Solutions Manual to Pattern Recognition and Machine Learning

Hiromichi Inawashiro

October 11, 2025

Contents

1 Introduction **1**

2 Probability Distributions **43**

3 Linear Models for Regression **106**

4 Linear Models for Classification **131**

5 Neural Networks **157**

6 Kernel Methods **191**

7 Sparse Kernel Machines **220**

1 Introduction

1.1

Let

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(y(x_n, \mathbf{w}) - t_n\right)^2. \tag{1.1}$$

Setting the derivative with respect to $\mathbf{w}$ to zero gives

$$\mathbf{0} = \sum_{n=1}^{N}\frac{\partial y(x_n, \mathbf{w})}{\partial \mathbf{w}}\left(y(x_n, \mathbf{w}) - t_n\right). \tag{1.2}$$

If

$$y(x_n, \mathbf{w}) = \mathbf{w}^\intercal \boldsymbol{\phi}(x_n), \tag{1.3}$$

then

$$\mathbf{0} = \sum_{n=1}^{N}\boldsymbol{\phi}(x_n)\left(\mathbf{w}^\intercal\boldsymbol{\phi}(x_n) - t_n\right). \tag{1.4}$$

Then,

$$\left(\sum_{n=1}^{N}\boldsymbol{\phi}(x_n)\boldsymbol{\phi}(x_n)^\intercal\right)\mathbf{w} = \sum_{n=1}^{N}t_n\boldsymbol{\phi}(x_n). \tag{1.5}$$

Therefore,

$$\operatorname*{argmin}_{\mathbf{w}} E(\mathbf{w}) = \mathbf{A}^{-1}\mathbf{v}, \tag{1.6}$$

where

$$\begin{aligned}\mathbf{A} &= \sum_{n=1}^{N}\boldsymbol{\phi}(x_n)\boldsymbol{\phi}(x_n)^\intercal,\\ \mathbf{v} &= \sum_{n=1}^{N}t_n\boldsymbol{\phi}(x_n).\end{aligned} \tag{1.7}$$

If

$$\boldsymbol{\phi}(x_n) = \begin{bmatrix}1\\ x_n\\ \vdots\\ x_n^M\end{bmatrix},$$

then

$$\begin{aligned} A_{mm'} &= \sum_{n=1}^{N} x_n^{m+m'}, \\ v_m &= \sum_{n=1}^{N} t_n x_n^m. \end{aligned} \tag{1.8}$$

1.2

Let

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N} (y(x_n, \mathbf{w}) - t_n)^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2. \tag{1.9}$$

Setting the derivative with respect to $\mathbf{w}$ to zero gives

$$\mathbf{0} = \sum_{n=1}^{N} \frac{\partial y(x_n, \mathbf{w})}{\partial \mathbf{w}} (y(x_n, \mathbf{w}) - t_n) + \lambda \mathbf{w}. \tag{1.10}$$

If

$$y(x_n, \mathbf{w}) = \mathbf{w}^\intercal \boldsymbol{\phi}(x_n), \tag{1.11}$$

then

$$\mathbf{0} = \sum_{n=1}^{N} \boldsymbol{\phi}(x_n) (\mathbf{w}^\intercal \boldsymbol{\phi}(x_n) - t_n) + \lambda \mathbf{w}. \tag{1.12}$$

Then,

$$\left(\sum_{n=1}^{N} \boldsymbol{\phi}(x_n) \boldsymbol{\phi}(x_n)^\intercal + \lambda \mathbf{I} \right) \mathbf{w} = \sum_{n=1}^{N} t_n \boldsymbol{\phi}(x_n). \tag{1.13}$$

Therefore,

$$\operatorname*{argmin}_{\mathbf{w}} E(\mathbf{w}) = \mathbf{A}^{-1}\mathbf{v}, \tag{1.14}$$

where

$$\begin{aligned} \mathbf{A} &= \sum_{n=1}^{N} \boldsymbol{\phi}(x_n) \boldsymbol{\phi}(x_n)^\intercal + \lambda \mathbf{I}, \\ \mathbf{v} &= \sum_{n=1}^{N} t_n \boldsymbol{\phi}(x_n). \end{aligned} \tag{1.15}$$

If

$$\boldsymbol{\phi}(x_n) = \begin{bmatrix} 1 \\ x_n \\ \vdots \\ x_n^M \end{bmatrix},$$

then

$$\begin{aligned} A_{mm'} &= \sum_{n=1}^{N} x_n^{m+m'} + \lambda I_{mm'}, \\ v_m &= \sum_{n=1}^{N} t_n x_n^m. \end{aligned} \tag{1.16}$$

1.3

Let

$$\begin{aligned} &p(a|r) = \frac{3}{10}, p(o|r) = \frac{2}{5}, p(l|r) = \frac{3}{10}, \\ &p(a|b) = \frac{1}{2}, p(o|b) = \frac{1}{2}, \\ &p(a|g) = \frac{3}{10}, p(o|g) = \frac{3}{10}, p(l|g) = \frac{2}{5}. \end{aligned} \tag{1.17}$$

Let

$$p(r) = \frac{1}{5}, p(b) = \frac{1}{5}, p(g) = \frac{3}{5}. \tag{1.18}$$

(a)

By the Bayes' theorem,

$$p(a) = p(a|r)p(r) + p(a|b)p(b) + p(a|g)p(g). \tag{1.19}$$

Therefore,

$$p(a) = \frac{17}{50}. \tag{1.20}$$

(b)

By the Bayes' thorem,

$$p(g|o) = \frac{p(g, o)}{p(o)}. \tag{1.21}$$

By the Bayes' throrem, the right hand side can be written as

$$\frac{p(o|g)p(g)}{p(o|r)p(r)+p(o|b)p(b)+p(o|g)p(g)}. \tag{1.22}$$

Therefore,

$$p(g|o)=\frac{1}{2}. \tag{1.23}$$

1.4

Let x and y be variables such that

$$x=g(y). \tag{1.24}$$

Let $\hat{x}$ and $\hat{y}$ be the locations of the maximum of p_x and p_y respcetively. Let us assume that there exists a positive ϵ such that if

$$|y-\hat{y}|<\epsilon, \tag{1.25}$$

then

$$g'(y)\neq 0. \tag{1.26}$$

(a)

Since

$$\int p_x(x)dx=\int p_x\left(g(y)\right)|g'(y)|dy, \tag{1.27}$$

we have

$$p_y(y)=p_x\left(g(y)\right)|g'(y)|. \tag{1.28}$$

Taking the derivative and substituting

$$y=\hat{y} \tag{1.29}$$

gives

$$0=g'(\hat{y})p'_x\left(g\left(\hat{y}\right)\right)+p_x\left(g\left(\hat{y}\right)\right)g''\left(\hat{y}\right). \tag{1.30}$$

Therefore, in general,

$$\hat{x}\neq g\left(\hat{y}\right). \tag{1.31}$$

(b)

By (a), if

$$g(y) = ay + b, \tag{1.32}$$

then

$$0 = ap'_x\left(g\left(\hat{y}\right)\right). \tag{1.33}$$

Therefore,

$$\hat{x} = g\left(\hat{y}\right). \tag{1.34}$$

1.5

We have

$$\operatorname{var} f(x) = \mathrm{E}\left(f(x) - \mathrm{E}\, f(x)\right)^2. \tag{1.35}$$

The right hand side can be written as

$$\mathrm{E}\left(\left(f(x)\right)^2 - 2f(x)\,\mathrm{E}\, f(x) + \left(\mathrm{E}\, f(x)\right)^2\right) = \mathrm{E}\left(f(x)\right)^2 - \left(\mathrm{E}\, f(x)\right)^2. \tag{1.36}$$

Therefore,

$$\operatorname{var} f(x) = \mathrm{E}\left(f(x)\right)^2 - \left(\mathrm{E}\, f(x)\right)^2. \tag{1.37}$$

1.6

We have

$$\operatorname{cov}(x, y) = \mathrm{E}\left(\left(x - \mathrm{E}\, x\right)\left(y - \mathrm{E}\, y\right)\right). \tag{1.38}$$

The right hand side can be written as

$$\mathrm{E}\, xy - \mathrm{E}\left(x\,\mathrm{E}\, y\right) - \mathrm{E}\left(y\,\mathrm{E}\, x\right) + \mathrm{E}\left(\mathrm{E}\, x\,\mathrm{E}\, y\right) = \mathrm{E}\, xy - \mathrm{E}\, x\,\mathrm{E}\, y. \tag{1.39}$$

The right hand side can be written as

$$\int xyp(x, y)dxdy - \int xp(x)dx \int yp(y)dy. \tag{1.40}$$

If x and y are independent, by the definition,

$$f(x, y) = f(x)f(y). \tag{1.41}$$

Then,

$$\int xyp(x, y)dxdy = \int p(x)dx \int p(y)dy. \tag{1.42}$$

Therefore,

$$\operatorname{cov}(x, y) = 0. \tag{1.43}$$

1.7

(a)

Let

$$I = \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}x^2\right) dx. \tag{1.44}$$

Then,

$$I^2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}\left(x^2+y^2\right)\right) dxdy. \tag{1.45}$$

By the transformation from Cartesian coordinates (x, y) to polar coordinates (r, θ), the right hand side can be written as

$$\int_0^{\infty}\int_0^{2\pi} \exp\left(-\frac{1}{2\sigma^2}r^2\right) \begin{vmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{vmatrix} drd\theta = 2\pi \int_0^{\infty} \exp\left(-\frac{1}{2\sigma^2}r^2\right) rdr. \tag{1.46}$$

By the transformation $s = \frac{r}{\sigma}$, the right hand side can be written as

$$2\pi\sigma^2 \int_0^{\infty} \exp\left(-\frac{1}{2}s^2\right) sds = 2\pi\sigma^2 \left[-\exp\left(-\frac{1}{2}s^2\right)\right]_0^{\infty}. \tag{1.47}$$

Therefore,

$$I = \left(2\pi\sigma^2\right)^{\frac{1}{2}}. \tag{1.48}$$

(b)

By the definition,

$$\mathcal{N}\left(x|\mu,\sigma^2\right) = \left(2\pi\sigma^2\right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right). \tag{1.49}$$

Then,

$$\int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu,\sigma^2\right) dx = \left(2\pi\sigma^2\right)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right) dx. \tag{1.50}$$

By the transformation $t = x - \mu$, the right hand side can be written as

$$\left(2\pi\sigma^2\right)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}t^2\right) dt = \left(2\pi\sigma^2\right)^{-\frac{1}{2}} I. \tag{1.51}$$

Therefore,

$$\int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu,\sigma^2\right) dx = 1. \tag{1.52}$$

1.8

(a)

Let x be a variable such that

$$p(x) = \mathcal{N}(x|\mu, \sigma^2). \tag{1.53}$$

Then,

$$\mathrm{E}\, x = \int_{-\infty}^{\infty} x\mathcal{N}\left(x|\mu, \sigma^2\right) dx. \tag{1.54}$$

The right hand side can be written as

$$\left(2\pi\sigma^2\right)^{-\frac{1}{2}} \int_{-\infty}^{\infty} x \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right) dx. \tag{1.55}$$

By the transformation

$$y = x - \mu, \tag{1.56}$$

the integral can be written as

$$\begin{aligned} &\int_{-\infty}^{\infty} (y+\mu) \exp\left(-\frac{1}{2\sigma^2}y^2\right) dy \\ &= \int_{-\infty}^{\infty} y \exp\left(-\frac{1}{2\sigma^2}y^2\right) dy + \mu \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}y^2\right) dy. \end{aligned} \tag{1.57}$$

By 1.7(a), the right hand side can be written as

$$\mu\left(2\pi\sigma^2\right)^{\frac{1}{2}}. \tag{1.58}$$

Therefore,

$$\mathrm{E}\, x = \mu. \tag{1.59}$$

(b)

By 1.7(b),

$$\int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) dx = 1, \tag{1.60}$$

so that

$$\left(2\pi\sigma^2\right)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right) dx = 1. \tag{1.61}$$

Taking the derivative with respect to σ^2 gives

$$\begin{aligned}&(2\pi)^{-\frac{1}{2}}\left(-\frac{1}{2}\right)\left(\sigma^2\right)^{-\frac{3}{2}}\int_{-\infty}^{\infty}\exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)dx\\&+\left(2\pi\sigma^2\right)^{-\frac{1}{2}}\int_{-\infty}^{\infty}\frac{1}{2}\left(\sigma^2\right)^{-2}(x-\mu)^2\exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)dx=0.\end{aligned}\tag{1.62}$$

The left hand side can be written as

$$\begin{aligned}&-\frac{1}{2}\left(\sigma^2\right)^{-1}\int_{-\infty}^{\infty}\mathcal{N}\left(x|\mu,\sigma^2\right)dx+\frac{1}{2}\left(\sigma^2\right)^{-2}\int_{-\infty}^{\infty}(x-\mu)^2\mathcal{N}\left(x|\mu,\sigma^2\right)dx\\&=-\frac{1}{2}\left(\sigma^2\right)^{-1}+\frac{1}{2}\left(\sigma^2\right)^{-2}\operatorname{var}x.\end{aligned}\tag{1.63}$$

Therefore,

$$\operatorname{var}x=\sigma^2.\tag{1.64}$$

1.9

(a)

Let x be a variable such that

$$p(x)=\mathcal{N}\left(x|\mu,\sigma^2\right).\tag{1.65}$$

Setting the derivative of the right hand side with respect to x to zero gives

$$0=\left(2\pi\sigma^2\right)^{-\frac{1}{2}}\left(-\frac{1}{\sigma^2}(x-\mu)\right)\exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right).\tag{1.66}$$

Therefore,

$$\operatorname{mode}x=\mu.\tag{1.67}$$

(b)

Let $\mathbf{x}$ be a variable such that

$$p(\mathbf{x})=\mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}\right).\tag{1.68}$$

Setting the derivative of the right hand side with respect to $\mathbf{x}$ to zero gives

$$\mathbf{0}=-(2\pi)^{-\frac{D}{2}}(\det\boldsymbol{\Sigma})^{-\frac{1}{2}}\left(\boldsymbol{\Sigma}^{-1}+\left(\boldsymbol{\Sigma}^{-1}\right)^{\intercal}\right)(\mathbf{x}-\boldsymbol{\mu})\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right).\tag{1.69}$$

Therefore,

$$\operatorname{mode} \mathbf{x} = \boldsymbol{\mu}. \tag{1.70}$$

1.10

(a)

We have

$$\mathrm{E}(x+y) = \iint (x+y)p(x,y)dxdy. \tag{1.71}$$

The right hand side can be written as

$$\int x \left(\int p(x,y)dy \right) dx + \int y \left(\int p(x,y)dx \right) dy = \int xp(x)dx + \int yp(y)dy. \tag{1.72}$$

The right hand side can be written as

$$\mathrm{E}\, x + \mathrm{E}\, y. \tag{1.73}$$

Therefore,

$$\mathrm{E}(x+y) = \mathrm{E}\, x + \mathrm{E}\, y. \tag{1.74}$$

(b)

We have

$$\operatorname{var}(x+y) = \mathrm{E}\left(x+y-\mathrm{E}(x+y)\right)^2 \tag{1.75}$$

The right hand side can be written as

$$\begin{aligned} &\mathrm{E}\left(x-\mathrm{E}\, x\right)^2 + 2\,\mathrm{E}\left(\left(x-\mathrm{E}\, x\right)\left(y-\mathrm{E}\, y\right)\right) + \mathrm{E}\left(y-\mathrm{E}\, y\right)^2 \\ &= \operatorname{var} x + 2\operatorname{cov}(x,y) + \operatorname{var} y. \end{aligned} \tag{1.76}$$

By 1.6, if x and y are independent, then

$$\operatorname{cov}(x,y) = 0. \tag{1.77}$$

Therefore,

$$\operatorname{var}(x+y) = \operatorname{var} x + \operatorname{var} y. \tag{1.78}$$

1.11

Let $x_1, \cdots, x_N$ be variables such that

$$p(x_n) = \mathcal{N}\left(x_n|\mu, \sigma^2\right). \tag{1.79}$$

Then,

$$\ln\left(\prod_{n=1}^{N} p(x_n)\right) = -\frac{N}{2}\ln\left(2\pi\sigma^2\right) - \frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n - \mu)^2. \tag{1.80}$$

Setting the derivatives with respect to μ and σ^2 to zero gives

$$\begin{aligned} 0 &= \frac{1}{\sigma^2}\sum_{n=1}^{N}(x_n - \mu), \\ 0 &= -\frac{N}{2\sigma^2} + \frac{1}{2\left(\sigma^2\right)^2}\sum_{n=1}^{N}(x_n - \mu)^2. \end{aligned} \tag{1.81}$$

Therefore, the maximum likelihood solutions for μ and σ^2 are given by

$$\begin{aligned} \mu_{\mathrm{ML}} &= \frac{1}{N}\sum_{n=1}^{N} x_n, \\ \sigma^2_{\mathrm{ML}} &= \frac{1}{N}\sum_{n=1}^{N}(x_n - \mu_{\mathrm{ML}})^2. \end{aligned} \tag{1.82}$$

1.12

(a)

Let x_n and $x_{n'}$ be independent variables such that

$$\begin{aligned} p(x_n) &= \mathcal{N}\left(x_n|\mu, \sigma^2\right), \\ p(x_{n'}) &= \mathcal{N}\left(x_{n'}|\mu, \sigma^2\right). \end{aligned} \tag{1.83}$$

Then,

$$\mathrm{E}\, x_n x_{n'} = \mu^2. \tag{1.84}$$

By the property

$$\mathrm{E}\, x_n^2 = \operatorname{var} x_n + \left(\mathrm{E}\, x_n\right)^2, \tag{1.85}$$

we have

$$\mathrm{E}\, x_n^2 = \sigma^2 + \mu^2. \tag{1.86}$$

Therefore,

$$\mathrm{E}\, x_n x_{n'} = \mu^2 + I_{nn'}\sigma^2. \tag{1.87}$$

(b)

Let $x_1, \cdots, x_N$ be independent variables such that

$$p(x_n) = \mathcal{N}\left(x_n|\mu, \sigma^2\right). \tag{1.88}$$

By 1.11, the maximum likelihood solution for μ is given by

$$\mu_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N} x_n. \tag{1.89}$$

Then,

$$\mathrm{E}\, \mu_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N} \mathrm{E}\, x_n. \tag{1.90}$$

Therefore,

$$\mathrm{E}\, \mu_{\mathrm{ML}} = \mu. \tag{1.91}$$

(c)

Let $x_1, \cdots, x_N$ be independent variables such that

$$p(x_n) = \mathcal{N}\left(x_n|\mu, \sigma^2\right). \tag{1.92}$$

By 1.11, the maximum likelihood solution for σ^2 is given by

$$\sigma^2_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N} \left(x_n - \mu_{\mathrm{ML}}\right)^2. \tag{1.93}$$

Then,

$$\mathrm{E}\, \sigma^2_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N} \mathrm{E}\left(x_n - \mu_{\mathrm{ML}}\right)^2. \tag{1.94}$$

The right hand side can be writen as

$$\begin{aligned}&\frac{1}{N}\sum_{n=1}^{N}\mathrm{E}\left(x_n^2-2\mu_{\mathrm{ML}}x_n+\mu_{\mathrm{ML}}^2\right)\\=&\frac{1}{N}\sum_{n=1}^{N}\mathrm{E}\,x_n^2-\frac{2}{N}\,\mathrm{E}\left(\mu_{\mathrm{ML}}\left(\sum_{n=1}^{N}x_n\right)\right)+\mathrm{E}\,\mu_{\mathrm{ML}}^2.\end{aligned}\tag{1.95}$$

The first term of the right hand side can be written as

$$\frac{1}{N}\sum_{n=1}^{N}\left(\mu^2+\sigma^2\right)=\mu^2+\sigma^2,\tag{1.96}$$

while, by 1.11, the second and third terms can be writen as

$$-\frac{2}{N}\,\mathrm{E}\left(N\left(\frac{1}{N}\sum_{n=1}^{N}x_n\right)^2\right)+\mathrm{E}\left(\frac{1}{N}\sum_{n=1}^{N}x_n\right)^2=-\,\mathrm{E}\left(\frac{1}{N}\sum_{n=1}^{N}x_n\right)^2.\tag{1.97}$$

By (a), the right hand side can be written as

$$\begin{aligned}&-\frac{1}{N^2}\sum_{n=1}^{N}\mathrm{E}\,x_n^2-\frac{2}{N^2}\sum_{1\le n<n'\le N}\mathrm{E}\,x_nx_{n'}\\=&-\frac{1}{N^2}N\left(\mu^2+\sigma^2\right)-\frac{2}{N^2}\frac{N(N-1)}{2}\mu^2.\end{aligned}\tag{1.98}$$

The right hand side can be written as

$$-\frac{1}{N}\left(\mu^2+\sigma^2\right)-\frac{N-1}{N}\mu^2=-\mu^2-\frac{1}{N}\sigma^2.\tag{1.99}$$

Then,

$$\mathrm{E}\,\sigma_{\mathrm{ML}}^2=\mu^2+\sigma^2-\mu^2-\frac{1}{N}\sigma^2.\tag{1.100}$$

Therefore,

$$\mathrm{E}\,\sigma_{\mathrm{ML}}^2=\frac{N-1}{N}\sigma^2.\tag{1.101}$$

1.13

Let $x_1, \cdots, x_N$ be variables such that

$$\begin{aligned} \mathrm{E}\, x_n &= \mu, \\ \mathrm{var}\, x_n &= \sigma^2. \end{aligned} \tag{1.102}$$

We have

$$\mathrm{E}\left(\frac{1}{N}\sum_{n=1}^{N}(x_n-\mu)^2\right) = \frac{1}{N^2}\sum_{n=1}^{N}\mathrm{E}\,(x_n-\mu)^2\,. \tag{1.103}$$

The right hand side can be writen as

$$\frac{1}{N^2}\sum_{n=1}^{N}\mathrm{var}\, x_n = \frac{\sigma^2}{N}. \tag{1.104}$$

Therefore,

$$\mathrm{E}\left(\frac{1}{N}\sum_{n=1}^{N}(x_n-\mu)^2\right) = \frac{\sigma^2}{N}. \tag{1.105}$$

1.14

Let

$$\begin{aligned} w^{\mathrm{S}}_{dd'} &= \frac{1}{2}(w_{dd'} + w_{d'd}), \\ w^{\mathrm{A}}_{dd'} &= \frac{1}{2}(w_{dd'} - w_{d'd}). \end{aligned} \tag{1.106}$$

(a)

We have

$$\begin{aligned} w_{dd'} &= w^{\mathrm{S}}_{dd'} + w^{\mathrm{A}}_{dd'}, \\ w^{\mathrm{S}}_{dd'} &= w^{\mathrm{S}}_{d'd}, \\ w^{\mathrm{A}}_{dd'} &= -w^{\mathrm{A}}_{d'd}. \end{aligned} \tag{1.107}$$

(b)

We have

$$\sum_{d=1}^{D}\sum_{d'=1}^{D} w^{\mathrm{A}}_{dd'} x_d x_{d'} = \frac{1}{2}\sum_{d=1}^{D}\sum_{d'=1}^{D}(w_{dd'} - w_{d'd})x_d x_{d'}. \tag{1.108}$$

The right hand side can be written as

$$\frac{1}{2}\left(\sum_{d=1}^{D}\sum_{d'=1}^{D} w_{dd'}x_d x_{d'} - \sum_{d=1}^{D}\sum_{d'=1}^{D} w_{d'd}x_d x_{d'}\right) = 0. \tag{1.109}$$

Therefore,

$$\sum_{d=1}^{D}\sum_{d'=1}^{D} w^{\mathrm{A}}_{dd'}x_d x_{d'} = 0. \tag{1.110}$$

(c)

We have

$$\sum_{d=1}^{D}\sum_{d'=1}^{D} w_{dd'}x_d x_{d'} = \sum_{d=1}^{D}\sum_{d'=1}^{D} \left(w^{\mathrm{S}}_{dd'} + w^{\mathrm{A}}_{dd'}\right) x_d x_{d'}. \tag{1.111}$$

By (b), the right hand side can be written as

$$\sum_{d=1}^{D}\sum_{d'=1}^{D} w^{\mathrm{S}}_{dd'}x_d x_{d'} + \sum_{d=1}^{D}\sum_{d'=1}^{D} w^{\mathrm{A}}_{dd'}x_d x_{d'} = \sum_{d=1}^{D}\sum_{d'=1}^{D} w^{\mathrm{S}}_{dd'}x_d x_{d'}, \tag{1.112}$$

Therefore,

$$\sum_{d=1}^{D}\sum_{d'=1}^{D} w_{dd'}x_d x_{d'} = \sum_{d=1}^{D}\sum_{d'=1}^{D} w^{\mathrm{S}}_{dd'}x_d x_{d'}. \tag{1.113}$$

(d)

Since $\mathbf{W}^{\mathrm{S}}$ is a $D\times D$ symmetric matrix, its number of independent parameters is $\frac{D(D+1)}{2}$.

1.15

(a)

Let $n(D, M)$ be the number of independent parameters of a polynomial in D dimensions and M orders. Then

$$n(1, M) = n(1, M-1) = 1. \tag{1.114}$$

Let us assume that

$$n(D, M) = \sum_{d=1}^{D} n(d, M-1). \tag{1.115}$$

The independent terms of a polynomial in $D+1$ dimensions and M orders can be split into 1. the ones of a polynomial in D dimensions and M orders and 2. the ones generated by multiplying the ones in $D+1$ dimensions and M orders by the $D+1$th variable. Then,

$$n(D+1, M) = n(D, M) + n(D+1, M-1), \tag{1.116}$$

so that

$$n(D+1, M) = \sum_{d=1}^{D+1} n(d, M-1). \tag{1.117}$$

Therefore, the assumption is proved by induction on D.

(b)

We have

$$\sum_{d=1}^{1} \frac{(d+M-2)!}{(d-1)!(M-1)!} = 1. \tag{1.118}$$

Let us assume that

$$\sum_{d=1}^{D} \frac{(d+M-2)!}{(d-1)!(M-1)!} = \frac{(D+M-1)!}{(D-1)!M!}. \tag{1.119}$$

Then,

$$\sum_{d=1}^{D+1} \frac{(d+M-2)!}{(d-1)!(M-1)!} = \frac{(D+M-1)!}{(D-1)!M!} + \frac{(D+M-1)!}{D!(M-1)!}. \tag{1.120}$$

The right hand side can be written as

$$\frac{D(D+M-1)! + M(D+M-1)!}{D!M!} = \frac{(D+M)!}{D!M!}. \tag{1.121}$$

Therefore, the assumption is proved by induction on D.

(c)

By 1.14(d),

$$n(D,2) = \frac{D(D+1)}{2}. \tag{1.122}$$

Let us assume that

$$n(D,M) = \frac{(D+M-1)!}{(D-1)!M!}. \tag{1.123}$$

By (a),

$$n(D,M+1) = \sum_{d=1}^{D} n(d,M). \tag{1.124}$$

By the assumption and (b), the right hand side can be written as

$$\sum_{d=1}^{D} \frac{(d+M-1)!}{(d-1)!M!} = \frac{(D+M)!}{(D-1)!(M+1)!}. \tag{1.125}$$

Therefore, the assumption is proved by induction on M.

1.16

(a)

Let $N(D,M)$ be the number of independent parameters in all of the terms up to and including the ones of D dimensions and M orders. By 1.15,

$$N(D,M) = \sum_{m=0}^{M} n(D,m), \tag{1.126}$$

where

$$n(D,m) = \frac{(D+m-1)!}{(D-1)!m!}. \tag{1.127}$$

(b)

By (a),

$$N(D,0) = 1. \tag{1.128}$$

Let us assume that

$$\sum_{m=0}^{M} n(D,m) = \frac{(D+M)!}{D!M!}. \tag{1.129}$$

Then,

$$\sum_{m=0}^{M+1} n(D,m) = \frac{(D+M)!}{D!M!} + \frac{(D+M)!}{(D-1)!(M+1)!}. \tag{1.130}$$

The right hand side can be written as

$$\frac{(M+1)(D+M)! + D(D+M)!}{D!(M+1)!} = \frac{(D+M+1)!}{D!(M+1)!}. \tag{1.131}$$

Then, the assumption is proved by induction on M. Therefore,

$$N(D,M) = \frac{(D+M)!}{D!M!}. \tag{1.132}$$

(c)

By the approximation

$$n! \simeq n^n \exp(-n), \tag{1.133}$$

we have

$$\frac{(D+M)!}{D!M!} \simeq \frac{(D+M)^{D+M}}{D^D M^M}. \tag{1.134}$$

The right hand side can be written as

$$D^M \left(1 + \frac{M}{D}\right)^D \left(\frac{1}{M} + \frac{1}{D}\right)^M = M^D \left(1 + \frac{D}{M}\right)^M \left(\frac{1}{D} + \frac{1}{M}\right)^D. \tag{1.135}$$

Therefore,

$$N(D,M) \simeq \begin{cases} D^M, & D \gg M, \\ M^D, & M \gg D. \end{cases} \tag{1.136}$$

(d)

By (b),

$$\begin{aligned} N(10,3) &= 286, \\ N(100,3) &= 176851, \\ N(1000,3) &= 167668501. \end{aligned} \tag{1.137}$$

1.17

Let

$$\Gamma(x) = \int_0^\infty u^{x-1} \exp(-u) du. \tag{1.138}$$

(a)

We have

$$\Gamma(x+1) = \int_0^\infty u^x \exp(-u) du. \tag{1.139}$$

The right hand side can be written as

$$[-u^x \exp(-u)]_{u=0}^{u=\infty} + \int_0^\infty x u^{x-1} \exp(-u) du = x\Gamma(x). \tag{1.140}$$

Therefore,

$$\Gamma(x+1) = x\Gamma(x). \tag{1.141}$$

(b)

We have

$$\Gamma(1) = \int_0^\infty \exp(-u) du, \tag{1.142}$$

so that

$$\Gamma(1) = 0!. \tag{1.143}$$

For a positive integer x, let us assume that

$$\Gamma(x) = (x-1)!. \tag{1.144}$$

By (a),

$$\Gamma(x+1) = x\Gamma(x), \tag{1.145}$$

so that

$$\Gamma(x+1) = x!. \tag{1.146}$$

Therefore, the assumption is proved by induction on x.

1.18

(a)

Let

$$\prod_{d=1}^{D} \int_{-\infty}^{\infty} \exp\left(-x_d^2\right) dx_i = S_D \int_0^\infty \exp\left(-r^2\right) r^{D-1} dr, \tag{1.147}$$

where S_D is the surface area of a sphere of unit raidus in D dimensions. By 1.7, the left hand side can be written as $\pi^{\frac{D}{2}}$. By the transformation

$$s = r^2, \tag{1.148}$$

the right hand side can be written as

$$\frac{S_D}{2}\int_0^\infty \exp(-s)s^{\frac{D-1}{2}}s^{-\frac{1}{2}}ds = \frac{S_D}{2}\Gamma\left(\frac{D}{2}\right). \tag{1.149}$$

Therefore,

$$S_D = \frac{2\pi^{\frac{D}{2}}}{\Gamma\left(\frac{D}{2}\right)}. \tag{1.150}$$

(b)

The volume of the sphere can can be written as

$$V_D = S_D\int_0^1 r^{D-1}dr. \tag{1.151}$$

Therefore,

$$V_D = \frac{S_D}{D}. \tag{1.152}$$

(c)

By (a) and (b),

$$\begin{aligned} S_2 &= 2\pi, \\ V_2 &= \pi. \end{aligned} \tag{1.153}$$

Similarly,

$$\begin{aligned} S_3 &= 4\pi, \\ V_3 &= \frac{4}{3}\pi. \end{aligned} \tag{1.154}$$

1.19

(a)

The volume of a cube of side 2 in D dimensions is 2^D. By 1.18, the ratio of the volume of the cocentric sphere of radius 1 divided by the volume of the

cube is given by

$$\frac{V_D}{2^D} = \frac{\pi^{\frac{D}{2}}}{D2^{D-1}\Gamma\left(\frac{D}{2}\right)}. \tag{1.155}$$

(b)

By (a) and the Stering's formula

$$\Gamma(x+1) \simeq (2\pi)^{\frac{1}{2}} \exp(-x) x^{\frac{x+1}{2}}, \tag{1.156}$$

we have

$$\frac{V_D}{2^D} \simeq \frac{\pi^{\frac{D}{2}}}{D2^{D-1}(2\pi)^{\frac{1}{2}} \exp\left(1-\frac{D}{2}\right)\left(\frac{D}{2}-1\right)^{\frac{D}{4}}}. \tag{1.157}$$

The right hand side can be written as

$$\frac{1}{2e(2\pi)^{\frac{1}{2}}} \frac{1}{D} \left(\frac{e^2\pi^2}{8D-16}\right)^{\frac{D}{4}}. \tag{1.158}$$

Therefore,

$$\lim_{D\to\infty} \frac{V_D}{2^D} = 0. \tag{1.159}$$

(c)

The ratio of the distance from the center of the cube to one of the corners divided by the perpendicular distance to one of the sides is given by

$$\frac{\sqrt{\sum_{i=1}^{D} 1^2}}{1} = \sqrt{D}. \tag{1.160}$$

Therefore, the ratio goes to ∞ as $D \to \infty$.

1.20

Let $\mathbf{x}$ be a variable in D dimensions such that

$$p(\mathbf{x}) = (2\pi\sigma^2)^{-\frac{D}{2}} \exp\left(-\frac{\|\mathbf{x}\|^2}{2\sigma^2}\right). \tag{1.161}$$

(a)

We have

$$\int_{r\leq\|\mathbf{x}\|\leq r+\epsilon} p(\mathbf{x})d\mathbf{x} = \int_{r}^{r+\epsilon}\int (2\pi\sigma^2)^{-\frac{D}{2}} \exp\left(-\frac{r'^2}{2\sigma^2}\right) Jdr'd\boldsymbol{\phi}, \tag{1.162}$$

where $\boldsymbol{\phi}$ is the vector of the angular components of the polar corrdinate and J is the Jacobian of the transformation from the Cartesian to polar coordinate. For a sufficiently small ϵ, the right hand side can be approximated as

$$\begin{aligned} &(2\pi\sigma^2)^{-\frac{D}{2}} \exp\left(-\frac{r^2}{2\sigma^2}\right) \int_{r}^{r+\epsilon}\int Jdr'd\boldsymbol{\phi} \\ =&(2\pi\sigma^2)^{-\frac{D}{2}} \exp\left(-\frac{r^2}{2\sigma^2}\right) \int_{r\leq\|\mathbf{x}\|\leq r+\epsilon} d\mathbf{x}. \end{aligned} \tag{1.163}$$

Therefore,

$$\int_{r\leq\|\mathbf{x}\|\leq r+\epsilon} p(\mathbf{x})d\mathbf{x} \simeq p(r)\epsilon, \tag{1.164}$$

where

$$p(r) = (2\pi\sigma^2)^{-\frac{D}{2}} S_D r^{D-1} \exp\left(-\frac{r^2}{2\sigma^2}\right), \tag{1.165}$$

and S_D is the surface area of a unit sphere in D dimensions.

(b)

Setting the derivative of $p(r)$ to zero gives

$$0 = (2\pi\sigma^2)^{-\frac{D}{2}} S_D \left((D-1)r^{D-2} - \frac{r^D}{\sigma^2}\right) \exp\left(-\frac{r^2}{2\sigma^2}\right). \tag{1.166}$$

Therefore, $p(r)$ is maximised at a sigle stationary point

$$\hat{r} = \sqrt{D-1}\sigma. \tag{1.167}$$

(c)

We have

$$\frac{p\left(\hat{r}+\epsilon\right)}{p(\hat{r})} = \left(\frac{\hat{r}+\epsilon}{\hat{r}}\right)^{D-1} \exp\left(-\frac{2\hat{r}\epsilon+\epsilon^2}{2\sigma^2}\right). \tag{1.168}$$

By (b), the right hand side can be written as

$$\begin{aligned} &\exp\left((D-1)\ln\left(1+\frac{\epsilon}{\hat{r}}\right)-\frac{2\hat{r}\epsilon+\epsilon^2}{2\sigma^2}\right) \\ =&\exp\left(\frac{\hat{r}^2}{\sigma^2}\ln\left(1+\frac{\epsilon}{\hat{r}}\right)-\frac{2\hat{r}\epsilon+\epsilon^2}{2\sigma^2}\right). \end{aligned} \tag{1.169}$$

By the Taylor series

$$\ln(1+x)=x-\frac{1}{2}x^2+o\left(x^3\right), \tag{1.170}$$

the right hand side can be approximated as

$$\exp\left(\frac{\hat{r}^2}{\sigma^2}\left(\frac{\epsilon}{\hat{r}}-\frac{\epsilon^2}{2\hat{r}^2}\right)-\frac{2\hat{r}\epsilon+\epsilon^2}{2\sigma^2}\right)=\exp\left(-\frac{\epsilon^2}{\sigma^2}\right). \tag{1.171}$$

Therefore,

$$p\left(\hat{r}+\epsilon\right)\simeq p\left(\hat{r}\right)\exp\left(-\frac{\epsilon^2}{\sigma^2}\right). \tag{1.172}$$

(d)

Let $\hat{\mathbf{r}}$ be a vector of length $\hat{r}$. We have

$$\frac{p(\mathbf{0})}{p\left(\hat{\mathbf{r}}\right)}=\exp\left(\frac{\hat{r}^2}{2\sigma^2}\right). \tag{1.173}$$

By (b), the right hand side can be written as

$$\exp\left(\frac{D-1}{2}\right). \tag{1.174}$$

Therefore,

$$\frac{p(\mathbf{0})}{p\left(\hat{\mathbf{r}}\right)}=\exp\left(\frac{D-1}{2}\right). \tag{1.175}$$

1.21

(a)

If $0\leq a\leq b$, then

$$0\leq a(b-a). \tag{1.176}$$

Therefore,

$$a\leq(ab)^{\frac{1}{2}}. \tag{1.177}$$

(b)

For a two-class classification problem of $\mathbf{x}$, let the classes be $\mathcal{C}_1$ and $\mathcal{C}_2$ and let the decision regions be $\mathcal{R}_1$ and $\mathcal{R}_2$. Let us choose the decision regions to minimise the probability of misclassification. Then,

$$\begin{aligned} p(\mathbf{x}, \mathcal{C}_1) > p(\mathbf{x}, \mathcal{C}_2) \Rightarrow \mathbf{x} \in \mathcal{C}_1, \\ p(\mathbf{x}, \mathcal{C}_2) > p(\mathbf{x}, \mathcal{C}_1) \Rightarrow \mathbf{x} \in \mathcal{C}_2. \end{aligned} \tag{1.178}$$

By (a),

$$\begin{aligned} \int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2) d\mathbf{x} \leq \int_{\mathcal{R}_1} (p(\mathbf{x}, \mathcal{C}_1) p(\mathbf{x}, \mathcal{C}_2))^{\frac{1}{2}} \, d\mathbf{x}, \\ \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1) d\mathbf{x} \leq \int_{\mathcal{R}_2} (p(\mathbf{x}, \mathcal{C}_1) p(\mathbf{x}, \mathcal{C}_2))^{\frac{1}{2}} \, d\mathbf{x}. \end{aligned} \tag{1.179}$$

Therefore,

$$\int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2) d\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1) d\mathbf{x} \leq \int (p(\mathbf{x}, \mathcal{C}_1) p(\mathbf{x}, \mathcal{C}_2))^{\frac{1}{2}} \, d\mathbf{x}. \tag{1.180}$$

1.22

Let

$$\mathrm{E}\, L = \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(\mathbf{x}, \mathcal{C}_k) d\mathbf{x}. \tag{1.181}$$

If

$$L_{kj} = 1 - I_{kj}, \tag{1.182}$$

then the right hand side can be written as

$$\sum_k \sum_j \int_{\mathcal{R}_j} (p(\mathbf{x}, \mathcal{C}_k) - p(\mathbf{x}, \mathcal{C}_j)) \, d\mathbf{x} = \sum_j \int_{\mathcal{R}_j} \left(\sum_k p(\mathbf{x}, \mathcal{C}_k) - p(\mathbf{x}, \mathcal{C}_j) \right) d\mathbf{x}. \tag{1.183}$$

The right hand side can be written as

$$\sum_j \int_{\mathcal{R}_j} (p(\mathbf{x}) - p(\mathbf{x}, \mathcal{C}_j)) \, d\mathbf{x} = 1 - \sum_j \int_{\mathcal{R}_j} p(\mathbf{x}, \mathcal{C}_j) d\mathbf{x}. \tag{1.184}$$

Then,

$$\mathrm{E}\, L = 1 - \sum_j \int_{\mathcal{R}_j} p(\mathcal{C}_j | \mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \tag{1.185}$$

Therefore, minimising $\mathrm{E}\,L$ reduces to choosing the criterion to maximise the posterior probatility $p(\mathcal{C}_j|\mathbf{x})$.

