Review

- Univariate Normal: $\mathcal{N}(x;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$
- Multivariate Normal: $\mathcal{N}(\mathbf{x};\boldsymbol{\mu},\Sigma) = \frac{1}{det(2\pi\Sigma)} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})}$
- Covariance matrices are Hermitian and thus can be diagonalized by its eigenvectors. Covariance matrices are positive semi-definite (eigenvalues ≥ 0)
- Independence: $p(x,y) = p(x)p(y)$, $X \perp\!\!\!\perp Y$
- Markov property and conditional independence: $p(x,y|z) = p(x|z)p(y|z)$, $X \perp\!\!\!\perp Y|Z, X \leftrightarrow Z \leftrightarrow Y$

Remark

Note that $\mathcal{N}(\mathbf{x};\boldsymbol{\mu},\Sigma) = \mathcal{N}(\boldsymbol{\mu};\mathbf{x},\Sigma)$. It is trivial but quite useful

Inference

o: (Observed) evidence, θ: Parameter, x: prediction

Maximum Likelihood (ML)

$\hat{x} = \arg\max_x p(x|\hat{\theta}), \hat{\theta} = \arg\max_\theta p(o|\theta)$

Maximum A Posteriori (MAP)

$\hat{x} = \arg\max_x p(x|\hat{\theta}), \hat{\theta} = \arg\max_\theta p(\theta|o)$

Bayesian

$$\hat{x} = \sum_x x \underbrace{\sum_\theta p(x|\theta)p(\theta|o)}_{p(x|o)}$$

where $p(\theta|o) = \frac{p(o|\theta)p(\theta)}{p(o)} \propto p(o|\theta)\underbrace{p(\theta)}_{prior}$

Covariance matrices

Definition (Covariance matrices)

Recall that for a vector random variable $\boldsymbol{X} = [X_1, X_2, \cdots, X_n]^T$, the covariance matrix $\Sigma \triangleq E[(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^T]$

Remark

Covariance matrices are always positive semi-definite since $\forall u$, $u^T \Sigma u = E[u^T (\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^T u] = E[\|(\boldsymbol{X} - \boldsymbol{\mu})^T u\|^2] \geq 0$

Remark

In general, we usually would like to assume Σ *to be strictly positive definite. Because otherwise it means that some of its eigenvalues are zero and so in some dimension, there is actually no variation and is just constant along that dimension. Representing those dimension as random variable is troublesome since "*$1/\sigma^2$*" which occurs often will become infinite. Instead we can always simply strip away those dimensions to avoid complications*

Eigenvectors and eigenvalues of covariance matrices

- WLOG, let's assume $\mathbf{X} = [X_1, X_2, \cdots, X_n]^T$ is zero mean. So the covariance matrix $\Sigma_X = E[\mathbf{X}\mathbf{X}^T]$

Eigenvectors and eigenvalues of covariance matrices

- WLOG, let's assume $\mathbf{X} = [X_1, X_2, \cdots, X_n]^T$ is zero mean. So the covariance matrix $\Sigma_X = E[\mathbf{X}\mathbf{X}^T]$
- Covariance matrices are real symmetric (hence Hermitian) and so can be diagonalized by its eigenvectors. That is,
  - $P^T \Sigma_X P = D$, where $P = [u_1, u_2, \cdots, u_n]$ with u_k being eigenvectors of Σ and D is a diagonal matrix with eigenvalues $\lambda_1, \lambda_2, \cdots, \lambda_n$ as the diagonal elements

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- Let $\mathbf{Y} = P^T \mathbf{X}$, note that the covariance matrix of $\mathbf{Y}$

$$\Sigma_Y = E[\mathbf{Y}\mathbf{Y}^T] = E[P^T \mathbf{X}\mathbf{X}^T P] = P^T E[\mathbf{X}\mathbf{X}^T] P = P^T \Sigma_X P = D$$

is diagonalized

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  - $P^T \Sigma_X P = D$, where $P = [u_1, u_2, \cdots, u_n]$ with u_k being eigenvectors of Σ and D is a diagonal matrix with eigenvalues $\lambda_1, \lambda_2, \cdots, \lambda_n$ as the diagonal elements
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  is diagonalized
  - So the variance of Y_k is simply λ_k
  - $E[Y_i Y_j] = 0$ for $i \neq j$. That is, $Y_i \perp\!\!\!\perp Y_j$ for $i \neq j$

Marginalization of normal distribution

- Consider $\mathbf{Z} \sim \mathcal{N}(\boldsymbol{\mu}_{\mathbf{Z}}, \Sigma_{\mathbf{Z}})$ and let say $\mathbf{X}$ is a segment of $\mathbf{Z}$. That is, $\mathbf{Z} = \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix}$ for some $\mathbf{Y}$. Then how should $\mathbf{X}$ behave?

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- We can find the pdf of $\mathbf{X}$ by just marginalizing that of $\mathbf{Z}$. That is

$$\begin{aligned} p(\mathbf{x}) &= \int p(\mathbf{x}, \mathbf{y}) d\mathbf{y} \\ &= \frac{1}{\sqrt{\det(2\pi\Sigma)}} \int \exp\left(-\frac{1}{2} \begin{pmatrix} \mathbf{x} - \boldsymbol{\mu}_\mathbf{X} \\ \mathbf{y} - \boldsymbol{\mu}_\mathbf{Y} \end{pmatrix}^T \Sigma^{-1} \begin{pmatrix} \mathbf{x} - \boldsymbol{\mu}_\mathbf{X} \\ \mathbf{y} - \boldsymbol{\mu}_\mathbf{Y} \end{pmatrix} \right) d\mathbf{y} \end{aligned}$$

Marginalization of normal distribution

- Denote Σ^{-1} as Λ (also known as the precision matrix). And partition both Σ and Λ into $\Sigma = \begin{pmatrix} \Sigma_{\mathbf{XX}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{YX}} & \Sigma_{\mathbf{YY}} \end{pmatrix}$ and $\Lambda = \begin{pmatrix} \Lambda_{\mathbf{XX}} & \Lambda_{\mathbf{XY}} \\ \Lambda_{\mathbf{YX}} & \Lambda_{\mathbf{YY}} \end{pmatrix}$

