,j} = \text{Cov}(X_i, X_j) = 0$$

why?

marginalize  $\mathcal{N}(\mu, \Sigma)$  to get  $\begin{bmatrix} X_i \\ X_j \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_i \\ \mu_j \end{bmatrix}, \begin{bmatrix} \sigma_i^2, & \mathbf{0} \\ \mathbf{0}, & \sigma_j^2 \end{bmatrix}\right) = \mathcal{N}(x_i; \mu_i, \sigma_i^2)\mathcal{N}(x_j; \mu_j, \sigma_j^2)$

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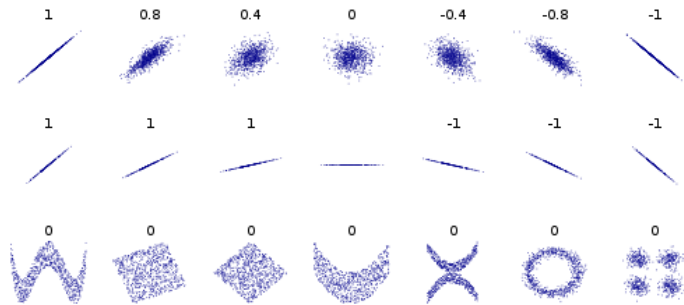


image from wikipedia

*Gaussian is special in this sense*

**correlation:** normalized covariance

$$\rho(X_i, X_j) = \frac{\text{Cov}(X_i, X_j)}{\sqrt{\text{Var}(X_i)\text{Var}(X_j)}}$$

# Conditional independencies: *information form*

zeros of the **precision matrix** mean conditional independence

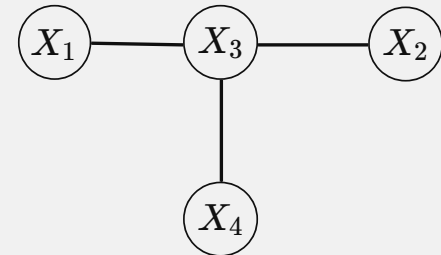
$$X_i \perp X_j \mid \mathbf{X} - \{X_i, X_j\} \Leftrightarrow \Lambda_{i,j} = 0$$

$\Lambda \neq 0$  adjacency matrix in the *Markov network* (**Gaussian MRF**)

$$p(\mathbf{x}; \eta, \Lambda) = \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \exp\left(-\frac{1}{2}\mathbf{x}^T \Lambda \mathbf{x} + \eta \mathbf{x} - \frac{1}{2}\eta^T \Lambda \eta\right)$$

why?

$$\Lambda = \begin{bmatrix} \Lambda_{11}, & 0, & \Lambda_{1,3}, & 0 \\ 0, & \Lambda_{2,2}, & \Lambda_{2,3}, & 0 \\ \Lambda_{3,1}, & \Lambda_{3,2}, & \Lambda_{3,3}, & \Lambda_{3,4} \\ 0, & 0, & \Lambda_{4,3}, & \Lambda_{4,4} \end{bmatrix}$$





# Conditional independencies: *information form*

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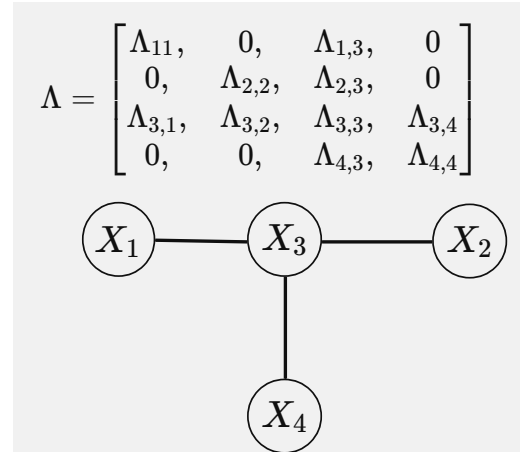
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**why?** write it as the product of factors:

$$\begin{array}{l} \text{corresponding} \\ \text{potentials} \end{array} \left| \begin{array}{l} \psi_{i,j}(x_i, x_j) = -x_i \Lambda_{i,j} x_j \\ \psi_i(x_i) = -\frac{1}{2} \Lambda_{i,i} x_i^2 + \eta_i x_i \end{array} \right.$$