1.23

Let

$$\mathrm{E}\,L = \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(\mathbf{x}, \mathcal{C}_k) d\mathbf{x}. \tag{1.186}$$

The right hand side can be written as

$$\sum_j \int_{\mathcal{R}_j} \sum_k L_{kj} p(\mathbf{x}, \mathcal{C}_k) d\mathbf{x} = \sum_j \int_{\mathcal{R}_j} \left(\sum_k L_{kj} p(\mathcal{C}_k|\mathbf{x}) \right) p(\mathbf{x}) d\mathbf{x}. \tag{1.187}$$

Then,

$$\mathrm{E}\,L = \sum_j \int_{\mathcal{R}_j} \left(\sum_k L_{kj} p(\mathcal{C}_k|\mathbf{x}) \right) p(\mathbf{x}) d\mathbf{x}. \tag{1.188}$$

Therefore, minimising $\mathrm{E}\,L$ reduces to minimising $\sum_k L_{kj} p(\mathcal{C}_k|\mathbf{x})$.

1.24 (Incomplete)

Let

$$\mathrm{E}\,L = \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(\mathbf{x}, \mathcal{C}_k) d\mathbf{x} + \lambda \int_{\forall k p(\mathcal{C}_k|\mathbf{x}) < \theta} p(\mathbf{x}) d\mathbf{x}. \tag{1.189}$$

1.25

Let

$$\mathrm{E}\,L(\mathbf{t}, \mathbf{y}(\mathbf{x})) = \iint \|\mathbf{y}(\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}. \tag{1.190}$$

Setting the derivative with respect to $\mathbf{y}(\mathbf{x})$ to zero gives

$$\mathbf{0} = 2 \int (\mathbf{y}(\mathbf{x}) - \mathbf{t})\, p(\mathbf{x}, \mathbf{t}) d\mathbf{t}. \tag{1.191}$$

The integral of the right hand side can be written as

$$\mathbf{y}(\mathbf{x}) \int p(\mathbf{x}, \mathbf{t}) d\mathbf{t} - \int \mathbf{t} p(\mathbf{x}, \mathbf{t}) d\mathbf{t} = \mathbf{y}(\mathbf{x}) p(\mathbf{x}) - p(\mathbf{x}) \int \mathbf{t} p(\mathbf{t}|\mathbf{x}) d\mathbf{t}. \tag{1.192}$$

The integral in the second term of the right hand side can be written as $\mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})$. Then, the right hand side can be written as

$$\mathbf{0} = p(\mathbf{x}) \left(\mathbf{y}(\mathbf{x}) - \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) \right). \tag{1.193}$$

Therefore,

$$\underset{\mathbf{y}(\mathbf{x})}{\operatorname{argmin}} \, \mathrm{E}\, L(\mathbf{t}, \mathbf{y}(\mathbf{x})) = \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}). \tag{1.194}$$

For a single target variable t, it reduces to

$$\underset{\mathbf{y}(\mathbf{x})}{\operatorname{argmin}} \, \mathrm{E}\, L(t, \mathbf{y}(\mathbf{x})) = \mathrm{E}_{t}(t|\mathbf{x}). \tag{1.195}$$

1.26

Let

$$\mathrm{E}\, L(\mathbf{t}, \mathbf{y}(\mathbf{x})) = \iint \|\mathbf{y}(\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}. \tag{1.196}$$

The right hand side can be written as

$$\begin{aligned} & \iint \|\mathbf{y}(\mathbf{x}) - \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) + \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t} \\ = & \iint \|\mathbf{y}(\mathbf{x}) - \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t} \\ & + 2 \iint \left(\mathbf{y}(\mathbf{x}) - \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\right)^{\mathsf{T}} \left(\mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}\right) p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t} \\ & + \iint \|\mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}. \end{aligned} \tag{1.197}$$

Let us look at each term of the right hand side. The first term can be written as

$$\int \|\mathbf{y}(\mathbf{x}) - \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\|^2 \left(\int p(\mathbf{x}, \mathbf{t}) d\mathbf{t} \right) d\mathbf{x} = \int \|\mathbf{y}(\mathbf{x}) - \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\|^2 p(\mathbf{x}) d\mathbf{x}. \tag{1.198}$$

The integral of the second term can be written as

$$\int \left(\mathbf{y}(\mathbf{x}) - \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\right)^{\mathsf{T}} \left(\int \left(\mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}\right) p(\mathbf{t}|\mathbf{x}) d\mathbf{t} \right) p(\mathbf{x}) d\mathbf{x}. \tag{1.199}$$

Since

$$\int \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})p(\mathbf{t}|\mathbf{x})d\mathbf{t} = \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\frac{\int p(\mathbf{x},\mathbf{t})d\mathbf{t}}{p(\mathbf{x})}, \qquad \int \mathbf{t}p(\mathbf{t}|\mathbf{x})d\mathbf{t} = \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}), \tag{1.200}$$

the second term is zero. The third term can be written as

$$\int \left(\int \|\mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{t}|\mathbf{x})d\mathbf{t} \right) p(\mathbf{x})d\mathbf{x} = \int \mathrm{var}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})p(\mathbf{x})d\mathbf{x}. \tag{1.201}$$

Then,

$$\mathrm{E}\, L(\mathbf{t}, \mathbf{y}(\mathbf{x})) = \int \|\mathbf{y}(\mathbf{x}) - \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\|^2 p(\mathbf{x})d\mathbf{x} + \int \mathrm{var}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})p(\mathbf{x})d\mathbf{x}. \tag{1.202}$$

Therefore,

$$\underset{\mathbf{y}(\mathbf{x})}{\mathrm{argmin}}\, \mathrm{E}\, L(\mathbf{t}, \mathbf{y}(\mathbf{x})) = \mathrm{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}). \tag{1.203}$$

1.27 (Incomplete)

(a)

Let

$$\mathrm{E}\, L_q = \int \int |y(\mathbf{x}) - t|^q p(\mathbf{x}, t)d\mathbf{x}dt. \tag{1.204}$$

Setting the derivative with respect to $y(\mathbf{x})$ to zero gives

$$0 = qp(\mathbf{x}) \int |y(\mathbf{x}) - t|^{q-1} \,\mathrm{sign}(y(\mathbf{x}) - t)p(t|\mathbf{x})dt. \tag{1.205}$$

Therefore,

$$\underset{y(\mathbf{x})}{\mathrm{argmin}}\, \mathrm{E}\, L_q = \left\{ y(\mathbf{x}) \mid \int |y(\mathbf{x}) - t|^{q-1} \,\mathrm{sign}(y(\mathbf{x}) - t)p(t|\mathbf{x})dt = 0 \right\}. \tag{1.206}$$

(b)

We have

$$\mathrm{E}\, L_1 = \int \left(\int \mathrm{sign}(y(\mathbf{x}) - t) p(t|\mathbf{x}) dt \right) p(\mathbf{x}) d\mathbf{x}. \tag{1.207}$$

The integral of the right hand side with respect to t can be written as

$$\int_{y(\mathbf{x})}^{\infty} p(t|\mathbf{x}) dt - \int_{-\infty}^{y(\mathbf{x})} p(t|\mathbf{x}) dt. \tag{1.208}$$

Therefore,

$$\underset{y(\mathbf{x})}{\mathrm{argmin}}\, \mathrm{E}\, L_1 = \mathrm{median}(t|\mathbf{x}). \tag{1.209}$$

(c)

We have

$$\lim_{q \to 0} \left(\underset{y(\mathbf{x})}{\mathrm{argmin}}\, \mathrm{E}\, L_q \right) = \mathrm{mode}(t|\mathbf{x})? \tag{1.210}$$

1.28

(a)

Let us assume that

$$p(x, y) = p(x)p(y) \Rightarrow h(x, y) = h(x) + h(y). \tag{1.211}$$

Then,

$$h\left(p^2\right) = 2h(p). \tag{1.212}$$

Let us assume that, for a positive integer n,

$$h\left(p^n\right) = nh(p). \tag{1.213}$$

Then, by the first assumption,

$$h\left(p^{n+1}\right) = h\left(p^n\right) + h(p), \tag{1.214}$$

so that

$$h\left(p^{n+1}\right) = (n+1)h(p). \tag{1.215}$$

Therefore, the second assumption is proved by induction on n.

(b)

For positive integers m and n,

$$h\left(p^n\right) = h\left(p^{\frac{n}{m}m}\right). \tag{1.216}$$

By the second assumption in (a), the left hand side can be written as $nh(p)$. By the first assumption in (a), the right hand side can be written as $mh\left(p^{\frac{n}{m}}\right)$. Therefore,

$$h\left(p^{\frac{n}{m}}\right) = \frac{n}{m}h(p). \tag{1.217}$$

(c)

By the continuity, for a positive real number a,

$$h\left(p^a\right) = ah(p). \tag{1.218}$$

Taking the derivative with respect to a and substituting $a = 1$ gives

$$(p \ln p)h'(p) = h(p). \tag{1.219}$$

Then,

$$\int \frac{h'(p)}{h(p)}dp = \int \frac{1}{p \ln p}dp + \text{const}. \tag{1.220}$$

Ignorting the constants, the left hand side can be written as $\ln h(p)$ and the right hand side can be written as $\ln(\ln p)$. Therefore,

$$h(p) \propto \ln p. \tag{1.221}$$

1.29

Let x be an M-state discrete random variable. Then, the entropy is given by

$$\mathrm{H}(x) = -\sum_{m=1}^{M} p(x_m) \ln p(x_m), \tag{1.222}$$

where

$$\sum_{m=1}^{M} p(x_m) = 1. \tag{1.223}$$

By the Jensen's inequality,

$$\sum_{m=1}^{M} p(x_i) \ln \frac{1}{p(x_m)} \leq \ln \left(\sum_{m=1}^{M} 1 \right). \tag{1.224}$$

Therefore,

$$\mathrm{H}(x) \leq \ln M. \tag{1.225}$$

1.30

Let

$$\begin{aligned} p(x) &= \mathcal{N}\left(x|\mu, \sigma^2\right), \\ q(x) &= \mathcal{N}\left(x|m, s^2\right). \end{aligned} \tag{1.226}$$

Then, the Kullback-Leibler divergence is given by

$$\mathrm{KL}\left(p||q\right) = -\int p(x) \ln \frac{q(x)}{p(x)} dx. \tag{1.227}$$

The right hand side can be written as

$$\begin{aligned} &-\int_{-\infty}^{\infty} p(x) \ln \frac{\left(2\pi s^2\right)^{-\frac{1}{2}} \exp\left(-\frac{(x-m)^2}{2s^2}\right)}{\left(2\pi\sigma^2\right)^{-\frac{1}{2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)} dx \\ =&-\int_{-\infty}^{\infty} p(x) \left(-\frac{1}{2} \ln \frac{s^2}{\sigma^2} - \frac{(x-m)^2}{2s^2} + \frac{(x-\mu)^2}{2\sigma^2} \right) dx. \end{aligned} \tag{1.228}$$

The right hand side can be written as

$$\ln \frac{s}{\sigma} \int_{-\infty}^{\infty} p(x) dx + \frac{1}{2s^2} \int_{-\infty}^{\infty} (x-m)^2 p(x) dx - \frac{1}{2\sigma^2} \int_{-\infty}^{\infty} (x-\mu)^2 p(x) dx. \tag{1.229}$$

The integral of the second term can be written as

$$\begin{aligned} &\int_{-\infty}^{\infty} (x-\mu+\mu-m)^2 p(x) dx \\ =&\int_{-\infty}^{\infty} (x-\mu)^2 p(x) dx + 2(\mu-m) \int_{-\infty}^{\infty} (x-\mu) p(x) dx \\ &+ (\mu-m)^2 \int_{-\infty}^{\infty} p(x) dx. \end{aligned} \tag{1.230}$$

Therefore,

$$\mathrm{KL}\left(p||q\right) = \ln \frac{s}{\sigma} + \frac{\sigma^2 + (\mu-m)^2}{2s^2} - \frac{1}{2}. \tag{1.231}$$

1.31

Let $\mathbf{x}$ and $\mathbf{y}$ be two variables. We have

$$\begin{aligned} \mathrm{H}(\mathbf{x}) &= -\int p(\mathbf{x}) \ln p(\mathbf{x}) d\mathbf{x}, \\ \mathrm{H}(\mathbf{y}) &= -\int p(\mathbf{y}) \ln p(\mathbf{y}) d\mathbf{y}, \\ \mathrm{H}(\mathbf{x}, \mathbf{y}) &= -\iint p(\mathbf{x}, \mathbf{y}) \ln p(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}. \end{aligned} \tag{1.232}$$

Since

$$\begin{aligned} \mathrm{H}(\mathbf{x}) &= -\int \left(\int p(\mathbf{x}, \mathbf{y}) d\mathbf{y} \right) \ln p(\mathbf{x}) d\mathbf{x}, \\ \mathrm{H}(\mathbf{y}) &= -\int \left(\int p(\mathbf{x}, \mathbf{y}) d\mathbf{x} \right) \ln p(\mathbf{y}) d\mathbf{y}, \end{aligned} \tag{1.233}$$

we have

$$\mathrm{H}(\mathbf{x}) + \mathrm{H}(\mathbf{y}) - \mathrm{H}(\mathbf{x}, \mathbf{y}) = -\iint p(\mathbf{x}, \mathbf{y}) \ln \frac{p(\mathbf{x}) p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} d\mathbf{x} d\mathbf{y}. \tag{1.234}$$

Since

$$\iint p(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y} = 1, \tag{1.235}$$

the Jensen's inequality can be used to have

$$-\iint p(\mathbf{x}, \mathbf{y}) \ln \frac{p(\mathbf{x}) p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} d\mathbf{x} d\mathbf{y} \geq -\ln \left(\iint p(\mathbf{x}) p(\mathbf{y}) d\mathbf{x} d\mathbf{y} \right). \tag{1.236}$$

The right hand side can be written as

$$-\ln \left(\int p(\mathbf{x}) d\mathbf{x} \int p(\mathbf{y}) d\mathbf{y} \right) = 0. \tag{1.237}$$

Therefore,

$$\mathrm{H}(\mathbf{x}, \mathbf{y}) \leq \mathrm{H}(\mathbf{x}) + \mathrm{H}(\mathbf{y}). \tag{1.238}$$

1.32

Let $\mathbf{x}$ and $\mathbf{y}$ be variables such that

$$\mathbf{y} = \mathbf{A}\mathbf{x}, \tag{1.239}$$

where $\mathbf{A}$ is a nonsingular matrix. We have

$$\int p_x(\mathbf{x})d\mathbf{x} = \int p_x\left(\mathbf{A}^{-1}\mathbf{y}\right)\left|\det \mathbf{A}^{-1}\right|d\mathbf{y}. \tag{1.240}$$

Then,

$$p_y(\mathbf{y}) = p_x\left(\mathbf{A}^{-1}\mathbf{y}\right)\left|\det \mathbf{A}^{-1}\right|. \tag{1.241}$$

We have

$$\mathrm{H}(\mathbf{y}) = -\int p_y(\mathbf{y}) \ln p_y(\mathbf{y})d\mathbf{y}. \tag{1.242}$$

The right hand side can be written as

$$\begin{aligned} &-\int p_y(\mathbf{y}) \ln \left(p_x\left(\mathbf{A}^{-1}\mathbf{y}\right)\left|\det \mathbf{A}^{-1}\right|\right) d\mathbf{y} \\ =&-\int p_y(\mathbf{y}) \ln p_x\left(\mathbf{A}^{-1}\mathbf{y}\right) d\mathbf{y} + \ln\left|\det \mathbf{A}\right| \int p_y(\mathbf{y})d\mathbf{y}. \end{aligned} \tag{1.243}$$

The first term can be written as

$$-\left|\det \mathbf{A}^{-1}\right| \int p_x\left(\mathbf{A}^{-1}\mathbf{y}\right) \ln p_x\left(\mathbf{A}^{-1}\mathbf{y}\right) d\mathbf{y}. \tag{1.244}$$

By the transformation

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{y}, \tag{1.245}$$

it can be written as

$$-\int p_x(\mathbf{x}) \ln p_x(\mathbf{x})d\mathbf{x} = \mathrm{H}(\mathbf{x}). \tag{1.246}$$

Therefore,

$$\mathrm{H}(\mathbf{y}) = \mathrm{H}(\mathbf{x}) + \ln\left|\det \mathbf{A}\right|. \tag{1.247}$$

1.33

Let x and y be two discrete variables with K and L states. Then,

$$\mathrm{H}(y|x) = -\sum_{k=1}^{K}\sum_{l=1}^{L} p(x_k, y_l) \ln p(y_l|x_k). \tag{1.248}$$

If

$$\mathrm{H}(y|x) = 0, \tag{1.249}$$

then

$$0 = -\sum_{k=1}^{K} p(x_k) \sum_{l=1}^{L} p(y_l|x_k) \ln p(y_l|x_k). \tag{1.250}$$

Since

$$\begin{aligned} p(x_k) &\geq 0, \\ p(y_l|x_k) \ln p(y_l|x_k) &\leq 0, \end{aligned} \tag{1.251}$$

the equation reduces to

$$p(y_l|x_k) \ln p(y_l|x_k) = 0. \tag{1.252}$$

Then,

$$p(y_l|x_k) = \begin{cases} 1, \\ 0. \end{cases} \tag{1.253}$$

Since

$$\sum_{l=1}^{L} p(y_l|x_k) = 1, \tag{1.254}$$

we have

$$p(y_l|x_k) = \begin{cases} 1, & \text{if } K = 1, \\ 0, & \text{otherwise.} \end{cases} \tag{1.255}$$

1.34

Let x be a variable. We have

$$\mathrm{H}(x) = -\int_{-\infty}^{\infty} p(x) \ln p(x) dx. \tag{1.256}$$

In order to maximise $\mathrm{H}(x)$ with the constratints

$$\begin{aligned}\int_{-\infty}^{\infty} p(x)dx &= 1,\\ \int_{-\infty}^{\infty} xp(x)dx &= \mu,\\ \int_{-\infty}^{\infty} (x-\mu)^2 p(x)dx &= \sigma^2,\end{aligned} \tag{1.257}$$

let

$$\begin{aligned}L(p) =&\mathrm{H}(x) + \lambda_1\left(\int_{-\infty}^{\infty} p(x)dx - 1\right) + \lambda_2\left(\int_{-\infty}^{\infty} xp(x)dx - \mu\right)\\ &+ \lambda_3\left(\int_{-\infty}^{\infty} (x-\mu)^2 p(x)dx - \sigma^2\right).\end{aligned} \tag{1.258}$$

Setting the variation with respect to p to zero gives

$$0 = -\ln p - 1 + \lambda_1 + \lambda_2 x + \lambda_3 (x-\mu)^2. \tag{1.259}$$

Then,

$$p(x) = \exp\left(-1 + \lambda_1 + \lambda_2 x + \lambda_3 (x-\mu)^2\right), \tag{1.260}$$

so that

$$p(x) = c\exp\left(\lambda_3\left(x - \left(\mu - \frac{\lambda_2}{2\lambda_3}\right)\right)^2\right), \tag{1.261}$$

where

$$c = \exp\left(-1 + \lambda_1 - \frac{\lambda_2^2}{4\lambda_3}\right). \tag{1.262}$$

Substituting it to the constraints gives

$$\begin{aligned}c\int_{-\infty}^{\infty} \exp\left(\lambda_3\left(x - \left(\mu - \frac{\lambda_2}{2\lambda_3}\right)\right)^2\right) dx &= 1,\\ c\int_{-\infty}^{\infty} x\exp\left(\lambda_3\left(x - \left(\mu - \frac{\lambda_2}{2\lambda_3}\right)\right)^2\right) dx &= \mu,\\ c\int_{-\infty}^{\infty} (x-\mu)^2\exp\left(\lambda_3\left(x - \left(\mu - \frac{\lambda_2}{2\lambda_3}\right)\right)^2\right) dx &= \sigma^2.\end{aligned} \tag{1.263}$$

By the transformation

$$y = (-\lambda_3)^{\frac{1}{2}} \left(x - \left(\mu - \frac{\lambda_2}{2\lambda_3} \right) \right), \tag{1.264}$$

they can be written as

$$\begin{aligned} c \int_{-\infty}^{\infty} \exp\left(-y^2\right) (-\lambda_3)^{-\frac{1}{2}} dy &= 1, \\ c \int_{-\infty}^{\infty} \left((-\lambda_3)^{-\frac{1}{2}} y + \mu - \frac{\lambda_2}{2\lambda_3} \right) \exp\left(-y^2\right) (-\lambda_3)^{-\frac{1}{2}} dy &= \mu, \\ c \int_{-\infty}^{\infty} \left((-\lambda_3)^{-\frac{1}{2}} y - \frac{\lambda_2}{2\lambda_3} \right)^2 \exp\left(-y^2\right) (-\lambda_3)^{-\frac{1}{2}} dy &= \sigma^2. \end{aligned} \tag{1.265}$$

Since

$$\begin{aligned} \int_{-\infty}^{\infty} \exp\left(-y^2\right) dy &= \Gamma\left(\frac{1}{2}\right), \\ \int_{-\infty}^{\infty} y \exp\left(-y^2\right) dy &= 0, \\ \int_{-\infty}^{\infty} y^2 \exp\left(-y^2\right) dy &= \Gamma\left(\frac{3}{2}\right), \end{aligned} \tag{1.266}$$

they can be written as

$$\begin{aligned} c(-\lambda_3)^{-\frac{1}{2}} \Gamma\left(\frac{1}{2}\right) &= 1, \\ c\left(\mu - \frac{\lambda_2}{2\lambda_3}\right) (-\lambda_3)^{-\frac{1}{2}} \Gamma\left(\frac{1}{2}\right) &= \mu, \\ c\left((-\lambda_3)^{-\frac{3}{2}} \Gamma\left(\frac{3}{2}\right) + (-\lambda_3)^{-\frac{1}{2}} \frac{\lambda_2^2}{4\lambda_3^2} \Gamma\left(\frac{1}{2}\right) \right) &= \sigma^2. \end{aligned} \tag{1.267}$$

Then,

$$\begin{aligned} \lambda_1 &= 1 - \frac{1}{2} \ln\left(2\pi\sigma^2\right), \\ \lambda_2 &= 0, \\ \lambda_3 &= -\frac{1}{2\sigma^2}. \end{aligned} \tag{1.268}$$

Therefore,

$$p(x) = \left(2\pi\sigma^2\right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2\sigma^2} (x - \mu)^2 \right). \tag{1.269}$$

1.35

Let x be a variable such that

$$p(x) = \mathcal{N}\left(x|\mu, \sigma^2\right). \tag{1.270}$$

Then,

$$\mathrm{H}(x) = -\int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) \ln \mathcal{N}\left(x|\mu, \sigma^2\right) dx. \tag{1.271}$$

The right hand side can be written as

$$\begin{aligned} &-\int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) \left(-\frac{1}{2}\ln\left(2\pi\sigma^2\right) - \frac{1}{2\sigma^2}(x-\mu)^2\right) dx \\ =&\frac{1}{2}\ln\left(2\pi\sigma^2\right) \int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) dx + \frac{1}{2\sigma^2}\int_{-\infty}^{\infty} (x-\mu)^2 \mathcal{N}\left(x|\mu, \sigma^2\right) dx. \end{aligned} \tag{1.272}$$

Therefore,

$$\mathrm{H}(x) = \frac{1}{2}\left(1 + \ln\left(2\pi\sigma^2\right)\right). \tag{1.273}$$

1.36 (Incomplete)

Let f be a strictly convex function. Then,

$$f\left(\lambda a + (1-\lambda)b\right) \leq \lambda f(a) + (1-\lambda) f(b), \tag{1.274}$$

where $a \leq b$ and $0 \leq \lambda \leq 1$. Let

$$x = \lambda a + (1-\lambda)b. \tag{1.275}$$

Then, the inequality can be written as

$$f(x) \leq \frac{b-x}{b-a} f(a) + \frac{x-a}{b-a} f(b). \tag{1.276}$$

Let

$$g(x) = \frac{b-x}{b-a} f(a) + \frac{x-a}{b-a} f(b) - f(x). \tag{1.277}$$

Then,

$$g(x) \geq 0. \tag{1.278}$$

Additionally, for $x > a$,

$$g(x) = (x-a)\left(\frac{f(b)-f(a)}{b-a} - \frac{f(x)-f(a)}{x-a}\right). \tag{1.279}$$

By the mean value theorem, there exists c and y such that $a \leq c \leq b$, $a \leq y \leq x$ and

$$\begin{aligned} f'(c) &= \frac{f(b)-f(a)}{b-a}, \\ f'(y) &= \frac{f(x)-f(a)}{x-a}. \end{aligned} \tag{1.280}$$

Then, for $x > a$, the inequality reduces to

$$f'(y) \leq f'(c). \tag{1.281}$$

1.37

Let $\mathbf{x}$ and $\mathbf{y}$ be two variables. We have

$$\mathrm{H}(\mathbf{x},\mathbf{y}) = -\iint p(\mathbf{x},\mathbf{y}) \ln p(\mathbf{x},\mathbf{y}) d\mathbf{x} d\mathbf{y}. \tag{1.282}$$

The right hand side can be written as

$$\begin{aligned} &-\iint p(\mathbf{x},\mathbf{y}) \left(\ln p(\mathbf{y}|\mathbf{x}) + \ln p(\mathbf{x})\right) d\mathbf{x} d\mathbf{y} \\ =&-\iint p(\mathbf{x},\mathbf{y}) \ln p(\mathbf{y}|\mathbf{x}) d\mathbf{x} d\mathbf{y} - \int \left(\int p(\mathbf{x},\mathbf{y}) d\mathbf{y}\right) \ln p(\mathbf{x}) d\mathbf{x}. \end{aligned} \tag{1.283}$$

By the definition, the first and second terms of the right hand side can be written as $\mathrm{H}(\mathbf{y}|\mathbf{x})$ and $\mathrm{H}(\mathbf{x})$. Therefore,

$$\mathrm{H}(\mathbf{x},\mathbf{y}) = \mathrm{H}(\mathbf{y}|\mathbf{x}) + \mathrm{H}(\mathbf{x}). \tag{1.284}$$

1.38

Let f be a strictly convex function. Then,

$$f\left(\lambda x_1 + (1-\lambda)x_2\right) \leq \lambda f(x_1) + (1-\lambda) f(x_2), \tag{1.285}$$

where

$$0 \leq \lambda \leq 1. \tag{1.286}$$

Let us assume that

$$f\left(\sum_{m=1}^{M} \lambda_m x_m\right) \leq \sum_{m=1}^{M} \lambda_m f(x_m), \tag{1.287}$$

where

$$\begin{aligned} \sum_{m=1}^{M} \lambda_m &= 1, \\ \lambda_m &\geq 0. \end{aligned} \tag{1.288}$$

Since f is strictly convex,

$$f\left(\sum_{m=1}^{M+1} \lambda_m x_m\right) \leq \lambda_{M+1} f(x_{M+1}) + (1-\lambda_{M+1}) f\left(\sum_{m=1}^{M} \frac{\lambda_m}{1-\lambda_{M+1}} x_m\right), \tag{1.289}$$

where

$$\begin{aligned} \sum_{m=1}^{M+1} \lambda_m &= 1, \\ \lambda_m &\geq 0. \end{aligned} \tag{1.290}$$

By the assumption,

$$f\left(\sum_{m=1}^{M} \frac{\lambda_m}{1-\lambda_{M+1}} x_m\right) \leq \sum_{m=1}^{M} \frac{\lambda_m}{1-\lambda_{M+1}} f(x_m). \tag{1.291}$$

Then,

$$f\left(\sum_{m=1}^{M+1} \lambda_m x_m\right) \leq \lambda_{M+1} f(x_{M+1}) + (1-\lambda_{M+1}) \sum_{m=1}^{M} \frac{\lambda_m}{1-\lambda_{M+1}} f(x_m), \tag{1.292}$$

so that

$$f\left(\sum_{m=1}^{M+1} \lambda_m x_m\right) \leq \sum_{m=1}^{M+1} \lambda_m f(x_m). \tag{1.293}$$

Therefore, the assumption is proved by induction on M.

1.39

Let x and y be two binary variables where

$$\begin{aligned} p(x=0,y=0) &= \frac{1}{3}, \\ p(x=0,y=1) &= \frac{1}{3}, \\ p(x=1,y=0) &= 0, \\ p(x=1,y=1) &= \frac{1}{3}. \end{aligned} \tag{1.294}$$

(a)

We have

$$\mathrm{H}(x) = -\sum_{x} p(x) \ln p(x). \tag{1.295}$$

We have

$$\begin{aligned} p(x=0) &= p(x=0,y=0) + p(x=0,y=1), \\ p(x=1) &= p(x=1,y=0) + p(x=1,y=1). \end{aligned} \tag{1.296}$$

Then,

$$\begin{aligned} p(x=0) &= \frac{2}{3}, \\ p(x=1) &= \frac{1}{3}. \end{aligned} \tag{1.297}$$

Therefore,

$$\mathrm{H}(x) = \ln 3 - \frac{2}{3} \ln 2. \tag{1.298}$$

(b)

We have

$$\mathrm{H}(y) = -\sum_{y} p(y) \ln p(y). \tag{1.299}$$

We have

$$\begin{aligned} p(y=0) &= p(x=0,y=0) + p(x=1,y=0), \\ p(y=1) &= p(x=0,y=1) + p(x=1,y=1). \end{aligned} \tag{1.300}$$

Then,

$$\begin{aligned} p(y=0) &= \frac{1}{3}, \\ p(y=1) &= \frac{2}{3}. \end{aligned} \tag{1.301}$$

Therefore,

$$\mathrm{H}(y) = \ln 3 - \frac{2}{3}\ln 2. \tag{1.302}$$

(c)

We have

$$\mathrm{H}(y|x) = -\sum_{x,y} p(x,y) \ln p(y|x). \tag{1.303}$$

By the Bayes' theorem,

$$\begin{aligned} p(y=0|x=0) &= \frac{p(x=0,y=0)}{p(x=0)}, \\ p(y=0|x=1) &= \frac{p(x=1,y=0)}{p(x=1)}, \\ p(y=1|x=0) &= \frac{p(x=0,y=1)}{p(x=0)}, \\ p(y=1|x=1) &= \frac{p(x=1,y=1)}{p(x=1)}. \end{aligned} \tag{1.304}$$

Then,

$$\begin{aligned} p(y=0|x=0) &= \frac{1}{2}, \\ p(y=0|x=1) &= 0, \\ p(y=1|x=0) &= \frac{1}{2}, \\ p(y=1|x=1) &= 1. \end{aligned} \tag{1.305}$$

Therefore,

$$\mathrm{H}(y|x) = \frac{2}{3}\ln 2. \tag{1.306}$$

(d)

We have

$$\mathrm{H}(x|y) = -\sum_{x,y} p(x,y) \ln p(x|y). \tag{1.307}$$

By the Bayes' theorem,

$$\begin{aligned} p(x=0|y=0) &= \frac{p(x=0,y=0)}{p(y=0)}, \\ p(x=0|y=1) &= \frac{p(x=0,y=1)}{p(y=1)}, \\ p(x=1|y=0) &= \frac{p(x=1,y=0)}{p(y=0)}, \\ p(x=1|y=1) &= \frac{p(x=1,y=1)}{p(y=1)}. \end{aligned} \tag{1.308}$$

Then,

$$\begin{aligned} p(x=0|y=0) &= 1, \\ p(x=0|y=1) &= \frac{1}{2}, \\ p(x=1|y=0) &= 0, \\ p(x=1|y=1) &= \frac{1}{2}. \end{aligned} \tag{1.309}$$

Therefore,

$$\mathrm{H}(x|y) = \frac{2}{3} \ln 2. \tag{1.310}$$

(e)

We have

$$\mathrm{H}(x,y) = -\sum_{x,y} p(x,y) \ln p(x,y). \tag{1.311}$$

Therefore,

$$\mathrm{H}(x,y) = \ln 3. \tag{1.312}$$

(f)

We have

$$\mathrm{I}(x,y) = -\sum_{x,y} p(x,y) \ln \frac{p(x)p(y)}{p(x,y)}. \tag{1.313}$$

The right hand side can be written as

$$\mathrm{H}(x) + \mathrm{H}(y) - \mathrm{H}(x,y). \tag{1.314}$$

Therefore,

$$\mathrm{I}(x,y) = \ln 3 - \frac{4}{3} \ln 2. \tag{1.315}$$

1.40

Let $\lambda_1, \cdots, \lambda_M$ and $x_1, \cdots, x_M$ be numbers such that

$$\begin{aligned} \sum_{m=1}^{M} \lambda_m &= 1, \\ \lambda_m &\geq 0, \\ x_m &> 0. \end{aligned} \tag{1.316}$$

By the Jensen's inequality,

$$\sum_{m=1}^{M} \lambda_m \ln x_m \leq \ln \left(\sum_{m=1}^{M} \lambda_m x_m \right), \tag{1.317}$$

so that

$$\prod_{m=1}^{M} x_m^{\lambda_m} \leq \sum_{m=1}^{M} \lambda_m x_m. \tag{1.318}$$

Substituting

$$\lambda_m = \frac{1}{M} \tag{1.319}$$

to the inequality gives

$$\left(\prod_{m=1}^{M} x_m \right)^{\frac{1}{M}} \leq \frac{1}{M} \sum_{m=1}^{M} x_m. \tag{1.320}$$

1.41

Let $\mathbf{x}$ and $\mathbf{y}$ be variables.

(a)

We have

$$\mathrm{I}(\mathbf{x}, \mathbf{y}) = -\iint p(\mathbf{x}, \mathbf{y}) \ln \frac{p(\mathbf{x})p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} d\mathbf{x}d\mathbf{y}. \tag{1.321}$$

By the Bayes' theorem, the right hand side can be written as

$$\begin{aligned} &-\iint p(\mathbf{x}, \mathbf{y}) \left(\ln p(\mathbf{x}) + \ln \frac{p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} \right) d\mathbf{x}d\mathbf{y} \\ =&-\iint p(\mathbf{x}, \mathbf{y}) \left(\ln p(\mathbf{x}) - \ln p(\mathbf{x}|\mathbf{y}) \right) d\mathbf{x}d\mathbf{y}. \end{aligned} \tag{1.322}$$

The right hand side can be written as

$$-\int \left(\int p(\mathbf{x}, \mathbf{y}) d\mathbf{y} \right) \ln p(\mathbf{x}) d\mathbf{x} + \iint p(\mathbf{x}, \mathbf{y}) \ln p(\mathbf{x}|\mathbf{y}) d\mathbf{x}d\mathbf{y}. \tag{1.323}$$

Therefore,

$$\mathrm{I}(\mathbf{x}, \mathbf{y}) = \mathrm{H}(\mathbf{x}) - \mathrm{H}(\mathbf{x}|\mathbf{y}). \tag{1.324}$$

(b)

We have

$$\mathrm{I}(\mathbf{x}, \mathbf{y}) = \mathrm{I}(\mathbf{y}, \mathbf{x}). \tag{1.325}$$

By (a), the right hand side can be written as

$$\mathrm{H}(\mathbf{y}) - \mathrm{H}(\mathbf{y}|\mathbf{x}). \tag{1.326}$$

Therefore,

$$\mathrm{I}(\mathbf{x}, \mathbf{y}) = \mathrm{H}(\mathbf{y}) - \mathrm{H}(\mathbf{y}|\mathbf{x}). \tag{1.327}$$

2 Probability Distributions

2.1

Let x be a variable such that

$$\begin{aligned} x &\in \{0, 1\}, \\ p(x) &= \mu^x (1 - \mu)^{1-x}. \end{aligned} \tag{2.1}$$

(a)

We have

$$\sum_x p(x) = 1 - \mu + \mu. \tag{2.2}$$

Therefore,

$$\sum_x p(x) = 1. \tag{2.3}$$

(b)

We have

$$\begin{aligned} \mathrm{E}\, x &= \sum_x x p(x), \\ \mathrm{E}\, x^2 &= \sum_x x^2 p(x), \end{aligned} \tag{2.4}$$

Then,

$$\begin{aligned} \mathrm{E}\, x &= \mu, \\ \mathrm{E}\, x^2 &= \mu. \end{aligned} \tag{2.5}$$

We have

$$\mathrm{var}\, x = \mathrm{E}\, x^2 - (\mathrm{E}\, x)^2 . \tag{2.6}$$

Therefore,

$$\mathrm{var}\, x = \mu(1 - \mu). \tag{2.7}$$

(c)

We have

$$\mathrm{H}(x) = -\sum_x p(x) \ln p(x). \tag{2.8}$$

Therefore,

$$\mathrm{H}(x) = -\mu \ln \mu - (1-\mu)\ln(1-\mu). \tag{2.9}$$

2.2

Let x be a variable such that

$$\begin{aligned} x &\in \{-1, 1\}, \\ p(x) &= \left(\frac{1-\mu}{2}\right)^{\frac{1-x}{2}} \left(\frac{1+\mu}{2}\right)^{\frac{1+x}{2}}. \end{aligned} \tag{2.10}$$

(a)

We have

$$\sum_x p(x) = \frac{1-\mu}{2} + \frac{1+\mu}{2}. \tag{2.11}$$

Therefore,

$$\sum_x p(x) = 1. \tag{2.12}$$

(b)

We have

$$\begin{aligned} \mathrm{E}\, x &= \sum_x x p(x), \\ \mathrm{E}\, x^2 &= \sum_x x^2 p(x). \end{aligned} \tag{2.13}$$

The right hand sides can be written as

$$\begin{aligned} -\frac{1-\mu}{2} + \frac{1+\mu}{2} &= \mu, \\ \frac{1-\mu}{2} + \frac{1+\mu}{2} &= 1. \end{aligned} \tag{2.14}$$

Then,

$$\begin{aligned} \mathrm{E}\, x &= \mu, \\ \mathrm{E}\, x^2 &= 1. \end{aligned} \tag{2.15}$$

We have

$$\operatorname{var} x = \mathrm{E}\, x^2 - (\mathrm{E}\, x)^2. \tag{2.16}$$

Therefore,

$$\operatorname{var} x = 1 - \mu^2. \tag{2.17}$$

(c)

We have

$$\mathrm{H}(x) = -\sum_x p(x|\mu) \ln p(x|\mu). \tag{2.18}$$

Therefore,

$$\mathrm{H}(x) = -\frac{1-\mu}{2} \ln \frac{1-\mu}{2} - \frac{1+\mu}{2} \ln \frac{1+\mu}{2}. \tag{2.19}$$

2.3

(a)

We have

$$\begin{aligned} \binom{N}{n} &= \frac{N!}{n!(N-n)!}, \\ \binom{N}{n-1} &= \frac{N!}{(n-1)!(N-n+1)!} \end{aligned} \tag{2.20}$$

Then,

$$\binom{N}{n} + \binom{N}{n-1} = \frac{(N-n+1)N! + nN!}{n!(N-n+1)!}. \tag{2.21}$$

The right hand side can be written as

$$\frac{(N+1)!}{n!(N+1-n)!} = \binom{N+1}{n}. \tag{2.22}$$

Therefore,

$$\binom{N}{n} + \binom{N}{n-1} = \binom{N+1}{n}. \tag{2.23}$$

(b)

We have

$$1 + x = \sum_{n=0}^{1} \binom{1}{n} x^n. \tag{2.24}$$

Let us assume that

$$(1+x)^N = \sum_{n=0}^{N} \binom{N}{n} x^n. \tag{2.25}$$

Then,

$$(1+x)^{N+1} = \sum_{n=0}^{N} \binom{N}{n} x^n + \sum_{n=0}^{N} \binom{N}{n} x^{n+1}. \tag{2.26}$$

By (a), the right hand side can be written as

$$\sum_{n=0}^{N} \binom{N}{n} x^n + \sum_{n=1}^{N+1} \binom{N}{n-1} x^n = 1 + x^{N+1} + \sum_{n=1}^{N} \binom{N+1}{n} x^n. \tag{2.27}$$

Then,

$$(1+x)^{N+1} = \sum_{n=0}^{N+1} \binom{N+1}{n} x^n. \tag{2.28}$$

Therefore, the assumption is proved by induction on N.