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- Then we have

$$p(\mathbf{x}) = \frac{1}{\sqrt{\det(2\pi\Sigma)}} \int \exp\left(-\frac{1}{2}\left[(\mathbf{x}-\mu_{\mathbf{X}})^T\Lambda_{\mathbf{XX}}(\mathbf{x}-\mu_{\mathbf{X}}) + (\mathbf{y}-\mu_{\mathbf{Y}})^T\Lambda_{\mathbf{YX}}(\mathbf{x}-\mu_{\mathbf{X}}) + (\mathbf{x}-\mu_{\mathbf{X}})^T\Lambda_{\mathbf{XY}}(\mathbf{y}-\mu_{\mathbf{Y}}) + (\mathbf{y}-\mu_{\mathbf{Y}})^T\Lambda_{\mathbf{YY}}(\mathbf{y}-\mu_{\mathbf{Y}})\right]\right) d\mathbf{y}$$

$$= \frac{e^{-\frac{(\mathbf{x}-\mu_{\mathbf{X}})^T\Lambda_{\mathbf{XX}}(\mathbf{x}-\mu_{\mathbf{X}})}{2}}}{\sqrt{\det(2\pi\Sigma)}} \int \exp\left(-\frac{1}{2}\left[(\mathbf{y}-\mu_{\mathbf{Y}})^T\Lambda_{\mathbf{YX}}(\mathbf{x}-\mu_{\mathbf{X}}) + (\mathbf{x}-\mu_{\mathbf{X}})^T\Lambda_{\mathbf{XY}}(\mathbf{y}-\mu_{\mathbf{Y}}) + (\mathbf{y}-\mu_{\mathbf{Y}})^T\Lambda_{\mathbf{YY}}(\mathbf{y}-\mu_{\mathbf{Y}})\right]\right) d\mathbf{y}$$

Marginalization of normal distribution

To proceed, let's apply the completing square trick on $(\mathbf{y}-\mu_{\mathbf{Y}})^T\Lambda_{\mathbf{YX}}(\mathbf{x}-\mu_{\mathbf{X}})+(\mathbf{x}-\mu_{\mathbf{X}})^T\Lambda_{\mathbf{XY}}(\mathbf{y}-\mu_{\mathbf{Y}})+(\mathbf{y}-\mu_{\mathbf{Y}})^T\Lambda_{\mathbf{YY}}(\mathbf{y}-\mu_{\mathbf{Y}})$. For the ease of exposition, let us denote $\tilde{\mathbf{x}}$ as $\mathbf{x}-\mu_{\mathbf{X}}$ and $\tilde{\mathbf{y}}$ as $\mathbf{y}-\mu_{\mathbf{Y}}$. We have

Marginalization of normal distribution

To proceed, let's apply the completing square trick on $(\mathbf{y}-\boldsymbol{\mu}_\mathbf{Y})^T\Lambda_{\mathbf{YX}}(\mathbf{x}-\boldsymbol{\mu}_\mathbf{X})+(\mathbf{x}-\boldsymbol{\mu}_\mathbf{X})^T\Lambda_{\mathbf{XY}}(\mathbf{y}-\boldsymbol{\mu}_\mathbf{Y})+(\mathbf{y}-\boldsymbol{\mu}_\mathbf{Y})^T\Lambda_{\mathbf{YY}}(\mathbf{y}-\boldsymbol{\mu}_\mathbf{Y})$. For the ease of exposition, let us denote $\tilde{\mathbf{x}}$ as $\mathbf{x}-\boldsymbol{\mu}_\mathbf{X}$ and $\tilde{\mathbf{y}}$ as $\mathbf{y}-\boldsymbol{\mu}_\mathbf{Y}$. We have

$$
\begin{aligned}
&\tilde{\mathbf{y}}^T\Lambda_{\mathbf{YX}}\tilde{\mathbf{x}}+\tilde{\mathbf{x}}^T\Lambda_{\mathbf{XY}}\tilde{\mathbf{y}}+\tilde{\mathbf{y}}^T\Lambda_{\mathbf{YY}}\tilde{\mathbf{y}}\\
=&(\tilde{\mathbf{y}}+\Lambda_{\mathbf{YY}}^{-1}\Lambda_{\mathbf{YX}}\tilde{\mathbf{x}})^T\Lambda_{\mathbf{YY}}(\tilde{\mathbf{y}}+\Lambda_{\mathbf{YY}}^{-1}\Lambda_{\mathbf{YX}}\tilde{\mathbf{x}})-\tilde{\mathbf{x}}^T\Lambda_{\mathbf{XY}}\Lambda_{\mathbf{YY}}^{-1}\Lambda_{\mathbf{YX}}\tilde{\mathbf{x}},
\end{aligned}
$$

where we use the fact that $\Lambda=\Sigma^{-1}$ is symmetric and so $\Lambda_{\mathbf{XY}}=\Lambda_{\mathbf{YX}}$

Marginalization of normal distribution

$$p(\mathbf{x}) = \frac{e^{-\frac{\tilde{\mathbf{x}}^T(\Lambda_{\mathbf{XX}} - \Lambda_{\mathbf{XY}}\Lambda_{\mathbf{YY}}^{-1}\Lambda_{\mathbf{YX}})\tilde{\mathbf{x}}}{2}}}{\sqrt{\det(2\pi\Sigma)}} \int e^{-\frac{(\tilde{\mathbf{y}}+\Lambda_{\mathbf{YY}}^{-1}\Lambda_{\mathbf{YX}}\tilde{\mathbf{x}})^T\Lambda_{\mathbf{YY}}(\tilde{\mathbf{y}}+\Lambda_{\mathbf{YY}}^{-1}\Lambda_{\mathbf{YX}}\tilde{\mathbf{x}})}{2}} d\mathbf{y}$$

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$$= \frac{\sqrt{\det(2\pi\Lambda_{\mathbf{YY}}^{-1})}}{\sqrt{\det(2\pi\Sigma)}} \exp\left(-\frac{\tilde{\mathbf{x}}^T(\Lambda_{\mathbf{XX}} - \Lambda_{\mathbf{XY}}\Lambda_{\mathbf{YY}}^{-1}\Lambda_{\mathbf{YX}})\tilde{\mathbf{x}}}{2}\right)$$

Marginalization of normal distribution

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$$\stackrel{(a)}{=} \frac{\sqrt{\det(2\pi\Lambda_{\mathbf{YY}}^{-1})}}{\sqrt{\det(2\pi\Sigma)}} \exp\left(-\frac{\tilde{\mathbf{x}}^T\Sigma_{\mathbf{XX}}^{-1}\tilde{\mathbf{x}}}{2}\right)$$

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$$\overset{(a)}{=} \frac{\sqrt{\det(2\pi\Lambda_{\mathbf{YY}}^{-1})}}{\sqrt{\det(2\pi\Sigma)}} \exp\left(-\frac{\tilde{\mathbf{x}}^T\Sigma_{\mathbf{XX}}^{-1}\tilde{\mathbf{x}}}{2}\right)$$

$$\overset{(b)}{=} \frac{1}{\sqrt{\det(2\pi\Sigma_{\mathbf{XX}})}} \exp\left(-\frac{\tilde{\mathbf{x}}^T\Sigma_{\mathbf{XX}}^{-1}\tilde{\mathbf{x}}}{2}\right)$$