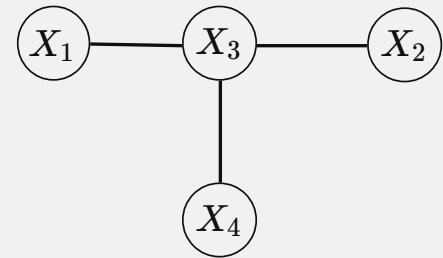
## Gaussian MRF: *information form*

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corresponding  
potentials

$$\begin{cases} \psi_{i,j}(X_i, X_j) = -x_i \Lambda_{i,j} x_j \\ \psi_i(X_i) = -\Lambda_{i,i} x_i^2 + \eta_i x_i \end{cases}$$

$$\Lambda = \begin{bmatrix} \Lambda_{11} & 0 & \Lambda_{1,3} & 0 \\ 0 & \Lambda_{2,2} & \Lambda_{2,3} & 0 \\ \Lambda_{3,1} & \Lambda_{3,2} & \Lambda_{3,3} & \Lambda_{3,4} \\ 0 & 0 & \Lambda_{4,3} & \Lambda_{4,4} \end{bmatrix}$$



$\Lambda$  should be **positive definite**

- otherwise the partition function

$$Z = \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}\mathbf{x}^T \Lambda \mathbf{x} + \eta^T \mathbf{x}\right) d\mathbf{x} \text{ is not well-defined}$$

# Conditioning: information form

marginalization: easy in the moment form

**conditioning:** easy in the information form

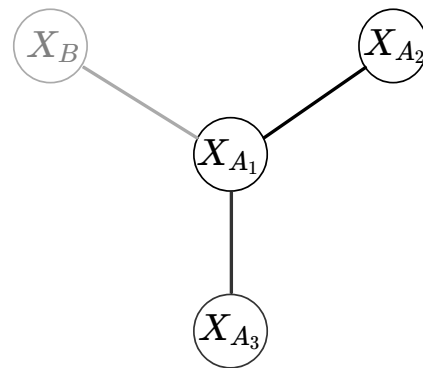
$$\mathbf{X}_A \mid \mathbf{X}_B \sim \mathcal{N}(\eta_{A|B}, \Lambda_{A|B})$$

why?

$$\Lambda_{A|B} = \Lambda_{AA}$$

$$\eta_{A|B} = \eta_A + \Lambda_{AB} \mathbf{X}_B$$

$$\begin{aligned} \mathbf{X} &= [\mathbf{X}_A, \mathbf{X}_B]^T \\ \eta &= [\eta_A, \eta_B]^T \\ \Lambda &= \begin{bmatrix} \Lambda_{AA} & \Lambda_{AB} \\ \Lambda_{BA} & \Lambda_{BB} \end{bmatrix} \end{aligned}$$



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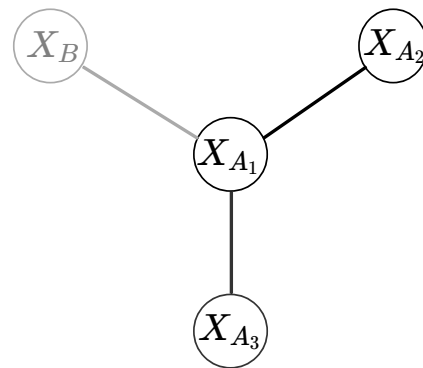
$$\Lambda = \begin{bmatrix} \Lambda_{AA} & \Lambda_{AB} \\ \Lambda_{BA} & \Lambda_{BB} \end{bmatrix}$$

not so easy in the moment form!