(c)

Let n be a variable such that

$$p(n) = \binom{N}{n} \mu^n (1-\mu)^{N-n}. \tag{2.29}$$

Then,

$$\sum_{n=0}^{N} p(n) = \sum_{n=0}^{N} \binom{N}{n} \mu^n (1-\mu)^{N-n}. \tag{2.30}$$

By (b), the right hand side can be written as

$$(1-\mu)^N \sum_{n=0}^{N} \binom{N}{n} \left(\frac{\mu}{1-\mu}\right)^n = (1-\mu)^N \left(1 + \frac{\mu}{1-\mu}\right)^N. \tag{2.31}$$

Therefore,

$$\sum_{n=0}^{N} p(n) = 1. \tag{2.32}$$

2.4

Let n be a variable such that

$$p(n) = \binom{N}{n}\mu^n(1-\mu)^{N-n}. \tag{2.33}$$

(a)

We have

$$\mathrm{E}\, n = \sum_{n=0}^{N} n\binom{N}{n}\mu^n(1-\mu)^{N-n}. \tag{2.34}$$

By 2.3(c),

$$\sum_{n=0}^{N}\binom{N}{n}\mu^n(1-\mu)^{N-n} = 1. \tag{2.35}$$

Taking the derivative with respect to μ gives

$$\sum_{n=0}^{N} n\binom{N}{n}\mu^{n-1}(1-\mu)^{N-n} - \sum_{n=0}^{N}(N-n)\binom{N}{n}\mu^n(1-\mu)^{N-n-1} = 0. \tag{2.36}$$

The first term of the left hand side can be written as

$$\frac{1}{\mu}\sum_{n=0}^{N} np(n) = \frac{1}{\mu}\mathrm{E}\, n. \tag{2.37}$$

Since

$$(N-n)\binom{N}{n} = N\binom{N-1}{n}, \tag{2.38}$$

the second term can be written as

$$-N\sum_{n=0}^{N-1}\binom{N-1}{n}\mu^n(1-\mu)^{N-n-1} = -N. \tag{2.39}$$

Therefore,

$$\mathrm{E}\, n = N\mu. \tag{2.40}$$

(b)

By 2.3(c),

$$\sum_{n=0}^{N} \binom{N}{n} \mu^n (1-\mu)^{N-n} = 1. \tag{2.41}$$

Taking the second derivative with respect to μ gives

$$\begin{aligned} &\sum_{n=0}^{N} n(n-1) \binom{N}{n} \mu^{n-2} (1-\mu)^{N-n} \\ &- 2 \sum_{n=0}^{N} n(N-n) \binom{N}{n} \mu^{n-1} (1-\mu)^{N-n-1} \\ &+ \sum_{n=0}^{N} (N-n)(N-n-1) \binom{N}{n} \mu^n (1-\mu)^{N-n-2} = 0. \end{aligned} \tag{2.42}$$

The first term of the left hand side can be written as

$$\frac{1}{\mu^2} \sum_{n=0}^{N} n(n-1) p(n) = \frac{1}{\mu^2} \operatorname{E} n(n-1). \tag{2.43}$$

Since

$$\begin{aligned} n(N-n) \binom{N}{n} &= N(N-1) \binom{N-2}{n-1}, \\ (N-n)(N-n-1) \binom{N}{n} &= N(N-1) \binom{N-2}{n}, \end{aligned} \tag{2.44}$$

the second and third terms can be written as

$$\begin{aligned} -2N(N-1) \sum_{n=1}^{N-1} \binom{N-2}{n-1} \mu^{n-1} (1-\mu)^{N-n-1} &= -2N(N-1), \\ N(N-1) \sum_{n=0}^{N} \binom{N-2}{n} \mu^n (1-\mu)^{N-n-2} &= N(N-1). \end{aligned} \tag{2.45}$$

Then,

$$\operatorname{E} n(n-1) = N(N-1)\mu^2. \tag{2.46}$$

We have

$$\operatorname{var} n = \operatorname{E} n(n-1) + \operatorname{E} n - (\operatorname{E} n)^2. \tag{2.47}$$

Therefore,

$$\operatorname{var} n = N\mu(1-\mu). \tag{2.48}$$

2.5

We have

$$\Gamma(a)\Gamma(b) = \int_0^\infty x^{a-1}\exp(-x)dx \int_0^\infty y^{b-1}\exp(-y)dy. \tag{2.49}$$

By the transformation

$$t = x + y, \tag{2.50}$$

the right hand side can be written as

$$\begin{aligned} &\int_0^\infty x^{a-1}\left(\int_x^\infty (t-x)^{b-1}\exp(-t)dt\right)dx \\ =&\int_0^\infty \left(\int_0^t x^{a-1}(t-x)^{b-1}dx\right)\exp(-t)dt. \end{aligned} \tag{2.51}$$

By the transformation

$$x = t\mu, \tag{2.52}$$

the right hand side can be written as

$$\begin{aligned} &\int_0^\infty \left(\int_0^1 (t\mu)^{a-1}t^{b-1}(1-\mu)^{b-1}td\mu\right)\exp(-t)dt \\ =&\int_0^1 \mu^{a-1}(1-\mu)^{b-1}d\mu \int_0^\infty t^{a+b-1}\exp(-t)dt. \end{aligned} \tag{2.53}$$

Then,

$$\Gamma(a)\Gamma(b) = \Gamma(a+b)\int_0^1 \mu^{a-1}(1-\mu)^{b-1}d\mu. \tag{2.54}$$

Therefore,

$$\int_0^1 \mu^{a-1}(1-\mu)^{b-1}d\mu = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}. \tag{2.55}$$

2.6

Let μ be a variable such that

$$p(\mu) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\mu^{a-1}(1-\mu)^{b-1}. \tag{2.56}$$

(a)

We have

$$\begin{aligned} \mathrm{E}\,\mu &= \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \int_0^1 \mu^a (1-\mu)^{b-1} d\mu, \\ \mathrm{E}\,\mu^2 &= \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \int_0^1 \mu^{a+1} (1-\mu)^{b-1} d\mu. \end{aligned} \tag{2.57}$$

By 2.5,

$$\begin{aligned} \int_0^1 \mu^a (1-\mu)^{b-1} d\mu &= \frac{\Gamma(a+1)\Gamma(b)}{\Gamma(a+b+1)}, \\ \int_0^1 \mu^{a+1} (1-\mu)^{b-1} d\mu &= \frac{\Gamma(a+2)\Gamma(b)}{\Gamma(a+b+2)}. \end{aligned} \tag{2.58}$$

Therefore,

$$\begin{aligned} \mathrm{E}\,\mu &= \frac{a}{a+b}, \\ \mathrm{E}\,\mu^2 &= \frac{a(a+1)}{(a+b)(a+b+1)}. \end{aligned} \tag{2.59}$$

(b)

We have

$$\operatorname{var}\mu = \mathrm{E}\,\mu^2 - (\mathrm{E}\mu)^2 . \tag{2.60}$$

By (a), the right hand side can be written as

$$\frac{a(a+1)}{(a+b)(a+b+1)} - \left(\frac{a}{a+b}\right)^2 = \frac{a(a+1)(a+b) - a^2(a+b+1)}{(a+b)^2(a+b+1)}. \tag{2.61}$$

Therefore,

$$\operatorname{var}\mu = \frac{ab}{(a+b)^2(a+b+1)}. \tag{2.62}$$

(c)

Setting the derivative of p with respect to μ to zero gives

$$0 = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \mu^{a-1}(1-\mu)^{b-1} \left(\frac{a-1}{\mu} - \frac{b-1}{1-\mu}\right). \tag{2.63}$$

Therefore,

$$\operatorname{mode}\mu = \frac{a-1}{a+b-2}. \tag{2.64}$$

2.7

Let m and l be variables such that

$$\begin{aligned} p(m, l|\mu) &= \binom{m+l}{m} \mu^m (1-\mu)^l, \\ p(\mu) &= \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \mu^{a-1} (1-\mu)^{b-1}. \end{aligned} \tag{2.65}$$

By 2.6,

$$\mathrm{E}\,\mu = \frac{a}{a+b}. \tag{2.66}$$

Setting the derivative of $p(m, l|\mu)$ with respect to μ to zero gives

$$0 = \binom{m+l}{m} \mu^m (1-\mu)^l \left(\frac{m}{\mu} + \frac{l}{1-\mu} \right). \tag{2.67}$$

Then, the maximum likelihood solution for μ is given by

$$\mu_{\mathrm{ML}} = \frac{m}{m+l}. \tag{2.68}$$

By the Bayes' thereorem,

$$p(\mu|m, l)p(m, l) = p(m, l|\mu)p(\mu). \tag{2.69}$$

Then, by 2.5,

$$p(\mu|m, l) = \frac{\Gamma(m+l+a+b)}{\Gamma(m+a)\Gamma(l+b)} \mu^{m+a-1} (1-\mu)^{l+b-1}. \tag{2.70}$$

The, by 2.6,

$$\mathrm{E}(\mu|m, l) = \frac{m+a}{m+l+a+b}. \tag{2.71}$$

Therefore,

$$\mathrm{E}(\mu|m, l) = \lambda \mu_{\mathrm{ML}} + (1-\lambda)\,\mathrm{E}\,\mu, \tag{2.72}$$

where

$$\lambda = \frac{m+l}{m+l+a+b}. \tag{2.73}$$

2.8

Let x and y be variables.

(a)

By the definition,

$$\mathrm{E}\, x = \int x p(x) dx. \tag{2.74}$$

The right hand side can be written as

$$\int x \left(\int p(x, y) dy \right) dx = \int \left(\int x p(x|y) dx \right) p(y) dy. \tag{2.75}$$

Therefore,

$$\mathrm{E}\, x = \mathrm{E}_y \left(\mathrm{E}_x (x|y) \right). \tag{2.76}$$

(b)

By the definition,

$$\mathrm{var}\, x = \mathrm{E} \left(x - \mathrm{E}\, x \right)^2. \tag{2.77}$$

By (a), the right hand side can be written as

$$\mathrm{E}_y \left(\mathrm{E}_x \left((x - \mathrm{E}\, x)^2 | y \right) \right) = \mathrm{E}_y \left(\mathrm{E}_x \left((x - \mathrm{E}_x(x|y) + \mathrm{E}_x(x|y) - \mathrm{E}\, x)^2 | y \right) \right). \tag{2.78}$$

The right hand side can be written as

$$\begin{aligned} &\mathrm{E}_y \left(\mathrm{E}_x \left((x - \mathrm{E}_x(x|y))^2 | y \right) \right) \\ &+ 2\, \mathrm{E}_y \left(\left((\mathrm{E}_x(x|y) - \mathrm{E}\, x)\, \mathrm{E}_x \left(x - \mathrm{E}_x(x|y) \right) | y \right) \right) \\ &+ \mathrm{E}_y \left((\mathrm{E}_x(x|y) - \mathrm{E}\, x)^2 | y \right). \end{aligned} \tag{2.79}$$

Let us look at each term of the right hand side. By the definition, the first term can be written as $\mathrm{E}_y \left(\mathrm{var}_x(x|y) \right)$. The second term can be written as

$$2\, \mathrm{E}_y \left((\mathrm{E}_x(x|y) - \mathrm{E}\, x) \left(\mathrm{E}_x(x|y) - \mathrm{E}_x(x|y) \right) \right) = 0. \tag{2.80}$$

By (a), the third term can be written as

$$\mathrm{E}_y \left(\mathrm{E}_x(x|y) - \mathrm{E}_y \left(\mathrm{E}_x(x|y) \right) \right)^2 = \mathrm{var}_y \left(\mathrm{E}_x(x|y) \right). \tag{2.81}$$

Therefore,

$$\mathrm{var}\, x = \mathrm{E}_y \left(\mathrm{var}_x(x|y) \right) + \mathrm{var}_y \left(\mathrm{E}_x(x|y) \right). \tag{2.82}$$

2.9 (Incomplete)

For a vector $\boldsymbol{\mu}$ in 2 dimensions, by 2.5,

$$\int_{\substack{\mu_1+\mu_2=1 \\ \mu_1\geq 0,\mu_2\geq 0}} \mu_1^{\alpha_1-1}\mu_2^{\alpha_2-1}d\boldsymbol{\mu} = \frac{\Gamma(\alpha_1)\Gamma(\alpha_2)}{\Gamma(\alpha_1+\alpha_2)}.$$

For a vector $\boldsymbol{\mu}$ in M dimensions, let us assume that

$$\int_{\substack{\sum_{m=1}^{M}\mu_m=1 \\ \mu_m\geq 0}} \prod_{m=1}^{M}\mu_m^{\alpha_m-1}d\boldsymbol{\mu} = \frac{\prod_{m=1}^{M}\Gamma(\alpha_m)}{\Gamma(\sum_{m=1}^{M}\alpha_m)}.$$

Under the constraint

$$\sum_{m=1}^{M+1}\mu_m = 1, \tag{2.83}$$

we have

$$\int_0^c \prod_{m=1}^{M+1}\mu_m^{\alpha_m-1}d\mu_{M+1} = \left(\prod_{m=1}^{M-1}{\mu_m}^{\alpha_m-1}\right)\int_0^c \mu_{M+1}^{\alpha_{M+1}-1}\left(c-\mu_{M+1}\right)^{\alpha_M-1}d\mu_{M+1}, \tag{2.84}$$

where

$$c = 1-\sum_{m=1}^{M-1}\mu_m. \tag{2.85}$$

By the transformation

$$\mu'_{M+1} = \frac{\mu_{M+1}}{c}, \tag{2.86}$$

the integral of the right hand side can be written as

$$\begin{aligned}&\int_0^1 (c\mu'_{M+1})^{\alpha_{M+1}-1}\left(c(1-\mu'_{M+1})\right)^{\alpha_M-1}c d\mu'_{M+1}\\ =&c^{\alpha_M+\alpha_{M+1}-1}\int_0^1 {\mu'_{M+1}}^{\alpha_{M+1}-1}(1-\mu'_{M+1})^{\alpha_M-1}d\mu'_{M+1}.\end{aligned} \tag{2.87}$$

By 2.5, the integral of the right hand side can be written as

$$\frac{\Gamma(\alpha_M)\Gamma(\alpha_{M+1})}{\Gamma(\alpha_M+\alpha_{M+1})}. \tag{2.88}$$

Then,

$$\int_0^c \prod_{m=1}^{M+1} \mu_m^{\alpha_m - 1} d\mu_{M+1} = \left(\prod_{m=1}^{M-1} {\mu_m}^{\alpha_m - 1} \right) c^{\alpha_M + \alpha_{M+1} - 1} \frac{\Gamma(\alpha_M)\Gamma(\alpha_{M+1})}{\Gamma(\alpha_M + \alpha_{M+1})}. \quad (2.89)$$

For a vector $\boldsymbol{\mu}$ in M dimensions, by the assumption,

$$\int_{\substack{\sum_{m=1}^{M} \mu_m = 1 \\ \mu_m \geq 0}} \left(\prod_{m=1}^{M-1} {\mu_m}^{\alpha_m - 1} \right) \mu_M^{\alpha_M + \alpha_{M+1} - 1} d\boldsymbol{\mu} = \frac{\left(\prod_{m=1}^{M-1} \Gamma(\alpha_m) \right) \Gamma(\alpha_M + \alpha_{M+1})}{\Gamma(\sum_{m=1}^{M+1} \alpha_m)}.$$

Then, for a vector $\boldsymbol{\mu}$ in $M+1$ dimensions,

$$\int_{\substack{\sum_{m=1}^{M+1} \mu_m = 1 \\ \mu_m \geq 0}} \prod_{m=1}^{M+1} \mu_m^{\alpha_m - 1} d\boldsymbol{\mu} = \frac{\Gamma(\alpha_M)\Gamma(\alpha_{M+1})}{\Gamma(\alpha_M + \alpha_{M+1})} \frac{\left(\prod_{m=1}^{M-1} \Gamma(\alpha_k) \right) \Gamma(\alpha_M + \alpha_{M+1})}{\Gamma(\sum_{m=1}^{M+1} \alpha_m)} ?$$

The right hand side can be written as

$$\frac{\prod_{m=1}^{M+1} \Gamma(\alpha_m)}{\Gamma(\sum_{m=1}^{M+1} \alpha_m)}. \quad (2.90)$$

Therefore, the assumption is proved by induction on M.

2.10

Let $\boldsymbol{\mu}$ be a vector such that

$$p(\boldsymbol{\mu}) = \frac{\Gamma(\sum_{k=1}^{K} \alpha_k)}{\prod_{k=1}^{K} \Gamma(\alpha_k)} \prod_{k=1}^{K} \mu_k^{\alpha_k - 1}. \quad (2.91)$$

Then, by the definition,

$$\begin{aligned} \mathrm{E}\, \mu_k &= \int \mu_k p(\boldsymbol{\mu}) d\boldsymbol{\mu}, \\ \mathrm{E}\, \mu_k^2 &= \int \mu_k^2 p(\boldsymbol{\mu}) d\boldsymbol{\mu}, \\ \mathrm{E}\, \mu_k \mu_{k'} &= \int \mu_k \mu_{k'} p(\boldsymbol{\mu}) d\boldsymbol{\mu}. \end{aligned} \quad (2.92)$$

Let $k \neq k'$. Then, by 2.9, the right hand sides can be written as

$$\begin{aligned}
\frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \frac{\frac{\Gamma(\alpha_k+1)}{\Gamma(\alpha_k)} \prod_{k=1}^K \Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^K \alpha_k + 1)} &= \frac{\alpha_k}{\sum_{k=1}^K \alpha_k}, \\
\frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \frac{\frac{\Gamma(\alpha_k+2)}{\Gamma(\alpha_k)} \prod_{k=1}^K \Gamma(\alpha_k)}{\Gamma\left(\sum_{k=1}^K \alpha_k + 2\right)} &= \frac{\alpha_k(\alpha_k+1)}{\sum_{k=1}^K \alpha_k(\sum_{k=1}^K \alpha_k + 1)}, \\
\frac{\Gamma\left(\sum_{k=1}^K \alpha_k\right)}{\prod_{k=1}^K \Gamma(\alpha_k)} \frac{\frac{\Gamma(\alpha_k+1)\Gamma(\alpha_{k'}+1)}{\Gamma(\alpha_k)\Gamma(\alpha_{k'})} \prod_{k=1}^K \Gamma(\alpha_k)}{\Gamma\left(\sum_{k=1}^K \alpha_k + 2\right)} &= \frac{\alpha_k \alpha_{k'}}{\sum_{k=1}^K \alpha_k(\sum_{k=1}^K \alpha_k + 1)}.
\end{aligned} \tag{2.93}$$

Then,

$$\begin{aligned}
\mathrm{E}\,\mu_k &= \frac{\alpha_k}{\sum_{k=1}^K \alpha_k}. \\
\mathrm{E}\,\mu_k^2 &= \frac{\alpha_k(\alpha_k+1)}{\sum_{k=1}^K \alpha_k \left(\sum_{k=1}^K \alpha_k + 1\right)}, \\
\mathrm{E}\,\mu_k\mu_{k'} &= \frac{\alpha_k \alpha_{k'}}{\sum_{k=1}^K \alpha_k \left(\sum_{k=1}^K \alpha_k + 1\right)}.
\end{aligned} \tag{2.94}$$

Since

$$\begin{aligned}
\mathrm{var}\,\mu_k &= \mathrm{E}\,\mu_k^2 - (\mathrm{E}\,\mu_k)^2, \\
\mathrm{cov}\,(\mu_k, \mu_{k'}) &= \mathrm{E}\,\mu_k\mu_{k'} - \mathrm{E}\,\mu_k\,\mathrm{E}\,\mu_{k'},
\end{aligned} \tag{2.95}$$

we have

$$\begin{aligned}
\mathrm{var}\,\mu_k &= \frac{\alpha_k \left(\left(\sum_{k=1}^K \alpha_k\right) - \alpha_k\right)}{(\sum_{k=1}^K \alpha_k)^2(\sum_{k=1}^K \alpha_k + 1)}, \\
\mathrm{cov}(\mu_k, \mu_{k'}) &= -\frac{\alpha_k \alpha_{k'}}{(\sum_{k=1}^K \alpha_k)^2(\sum_{k=1}^K \alpha_k + 1)}.
\end{aligned} \tag{2.96}$$

2.11

Let $\boldsymbol{\mu}$ be a variable such that

$$p(\boldsymbol{\mu}) = \frac{\Gamma\left(\sum_{k=1}^K \alpha_k\right)}{\prod_{k=1}^K \Gamma(\alpha_k)} \prod_{k=1}^K \mu_k^{\alpha_k - 1}. \tag{2.97}$$

Then, by the definition,

$$\mathrm{E} \ln \mu_k = \int (\ln \mu_k)\, p(\boldsymbol{\mu}) d\boldsymbol{\mu}. \tag{2.98}$$

Since

$$\frac{\partial}{\partial \alpha_k} p(\boldsymbol{\mu}) = \left(\frac{\Gamma'\left(\sum_{k=1}^K \alpha_k\right)}{\Gamma\left(\sum_{k=1}^K \alpha_k\right)} - \frac{\Gamma'(\alpha_k)}{\Gamma(\alpha_k)} + \ln \mu_k \right) p(\boldsymbol{\mu}), \tag{2.99}$$

we have

$$\mathrm{E} \ln \mu_k = \frac{\partial}{\partial \alpha_k} \int p(\boldsymbol{\mu}) d\boldsymbol{\mu} + \left(\psi(\alpha_k) - \psi\left(\sum_{k=1}^K \alpha_k \right) \right) \int p(\boldsymbol{\mu}) d\boldsymbol{\mu}, \tag{2.100}$$

where

$$\psi(a) = \frac{d}{da} \ln \Gamma(a). \tag{2.101}$$

Therefore,

$$\mathrm{E} \ln \mu_k = \psi(\alpha_k) - \psi\left(\sum_{k=1}^K \alpha_k \right). \tag{2.102}$$

2.12

Let x be a variable such that

$$p(x) = \frac{1}{b-a}, \tag{2.103}$$

where $a < b$. Then

$$\int_a^b p(x) dx = 1. \tag{2.104}$$

Then, by the definition,

$$\begin{aligned} \mathrm{E}\, x &= \frac{1}{b-a} \int_a^b x dx, \\ \mathrm{E}\, x^2 &= \frac{1}{b-a} \int_a^b x^2 dx. \end{aligned} \tag{2.105}$$

Then,

$$\begin{aligned} \mathrm{E}\, x &= \frac{1}{2}(a+b), \\ \mathrm{E}\, x^2 &= \frac{1}{3}\left(a^2 + ab + b^2\right). \end{aligned} \tag{2.106}$$

Since

$$\mathrm{var}\, x = \mathrm{E}\, x^2 - (\mathrm{E}\, x)^2, \tag{2.107}$$

we have

$$\mathrm{var}\, x = \frac{1}{12}(b-a)^2. \tag{2.108}$$

2.13

Let $\mathbf{x}$ be a variable in D dimensions and let

$$\begin{aligned} p(\mathbf{x}) &= \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}), \\ q(\mathbf{x}) &= \mathcal{N}(\mathbf{x}|\mathbf{m}, \mathbf{L}). \end{aligned} \tag{2.109}$$

Then, by the definition, the Kulleback-Leibler divergence is given by

$$\mathrm{KL}(p||q) = -\int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) \ln \frac{\mathcal{N}(\mathbf{x}|\mathbf{m}, \mathbf{L})}{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})} d\mathbf{x}. \tag{2.110}$$

Note that

$$\ln \frac{\mathcal{N}(\mathbf{x}|\mathbf{m}, \mathbf{L})}{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})} = \ln \frac{(2\pi)^{-\frac{D}{2}} |\det \mathbf{L}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mathbf{m})^\intercal \mathbf{L}^{-1}(\mathbf{x}-\mathbf{m})\right)}{(2\pi)^{-\frac{D}{2}} |\det \boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)}. \tag{2.111}$$

The right hand side can be written as

$$\frac{1}{2} \ln \left| \frac{\det \boldsymbol{\Sigma}}{\det \mathbf{L}} \right| + \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}) - \frac{1}{2}(\mathbf{x}-\mathbf{m})^\intercal \mathbf{L}^{-1}(\mathbf{x}-\mathbf{m}). \tag{2.112}$$

Then, the integral can be written as

$$\begin{aligned} &\frac{1}{2} \ln \left| \frac{\det \boldsymbol{\Sigma}}{\det \mathbf{L}} \right| \int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x} \\ &+ \frac{1}{2} \int (\mathbf{x}-\boldsymbol{\mu})^\intercal \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x} \\ &- \frac{1}{2} \int (\mathbf{x}-\mathbf{m})^\intercal \mathbf{L}^{-1}(\mathbf{x}-\mathbf{m}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x}. \end{aligned} \tag{2.113}$$

Let us look at the integral of each term. The integral of the first term is 1. Since

$$\int (\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})d\mathbf{x} = \boldsymbol{\Sigma}, \tag{2.114}$$

we have

$$\int (\mathbf{x}-\boldsymbol{\mu})^{\intercal}(\mathbf{x}-\boldsymbol{\mu})\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})d\mathbf{x} = \operatorname{tr}\boldsymbol{\Sigma}. \tag{2.115}$$

Then, the integral of the second term can be written as

$$\operatorname{tr}\left(\boldsymbol{\Sigma}^{-1}\boldsymbol{\Sigma}\right) = D. \tag{2.116}$$

Since

$$(\mathbf{x}-\mathbf{m})^{\intercal}\mathbf{L}^{-1}(\mathbf{x}-\mathbf{m}) = (\mathbf{x}-\boldsymbol{\mu}+\boldsymbol{\mu}-\mathbf{m})^{\intercal}\mathbf{L}^{-1}(\mathbf{x}-\boldsymbol{\mu}+\boldsymbol{\mu}-\mathbf{m}), \tag{2.117}$$

the integral of the third term can be written as

$$\begin{aligned}
&\int (\mathbf{x}-\boldsymbol{\mu})^{\intercal}\mathbf{L}^{-1}(\mathbf{x}-\boldsymbol{\mu})\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})d\mathbf{x} \\
&+ 2(\boldsymbol{\mu}-\mathbf{m})^{\intercal}\mathbf{L}^{-1}\int (\mathbf{x}-\boldsymbol{\mu})\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})d\mathbf{x} \\
&+ (\boldsymbol{\mu}-\mathbf{m})^{\intercal}\mathbf{L}^{-1}(\boldsymbol{\mu}-\mathbf{m})\int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})d\mathbf{x} \\
=&\operatorname{tr}\left(\mathbf{L}^{-1}\boldsymbol{\Sigma}\right) + (\boldsymbol{\mu}-\mathbf{m})^{\intercal}\mathbf{L}^{-1}(\boldsymbol{\mu}-\mathbf{m}).
\end{aligned} \tag{2.118}$$

Therefore,

$$\mathrm{KL}(p||q) = \frac{1}{2}\left(\ln\left|\frac{\det\mathbf{L}}{\det\boldsymbol{\Sigma}}\right| - D + \operatorname{tr}\left(\mathbf{L}^{-1}\boldsymbol{\Sigma}\right) + (\boldsymbol{\mu}-\mathbf{m})^{\intercal}\mathbf{L}^{-1}(\boldsymbol{\mu}-\mathbf{m})\right). \tag{2.119}$$

2.14

Let $\mathbf{x}$ be a variable in D dimensions. By the definition, the entropy is given by

$$\mathrm{H}(\mathbf{x}) = -\int p(\mathbf{x})\ln p(\mathbf{x})d\mathbf{x}. \tag{2.120}$$

In order to maximise H(x) with the constratints

$$\begin{aligned} \int p(\mathbf{x})d\mathbf{x} &= 1, \\ \int \mathbf{x}p(\mathbf{x})d\mathbf{x} &= \boldsymbol{\mu}, \\ \int (\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\intercal p(\mathbf{x})d\mathbf{x} &= \boldsymbol{\Sigma}, \end{aligned} \tag{2.121}$$

let

$$\begin{aligned} L(p) =& \mathrm{H}(\mathbf{x}) + \lambda\left(\int p(\mathbf{x})d\mathbf{x} - 1\right) + \mathbf{l}^\intercal\left(\int \mathbf{x}p(\mathbf{x})d\mathbf{x} - \boldsymbol{\mu}\right) \\ &+ \mathbf{m}^\intercal\left(\int (\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\intercal p(\mathbf{x})d\mathbf{x} - \boldsymbol{\Sigma}\right)\mathbf{m}. \end{aligned} \tag{2.122}$$

Setting the variation with respect to p to zero gives

$$0 = -\ln p(\mathbf{x}) - 1 + \lambda + \mathbf{l}^\intercal\mathbf{x} + \mathbf{m}^\intercal(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\intercal\mathbf{m}. \tag{2.123}$$

Then,

$$p(\mathbf{x}) = \exp\left(-1 + \lambda + \mathbf{l}^\intercal\mathbf{x} + \mathbf{m}^\intercal(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\intercal\mathbf{m}\right), \tag{2.124}$$

so that

$$p(\mathbf{x}) = c\exp\left(-\left(\mathbf{x}-\boldsymbol{\mu}-\mathbf{M}\mathbf{l}\right)^\intercal\mathbf{M}^{-1}\left(\mathbf{x}-\boldsymbol{\mu}-\mathbf{M}\mathbf{l}\right)\right), \tag{2.125}$$

where

$$\begin{aligned} c &= \exp\left(-1 + \lambda - \mathbf{l}^\intercal\mathbf{M}\mathbf{l}\right), \\ \mathbf{M} &= -\left(\mathbf{m}\mathbf{m}^\intercal\right)^{-1}. \end{aligned} \tag{2.126}$$

Substituting it to the constraints and the transformation

$$\mathbf{y} = \mathbf{x} - \boldsymbol{\mu} - \mathbf{M}\mathbf{l} \tag{2.127}$$

gives

$$\begin{aligned} c\int \exp\left(-\mathbf{y}^\intercal\mathbf{M}^{-1}\mathbf{y}\right)d\mathbf{y} &= 1, \\ c\int \left(\mathbf{y}+\boldsymbol{\mu}+\mathbf{M}\mathbf{l}\right)\exp\left(-\mathbf{y}^\intercal\mathbf{M}^{-1}\mathbf{y}\right)d\mathbf{y} &= \boldsymbol{\mu}, \\ c\int \left(\mathbf{y}+\mathbf{M}\mathbf{l}\right)\left(\mathbf{y}+\mathbf{M}\mathbf{l}\right)^\intercal\exp\left(-\mathbf{y}^\intercal\mathbf{M}^{-1}\mathbf{y}\right)d\mathbf{y} &= \boldsymbol{\Sigma}. \end{aligned} \tag{2.128}$$

Since

$$\begin{aligned}\int \exp\left(-\mathbf{y}^\intercal\mathbf{y}\right) d\mathbf{y} &= \left(\Gamma\left(\frac{1}{2}\right)\right)^D,\\ \int \mathbf{y}\exp\left(-\mathbf{y}^\intercal\mathbf{y}\right) d\mathbf{y} &= \mathbf{0},\\ \int \mathbf{y}\mathbf{y}^\intercal\exp\left(-\mathbf{y}^\intercal\mathbf{y}\right) d\mathbf{y} &= \Gamma\left(\frac{3}{2}\right)\left(\Gamma\left(\frac{1}{2}\right)\right)^{D-1}\mathbf{I},\end{aligned} \tag{2.129}$$

they can be written as

$$\begin{aligned} c\left(\Gamma\left(\frac{1}{2}\right)\right)^D |\det\mathbf{M}|^{\frac{1}{2}} &= 1,\\ c(\boldsymbol{\mu}+\mathbf{M}\mathbf{l})\left(\Gamma\left(\frac{1}{2}\right)\right)^D |\det\mathbf{M}|^{\frac{1}{2}} &= \boldsymbol{\mu},\\ c\left(\Gamma\left(\frac{3}{2}\right)\left(\Gamma\left(\frac{1}{2}\right)\right)^{D-1}\mathbf{M} + \mathbf{M}\mathbf{l}(\mathbf{M}\mathbf{l})^\intercal\left(\Gamma\left(\frac{1}{2}\right)\right)^D\right)|\det\mathbf{M}|^{\frac{1}{2}} &= \boldsymbol{\Sigma}.\end{aligned} \tag{2.130}$$

Then,

$$\begin{aligned}\lambda &= 1 - \frac{D}{2}\ln\pi - \frac{1}{2}\ln|\det\mathbf{M}|,\\ \mathbf{l} &= \mathbf{0},\\ \mathbf{M} &= 2\boldsymbol{\Sigma}.\end{aligned} \tag{2.131}$$

Therefore,

$$p(\mathbf{x}) = (2\pi)^{-\frac{D}{2}}|\det\boldsymbol{\Sigma}|^{-\frac{1}{2}}\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right). \tag{2.132}$$

2.15

Let $\mathbf{x}$ be a variable in D dimensions such that

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}). \tag{2.133}$$

Then, by the definition, the entropy is given by

$$\mathrm{H}(\mathbf{x}) = -\int \mathcal{N}(\mathbf{x}|\mu,\boldsymbol{\Sigma})\ln\mathcal{N}(\mathbf{x}|\mu,\boldsymbol{\Sigma})d\mathbf{x}. \tag{2.134}$$

The right hand side can be written as

$$\begin{aligned}
&-\int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})\left(-\frac{D}{2}\ln(2\pi)-\frac{1}{2}\ln|\det\boldsymbol{\Sigma}|-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)d\mathbf{x}\\
&=\left(\frac{D}{2}\ln(2\pi)+\frac{1}{2}\ln|\det\boldsymbol{\Sigma}|\right)\int\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})d\mathbf{x}\\
&+\frac{1}{2}\int(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})d\mathbf{x}.
\end{aligned} \tag{2.135}$$

Let us look at each integral of the right hand side. The first integral is 1. Since

$$\int(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})d\mathbf{x}=\boldsymbol{\Sigma}, \tag{2.136}$$

we have

$$\int(\mathbf{x}-\boldsymbol{\mu})^{\intercal}(\mathbf{x}-\boldsymbol{\mu})\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})d\mathbf{x}=\operatorname{tr}\boldsymbol{\Sigma}. \tag{2.137}$$

Then, the second integral can be written as

$$\operatorname{tr}\left(\boldsymbol{\Sigma}^{-1}\boldsymbol{\Sigma}\right)=D. \tag{2.138}$$

Therefore,

$$\mathrm{H}(\mathbf{x})=\frac{D}{2}\left(1+\ln(2\pi)\right)+\frac{1}{2}\ln|\det\boldsymbol{\Sigma}|. \tag{2.139}$$

2.16

Let x be a variable such that

$$x=x_1+x_2, \tag{2.140}$$

where

$$\begin{aligned}
p(x_1)&=\mathcal{N}\left(x_1|\mu_1,\tau_1^{-1}\right),\\
p(x_2)&=\mathcal{N}\left(x_2|\mu_2,\tau_2^{-1}\right).
\end{aligned} \tag{2.141}$$

By marginalisation,

$$p(x)=\int_{-\infty}^{\infty}p(x|x_2)p(x_2)dx_2. \tag{2.142}$$

The right hand side can be written as

$$\begin{aligned}&\int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu_1+x_2,\tau_1^{-1}\right)\mathcal{N}\left(x_2|\mu_2,\tau_2^{-1}\right)dx_2\\&=\int_{-\infty}^{\infty}\left(\frac{\tau_1}{2\pi}\right)^{\frac{1}{2}}\exp\left(-\frac{\tau_1}{2}(x-\mu_1-x_2)^2\right)\left(\frac{\tau_2}{2\pi}\right)^{\frac{1}{2}}\exp\left(-\frac{\tau_2}{2}(x_2-\mu_2)^2\right)dx_2.\end{aligned} \tag{2.143}$$

The logarithm of the integrand except the terms independent of x and z is given by

$$\begin{aligned}&-\frac{\tau_1+\tau_2}{2}\left(x_2-\frac{\tau_1(x-\mu_1)+\tau_2\mu_2}{\tau_1+\tau_2}\right)^2-\frac{\tau_1}{2}(x-\mu_1)^2-\frac{\tau_2}{2}\mu_2^2\\&+\frac{\tau_1+\tau_2}{2}\left(\frac{\tau_1(x-\mu_1)+\tau_2\mu_2}{\tau_1+\tau_2}\right)^2\\&=-\frac{\tau_1+\tau_2}{2}\left(x_2-\frac{\tau_1(x-\mu_1)+\tau_2\mu_2}{\tau_1+\tau_2}\right)^2-\frac{\tau_1\tau_2}{2(\tau_1+\tau_2)}(x-\mu_1-\mu_2)^2.\end{aligned} \tag{2.144}$$

Then,

$$p(x)=\mathcal{N}\left(x|\mu_1+\mu_2,\tau_1^{-1}+\tau_2^{-1}\right). \tag{2.145}$$