Marginalization of normal distribution

$$p(\mathbf{x}) = \frac{e^{-\frac{\tilde{\mathbf{x}}^T(\Lambda_{\mathbf{XX}}-\Lambda_{\mathbf{XY}}\Lambda_{\mathbf{YY}}^{-1}\Lambda_{\mathbf{YX}})\tilde{\mathbf{x}}}{2}}}{\sqrt{\det(2\pi\Sigma)}} \int e^{-\frac{(\tilde{\mathbf{y}}+\Lambda_{\mathbf{YY}}^{-1}\Lambda_{\mathbf{YX}}\tilde{\mathbf{x}})^T\Lambda_{\mathbf{YY}}(\tilde{\mathbf{y}}+\Lambda_{\mathbf{YY}}^{-1}\Lambda_{\mathbf{YX}}\tilde{\mathbf{x}})}{2}} d\mathbf{y}$$

$$= \frac{\sqrt{\det(2\pi\Lambda_{\mathbf{YY}}^{-1})}}{\sqrt{\det(2\pi\Sigma)}} \exp\left(-\frac{\tilde{\mathbf{x}}^T(\Lambda_{\mathbf{XX}}-\Lambda_{\mathbf{XY}}\Lambda_{\mathbf{YY}}^{-1}\Lambda_{\mathbf{YX}})\tilde{\mathbf{x}}}{2}\right)$$

$$\stackrel{(a)}{=} \frac{\sqrt{\det(2\pi\Lambda_{\mathbf{YY}}^{-1})}}{\sqrt{\det(2\pi\Sigma)}} \exp\left(-\frac{\tilde{\mathbf{x}}^T\Sigma_{\mathbf{XX}}^{-1}\tilde{\mathbf{x}}}{2}\right)$$

$$\stackrel{(b)}{=} \frac{1}{\sqrt{\det(2\pi\Sigma_{\mathbf{XX}})}} \exp\left(-\frac{\tilde{\mathbf{x}}^T\Sigma_{\mathbf{XX}}^{-1}\tilde{\mathbf{x}}}{2}\right)$$

$$= \frac{1}{\sqrt{\det(2\pi\Sigma_{\mathbf{XX}})}} \exp\left(-\frac{(\mathbf{x}-\mu_{\mathbf{X}})^T\Sigma_{\mathbf{XX}}^{-1}(\mathbf{x}-\mu_{\mathbf{X}})}{2}\right),$$

where (a) and (b) will be shown next

(a) $\Sigma_{XX}^{-1} = \Lambda_{XX} - \Lambda_{XY}\Lambda_{YY}^{-1}\Lambda_{YX}$

Proof.

Since $\Lambda = \Sigma^{-1}$, we have $\Sigma_{XX}\Lambda_{XY} + \Sigma_{XY}\Lambda_{YY} = 0$ and $\Sigma_{XX}\Lambda_{XX} + \Sigma_{XY}\Lambda_{YX} = I$. Insert an identity into the latter equation, we have $\Sigma_{XX}\Lambda_{XX} + \Sigma_{XY}(\Lambda_{YY}\Lambda_{YY}^{-1})\Lambda_{YX} = \Sigma_{XX}\Lambda_{XX} - (\Sigma_{XX}\Lambda_{XY})\Lambda_{YY}^{-1}\Lambda_{YX} = \Sigma_{XX}(\Lambda_{XX} - \Lambda_{XY}\Lambda_{YY}^{-1}\Lambda_{YX}) = I$. □

Remark

By symmetry, we also have

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

(b') $\det(\Sigma) = \det(\Sigma_{\mathbf{YY}}) \det(\Lambda_{\mathbf{XX}}^{-1})$

Proof.

$$\det(\Sigma) = \det \begin{pmatrix} \Sigma_{\mathbf{XX}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{YX}} & \Sigma_{\mathbf{YY}} \end{pmatrix}$$

□

(b') $\det(\Sigma) = \det(\Sigma_{\mathbf{YY}})\det(\Lambda_{\mathbf{XX}}^{-1})$

Proof.

$$\det(\Sigma) = \det\begin{pmatrix}\Sigma_{\mathbf{XX}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{YX}} & \Sigma_{\mathbf{YY}}\end{pmatrix}$$

$$= \det\left(\begin{pmatrix} I & 0 \\ 0 & \Sigma_{\mathbf{YY}}\end{pmatrix}\begin{pmatrix}\Sigma_{\mathbf{XX}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & I\end{pmatrix}\right)$$

□

(b') $\det(\Sigma) = \det(\Sigma_{\mathbf{YY}}) \det(\Lambda_{\mathbf{XX}}^{-1})$

Proof.

$$\begin{aligned}
\det(\Sigma) &= \det \begin{pmatrix} \Sigma_{\mathbf{XX}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{YX}} & \Sigma_{\mathbf{YY}} \end{pmatrix} \\
&= \det \left(\begin{pmatrix} I & 0 \\ 0 & \Sigma_{\mathbf{YY}} \end{pmatrix} \begin{pmatrix} \Sigma_{\mathbf{XX}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & I \end{pmatrix} \right) \\
&= \det \left(\begin{pmatrix} I & 0 \\ 0 & \Sigma_{\mathbf{YY}} \end{pmatrix} \begin{pmatrix} I & \Sigma_{\mathbf{XY}} \\ 0 & I \end{pmatrix} \begin{pmatrix} \Sigma_{\mathbf{XX}} - \Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & 0 \\ \Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & I \end{pmatrix} \right)
\end{aligned}$$

□

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$$= \det \left(\begin{pmatrix} I & 0 \\ 0 & \Sigma_{\mathbf{YY}} \end{pmatrix} \begin{pmatrix} I & \Sigma_{\mathbf{XY}} \\ 0 & I \end{pmatrix} \begin{pmatrix} \Sigma_{\mathbf{XX}} - \Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & 0 \\ \Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & I \end{pmatrix} \right)$$

$$= \det \begin{pmatrix} I & 0 \\ 0 & \Sigma_{\mathbf{YY}} \end{pmatrix} \det \begin{pmatrix} I & \Sigma_{\mathbf{XY}} \\ 0 & I \end{pmatrix} \det \begin{pmatrix} \Sigma_{\mathbf{XX}} - \Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & 0 \\ \Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & I \end{pmatrix}$$