$$\mathbf{X}_A \mid \mathbf{X}_B \sim \mathcal{N}(\mu_{A|B}, \Sigma_{A|B})$$

$$\Sigma_{A|B} = \Sigma_{AA} - \Sigma_{AB} \Sigma_{BB}^{-1} \Sigma_{BA}$$

$$\mu_{A|B} = \mu_A - \Sigma_{AB} \Sigma_{BB}^{-1} (\mathbf{X}_B - \mu_B)$$

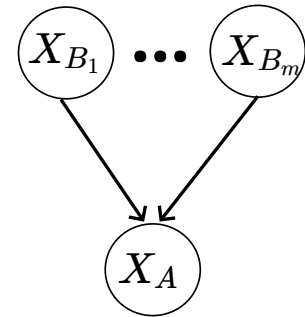


# Gaussian Bayesian network

an alternative representation for multivariate Gaussian

linear Gaussian CPD  $X_A | \mathbf{X}_B \sim \mathbf{w}^T \mathbf{X}_B + \mathcal{N}(\mu_0, \sigma_0^2)$

and  $\mathbf{X}_B \sim \mathcal{N}(\mu_B, \Sigma_B)$



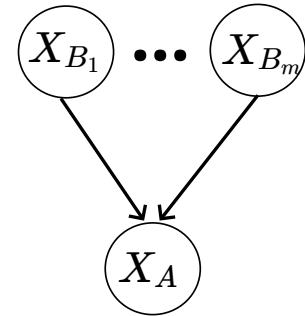
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joint dist.  $\Leftrightarrow$  conditional form (CPD)



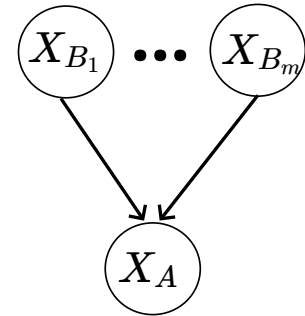
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joint dist.  $\Leftrightarrow$  conditional form (CPD)



$$X_0 \sim \mathcal{N}(\mu_0, \sigma_0^2)$$

$$X_1 = \mathbf{w}^T \mathbf{X}_B \sim \mathcal{N}(\mathbf{w}^T \mu_B, \mathbf{w}^T \Sigma_B \mathbf{w})$$

$$X_A = X_0 + X_1 \sim \mathcal{N}(\mu_0 + \mathbf{w}^T \mu_B, \sigma_0^2 + \mathbf{w}^T \Sigma_B \mathbf{w})$$

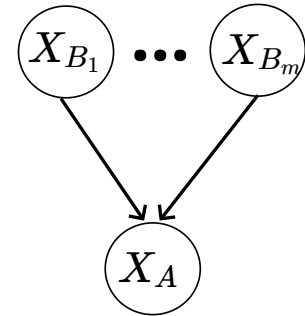
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and  $\mathbf{X}_B \sim \mathcal{N}(\mu_B, \Sigma_B)$

joint dist.  $\Leftrightarrow$  conditional form (CPD)



sum of two Gaussian RVs is a Gaussian RV

the pdf of the sum of RVs from the convolution of pdfs

$$X_0 \sim \mathcal{N}(\mu_0, \sigma_0^2)$$

$$X_1 = \mathbf{w}^T \mathbf{X}_B \sim \mathcal{N}(\mathbf{w}^T \mu_B, \mathbf{w}^T \Sigma_B \mathbf{w})$$

$$X_A = X_0 + X_1 \sim \mathcal{N}(\mu_0 + \mathbf{w}^T \mu_B, \sigma_0^2 + \mathbf{w}^T \Sigma_B \mathbf{w})$$



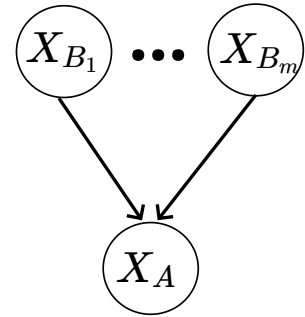
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an **alternative representation** for multivariate Gaussian