Therefore, by 1.35,

$$\mathrm{H}(x)=\frac{1}{2}\left(1+\ln(2\pi)+\ln\left(\tau_1^{-1}+\tau_2^{-1}\right)\right). \tag{2.146}$$

2.17

Let $\mathbf{\Sigma}$ be a matrix and

$$\begin{aligned}\mathbf{S}&=\frac{1}{2}\left(\mathbf{\Sigma}^{-1}+\left(\mathbf{\Sigma}^{-1}\right)^{\intercal}\right),\\\mathbf{A}&=\frac{1}{2}\left(\mathbf{\Sigma}^{-1}-\left(\mathbf{\Sigma}^{-1}\right)^{\intercal}\right).\end{aligned} \tag{2.147}$$

Then,

$$\mathbf{\Sigma}^{-1}=\mathbf{S}+\mathbf{A}, \tag{2.148}$$

so that

$$(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})=(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\mathbf{S}(\mathbf{x}-\boldsymbol{\mu})+(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\mathbf{A}(\mathbf{x}-\boldsymbol{\mu}). \tag{2.149}$$

The second term of the right hand side can be written as

$$\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal\left(\boldsymbol{\Sigma}^{-1}\right)^\intercal(\mathbf{x}-\boldsymbol{\mu}). \tag{2.150}$$

The second term of the right hand side can be written as

$$-\frac{1}{2}\left(\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)^\intercal(\mathbf{x}-\boldsymbol{\mu})=-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}). \tag{2.151}$$

Then,

$$(\mathbf{x}-\boldsymbol{\mu})^\intercal\mathbf{A}(\mathbf{x}-\boldsymbol{\mu})=0. \tag{2.152}$$

Therefore,

$$(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})=(\mathbf{x}-\boldsymbol{\mu})^\intercal\mathbf{S}(\mathbf{x}-\boldsymbol{\mu}). \tag{2.153}$$

2.18

(a)

Let $\boldsymbol{\Sigma}$ be a $D\times D$ real symmetric matrix such that

$$\boldsymbol{\Sigma}\mathbf{u}_d=\lambda_d\mathbf{u}_d, \tag{2.154}$$

where $\mathbf{u}_1,\cdots,\mathbf{u}_D$ are unit vectors. Then,

$$\overline{\mathbf{u}_d}^\intercal\boldsymbol{\Sigma}\mathbf{u}_d=\lambda_d, \tag{2.155}$$

where $\overline{\mathbf{u}_d}$ is the conjugate of $\mathbf{u}_d$. Since $\boldsymbol{\Sigma}$ is real and symmetric, the left hand side can be written as

$$\overline{\mathbf{u}_d}^\intercal\overline{\boldsymbol{\Sigma}}^\intercal\mathbf{u}_d=\left(\overline{\boldsymbol{\Sigma}}\,\overline{\mathbf{u}_d}\right)^\intercal\mathbf{u}_d. \tag{2.156}$$

The right hand side can be writtet as

$$\overline{\lambda_d}\,\overline{\mathbf{u}_d}^\intercal\mathbf{u}_d=\overline{\lambda_d}. \tag{2.157}$$

Therefore,

$$\lambda_d=\overline{\lambda_d}. \tag{2.158}$$

(b)

For $d \neq d'$, taking the inner product with $\mathbf{u}_d'$ on both sides of

$$\mathbf{\Sigma}\mathbf{u}_d = \lambda_d \mathbf{u}_d \tag{2.159}$$

gives

$$\mathbf{u}_{d'}^\intercal \mathbf{\Sigma}\mathbf{u}_d = \lambda_d \mathbf{u}_{d'}^\intercal \mathbf{u}_d. \tag{2.160}$$

Since $\mathbf{\Sigma}$ is symmetric, the left hand side can be written as

$$\mathbf{u}_{d'}^\intercal \mathbf{\Sigma}^\intercal \mathbf{u}_d = (\mathbf{\Sigma}\mathbf{u}_{d'})^\intercal \mathbf{u}_d. \tag{2.161}$$

The right hand side can be written as $\lambda_{d'}\mathbf{u}_{d'}^\intercal \mathbf{u}_d$. Then,

$$\lambda_d \mathbf{u}_{d'}^\intercal \mathbf{u}_d = \lambda_{d'} \mathbf{u}_{d'}^\intercal \mathbf{u}_d. \tag{2.162}$$

Therefore, if $\lambda_d \neq \lambda_{d'}$, then

$$\mathbf{u}_{d'}^\intercal \mathbf{u}_d = 0. \tag{2.163}$$

2.19

Let $\mathbf{\Sigma}$ be a $D \times D$ real symmetric matrix such that

$$\mathbf{\Sigma}\mathbf{u}_d = \lambda_d \mathbf{u}_d, \tag{2.164}$$

where $\mathbf{u}_1, \cdots, \mathbf{u}_D$ are unit vectors. Let

$$\begin{aligned} \mathbf{\Lambda} &= \mathrm{diag}(\lambda_1, \cdots, \lambda_D), \\ \mathbf{U} &= [\mathbf{u}_1 \cdots \mathbf{u}_D]. \end{aligned} \tag{2.165}$$

Then

$$\mathbf{\Sigma}\mathbf{U} = \mathbf{U}\mathbf{\Lambda}. \tag{2.166}$$

By 2.18,

$$\mathbf{U}^\intercal \mathbf{U} = \mathbf{I}. \tag{2.167}$$

Then,

$$\begin{aligned} \mathbf{\Sigma} &= \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\intercal, \\ \mathbf{\Sigma}^{-1} &= \mathbf{U}\mathbf{\Lambda}^{-1}\mathbf{U}^\intercal, \end{aligned} \tag{2.168}$$

Therefore,

$$\begin{aligned} \mathbf{\Sigma} &= \sum_{d=1}^{D} \lambda_d \mathbf{u}_d \mathbf{u}_d^\intercal, \\ \mathbf{\Sigma}^{-1} &= \sum_{d=1}^{D} \frac{1}{\lambda_d} \mathbf{u}_d \mathbf{u}_d^\intercal. \end{aligned} \tag{2.169}$$

2.20

Let $\mathbf{\Sigma}$ be a $D \times D$ real symmetric matrix such that

$$\mathbf{\Sigma}\mathbf{u}_d = \lambda_d \mathbf{u}_d, \tag{2.170}$$

where $u_1, \cdots, u_D$ are unit vectors. Let

$$\begin{aligned} \mathbf{\Lambda} &= \mathrm{diag}(\lambda_1, \cdots, \lambda_D), \\ \mathbf{U} &= [\mathbf{u}_1 \cdots \mathbf{u}_D]. \end{aligned} \tag{2.171}$$

By 2.19,

$$\mathbf{a}^\intercal \mathbf{\Sigma} \mathbf{a} = \mathbf{b}^\intercal \mathbf{\Lambda} \mathbf{b}, \tag{2.172}$$

where

$$\mathbf{b} = \mathbf{U}^\intercal \mathbf{a}. \tag{2.173}$$

The right hand side can be written as $\sum_{d=1}^{D} \lambda_d b_d^2$. Therefore, the necessary and sufficient condition for

$$\mathbf{a}^\intercal \mathbf{\Sigma} \mathbf{a} > 0 \tag{2.174}$$

for any real vector $\mathbf{a}$ is

$$\lambda_d > 0. \tag{2.175}$$

2.21

Let $\mathbf{\Sigma}$ be a $D \times D$ real symmetric matrix. Then the number of independent parameters is $\frac{D(D+1)}{2}$.

2.22

Let $\mathbf{\Sigma}$ be a $D \times D$ symmetric matrix and

$$\mathbf{\Sigma}\mathbf{\Lambda} = \mathbf{I}. \tag{2.176}$$

Taking the transpose of the both sides gives

$$\mathbf{\Lambda}^\intercal \mathbf{\Sigma} = \mathbf{I}. \tag{2.177}$$

Therefore,

$$\mathbf{\Lambda}^\intercal = \mathbf{\Lambda}. \tag{2.178}$$

2.23

Let $\mathbf{\Sigma}$ be a $D \times D$ real symmetric matrix such that

$$\mathbf{\Sigma}\mathbf{u}_d = \lambda_d \mathbf{u}_d, \tag{2.179}$$

where $u_1, \cdots, u_D$ are unit vectors. Let

$$\begin{aligned} \mathbf{\Lambda}' &= \mathrm{diag}\left(\lambda_1^{-\frac{1}{2}}, \cdots, \lambda_D^{-\frac{1}{2}}\right), \\ \mathbf{U} &= [\mathbf{u}_1 \cdots \mathbf{u}_D]. \end{aligned} \tag{2.180}$$

By 2.19,

$$\int_{(\mathbf{x}-\boldsymbol{\mu})^\intercal \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})=\Delta} d\mathbf{x} = \int_{(\mathbf{x}-\boldsymbol{\mu})^\intercal \mathbf{U}\mathbf{\Lambda}'\mathbf{\Lambda}'^\intercal \mathbf{U}^\intercal(\mathbf{x}-\boldsymbol{\mu})=\Delta} d\mathbf{x}. \tag{2.181}$$

By the transformation

$$\mathbf{y} = \mathbf{\Lambda}'^\intercal \mathbf{U}^\intercal(\mathbf{x} - \boldsymbol{\mu}) \tag{2.182}$$

and the property

$$\mathbf{U}^\intercal \mathbf{U} = \mathbf{I}, \tag{2.183}$$

the right hand side can be written as

$$\int_{\|\mathbf{y}\|^2=\Delta} \left|\det\left(\mathbf{U}\mathbf{\Lambda}'^{-1}\right)\right| d\mathbf{y} = |\det \mathbf{\Sigma}|^{\frac{1}{2}} \int_{\|\mathbf{y}\|^2=\Delta} d\mathbf{y}. \tag{2.184}$$

Therefore,

$$\int_{(\mathbf{x}-\boldsymbol{\mu})^\intercal \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})=\Delta} d\mathbf{x} = |\det \mathbf{\Sigma}|^{\frac{1}{2}} \Delta^D V_D, \tag{2.185}$$

where

$$V_D = \int_{\|\mathbf{x}\|=1} d\mathbf{x}. \tag{2.186}$$

2.24

Let $\mathbf{A}$ be a square matrix and $\mathbf{D}$ be an invertible matrix. We have

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{B}\mathbf{D}^{-1} \\ \mathbf{O} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C} & \mathbf{O} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}. \tag{2.187}$$

The right hand side can be written as

$$\begin{bmatrix} \mathbf{I} & \mathbf{B}\mathbf{D}^{-1} \\ \mathbf{O} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C} & \mathbf{O} \\ \mathbf{O} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{O} \\ \mathbf{D}^{-1}\mathbf{C} & \mathbf{I} \end{bmatrix}. \tag{2.188}$$

Then,

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{I} & \mathbf{O} \\ -\mathbf{D}^{-1}\mathbf{C} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{M} & \mathbf{O} \\ \mathbf{O} & \mathbf{D}^{-1} \end{bmatrix} \begin{bmatrix} \mathbf{I} & -\mathbf{B}\mathbf{D}^{-1} \\ \mathbf{O} & \mathbf{I} \end{bmatrix}, \tag{2.189}$$

where

$$\mathbf{M} = \left(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}\right)^{-1}. \tag{2.190}$$

Therefore,

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{M} & -\mathbf{B}\mathbf{D}^{-1}\mathbf{M} \\ -\mathbf{D}^{-1}\mathbf{C}\mathbf{M} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{C}\mathbf{M}\mathbf{B}\mathbf{D}^{-1} \end{bmatrix}. \tag{2.191}$$

2.25

Let $\mathbf{x}$ be a variable such that

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}), \tag{2.192}$$

where

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \\ \mathbf{x}_c \end{bmatrix}, \boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \\ \boldsymbol{\mu}_c \end{bmatrix}, \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} & \boldsymbol{\Sigma}_{ac} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} & \boldsymbol{\Sigma}_{bc} \\ \boldsymbol{\Sigma}_{ca} & \boldsymbol{\Sigma}_{cb} & \boldsymbol{\Sigma}_{cc} \end{bmatrix}.$$

Let

$$\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}, \tag{2.193}$$

where

$$\boldsymbol{\Lambda} = \begin{bmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} & \boldsymbol{\Lambda}_{ac} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} & \boldsymbol{\Lambda}_{bc} \\ \boldsymbol{\Lambda}_{ca} & \boldsymbol{\Lambda}_{cb} & \boldsymbol{\Lambda}_{cc} \end{bmatrix}.$$

Then, the logarithm of $p(\mathbf{x})$ except the terms independent of $\mathbf{x}_a$ can be written as

$$\begin{aligned} &-\frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_a)^\intercal \boldsymbol{\Lambda}_{aa}(\mathbf{x}_a - \boldsymbol{\mu}_a) - \frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_a)^\intercal \boldsymbol{\Lambda}_{ab}(\mathbf{x}_b - \boldsymbol{\mu}_b) \\ &-\frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_a)^\intercal \boldsymbol{\Lambda}_{ac}(\mathbf{x}_c - \boldsymbol{\mu}_c) - \frac{1}{2}(\mathbf{x}_b - \boldsymbol{\mu}_b)^\intercal \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a) \\ &-\frac{1}{2}(\mathbf{x}_c - \boldsymbol{\mu}_c)^\intercal \boldsymbol{\Lambda}_{ca}(\mathbf{x}_a - \boldsymbol{\mu}_a). \end{aligned} \tag{2.194}$$

Except the terms independent of $\mathbf{x}_a$, it can be written as

$$-\frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_{a|b,c})^\intercal \boldsymbol{\Sigma}_{a|b,c}^{-1}(\mathbf{x}_a - \boldsymbol{\mu}_{a|b,c}), \tag{2.195}$$

where

$$\begin{aligned} \boldsymbol{\mu}_{a|b,c} &= \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ab}(\mathbf{x}_b - \boldsymbol{\mu}_b) - \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ac}(\mathbf{x}_c - \boldsymbol{\mu}_c), \\ \boldsymbol{\Sigma}_{a|b,c} &= \boldsymbol{\Lambda}_{aa}^{-1}. \end{aligned} \tag{2.196}$$

Then,

$$p(\mathbf{x}_a|\mathbf{x}_b, \mathbf{x}_c) = \mathcal{N}(\mathbf{x}_a|\boldsymbol{\mu}_{a|b,c}, \boldsymbol{\Sigma}_{a|b,c}). \tag{2.197}$$

By marginalisation,

$$p(\mathbf{x}_a|\mathbf{x}_b) = \int p(\mathbf{x}_a|\mathbf{x}_b, \mathbf{x}_c)p(\mathbf{x}_c)d\mathbf{x}_c. \tag{2.198}$$

The integrand of the right hand side except the terms independet of $\mathbf{x}_c$ can be written as

$$\begin{aligned} &-\frac{1}{2}\left(\mathbf{x}_a - \boldsymbol{\mu}_{a|b,c}\right)^\intercal \boldsymbol{\Sigma}_{a|b,c}^{-1}\left(\mathbf{x}_a - \boldsymbol{\mu}_{a|b,c}\right) - \frac{1}{2}(\mathbf{x}_c - \boldsymbol{\mu}_c)^\intercal \boldsymbol{\Lambda}_{cc}(\mathbf{x}_c - \boldsymbol{\mu}_c) \\ &= -\frac{1}{2}\mathbf{v}^\intercal \mathbf{M}\mathbf{v}, \end{aligned} \tag{2.199}$$

where

$$\begin{aligned} \mathbf{v} &= \begin{bmatrix} \mathbf{x}_c - \boldsymbol{\mu}_c \\ \mathbf{x}_a - \boldsymbol{\mu}_a + \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ab}\left(\mathbf{x}_b - \boldsymbol{\mu}_b\right) \end{bmatrix}, \\ \mathbf{M} &= \begin{bmatrix} \boldsymbol{\Lambda}_{cc} + \boldsymbol{\Lambda}_{ac}^\intercal \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ac} & \boldsymbol{\Lambda}_{ac}^\intercal \\ \boldsymbol{\Lambda}_{ac} & \boldsymbol{\Lambda}_{aa} \end{bmatrix}. \end{aligned} \tag{2.200}$$

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \boldsymbol{\Lambda}_{cc}^{-1} & -\boldsymbol{\Lambda}_{cc}^{-1}\boldsymbol{\Lambda}_{ac}^\intercal \boldsymbol{\Lambda}_{aa}^{-1} \\ -\boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ac}\boldsymbol{\Lambda}_{cc}^{-1} & \boldsymbol{\Lambda}_{aa}^{-1} + \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ac}\boldsymbol{\Lambda}_{cc}^{-1}\boldsymbol{\Lambda}_{ac}^\intercal \boldsymbol{\Lambda}_{aa}^{-1} \end{bmatrix}. \tag{2.201}$$

Therefore,

$$p(\mathbf{x}_a|\mathbf{x}_b) = \mathcal{N}(\mathbf{x}_a|\boldsymbol{\mu}_{a|b}, \boldsymbol{\Sigma}_{a|b}), \tag{2.202}$$

where

$$\begin{aligned} \boldsymbol{\mu}_{a|b} &= \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ab}\left(\mathbf{x}_b - \boldsymbol{\mu}_b\right), \\ \boldsymbol{\Sigma}_{a|b} &= \boldsymbol{\Lambda}_{aa}^{-1} + \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ac}\boldsymbol{\Lambda}_{cc}^{-1}\boldsymbol{\Lambda}_{ac}^\intercal \boldsymbol{\Lambda}_{aa}^{-1}. \end{aligned} \tag{2.203}$$

2.26

Let $\mathbf{A}$ be a square matrix and $\mathbf{C}$ be an invertible matrix. By 2.24,

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{D} & -\mathbf{C}^{-1} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{M} & \mathbf{MBC} \\ \mathbf{CDM} & -\mathbf{C} + \mathbf{CDMBC} \end{bmatrix}, \tag{2.204}$$

where

$$\mathbf{M} = (\mathbf{A} + \mathbf{BCD})^{-1}. \tag{2.205}$$

By 2.24,

$$\begin{bmatrix} -\mathbf{C}^{-1} & \mathbf{D} \\ \mathbf{B} & \mathbf{A} \end{bmatrix}^{-1} = \begin{bmatrix} -\mathbf{N} & \mathbf{NDA}^{-1} \\ \mathbf{A}^{-1}\mathbf{BN} & \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{BNDA}^{-1} \end{bmatrix}, \tag{2.206}$$

where

$$\mathbf{N} = \left(\mathbf{C}^{-1} + \mathbf{DA}^{-1}\mathbf{B}\right)^{-1}. \tag{2.207}$$

Therefore,

$$\mathbf{M} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{BNDA}^{-1}. \tag{2.208}$$

2.27

(a)

Let $\mathbf{x}$ and $\mathbf{z}$ be two variables. By the definition,

$$\mathrm{E}(\mathbf{x} + \mathbf{z}) = \int\int (\mathbf{x} + \mathbf{z}) p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z}. \tag{2.209}$$

The right hand side can be written as

$$\int \mathbf{x} \left(\int p(\mathbf{x}, \mathbf{z}) d\mathbf{z} \right) d\mathbf{x} + \int \mathbf{z} \left(\int p(\mathbf{x}, \mathbf{z}) d\mathbf{x} \right) d\mathbf{z} = \int \mathbf{x} p(\mathbf{x}) d\mathbf{x} + \int \mathbf{z} p(\mathbf{z}) d\mathbf{z}. \tag{2.210}$$

Therefore,

$$\mathrm{E}(\mathbf{x} + \mathbf{z}) = \mathrm{E}\,\mathbf{x} + \mathrm{E}\,\mathbf{z}. \tag{2.211}$$

(b)

Let $\mathbf{x}$ and $\mathbf{z}$ be two independent variables. By the definition,

$$\operatorname{cov}(\mathbf{x}+\mathbf{z}) = \int\int (\mathbf{x}+\mathbf{z}-\mathrm{E}(\mathbf{x}+\mathbf{z}))\,(\mathbf{x}+\mathbf{z}-\mathrm{E}(\mathbf{x}+\mathbf{z}))^{\intercal}\, p(\mathbf{x},\mathbf{z})d\mathbf{x}d\mathbf{z}. \tag{2.212}$$

The right hand side can be written as

$$\begin{aligned}&\int\int (\mathbf{x}-\mathrm{E}\,\mathbf{x})\,(\mathbf{x}-\mathrm{E}\,\mathbf{x})^{\intercal}\, p(\mathbf{x},\mathbf{z})d\mathbf{x}d\mathbf{z} + \int\int (\mathbf{x}-\mathrm{E}\,\mathbf{x})\,(\mathbf{z}-\mathrm{E}\,\mathbf{z})^{\intercal}\, p(\mathbf{x},\mathbf{z})d\mathbf{x}d\mathbf{z}\\ &+\int\int (\mathbf{z}-\mathrm{E}\,\mathbf{z})\,(\mathbf{x}-\mathrm{E}\,\mathbf{x})^{\intercal}\, p(\mathbf{x},\mathbf{z})d\mathbf{x}d\mathbf{z} + \int\int (\mathbf{z}-\mathrm{E}\,\mathbf{z})\,(\mathbf{z}-\mathrm{E}\,\mathbf{z})^{\intercal}\, p(\mathbf{x},\mathbf{z})d\mathbf{x}d\mathbf{z}.\end{aligned} \tag{2.213}$$

Each term can be written as

$$\begin{aligned}\int (\mathbf{x}-\mathrm{E}\,\mathbf{x})\,(\mathbf{x}-\mathrm{E}\,\mathbf{x})^{\intercal}\left(\int p(\mathbf{x},\mathbf{z})d\mathbf{z}\right)d\mathbf{x} &= \int (\mathbf{x}-\mathrm{E}\,\mathbf{x})\,(\mathbf{x}-\mathrm{E}\,\mathbf{x})^{\intercal}\, p(\mathbf{x})d\mathbf{x},\\ \int (\mathbf{x}-\mathrm{E}\,\mathbf{x})p(\mathbf{x})d\mathbf{x}\int (\mathbf{z}-\mathrm{E}\,\mathbf{z})^{\intercal}p(\mathbf{z})d\mathbf{z} &= (\mathrm{E}\,\mathbf{x}-\mathrm{E}\,\mathbf{x})(\mathrm{E}\,\mathbf{z}-\mathrm{E}\,\mathbf{z})^{\intercal},\\ \int (\mathbf{z}-\mathrm{E}\,\mathbf{z})p(\mathbf{z})d\mathbf{z}\int (\mathbf{x}-\mathrm{E}\,\mathbf{x})^{\intercal}p(\mathbf{x})d\mathbf{x} &= (\mathrm{E}\,\mathbf{z}-\mathrm{E}\,\mathbf{z})(\mathrm{E}\,\mathbf{x}-\mathrm{E}\,\mathbf{x})^{\intercal},\\ \int (\mathbf{z}-\mathrm{E}\,\mathbf{z})\,(\mathbf{z}-\mathrm{E}\,\mathbf{z})^{\intercal}\left(\int p(\mathbf{x},\mathbf{z})d\mathbf{x}\right)d\mathbf{z} &= \int (\mathbf{z}-\mathrm{E}\,\mathbf{z})\,(\mathbf{z}-\mathrm{E}\,\mathbf{z})^{\intercal}\, p(\mathbf{z})d\mathbf{z}.\end{aligned} \tag{2.214}$$

Therefore,

$$\operatorname{cov}(\mathbf{x}+\mathbf{z}) = \operatorname{cov}\mathbf{x} + \operatorname{cov}\mathbf{z}. \tag{2.215}$$

2.28

Let $\mathbf{z}$ be a variable such that

$$\begin{aligned}\mathbf{z} &= \begin{bmatrix}\mathbf{x}\\ \mathbf{y}\end{bmatrix},\\ \mathrm{E}\,\mathbf{z} &= \begin{bmatrix}\boldsymbol{\mu}\\ \mathbf{A}\boldsymbol{\mu}+\mathbf{b}\end{bmatrix},\\ \operatorname{cov}\mathbf{z} &= \begin{bmatrix}\boldsymbol{\Lambda}^{-1} & \boldsymbol{\Lambda}^{-1}\mathbf{A}^{\intercal}\\ \mathbf{A}\boldsymbol{\Lambda}^{-1} & \mathbf{L}^{-1}+\mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\intercal}\end{bmatrix},\end{aligned} \tag{2.216}$$

where $\mathbf{x}$ and $\mathbf{y}$ are Gaussian variables. By 2.29,

$$(\operatorname{cov} \mathbf{z})^{-1} = \begin{bmatrix} \mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A} & -\mathbf{A}^\intercal \mathbf{L} \\ -\mathbf{L}\mathbf{A} & \mathbf{L} \end{bmatrix}.$$

Then, $\ln p(\mathbf{z})$ except the terms independent of $\mathbf{x}$ and $\mathbf{y}$ is given by

$$\begin{aligned} &-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \left(\mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)(\mathbf{x}-\boldsymbol{\mu}) + \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \mathbf{A}^\intercal \mathbf{L}(\mathbf{y}-\mathbf{A}\boldsymbol{\mu}-\mathbf{b}) \\ &+\frac{1}{2}(\mathbf{y}-\mathbf{A}\boldsymbol{\mu}-\mathbf{b})^\intercal \mathbf{L}\mathbf{A}(\mathbf{x}-\boldsymbol{\mu}) - \frac{1}{2}(\mathbf{y}-\mathbf{A}\boldsymbol{\mu}-\mathbf{b})^\intercal \mathbf{L}(\mathbf{y}-\mathbf{A}\boldsymbol{\mu}-\mathbf{b}) \\ =&-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \left(\mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)(\mathbf{x}-\boldsymbol{\mu}) + \\ &-\frac{1}{2}\left(\mathbf{y}-\mathbf{A}\boldsymbol{\mu}-\mathbf{b}-\mathbf{A}(\mathbf{x}-\boldsymbol{\mu})\right)^\intercal \mathbf{L}\left(\mathbf{y}-\mathbf{A}\boldsymbol{\mu}-\mathbf{b}-\mathbf{A}(\mathbf{x}-\boldsymbol{\mu})\right) \\ &+\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \mathbf{A}^\intercal \mathbf{L}\mathbf{A}(\mathbf{x}-\boldsymbol{\mu}). \end{aligned} \tag{2.217}$$

The right hand side can be written as

$$-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \mathbf{\Lambda}(\mathbf{x}-\boldsymbol{\mu}) - \frac{1}{2}\left(\mathbf{y}-\mathbf{A}\mathbf{x}-\mathbf{b}\right)^\intercal \mathbf{L}\left(\mathbf{y}-\mathbf{A}\mathbf{x}-\mathbf{b}\right). \tag{2.218}$$

Therefore,

$$\begin{aligned} p(\mathbf{x}) &= \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, \mathbf{\Lambda}^{-1}\right), \\ p(\mathbf{y}|\mathbf{x}) &= \mathcal{N}\left(\mathbf{y}|\mathbf{A}\mathbf{x}+\mathbf{b}, \mathbf{L}^{-1}\right). \end{aligned} \tag{2.219}$$

2.29

Let

$$\mathbf{R} = \begin{bmatrix} \mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A} & -\mathbf{A}^\intercal \mathbf{L} \\ -\mathbf{L}\mathbf{A} & \mathbf{L} \end{bmatrix}. \tag{2.220}$$

By 2.24,

$$\mathbf{R}^{-1} = \begin{bmatrix} \mathbf{\Lambda}^{-1} & \mathbf{\Lambda}^{-1}\mathbf{A}^\intercal \\ \mathbf{A}\mathbf{\Lambda}^{-1} & \mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1}\mathbf{A}^\intercal \end{bmatrix}. \tag{2.221}$$

2.30

Let

$$\mathbf{R}^{-1} = \begin{bmatrix} \mathbf{\Lambda}^{-1} & \mathbf{\Lambda}^{-1}\mathbf{A}^\intercal \\ \mathbf{A}\mathbf{\Lambda}^{-1} & \mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1}\mathbf{A}^\intercal \end{bmatrix}. \tag{2.222}$$

Then,

$$\mathbf{R}^{-1}\begin{bmatrix}\boldsymbol{\Lambda}\boldsymbol{\mu}-\mathbf{A}^{\intercal}\mathbf{L}\mathbf{b}\\ \mathbf{L}\mathbf{b}\end{bmatrix}=\begin{bmatrix}\boldsymbol{\mu}\\ \mathbf{A}\boldsymbol{\mu}+\mathbf{b}\end{bmatrix}. \tag{2.223}$$

2.31

Let $\mathbf{y}$ be a variable such that

$$\mathbf{y}=\mathbf{x}+\mathbf{z}, \tag{2.224}$$

where

$$\begin{aligned} p(\mathbf{x})&=\mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}_{\mathbf{x}},\boldsymbol{\Sigma}_{\mathbf{x}}\right),\\ p(\mathbf{z})&=\mathcal{N}\left(\mathbf{z}|\boldsymbol{\mu}_{\mathbf{z}},\boldsymbol{\Sigma}_{\mathbf{z}}\right). \end{aligned} \tag{2.225}$$

By marginalisation,

$$p(\mathbf{y})=\int p(\mathbf{y}|\mathbf{x})p(\mathbf{x})d\mathbf{x}. \tag{2.226}$$

The right hand side can be written as

$$\int\mathcal{N}\left(\mathbf{y}|\mathbf{x}+\boldsymbol{\mu}_{\mathbf{z}},\boldsymbol{\Sigma}_{\mathbf{z}}\right)\mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}_{\mathbf{x}},\boldsymbol{\Sigma}_{\mathbf{x}}\right)d\mathbf{x}. \tag{2.227}$$

The logarithm of the integrand except the terms independent of $\mathbf{x}$ and $\mathbf{y}$ is given by

$$-\frac{1}{2}\left(\mathbf{y}-\mathbf{x}-\boldsymbol{\mu}_{\mathbf{z}}\right)^{\intercal}\boldsymbol{\Sigma}_{\mathbf{z}}^{-1}\left(\mathbf{y}-\mathbf{x}-\boldsymbol{\mu}_{\mathbf{z}}\right)-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_{\mathbf{x}})^{\intercal}\boldsymbol{\Sigma}_{\mathbf{x}}^{-1}(\mathbf{x}-\boldsymbol{\mu}_{\mathbf{x}}). \tag{2.228}$$

The terms except the ones independent of $\mathbf{x}$ and $\mathbf{y}$ can be written as

$$-\frac{1}{2}\mathbf{u}^{\intercal}\mathbf{R}\mathbf{u}+\mathbf{u}^{\intercal}\mathbf{v}=-\frac{1}{2}\left(\mathbf{u}-\mathbf{R}^{-1}\mathbf{v}\right)^{\intercal}\mathbf{R}\left(\mathbf{u}-\mathbf{R}^{-1}\mathbf{v}\right)+\frac{1}{2}\mathbf{v}^{\intercal}\mathbf{R}^{-1}\mathbf{v}, \tag{2.229}$$

where

$$\begin{aligned} \mathbf{u}&=\begin{bmatrix}\mathbf{x}\\ \mathbf{y}\end{bmatrix},\\ \mathbf{R}&=\begin{bmatrix}\boldsymbol{\Sigma}_{\mathbf{x}}^{-1}+\boldsymbol{\Sigma}_{\mathbf{z}}^{-1} & -\boldsymbol{\Sigma}_{\mathbf{z}}^{-1}\\ -\boldsymbol{\Sigma}_{\mathbf{z}}^{-1} & \boldsymbol{\Sigma}_{\mathbf{z}}^{-1}\end{bmatrix},\\ \mathbf{v}&=\begin{bmatrix}\boldsymbol{\Sigma}_{\mathbf{x}}^{-1}\boldsymbol{\mu}_{\mathbf{x}}-\boldsymbol{\Sigma}_{\mathbf{z}}^{-1}\boldsymbol{\mu}_{\mathbf{z}}\\ \boldsymbol{\Sigma}_{\mathbf{z}}^{-1}\boldsymbol{\mu}_{\mathbf{z}}\end{bmatrix}, \end{aligned} \tag{2.230}$$

By 2.29 and 2.30,

$$\begin{aligned}\mathbf{R}^{-1} &= \begin{bmatrix}\boldsymbol{\Sigma}_{\mathbf{x}} & \boldsymbol{\Sigma}_{\mathbf{x}} \\ \boldsymbol{\Sigma}_{\mathbf{x}} & \boldsymbol{\Sigma}_{\mathbf{x}} + \boldsymbol{\Sigma}_{\mathbf{z}}\end{bmatrix}, \\ \mathbf{R}^{-1}\mathbf{v} &= \begin{bmatrix}\boldsymbol{\mu}_{\mathbf{x}} \\ \boldsymbol{\mu}_{\mathbf{x}} + \boldsymbol{\mu}_{\mathbf{z}}\end{bmatrix}.\end{aligned} \tag{2.231}$$

Therefore,

$$p(\mathbf{y}) = \mathcal{N}\left(\mathbf{y}|\boldsymbol{\mu}_{\mathbf{x}} + \boldsymbol{\mu}_{\mathbf{z}}, \boldsymbol{\Sigma}_{\mathbf{x}} + \boldsymbol{\Sigma}_{\mathbf{z}}\right). \tag{2.232}$$

2.32

Let $\mathbf{x}$ and $\mathbf{y}$ be variables such that

$$\begin{aligned}p(\mathbf{x}) &= \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}\right), \\ p(\mathbf{y}|\mathbf{x}) &= \mathcal{N}\left(\mathbf{y}|\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1}\right).\end{aligned} \tag{2.233}$$

By the Bayes' theorem,

$$p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) = p(\mathbf{x}|\mathbf{y})p(\mathbf{y}). \tag{2.234}$$

The logarithm of the left hand side except the terms independent of $\mathbf{x}$ and $\mathbf{y}$ can be written as

$$\begin{aligned}&-\frac{1}{2}\left(\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b}\right)^{\intercal}\mathbf{L}\left(\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b}\right) - \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\intercal}\boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu}) \\ =&-\frac{1}{2}\left(\mathbf{y} - \mathbf{A}(\mathbf{x} - \boldsymbol{\mu}) - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}\right)^{\intercal}\mathbf{L}\left(\mathbf{y} - \mathbf{A}(\mathbf{x} - \boldsymbol{\mu}) - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}\right) \\ &-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\intercal}\boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu}).\end{aligned} \tag{2.235}$$

The right hand side can be written as

$$\begin{aligned}&-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\intercal}\left(\boldsymbol{\Lambda} + \mathbf{A}^{\intercal}\mathbf{L}\mathbf{A}\right)(\mathbf{x} - \boldsymbol{\mu}) + (\mathbf{x} - \boldsymbol{\mu})^{\intercal}\mathbf{A}^{\intercal}\mathbf{L}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}) \\ &-\frac{1}{2}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})^{\intercal}\mathbf{L}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}) \\ =&-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu} - \mathbf{z})^{\intercal}\left(\boldsymbol{\Lambda} + \mathbf{A}^{\intercal}\mathbf{L}\mathbf{A}\right)(\mathbf{x} - \boldsymbol{\mu} - \mathbf{z}) + \frac{1}{2}\mathbf{z}^{\intercal}\left(\boldsymbol{\Lambda} + \mathbf{A}^{\intercal}\mathbf{L}\mathbf{A}\right)\mathbf{z} \\ &-\frac{1}{2}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})^{\intercal}\mathbf{L}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}),\end{aligned} \tag{2.236}$$

where

$$\mathbf{z} = \left(\mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)^{-1} \mathbf{A}^\intercal \mathbf{L} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}). \tag{2.237}$$

The right hand side can be written as

$$\begin{aligned} &-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu} - \mathbf{z})^\intercal \left(\mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right) (\mathbf{x} - \boldsymbol{\mu} - \mathbf{z}) \\ &-\frac{1}{2}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})^\intercal \mathbf{M} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}), \end{aligned} \tag{2.238}$$

where

$$\mathbf{M} = \mathbf{L} - \mathbf{L}\mathbf{A} \left(\mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)^{-1} \mathbf{A}^\intercal \mathbf{L}. \tag{2.239}$$

We have

$$\boldsymbol{\mu} + \mathbf{z} = \left(\mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)^{-1} \left(\left(\mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right) \boldsymbol{\mu} + \mathbf{A}^\intercal \mathbf{L} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})\right). \tag{2.240}$$

Then,

$$\boldsymbol{\mu} + \mathbf{z} = \left(\mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)^{-1} \left(\mathbf{A}^\intercal \mathbf{L} (\mathbf{y} - \mathbf{b}) + \mathbf{\Lambda}\boldsymbol{\mu}\right). \tag{2.241}$$

By 2.26,

$$\left(\mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)^{-1} = \mathbf{\Lambda}^{-1} - \mathbf{\Lambda}^{-1} \mathbf{A}^\intercal \left(\mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal\right)^{-1} \mathbf{A}\mathbf{\Lambda}^{-1}. \tag{2.242}$$

Then,

$$\mathbf{M} = \mathbf{L} - \mathbf{L}\mathbf{A} \left(\mathbf{\Lambda}^{-1} - \mathbf{\Lambda}^{-1} \mathbf{A}^\intercal \left(\mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal\right)^{-1} \mathbf{A}\mathbf{\Lambda}^{-1}\right) \mathbf{A}^\intercal \mathbf{L}. \tag{2.243}$$

The right hand side can be written as

$$\begin{aligned} &\mathbf{L} - \mathbf{L} \left(\mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal - \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal \left(\mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal\right)^{-1} \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal\right) \mathbf{L} \\ =&\mathbf{L} - \mathbf{L}\mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal \left(\mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal\right)^{-1} \left(\mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal - \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal\right) \mathbf{L}. \end{aligned} \tag{2.244}$$

The right hand side can be written as

$$\begin{aligned} &\mathbf{L} - \mathbf{L}\mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal \left(\mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal\right)^{-1} \\ =&\mathbf{L} \left(\mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal - \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal\right) \left(\mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal\right)^{-1}. \end{aligned} \tag{2.245}$$

Then,

$$\mathbf{M} = \left(\mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal\right)^{-1}. \tag{2.246}$$

Therefore,

$$\begin{aligned} p(\mathbf{x}|\mathbf{y}) &= \mathcal{N}\left(\mathbf{x}| \left(\mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)^{-1} \left(\mathbf{A}^\intercal \mathbf{L} (\mathbf{y} - \mathbf{b}) + \mathbf{\Lambda}\boldsymbol{\mu}\right), \left(\mathbf{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)^{-1}\right), \\ p(\mathbf{y}) &= \mathcal{N}\left(\mathbf{y}|\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^\intercal\right). \end{aligned} \tag{2.247}$$

2.33

Refer to 2.32, while a different approach is presented below.

