Gaussian Identities (cont.)

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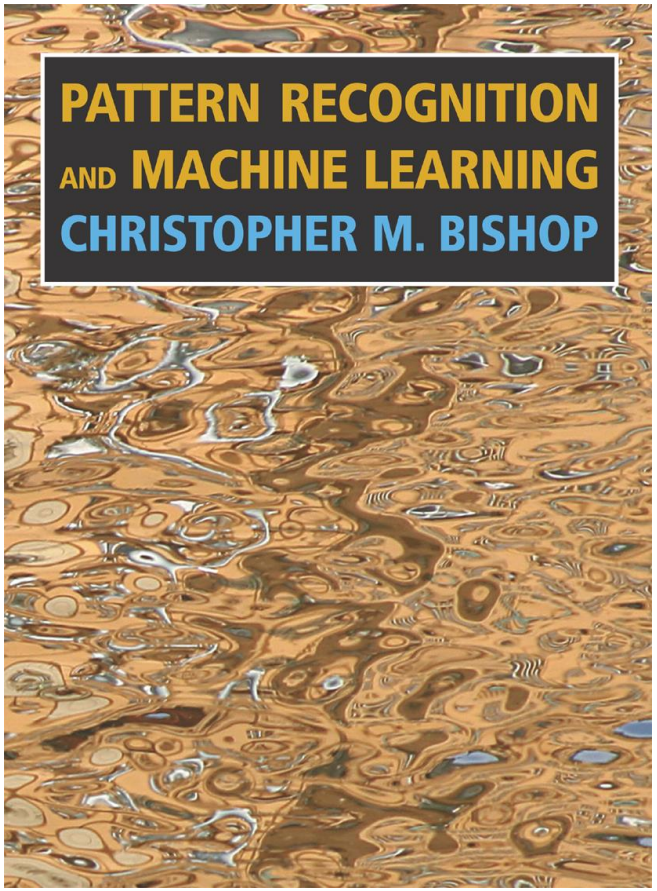
Office Hour: Wednesday 4pm-5pm

NO LAB this week.

Reference



Today's class *roughly* follows Chapter 2.3-2.34

Pattern Recognition and Machine Learning

Christopher Bishop, 2006

Recap

- $N_{\boldsymbol{x}}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) := \frac{1}{(2\pi)^{\frac{d}{2}} |\boldsymbol{\Sigma}|^{\frac{1}{2}}} \cdot \exp\left[-\frac{(\boldsymbol{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\boldsymbol{x}-\boldsymbol{\mu})}{2}\right]$
- MVNs are multi-dimensional generalizations of univariate normal distributions, in the sense that:
- $\boldsymbol{\Sigma}^{-1} = \boldsymbol{U}\boldsymbol{D}\mathbf{U}^\top$
  - Eigen-decomposition, $\boldsymbol{D}$ is diagonal.
  - $\boldsymbol{U} \in R^{d \times d}, \boldsymbol{U}\boldsymbol{U}^\top = \boldsymbol{U}^\top \boldsymbol{U} = \boldsymbol{I}$
- $\boldsymbol{y} = \boldsymbol{U}^\top (\boldsymbol{x} - \boldsymbol{\mu})$.
- $p(\boldsymbol{y}) = \prod_i N_{\boldsymbol{y}}(\mathbf{0}, d_i)$, $\frac{1}{d_i}$ is i-th diagonal-elem. of $\boldsymbol{D}$.
- Use this to generate samples of MVN using uni-normal!

