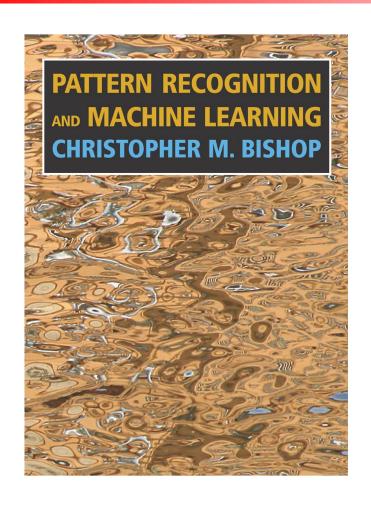
# Gaussian Identities (cont.)

Song Liu (song.liu@bristol.ac.uk)

Office Hour: Wednesday 4pm-5pm

NOT LAB this week.

#### Reference



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

Pattern Recognition and Machine Learning

Christopher Bishop, 2006

## Recap

• 
$$N_{\mathbf{x}}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \coloneqq \frac{1}{(2\pi)^{\frac{d}{2}|\boldsymbol{\Sigma}|^{\frac{1}{2}}}} \cdot \exp\left[-\frac{(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}{2}\right]$$

- MVNs are multi-dimensional generalizations of univariate normal distributions, in the sense that:
- $\Sigma^{-1} = UDU^{\top}$ 
  - Eigen-decomposition, **D** is diagonal.
  - $\boldsymbol{U} \in R^{d \times d}$ ,  $\boldsymbol{U} \boldsymbol{U}^{\top} = \boldsymbol{U}^{\top} \boldsymbol{U} = \boldsymbol{I}$
- $\mathbf{y} = \mathbf{U}^{\mathsf{T}}(\mathbf{x} \boldsymbol{\mu}).$
- $p(y) = \prod_i N_y(\mathbf{0}, \sigma_i^2), \sigma_i^2$  is *i*-th eigenvalue of  $\Sigma$ .
- Use this to generate samples of MVN using uni-normal!

## Recap

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

#### Moments of MVN.

- $\mathbb{E}[x] = \mu$ 
  - Apply the transform  $z = x \mu$ .

• 
$$\int_{-\infty}^{0} \exp\left[-\frac{z\Sigma^{-1}z}{2}\right] z dz = -\int_{0}^{\infty} \exp\left[-\frac{z\Sigma^{-1}z}{2}\right] z dz$$

- $\mathbb{E}[xx^{\mathsf{T}}] = \mu^{\mathsf{T}}\mu + \Sigma$ 
  - Apply the transform  $z = x \mu$ .
  - Use z = Uy and  $UU^{T} = I$ .

#### Partitioned MVNs

#### • Given:

• 
$$p(\mathbf{x}_a, \mathbf{x}_b) = N_{\mathbf{x}_a, \mathbf{x}_b} \begin{pmatrix} \mathbf{\mu}_a \\ \mathbf{\mu}_b \end{pmatrix}, \begin{bmatrix} \mathbf{\Sigma}_{aa}, \mathbf{\Sigma}_{ab} \\ \mathbf{\Sigma}_{ba}, \mathbf{\Sigma}_{bb} \end{bmatrix}$$

- Represent  $p(x_a|x_b)$  and  $p(x_a)$  using  $\frac{\mu_a}{\mu_b}$  and  $\frac{\Sigma_{aa}, \Sigma_{ab}}{\Sigma_{ba}, \Sigma_{bb}}$ .
- Partitioned MVN formulas have huge applications in Bayesian regression, Gaussian graphical models etc.
- For simplicity, we let  $\Sigma^{-1} = \Theta = \begin{bmatrix} \Theta_{aa}, \Theta_{ab} \\ \Theta_{ba}, \Theta_{bb} \end{bmatrix}$ .