□

(b') $\det(\Sigma) = \det(\Sigma_{\mathbf{YY}})\det(\Lambda_{\mathbf{XX}}^{-1})$

Proof.

$$\begin{aligned}
\det(\Sigma) &= \det\begin{pmatrix} \Sigma_{\mathbf{XX}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{YX}} & \Sigma_{\mathbf{YY}} \end{pmatrix} \\
&= \det\left(\begin{pmatrix} I & 0 \\ 0 & \Sigma_{\mathbf{YY}} \end{pmatrix}\begin{pmatrix} \Sigma_{\mathbf{XX}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & I \end{pmatrix}\right) \\
&= \det\left(\begin{pmatrix} I & 0 \\ 0 & \Sigma_{\mathbf{YY}} \end{pmatrix}\begin{pmatrix} I & \Sigma_{\mathbf{XY}} \\ 0 & I \end{pmatrix}\begin{pmatrix} \Sigma_{\mathbf{XX}} - \Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & 0 \\ \Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & I \end{pmatrix}\right) \\
&= \det\begin{pmatrix} I & 0 \\ 0 & \Sigma_{\mathbf{YY}} \end{pmatrix}\det\begin{pmatrix} I & \Sigma_{\mathbf{XY}} \\ 0 & I \end{pmatrix}\det\begin{pmatrix} \Sigma_{\mathbf{XX}} - \Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & 0 \\ \Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & I \end{pmatrix} \\
&= \det\Sigma_{\mathbf{YY}}\det(\Sigma_{\mathbf{XX}} - \Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}})
\end{aligned}$$

□

(b') $\det(\Sigma) = \det(\Sigma_{\mathbf{YY}}) \det(\Lambda_{\mathbf{XX}}^{-1})$

Proof.

$$\begin{aligned}
\det(\Sigma) &= \det \begin{pmatrix} \Sigma_{\mathbf{XX}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{YX}} & \Sigma_{\mathbf{YY}} \end{pmatrix} \\
&= \det \left(\begin{pmatrix} I & 0 \\ 0 & \Sigma_{\mathbf{YY}} \end{pmatrix} \begin{pmatrix} \Sigma_{\mathbf{XX}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & I \end{pmatrix} \right) \\
&= \det \left(\begin{pmatrix} I & 0 \\ 0 & \Sigma_{\mathbf{YY}} \end{pmatrix} \begin{pmatrix} I & \Sigma_{\mathbf{XY}} \\ 0 & I \end{pmatrix} \begin{pmatrix} \Sigma_{\mathbf{XX}} - \Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & 0 \\ \Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & I \end{pmatrix} \right) \\
&= \det \begin{pmatrix} I & 0 \\ 0 & \Sigma_{\mathbf{YY}} \end{pmatrix} \det \begin{pmatrix} I & \Sigma_{\mathbf{XY}} \\ 0 & I \end{pmatrix} \det \begin{pmatrix} \Sigma_{\mathbf{XX}} - \Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & 0 \\ \Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}} & I \end{pmatrix} \\
&= \det \Sigma_{\mathbf{YY}} \det(\Sigma_{\mathbf{XX}} - \Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}}) \\
&= \det \Sigma_{\mathbf{YY}} \det \Lambda_{\mathbf{XX}}^{-1},
\end{aligned}$$

where the last equality is from (a) □

(b) $\det(a\Sigma) = \det(a\Sigma_{\mathbf{YY}})\det(a\Lambda_{\mathbf{XX}}^{-1})$ for any constant a

Proof.

Note that since the width (height) of Σ is equal to the sum of the widths of $\Sigma_{\mathbf{XX}}$ and $\Sigma_{\mathbf{YY}}$. The equation below follows immediately □

Remark

Note that by symmetry, we also have $\det(a\Sigma) = \det(a\Sigma_{\mathbf{XX}})\det(a\Lambda_{\mathbf{YY}}^{-1})$ *for any constant a. Take* $a = 2\pi$ *and that is exactly what we need for (b)*

Conditioning of normal distribution

- Consider the same $\mathbf{Z} \sim \mathcal{N}(\mu_{\mathbf{Z}}, \Sigma_{\mathbf{Z}})$ and $\mathbf{Z} = \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix}$. What will $\mathbf{X}$ be like if $\mathbf{Y}$ is observed to be $\mathbf{y}$?

Conditioning of normal distribution

- Consider the same $\mathbf{Z} \sim \mathcal{N}(\boldsymbol{\mu}_{\mathbf{Z}}, \Sigma_{\mathbf{Z}})$ and $\mathbf{Z} = \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix}$. What will $\mathbf{X}$ be like if $\mathbf{Y}$ is observed to be $\mathbf{y}$?
- Basically, we want to find $p(\mathbf{x}|\mathbf{y}) = p(\mathbf{x}, \mathbf{y})/p(\mathbf{y})$

Conditioning of normal distribution

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- Basically, we want to find $p(\mathbf{x}|\mathbf{y}) = p(\mathbf{x}, \mathbf{y})/p(\mathbf{y})$
- From previous result, we have $p(\mathbf{y}) = \mathcal{N}(\mathbf{y}; \boldsymbol{\mu}_\mathbf{Y}, \Sigma_\mathbf{YY})$. Therefore,

$$
\begin{aligned}
p(\mathbf{x}|\mathbf{y}) &\propto \exp\left(-\frac{1}{2}\left[\begin{pmatrix} \tilde{\mathbf{x}} \\ \tilde{\mathbf{y}} \end{pmatrix}^T \Sigma^{-1} \begin{pmatrix} \tilde{\mathbf{x}} \\ \tilde{\mathbf{y}} \end{pmatrix} - \tilde{\mathbf{y}}^T \Sigma_\mathbf{YY}^{-1} \tilde{\mathbf{y}}\right]\right) \\
&\propto \exp\left(-\frac{1}{2}[\tilde{\mathbf{x}}^T \Lambda_\mathbf{XX} \tilde{\mathbf{x}} + \tilde{\mathbf{x}}^T \Lambda_\mathbf{XY} \tilde{\mathbf{y}} + \tilde{\mathbf{y}}^T \Lambda_\mathbf{YX} \tilde{\mathbf{x}}]\right),
\end{aligned}
$$

where we use $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{y}}$ as shorthands of $\mathbf{x} - \boldsymbol{\mu}_\mathbf{X}$ and $\mathbf{y} - \boldsymbol{\mu}_\mathbf{Y}$ as before