Let $\mathbf{x}$ and $\mathbf{y}$ be variables such that

$$\begin{aligned} p(\mathbf{x}) &= \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}\right), \\ p(\mathbf{y}|\mathbf{x}) &= \mathcal{N}\left(\mathbf{y}|\mathbf{A}\mathbf{x}+\mathbf{b}, \mathbf{L}^{-1}\right). \end{aligned} \tag{2.248}$$

By the Bayes' theorem,

$$p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) = p(\mathbf{x}|\mathbf{y})p(\mathbf{y}). \tag{2.249}$$

The logarithm of the left hand side except the terms independent of $\mathbf{x}$ and $\mathbf{y}$ can be written as

$$-\frac{1}{2}\left(\mathbf{y}-\mathbf{A}\mathbf{x}-\mathbf{b}\right)^{\intercal}\mathbf{L}\left(\mathbf{y}-\mathbf{A}\mathbf{x}-\mathbf{b}\right) - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu}). \tag{2.250}$$

The terms except the ones independent of $\mathbf{x}$ and $\mathbf{y}$ can be written as

$$-\frac{1}{2}\begin{bmatrix}\mathbf{x}\\ \mathbf{y}\end{bmatrix}^{\intercal}\begin{bmatrix}\boldsymbol{\Lambda}+\mathbf{A}^{\intercal}\mathbf{L}\mathbf{A} & -\mathbf{A}^{\intercal}\mathbf{L}\\ -\mathbf{L}\mathbf{A} & \mathbf{L}\end{bmatrix}\begin{bmatrix}\mathbf{x}\\ \mathbf{y}\end{bmatrix} + \begin{bmatrix}\mathbf{x}\\ \mathbf{y}\end{bmatrix}^{\intercal}\begin{bmatrix}-\mathbf{A}^{\intercal}\mathbf{L}\mathbf{b}+\boldsymbol{\Lambda}\boldsymbol{\mu}\\ \mathbf{L}\mathbf{b}\end{bmatrix}. \tag{2.251}$$

By 2.24,

$$\begin{bmatrix}\boldsymbol{\Lambda}+\mathbf{A}^{\intercal}\mathbf{L}\mathbf{A} & -\mathbf{A}^{\intercal}\mathbf{L}\\ -\mathbf{L}\mathbf{A} & \mathbf{L}\end{bmatrix}^{-1} = \begin{bmatrix}\boldsymbol{\Lambda}^{-1} & \boldsymbol{\Lambda}^{-1}\mathbf{A}^{\intercal}\\ \mathbf{A}\boldsymbol{\Lambda}^{-1} & \mathbf{L}^{-1}+\mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\intercal}\end{bmatrix}, \tag{2.252}$$

so that

$$\begin{bmatrix}\boldsymbol{\Lambda}+\mathbf{A}^{\intercal}\mathbf{L}\mathbf{A} & -\mathbf{A}^{\intercal}\mathbf{L}\\ -\mathbf{L}\mathbf{A} & \mathbf{L}\end{bmatrix}^{-1}\begin{bmatrix}-\mathbf{A}^{\intercal}\mathbf{L}\mathbf{b}+\boldsymbol{\Lambda}\boldsymbol{\mu}\\ \mathbf{L}\mathbf{b}\end{bmatrix} = \begin{bmatrix}\boldsymbol{\mu}\\ \mathbf{A}\boldsymbol{\mu}+\mathbf{b}\end{bmatrix}. \tag{2.253}$$

Then,

$$p(\mathbf{y}) = \mathcal{N}\left(\mathbf{y}|\mathbf{A}\boldsymbol{\mu}+\mathbf{b}, \mathbf{L}^{-1}+\mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\intercal}\right). \tag{2.254}$$

By 2.25,

$$p(\mathbf{x}|\mathbf{y}) = \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}+\left(\boldsymbol{\Lambda}+\mathbf{A}^{\intercal}\mathbf{L}\mathbf{A}\right)^{-1}\mathbf{A}^{\intercal}\mathbf{L}\left(\mathbf{y}-\mathbf{A}\boldsymbol{\mu}-\mathbf{b}\right), \left(\boldsymbol{\Lambda}+\mathbf{A}^{\intercal}\mathbf{L}\mathbf{A}\right)^{-1}\right). \tag{2.255}$$

We have

$$\begin{aligned}&\boldsymbol{\mu} + \left(\boldsymbol{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)^{-1} \mathbf{A}^\intercal \mathbf{L} \left(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}\right) \\ =& \left(\boldsymbol{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)^{-1} \left(\boldsymbol{\Lambda}\boldsymbol{\mu} + \mathbf{A}^\intercal \mathbf{L}(\mathbf{y} - \mathbf{b})\right).\end{aligned} \tag{2.256}$$

Therefore,

$$p(\mathbf{x}|\mathbf{y}) = \mathcal{N}\left(\mathbf{x}| \left(\boldsymbol{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)^{-1} \left(\boldsymbol{\Lambda}\boldsymbol{\mu} + \mathbf{A}^\intercal \mathbf{L}(\mathbf{y} - \mathbf{b})\right), \left(\boldsymbol{\Lambda} + \mathbf{A}^\intercal \mathbf{L} \mathbf{A}\right)^{-1}\right). \tag{2.257}$$

2.34

Let $\mathbf{x}_1, \cdots, \mathbf{x}_N$ be variables such that

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}). \tag{2.258}$$

Then,

$$\ln\left(\prod_{n=1}^{N} p(\mathbf{x}_n)\right) = -\frac{ND}{2}\ln(2\pi) - \frac{N}{2}\ln|\det \boldsymbol{\Sigma}| - \frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_n - \boldsymbol{\mu})^\intercal \boldsymbol{\Sigma}^{-1}(\mathbf{x}_n - \boldsymbol{\mu}). \tag{2.259}$$

By 3.21(a), setting the derivatives with respect to $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ to zero gives

$$\begin{aligned}\mathbf{0} &= \sum_{n=1}^{N}\left(\boldsymbol{\Sigma}^{-1} + \left(\boldsymbol{\Sigma}^{-1}\right)^\intercal\right)(\mathbf{x}_n - \boldsymbol{\mu}), \\ \mathbf{O} &= -\frac{N}{2}\left(\boldsymbol{\Sigma}^{-1}\right)^\intercal + \frac{1}{2}\left(\boldsymbol{\Sigma}^{-1}\right)^2 \sum_{n=1}^{N}(\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{x}_n - \boldsymbol{\mu})^\intercal.\end{aligned} \tag{2.260}$$

Therefore, the maximum likelihood solutions for $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are given by

$$\begin{aligned}\boldsymbol{\mu}_{\mathrm{ML}} &= \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n, \\ \boldsymbol{\Sigma}_{\mathrm{ML}} &= \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})(\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})^\intercal.\end{aligned} \tag{2.261}$$

2.35

(a)

Let $\mathbf{x}$ be a variable such that

$$p(\mathbf{x}) = \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}\right). \tag{2.262}$$

Then,

$$\mathrm{E}\,\mathbf{x}\mathbf{x}^\intercal = \mathrm{E}(\mathbf{x}-\boldsymbol{\mu}+\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu}+\boldsymbol{\mu})^\intercal. \tag{2.263}$$

The right hand side can be written as

$$\mathrm{E}(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\intercal + \boldsymbol{\mu}\,\mathrm{E}(\mathbf{x}-\boldsymbol{\mu})^\intercal + \mathrm{E}(\mathbf{x}-\boldsymbol{\mu})\boldsymbol{\mu}^\intercal + \boldsymbol{\mu}\boldsymbol{\mu}^\intercal. \tag{2.264}$$

Since

$$\begin{aligned} \mathrm{E}\,\mathbf{x} &= \boldsymbol{\mu}, \\ \mathrm{cov}\,\mathbf{x} &= \boldsymbol{\Sigma}, \end{aligned} \tag{2.265}$$

The right hand side can be written as $\boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^\intercal$. Therefore,

$$\mathrm{E}\,\mathbf{x}\mathbf{x}^\intercal = \boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^\intercal. \tag{2.266}$$

(b)

Let $\mathbf{x}_n$ and $\mathbf{x}_m$ be independent variables such that

$$\begin{aligned} p(\mathbf{x}_n) &= \mathcal{N}\left(\mathbf{x_n}|\boldsymbol{\mu}, \boldsymbol{\Sigma}\right), \\ p(\mathbf{x}_m) &= \mathcal{N}\left(\mathbf{x_m}|\boldsymbol{\mu}, \boldsymbol{\Sigma}\right). \end{aligned} \tag{2.267}$$

If $n \neq m$, then

$$\mathrm{E}\,\mathbf{x}_n\mathbf{x}_m^\intercal = \mathrm{E}\,\mathbf{x}_n\,\mathrm{E}\,\mathbf{x}_m^\intercal. \tag{2.268}$$

The right hand side can be written as $\boldsymbol{\mu}\boldsymbol{\mu}^\intercal$. Therefore, by (a),

$$\mathrm{E}\,\mathbf{x}_n\mathbf{x}_m^\intercal = I_{nm}\boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^\intercal. \tag{2.269}$$

(c)

Let $\mathbf{x}_1, \cdots, \mathbf{x}_N$ be variables such that

$$p(\mathbf{x}_n) = \mathcal{N}\left(\mathbf{x}_n|\boldsymbol{\mu}, \boldsymbol{\Sigma}\right). \tag{2.270}$$

By 2.34, the maximum likelihood solutions for $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are given by

$$\begin{aligned} \boldsymbol{\mu}_{\mathrm{ML}} &= \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n, \\ \boldsymbol{\Sigma}_{\mathrm{ML}} &= \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})(\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})^\intercal. \end{aligned} \tag{2.271}$$

Then,

$$\mathrm{E}\,\boldsymbol{\Sigma}_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N}\mathrm{E}(\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})(\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})^{\intercal}. \tag{2.272}$$

The right hand side can be written as

$$\begin{aligned}&\frac{1}{N}\sum_{n=1}^{N}\mathrm{E}\,\mathbf{x}_n\mathbf{x}_n^{\intercal} - \frac{1}{N^2}\sum_{n=1}^{N}\mathrm{E}\left(\sum_{n=1}^{N}\mathbf{x_n}\right)\mathbf{x}_n^{\intercal} - \frac{1}{N^2}\sum_{n=1}^{N}\mathrm{E}\,\mathbf{x}_n\left(\sum_{n=1}^{N}\mathbf{x_n}\right)^{\intercal}\\ &+ \frac{1}{N^3}\sum_{n=1}^{N}\mathrm{E}\left(\sum_{n=1}^{N}\mathbf{x_n}\right)\left(\sum_{n=1}^{N}\mathbf{x_n}\right)^{\intercal}.\end{aligned} \tag{2.273}$$

By (b), the first term can be written as $\boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^{\intercal}$. By (b), the second and third terms can be written as

$$-\frac{1}{N}\left((\boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^{\intercal}) + (N-1)\boldsymbol{\mu}\boldsymbol{\mu}^{\intercal}\right) = -\frac{1}{N}\boldsymbol{\Sigma} - \boldsymbol{\mu}\boldsymbol{\mu}^{\intercal}. \tag{2.274}$$

By (b), the fourth term can be written as

$$\frac{1}{N^2}\left(N\left(\boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^{\intercal}\right) + N(N-1)\boldsymbol{\mu}\boldsymbol{\mu}^{\intercal}\right) = \frac{1}{N}\boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^{\intercal}. \tag{2.275}$$

Then,

$$\mathrm{E}\,\boldsymbol{\Sigma}_{\mathrm{ML}} = (\boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^{\intercal}) + 2\left(-\frac{1}{N}\boldsymbol{\Sigma} - \boldsymbol{\mu}\boldsymbol{\mu}^{\intercal}\right) + \frac{1}{N}\boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^{\intercal}. \tag{2.276}$$

Therefore,

$$\mathrm{E}\,\boldsymbol{\Sigma}_{\mathrm{ML}} = \frac{N-1}{N}\boldsymbol{\Sigma}. \tag{2.277}$$

2.36

Let $x_1, \cdots, x_N$ be variables such that

$$p(x_n) = \mathcal{N}\left(x_n|\mu, \sigma^2\right). \tag{2.278}$$

Let us assume that μ is known. By 2.34, the maximum likelihood solution for σ^2 is given by

$${\sigma^2_{\mathrm{ML}}}^{(N)} = \frac{1}{N}\sum_{n=1}^{N}(x_n - \mu)^2. \tag{2.279}$$

The right hand side can be written as

$$\frac{1}{N}(x_N-\mu)^2+\frac{1}{N}\sum_{n=1}^{N-1}(x_n-\mu)^2=\frac{1}{N}(x_N-\mu)^2+\frac{N-1}{N}{\sigma^2_{\mathrm{ML}}}^{(N-1)}. \quad (2.280)$$

Then,

$${\sigma^2_{\mathrm{ML}}}^{(N)}={\sigma^2_{\mathrm{ML}}}^{(N-1)}+\frac{1}{N}\left((x_N-\mu)^2-{\sigma^2_{\mathrm{ML}}}^{(N-1)}\right). \quad (2.281)$$

We have

$$\frac{\partial}{\partial\sigma^2}\left(-\ln p(x_n)\right)=\frac{1}{2\sigma^2}-\frac{1}{2\left(\sigma^2\right)^2}(x_n-\mu)^2. \quad (2.282)$$

Therefore,

$${\sigma^2_{\mathrm{ML}}}^{(N)}={\sigma^2_{\mathrm{ML}}}^{(N-1)}-\frac{2\left({\sigma^2_{\mathrm{ML}}}^{(N-1)}\right)^2}{N}\left(\frac{\partial}{\partial\sigma^2}\left(-\ln p(x_N)\right)\right)\Big|_{\sigma^2={\sigma^2_{\mathrm{ML}}}^{(N-1)}}. \quad (2.283)$$

2.37

Let $\mathbf{x}_1,\cdots,\mathbf{x}_N$ be variables such that

$$p(\mathbf{x}_n)=\mathcal{N}\left(\mathbf{x}_n|\boldsymbol{\mu},\boldsymbol{\Sigma}\right). \quad (2.284)$$

Let us assume that $\boldsymbol{\mu}$ is known. By 2.34, the maximum likelihood solution for $\boldsymbol{\Sigma}$ is given by

$$\boldsymbol{\Sigma}^{(N)}_{\mathrm{ML}}=\frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n-\boldsymbol{\mu})(\mathbf{x}_n-\boldsymbol{\mu})^{\intercal}. \quad (2.285)$$

The right hand side can be written as

$$\begin{aligned}&\frac{1}{N}(\mathbf{x}_N-\boldsymbol{\mu})(\mathbf{x}_N-\boldsymbol{\mu})^{\intercal}+\frac{1}{N}\sum_{n=1}^{N-1}(\mathbf{x}_n-\boldsymbol{\mu})(\mathbf{x}_n-\boldsymbol{\mu})^{\intercal}\\ =&\frac{1}{N}(\mathbf{x}_N-\boldsymbol{\mu})(\mathbf{x}_N-\boldsymbol{\mu})^{\intercal}+\frac{N-1}{N}\boldsymbol{\Sigma}^{(N-1)}_{\mathrm{ML}}.\end{aligned} \quad (2.286)$$

Then,

$$\boldsymbol{\Sigma}_{\mathrm{ML}}^{(N)} = \boldsymbol{\Sigma}_{\mathrm{ML}}^{(N-1)} + \frac{1}{N}\left((\mathbf{x}_N - \boldsymbol{\mu})(\mathbf{x}_N - \boldsymbol{\mu})^{\intercal} - \boldsymbol{\Sigma}_{\mathrm{ML}}^{(N-1)}\right). \tag{2.287}$$

By 3.21(a), we have

$$\frac{\partial}{\partial \boldsymbol{\Sigma}}\left(-\ln p(x_n)\right) = -\frac{1}{2}\left(\boldsymbol{\Sigma}^{-1}\right)^{\intercal} + \frac{1}{2}\left(\boldsymbol{\Sigma}^{-1}\right)^2 (\mathbf{x}_N - \boldsymbol{\mu})(\mathbf{x}_N - \boldsymbol{\mu})^{\intercal}. \tag{2.288}$$

Therefore,

$$\boldsymbol{\Sigma}_{\mathrm{ML}}^{(N)} = \boldsymbol{\Sigma}_{\mathrm{ML}}^{(N-1)} - \frac{\left(\boldsymbol{\Sigma}_{\mathrm{ML}}^{(N-1)}\right)^2}{N}\left(\frac{\partial}{\partial \boldsymbol{\Sigma}}\left(-\ln p\left(\mathbf{x}_N\right)\right)\right)\Big|_{\boldsymbol{\Sigma}=\boldsymbol{\Sigma}_{\mathrm{ML}}^{(N-1)}}. \tag{2.289}$$

2.38

Let $x_1, \cdots, x_N$ be variables such that

$$\begin{aligned} p(x_n|\mu) &= \mathcal{N}\left(x_n|\mu, \sigma^2\right), \\ p(\mu) &= \mathcal{N}\left(\mu|\mu_0, \sigma_0^2\right). \end{aligned} \tag{2.290}$$

By the Bayes' theorem,

$$p(\mu|\mathbf{x})p(\mathbf{x}) = p(\mathbf{x}|\mu)p(\mu). \tag{2.291}$$

The logarithm of the right hand side excpt the terms independent of $\mathbf{x}$ and μ can be written as

$$-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n - \mu)^2 - \frac{1}{2\sigma_0^2}(\mu - \mu_0)^2. \tag{2.292}$$

By 2.34, the maximum likelihood solution for μ is given by

$$\mu_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N} x_n. \tag{2.293}$$

Then, the first term can be written as

$$\begin{aligned} &-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n - \mu_{\mathrm{ML}} + \mu_{\mathrm{ML}} - \mu)^2 \\ =&-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n - \mu_{\mathrm{ML}})^2 - \frac{\mu_{\mathrm{ML}} - \mu}{\sigma^2}\sum_{n=1}^{N}(x_n - \mu_{\mathrm{ML}}) - \frac{N}{2\sigma^2}(\mu_{\mathrm{ML}} - \mu)^2. \end{aligned} \tag{2.294}$$

Since the second term of the right hand side is zero, the logarithm except the terms independent of $\mathbf{x}$ and μ can be written as

$$\begin{aligned} &-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n-\mu_{\mathrm{ML}})^2-\frac{N}{2\sigma^2}(\mu_{\mathrm{ML}}-\mu)^2-\frac{1}{2\sigma_0^2}(\mu-\mu_0)^2 \\ =&-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n-\mu_{\mathrm{ML}})^2-\frac{1}{2\sigma_N^2}\left(\mu-\mu_N\right)^2+\frac{\mu_N^2}{2\sigma_N^2}-\frac{N\mu_{\mathrm{ML}}^2}{2\sigma^2}-\frac{\mu_0^2}{2\sigma_0^2}, \end{aligned} \tag{2.295}$$

where

$$\begin{aligned} \mu_N &= \frac{N\sigma_0^2}{N\sigma_0^2+\sigma^2}\mu_{\mathrm{ML}}+\frac{\sigma^2}{N\sigma_0^2+\sigma^2}\mu_0, \\ \sigma_N^2 &= \frac{\sigma^2\sigma_0^2}{N\sigma_0^2+\sigma^2}. \end{aligned} \tag{2.296}$$

Therefore,

$$p(\mu|\mathbf{x})=\mathcal{N}\left(\mu|\mu_N,\sigma_N^2\right). \tag{2.297}$$

2.39

Let $x_1,\cdots,x_N$ be variables such that

$$\begin{aligned} p(x_n|\mu)&=\mathcal{N}\left(x_n|\mu,\sigma^2\right), \\ p(\mu)&=\mathcal{N}\left(\mu|\mu_0,\sigma_0^2\right). \end{aligned} \tag{2.298}$$

(a)

By 2.38,

$$p(\mu|\mathbf{x})=\mathcal{N}\left(\mu|\mu_N,\sigma_N^2\right), \tag{2.299}$$

where

$$\begin{aligned} \mu_N &= \frac{\sigma_0^2}{N\sigma_0^2+\sigma^2}\sum_{n=1}^{N}x_n+\frac{\sigma^2}{N\sigma_0^2+\sigma^2}\mu_0, \\ \sigma_N^2 &= \frac{\sigma^2\sigma_0^2}{N\sigma_0^2+\sigma^2}. \end{aligned} \tag{2.300}$$

Then,

$$\frac{1}{\sigma_N^2}=\frac{(N-1)\sigma_0^2+\sigma^2}{\sigma^2\sigma_0^2}+\frac{1}{\sigma^2}. \tag{2.301}$$

Therefore,

$$\frac{1}{\sigma_N^2} = \frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}. \tag{2.302}$$

We have

$$\frac{\mu_N}{\sigma_N^2} = \frac{1}{\sigma^2}\sum_{n=1}^{N} x_n + \frac{\mu_0}{\sigma_0^2}, \tag{2.303}$$

so that

$$\frac{\mu_{N-1}}{\sigma_{N-1}^2} = \frac{1}{\sigma^2}\sum_{n=1}^{N-1} x_n + \frac{\mu_0}{\sigma_0^2}. \tag{2.304}$$

Therefore,

$$\frac{\mu_N}{\sigma_N^2} = \frac{\mu_{N-1}}{\sigma_{N-1}^2} + \frac{x_N}{\sigma^2}. \tag{2.305}$$

(b)

By the Bayes' theorem,

$$p(\mu|\mathbf{x}_N)p(\mathbf{x}_N) = p(\mathbf{x}_N|\mu)p(\mu). \tag{2.306}$$

Since x_N and $\mathbf{x}_{N-1}$ are independent, it can be written as

$$p(\mu|\mathbf{x}_N)p(x_N)p(\mathbf{x}_{N-1}) = p(x_N|\mu)p(\mathbf{x}_{N-1}|\mu)p(\mu). \tag{2.307}$$

By the Bayes' theorem, the right hand side can be written as

$$p(x_N|\mu)p(\mu|\mathbf{x}_{N-1})p(\mathbf{x}_{N-1}). \tag{2.308}$$

Then,

$$p(\mu|\mathbf{x}_N)p(x_N) = p(\mu|\mathbf{x}_{N-1})p(x_N|\mu). \tag{2.309}$$

The logarithm of the integrand of the right hand side except the terms independent of μ or x_N can be written as

$$\begin{aligned}
&-\frac{1}{2\sigma_{N-1}^2}(\mu-\mu_{N-1})^2 - \frac{1}{2\sigma^2}(x_N-\mu)^2 \\
=&-\frac{1}{2}\left(\frac{1}{\sigma_{N-1}^2}+\frac{1}{\sigma^2}\right)\left(\mu - \frac{\frac{1}{\sigma_{N-1}^2}}{\frac{1}{\sigma_{N-1}^2}+\frac{1}{\sigma^2}}\mu_{N-1} - \frac{\frac{1}{\sigma^2}}{\frac{1}{\sigma_{N-1}^2}+\frac{1}{\sigma^2}}x_N\right)^2 \\
&+\frac{1}{2}\left(\frac{1}{\sigma_{N-1}^2}+\frac{1}{\sigma^2}\right)\left(\frac{\frac{1}{\sigma_{N-1}^2}}{\frac{1}{\sigma_{N-1}^2}+\frac{1}{\sigma^2}}\mu_{N-1} + \frac{\frac{1}{\sigma^2}}{\frac{1}{\sigma_{N-1}^2}+\frac{1}{\sigma^2}}x_N\right)^2 - \frac{\mu_{N-1}^2}{2\sigma_{N-1}^2} - \frac{x_N^2}{2\sigma^2}.
\end{aligned} \tag{2.310}$$

Then,

$$\begin{aligned}\mu_N &= \frac{\frac{1}{\sigma^2_{N-1}}}{\frac{1}{\sigma^2_{N-1}}+\frac{1}{\sigma^2}}\mu_{N-1} + \frac{\frac{1}{\sigma^2}}{\frac{1}{\sigma^2_{N-1}}+\frac{1}{\sigma^2}}x_N, \\ \sigma^2_N &= \frac{1}{\frac{1}{\sigma^2_{N-1}}+\frac{1}{\sigma^2}}.\end{aligned} \tag{2.311}$$

Therefore,

$$\begin{aligned}\frac{\mu_N}{\sigma^2_N} &= \frac{\mu_{N-1}}{\sigma^2_{N-1}} + \frac{x_N}{\sigma^2}, \\ \frac{1}{\sigma^2_N} &= \frac{1}{\sigma^2_{N-1}} + \frac{1}{\sigma^2}.\end{aligned} \tag{2.312}$$

2.40

Let $\mathbf{x}_1, \cdots, \mathbf{x}_N$ be variables such that

$$\begin{aligned}p(\mathbf{x}_n|\boldsymbol{\mu}) &= \mathcal{N}\left(\mathbf{x}_n|\boldsymbol{\mu}, \boldsymbol{\Sigma}\right), \\ p(\boldsymbol{\mu}) &= \mathcal{N}\left(\boldsymbol{\mu}|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0\right).\end{aligned} \tag{2.313}$$

By 2.34, the maximum likelihood solution for $\boldsymbol{\mu}$ is given by

$$\boldsymbol{\mu}_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n, \tag{2.314}$$

By the Bayes' theorem,

$$p(\boldsymbol{\mu}|\mathbf{X})p(\mathbf{X}) = p(\mathbf{X}|\boldsymbol{\mu})p(\boldsymbol{\mu}). \tag{2.315}$$

The logarithm of the right hand side excpt the terms independent of $\mathbf{X}$ and $\boldsymbol{\mu}$ can be written as

$$-\frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_n-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n-\boldsymbol{\mu}) - \frac{1}{2}(\boldsymbol{\mu}-\boldsymbol{\mu}_0)\boldsymbol{\Sigma}_0^{-1}(\boldsymbol{\mu}-\boldsymbol{\mu}_0)^{\intercal}. \tag{2.316}$$

The first term can be written as

$$\begin{aligned}
&-\frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_n-\boldsymbol{\mu}_{\mathrm{ML}}+\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n-\boldsymbol{\mu}_{\mathrm{ML}}+\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})\\
=&-\frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_n-\boldsymbol{\mu}_{\mathrm{ML}})^{\intercal}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n-\boldsymbol{\mu}_{\mathrm{ML}})-(\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Sigma}^{-1}\sum_{n=1}^{N}(\mathbf{x}_n-\boldsymbol{\mu}_{\mathrm{ML}})\\
&-\frac{N}{2}(\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu}).
\end{aligned}\tag{2.317}$$

The second term of the right hand side is zero. Then, the logarithm except the terms independent of $\mathbf{X}$ and $\boldsymbol{\mu}$ can be written as

$$\begin{aligned}
&-\frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_n-\boldsymbol{\mu}_{\mathrm{ML}})^{\intercal}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n-\boldsymbol{\mu}_{\mathrm{ML}})-\frac{N}{2}(\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})\\
&-\frac{1}{2}(\boldsymbol{\mu}-\boldsymbol{\mu}_0)\boldsymbol{\Sigma}_0^{-1}(\boldsymbol{\mu}-\boldsymbol{\mu}_0)^{\intercal}\\
=&-\frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_n-\boldsymbol{\mu}_{\mathrm{ML}})^{\intercal}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n-\boldsymbol{\mu}_{\mathrm{ML}})-\frac{1}{2}(\boldsymbol{\mu}-\boldsymbol{\mu}_N)^{\intercal}\boldsymbol{\Sigma}_N^{-1}(\boldsymbol{\mu}-\boldsymbol{\mu}_N)\\
&+\frac{1}{2}\boldsymbol{\mu}_N^{\intercal}\boldsymbol{\Sigma}_N^{-1}\boldsymbol{\mu}_N-\frac{N}{2}\boldsymbol{\mu}_{\mathrm{ML}}^{\intercal}\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{\mathrm{ML}},
\end{aligned}\tag{2.318}$$

where

$$\begin{aligned}
\boldsymbol{\mu}_N&=\left(N\boldsymbol{\Sigma}^{-1}+\boldsymbol{\Sigma}_0^{-1}\right)^{-1}\left(N\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{\mathrm{ML}}+\boldsymbol{\Sigma}_0^{-1}\boldsymbol{\mu}_0\right),\\
\boldsymbol{\Sigma}_N&=\left(N\boldsymbol{\Sigma}^{-1}+\boldsymbol{\Sigma}_0^{-1}\right)^{-1}.
\end{aligned}\tag{2.319}$$

Therefore,

$$p(\boldsymbol{\mu}|\mathbf{X})=\mathcal{N}(\boldsymbol{\mu}|\boldsymbol{\mu}_N,\boldsymbol{\Sigma}_N).\tag{2.320}$$

2.41

By the definition,

$$\mathrm{Gam}(\lambda|a,b)=\frac{b^a}{\Gamma(a)}\lambda^{a-1}\exp(-b\lambda).\tag{2.321}$$

Then,

$$\int_0^\infty \mathrm{Gam}(\lambda|a,b)d\lambda=\frac{b^a}{\Gamma(a)}\int_0^\infty \lambda^{a-1}\exp(-b\lambda)d\lambda.\tag{2.322}$$

By the transformation

$$\lambda' = b\lambda, \tag{2.323}$$

the right hand side can be written as

$$\frac{b^a}{\Gamma(a)} \int_0^\infty \left(\frac{\lambda'}{b}\right)^{a-1} \exp(-\lambda') \frac{1}{b} d\lambda' = \frac{1}{\Gamma(a)} \int_0^\infty \lambda'^{a-1} \exp(-\lambda') d\lambda'. \tag{2.324}$$

The right hand side can be written as

$$\frac{1}{\Gamma(a)} \Gamma(a) = 1. \tag{2.325}$$

Therefore,

$$\int_0^\infty \mathrm{Gam}(\lambda|a, b) d\lambda = 1. \tag{2.326}$$

2.42

Let λ be a variable such that

$$p(\lambda) = \mathrm{Gam}(\lambda|a, b). \tag{2.327}$$

By the definition,

$$\mathrm{Gam}(\lambda|a, b) = \frac{b^a}{\Gamma(a)} \lambda^{a-1} \exp(-b\lambda). \tag{2.328}$$

(a)

We have

$$\mathrm{E}\,\lambda = \frac{b^a}{\Gamma(a)} \int_0^\infty \lambda^a \exp\left(-\frac{\lambda}{b}\right) d\lambda. \tag{2.329}$$

By the transformation

$$\lambda' = b\lambda, \tag{2.330}$$

the right hand side can be written as

$$\frac{b^a}{\Gamma(a)} \int_0^\infty \left(\frac{\lambda'}{b}\right)^{a} \exp(-\lambda') \frac{1}{b} d\lambda' = \frac{1}{b\Gamma(a)} \int_0^\infty \lambda'^{a} \exp(-\lambda') d\lambda'. \tag{2.331}$$

The right hand side can be written as

$$\frac{1}{b\Gamma(a)} \Gamma(a+1) = \frac{a}{b}. \tag{2.332}$$

Therefore,

$$\mathrm{E}\,\lambda = \frac{a}{b}. \tag{2.333}$$

(b)

We have

$$\mathrm{E}\,\lambda^2 = \frac{b^a}{\Gamma(a)} \int_0^\infty \lambda^{a+1} \exp\left(-\frac{\lambda}{b}\right) d\lambda. \tag{2.334}$$

By the transformation

$$\lambda' = b\lambda, \tag{2.335}$$

the right hand side can be written as

$$\frac{b^a}{\Gamma(a)} \int_0^\infty \left(\frac{\lambda'}{b}\right)^{a+1} \exp(-\lambda')\frac{1}{b} d\lambda' = \frac{1}{b^2\Gamma(a)} \int_0^\infty \lambda'^{a+1} \exp(-\lambda') d\lambda'. \tag{2.336}$$

The right hand side can be written as

$$\frac{1}{b^2\Gamma(a)}\Gamma(a+2) = \frac{a(a+1)}{b^2}. \tag{2.337}$$

Then,

$$\mathrm{E}\,\lambda^2 = \frac{a(a+1)}{b^2}. \tag{2.338}$$

We have

$$\mathrm{var}\,\lambda = \mathrm{E}\,\lambda^2 - (\mathrm{E}\,\lambda)^2. \tag{2.339}$$

Therefore,

$$\mathrm{var}\,\lambda = \frac{a}{b^2}. \tag{2.340}$$

(c)

Setting the derivative of $\mathrm{Gam}(\lambda|a,b)$ with respect to λ to zero gives

$$0 = \frac{b^a}{\Gamma(a)} \left(\frac{a-1}{\lambda} - b\right) \lambda^{a-1} \exp\left(-\frac{\lambda}{b}\right). \tag{2.341}$$

Therefore,

$$\mathrm{mode}\,\lambda = \frac{a-1}{b}. \tag{2.342}$$

2.43

Let

$$p\left(x|\sigma^2, q\right) = \frac{q}{2\Gamma(\frac{1}{q})} \left(2\sigma^2\right)^{-\frac{1}{q}} \exp\left(-\frac{|x|^q}{2\sigma^2}\right). \tag{2.343}$$

(a)

We have

$$\int_{-\infty}^{\infty} p\left(x|\sigma^2, q\right) dx = \frac{q}{\Gamma(\frac{1}{q})} \left(2\sigma^2\right)^{-\frac{1}{q}} \int_0^{\infty} \exp\left(-\frac{x^q}{2\sigma^2}\right) dx. \tag{2.344}$$

By the transformation

$$x' = \frac{x^q}{2\sigma^2}, \tag{2.345}$$

the right hand side can be written as

$$\begin{aligned} &\frac{q}{\Gamma(\frac{1}{q})} \left(2\sigma^2\right)^{-\frac{1}{q}} \int_0^{\infty} \exp(-x') \left(2\sigma^2\right)^{\frac{1}{q}} \frac{1}{q} x^{\frac{1}{q}-1} dx' \\ =&\frac{1}{\Gamma(\frac{1}{q})} \int_0^{\infty} x^{\frac{1}{q}-1} \exp(-x') dx'. \end{aligned} \tag{2.346}$$

The right hand side can be written as

$$\frac{1}{\Gamma(\frac{1}{q})} \Gamma\left(\frac{1}{q}\right) = 1. \tag{2.347}$$

Therefore,

$$\int_{-\infty}^{\infty} p\left(x|\sigma^2, q\right) dx = 1. \tag{2.348}$$

(b)

We have

$$p\left(x|\sigma^2, 2\right) = \frac{1}{\Gamma(\frac{1}{2})} \left(2\sigma^2\right)^{-\frac{1}{2}} \exp\left(-\frac{x^2}{2\sigma^2}\right). \tag{2.349}$$

Therefore,

$$p\left(x|\sigma^2, 2\right) = \mathcal{N}\left(x|0, \sigma^2\right). \tag{2.350}$$

(c)

Let $\mathbf{t} = (t_1, \cdots, t_N)^\intercal$ and $\mathbf{X} = \{\mathbf{x}_1, \cdots, \mathbf{x}_N\}$ such that

$$t_n = y(\mathbf{x}_n, \mathbf{w}) + \epsilon_n, \tag{2.351}$$

where

$$p(\epsilon_n) = p\left(\epsilon_n|\sigma^2, q\right). \tag{2.352}$$

Then, the logarithm of $p(\epsilon_n)$ except the terms independent of $\mathbf{w}$ and σ^2 can be written as

$$-\frac{|\epsilon_n|^q}{2\sigma^2} - \frac{1}{q}\ln\left(2\sigma^2\right). \tag{2.353}$$

Therefore, the logarithm of $p\left(\mathbf{t}|\mathbf{X}, \mathbf{w}, \sigma^2\right)$ except the terms independent of $\mathbf{w}$ and σ^2 can be written as

$$-\frac{1}{2\sigma^2}\sum_{n=1}^{N}|y(\mathbf{x}_n, \mathbf{w}) - t_n|^q - \frac{N}{q}\ln\left(2\sigma^2\right). \tag{2.354}$$

2.44

Let $x_1, \cdots, x_N$ be variables such that

$$\begin{aligned} p(x_n|\mu, \tau) &= \mathcal{N}\left(x_n|\mu, \tau^{-1}\right), \\ p(\mu, \tau) &= \mathcal{N}\left(\mu|\mu_0, (\beta\tau)^{-1}\right)\mathrm{Gam}(\tau|a, b). \end{aligned} \tag{2.355}$$

By the Bayes' theorem,

$$p(\mu, \tau|\mathbf{x})p(\mathbf{x}) = p(\mathbf{x}|\mu, \tau)p(\mu, \tau). \tag{2.356}$$

The logarithm of the right hand side except the terms independent of $\mathbf{x}$, μ and τ can be written as

$$\begin{aligned} &\frac{N}{2}\ln\tau - \frac{\tau}{2}\sum_{n=1}^{N}(x_n - \mu)^2 + \frac{1}{2}\ln\tau - \frac{\beta\tau}{2}(\mu - \mu_0)^2 + (a-1)\ln\tau - b\tau \\ &= \left(a + \frac{N-1}{2}\right)\ln\tau - \frac{\tau}{2}\sum_{n=1}^{N}(x_n - \mu)^2 - \frac{\beta\tau}{2}(\mu - \mu_0)^2 - b\tau. \end{aligned} \tag{2.357}$$

Let

$$\bar{x} = \frac{1}{N}\sum_{n=1}^{N}x_n. \tag{2.358}$$

Then,

$$\sum_{n=1}^{N}(x_n - \mu)^2 = \sum_{n=1}^{N}(x_n - \bar{x} + \bar{x} - \mu)^2. \tag{2.359}$$

The right hand side can be written as

$$\begin{aligned}&\sum_{n=1}^{N}(x_n-\bar{x})^2+2(\bar{x}-\mu)\sum_{n=1}^{N}(x_n-\bar{x})+N(\bar{x}-\mu)^2\\=&\sum_{n=1}^{N}(x_n-\bar{x})^2+N(\bar{x}-\mu)^2.\end{aligned}\tag{2.360}$$

Then, the logarithm except the terms independent of $\mathbf{x}$, μ and τ can be written as

$$\left(a+\frac{N-1}{2}\right)\ln\tau-\frac{N\tau}{2}(\bar{x}-\mu)^2-\frac{\beta\tau}{2}(\mu-\mu_0)^2-b\tau-\frac{\tau}{2}\sum_{n=1}^{N}(x_n-\bar{x})^2.\tag{2.361}$$

The second and third terms can be written as

$$\begin{aligned}&-\frac{N\tau}{2}(\bar{x}-\mu)^2-\frac{\beta\tau}{2}(\mu-\mu_0)^2\\=&-\frac{(N+\beta)\tau}{2}\left(\mu-\frac{N\bar{x}+\beta\mu_0}{N+\beta}\right)^2+\frac{(N\bar{x}+\beta\mu_0)^2\tau}{2(N+\beta)}-\frac{N\tau}{2}\bar{x}^2-\frac{\beta\tau}{2}\mu_0^2.\end{aligned}\tag{2.362}$$

The second, third and forth terms on the right hand side can be written as

$$\frac{(N\bar{x}+\beta\mu_0)^2\tau-(N+\beta)N\tau\bar{x}^2-(N+\beta)\beta\tau\mu_0^2}{2(N+\beta)}=-\frac{N\beta\tau(\bar{x}-\mu_0)^2}{2(N+\beta)}.\tag{2.363}$$

Then, the logrithm except the terms independent of $\mathbf{x}$, μ and τ can be written as

$$\begin{aligned}&-\frac{(N+\beta)\tau}{2}\left(\mu-\frac{N\bar{x}+\beta\mu_0}{N+\beta}\right)^2\\&+\left(a+\frac{N-1}{2}\right)\ln\tau-\left(b+\frac{N\beta(\bar{x}-\mu_0)^2}{2(N+\beta)}+\frac{1}{2}\sum_{n=1}^{N}(x_n-\bar{x})^2\right)\tau.\end{aligned}\tag{2.364}$$

Therefore,

$$p(\mu,\tau|\mathbf{x})=\mathcal{N}\left(\mu|\mu_N,\tau_N^{-1}\right)\mathrm{Gam}\left(\tau|a_N,b_N\right),\tag{2.365}$$

where

$$\begin{aligned}\mu_N &= \frac{N\bar{x} + \beta\mu_0}{N+\beta},\\ \tau_N &= (N+\beta)\tau,\\ a_N &= a + \frac{N+1}{2},\\ b_N &= b + \frac{N\beta(\bar{x}-\mu_0)^2}{2(N+\beta)} + \frac{1}{2}\sum_{n=1}^{N}(x_n - \bar{x})^2.\end{aligned} \tag{2.366}$$

2.45

Let $\mathbf{x}_1, \cdots, \mathbf{x}_N$ be variables in D dimensions such that

$$\begin{aligned}p(\mathbf{x}_n|\mathbf{\Lambda}) &= \mathcal{N}\left(\mathbf{x}_n|\boldsymbol{\mu}, \mathbf{\Lambda}^{-1}\right),\\ p(\mathbf{\Lambda}) &= \mathcal{W}(\mathbf{\Lambda}|\mathbf{W}, \nu),\end{aligned} \tag{2.367}$$

where

$$\mathcal{W}(\mathbf{\Lambda}|\mathbf{W}, \nu) = B(\mathbf{W}, \nu)|\det \mathbf{\Lambda}|^{\frac{\nu-D-1}{2}} \exp\left(-\frac{1}{2}\operatorname{tr}\left(\mathbf{W}^{-1}\mathbf{\Lambda}\right)\right). \tag{2.368}$$

By the Bayes' theorem,

$$p(\mathbf{\Lambda}|\mathbf{X})p(\mathbf{X}) = p(\mathbf{X}|\mathbf{\Lambda})p(\mathbf{\Lambda}). \tag{2.369}$$

The logarithm of the right hand side except the terms independent of $\mathbf{\Lambda}$ can be written as

$$\begin{aligned}&-\frac{N}{2}\ln\left|\det\left(\mathbf{\Lambda}^{-1}\right)\right| - \frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_n - \boldsymbol{\mu})^{\intercal}\mathbf{\Lambda}(\mathbf{x}_n - \boldsymbol{\mu})\\ &+\frac{\nu-D-1}{2}\ln|\det\mathbf{\Lambda}| - \frac{1}{2}\operatorname{tr}\left(\mathbf{W}^{-1}\mathbf{\Lambda}\right)\\ =&\frac{\nu+N-D-1}{2}\ln|\det\mathbf{\Lambda}| - \frac{1}{2}\operatorname{tr}\left(\left(\mathbf{W}^{-1}+\mathbf{S}\right)\mathbf{\Lambda}\right),\end{aligned} \tag{2.370}$$

where

$$\mathbf{S} = \sum_{n=1}^{N}(\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{x}_n - \boldsymbol{\mu})^{\intercal}. \tag{2.371}$$

Then,

$$p(\mathbf{\Lambda}|\mathbf{X}) = \mathcal{W}\left(\mathbf{\Lambda}|\left(\mathbf{W}^{-1}+\mathbf{S}\right)^{-1}, \nu+N\right). \tag{2.372}$$

Therefore, $\mathcal{W}$ is a conjugate prior distribution of $\mathbf{\Lambda}$.