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and  $\mathbf{X}_B \sim \mathcal{N}(\mu_B, \Sigma_B)$

joint dist.  $\Leftrightarrow$  conditional form (CPD)

marginal over  $X_A$  is  $X_A \sim \mathcal{N}(\mu_0 + \mathbf{w}^T \mu_B, \sigma_0^2 + \mathbf{w}^T \Sigma_B \mathbf{w})$



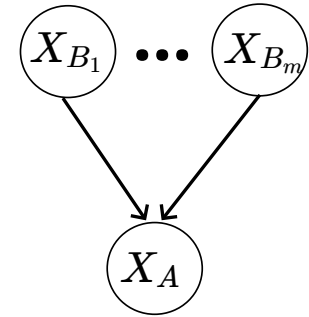
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linear Gaussian CPD  $X_A | \mathbf{X}_B \sim \mathbf{w}^T \mathbf{X}_B + \mathcal{N}(\mu_0, \sigma_0^2)$

and  $\mathbf{X}_B \sim \mathcal{N}(\mu_B, \Sigma_B)$

joint dist.  $\Leftrightarrow$  conditional form (CPD)



marginal over  $X_A$  is  $X_A \sim \mathcal{N}(\mu_0 + \mathbf{w}^T \mu_B, \sigma_0^2 + \mathbf{w}^T \Sigma_B \mathbf{w})$

joint dist. is  $(X_A, \mathbf{X}_B) \sim \mathcal{N} \left( \begin{bmatrix} \mu_0 + \mathbf{w}^T \mu_B \\ \mu_B \end{bmatrix}, \begin{bmatrix} \sigma_0^2 + \mathbf{w}^T \Sigma_B \mathbf{w}, & \mathbf{w}^T \Sigma_B \\ \Sigma_B \mathbf{w}, & \Sigma_B \end{bmatrix} \right)$

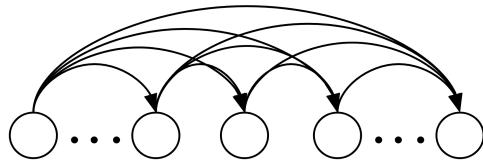
all the other elements follow from the marginals

$$\text{Cov}(X_A, X_{B,i}) = \sum_j w_j \text{Cov}(X_{B,j}, X_{B,i})$$

# Gaussian Bayesian network

an alternative representation for multivariate Gaussian

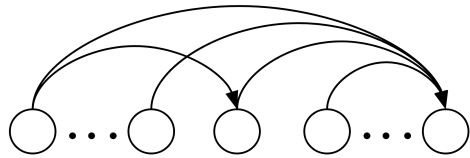
linear Gaussian CPD  $X_i | Pa_{X_i} \sim \mathbf{w}_i^T Pa_{X_i} + \mathcal{N}(\mu_i, \sigma_i^2)$



**worst case:**  $\mathcal{O}(n)$  parameters per node

- even if  $\Sigma$  is sparse!

**generally:**

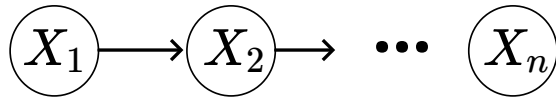


- DAG structure depends on the ordering
- v-structures  $X_k \perp X_j \Rightarrow \Sigma_{k,j} = 0$
- d-separation to find the sparsity of  $\Sigma$

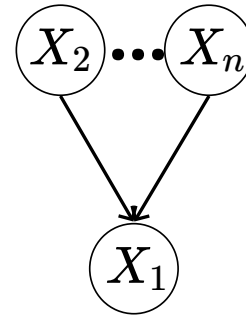
# quiz

what is the sparsity patterns of  $\Sigma$ ,  $\Lambda$ , and  $\mathbf{w}^i$  in Gaussian BN?

case 1



case 2



# Summary

- **multivariate Gaussian:**
  - mean param. (moment form)  $\Sigma, \mu$ 
    - useful for marginalization
    - sparsity  $\Leftrightarrow$  *marginal* independence



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# Summary

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    - sparsity  $\Leftrightarrow$  *conditional* independence
- **Gaussian Bayesian network (linear Gaussian CPD)**
- **Gaussian MRF (using information form)**