Conditioning of normal distribution

- Completing the square for $\tilde{\mathbf{x}}$, we have

$$p(\mathbf{x}|\mathbf{y}) \propto \exp\left(-\frac{1}{2}(\tilde{\mathbf{x}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}\tilde{\mathbf{y}})^T\Lambda_{\mathbf{XX}}(\tilde{\mathbf{x}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}\tilde{\mathbf{y}})\right)$$

$$= \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_{\mathbf{X}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}(\mathbf{y} - \boldsymbol{\mu}_{\mathbf{Y}}))^T\Lambda_{\mathbf{XX}}\right.$$

$$\left.(\mathbf{x} - \boldsymbol{\mu}_{\mathbf{X}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}(\mathbf{y} - \boldsymbol{\mu}_{\mathbf{Y}}))\right)$$

Conditioning of normal distribution

- Completing the square for $\tilde{\mathbf{x}}$, we have

$$p(\mathbf{x}|\mathbf{y}) \propto \exp\left(-\frac{1}{2}(\tilde{\mathbf{x}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}\tilde{\mathbf{y}})^T\Lambda_{\mathbf{XX}}(\tilde{\mathbf{x}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}\tilde{\mathbf{y}})\right)$$
$$= \exp\left(-\frac{1}{2}(\mathbf{x} - \mu_{\mathbf{X}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}(\mathbf{y} - \mu_{\mathbf{Y}}))^T\Lambda_{\mathbf{XX}} (\mathbf{x} - \mu_{\mathbf{X}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}(\mathbf{y} - \mu_{\mathbf{Y}}))\right)$$

- Therefore $\mathbf{X}|\mathbf{y}$ is Gaussian distributed with mean $\mu_{\mathbf{X}} - \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}(\mathbf{y} - \mu_{\mathbf{Y}})$ and covariance $\Lambda_{\mathbf{XX}}^{-1}$

Conditioning of normal distribution

- Completing the square for $\tilde{\mathbf{x}}$, we have

$$p(\mathbf{x}|\mathbf{y}) \propto \exp\left(-\frac{1}{2}(\tilde{\mathbf{x}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}\tilde{\mathbf{y}})^T \Lambda_{\mathbf{XX}}(\tilde{\mathbf{x}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}\tilde{\mathbf{y}})\right)$$
$$= \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_{\mathbf{X}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}(\mathbf{y} - \boldsymbol{\mu}_{\mathbf{Y}}))^T \Lambda_{\mathbf{XX}} (\mathbf{x} - \boldsymbol{\mu}_{\mathbf{X}} + \Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}}(\mathbf{y} - \boldsymbol{\mu}_{\mathbf{Y}}))\right)$$

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- Note that since $\Lambda_{\mathbf{XX}}\Sigma_{\mathbf{XY}} + \Lambda_{\mathbf{XY}}\Sigma_{\mathbf{YY}} = 0$, $\Lambda_{\mathbf{XX}}^{-1}\Lambda_{\mathbf{XY}} = -\Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}$ and from (a), we have

$$\mathbf{X}|\mathbf{y} \sim \mathcal{N}(\boldsymbol{\mu}_{\mathbf{X}} + \Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}(\mathbf{y} - \boldsymbol{\mu}_{\mathbf{Y}}), \Sigma_{\mathbf{XX}} - \Sigma_{\mathbf{XY}}\Sigma_{\mathbf{YY}}^{-1}\Sigma_{\mathbf{YX}})$$

Interpretation of conditioning

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  - In particular, if **X** and **Y** are negatively correlated, the sign of the adjustment will be reversed
- As for the variance of the conditioned variable, it always decreases and the decrease is larger if $\Sigma_{\mathbf{YY}}$ is smaller and $\Sigma_{\mathbf{XY}}$ is larger (**X** and **Y** are more correlated)

$X \perp\!\!\!\perp Y|Z$ if $\rho_{XZ}\rho_{YZ} = \rho_{XY}$

Corollary

Given multivariate Gaussian variables X, Y and Z, we have X and Y are conditionally independent given Z if $\rho_{XZ}\rho_{YZ} = \rho_{XY}$, where $\rho_{XZ} = \frac{E[(X-E(X))(Z-E(Z))]}{\sqrt{E[(X-E(X))^2]E[(Z-E(Z))^2]}}$ is the correlation coefficent between X and Z. Similarly, ρ_{YZ} and ρ_{XY} are the correlation coefficients between Y and Z, and X and Y, respectively.

$X \perp\!\!\!\perp Y|Z$ if $\rho_{XZ}\rho_{YZ} = \rho_{XY}$

Proof.

- Without loss of generality, we can assume the variables with mean 0 and variance 1. Thus, $\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} \sim \mathcal{N}(\mathbf{0}, \Sigma)$, where $\Sigma = \begin{pmatrix} 1 & \rho_{XY} & \rho_{XZ} \\ \rho_{XY} & 1 & \rho_{YZ} \\ \rho_{XZ} & \rho_{YZ} & 1 \end{pmatrix}$

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- Then from the conditioning result, we have

$$\Sigma_{\left(\begin{smallmatrix} X \\ Y \end{smallmatrix}\right)|Z} = \begin{pmatrix} 1 & \rho_{XY} \\ \rho_{XY} & 1 \end{pmatrix} - \begin{pmatrix} \rho_{XZ} & \rho_{YZ} \end{pmatrix} \sigma_{YY}^{-1} \begin{pmatrix} \rho_{XZ} \\ \rho_{YZ} \end{pmatrix}$$
$$= \begin{pmatrix} 1 - \rho_{XZ}^2 & \rho_{XY} - \rho_{XZ}\rho_{YZ} \\ \rho_{XY} - \rho_{XZ}\rho_{YZ} & 1 - \rho_{YZ}^2 \end{pmatrix}$$

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- Therefore, X and Y are uncorrelated given Z when $\sigma_{XY|Z} = \rho_{XY} - \rho_{XZ}\rho_{YZ} = 0$ or $\rho_{XY} = \rho_{XZ}\rho_{YZ}$. Since for Gaussian variables, uncorrelatedness implies independence. This concludes the proof.

□

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$$\begin{aligned} p(\mathbf{y}_1, \mathbf{y}_2|\mathbf{x}) &= p(\mathbf{y}_1|\mathbf{x})p(\mathbf{y}_2|\mathbf{x}) \\ &= \mathcal{N}(\mathbf{y}_1; \mathbf{x}, \Sigma_{\mathbf{Y}_1})\mathcal{N}(\mathbf{y}_2; \mathbf{x}, \Sigma_{\mathbf{Y}_2}). \end{aligned}$$

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- Essentially, we just need to compute the product of two Gaussian pdfs. Such computation is very useful and it occurs often when one needs to perform inference

Product of normal distributions

As in previous cases, the product turns out to be normal also. However, unlike them, the product is not a pdf and so it does not normalize to 1. So we have to compute both the scaling factor and the exponent explicitly. Let us start with the exponent.