2.46

Let x be a variable such that

$$\begin{aligned} p(x|\tau) &= \mathcal{N}\left(x|\mu, \tau^{-1}\right), \\ p(\tau) &= \mathrm{Gam}(\tau|a, b). \end{aligned} \tag{2.373}$$

By marginalisation,

$$p(x) = \int_0^\infty p(x|\tau)p(\tau)d\tau. \tag{2.374}$$

The right hand side can be written as

$$\begin{aligned} &\int_0^\infty \left(2\pi\tau^{-1}\right)^{-\frac{1}{2}} \exp\left(-\frac{\tau}{2}(x-\mu)^2\right) \frac{b^a}{\Gamma(a)}\tau^{a-1}\exp(-b\tau)d\tau \\ =&(2\pi)^{-\frac{1}{2}}\frac{b^a}{\Gamma(a)}\int_0^\infty \tau^{a-\frac{1}{2}} \exp\left(-\left(b+\frac{(x-\mu)^2}{2}\right)\tau\right)d\tau. \end{aligned} \tag{2.375}$$

By the transformation

$$\tau' = \left(b+\frac{(x-\mu)^2}{2}\right)\tau, \tag{2.376}$$

the integral of the right hand side can be written as

$$\begin{aligned} &\int_0^\infty \left(\frac{\tau'}{b+\frac{(x-\mu)^2}{2}}\right)^{a-\frac{1}{2}} \exp(-\tau')\frac{1}{b+\frac{(x-\mu)^2}{2}}d\tau' \\ =&\Gamma\left(a+\frac{1}{2}\right)\left(b+\frac{(x-\mu)^2}{2}\right)^{-a-\frac{1}{2}}. \end{aligned} \tag{2.377}$$

Then,

$$p(x) = (2\pi)^{-\frac{1}{2}}\frac{\Gamma(a+\frac{1}{2})}{\Gamma(a)}b^a\left(b+\frac{(x-\mu)^2}{2}\right)^{-a-\frac{1}{2}}. \tag{2.378}$$

By the transformation

$$\begin{aligned} \nu &= 2a, \\ \lambda &= \frac{a}{b}, \end{aligned} \tag{2.379}$$

the right hand side can be written as

$$\begin{aligned}&(2\pi)^{-\frac{1}{2}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\left(\frac{\nu}{2\lambda}\right)^{-\frac{1}{2}}\left(1+\frac{(x-\mu)^2}{\frac{\nu}{\lambda}}\right)^{-\frac{\nu+1}{2}}\\ =&\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\left(\frac{\lambda}{\pi\nu}\right)^{\frac{1}{2}}\left(1+\frac{\lambda}{\nu}(x-\mu)^2\right)^{-\frac{\nu+1}{2}}.\end{aligned} \tag{2.380}$$

Therefore,

$$p(x)=\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\left(\frac{\lambda}{\pi\nu}\right)^{\frac{1}{2}}\left(1+\frac{\lambda}{\nu}(x-\mu)^2\right)^{-\frac{\nu+1}{2}}. \tag{2.381}$$

2.47

Let

$$\mathrm{St}(x|\mu,\lambda,\nu)=\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\left(\frac{\lambda}{\pi\nu}\right)^{\frac{1}{2}}\left(1+\frac{\lambda}{\nu}(x-\mu)^2\right)^{-\frac{\nu+1}{2}}. \tag{2.382}$$

By the transformation

$$\frac{1}{y}=\frac{\lambda}{\nu}(x-\mu)^2, \tag{2.383}$$

the right hand side except the terms independent of x can be written as

$$\left(1+\frac{1}{y}\right)^{-\frac{\lambda(x-\mu)^2}{2}y-\frac{1}{2}}. \tag{2.384}$$

By the property

$$\lim_{x\to\infty}\left(1+\frac{1}{x}\right)^{x}=e, \tag{2.385}$$

we have

$$\lim_{y\to\infty}\left(1+\frac{1}{y}\right)^{-\frac{\lambda(x-\mu)^2}{2}y-\frac{1}{2}}=\exp\left(-\frac{\lambda}{2}(x-\mu)^2\right). \tag{2.386}$$

Therefore,

$$\lim_{\nu\to\infty}\mathrm{St}(x|\mu,\lambda,\nu)=\mathcal{N}(x|\mu,\lambda^{-1}). \tag{2.387}$$

2.48

Let $\mathbf{x}$ be a variable in D dimensions such that

$$\begin{aligned} p(\mathbf{x}|\eta) &= \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, (\eta\boldsymbol{\Lambda})^{-1}\right), \\ p(\eta) &= \mathrm{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right). \end{aligned} \tag{2.388}$$

By marginalisation,

$$p(\mathbf{x}) = \int_0^\infty p(\mathbf{x}|\eta)p(\eta)d\eta. \tag{2.389}$$

The right hand side can be written as

$$\begin{aligned} &\int_0^\infty (2\pi)^{-\frac{D}{2}} \left|\det(\eta\boldsymbol{\Lambda})^{-1}\right|^{-\frac{1}{2}} \exp\left(-\frac{\eta}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})\right) \frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})}\eta^{\frac{\nu}{2}-1}\exp\left(-\frac{\nu}{2}\eta\right)d\eta \\ =&(2\pi)^{-\frac{D}{2}}\frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})}|\det\boldsymbol{\Lambda}|^{\frac{1}{2}}\int_0^\infty \eta^{\frac{D+\nu}{2}-1}\exp\left(-\frac{\nu+(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}{2}\eta\right)d\eta. \end{aligned} \tag{2.390}$$

By the transformation

$$\eta' = \frac{\nu+(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}{2}\eta, \tag{2.391}$$

the integral of the right hand side can be written as

$$\begin{aligned} &\int_0^\infty \left(\frac{2\eta'}{\nu+(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}\right)^{\frac{D+\nu}{2}-1}\exp(-\eta')\frac{2}{\nu+(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}d\eta' \\ =&\left(\frac{2}{\nu+(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}\right)^{\frac{D+\nu}{2}}\int_0^\infty {\eta'}^{\frac{D+\nu}{2}-1}\exp(-\eta')d\eta'. \end{aligned} \tag{2.392}$$

Then,

$$p(\mathbf{x}) = (2\pi)^{-\frac{D}{2}}\frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})}|\det\boldsymbol{\Lambda}|^{\frac{1}{2}}\left(\frac{2}{\nu+(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}\right)^{\frac{D+\nu}{2}}\Gamma\left(\frac{D+\nu}{2}\right). \tag{2.393}$$

The right hand side can be written as

$$\begin{aligned} &(2\pi)^{-\frac{D}{2}}\frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})}|\det\boldsymbol{\Lambda}|^{\frac{1}{2}}\left(\frac{\nu}{2}\right)^{-\frac{D}{2}}\left(\frac{\nu}{2}\right)^{\frac{D+\nu}{2}}\left(\frac{2}{\nu+(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}\right)^{\frac{D+\nu}{2}} \\ =&(2\pi)^{-\frac{D}{2}}\frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})}|\det\boldsymbol{\Lambda}|^{\frac{1}{2}}\left(\frac{\nu}{2}\right)^{-\frac{D}{2}}\left(1+\frac{(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}{\nu}\right)^{-\frac{D+\nu}{2}}. \end{aligned} \tag{2.394}$$

Therefore,

$$p(\mathbf{x}) = \frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})} \frac{|\det \mathbf{\Lambda}|^{\frac{1}{2}}}{(\pi\nu)^{\frac{D}{2}}} \left(1 + \frac{(\mathbf{x}-\boldsymbol{\mu})^\intercal \mathbf{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}{\nu}\right)^{-\frac{D+\nu}{2}}. \tag{2.395}$$

2.49

Let $\mathbf{x}$ be a variable such that

$$p(\mathbf{x}) = \mathrm{St}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{\Lambda}, \nu), \tag{2.396}$$

where

$$\mathrm{St}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{\Lambda}, \nu) = \int \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, (\eta\mathbf{\Lambda})^{-1}\right) \mathrm{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta. \tag{2.397}$$

(a)

We have

$$\mathrm{E}\,\mathbf{x} = \int \mathbf{x}\mathrm{St}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{\Lambda}, \nu) d\mathbf{x}. \tag{2.398}$$

The right hand side can be written as

$$\begin{aligned} &\int \mathbf{x} \left(\int \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, (\eta\mathbf{\Lambda})^{-1}\right) \mathrm{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta \right) d\mathbf{x} \\ &= \int \left(\int \mathbf{x} \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, (\eta\mathbf{\Lambda})^{-1}\right) d\mathbf{x} \right) \mathrm{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta. \end{aligned} \tag{2.399}$$

The right hand side can be written as

$$\boldsymbol{\mu} \int \mathrm{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta = \boldsymbol{\mu}. \tag{2.400}$$

Therefore,

$$\mathrm{E}\,\mathbf{x} = \boldsymbol{\mu}. \tag{2.401}$$

(b)

By (a), we have

$$\mathrm{cov}\,\mathbf{x} = \int (\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\intercal \mathrm{St}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{\Lambda}, \nu) d\mathbf{x}. \tag{2.402}$$

The right hand side can be written as

$$\begin{aligned}&\int (\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\left(\int \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu},(\eta\boldsymbol{\Lambda})^{-1}\right)\mathrm{Gam}\left(\eta\,|\,\frac{\nu}{2},\frac{\nu}{2}\right)d\eta\right)d\mathbf{x}\\ =&\int\left(\int (\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu},(\eta\boldsymbol{\Lambda})^{-1}\right)d\mathbf{x}\right)\mathrm{Gam}\left(\eta\,|\,\frac{\nu}{2},\frac{\nu}{2}\right)d\eta.\end{aligned} \tag{2.403}$$

The right hand side can be written as

$$\int (\eta\boldsymbol{\Lambda})^{-1}\mathrm{Gam}\left(\eta\,|\,\frac{\nu}{2},\frac{\nu}{2}\right)d\eta=\frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})}\left(\int \eta^{\frac{\nu}{2}-2}\exp\left(-\frac{\nu}{2}\eta\right)d\eta\right)\boldsymbol{\Lambda}^{-1}. \tag{2.404}$$

By the transformation

$$\eta'=\frac{\nu}{2}\eta, \tag{2.405}$$

the integral of the right hand side can be written as

$$\int\left(\frac{2}{\nu}\eta'\right)^{\frac{\nu}{2}-2}\exp(-\eta')\frac{2}{\nu}d\eta'=\left(\frac{2}{\nu}\right)^{\frac{\nu}{2}-1}\Gamma\left(\frac{\nu}{2}-1\right). \tag{2.406}$$

Then,

$$\mathrm{cov}\,\mathbf{x}=\frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})}\left(\frac{2}{\nu}\right)^{\frac{\nu}{2}-1}\Gamma\left(\frac{\nu}{2}-1\right)\boldsymbol{\Lambda}^{-1}. \tag{2.407}$$

Therefore,

$$\mathrm{cov}\,\mathbf{x}=\frac{\nu}{\nu-2}\boldsymbol{\Lambda}^{-1}. \tag{2.408}$$

(c)

Setting the derivative of $p(\mathbf{x})$ to zero gives

$$\mathbf{0}=-\frac{1}{2}\left(\boldsymbol{\Lambda}+\boldsymbol{\Lambda}^{\intercal}\right)(\mathbf{x}-\boldsymbol{\mu})\int \eta\mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu},(\eta\boldsymbol{\Lambda})^{-1}\right)\mathrm{Gam}\left(\eta\,|\,\frac{\nu}{2},\frac{\nu}{2}\right)d\eta. \tag{2.409}$$

Therefore,

$$\mathrm{mode}\,\mathbf{x}=\boldsymbol{\mu}. \tag{2.410}$$

2.50

Let

$$\mathrm{St}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Lambda},\nu)=\frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})}\frac{(\det\boldsymbol{\Lambda})^{\frac{1}{2}}}{(\pi\nu)^{\frac{D}{2}}}\left(1+\frac{(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}{\nu}\right)^{-\frac{D+\nu}{2}}. \quad (2.411)$$

By the transformation

$$y=\frac{\nu}{(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}, \quad (2.412)$$

the right hand side except the terms independent of $\mathbf{x}$ can be written as

$$\left(1+\frac{1}{y}\right)^{-\frac{(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}{2}y-\frac{D}{2}}. \quad (2.413)$$

By the property

$$\lim_{x\to\infty}\left(1+\frac{1}{x}\right)^{x}=e, \quad (2.414)$$

we have

$$\lim_{y\to\infty}\left(1+\frac{1}{y}\right)^{-\frac{(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}{2}y-\frac{D}{2}}=\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})\right). \quad (2.415)$$

Therefore,

$$\lim_{\nu\to\infty}\mathrm{St}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Lambda},\nu)=\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Lambda}^{-1}). \quad (2.416)$$

2.51

(a)

We have

$$\exp(iA)\exp(-iA)=1. \quad (2.417)$$

The left hand side can be written as

$$(\cos A+i\sin A)(\cos A-i\sin A)=\cos^2 A+\sin^2 A. \quad (2.418)$$

Therefore,

$$\cos^2 A+\sin^2 A=1. \quad (2.419)$$

(b)

We have

$$\cos(A-B) = \mathrm{Re}\left(\exp\left(i(A-B)\right)\right). \tag{2.420}$$

The right hand side can be written as

$$\mathrm{Re}\left(\exp(iA)\exp(-iB)\right) = \mathrm{Re}\left((\cos A + i\sin A)(\cos B - i\sin B)\right). \tag{2.421}$$

Therefore,

$$\cos(A-B) = \cos A\cos B + \sin A\sin B. \tag{2.422}$$

(c)

We have

$$\sin(A-B) = \mathrm{Im}\left(\exp\left(i(A-B)\right)\right). \tag{2.423}$$

The right hand side can be written as

$$\mathrm{Im}\left(\exp(iA)\exp(-iB)\right) = \left((\cos A + i\sin A)(\cos B - i\sin B)\right). \tag{2.424}$$

Therefore,

$$\sin(A-B) = \sin A\cos B - \cos A\sin B. \tag{2.425}$$

2.52

Let

$$f(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)}\exp\left(m\cos(\theta-\theta_0)\right), \tag{2.426}$$

where

$$I_0(m) = \frac{1}{2\pi}\int_0^{2\pi}\exp(m\cos\theta)d\theta. \tag{2.427}$$

By the Taylor series

$$\cos\alpha = 1 - \frac{1}{2}\alpha^2 + O\left(\alpha^4\right), \tag{2.428}$$

the right hand side can be written as

$$\begin{aligned}&\frac{\exp\left(m\left(1-\frac{1}{2}(\theta-\theta_0)^2 + O\left((\theta-\theta_0)^4\right)\right)\right)}{\int_0^{2\pi}\exp\left(m\left(1-\frac{1}{2}\theta^2+O(\theta^4)\right)\right)d\theta}\\ =&\exp\left(-\frac{m}{2}(\theta-\theta_0)^2\right)\frac{\exp\left(mO\left((\theta-\theta_0)^4\right)\right)}{\int_0^{2\pi}\exp\left(m\left(-\frac{1}{2}\theta^2+O(\theta^4)\right)\right)d\theta}.\end{aligned} \tag{2.429}$$

Therefore,

$$\lim_{m\to\infty} f(\theta|\theta_0, m) = \mathcal{N}\left(\theta|\theta_0, m^{-1}\right). \tag{2.430}$$

2.53

Let

$$\sum_{n=1}^{N} \sin(\theta_n - \theta_0) = 0. \tag{2.431}$$

The left hand side can be written as

$$\sum_{n=1}^{N} (\sin\theta_n \cos\theta_0 - \cos\theta_n \sin\theta_0) = \cos\theta_0 \sum_{n=1}^{N} \sin\theta_n - \sin\theta_0 \sum_{n=1}^{N} \cos\theta_n. \tag{2.432}$$

Therefore,

$$\theta_0 = \arctan\left(\frac{\sum_{n=1}^{N} \sin\theta_n}{\sum_{n=1}^{N} \cos\theta_n}\right). \tag{2.433}$$

2.54

Let

$$f(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp\left(m\cos(\theta - \theta_0)\right), \tag{2.434}$$

where

$$I_0(m) = \frac{1}{2\pi} \int_0^{2\pi} \exp(m\cos\theta) d\theta. \tag{2.435}$$

Setting the first and seconnd derivatives with respect to θ to zero gives

$$\begin{aligned} 0 &= -m\sin(\theta - \theta_0) f(\theta|\theta_0, m), \\ 0 &= \left(m^2 \sin^2(\theta - \theta_0) - m\cos(\theta - \theta_0)\right) f(\theta|\theta_0, m). \end{aligned} \tag{2.436}$$

Therefore,

$$\begin{aligned} \underset{\theta}{\operatorname{argmax}}\, f(\theta|\theta_0, m) &= \theta_0, \\ \underset{\theta}{\operatorname{argmin}}\, f(\theta|\theta_0, m) &= \theta_0 - \pi\,\mathrm{sgn}(\theta_0 - \pi). \end{aligned} \tag{2.437}$$

2.55

(a)

Let $\theta_1, \cdots, \theta_N$ be variables such that

$$p(\theta_n) = f(\theta_n|\theta_0, m), \tag{2.438}$$

where

$$f(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp\left(m\cos(\theta - \theta_0)\right),$$
$$I_0(m) = \frac{1}{2\pi}\int_0^{2\pi} \exp(m\cos\theta)d\theta. \tag{2.439}$$

Then,

$$\ln\left(\prod_{n=1}^{N} p(\theta_n|\theta_0, m)\right) = -\frac{N}{2}\ln\left(2\pi I_0(m)\right) + m\sum_{n=1}^{N}\cos(\theta_n - \theta_0). \tag{2.440}$$

Setting the derivative with respect to θ_0 to zero gives

$$0 = m\sum_{n=1}^{N}\sin(\theta_n - \theta_0). \tag{2.441}$$

Therefore, by 2.53, the maximum likelihood solution for θ_0 is given by

$$\theta_0^{\mathrm{ML}} = \arctan\left(\frac{\sum_{n=1}^{N}\sin\theta_n}{\sum_{n=1}^{N}\cos\theta_n}\right). \tag{2.442}$$

(b)

Let

$$\bar{r}\cos\bar{\theta} = \frac{1}{N}\sum_{n=1}^{N}\cos\theta_n,$$
$$\bar{r}\sin\bar{\theta} = \frac{1}{N}\sum_{n=1}^{N}\sin\theta_n. \tag{2.443}$$

By (a),

$$\bar{\theta} = \theta_0^{\mathrm{ML}}. \tag{2.444}$$

We have

$$\frac{1}{N}\sum_{n=1}^{N}\cos\left(\theta_n - \theta_0^{\mathrm{ML}}\right) = \left(\frac{1}{N}\sum_{n=1}^{N}\cos\theta_n\right)\cos\theta_0^{\mathrm{ML}} + \left(\frac{1}{N}\sum_{n=1}^{N}\sin\theta_n\right)\sin\theta_0^{\mathrm{ML}}. \tag{2.445}$$

The right hand side can be written as

$$\bar{r}\cos^2\bar{\theta} + \bar{r}\sin^2\bar{\theta} = \bar{r}. \tag{2.446}$$

Therefore,

$$\frac{1}{N}\sum_{n=1}^{N}\cos\left(\theta_n - \theta_0^{\mathrm{ML}}\right) = \bar{r}. \tag{2.447}$$

2.56

(a)

Let

$$\mathrm{Beta}(\mu|a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\mu^{a-1}(1-\mu)^{b-1}. \tag{2.448}$$

The right hand side can be written as

$$\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\exp\left((a-1)\ln\mu + (b-1)\ln(1-\mu)\right) \tag{2.449}$$

Therefore, the natural parameters are given by

$$\boldsymbol{\eta} = \begin{bmatrix} a-1 \\ b-1 \end{bmatrix}.$$

(b)

Let

$$\mathrm{Gam}(\lambda|a,b) = \frac{b^a}{\Gamma(a)}\lambda^{a-1}\exp(-b\lambda). \tag{2.450}$$

The right hand side can be written as

$$\frac{b^a}{\Gamma(a)}\exp\left((a-1)\ln\lambda - b\lambda\right). \tag{2.451}$$

Therefore, the natural parameters are given by

$$\boldsymbol{\eta} = \begin{bmatrix} a-1 \\ -b \end{bmatrix}.$$

(c)

Let

$$f(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp\left(m\cos(\theta - \theta_0)\right), \tag{2.452}$$

where

$$I_0(m) = \frac{1}{2\pi}\int_0^{2\pi} \exp(m\cos\theta)d\theta, \tag{2.453}$$

the right hand side can be written as

$$\frac{1}{2\pi I_0(m)} \exp(m\cos\theta_0\cos\theta + m\sin\theta_0\sin\theta). \tag{2.454}$$

Therefore, the natural parameters are given by

$$\boldsymbol{\eta} = \begin{bmatrix} m\cos\theta_0 \\ m\sin\theta_0 \end{bmatrix}.$$

2.57

By the definition,

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}}(\det\boldsymbol{\Sigma})^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right). \tag{2.455}$$

Therefore,

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = h(\mathbf{x})g(\boldsymbol{\eta})\exp\left(\boldsymbol{\eta}^\intercal\mathbf{u}(\mathbf{x})\right), \tag{2.456}$$

where

$$\begin{aligned} h(\mathbf{x}) &= (2\pi)^{-\frac{D}{2}}, \\ g(\boldsymbol{\eta}) &= (\det(-2\boldsymbol{\eta}_2))^{-\frac{1}{2}} \exp\left(\frac{1}{4}\boldsymbol{\eta}_1^\intercal\boldsymbol{\eta}_2^{-1}\boldsymbol{\eta}_1\right), \\ \boldsymbol{\eta} &= \begin{bmatrix} \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} \\ -\frac{1}{2}\boldsymbol{\Sigma}^{-1} \end{bmatrix}, \\ \mathbf{u}(\mathbf{x}) &= \begin{bmatrix} \mathbf{x} \\ \mathbf{x}\mathbf{x}^\intercal \end{bmatrix}. \end{aligned}$$

2.58

Let $\mathbf{x}$ be a variable such that

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta}) \exp\left(\boldsymbol{\eta}^\intercal \mathbf{u}(\mathbf{x})\right). \tag{2.457}$$

Then, taking the first derivative of

$$\int p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} = 1 \tag{2.458}$$

with respect to $\boldsymbol{\eta}$ gives

$$\nabla g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp\left(\boldsymbol{\eta}^\intercal \mathbf{u}(\mathbf{x})\right) d\mathbf{x} + g(\boldsymbol{\eta}) \int \mathbf{u}(\mathbf{x}) h(\mathbf{x}) \exp\left(\boldsymbol{\eta}^\intercal \mathbf{u}(\mathbf{x})\right) d\mathbf{x} = \mathbf{0}. \tag{2.459}$$

The left hand side can be written as

$$\frac{\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} \int p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} + \int \mathbf{u}(\mathbf{x}) p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} = \frac{\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} + \mathrm{E}\,\mathbf{u}(\mathbf{x}). \tag{2.460}$$

Therefore,

$$\mathrm{E}\,\mathbf{u}(\mathbf{x}) = -\frac{\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})}. \tag{2.461}$$

Thus,

$$\mathrm{E}\,\mathbf{u}(\mathbf{x}) = -\nabla \ln g(\boldsymbol{\eta}). \tag{2.462}$$

Taking the second derivative with respect to $\boldsymbol{\eta}$ gives

$$\begin{aligned}\nabla\nabla g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp\left(\boldsymbol{\eta}^\intercal \mathbf{u}(\mathbf{x})\right) d\mathbf{x} + 2\nabla g(\boldsymbol{\eta}) \int \mathbf{u}(\mathbf{x})^\intercal h(\mathbf{x}) \exp\left(\boldsymbol{\eta}^\intercal \mathbf{u}(\mathbf{x})\right) d\mathbf{x} \\ + g(\boldsymbol{\eta}) \int \mathbf{u}(\mathbf{x})\mathbf{u}(\mathbf{x})^\intercal h(\mathbf{x}) \exp\left(\boldsymbol{\eta}^\intercal \mathbf{u}(\mathbf{x})\right) d\mathbf{x} = \mathbf{O}.\end{aligned} \tag{2.463}$$

The left hand side can be written as

$$\begin{aligned}&\frac{\nabla\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} \int p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} + \frac{2\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} \int \mathbf{u}(\mathbf{x})^\intercal p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} + \int \mathbf{u}(\mathbf{x})\mathbf{u}(\mathbf{x})^\intercal p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} \\ =&\frac{\nabla\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} - 2\,\mathrm{E}\,\mathbf{u}(\mathbf{x})\,\mathrm{E}\,\mathbf{u}(\mathbf{x})^\intercal + \mathrm{E}\left(\mathbf{u}(\mathbf{x})\mathbf{u}(\mathbf{x})^\intercal\right).\end{aligned} \tag{2.464}$$

Therefore,

$$\mathrm{E}\left(\mathbf{u}(\mathbf{x})\mathbf{u}(\mathbf{x})^\intercal\right) = -\frac{\nabla\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} + \frac{2\nabla g(\boldsymbol{\eta})(\nabla g(\boldsymbol{\eta}))^\intercal}{g^2(\boldsymbol{\eta})}. \tag{2.465}$$

By the definition,

$$\operatorname{cov}\mathbf{u}(\mathbf{x}) = \mathrm{E}\left(\mathbf{u}(\mathbf{x})\mathbf{u}(\mathbf{x})^\intercal\right) - \mathrm{E}\,\mathbf{u}(\mathbf{x})\,\mathrm{E}\,\mathbf{u}(\mathbf{x})^\intercal. \tag{2.466}$$

Thus,

$$\operatorname{cov}\mathbf{u}(\mathbf{x}) = -\frac{\nabla\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} + \frac{\nabla g(\boldsymbol{\eta})(\nabla g(\boldsymbol{\eta}))^\intercal}{g^2(\boldsymbol{\eta})}. \tag{2.467}$$

Hence,

$$\operatorname{cov}\mathbf{u}(\mathbf{x}) = -\nabla\nabla \ln g(\boldsymbol{\eta}). \tag{2.468}$$

2.59

Let

$$p(x|\sigma) = \frac{1}{\sigma} f\left(\frac{x}{\sigma}\right). \tag{2.469}$$

Then

$$\int p(x|\sigma)dx = \frac{1}{\sigma}\int f\left(\frac{x}{\sigma}\right)dx. \tag{2.470}$$

By the transformation

$$x' = \frac{x}{\sigma}, \tag{2.471}$$

the right hand side can be written as

$$\frac{1}{\sigma}\int f(x')\sigma dx' = \int f(x')dx'. \tag{2.472}$$

Therefore, $p(x|\sigma)$ will be normalised if $f(x)$ is normalised.

2.60

Let $\mathbf{x}$ be a variable such that

$$\mathbf{x} \in \mathcal{R}_i \Rightarrow p(\mathbf{x}) = h_i, \tag{2.473}$$

where

$$\int_{\mathcal{R}_i} d\mathbf{x} = \Delta_i. \tag{2.474}$$

Since

$$\int p(\mathbf{x})d\mathbf{x} = 1, \tag{2.475}$$

we have

$$\sum_i h_i \Delta_i = 1. \tag{2.476}$$

Let N be the total number of observations and n_i be the number of observations which fall in $\mathcal{R}_i$. Then, the logarithm of the likelihood is given by

$$\ln\left(\prod_i {h_i}^{n_i}\right) = \sum_i n_i \ln h_i, \tag{2.477}$$

where

$$\sum_i n_i = N. \tag{2.478}$$

Setting the derivatives of

$$\sum_i n_i \ln h_i + \lambda\left(\sum_i h_i \Delta_i - 1\right) \tag{2.479}$$

with respect to h_i and λ to zero gives

$$\begin{aligned} \frac{n_i}{h_i} + \lambda\Delta_i &= 0, \\ \sum_i h_i \Delta_i - 1 &= 0. \end{aligned} \tag{2.480}$$

Then,

$$\begin{aligned} \lambda &= -N, \\ h_i &= \frac{n_i}{N\Delta_i}. \end{aligned} \tag{2.481}$$

Therefore, the maximum likelihood estimator for the $\{h_i\}$ is $\frac{n_i}{N\Delta_i}$.

2.61 (Incomplete)

Let $\mathbf{x}$ be a variable and $\mathbf{x}_1, \cdots, \mathbf{x}_N$ be observations. Let

$$p(\mathbf{x}) = \frac{K}{NV(\mathbf{x})}, \tag{2.482}$$

where

$$V(\mathbf{x}) = \int_{\|\mathbf{x}'-\mathbf{x}\| \leq \|\mathbf{x}_{(K)}-\mathbf{x}\|} d\mathbf{x}', \tag{2.483}$$

K is a constant and $\mathbf{x}_{(K)}$ is the Kth nearest observation from the point $\mathbf{x}$.

3 Linear Models for Regression

3.1

By the definition,

$$\tanh a = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)}. \tag{3.1}$$

The right hand side can be written as

$$\frac{1 - \exp(-2a)}{1 + \exp(-2a)} = \frac{2}{1 + \exp(-2a)} - 1. \tag{3.2}$$

Therefore,

$$\tanh a = 2\sigma(2a) - 1, \tag{3.3}$$

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}. \tag{3.4}$$

Let

$$y(x_n, \mathbf{w}) = w_0 + \sum_{m=1}^{M} w_j \sigma\left(\frac{x - \mu_j}{s}\right). \tag{3.5}$$

By the result above, the right hand side can be written as

$$w_0 + \sum_{m=1}^{M} w_m \frac{1 + \tanh\left(\frac{x-\mu_m}{2s}\right)}{2} = w_0 + \frac{1}{2}\sum_{m=1}^{M} w_m + \frac{1}{2}\sum_{m=1}^{M} w_m \tanh\left(\frac{x - \mu_m}{2s}\right). \tag{3.6}$$

Therefore, $y(x_n, \mathbf{w})$ is equivalent to

$$y(x_n, \mathbf{u}) = u_0 + \sum_{m=1}^{M} u_m \tanh\left(\frac{x - \mu_m}{2s}\right), \tag{3.7}$$

where

$$\begin{aligned} u_0 &= w_0 + \frac{1}{2}\sum_{m=1}^{M} w_m, \\ u_m &= \frac{1}{2} w_m. \end{aligned} \tag{3.8}$$

3.2 (Incomplete)

Let $\mathbf{\Phi}$ be an $N \times M$ matarix. Then, for any vector $\mathbf{v}$ in N dimensions,

$$\mathbf{\Phi} \left(\mathbf{\Phi}^\intercal \mathbf{\Phi} \right)^{-1} \mathbf{\Phi}^\intercal \mathbf{v} \tag{3.9}$$

is a projection of $\mathbf{v}$ onto the space spanned by the columns of $\mathbf{\Phi}$?

Additionally, for a vector $\mathbf{t}$ in N dimensions,

$$\left(\mathbf{\Phi}^\intercal \mathbf{\Phi} \right)^{-1} \mathbf{\Phi}^\intercal \mathbf{t} \tag{3.10}$$

is an orthogonal projection of $\mathbf{t}$ onto the space spanned by the columns of $\mathbf{\Phi}$?