Recap

- **Mahalanobis distance,** $(\boldsymbol{x}-\boldsymbol{\mu})^{\top}\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})$
  - Distance between a point $\boldsymbol{x}$ to the center of $N_{\boldsymbol{x}}(\boldsymbol{\mu},\boldsymbol{\Sigma})$,
  - Distance between $\boldsymbol{x}$ and $\boldsymbol{\mu}$ rotated by $\boldsymbol{U}$.
  - Can be used to define the **confidence region.**

- **Moments of MVN.**
  - $\mathbb{E}[\boldsymbol{x}]=\boldsymbol{\mu}$
    - Apply the transform $\boldsymbol{z}=\boldsymbol{x}-\boldsymbol{\mu}$.
    - $\int_{-\infty}^{\mathbf{0}}\exp\left[-\frac{\boldsymbol{z}\boldsymbol{\Sigma}^{-1}\boldsymbol{z}}{2}\right]\boldsymbol{z}d\boldsymbol{z}=-\int_{\mathbf{0}}^{\infty}\exp\left[-\frac{\boldsymbol{z}\boldsymbol{\Sigma}^{-1}\boldsymbol{z}}{2}\right]\boldsymbol{z}\,d\boldsymbol{z}$
  - $\mathbb{E}[\boldsymbol{x}\boldsymbol{x}^{\top}]=\boldsymbol{\mu}^{\top}\boldsymbol{\mu}+\boldsymbol{\Sigma}$
    - Apply the transform $\boldsymbol{z}=\boldsymbol{x}-\boldsymbol{\mu}$.
    - Use $\boldsymbol{z}=\boldsymbol{U}\boldsymbol{y}$ and $\boldsymbol{U}\boldsymbol{U}^{\top}=\boldsymbol{I}$.

Partitioned MVNs

- **Given:**
- $p(\boldsymbol{x}_a, \boldsymbol{x}_b) = N_{\boldsymbol{x}_a, \boldsymbol{x}_b}\left(\begin{bmatrix}\boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b\end{bmatrix}, \begin{bmatrix}\boldsymbol{\Sigma}_{aa}, \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba}, \boldsymbol{\Sigma}_{bb}\end{bmatrix}\right)$
- Represent $p(\boldsymbol{x}_a|\boldsymbol{x}_b)$ and $p(\boldsymbol{x}_a)$ using $\begin{matrix}\boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b\end{matrix}$ and $\begin{matrix}\boldsymbol{\Sigma}_{aa}, \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba}, \boldsymbol{\Sigma}_{bb}\end{matrix}$.

- Partitioned MVN formulas have huge applications in Bayesian regression, Gaussian graphical models etc.
- For simplicity, we let $\boldsymbol{\Sigma}^{-1} = \boldsymbol{\Theta} = \begin{bmatrix}\boldsymbol{\Theta}_{aa}, \boldsymbol{\Theta}_{ab} \\ \boldsymbol{\Theta}_{ba}, \boldsymbol{\Theta}_{bb}\end{bmatrix}$.

Proof Walkthrough

- You can prove by following the def. of conditional dist.
- **However, observe:**

Quadratic term

$$\log N_{\boldsymbol{x}}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{-\begin{bmatrix} \boldsymbol{x}_a - \boldsymbol{\mu}_a \\ \boldsymbol{x}_b - \boldsymbol{\mu}_b \end{bmatrix}^\top \begin{bmatrix} \boldsymbol{\Theta}_{aa}, \boldsymbol{\Theta}_{ab} \\ \boldsymbol{\Theta}_{ba}, \boldsymbol{\Theta}_{bb} \end{bmatrix} \begin{bmatrix} \boldsymbol{x}_a - \boldsymbol{\mu}_a \\ \boldsymbol{x}_b - \boldsymbol{\mu}_b \end{bmatrix}}{2} + \text{const.}$$

- $\log N_{\boldsymbol{x}}$ is merely a quadratic function w.r.t $\boldsymbol{x}$ + const.
- Expanding quad. term only leads to quad./linear terms.
  - w.r.t. $\boldsymbol{x}_a, \boldsymbol{x}_b$
- $\Rightarrow P(\boldsymbol{x}_a | \boldsymbol{x}_b)$ is an MVN (not rigorously speaking).