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&\propto \exp\left(-\frac{1}{2}[\mathbf{x}^T(\Lambda_{\mathbf{Y}_1}+\Lambda_{\mathbf{Y}_2})\mathbf{x}-(\mathbf{y}_2^T\Lambda_{\mathbf{Y}_2}+\mathbf{y}_1^T\Lambda_{\mathbf{Y}_1})\mathbf{x}-\mathbf{x}^T(\Lambda_{\mathbf{Y}_2}\mathbf{y}_2+\Lambda_{\mathbf{Y}_1}\mathbf{y}_1)]\right)
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$$\propto e^{-\frac{1}{2}[(\mathbf{x}-(\Lambda_{\mathbf{Y}_1}+\Lambda_{\mathbf{Y}_2})^{-1}(\Lambda_{\mathbf{Y}_2}\mathbf{y}_2+\Lambda_{\mathbf{Y}_1}\mathbf{y}_1))^T(\Lambda_{\mathbf{Y}_1}+\Lambda_{\mathbf{Y}_2})(\mathbf{x}-(\Lambda_{\mathbf{Y}_1}+\Lambda_{\mathbf{Y}_2})^{-1}(\Lambda_{\mathbf{Y}_2}\mathbf{y}_2+\Lambda_{\mathbf{Y}_1}\mathbf{y}_1))]}$$

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\end{aligned}$$

Therefore,

$$\begin{aligned}
&\mathcal{N}(\mathbf{y}_1; \mathbf{x}, \Sigma_{\mathbf{Y}_1})\mathcal{N}(\mathbf{y}_2; \mathbf{x}, \Sigma_{\mathbf{Y}_2}) \\
= &K(\mathbf{y}_1, \mathbf{y}_2, \Sigma_{\mathbf{Y}_1}, \Sigma_{\mathbf{Y}_2})\mathcal{N}(\mathbf{x}; (\Lambda_{\mathbf{Y}_1}+\Lambda_{\mathbf{Y}_2})^{-1}(\Lambda_{\mathbf{Y}_2}\mathbf{y}_2 + \Lambda_{\mathbf{Y}_1}\mathbf{y}_1), (\Lambda_{\mathbf{Y}_2}+\Lambda_{\mathbf{Y}_1})^{-1})
\end{aligned}$$

for some scaling factor $K(\mathbf{y}_1, \mathbf{y}_2, \Sigma_{\mathbf{Y}_1}, \Sigma_{\mathbf{Y}_2})$ independent of $\mathbf{x}$.

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- One can compute the scaling factor $K(\mathbf{y}_1, \mathbf{y}_2, \Sigma_{\mathbf{Y}_1}, \Sigma_{\mathbf{Y}_2})$ directly

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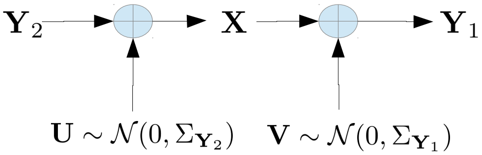
- However, it is much easier to take advantage for the following setup when $\mathbf{X} \perp\!\!\!\perp \mathbf{Y_1} | \mathbf{Y_2}$ as shown below



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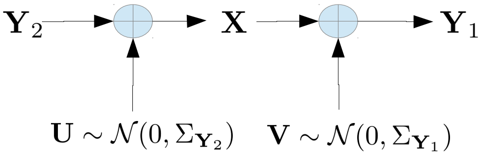
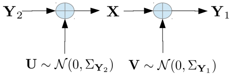


- Since $\mathcal{N}(\mathbf{y}_2; \mathbf{x}, \Sigma_{\mathbf{Y}_2}) = \mathcal{N}(\mathbf{x}; \mathbf{y}_2, \Sigma_{\mathbf{Y}_2})$ and $\mathbf{X} \perp\!\!\!\perp \mathbf{Y_1} | \mathbf{Y_2}$, we have

$$\mathcal{N}(\mathbf{y}_1; \mathbf{x}, \Sigma_{\mathbf{Y}_1})\mathcal{N}(\mathbf{y}_2; \mathbf{x}, \Sigma_{\mathbf{Y}_2}) = \mathcal{N}(\mathbf{y}_1; \mathbf{x}, \Sigma_{\mathbf{Y}_1})\mathcal{N}(\mathbf{x}; \mathbf{y}_2, \Sigma_{\mathbf{Y}_2}) = p(\mathbf{y}_1, \mathbf{x} | \mathbf{y}_2)$$

Product of normal distributions

- Then, marginalizing $\mathbf{x}$ out from $p(\mathbf{y}_1, \mathbf{x}|\mathbf{y}_2)$, we have



  $p(\mathbf{y}_1|\mathbf{y}_2) = \int p(\mathbf{y}_1, \mathbf{x}|\mathbf{y}_2) d\mathbf{x}$. However, from the figure,

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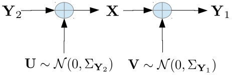

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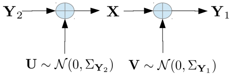

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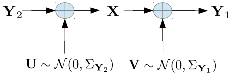

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$$\mathcal{N}(\mathbf{y}_1; \mathbf{x}, \Sigma_{\mathbf{Y}_1})\mathcal{N}(\mathbf{y}_2; \mathbf{x}, \Sigma_{\mathbf{Y}_2})$$

$$= \mathcal{N}(\mathbf{y}_1; \mathbf{y}_2, \Sigma_{\mathbf{Y}_2} + \Sigma_{\mathbf{Y}_1})\mathcal{N}(\mathbf{x}; (\Lambda_{\mathbf{Y}_1} + \Lambda_{\mathbf{Y}_2})^{-1}(\Lambda_{\mathbf{Y}_2}\mathbf{y}_2 + \Lambda_{\mathbf{Y}_1}y), (\Lambda_{\mathbf{Y}_2} + \Lambda_{\mathbf{Y}_1})^{-1})$$

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- The scaling factor, $\mathcal{N}(\mathbf{y}_1; \mathbf{y}_2, \Sigma_{\mathbf{Y}_2} + \Sigma_{\mathbf{Y}_1})$, can be interpreted as how much one can believe on the overall likelihood.
  - The value is reasonable since when the two observations are far away with respect to the overall variance $\Sigma_{\mathbf{Y}_2} + \Sigma_{\mathbf{Y}_1}$, the likelihood will become less reliable
  - The scaling factor is especially useful when we deal with mixture of Gaussian to be discussed next