3.3

Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} r_n \left(t_n - \mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n) \right)^2 . \tag{3.11}$$

The right hand side can be written as

$$\frac{1}{2} \| \mathbf{t}' - \mathbf{\Phi}' \mathbf{w} \|^2, \tag{3.12}$$

where

$$\mathbf{t}' = \begin{bmatrix} \sqrt{r_1} t_1 \\ \vdots \\ \sqrt{r_N} t_N \end{bmatrix}, \mathbf{\Phi}' = \begin{bmatrix} \sqrt{r_1} \boldsymbol{\phi}(\mathbf{x}_1)^\intercal \\ \vdots \\ \sqrt{r_N} \boldsymbol{\phi}(\mathbf{x}_N)^\intercal \end{bmatrix}.$$

Setting the derivative with respect to $\mathbf{w}$ to zero gives

$$\mathbf{0} = -\mathbf{\Phi}'^\intercal (\mathbf{t}' - \mathbf{\Phi}' \mathbf{w}). \tag{3.13}$$

Therefore,

$$\operatorname*{argmin}_{\mathbf{w}} E(\mathbf{w}) = \left(\mathbf{\Phi}'^\intercal \mathbf{\Phi}' \right)^{-1} \mathbf{\Phi}'^\intercal \mathbf{t}'. \tag{3.14}$$

3.4 (Incomplete)

Let

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(y(\mathbf{x}_n, \mathbf{w}) - t_n\right)^2, \tag{3.15}$$

where

$$\begin{aligned} y(\mathbf{x}, \mathbf{w}) &= w_0 + \sum_{m=1}^{M} w_m(x_m + \epsilon_m), \\ p(\epsilon_m) &= \mathcal{N}\left(\epsilon_m | 0, \sigma^2\right). \end{aligned} \tag{3.16}$$

Setting the derivative with respect to $\mathbf{w}$ to zero gives

$$\mathbf{0} = \sum_{n=1}^{N}\begin{bmatrix} 1 \\ \mathbf{x}_n + \boldsymbol{\epsilon}_n \end{bmatrix}\left(y(\mathbf{x}_n, \mathbf{w}) - t_n\right).$$

The right hand side can be written as

$$\sum_{n=1}^{N}\begin{bmatrix} 1 \\ \mathbf{x}_n \end{bmatrix}\left(y(\mathbf{x}_n, \mathbf{w}) - t_n\right) + \sum_{n=1}^{N}\begin{bmatrix} 0 \\ \boldsymbol{\epsilon}_n \end{bmatrix}\left(y(\mathbf{x}_n, \mathbf{w}) - t_n\right).$$

3.5

Let

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(t_n - \mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n)\right)^2. \tag{3.17}$$

Then, the minimisation of $E(\mathbf{w})$ under the constraint

$$\sum_{m=1}^{M}|w_m|^q \leq \eta \tag{3.18}$$

reduces to the minimisation of

$$E(\mathbf{w}) + \lambda\left(\sum_{m=1}^{M}|w_m|^q - \eta\right) \tag{3.19}$$

with respect to $\mathbf{w}$ and λ. Then,

$$\eta = \sum_{m=1}^{M}|w_m^*(\lambda)|^q, \tag{3.20}$$

where

$$\mathbf{w}^*(\lambda) = \underset{\mathbf{w}}{\operatorname{argmin}} \left(E(\mathbf{w}) + \lambda \left(\sum_{m=1}^{M} |w_m|^q - \eta \right) \right). \tag{3.21}$$

3.6

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables in D dimensions such that

$$p(\mathbf{t}_n|\mathbf{y}_n) = \mathcal{N}\left(\mathbf{t}_n|\mathbf{y}_n, \boldsymbol{\Sigma}\right), \tag{3.22}$$

where

$$\mathbf{y}_n = \mathbf{W}^\intercal \boldsymbol{\phi}(\mathbf{x}_n). \tag{3.23}$$

Then,

$$\begin{aligned} \ln p(\mathbf{T}|\mathbf{Y}) = &- \frac{ND}{2} \ln(2\pi) - \frac{N}{2} \ln(\det \boldsymbol{\Sigma}) \\ &- \frac{1}{2} \sum_{n=1}^{N} \left(\mathbf{t}_n - \mathbf{W}^\intercal \boldsymbol{\phi}(\mathbf{x}_n)\right)^\intercal \boldsymbol{\Sigma}^{-1} \left(\mathbf{t}_n - \mathbf{W}^\intercal \boldsymbol{\phi}(\mathbf{x}_n)\right). \end{aligned} \tag{3.24}$$

By 3.21(a), setting the derivatives with respect to $\mathbf{W}$ and $\boldsymbol{\Sigma}$ to zero gives

$$\begin{aligned} \mathbf{O} &= -\frac{1}{2} \left(\boldsymbol{\Sigma}^{-1} + \left(\boldsymbol{\Sigma}^{-1}\right)^\intercal\right) \sum_{n=1}^{N} \left(\mathbf{t}_n - \mathbf{W}^\intercal \boldsymbol{\phi}(\mathbf{x}_n)\right) \left(\boldsymbol{\phi}(\mathbf{x}_n)\right)^\intercal, \\ \mathbf{O} &= -\frac{N}{2} \left(\boldsymbol{\Sigma}^{-1}\right)^\intercal + \frac{1}{2} \left(\boldsymbol{\Sigma}^{-1}\right)^2 \sum_{n=1}^{N} \left(\mathbf{t}_n - \mathbf{W}^\intercal \boldsymbol{\phi}(\mathbf{x}_n)\right) \left(\mathbf{t}_n - \mathbf{W}^\intercal \boldsymbol{\phi}(\mathbf{x}_n)\right)^\intercal. \end{aligned} \tag{3.25}$$

Therefore, the maximum likelihood solutions for $\mathbf{W}$ and $\boldsymbol{\Sigma}$ are given by

$$\begin{aligned} \mathbf{W}_{\mathrm{ML}} &= \left(\boldsymbol{\Phi}^\intercal \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^\intercal \mathbf{t}, \\ \boldsymbol{\Sigma}_{\mathrm{ML}} &= \frac{1}{N} \sum_{n=1}^{N} \left(\mathbf{t}_n - \mathbf{W}_{\mathrm{ML}}^\intercal \boldsymbol{\phi}(\mathbf{x}_n)\right) \left(\mathbf{t}_n - \mathbf{W}_{\mathrm{ML}}^\intercal \boldsymbol{\phi}(\mathbf{x}_n)\right)^\intercal. \end{aligned} \tag{3.26}$$

3.7

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal \boldsymbol{\phi}_n, \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0). \end{aligned} \tag{3.27}$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{t})p(\mathbf{t}) = p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \tag{3.28}$$

The logarithm of the right hand side except the terms independent of $\mathbf{t}$ and $\mathbf{w}$ can be written as

$$\begin{aligned} &-\frac{\beta}{2}\sum_{n=1}^{N}(t_n - \mathbf{w}^\intercal\boldsymbol{\phi}_n)^2 - \frac{1}{2}(\mathbf{w}-\mathbf{m}_0)^\intercal\mathbf{S}_0^{-1}(\mathbf{w}-\mathbf{m}_0) \\ =&-\frac{1}{2}\begin{bmatrix}\mathbf{w}\\ \mathbf{t}\end{bmatrix}^\intercal\begin{bmatrix}\mathbf{S}_0^{-1}+\beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi} & -\beta\boldsymbol{\Phi}^\intercal\\ -\beta\boldsymbol{\Phi} & \beta\mathbf{I}\end{bmatrix}\begin{bmatrix}\mathbf{w}\\ \mathbf{t}\end{bmatrix} + \begin{bmatrix}\mathbf{w}\\ \mathbf{t}\end{bmatrix}^\intercal\begin{bmatrix}\mathbf{S}_0^{-1}\mathbf{m}_0\\ \mathbf{0}\end{bmatrix}. \end{aligned} \tag{3.29}$$

Therefore,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m},\mathbf{S}), \tag{3.30}$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S}\left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\boldsymbol{\Phi}^\intercal\mathbf{t}\right), \\ \mathbf{S} &= \left(\mathbf{S}_0^{-1}+\beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi}\right)^{-1}. \end{aligned} \tag{3.31}$$

3.8

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}_n, \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{m}_0,\mathbf{S}_0). \end{aligned} \tag{3.32}$$

By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m},\mathbf{S}), \tag{3.33}$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S}\left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\boldsymbol{\Phi}^\intercal\mathbf{t}\right), \\ \mathbf{S} &= \left(\mathbf{S}_0^{-1}+\beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi}\right)^{-1}. \end{aligned} \tag{3.34}$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{t}')p(\mathbf{t}') = p(\mathbf{t}'|\mathbf{w})p(\mathbf{w}), \tag{3.35}$$

where

$$\mathbf{t}' = \begin{bmatrix}\mathbf{t}\\ t_{N+1}\end{bmatrix}. \tag{3.36}$$

Since $\mathbf{t}$ and t_{N+1} are independent, it can be written as

$$p(\mathbf{w}|\mathbf{t}')p(t_{N+1})p(\mathbf{t}) = p(t_{N+1}|\mathbf{w})p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \tag{3.37}$$

By the Bayes' theorem, the right hand side can be written as

$$p(t_{N+1}|\mathbf{w})p(\mathbf{w}|\mathbf{t})p(\mathbf{t}). \tag{3.38}$$

Then,

$$p(\mathbf{w}|\mathbf{t}')p(t_{N+1}) = p(\mathbf{w}|\mathbf{t})p(t_{N+1}|\mathbf{w}). \tag{3.39}$$

The logarithm of the right hand side except the terms independent of $\mathbf{w}$ can be written as

$$\begin{aligned} &-\frac{1}{2}\left(\mathbf{w}-\mathbf{m}\right)^{\intercal}\mathbf{S}^{-1}\left(\mathbf{w}-\mathbf{m}\right)-\frac{\beta}{2}\left(t_{N+1}-\mathbf{w}^{\intercal}\boldsymbol{\phi}_{N+1}\right)^{2} \\ =&-\frac{1}{2}\begin{bmatrix}\mathbf{w}\\ t_{N+1}\end{bmatrix}^{\intercal}\begin{bmatrix}\mathbf{S}^{-1}+\beta\boldsymbol{\phi}_{N+1}\boldsymbol{\phi}_{N+1}^{\intercal} & -\beta\boldsymbol{\phi}_{N+1}\\ -\beta\boldsymbol{\phi}_{N+1}^{\intercal} & \beta\end{bmatrix}\begin{bmatrix}\mathbf{w}\\ t_{N+1}\end{bmatrix} \\ &+\begin{bmatrix}\mathbf{w}\\ t_{N+1}\end{bmatrix}^{\intercal}\begin{bmatrix}\mathbf{S}^{-1}\mathbf{m}\\ 0\end{bmatrix}-\frac{1}{2}\mathbf{m}^{\intercal}\mathbf{S}^{-1}\mathbf{m}. \end{aligned} \tag{3.40}$$

Then,

$$p(\mathbf{w}|\mathbf{t}') = \mathcal{N}\left(\mathbf{w}|\mathbf{m}',\mathbf{S}'\right), \tag{3.41}$$

where

$$\begin{aligned} \mathbf{m}' &= \mathbf{S}'\left(\mathbf{S}^{-1}\mathbf{m}+\beta t_{N+1}\boldsymbol{\phi}_{N+1}\right), \\ \mathbf{S}' &= \left(\mathbf{S}^{-1}+\beta\boldsymbol{\phi}_{N+1}\boldsymbol{\phi}_{N+1}^{\intercal}\right)^{-1}. \end{aligned} \tag{3.42}$$

We have

$$\mathbf{S}^{-1}\mathbf{m}+\beta t_{N+1}\boldsymbol{\phi}_{N+1} = \mathbf{S}_0^{-1}\mathbf{m}_0+\beta\boldsymbol{\Phi}'^{\intercal}\mathbf{t}', \tag{3.43}$$

and

$$\mathbf{S}^{-1}+\beta\boldsymbol{\phi}_{N+1}\boldsymbol{\phi}_{N+1}^{\intercal} = \mathbf{S}_0^{-1}+\beta\boldsymbol{\Phi}'^{\intercal}\boldsymbol{\Phi}', \tag{3.44}$$

where

$$\boldsymbol{\Phi}' = \begin{bmatrix}\boldsymbol{\Phi}\\ \boldsymbol{\phi}_{N+1}^{\intercal}\end{bmatrix}. \tag{3.45}$$

Therefore,

$$\begin{aligned} \mathbf{m}' &= \mathbf{S}'\left(\mathbf{S}_0^{-1}\mathbf{m}_0+\beta\boldsymbol{\Phi}'^{\intercal}\mathbf{t}'\right), \\ \mathbf{S}' &= \left(\mathbf{S}_0^{-1}+\beta\boldsymbol{\Phi}'^{\intercal}\boldsymbol{\Phi}'\right)^{-1}. \end{aligned} \tag{3.46}$$

3.9

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}_n, \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0). \end{aligned} \tag{3.47}$$

Then, by 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{S}), \tag{3.48}$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S}\left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\boldsymbol{\Phi}^\intercal\mathbf{t}\right), \\ \mathbf{S} &= \left(\mathbf{S}_0^{-1} + \beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi}\right)^{-1}. \end{aligned} \tag{3.49}$$

Let

$$\mathbf{t}' = \begin{bmatrix} \mathbf{t} \\ t_{N+1} \end{bmatrix}, \boldsymbol{\Phi} = \begin{bmatrix} \boldsymbol{\Phi} \\ \boldsymbol{\phi}_{N+1}^\intercal \end{bmatrix}. \tag{3.50}$$

Therefore,

$$p(\mathbf{w}|\mathbf{t}') = \mathcal{N}\left(\mathbf{w}|\mathbf{m}', \mathbf{t}'\right), \tag{3.51}$$

where

$$\begin{aligned} \mathbf{m}' &= \mathbf{S}'\left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\boldsymbol{\Phi}'^\intercal\mathbf{t}'\right), \\ \mathbf{S}' &= \left(\mathbf{S}_0^{-1} + \beta\boldsymbol{\Phi}'^\intercal\boldsymbol{\Phi}'\right)^{-1}. \end{aligned} \tag{3.52}$$

3.10

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}_n, \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}\left(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0\right). \end{aligned} \tag{3.53}$$

By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}\left(\mathbf{w}|\mathbf{m}, \mathbf{S}\right), \tag{3.54}$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S}\left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\boldsymbol{\Phi}^\intercal\mathbf{t}\right), \\ \mathbf{S} &= \left(\mathbf{S}_0^{-1} + \beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi}\right)^{-1}. \end{aligned} \tag{3.55}$$

By marginalisation,

$$p(t_{N+1}|\mathbf{t}) = \int p(t_{N+1}|\mathbf{w})p(\mathbf{w}|\mathbf{t})d\mathbf{w}. \tag{3.56}$$

The logarithm of the integrand of the right hand side except the terms independent of t_{N+1} and $\mathbf{w}$ can be written as

$$\begin{aligned}
&-\frac{\beta}{2}\left(t_{N+1}-\mathbf{w}^\intercal\boldsymbol{\phi}_{N+1}\right)^2-\frac{1}{2}(\mathbf{w}-\mathbf{m})^\intercal\mathbf{S}^{-1}(\mathbf{w}-\mathbf{m})\\
=&-\frac{1}{2}\begin{bmatrix}\mathbf{w}\\ t_{N+1}\end{bmatrix}^\intercal\begin{bmatrix}\mathbf{S}^{-1}+\beta\boldsymbol{\phi}_{N+1}\boldsymbol{\phi}_{N+1}^\intercal & -\beta\boldsymbol{\phi}_{N+1}\\ -\beta\boldsymbol{\phi}_{N+1}^\intercal & \beta\end{bmatrix}\begin{bmatrix}\mathbf{w}\\ t_{N+1}\end{bmatrix}\\
&+\begin{bmatrix}\mathbf{w}\\ t_{N+1}\end{bmatrix}^\intercal\begin{bmatrix}\mathbf{S}^{-1}\mathbf{m}\\ 0\end{bmatrix}-\frac{1}{2}\mathbf{m}^\intercal\mathbf{S}^{-1}\mathbf{m}.
\end{aligned}\tag{3.57}$$

By 2.24,

$$\begin{bmatrix}\mathbf{S}^{-1}+\beta\boldsymbol{\phi}_{N+1}\boldsymbol{\phi}_{N+1}^\intercal & -\beta\boldsymbol{\phi}_{N+1}\\ -\beta\boldsymbol{\phi}_{N+1}^\intercal & \beta\end{bmatrix}^{-1}=\begin{bmatrix}\mathbf{S} & \mathbf{S}\boldsymbol{\phi}_{N+1}\\ \boldsymbol{\phi}_{N+1}^\intercal\mathbf{S} & \beta^{-1}+\boldsymbol{\phi}_{N+1}^\intercal\mathbf{S}\boldsymbol{\phi}_{N+1}\end{bmatrix}.\tag{3.58}$$

Then,

$$\begin{bmatrix}\mathbf{S}^{-1}+\beta\boldsymbol{\phi}_{N+1}\boldsymbol{\phi}_{N+1}^\intercal & \beta\boldsymbol{\phi}_{N+1}\\ \beta\boldsymbol{\phi}_{N+1}^\intercal & \beta\end{bmatrix}^{-1}\begin{bmatrix}\mathbf{S}^{-1}\mathbf{m}\\ 0\end{bmatrix}=\begin{bmatrix}\mathbf{m}\\ \mathbf{m}^\intercal\boldsymbol{\phi}_{N+1}\end{bmatrix}.\tag{3.59}$$

Therefore,

$$p(t_{N+1}|\mathbf{t})=\mathcal{N}\left(t_{N+1}|\mathbf{m}^\intercal\boldsymbol{\phi}_{N+1},\sigma^2\right),\tag{3.60}$$

where

$$\sigma^2=\beta^{-1}+\boldsymbol{\phi}_{N+1}^\intercal\mathbf{S}\boldsymbol{\phi}_{N+1}.\tag{3.61}$$

3.11

Let $t_1,\cdots,t_N$ be a variable such that

$$\begin{aligned}
p(t_n|\mathbf{w})&=\mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}_n,\beta^{-1}\right),\\
p(\mathbf{w})&=\mathcal{N}\left(\mathbf{w}|\mathbf{m}_0,\mathbf{S}_0\right).
\end{aligned}\tag{3.62}$$

By 3.10,

$$p(t_{N+1}|\mathbf{t})=\mathcal{N}\left(t_{N+1}|\mathbf{m}^\intercal\boldsymbol{\phi}_{N+1},\sigma^2\right),\tag{3.63}$$

where

$$\begin{aligned}
\mathbf{m}&=\mathbf{S}\left(\mathbf{S}_0^{-1}\mathbf{m}_0+\beta\boldsymbol{\Phi}^\intercal\mathbf{t}\right),\\
\mathbf{S}&=\left(\mathbf{S}_0^{-1}+\beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi}\right)^{-1},\\
\sigma^2&=\beta^{-1}+\boldsymbol{\phi}_{N+1}^\intercal\mathbf{S}\boldsymbol{\phi}_{N+1}.
\end{aligned}\tag{3.64}$$

Then,

$$\sigma^2 - \sigma'^2 = \boldsymbol{\phi}^\intercal \left(\mathbf{S} - \mathbf{S}'\right) \boldsymbol{\phi}. \tag{3.65}$$

We have

$$\mathbf{S}' = \left(\mathbf{S}^{-1} + \beta \boldsymbol{\phi}_{N+1} \boldsymbol{\phi}_{N+1}^\intercal\right)^{-1}. \tag{3.66}$$

By 2.24,

$$\begin{bmatrix} \mathbf{S}^{-1} & \beta\boldsymbol{\phi}_{N+1} \\ \beta\boldsymbol{\phi}_{N+1}^\intercal & -\beta \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{S}' & \mathbf{S}'\boldsymbol{\phi}_{N+1} \\ \boldsymbol{\phi}_{N+1}^\intercal \mathbf{S}' & -\beta^{-1} + \boldsymbol{\phi}_{N+1}^\intercal \mathbf{S}' \boldsymbol{\phi}_{N+1} \end{bmatrix}, \tag{3.67}$$

and

$$\begin{bmatrix} -\beta & \beta\boldsymbol{\phi}_{N+1}^\intercal \\ \beta\boldsymbol{\phi}_{N+1} & \mathbf{S}^{-1} \end{bmatrix}^{-1} = \begin{bmatrix} -c & \beta c \boldsymbol{\phi}_{N+1}^\intercal \mathbf{S} \\ \beta c \mathbf{S}\boldsymbol{\phi}_{N+1} & \mathbf{S} - \beta^2 c \mathbf{S}\boldsymbol{\phi}_{N+1}\boldsymbol{\phi}_{N+1}^\intercal \mathbf{S} \end{bmatrix}, \tag{3.68}$$

where

$$c = \left(\beta + \beta^2 \boldsymbol{\phi}_{N+1}^\intercal \mathbf{S} \boldsymbol{\phi}_{N+1}\right)^{-1}. \tag{3.69}$$

Then,

$$\mathbf{S}' = \mathbf{S} - \beta^2 c \mathbf{S}\boldsymbol{\phi}_{N+1}\boldsymbol{\phi}_{N+1}^\intercal \mathbf{S}. \tag{3.70}$$

Then,

$$\boldsymbol{\phi}(\mathbf{x})^\intercal (\mathbf{S}_N - \mathbf{S}_{N+1}) \boldsymbol{\phi}(\mathbf{x}) = \frac{\beta \left(\boldsymbol{\phi}(\mathbf{x})^\intercal \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}_{N+1})\right)^2}{1 + \beta \boldsymbol{\phi}(\mathbf{x}_{N+1}) \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}_{N+1})^\intercal}. \tag{3.71}$$

Therefore,

$$\sigma_{N+1}^2(\mathbf{x}) \leq \sigma_N^2(\mathbf{x}). \tag{3.72}$$

3.12

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}, \beta) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right), \\ p(\mathbf{w}, \beta) &= \mathcal{N}\left(\mathbf{w}|\mathbf{m}_0, \beta^{-1}\mathbf{S}_0\right) \mathrm{Gam}(\beta|a_0, b_0), \end{aligned} \tag{3.73}$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. By the Bayes' theorem,

$$p(\mathbf{w}, \beta|\mathbf{t}) p(\mathbf{t}) = p(\mathbf{t}|\mathbf{w}, \beta) p(\mathbf{w}, \beta). \tag{3.74}$$

The logarithm of the right hand side except the terms independent of $\mathbf{t}$, $\mathbf{w}$ and β can be written as

$$\begin{aligned}
&-\frac{N}{2}\ln\beta^{-1}-\frac{\beta}{2}\sum_{n=1}^{N}\left(t_n-\mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n)\right)^2-\frac{M}{2}\ln\beta^{-1}-\frac{\beta}{2}(\mathbf{w}-\mathbf{m}_0)^\intercal\mathbf{S}_0^{-1}(\mathbf{w}-\mathbf{m}_0)\\
&+(a_0-1)\ln\beta-b_0\beta\\
=&-\frac{M}{2}\ln\beta-\frac{\beta}{2}\mathbf{w}^\intercal\left(\mathbf{S}_0^{-1}+\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi}\right)\mathbf{w}+\beta\mathbf{w}^\intercal\left(\mathbf{S}_0^{-1}\mathbf{m}_0+\boldsymbol{\Phi}^\intercal\mathbf{t}\right)-\frac{\beta}{2}\|\mathbf{t}\|^2-\frac{\beta}{2}\mathbf{m}_0^\intercal\mathbf{S}_0^{-1}\mathbf{m}_0\\
&+\left(a_0+\frac{N}{2}-1\right)\ln\beta-b_0\beta.
\end{aligned}\tag{3.75}$$

The right hand side can be written as

$$-\frac{M}{2}\ln\beta-\frac{\beta}{2}(\mathbf{w}-\mathbf{m}_N)^\intercal\mathbf{S}_N^{-1}(\mathbf{w}-\mathbf{m}_N)+(a_N-1)\ln\beta-b_N\beta,\tag{3.76}$$

where

$$\begin{aligned}
\mathbf{m}_N&=\mathbf{S}_N\left(\mathbf{S}_0^{-1}\mathbf{m}_0+\boldsymbol{\Phi}^\intercal\mathbf{t}\right),\\
\mathbf{S}_N^{-1}&=\mathbf{S}_0^{-1}+\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi},\\
a_N&=a_0+\frac{N}{2},\\
b_N&=b_0+\frac{1}{2}\|\mathbf{t}\|^2+\frac{1}{2}\mathbf{m}_0^\intercal\mathbf{S}_0\mathbf{m}_0-\frac{1}{2}\mathbf{m}_N^\intercal\mathbf{S}_N^{-1}\mathbf{m}_N.
\end{aligned}\tag{3.77}$$

Therefore,

$$p(\mathbf{w},\beta|\mathbf{t})=\mathcal{N}\left(\mathbf{w}|\mathbf{m}_N,\beta^{-1}\mathbf{S}_N\right)\mathrm{Gam}(\beta|a_N,b_N).\tag{3.78}$$

Substituting it to the result of the Bayes' theorem above, we have

$$p(\mathbf{t})=\frac{\mathcal{N}\left(\mathbf{t}|\boldsymbol{\Phi}\mathbf{w},\beta^{-1}\mathbf{I}\right)\mathcal{N}\left(\mathbf{w}|\mathbf{m}_0,\beta^{-1}\mathbf{S}_0\right)\mathrm{Gam}(\beta|a_0,b_0)}{\mathcal{N}\left(\mathbf{w}|\mathbf{m}_N,\beta^{-1}\mathbf{S}_N\right)\mathrm{Gam}(\beta|a_N,b_N)}.\tag{3.79}$$

The logarithm of the right hand side can be written as

$$
\begin{aligned}
&-\frac{N}{2}\ln(2\pi)-\frac{N}{2}\ln\beta^{-1}-\frac{\beta}{2}\left(\mathbf{t}-\mathbf{\Phi}\mathbf{w}\right)^{\intercal}\left(\mathbf{t}-\mathbf{\Phi}\mathbf{w}\right)\\
&-\frac{M}{2}\ln(2\pi)-\frac{M}{2}\ln\beta^{-1}-\frac{1}{2}\det\mathbf{S}_0-\frac{\beta}{2}(\mathbf{w}-\mathbf{m}_0)^{\intercal}\mathbf{S}_0^{-1}(\mathbf{w}-\mathbf{m}_0)\\
&+a_0\ln b_0-\ln\Gamma(a_0)+(a_0-1)\ln\beta-b_0\beta\\
&+\frac{M}{2}\ln(2\pi)+\frac{M}{2}\ln\beta^{-1}+\frac{1}{2}\det\mathbf{S}_N+\frac{\beta}{2}(\mathbf{w}-\mathbf{m}_N)^{\intercal}\mathbf{S}_N^{-1}(\mathbf{w}-\mathbf{m}_0)\\
&-a_N\ln b_N+\ln\Gamma(a_N)-(a_N-1)\ln\beta+b_N\beta\\
=&-\frac{N}{2}\ln(2\pi)-\frac{1}{2}\det\mathbf{S}_0+a_0\ln b_0-\ln\Gamma(a_0)+\frac{1}{2}\det\mathbf{S}_N-a_N\ln b_N+\ln\Gamma(a_N).
\end{aligned}
\tag{3.80}
$$

Therefore,

$$
p(\mathbf{t})=(2\pi)^{-\frac{N}{2}}\left(\frac{\det\mathbf{S}_N}{\det\mathbf{S}_0}\right)^{\frac{1}{2}}\frac{\Gamma(a_N)}{\Gamma(a_0)}\frac{b_0^{a_0}}{b_N^{a_N}}. \tag{3.81}
$$

3.13

Let $t_1,\cdots,t_N$ be variables such that

$$
\begin{aligned}
p(t_n|\mathbf{w},\beta)&=\mathcal{N}\left(t_n|\mathbf{w}^{\intercal}\boldsymbol{\phi}(\mathbf{x}_n),\beta^{-1}\right),\\
p(\mathbf{w},\beta)&=\mathcal{N}\left(\mathbf{w}|\mathbf{m}_0,\beta^{-1}\mathbf{S}_0\right)\mathrm{Gam}(\beta|a_0,b_0),
\end{aligned}
\tag{3.82}
$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. Then, by 3.12,

$$
p(\mathbf{w},\beta|\mathbf{t})=\mathcal{N}\left(\mathbf{w}|\mathbf{m}_N,\beta^{-1}\mathbf{S}_N\right)\mathrm{Gam}(\beta|a_N,b_N), \tag{3.83}
$$

where

$$
\begin{aligned}
\mathbf{m}_N&=\mathbf{S}_N\left(\mathbf{S}_0^{-1}\mathbf{m}_0+\mathbf{\Phi}^{\intercal}\mathbf{t}\right),\\
\mathbf{S}_N^{-1}&=\mathbf{S}_0^{-1}+\mathbf{\Phi}^{\intercal}\mathbf{\Phi},\\
a_N&=a_0+\frac{N}{2},\\
b_N&=b_0+\frac{1}{2}\|\mathbf{t}\|^2+\frac{1}{2}\mathbf{m}_0^{\intercal}\mathbf{S}_0\mathbf{m}_0-\frac{1}{2}\mathbf{m}_N^{\intercal}\mathbf{S}_N^{-1}\mathbf{m}_N.
\end{aligned}
\tag{3.84}
$$

By marginalisation,

$$
p(t|\mathbf{t})=\int\int p(t|\mathbf{w},\beta)p(\mathbf{w},\beta|\mathbf{t})d\mathbf{w}d\beta. \tag{3.85}
$$

The right hand side can be written as

$$\int \left(\int \mathcal{N}\left(t|\mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}), \beta^{-1}\right) \mathcal{N}\left(\mathbf{w}|\mathbf{m}_N, \beta^{-1}\mathbf{S}_N\right) d\mathbf{w} \right) \mathrm{Gam}(\beta|a_N, b_N) d\beta. \tag{3.86}$$

The logarithm of the integrand with respect to $\mathbf{w}$ except the terms indepn-dent of $\mathbf{w}$ can be written as

$$-\frac{\beta}{2}\left(t - \mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x})\right)^2 - \frac{\beta}{2}(\mathbf{w} - \mathbf{m}_N)^\intercal \mathbf{S}_N^{-1}(\mathbf{w} - \mathbf{m}_N). \tag{3.87}$$

It can be written as

$$-\frac{\beta}{2}\begin{bmatrix}\mathbf{w}\\ t\end{bmatrix}^\intercal \begin{bmatrix}\mathbf{S}_N^{-1} + \boldsymbol{\phi}(\mathbf{x})\boldsymbol{\phi}(\mathbf{x})^\intercal & -\boldsymbol{\phi}(\mathbf{x})\\ -\boldsymbol{\phi}(\mathbf{x})^\intercal & 1\end{bmatrix}\begin{bmatrix}\mathbf{w}\\ t\end{bmatrix} + \beta \begin{bmatrix}\mathbf{w}\\ t\end{bmatrix}^\intercal \begin{bmatrix}\mathbf{S}_N^{-1}\mathbf{m}_N\\ 0\end{bmatrix} - \frac{\beta}{2}\mathbf{m}_N^\intercal \mathbf{S}_N^{-1}\mathbf{m}_N.$$

By 2.24,

$$\begin{bmatrix}\mathbf{S}_N^{-1} + \boldsymbol{\phi}(\mathbf{x})\boldsymbol{\phi}(\mathbf{x})^\intercal & -\boldsymbol{\phi}(\mathbf{x})\\ -\boldsymbol{\phi}(\mathbf{x})^\intercal & 1\end{bmatrix}^{-1} = \begin{bmatrix}\mathbf{S}_N & \mathbf{S}_N\boldsymbol{\phi}(\mathbf{x})\\ \boldsymbol{\phi}(\mathbf{x})^\intercal \mathbf{S}_N & 1 + \boldsymbol{\phi}(\mathbf{x})^\intercal \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})\end{bmatrix}.$$

Then,

$$\begin{bmatrix}\mathbf{S}_N^{-1} + \boldsymbol{\phi}(\mathbf{x})\boldsymbol{\phi}(\mathbf{x})^\intercal & -\boldsymbol{\phi}(\mathbf{x})\\ -\boldsymbol{\phi}(\mathbf{x})^\intercal & 1\end{bmatrix}^{-1} \begin{bmatrix}\mathbf{S}_N^{-1}\mathbf{m}_N\\ 0\end{bmatrix} = \begin{bmatrix}\mathbf{m}_N\\ \mathbf{m}_N^\intercal \boldsymbol{\phi}(\mathbf{x})\end{bmatrix}.$$

Therefore, the integral with respect to $\mathbf{w}$ can be written as

$$\mathcal{N}\left(t|\mathbf{m}_N^\intercal \boldsymbol{\phi}(\mathbf{x}), \beta^{-1}\left(1 + \boldsymbol{\phi}(\mathbf{x})^\intercal \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})\right)\right). \tag{3.88}$$

Then, the logarithm of the integrand with respect to β except the terms independent of β can be written as

$$\begin{aligned}&-\frac{1}{2}\ln\beta^{-1} - \frac{\beta}{2\left(1 + \boldsymbol{\phi}(\mathbf{x})^\intercal \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})\right)}\left(t - \mathbf{m}_N^\intercal \boldsymbol{\phi}(\mathbf{x})\right)^2 + (a_N - 1)\ln\beta - b_N\beta\\ &= \left(a_N + \frac{1}{2} - 1\right)\ln\beta - \left(b_N + \frac{\left(t - \mathbf{m}_N^\intercal \boldsymbol{\phi}(\mathbf{x})\right)^2}{2\left(1 + \boldsymbol{\phi}(\mathbf{x})^\intercal \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})\right)}\right)\beta.\end{aligned} \tag{3.89}$$

Therefore, the integral with respect to β except the terms independent of t can be written as

$$\left(b_N + \frac{\left(t - \mathbf{m}_N^\intercal \boldsymbol{\phi}(\mathbf{x})\right)^2}{2\left(1 + \boldsymbol{\phi}(\mathbf{x})^\intercal \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})\right)}\right)^{-a_N - \frac{1}{2}}. \tag{3.90}$$

Thus,

$$p(t|\mathbf{x}, \mathbf{t}) = \mathrm{St}(t|\mu, \lambda, \nu), \tag{3.91}$$

where

$$\begin{aligned} \mu &= \mathbf{m}_N^\intercal \boldsymbol{\phi}(\mathbf{x}), \\ \lambda &= \frac{a_N}{b_N} \left(1 + \boldsymbol{\phi}(\mathbf{x})^\intercal \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})\right)^{-1}, \\ \nu &= 2a_N. \end{aligned} \tag{3.92}$$

3.14 (Incomplete)

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \tag{3.93}$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. Then, by 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.94}$$

where

$$\begin{aligned} \mathbf{m}_N &= \beta \mathbf{S}_N \boldsymbol{\Phi}^\intercal \mathbf{t}, \\ \mathbf{S}_N^{-1} &= \alpha \mathbf{I} + \beta \boldsymbol{\Phi}^\intercal \boldsymbol{\Phi}. \end{aligned} \tag{3.95}$$

Let

$$y(\mathbf{x}, \mathbf{w}) = \mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}). \tag{3.96}$$

Then,

$$y(\mathbf{x}, \mathbf{m}_N) = \sum_{n=1}^{N} k(\mathbf{x}, \mathbf{x}_n) t_n, \tag{3.97}$$

where

$$k(\mathbf{x}, \mathbf{x}') = \beta \boldsymbol{\phi}(\mathbf{x})^\intercal \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}'). \tag{3.98}$$

Let us suppose that $\phi_j(\mathbf{x})$ are linearly independent, $N > M$ and

$$\phi_0(\mathbf{x}) = 1. \tag{3.99}$$

Then, we can construct a new basis set $\psi_j(\mathbf{x})$ such that

$$\boldsymbol{\Psi}^\intercal \boldsymbol{\Psi} = \mathbf{I}? \tag{3.100}$$

$$\sum_{n=1}^{N} \psi_j(\mathbf{x}_n)\psi_k(\mathbf{x}_n) = I_{jk}? \tag{3.101}$$

where

$$\boldsymbol{\Psi} = \begin{bmatrix} \boldsymbol{\psi}(\mathbf{x}_1)^\intercal \\ \vdots \\ \boldsymbol{\psi}(\mathbf{x}_N)^\intercal \end{bmatrix}$$

and

$$\psi_0(\mathbf{x}) = 1. \tag{3.102}$$

Under the basis set, if $\alpha = 0$, then

$$\mathbf{S}_N^{-1} = \beta\mathbf{I}, \tag{3.103}$$

so that

$$k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\psi}(\mathbf{x})^\intercal\boldsymbol{\psi}(\mathbf{x}'). \tag{3.104}$$

Then,

$$\sum_{n=1}^{N} k(\mathbf{x}, \mathbf{x}_n) = \sum_{n=1}^{N}\sum_{j=0}^{M-1} \psi_j(\mathbf{x})\psi_j(\mathbf{x}_n) = 1? \tag{3.105}$$

3.15

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \tag{3.106}$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.107}$$

where

$$\begin{aligned} \mathbf{m}_N &= \beta\mathbf{S}_N\boldsymbol{\Phi}^\intercal\mathbf{t}, \\ \mathbf{S}_N^{-1} &= \alpha\mathbf{I} + \beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi}. \end{aligned} \tag{3.108}$$

By 3.19,

$$\ln p(\mathbf{t}) = \frac{M}{2}\ln\alpha + \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi) + \frac{1}{2}\ln(\det\mathbf{S}_N) - E(\mathbf{m}_N), \tag{3.109}$$

where

$$E(\mathbf{m}_N) = \frac{\beta}{2}\|\mathbf{t} - \mathbf{\Phi}\mathbf{m}_N\|^2 + \frac{\alpha}{2}\mathbf{m}_N^\intercal \mathbf{m}_N. \tag{3.110}$$

By 3.22, setting the derivatives of $\ln p(\mathbf{t})$ with respect to α and β to zero gives

$$\begin{aligned} \alpha &= \frac{\gamma}{\mathbf{m}_N^\intercal \mathbf{m}_N}, \\ \beta &= \frac{N - \gamma}{\|\mathbf{t} - \mathbf{\Phi}\mathbf{m}_N\|^2}, \end{aligned} \tag{3.111}$$

where

$$\gamma = \sum_{m=1}^{M} \frac{\lambda_m}{\alpha + \lambda_m} \tag{3.112}$$

and $\lambda_1, \cdots, \lambda_M$ are the eigenvalues of $\beta\mathbf{\Phi}^\intercal\mathbf{\Phi}$. If α and β are set as above, then

$$E(\mathbf{m}_N) = \frac{N}{2}. \tag{3.113}$$

3.16

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \tag{3.114}$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. By the Bayes' theorem,

$$p(\mathbf{t}, \mathbf{w}) = p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \tag{3.115}$$

Integrating both sides with respect to $\mathbf{w}$ gives

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}. \tag{3.116}$$

The logarithm of the integrand of the right hand side except the terms independent of $\mathbf{w}$ can be written as

$$-\frac{\beta}{2}\sum_{n=1}^{N}\left(t_n - \mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n)\right)^2 - \frac{\alpha}{2}\mathbf{w}^\intercal\mathbf{w} = -\frac{1}{2}\begin{bmatrix}\mathbf{w}\\ \mathbf{t}\end{bmatrix}^\intercal \begin{bmatrix}\alpha\mathbf{I} + \beta\mathbf{\Phi}^\intercal\mathbf{\Phi} & -\beta\mathbf{\Phi}^\intercal \\ -\beta\mathbf{\Phi} & \beta\mathbf{I}\end{bmatrix}\begin{bmatrix}\mathbf{w}\\ \mathbf{t}\end{bmatrix}.$$

By 2.24,

$$\begin{bmatrix} \alpha\mathbf{I}+\beta\mathbf{\Phi}^\intercal\mathbf{\Phi} & -\beta\mathbf{\Phi}^\intercal \\ -\beta\mathbf{\Phi} & \beta\mathbf{I} \end{bmatrix}^{-1} = \begin{bmatrix} \alpha^{-1}\mathbf{I} & \alpha^{-1}\mathbf{\Phi}^\intercal \\ \alpha^{-1}\mathbf{\Phi} & \alpha^{-1}\mathbf{\Phi}\mathbf{\Phi}^\intercal+\beta^{-1}\mathbf{I} \end{bmatrix}.$$

Therefore,

$$p(\mathbf{t}) = \mathcal{N}\left(\mathbf{t}|\mathbf{0}, \alpha^{-1}\mathbf{\Phi}\mathbf{\Phi}^\intercal+\beta^{-1}\mathbf{I}\right). \tag{3.117}$$

3.17

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \tag{3.118}$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. By the Bayes' theorem,

$$p(\mathbf{t}, \mathbf{w}) = p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \tag{3.119}$$

Then,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}. \tag{3.120}$$

The logarithm of the integrand of the right hand side can be written as

$$-\frac{N}{2}\ln\left(2\pi\beta^{-1}\right)-\frac{\beta}{2}\sum_{n=1}^{N}\left(t_n-\mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n)\right)^2-\frac{M}{2}\ln\left(2\pi\right)-\frac{1}{2}\ln\left(\det\left(\alpha^{-1}\mathbf{I}\right)\right)-\frac{\alpha}{2}\mathbf{w}^\intercal\mathbf{w}. \tag{3.121}$$

Therefore,

$$p(\mathbf{t}) = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}}\left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}}\int \exp\left(-E(\mathbf{w})\right)d\mathbf{w}, \tag{3.122}$$

where

$$E(\mathbf{w}) = \frac{\beta}{2}\|\mathbf{t}-\mathbf{\Phi}\mathbf{w}\|^2+\frac{\alpha}{2}\mathbf{w}^\intercal\mathbf{w}. \tag{3.123}$$

3.18

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \tag{3.124}$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.125}$$

where

$$\begin{aligned} \mathbf{m}_N &= \beta \mathbf{S}_N \boldsymbol{\Phi}^\intercal \mathbf{t}, \\ \mathbf{S}_N^{-1} &= \alpha \mathbf{I} + \beta \boldsymbol{\Phi}^\intercal \boldsymbol{\Phi}. \end{aligned} \tag{3.126}$$

By 3.17,

$$p(\mathbf{t}) = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}} \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} \int \exp\left(-E(\mathbf{w})\right) d\mathbf{w}, \tag{3.127}$$

where

$$E(\mathbf{w}) = \frac{\beta}{2}\|\mathbf{t} - \boldsymbol{\Phi}\mathbf{w}\|^2 + \frac{\alpha}{2}\mathbf{w}^\intercal \mathbf{w}. \tag{3.128}$$

The first term of the definition of $E(\mathbf{w})$ can be written as

$$\begin{aligned} &\frac{\beta}{2}\|\mathbf{t} - \boldsymbol{\Phi}\mathbf{m}_N - \boldsymbol{\Phi}(\mathbf{w} - \mathbf{m}_N)\|^2 \\ =&\frac{\beta}{2}\|\mathbf{t} - \boldsymbol{\Phi}\mathbf{m}_N\|^2 - \beta(\mathbf{t} - \boldsymbol{\Phi}\mathbf{m}_N)^\intercal \boldsymbol{\Phi}(\mathbf{w} - \mathbf{m}_N) + \frac{\beta}{2}(\mathbf{w} - \mathbf{m}_N)^\intercal \boldsymbol{\Phi}^\intercal \boldsymbol{\Phi}(\mathbf{w} - \mathbf{m}_N). \end{aligned} \tag{3.129}$$

Similarly, the second term can be written as

$$\begin{aligned} &\frac{\alpha}{2}(\mathbf{w} - \mathbf{m}_N + \mathbf{m}_N)^\intercal (\mathbf{w} - \mathbf{m}_N + \mathbf{m}_N) \\ =&\frac{\alpha}{2}(\mathbf{w} - \mathbf{m}_N)^\intercal (\mathbf{w} - \mathbf{m}_N) + \alpha \mathbf{m}_N^\intercal (\mathbf{w} - \mathbf{m}_N) + \frac{\alpha}{2}\mathbf{m}_N^\intercal \mathbf{m}_N. \end{aligned} \tag{3.130}$$