Proof Walkthrough

- If $p(\boldsymbol{t}) = N_{\boldsymbol{t}}(\boldsymbol{\mu}; \boldsymbol{\Sigma})$, then

$$\log p(\boldsymbol{t}) = -\frac{\boldsymbol{t}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{t}}{2} + \boldsymbol{t}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu} + \text{const.}$$

- If we spot terms in $-\begin{bmatrix} \boldsymbol{x}_a - \boldsymbol{\mu}_a \\ \boldsymbol{x}_b - \boldsymbol{\mu}_b \end{bmatrix}^\top \begin{bmatrix} \boldsymbol{\Theta}_{aa}, \boldsymbol{\Theta}_{ab} \\ \boldsymbol{\Theta}_{ba}, \boldsymbol{\Theta}_{bb} \end{bmatrix} \begin{bmatrix} \boldsymbol{x}_a - \boldsymbol{\mu}_a \\ \boldsymbol{x}_b - \boldsymbol{\mu}_b \end{bmatrix} /2$ with respect to $\boldsymbol{x}_a$ which has the same form as those in , we can *directly identify* the covariance and mean for $p(\boldsymbol{x}_a | \boldsymbol{x}_b)$.

Proof Walkthrough

- The *quadratic term* w.r.t. $\boldsymbol{x}_a$ after expansion:
- $-\boldsymbol{x}_a^\top \boldsymbol{\Theta}_{aa} \boldsymbol{x}_a / 2 \Longrightarrow \mathrm{Cov}_{\boldsymbol{x}_a|\boldsymbol{x}_b}[\boldsymbol{x}_a] = [\boldsymbol{\Theta}_{aa}]^{-1}$.
- The *linear terms* w.r.t. $\boldsymbol{x}_\mathrm{a}$ after expansion:
- $-\boldsymbol{x}_a^\top \boldsymbol{\Theta}_{ab} \boldsymbol{x}_b + \boldsymbol{x}_a^\top \boldsymbol{\Theta}_{ab} \boldsymbol{\mu}_b + \boldsymbol{x}_a^\top \boldsymbol{\Theta}_{aa} \boldsymbol{\mu}_a$

- Collect terms: $\boldsymbol{x}_a^\top \boldsymbol{\Theta}_{aa} (\boldsymbol{\mu}_a - \boldsymbol{\Theta}_{aa}^{-1} \boldsymbol{\Theta}_{ab} \boldsymbol{x}_b + \boldsymbol{\Theta}_{aa}^{-1} \boldsymbol{\Theta}_{ab} \boldsymbol{\mu}_b)$
- Knowing $\mathrm{Cov}_{\boldsymbol{x}_a|\boldsymbol{x}_b}[\boldsymbol{x}_a] = [\boldsymbol{\Theta}_{aa}]^{-1} \Longrightarrow$

$$\mathbb{E}_{\boldsymbol{x}_a|\boldsymbol{x}_b}[\boldsymbol{x}_a] = \boldsymbol{\mu}_a - \boldsymbol{\Theta}_{aa}^{-1} \boldsymbol{\Theta}_{ab} \boldsymbol{x}_b + \boldsymbol{\Theta}_{aa}^{-1} \boldsymbol{\Theta}_{ab} \boldsymbol{\mu}_b$$

Conditional MVN formula

- $p(\boldsymbol{x}_a|\boldsymbol{x}_b) = N_{\boldsymbol{x}_a}(\boldsymbol{\mu}_a - \boldsymbol{\Theta}_{aa}^{-1}\boldsymbol{\Theta}_{ab}\boldsymbol{x}_b + \boldsymbol{\Theta}_{aa}^{-1}\boldsymbol{\Theta}_{ab}\boldsymbol{\mu}_b, \boldsymbol{\Theta}_{\boldsymbol{aa}}^{-1})$.

- You can use block matrix inversion formula to represent $\boldsymbol{\Theta}_{aa}, \boldsymbol{\Theta}_{ab}$ using $\boldsymbol{\Sigma}_{aa}, \boldsymbol{\Sigma}_{ab}$ and $\boldsymbol{\Sigma}_{bb}$.
- **See 2.76 in PRML**

- However, this formula is most easily expressed using block matrices of $\boldsymbol{\Theta}$.