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

$$\log N_{x}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \begin{bmatrix} \boldsymbol{x}_{a} - \boldsymbol{\mu}_{a} \\ \boldsymbol{x}_{b} - \boldsymbol{\mu}_{b} \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \boldsymbol{\Theta}_{aa}, \boldsymbol{\Theta}_{ab} \\ \boldsymbol{\Theta}_{ba}, \boldsymbol{\Theta}_{bb} \end{bmatrix} \begin{bmatrix} \boldsymbol{x}_{a} - \boldsymbol{\mu}_{a} \\ \boldsymbol{x}_{b} - \boldsymbol{\mu}_{b} \end{bmatrix} + \text{const}$$

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

• If  $p(t) = N_t(\mu; \Sigma)$ , then  $\log p(t) = -\frac{t^{\top} \Sigma^{-1} t}{2} + t^{\top} \Sigma^{-1} \mu + \text{const.}$ 



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

- The quadratic term w.r.t.  $x_a$  after expansion:
- $-\mathbf{x}_a^{\mathsf{T}}\mathbf{\Theta}_{aa}\mathbf{x}_a/2 \Longrightarrow \mathrm{Cov}_{\mathbf{x}_a|\mathbf{x}_b}[\mathbf{x}_a] = [\mathbf{\Theta}_{aa}]^{-1}$ .
- The *linear terms* w.r.t.  $x_a$  after expansion:
- $\bullet \ -\boldsymbol{x}_{a}^{\mathsf{T}}\boldsymbol{\Theta}_{ab}\boldsymbol{x}_{b} + \boldsymbol{x}_{a}^{\mathsf{T}}\boldsymbol{\Theta}_{ab}\boldsymbol{\mu}_{b} + \boldsymbol{x}_{a}^{\mathsf{T}}\boldsymbol{\Theta}_{aa}\boldsymbol{\mu}_{a}$
- Collect terms:  $\mathbf{x}_a^{\mathsf{T}} \mathbf{\Theta}_{aa} (\boldsymbol{\mu}_a \mathbf{\Theta}_{aa}^{-1} \mathbf{\Theta}_{ab} \mathbf{x}_b + \mathbf{\Theta}_{aa}^{-1} \mathbf{\Theta}_{ab} \boldsymbol{\mu}_b)$
- Knowing  $Cov_{x_a|x_h}[x_a] = [\Theta_{aa}]^{-1} \Longrightarrow$

$$\mathbb{E}_{x_a|x_b}[x_a] = \mu_a - \Theta_{aa}^{-1}\Theta_{ab}x_b + \Theta_{aa}^{-1}\Theta_{ab}\mu_b$$

#### Conditional MVN formula

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

- You can use block matrix inversion formula to represent  $\Theta_{aa}$ ,  $\Theta_{ab}$  using  $\Sigma_{aa}$ ,  $\Sigma_{ab}$  and  $\Sigma_{bb}$ .
- See 2.76 in PRML

• However, this formula is most easily expressed using block matrices of  $\Theta$ .

# Partitioned MVNs (Marginal)

- How to represent  $p(x_a)$  using  $\frac{\mu_a}{\mu_b}$  and  $\frac{\Sigma_{aa}, \Sigma_{ab}}{\Sigma_{ba}, \Sigma_{bb}}$ ?
- First, we marginalize  $p(\mathbf{x}_a) = \int p(\mathbf{x}_a, \mathbf{x}_b) d\mathbf{x}_b$
- Write terms in  $\log p(x_a, x_b)$  w.r.t.  $x_b$  after expansion:

• 
$$-\mathbf{x}_b^{\mathsf{T}}\mathbf{\Theta}_{bb}\mathbf{x}_b/2 + \mathbf{x}_b^{\mathsf{T}}(\mathbf{\Theta}_{bb}\mathbf{\mu}_b - \mathbf{\Theta}_{ba}\mathbf{x}_a + \mathbf{\Theta}_{ba}\mathbf{\mu}_a)$$

$$= -(\boldsymbol{x}_b^{\mathsf{T}} - \boldsymbol{\Theta}_{bb}^{-1} \boldsymbol{m}) \boldsymbol{\Theta}_{bb} (\boldsymbol{x}_b - \boldsymbol{\Theta}_{bb}^{-1} \boldsymbol{m}) / 2 + \boldsymbol{m}^{\mathsf{T}} \boldsymbol{\Theta}_{bb}^{-1} \boldsymbol{m} / 2,$$

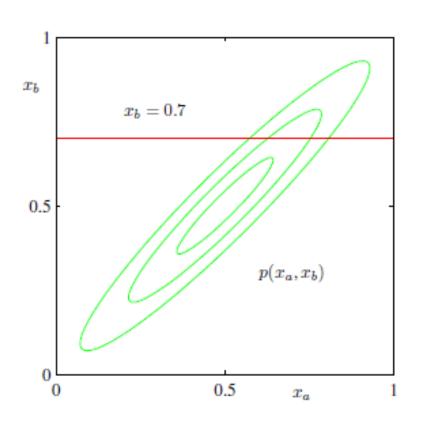
Completing the square!