Division of normal distributions

- To compute $\frac{\mathcal{N}(\mathbf{x};\boldsymbol{\mu}_1,\Sigma_1)}{\mathcal{N}(\mathbf{x};\boldsymbol{\mu}_2,\Sigma_2)}$, note that from the product formula earlier

$$\mathcal{N}(\mathbf{x};\boldsymbol{\mu}_2,\Sigma_2)\mathcal{N}(\mathbf{x};(\Lambda_1-\Lambda_2)^{-1}(\Lambda_1\boldsymbol{\mu}_1-\Lambda_2\boldsymbol{\mu}_2),(\Lambda_1-\Lambda_2)^{-1})$$
$$=\mathcal{N}(\boldsymbol{\mu}_1;(\Lambda_1-\Lambda_2)^{-1}(\Lambda_1\boldsymbol{\mu}_1-\Lambda_2\boldsymbol{\mu}_2),\Lambda_2^{-1}+(\Lambda_1-\Lambda_2)^{-1})\mathcal{N}(\mathbf{x};\boldsymbol{\mu}_1,\Sigma_1)$$

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- Therefore,

$$\frac{\mathcal{N}(\mathbf{x};\boldsymbol{\mu}_1,\Sigma_1)}{\mathcal{N}(\mathbf{x};\boldsymbol{\mu}_2,\Sigma_2)}=\frac{\mathcal{N}(\mathbf{x};(\Lambda_1-\Lambda_2)^{-1}(\Lambda_1\boldsymbol{\mu}_1-\Lambda_2\boldsymbol{\mu}_2),(\Lambda_1-\Lambda_2)^{-1})}{\mathcal{N}(\boldsymbol{\mu}_1,(\Lambda_1-\Lambda_2)^{-1}(\Lambda_1\boldsymbol{\mu}_1-\Lambda_2\boldsymbol{\mu}_2);\Lambda_2^{-1}+(\Lambda_1-\Lambda_2)^{-1})}$$
$$=\frac{\mathcal{N}(\mathbf{x};\boldsymbol{\mu},(\Lambda_1-\Lambda_2)^{-1})}{\mathcal{N}(\boldsymbol{\mu}_1;\boldsymbol{\mu},\Lambda_2^{-1}+(\Lambda_1-\Lambda_2)^{-1})},$$

where $\boldsymbol{\mu}=(\Lambda_1-\Lambda_2)^{-1}(\Lambda_1\boldsymbol{\mu}_1-\Lambda_2\boldsymbol{\mu}_2)$

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  where $\boldsymbol{\mu}=(\Lambda_1-\Lambda_2)^{-1}(\Lambda_1\boldsymbol{\mu}_1-\Lambda_2\boldsymbol{\mu}_2)$
- Note that the final pdf will be Gaussian-like if $\Lambda_1 \succeq \Lambda_2$. Otherwise, one can still write out the pdf using the precision matrix. But the covariance matrix will not be defined (Try plot some pdfs out yourselves)

Mixture of Gaussians

Consider an electrical system that outputs signal of different statistics when it is on and off

- When the system is on, the output signal S behaves like $\mathcal{N}(5, 1)$. When the system is off is off, S behaves like $\mathcal{N}(0, 1)$

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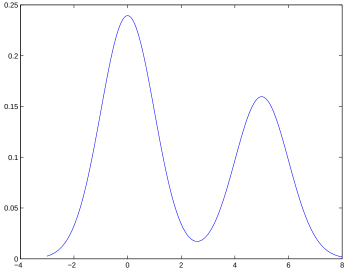
- If someone measuring the signal does not know the status of the system but only knows that the system is on 40% of the time, then to the observer, the signal S behaves like a mixture of Gaussians
- The pdf of S will be $0.4\mathcal{N}(s; 5, 1) + 0.6\mathcal{N}(s; 0, 1)$ as shown below



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- Let us illustrate this with the following example:
  - Consider two mixtures of Gaussian likelihood of x given two observations y_1 and y_2 as follows:

$$p(y_1|x) = 0.6\mathcal{N}(x; 0, 1) + 0.4\mathcal{N}(x; 5, 1);$$
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  What is the overall likelihood, $p(y_1, y_2|x)$?
- As usual, it is reasonable to assume the observations to be conditionally independent given x. Then,

$$\begin{aligned} p(y_1, y_2|x) &= p(y_1|x)p(y_2|x) \\ &= (0.6\mathcal{N}(x;0,1) + 0.4\mathcal{N}(x;5,1))(0.5\mathcal{N}(x;-2,1) + 0.5\mathcal{N}(x;4,1)) \\ &= 0.3\mathcal{N}(x;0,1)\mathcal{N}(x;-2,1) + 0.2\mathcal{N}(x;5,1)\mathcal{N}(x;-2,1) \\ &\quad + 0.3\mathcal{N}(x;0,1)\mathcal{N}(x;4,1) + 0.2\mathcal{N}(x;5,1)\mathcal{N}(x;4,1) \end{aligned}$$

Explosion of Gaussians

- The last step involves computing products of Gaussians but we have learned it in previous sections. Using the previous result,

$$\begin{aligned} p(y_1, y_2|x) = {} & 0.3\mathcal{N}(-2; 0, 2)\mathcal{N}(x; -1, 0.5) + 0.2\mathcal{N}(-2; 5, 2)\mathcal{N}(x; 1.5, 0.5) \\ & + 0.3\mathcal{N}(4; 0, 2)\mathcal{N}(x; 2, 0.5) + 0.2\mathcal{N}(4; 5, 2)\mathcal{N}(x; 4.5, 0.5). \end{aligned}$$

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- Let's repeat our discussion but with n observations instead. The overall likelihood will be a mixture of 2^n Gaussians!
  - Therefore, the computation will quickly become intractable as the number of observations increases
  - Fortunately, in reality, some of the Gaussians in the mixture tend to have a very small weight

Reduce number of components in Gaussian mixtures

- For instance, in our previous numerical example, if we continue our numerical computation for the two observation example, we have

$$\begin{aligned} p(y_1, y_2|x) = {} & 0.4163\mathcal{N}(x; -1, 0.5) + 3.5234 \times 10^{-6}\mathcal{N}(x; 1.5, 0.5) \\ & + 0.0202\mathcal{N}(x; 2, 0.5) + 0.5734\mathcal{N}(x; 4.5, 0.5). \end{aligned}$$

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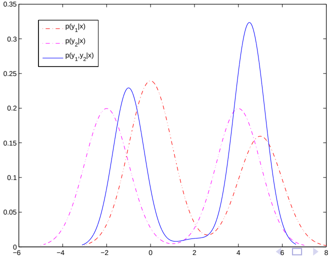
- We can see that the weight for the component at mean 1.5 is very small. And the component at mean 2 has a rather small weight also.
- Even with the four Gaussian components, the overall likelihood is essentially just a bimodal distribution as shown in the figure below