Partitioned MVNs (Marginal)

- How to represent $p(\boldsymbol{x}_a)$ using $\begin{matrix}\boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b\end{matrix}$ and $\begin{matrix}\boldsymbol{\Sigma}_{aa}, \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba}, \boldsymbol{\Sigma}_{bb}\end{matrix}$?

- First, we marginalize $p(\boldsymbol{x}_a) = \int p(\boldsymbol{x}_a, \boldsymbol{x}_b) d\boldsymbol{x}_b$
- Write terms in $\log p(\boldsymbol{x}_a, \boldsymbol{x}_b)$ w.r.t. $\boldsymbol{x}_b$ after expansion:
- $-\boldsymbol{x}_b^\top \boldsymbol{\Theta}_{bb} \boldsymbol{x}_b / 2 + \boldsymbol{x}_b^\top (\underbrace{\boldsymbol{\Theta}_{bb}\boldsymbol{\mu}_b - \boldsymbol{\Theta}_{ba}\boldsymbol{x}_a + \boldsymbol{\Theta}_{ba}\boldsymbol{\mu}_a}_{\boldsymbol{m}})$

$$= -\underbrace{\left(\boldsymbol{x}^\top - \boldsymbol{\Theta}_{bb}^{-1}\boldsymbol{m}\right)\boldsymbol{\Theta}_{bb}\left(\boldsymbol{x} - \boldsymbol{\Theta}_{bb}^{-1}\boldsymbol{m}\right)}/2 + \boldsymbol{m}^\top \boldsymbol{\Theta}_{bb}^{-1}\boldsymbol{m}/2,$$

Completing the square!

Proof Walkthrough

- Now we know
- $p(\boldsymbol{x}_a) = (\dots) \exp\left(\frac{\boldsymbol{m}^\top \boldsymbol{\Theta}_{bb}^{-1} \boldsymbol{m}}{2}\right) \int \exp\left[-\frac{(\boldsymbol{x}_b^\top - \boldsymbol{\Theta}_{bb}^{-1}\boldsymbol{m})\boldsymbol{\Theta}_{bb}(\boldsymbol{x}_b - \boldsymbol{\Theta}_{bb}^{-1}\boldsymbol{m})}{2}\right] \mathrm{d}\boldsymbol{x}_b$
- Inside integral, just a regular MVN w.r.t. $\boldsymbol{x}_b$ without normalizing constant, so
- $p(\boldsymbol{x}_a) = (\dots) \exp\left(\frac{\boldsymbol{m}^\top \boldsymbol{\Theta}_{bb}^{-1} \boldsymbol{m}}{2}\right) \cdot \mathrm{const}$
- Now, let us find all terms w.r.t. $\boldsymbol{x}_a$ in above expression.