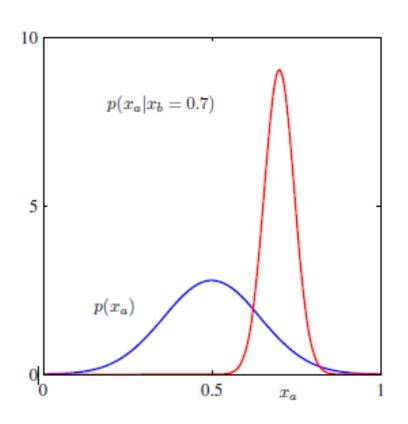
- Now we know
- $p(\mathbf{x}_a) =$   $(\dots) \exp\left(\frac{\mathbf{m}^{\mathsf{T}}\mathbf{\Theta}_{bb}^{-1}\mathbf{m}}{2}\right) \int \exp\left[-\frac{(\mathbf{x}_b^{\mathsf{T}} \mathbf{\Theta}_{bb}^{-1}\mathbf{m})\mathbf{\Theta}_{bb}(\mathbf{x}_b \mathbf{\Theta}_{bb}^{-1}\mathbf{m})}{2}\right] d\mathbf{x}_b$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

• 
$$\log p(x_a) = -\frac{x_a^{\mathsf{T}}(\Theta_{aa} - \Theta_{ab}\Theta_{bb}^{-1}\Theta_{ba})x_a}{+x_a^{\mathsf{T}}(\Theta_{aa} - \Theta_{ab}\Theta_{bb}^{-1}\Theta_{ba})\mu_a + \text{const}}$$

- Using the block matrix inversion formula,  $\Theta_{aa} \Theta_{ab}\Theta_{bb}^{-1}\Theta_{ba} = \Sigma_{aa}^{-1}$ .
- Therefore,  $p(x_a) = N_{x_a}(\mu_a, \Sigma_{aa})$
- The marginal of a joint MVN has mean and variance that is the same as the mean and variance of the partitioned MVN.

### Visualization

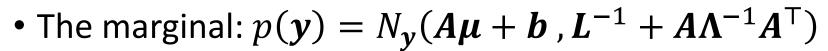




• PRML 2.9

#### Gaussian Linear Model

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



• The posterior:  $p(x|y) = N_x(\Sigma\{A^\top L(y-b) + \Lambda\mu\}, \Sigma)$  where  $\Sigma = (\Lambda + A^\top LA)^{-1}$ 

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

Read PRML, 2.3.3

#### Likelihood for MVN

• Given the dataset  $D := \{x_i\}_{i=1}^n$ , the likelihood function of MVN density can be written as

• 
$$L(\boldsymbol{\mu}, \boldsymbol{\Sigma}, D) = \sum_{i=1} \log N_{x_i}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$
  
=  $\operatorname{const} - \frac{n}{2} \log |\boldsymbol{\Sigma}| - \frac{\operatorname{tr}(\overline{X}\overline{X}^{\mathsf{T}}\boldsymbol{\Sigma}^{-1})}{2}$ 

- where  $\overline{X} = [(x_1 \mu) \dots (x_n \mu)] \in \mathbb{R}^{d \times n}$  is the "centralized" dataset.
- tr is the trace operator.

#### Maximum Likelihood Estimator

- $\max_{\mu, \Sigma} L(\mu, \Sigma, D) = \max_{\Sigma} \max_{\mu} L(\mu, \Sigma, D).$
- First, solve the inner max by

• 
$$\frac{\partial L(\mu, \Sigma, D)}{\partial \mu} = 0 \implies \mu_{\text{MLE}} := \frac{1}{n} \sum_{i=1}^{n} x_i$$

- Then, plug in  $\mu_{
  m MLE}$  and solve the outer max by
- $\bullet \frac{\partial L(\mu_{\text{MLE}}, \Sigma, D)}{\partial \Sigma} = 0 \Longrightarrow$
- $\Sigma_{\text{MLE}} := \frac{1}{n} \overline{X}_{\text{MLE}} \overline{X}_{\text{MLE}}^{\mathsf{T}}$ ,
- where  $\overline{X}_{\mathrm{MLE}}$ : =  $[(x_1 \mu_{\mathrm{MLE}}) ... (x_n \mu_{\mathrm{MLE}})]$