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- Therefore, we may approximate $p(y_1, y_2|x)$ with only two of its original component as $0.4163/(0.4163 + 0.5734)\mathcal{N}(x; -1, 0.5) + 0.5734/(0.4163 + 0.5734)\mathcal{N}(x; 4.5, 0.5) = 0.4206\mathcal{N}(x; -1, 0.5) + 0.5794\mathcal{N}(x; 4.5, 0.5)$

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- However, it is not always a good approximation strategy just to dump away the small components in a Gaussian mixture

Another example

Consider

$$p(x) = 0.1\mathcal{N}(x; -0.2, 1) + 0.1\mathcal{N}(x; -0.1, 1) + 0.1\mathcal{N}(x; 0, 1) + 0.1\mathcal{N}(x; 0.1, 1) + 0.1\mathcal{N}(x; 0.2, 1) + 0.5\mathcal{N}(x; 5, 1).$$

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- Let say we want to reduce $p(x)$ to only a mixture of two Gaussians. It is tempting to just dumping four smallest one and renormalized the weight. For example, if we choose to remove the first four components, we have

$$\hat{p}(x) = 1/6\mathcal{N}(x; 0.2, 1) + 5/6\mathcal{N}(x; 5, 1)$$

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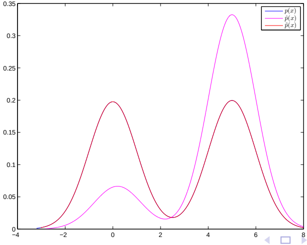
- The approximation $\hat{p}(x)$ is significantly different from $p(x)$ as shown below



Merging components

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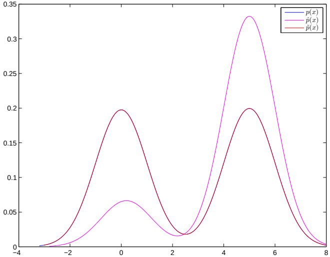
- Actually the first five components are so similar that their combined contribution can be accurately modeled as one Gaussian
- So rather than discarding the components, one can get a much more accurate approximation by merging them. The approximation is illustrated as $\tilde{p}(x)$ in the figure below



Merging components

To successfully obtain such approximation $\tilde{p}(x)$, we have to answer two questions:

- which components to merge?
- how to merge them?

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It is reasonable to pick similar components to merge. The question is how do will gauge the similarity between two components.

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$$\frac{\langle p(\mathbf{x}), q(\mathbf{x}) \rangle}{\sqrt{\langle p(\mathbf{x}), p(\mathbf{x}) \rangle \langle q(\mathbf{x}), q(\mathbf{x}) \rangle}} = \frac{\int p(\mathbf{x}) q(\mathbf{x}) d\mathbf{x}}{\sqrt{\int p(\mathbf{x})^2 d\mathbf{x} \int q(\mathbf{x})^2 d\mathbf{x}}} \leq 1$$

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- The inner product maximizes $(= 1)$ when $p(\mathbf{x}) = q(\mathbf{x})$. This suggests a very reasonable similarity measure between two pdfs

Similarity measure

- Let's define

$$Sim(p(\mathbf{x}), q(\mathbf{x})) \triangleq \frac{\int p(\mathbf{x})q(\mathbf{x})d\mathbf{x}}{\sqrt{\int p(\mathbf{x})^2 d\mathbf{x} \int q(\mathbf{x})^2 d\mathbf{x}}}$$

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- In particular, if $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_p, \Sigma_p)$ and $q(\mathbf{x}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_q, \Sigma_q)$, we have (please verify)

$$Sim(\mathcal{N}(\boldsymbol{\mu}_p, \Sigma_p), \mathcal{N}(\boldsymbol{\mu}_q, \Sigma_q)) = \frac{\mathcal{N}(\boldsymbol{\mu}_p; \boldsymbol{\mu}_q, \Sigma_p + \Sigma_q)}{\sqrt{\mathcal{N}(0; 0, 2\Sigma_p)\mathcal{N}(0; 0, 2\Sigma_q)}},$$

which can be computed very easily and is equal to one only when means and covariances are the same

How to Merge Components?

Say we have n components $\mathcal{N}(\boldsymbol{\mu}_1, \Sigma_1)$, $\mathcal{N}(\boldsymbol{\mu}_2, \Sigma_2)$, $\cdots$, $\mathcal{N}(\boldsymbol{\mu}_n, \Sigma_n)$ with weights $w_1, w_2, \cdots, w_n$. What should the combined component be like?

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- Combined component weight should equal to total weight $\sum_{i=1}^n w_i$
- Combined mean will simply be $\sum_{i=1}^n \hat{w}_i \boldsymbol{\mu}_i$, where $\hat{w}_i = \frac{w_i}{\sum_{i=1}^n w_i}$
- For combined covariance, it may be tempting to approximate it as $\sum_{i=1}^n \hat{w}_i \Sigma_i$.
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  - Because the weighted sum only counted the contribution of variation among each component, it did not take into account the variation due to different means across components.

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  - Instead, let's denote $\mathbf{X}$ as the variable sampled from the mixture. That is, $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}_i, \Sigma_i)$ with probability $\hat{w}_i$. Then, we have (please verify)

$$\begin{aligned}\Sigma &= E[\mathbf{X}\mathbf{X}^T] - E[\mathbf{X}]E[\mathbf{X}]^T \\ &= \sum_{i=1}^n \hat{w}_i(\Sigma_i + \boldsymbol{\mu}_i\boldsymbol{\mu}_i^T) - \sum_{i=1}^n \sum_{j=1}^n \hat{w}_i \hat{w}_j \boldsymbol{\mu}_i \boldsymbol{\mu}_j^T.\end{aligned}$$

Now, go back to our previous numerical example

- Recall that $p(x) = 0.1\mathcal{N}(x; -0.2, 1) + 0.1\mathcal{N}(x; -0.1, 1) + 0.1\mathcal{N}(x; 0, 1) + 0.1\mathcal{N}(x; 0.1, 1) + 0.1\mathcal{N}(x; 0.2, 1) + 0.5\mathcal{N}(x; 5, 1)$

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- If we merge the five smallest components (one can easily check that they are also more similar to each other than to the last component), we have $\tilde{p}(x) = 0.5\mathcal{N}(x; 0, 1.02) + 0.5\mathcal{N}(x; 5, 1)$ as shown again below. The approximate pdf is virtually indistinguishable from the original