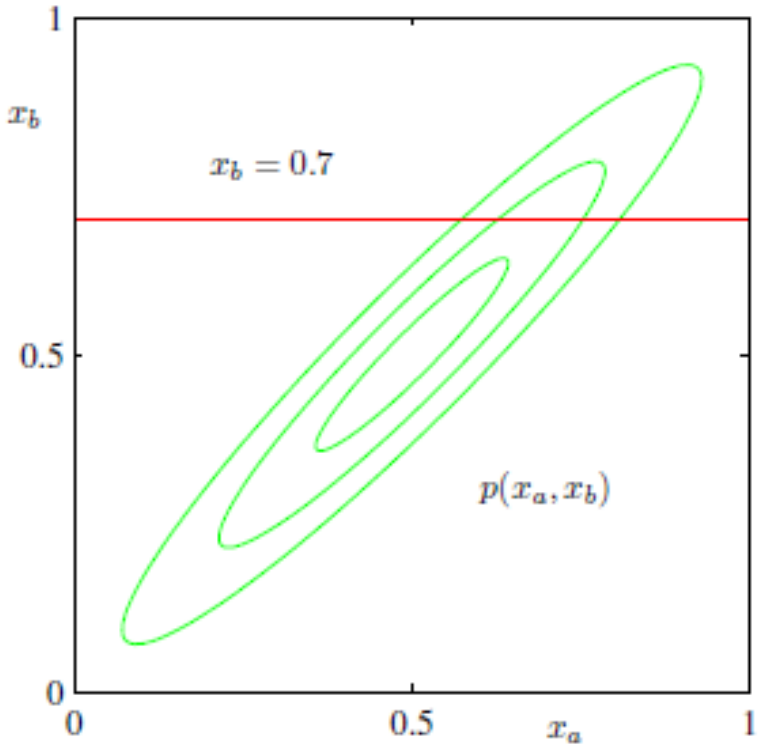
Proof Walkthrough

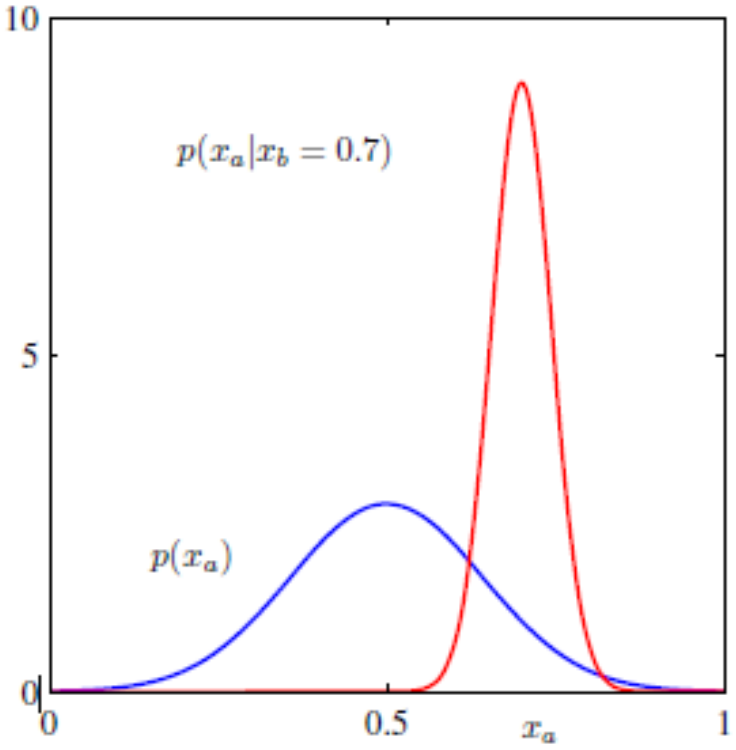
- $\log \boldsymbol{p}(\boldsymbol{x}_a) = -\frac{\boldsymbol{x}_a^\top \left(\boldsymbol{\Theta}_{aa} - \boldsymbol{\Theta}_{ab}\boldsymbol{\Theta}_{bb}^{-1}\boldsymbol{\Theta}_{ba}\right)\boldsymbol{x}_a}{2}$
  $+\boldsymbol{x}_a^\top \left(\boldsymbol{\Theta}_{aa} - \boldsymbol{\Theta}_{ab}\boldsymbol{\Theta}_{bb}^{-1}\boldsymbol{\Theta}_{ba}\right)\boldsymbol{\mu}_a + \text{const}$

- Using the block matrix inversion formula, $\boldsymbol{\Theta}_{aa} - \boldsymbol{\Theta}_{ab}\boldsymbol{\Theta}_{bb}^{-1}\boldsymbol{\Theta}_{ba} = \boldsymbol{\Sigma}_{aa}^{-1}$.
- Therefore, $\boldsymbol{p}(\boldsymbol{x}_a) = N_{\boldsymbol{x}_a}(\boldsymbol{\mu}_a, \boldsymbol{\Sigma}_{aa})$

- The marginal of a joint MVN has mean and variance that is the same as the mean and variance of the partitioned MVN.

Visualization





- PRML 2.9

Gaussian Linear Model

- The prior: $p(\boldsymbol{x}) = N_{\boldsymbol{x}}(\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1})$
- The Likelihood: $p(\boldsymbol{y}|\boldsymbol{x}) = N_{\boldsymbol{y}}(\boldsymbol{Ax} + \boldsymbol{b}, \boldsymbol{L}^{-1})$

Linear model

- The marginal: $p(\boldsymbol{y}) = N_{\boldsymbol{y}}(\boldsymbol{A\mu} + \boldsymbol{b}\ , \boldsymbol{L}^{-1} + \boldsymbol{A\Lambda}^{-1}\boldsymbol{A}^{\top})$
- The posterior: $p(\boldsymbol{x}|\boldsymbol{y}) = N_{\boldsymbol{x}}(\boldsymbol{\Sigma}\{\mathbf{A}^{\top}\boldsymbol{L}(\boldsymbol{y} - \boldsymbol{b}) + \boldsymbol{\Lambda\mu}\}, \boldsymbol{\Sigma})$

where $\boldsymbol{\Sigma} = (\boldsymbol{\Lambda} + \mathbf{A}^{\top}\mathbf{L}\mathbf{A})^{-1}$

Proof: 1. Calculate the joint $p(\boldsymbol{y}, \boldsymbol{x})$, 2. Use formula we just derived to obtain marginal and conditional dist.

Read PRML, 2.3.3

Likelihood for MVN

- Given the dataset $D \coloneqq \{\boldsymbol{x}_i\}_{i=1}^n$, the likelihood function of MVN density can be written as

- $$L(\boldsymbol{\mu}, \boldsymbol{\Sigma}, D) = \sum_{i=1} \log N_{\boldsymbol{x}_i}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$
$$= \text{const} - \frac{n}{2}\log|\Sigma| - \frac{\text{tr}\left(\overline{\boldsymbol{X}}\overline{\boldsymbol{X}}^\top \boldsymbol{\Sigma}^{-1}\right)}{2}$$

- where $\overline{\boldsymbol{X}} = [(\boldsymbol{x}_1 - \boldsymbol{\mu}) \dots (\boldsymbol{x}_n - \boldsymbol{\mu})] \in R^{d \times n}$ is the "centralized" dataset.
- tr is the trace operator.

Maximum Likelihood Estimator

- $\max_{\boldsymbol{\mu},\boldsymbol{\Sigma}} L(\boldsymbol{\mu},\boldsymbol{\Sigma},D) = \max_{\boldsymbol{\Sigma}} \max_{\boldsymbol{\mu}} L(\boldsymbol{\mu},\boldsymbol{\Sigma},D).$

- First, solve the inner max by
- $\frac{\partial L(\boldsymbol{\mu},\boldsymbol{\Sigma},D)}{\partial \boldsymbol{\mu}} = 0 \implies \boldsymbol{\mu}_{\mathrm{MLE}} := \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{x}_i$
- Then, plug in $\boldsymbol{\mu}_{\mathrm{MLE}}$ and solve the outer max by
- $\frac{\partial L(\boldsymbol{\mu}_{\mathrm{MLE}},\boldsymbol{\Sigma},D)}{\partial \boldsymbol{\Sigma}} = 0 \implies$
- $\boldsymbol{\Sigma}_{\mathrm{MLE}} := \frac{1}{n}\overline{\boldsymbol{X}}_{\mathrm{MLE}}\overline{\boldsymbol{X}}_{\mathrm{MLE}}^{\top}$,
- where $\overline{\boldsymbol{X}}_{\mathrm{MLE}} := [(\boldsymbol{x}_1 - \boldsymbol{\mu}_{\mathrm{MLE}}) \dots (\boldsymbol{x}_n - \boldsymbol{\mu}_{\mathrm{MLE}})]$