Here,

$$\begin{aligned} &- \beta(\mathbf{t} - \boldsymbol{\Phi}\mathbf{m}_N)^\intercal \boldsymbol{\Phi}(\mathbf{w} - \mathbf{m}_N) + \alpha \mathbf{m}_N^\intercal (\mathbf{w} - \mathbf{m}_N) \\ =&\left(-\beta \boldsymbol{\Phi}^\intercal \mathbf{t} + \beta \boldsymbol{\Phi}^\intercal \boldsymbol{\Phi}\mathbf{m}_N + \alpha \mathbf{m}_N\right)^\intercal (\mathbf{w} - \mathbf{m}_N). \end{aligned} \tag{3.131}$$

By the definitions of $\mathbf{m}_N$ and $\mathbf{S}_N$ above, the right hand can be written as

$$\left(-\beta \boldsymbol{\Phi}^\intercal \mathbf{t} + \mathbf{S}_N^{-1}\mathbf{m}_N\right)^\intercal (\mathbf{w} - \mathbf{m}_N) = 0. \tag{3.132}$$

Therefore,

$$E(\mathbf{w}) = E(\mathbf{m}_N) + \frac{1}{2}(\mathbf{w} - \mathbf{m}_N)^\intercal \mathbf{S}_N^{-1}(\mathbf{w} - \mathbf{m}_N). \tag{3.133}$$

3.19

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \tag{3.134}$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.135}$$

where

$$\begin{aligned} \mathbf{m}_N &= \beta\mathbf{S}_N\boldsymbol{\Phi}^\intercal\mathbf{t}, \\ \mathbf{S}_N^{-1} &= \alpha\mathbf{I} + \beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi}. \end{aligned} \tag{3.136}$$

By 3.17,

$$p(\mathbf{t}) = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}} \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} \int \exp\left(-E(\mathbf{w})\right) d\mathbf{w}, \tag{3.137}$$

where

$$E(\mathbf{w}) = \frac{\beta}{2}\|\mathbf{t} - \boldsymbol{\Phi}\mathbf{w}\|^2 + \frac{\alpha}{2}\mathbf{w}^\intercal\mathbf{w}. \tag{3.138}$$

By 3.18,

$$E(\mathbf{w}) = E(\mathbf{m}_N) + \frac{1}{2}(\mathbf{w} - \mathbf{m}_N)^\intercal\mathbf{S}_N^{-1}(\mathbf{w} - \mathbf{m}_N). \tag{3.139}$$

Therefore, the integral in the expression above of $p(\mathbf{t})$ can be written as

$$\begin{aligned} &\exp\left(-E(\mathbf{m}_N)\right) \int \exp\left(-\frac{1}{2}(\mathbf{w} - \mathbf{m}_N)^\intercal\mathbf{S}_N^{-1}(\mathbf{w} - \mathbf{m}_N)\right) d\mathbf{w} \\ =&(2\pi)^{\frac{M}{2}} (\det\mathbf{S}_N)^{\frac{1}{2}} \exp\left(-E(\mathbf{m}_N)\right). \end{aligned} \tag{3.140}$$

Thus,

$$\ln p(\mathbf{t}) = \frac{M}{2}\ln\alpha + \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi) + \frac{1}{2}\ln(\det\mathbf{S}_N) - E(\mathbf{m}_N). \tag{3.141}$$

3.20

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \tag{3.142}$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.143}$$

where

$$\begin{aligned} \mathbf{m}_N &= \beta \mathbf{S}_N \boldsymbol{\Phi}^\intercal \mathbf{t}, \\ \mathbf{S}_N^{-1} &= \alpha \mathbf{I} + \beta \boldsymbol{\Phi}^\intercal \boldsymbol{\Phi}. \end{aligned} \tag{3.144}$$

By 3.19,

$$\ln p(\mathbf{t}) = \frac{M}{2} \ln \alpha + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \mathbf{S}_N) - E(\mathbf{m}_N), \tag{3.145}$$

where

$$E(\mathbf{m}_N) = \frac{\beta}{2} \|\mathbf{t} - \boldsymbol{\Phi} \mathbf{m}_N\|^2 + \frac{\alpha}{2} \mathbf{m}_N^\intercal \mathbf{m}_N. \tag{3.146}$$

Let $\mathbf{u}_1, \cdots, \mathbf{u}_M$ be eigenvectors of $\beta \boldsymbol{\Phi}^\intercal \boldsymbol{\Phi}$ such that

$$\beta \boldsymbol{\Phi}^\intercal \boldsymbol{\Phi} \mathbf{u}_m = \lambda_m \mathbf{u}_m. \tag{3.147}$$

Then,

$$\mathbf{S}_N^{-1} \mathbf{u}_m = (\alpha + \lambda_m) \mathbf{u}_m, \tag{3.148}$$

so that

$$\det \mathbf{S}_N = \prod_{m=1}^{M} \frac{1}{\alpha + \lambda_m}. \tag{3.149}$$

Therefore, setting the derivative of $\ln p(\mathbf{t}|\alpha, \beta)$ with respect to α to zero gives

$$0 = \frac{M}{2\alpha} - \frac{1}{2} \sum_{m=1}^{M} \frac{1}{\alpha + \lambda_m} - \frac{1}{2} \mathbf{m}_N^\intercal \mathbf{m}_N. \tag{3.150}$$

Multiplying both sides by 2α gives

$$\alpha \mathbf{m}_N^\intercal \mathbf{m}_N = M - \sum_{m=1}^{M} \frac{\alpha}{\alpha + \lambda_m}. \tag{3.151}$$

The right hand side can be written as

$$\sum_{m=1}^{M} \left(1 - \frac{\alpha}{\alpha + \lambda_m}\right) = \sum_{m=1}^{M} \frac{\lambda_i}{\alpha + \lambda_m}. \tag{3.152}$$

Thus,

$$\alpha = \frac{\gamma}{\mathbf{m}_N^\intercal \mathbf{m}_N}, \tag{3.153}$$

where

$$\gamma = \sum_{m=1}^{M} \frac{\lambda_i}{\alpha + \lambda_m}. \tag{3.154}$$

3.21

(a)

Let $\mathbf{\Sigma}$ be a $M \times M$ real symmetric matrix such that

$$\mathbf{\Sigma}\mathbf{u}_m = \lambda_m \mathbf{u}_m, \tag{3.155}$$

where $\mathbf{u}_1, \cdots, \mathbf{u}_M$ are unit vectors. Let

$$\begin{aligned} \mathbf{\Lambda} &= \text{diag}(\lambda_1, \cdots, \lambda_M), \\ \mathbf{U} &= [\mathbf{u}_1 \cdots \mathbf{u}_M]. \end{aligned} \tag{3.156}$$

By 2.19,

$$\begin{aligned} \mathbf{\Sigma} &= \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\intercal, \\ \mathbf{U}^\intercal\mathbf{U} &= \mathbf{I}. \end{aligned} \tag{3.157}$$

Therefore,

$$\det \mathbf{\Sigma} = \prod_{m=1}^{M} \lambda_m, \tag{3.158}$$

so that

$$\ln(\det \mathbf{\Sigma}) = \sum_{m=1}^{M} \ln \lambda_i. \tag{3.159}$$

Then,

$$\frac{\partial}{\partial \alpha} \ln(\det \mathbf{\Sigma}) = \sum_{m=1}^{M} \frac{\partial \lambda_m}{\partial \alpha} \frac{1}{\lambda_m}. \tag{3.160}$$

Therefore,

$$\frac{\partial}{\partial \alpha} \ln(\det \mathbf{\Sigma}) = \text{tr}\left(\mathbf{\Lambda}^{-1} \frac{\partial \mathbf{\Lambda}}{\partial \alpha}\right). \tag{3.161}$$

The right hand side can be written as

$$\operatorname{tr}\left(\mathbf{U}\boldsymbol{\Lambda}^{-1}\mathbf{U}^{\intercal}\frac{\partial \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{\intercal}}{\partial\alpha}\right) = \operatorname{tr}\left(\boldsymbol{\Sigma}^{-1}\frac{\partial\boldsymbol{\Sigma}}{\partial\alpha}\right). \tag{3.162}$$

Therefore,

$$\frac{\partial}{\partial\alpha}\ln(\det\boldsymbol{\Sigma}) = \operatorname{tr}\left(\boldsymbol{\Sigma}^{-1}\frac{\partial\boldsymbol{\Sigma}}{\partial\alpha}\right). \tag{3.163}$$

(b)

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^{\intercal}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \tag{3.164}$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.165}$$

where

$$\begin{aligned} \mathbf{m}_N &= \beta\mathbf{S}_N\boldsymbol{\Phi}^{\intercal}\mathbf{t}, \\ \mathbf{S}_N^{-1} &= \alpha\mathbf{I} + \beta\boldsymbol{\Phi}^{\intercal}\boldsymbol{\Phi}. \end{aligned} \tag{3.166}$$

By 3.19,

$$\ln p(\mathbf{t}) = \frac{M}{2}\ln\alpha + \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi) + \frac{1}{2}\ln(\det\mathbf{S}_N) - E(\mathbf{m}_N), \tag{3.167}$$

where

$$E(\mathbf{m}_N) = \frac{\beta}{2}\|\mathbf{t} - \boldsymbol{\Phi}\mathbf{m}_N\|^2 + \frac{\alpha}{2}\mathbf{m}_N^{\intercal}\mathbf{m}_N. \tag{3.168}$$

By 3.21(a),

$$\frac{\partial}{\partial\alpha}\ln\left(\det\mathbf{S}_N^{-1}\right) = \operatorname{tr}\left(\mathbf{S}_N\right). \tag{3.169}$$

The right hand side can be written as

$$\sum_{m=1}^{M}\frac{1}{\alpha + \lambda_m}, \tag{3.170}$$

where $\lambda_1, \cdots, \lambda_M$ are eigenvalues of $\beta\mathbf{\Phi}^\intercal\mathbf{\Phi}$. Therefore, setting the derivative of $\ln p(\mathbf{t})$ with respect to α to zero gives

$$0 = \frac{M}{2\alpha} - \frac{1}{2}\sum_{m=1}^{M}\frac{1}{\alpha+\lambda_m} - \frac{1}{2}\mathbf{m}_N^\intercal\mathbf{m}_N, \tag{3.171}$$

Thus,

$$\alpha = \frac{\gamma}{\mathbf{m}_N^\intercal\mathbf{m}_N}, \tag{3.172}$$

where

$$\gamma = \sum_{m=1}^{M}\frac{\lambda_m}{\alpha+\lambda_m}. \tag{3.173}$$

3.22

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \tag{3.174}$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.175}$$

where

$$\begin{aligned} \mathbf{m}_N &= \beta\mathbf{S}_N\mathbf{\Phi}^\intercal\mathbf{t}, \\ \mathbf{S}_N^{-1} &= \alpha\mathbf{I} + \beta\mathbf{\Phi}^\intercal\mathbf{\Phi}. \end{aligned} \tag{3.176}$$

By 3.19,

$$\ln p(\mathbf{t}) = \frac{M}{2}\ln\alpha + \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi) + \frac{1}{2}\ln(\det\mathbf{S}_N) - E(\mathbf{m}_N), \tag{3.177}$$

where

$$E(\mathbf{m}_N) = \frac{\beta}{2}\|\mathbf{t} - \mathbf{\Phi}\mathbf{m}_N\|^2 + \frac{\alpha}{2}\mathbf{m}_N^\intercal\mathbf{m}_N. \tag{3.178}$$

By 3.21(a),

$$\frac{\partial}{\partial\beta}\ln\left(\det\mathbf{S}_N^{-1}\right) = \mathrm{tr}\left(\mathbf{S}_N\mathbf{\Phi}^\intercal\mathbf{\Phi}\right). \tag{3.179}$$

Since

$$\mathbf{S}_N \mathbf{\Phi}^\intercal \mathbf{\Phi} = \frac{1}{\beta} \left(\mathbf{I} - \alpha \mathbf{S}_N \right), \tag{3.180}$$

the right hand side can be written as

$$\frac{1}{\beta} \left(M - \alpha \sum_{m=1}^{M} \frac{1}{\alpha + \lambda_m} \right) = \frac{1}{\beta} \sum_{m=1}^{M} \frac{\lambda_m}{\alpha + \lambda_m}, \tag{3.181}$$

where $\lambda_1, \cdots, \lambda_M$ are eigenvalues of $\beta \mathbf{\Phi}^\intercal \mathbf{\Phi}$. Therefore, setting the derivative of $\ln p(\mathbf{t})$ with respect to β to zero gives

$$0 = \frac{N}{2\beta} - \frac{1}{2\beta} \sum_{m=1}^{M} \frac{\lambda_i}{\alpha + \lambda_m} - \frac{1}{2} \| \mathbf{t} - \mathbf{\Phi} \mathbf{m}_N \|^2. \tag{3.182}$$

Thus,

$$\beta = \frac{N - \gamma}{\| \mathbf{t} - \mathbf{\Phi} \mathbf{m}_N \|^2}, \tag{3.183}$$

where

$$\gamma = \sum_{m=1}^{M} \frac{\lambda_m}{\alpha + \lambda_m}. \tag{3.184}$$

3.23

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}, \beta) &= \mathcal{N} \left(t_n | \mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1} \right), \\ p(\mathbf{w}, \beta) &= \mathcal{N} \left(\mathbf{w} | \mathbf{m}_0, \beta^{-1} \mathbf{S}_0 \right) \mathrm{Gam}(\beta | a_0, b_0), \end{aligned} \tag{3.185}$$

where $\mathbf{w}$ and $\boldsymbol{\phi}$ are vectors in M dimensions. By marginalisation,

$$p(\mathbf{t}) = \int \int p(\mathbf{t} | \mathbf{w}, \beta) p(\mathbf{w}, \beta) d\mathbf{w} d\beta. \tag{3.186}$$

The right hand side can be written as

$$\int \left(\int \left(\prod_{n=1}^{N} \mathcal{N} \left(t_n | \mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1} \right) \right) \mathcal{N} \left(\mathbf{w} | \mathbf{m}_0, \beta^{-1} \mathbf{S}_0 \right) d\mathbf{w} \right) \mathrm{Gam}(\beta | a_0, b_0) d\beta. \tag{3.187}$$

The logarithm of the integrand with respect to $\mathbf{w}$ can be written as

$$\begin{aligned}
&-\frac{N}{2}\ln(2\pi)-\frac{N}{2}\ln\beta^{-1}-\frac{\beta}{2}\sum_{n=1}^{N}\left(t_n-\mathbf{w}^{\intercal}\boldsymbol{\phi}(\mathbf{x}_n)\right)^2\\
&-\frac{M}{2}\ln(2\pi)-\frac{1}{2}\ln\det\left(\beta^{-1}\mathbf{S}_0\right)-\frac{\beta}{2}(\mathbf{w}-\mathbf{m}_0)^{\intercal}\mathbf{S}_0^{-1}(\mathbf{w}-\mathbf{m}_0)\\
=&-\frac{N+M}{2}\ln(2\pi)+\frac{N+M}{2}\ln\beta-\frac{1}{2}\ln(\det\mathbf{S}_0)\\
&-\frac{\beta}{2}\mathbf{w}^{\intercal}\left(\mathbf{S}_0^{-1}+\boldsymbol{\Phi}^{\intercal}\boldsymbol{\Phi}\right)\mathbf{w}+\beta\mathbf{w}^{\intercal}\left(\mathbf{S}_0^{-1}\mathbf{m}_0+\boldsymbol{\Phi}^{\intercal}\mathbf{t}\right)-\frac{\beta}{2}\|\mathbf{t}\|^2-\frac{\beta}{2}\mathbf{m}_0^{\intercal}\mathbf{S}_0^{-1}\mathbf{m}_0.
\end{aligned}\tag{3.188}$$

The right hand side can be written as

$$\begin{aligned}
&-\frac{N+M}{2}\ln(2\pi)+\frac{N+M}{2}\ln\beta-\frac{1}{2}\ln(\det\mathbf{S}_0)\\
&-\frac{\beta}{2}\left(\mathbf{w}-\mathbf{m}_N\right)^{\intercal}\mathbf{S}_N^{-1}\left(\mathbf{w}-\mathbf{m}_N\right)+\frac{\beta}{2}\mathbf{m}_N^{\intercal}\mathbf{S}_N^{-1}\mathbf{m}_N-\frac{\beta}{2}\|\mathbf{t}\|^2-\frac{\beta}{2}\mathbf{m}_0^{\intercal}\mathbf{S}_0^{-1}\mathbf{m}_0,
\end{aligned}\tag{3.189}$$

where

$$\begin{aligned}
\mathbf{m}_N&=\mathbf{S}_N\left(\mathbf{S}_0^{-1}\mathbf{m}_0+\boldsymbol{\Phi}^{\intercal}\mathbf{t}\right),\\
\mathbf{S}_N^{-1}&=\mathbf{S}_0^{-1}+\boldsymbol{\Phi}^{\intercal}\boldsymbol{\Phi}.
\end{aligned}\tag{3.190}$$

Therefore, the logarithm of the integral with respect to $\mathbf{w}$ can be written as

$$\begin{aligned}
&-\frac{N}{2}\ln(2\pi)+\frac{N}{2}\ln\beta-\frac{1}{2}\ln(\det\mathbf{S}_0)+\frac{1}{2}\ln(\det\mathbf{S}_N)\\
&+\frac{\beta}{2}\mathbf{m}_N^{\intercal}\mathbf{S}_N^{-1}\mathbf{m}_N-\frac{\beta}{2}\|\mathbf{t}\|^2-\frac{\beta}{2}\mathbf{m}_0^{\intercal}\mathbf{S}_0^{-1}\mathbf{m}_0.
\end{aligned}\tag{3.191}$$

Then, the logarithm of the integrand with respect to β can be written as

$$\begin{aligned}
&-\frac{N}{2}\ln(2\pi)+\frac{N}{2}\ln\beta-\frac{1}{2}\ln(\det\mathbf{S}_0)+\frac{1}{2}\ln(\det\mathbf{S}_N)\\
&+\frac{\beta}{2}\mathbf{m}_N^{\intercal}\mathbf{S}_N^{-1}\mathbf{m}_N-\frac{\beta}{2}\|\mathbf{t}\|^2-\frac{\beta}{2}\mathbf{m}_0^{\intercal}\mathbf{S}_0^{-1}\mathbf{m}_0\\
&-\ln\Gamma(a_0)+a_0\ln b_0+(a_0-1)\ln\beta-b_0\beta\\
=&-\frac{N}{2}\ln(2\pi)-\frac{1}{2}\ln(\det\mathbf{S}_0)+\frac{1}{2}\ln(\det\mathbf{S}_N)\\
&-\ln\Gamma(a_0)+a_0\ln b_0+(a_N-1)\ln\beta-b_N\beta,
\end{aligned}\tag{3.192}$$

where

$$\begin{aligned} a_N &= a_0 + \frac{N}{2}, \\ b_N &= b_0 + \frac{\beta}{2}\|\mathbf{t}\|^2 + \frac{\beta}{2}\mathbf{m}_0^\intercal \mathbf{S}_0^{-1}\mathbf{m}_0 - \frac{\beta}{2}\mathbf{m}_N^\intercal \mathbf{S}_N^{-1}\mathbf{m}_N. \end{aligned} \tag{3.193}$$

Therefore, the logarithm of the integral with respect to β can be written as

$$-\frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln(\det \mathbf{S}_0) + \frac{1}{2}\ln(\det \mathbf{S}_N) - \ln\Gamma(a_0) + a_0 \ln b_0 + \ln\Gamma(a_N) - a_N \ln b_N. \tag{3.194}$$

Thus,

$$p(\mathbf{t}) = (2\pi)^{-\frac{N}{2}} \left(\frac{\det \mathbf{S}_N}{\det \mathbf{S}_0}\right)^{\frac{1}{2}} \frac{\Gamma(a_N)}{\Gamma(a_0)} \frac{{b_0}^{a_0}}{{b_N}^{a_N}}. \tag{3.195}$$

3.24

Refer to 3.12.

4 Linear Models for Classification

4.1

Let $x_1, \cdots, x_M$ and $y_1, \cdots, y_N$ be two sets of data points. Then, the corresponding convex hulls are defined as the sets of all points $\mathbf{x}$ and $\mathbf{y}$ such that

$$\begin{aligned} \mathbf{x} &= \sum_{m=1}^{M} \alpha_m \mathbf{x}_m, \\ \mathbf{y} &= \sum_{n=1}^{N} \beta_n \mathbf{y}_n, \end{aligned} \tag{4.1}$$

where

$$\begin{aligned} \sum_{m=1}^{M} \alpha_m = \sum_{n=1}^{N} \beta_n = 1, \\ \alpha_m \geq 0, \beta_n \geq 0. \end{aligned} \tag{4.2}$$

Let us assume that $\alpha_1, \cdots, \alpha_M$ and $\beta_1, \cdots, \beta_N$ below are subject to the constraints above.

If the convex hulls intersect, then there exist $\alpha_1, \cdots, \alpha_M$ and $\beta_1, \cdots, \beta_N$ such that

$$\sum_{m=1}^{M} \alpha_m \mathbf{x}_m = \sum_{n=1}^{N} \beta_n \mathbf{y}_n. \tag{4.3}$$

Then,

$$\sum_{m=1}^{M} \alpha_m \left(\hat{\mathbf{w}}^\intercal \mathbf{x}_m + w_0 \right) = \hat{\mathbf{w}}^\intercal \sum_{m=1}^{M} \alpha_m \mathbf{x}_m + w_0 \sum_m \alpha_m, \tag{4.4}$$

for any $\hat{\mathbf{w}}$ and w_0. The right hand side can be written as

$$\hat{\mathbf{w}}^\intercal \sum_{n=1}^{N} \beta_n \mathbf{y}_n + w_0 \sum_{n=1}^{N} \beta_n = \sum_{n=1}^{N} \beta_n \left(\hat{\mathbf{w}}^\intercal \mathbf{y}_n + w_0 \right). \tag{4.5}$$

Therefore, there do not exist $\hat{\mathbf{w}}$ and w_0 such that

$$\begin{aligned} \hat{\mathbf{w}}^\intercal \mathbf{x}_m + w_0 > 0, \\ \hat{\mathbf{w}}^\intercal \mathbf{y}_n + w_0 < 0. \end{aligned} \tag{4.6}$$

Conversely, if there exist $\hat{\mathbf{w}}$ and w_0 such that

$$\begin{aligned} \hat{\mathbf{w}}^\intercal \mathbf{x}_m + w_0 > 0, \\ \hat{\mathbf{w}}^\intercal \mathbf{y}_n + w_0 < 0, \end{aligned} \tag{4.7}$$

then

$$\begin{aligned} \sum_{m=1}^{M} \alpha_m \left(\hat{\mathbf{w}}^\intercal \mathbf{x}_m + w_0 \right) > 0, \\ \sum_{n=1}^{N} \beta_n \left(\hat{\mathbf{w}}^\intercal \mathbf{y}_n + w_0 \right) < 0. \end{aligned} \tag{4.8}$$

The left hand sides can be written as

$$\begin{aligned} \hat{\mathbf{w}}^\intercal \sum_{m=1}^{M} \alpha_m \mathbf{x}_m + w_0 \sum_{m=1}^{M} \alpha_m = \hat{\mathbf{w}}^\intercal \sum_{m=1}^{M} \alpha_m \mathbf{x}_m + w_0, \\ \hat{\mathbf{w}}^\intercal \sum_{n=1}^{N} \beta_n \mathbf{y}_n + w_0 \sum_{n=1}^{N} \beta_n = \hat{\mathbf{w}}^\intercal \sum_{n=1}^{N} \beta_n \mathbf{y}_n + w_0. \end{aligned} \tag{4.9}$$

Therefore, there do not exist $\alpha_1, \cdots, \alpha_M$ and $\beta_1, \cdots, \beta_N$ such that

$$\sum_{m=1}^{M} \alpha_m \mathbf{x}_m = \sum_{n=1}^{N} \beta_n \mathbf{y}_n. \tag{4.10}$$

Thus, the convex hulls do not intersect.

4.2 (Incomplete)

Let $\mathbf{x}_1, \cdots, \mathbf{x}_N$ and $\mathbf{w}_1, \cdots, \mathbf{w}_K$ are variables in M dimensions and $\mathbf{t}_1, \cdots, \mathbf{t}_N$ are ones in K dimensions. Let

$$E(\tilde{\mathbf{W}}) = \frac{1}{2} \operatorname{tr} \left((\tilde{\mathbf{X}}\tilde{\mathbf{W}} - \mathbf{T})^\intercal (\tilde{\mathbf{X}}\tilde{\mathbf{W}} - \mathbf{T}) \right), \tag{4.11}$$

where

$$\tilde{\mathbf{X}} = \begin{bmatrix} 1 & \mathbf{x}_1^\intercal \\ \vdots & \vdots \\ 1 & \mathbf{x}_N^\intercal \end{bmatrix},$$

$$\tilde{\mathbf{W}} = \begin{bmatrix} w_{10} & \cdots & w_{K0} \\ \mathbf{w}_1 & \cdots & \mathbf{w}_K \end{bmatrix}$$

and

$$\mathbf{T} = \begin{bmatrix} \mathbf{t}_1^\intercal \\ \vdots \\ \mathbf{t}_N^\intercal \end{bmatrix}.$$

Setting the derivative with respect to $\tilde{\mathbf{W}}$ to zero gives

$$\mathbf{O} = \tilde{\mathbf{X}}^\intercal(\tilde{\mathbf{X}}\tilde{\mathbf{W}} - \mathbf{T}). \tag{4.12}$$

Therefore,

$$\underset{\tilde{\mathbf{W}}}{\operatorname{argmin}} E(\tilde{\mathbf{W}}) = \left(\tilde{\mathbf{X}}^\intercal\tilde{\mathbf{X}}\right)^{-1}\tilde{\mathbf{X}}^\intercal\mathbf{T}. \tag{4.13}$$

Let $\tilde{\mathbf{W}}^*$ denote the least-square solution above. Then,

$$(\tilde{\mathbf{W}}^*)^\intercal\tilde{\mathbf{x}} - \mathbf{t}_n = \mathbf{T}^\intercal\tilde{\mathbf{X}}\left(\tilde{\mathbf{X}}^\intercal\tilde{\mathbf{X}}\right)^{-1}\tilde{\mathbf{x}} - \mathbf{t}_n, \tag{4.14}$$

where $\tilde{\mathbf{x}}$ is a vector in $M+1$ dimensions whose first element is 1. The right hand side can be written as

$$\mathbf{T}^\intercal\left(\tilde{\mathbf{X}}\left(\tilde{\mathbf{X}}^\intercal\tilde{\mathbf{X}}\right)^{-1}\tilde{\mathbf{x}} - \mathbf{v}_n\right) = \mathbf{0}? \tag{4.15}$$

where $\mathbf{v}_n$ is a vector in N dimensions whose n th element is 1 and other elements are zero. Therefore,

$$(\tilde{\mathbf{W}}^*)^\intercal\tilde{\mathbf{x}} - \mathbf{t}_n = \mathbf{0}. \tag{4.16}$$

Thus, if

$$\mathbf{a}^\intercal\mathbf{t}_n + b = 0, \tag{4.17}$$

then

$$\mathbf{a}^\intercal(\tilde{\mathbf{W}}^*)^\intercal\tilde{\mathbf{x}} + b = 0. \tag{4.18}$$

4.3 (Incomplete)

4.4

Let $\mathbf{x}_1, \cdots, \mathbf{x}_N$ be variables and let

$$\mathbf{m}_k = \frac{1}{N_k}\sum_{n\in\mathcal{C}_k}\mathbf{x}_n, \tag{4.19}$$

where N_k is the number of $\mathbf{x}_n$ such that n is in $\mathcal{C}_k$. Setting the derivatives of

$$\mathbf{w}^\intercal(\mathbf{m}_2 - \mathbf{m}_1) + \lambda\left(\|\mathbf{w}\|^2 - 1\right) \tag{4.20}$$

with respect to $\mathbf{w}$ and λ to zero gives

$$\begin{aligned} \mathbf{m}_2 - \mathbf{m}_1 + 2\lambda\mathbf{w} &= \mathbf{0}, \\ \|\mathbf{w}\|^2 - 1 &= 0. \end{aligned} \tag{4.21}$$

Therefore, $\mathbf{w}^\intercal(\mathbf{m}_2 - \mathbf{m}_1)$ under the constratint

$$\|\mathbf{w}\|^2 = 1 \tag{4.22}$$

is maximised if

$$\mathbf{w} \propto \mathbf{m}_2 - \mathbf{m}_1. \tag{4.23}$$

4.5

Let $\mathbf{x}_1, \cdots, \mathbf{x}_N$ be variables and let

$$\mathbf{m}_k = \frac{1}{N_k}\sum_{n\in\mathcal{C}_k}\mathbf{x}_n, \tag{4.24}$$

where N_k is the number of $\mathbf{x}_n$ such that n is in $\mathcal{C}_k$. Let

$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}, \tag{4.25}$$

where

$$\begin{aligned} s_k^2 &= \sum_{n\in\mathcal{C}_k}(y_n - m_k)^2, \\ y_n &= \mathbf{w}^\intercal\mathbf{x}_n, \\ m_k &= \mathbf{w}^\intercal\mathbf{m}_k. \end{aligned} \tag{4.26}$$

Then, $J(\mathbf{w})$ can be written as

$$\frac{\left(\mathbf{w}^\intercal(\mathbf{m}_2 - \mathbf{m}_1)\right)^2}{\sum_{n\in\mathcal{C}_1}\left(\mathbf{w}^\intercal(\mathbf{x}_n - \mathbf{m}_1)\right)^2 + \sum_{n\in\mathcal{C}_2}\left(\mathbf{w}^\intercal(\mathbf{x}_n - \mathbf{m}_2)\right)^2} = \frac{\mathbf{w}^\intercal\mathbf{S}_\mathrm{B}\mathbf{w}}{\mathbf{w}^\intercal\mathbf{S}_\mathrm{W}\mathbf{w}}, \tag{4.27}$$

where

$$\begin{aligned} \mathbf{S}_\mathrm{B} &= (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^\intercal, \\ \mathbf{S}_\mathrm{W} &= \sum_{n\in\mathcal{C}_1}(\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^\intercal + \sum_{n\in\mathcal{C}_2}(\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^\intercal. \end{aligned} \tag{4.28}$$

4.6

Let $\mathbf{x}_1, \cdots, \mathbf{x}_N$ be variables and let

$$\mathbf{m}_k = \frac{1}{N_k} \sum_{n \in \mathcal{C}_k} \mathbf{x}_n, \tag{4.29}$$

where N_k is the number of $\mathbf{x}_n$ such that n is in $\mathcal{C}_k$. Let

$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}, \tag{4.30}$$

where

$$\begin{aligned} s_k^2 &= \sum_{n \in \mathcal{C}_k} (y_n - m_k)^2, \\ y_n &= \mathbf{w}^\mathsf{T} \mathbf{x}_n, \\ m_k &= \mathbf{w}^\mathsf{T} \mathbf{m}_k. \end{aligned} \tag{4.31}$$

Then, by 4.5,

$$J(\mathbf{w}) = \frac{\mathbf{w}^\mathsf{T} \mathbf{S}_\mathrm{B} \mathbf{w}}{\mathbf{w}^\mathsf{T} \mathbf{S}_\mathrm{W} \mathbf{w}}, \tag{4.32}$$

where

$$\begin{aligned} \mathbf{S}_\mathrm{B} &= (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^\mathsf{T}, \\ \mathbf{S}_\mathrm{W} &= \sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^\mathsf{T} + \sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^\mathsf{T}. \end{aligned} \tag{4.33}$$

Let

$$E = \frac{1}{2} \sum_{n=1}^{N} \left(\mathbf{w}^\mathsf{T} \mathbf{x}_n + w_0 - t_n \right)^2, \tag{4.34}$$

where

$$t_n = \begin{cases} \frac{N}{N_1}, & n \in \mathcal{C}_1, \\ -\frac{N}{N_2}, & n \in \mathcal{C}_2. \end{cases} \tag{4.35}$$

Setting the derivative with respect to $\mathbf{w}$ and w_0 gives

$$\begin{aligned} 0 &= \sum_{n=1}^{N} \left(\mathbf{w}^\mathsf{T} \mathbf{x}_n + w_0 - t_n \right), \\ \mathbf{0} &= \sum_{n=1}^{N} \left(\mathbf{w}^\mathsf{T} \mathbf{x}_n + w_0 - t_n \right) \mathbf{x}_n. \end{aligned} \tag{4.36}$$

The right hand side of the first equation can be written as

$$\mathbf{w}^\intercal \sum_{n=1}^{N} \mathbf{x}_n + N w_0 - \sum_{n=1}^{N} t_n = N \left(\mathbf{w}^\intercal \mathbf{m} + w_0 \right), \tag{4.37}$$

where

$$\mathbf{m} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n. \tag{4.38}$$

Therefore,

$$w_0 = -\mathbf{w}^\intercal \mathbf{m}. \tag{4.39}$$

Then, the right hand side of the second equation above can be written as

$$\begin{aligned} &\sum_{n=1}^{N} \left(\mathbf{w}^\intercal \left(\mathbf{x}_n - \mathbf{m} \right) - t_n \right) \mathbf{x}_n \\ &= \sum_{n \in \mathcal{C}_1} \left(\mathbf{w}^\intercal (\mathbf{x}_n - \mathbf{m}) - \frac{N}{N_1} \right) \mathbf{x}_n + \sum_{n \in \mathcal{C}_2} \left(\mathbf{w}^\intercal (\mathbf{x}_n - \mathbf{m}) + \frac{N}{N_2} \right) \mathbf{x}_n. \end{aligned} \tag{4.40}$$

Since

$$\begin{aligned} \mathbf{m} &= \frac{N_1}{N} \mathbf{m}_1 + \frac{N_2}{N} \mathbf{m}_2, \\ \sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1) &= \mathbf{0}, \end{aligned} \tag{4.41}$$

the first term of the right hand side can be written as

$$\begin{aligned} &\sum_{n \in \mathcal{C}_1} \left(\mathbf{w}^\intercal \left(\mathbf{x}_n - \mathbf{m}_1 + \frac{N_2}{N} (\mathbf{m}_1 - \mathbf{m}_2) \right) - \frac{N}{N_1} \right) (\mathbf{x}_n - \mathbf{m}_1 + \mathbf{m}_1) \\ &= \left(\sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^\intercal \right) \mathbf{w} + \frac{N_1 N_2}{N} (\mathbf{m}_1 - \mathbf{m}_2) \mathbf{m}_1^\intercal \mathbf{w} - N \mathbf{m}_1. \end{aligned} \tag{4.42}$$

Similarly, the second term can be written as

$$\left(\sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^\intercal \right) \mathbf{w} + \frac{N_1 N_2}{N} (\mathbf{m}_2 - \mathbf{m}_1) \mathbf{m}_2^\intercal \mathbf{w} - N \mathbf{m}_2. \tag{4.43}$$

Therefore,

$$\mathbf{0} = \left(\sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^\intercal \right) \mathbf{w} + \frac{N_1 N_2}{N} (\mathbf{m}_1 - \mathbf{m}_2)\mathbf{m}_1^\intercal \mathbf{w} - N\mathbf{m}_1 + \left(\sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^\intercal \right) \mathbf{w} + \frac{N_1 N_2}{N} (\mathbf{m}_2 - \mathbf{m}_1)\mathbf{m}_2^\intercal \mathbf{w} - N\mathbf{m}_2. \tag{4.44}$$

Thus,

$$\left(\mathbf{S}_\mathrm{W} + \frac{N_1 N_2}{N} \mathbf{S}_\mathrm{B} \right) \mathbf{w} = N(\mathbf{m}_1 - \mathbf{m}_2). \tag{4.45}$$

4.7

Let

$$\sigma(a) = \frac{1}{1 + \exp(-a)}. \tag{4.46}$$

Then,

$$\sigma(-a) = \frac{1}{1 + \exp(a)}. \tag{4.47}$$

The right hand side can be written as

$$1 - \frac{\exp(a)}{1 + \exp(a)} = 1 - \frac{1}{1 + \exp(-a)}. \tag{4.48}$$

Therefore,

$$\sigma(-a) = 1 - \sigma(a). \tag{4.49}$$

Additionally,

$$\exp(-a) = \frac{1}{\sigma(a)} - 1. \tag{4.50}$$

Then,

$$a = -\ln \left(\frac{1}{\sigma(a)} - 1 \right). \tag{4.51}$$

Therefore,

$$\sigma^{-1}(y) = \ln \left(\frac{y}{1 - y} \right). \tag{4.52}$$

4.8

Let $\mathbf{x}$ be a variable in D dimensions such that

$$p(\mathbf{x}|\mathcal{C}_k) = \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}\right), \tag{4.53}$$

where

$$p(\mathcal{C}_1) + p(\mathcal{C}_2) = 1. \tag{4.54}$$

By the Bayes' theorem,

$$p(\mathcal{C}_1|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}. \tag{4.55}$$

The right hand side can be written as

$$\sigma(a) = \frac{1}{1 + \exp(-a)}, \tag{4.56}$$

where

$$a = \ln\left(\frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}\right). \tag{4.57}$$

Substituting the expressions above of $p(\mathbf{x}|\mathcal{C}_k)$, we have

$$\begin{aligned} a = &-\frac{D}{2}\ln(2\pi) - \frac{1}{2}\ln(\det\Sigma) - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_1)^\intercal\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_1) + \ln p(\mathcal{C}_1) \\ &+ \frac{D}{2}\ln(2\pi) + \frac{1}{2}\ln(\det\Sigma) + \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_2)^\intercal\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_2) - \ln p(\mathcal{C}_2). \end{aligned} \tag{4.58}$$

Therefore,

$$p(\mathcal{C}_1|\mathbf{x}) = \sigma\left(\mathbf{w}^\intercal\mathbf{x} + w_0\right), \tag{4.59}$$

where

$$\begin{aligned} \mathbf{w} &= \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2), \\ w_0 &= -\frac{1}{2}\boldsymbol{\mu}_1^\intercal\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^\intercal\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_2 + \ln p(\mathcal{C}_1) - \ln p(\mathcal{C}_2). \end{aligned} \tag{4.60}$$

4.9

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables in K dimensions such that

$$p(\mathbf{t}_n, \boldsymbol{\phi}_n) = \prod_{k=1}^{K}\left(p(\boldsymbol{\phi}_n, \mathcal{C}_k)\right)^{t_{nk}}, \tag{4.61}$$

where

$$\sum_{k=1}^{K} p(\mathcal{C}_k) = 1. \tag{4.62}$$

Then,

$$p(\mathbf{T}, \mathbf{\Phi}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \left(p(\boldsymbol{\phi}_n, \mathcal{C}_k)\right)^{t_{nk}}. \tag{4.63}$$

If

$$p(\mathcal{C}_k) = \pi_k, \tag{4.64}$$

then, by the Bayes' theorem,

$$\ln p(\mathbf{T}, \mathbf{\Phi}) = \sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \left(\ln \pi_k + \ln p(\boldsymbol{\phi}_n | \mathcal{C}_k)\right). \tag{4.65}$$

Setting the derivatives of

$$\ln p(\mathbf{T}, \mathbf{\Phi}) + \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right) \tag{4.66}$$

with respect to π_k and λ to zero gives

$$\begin{aligned} 0 &= \frac{1}{\pi_k} \sum_{n=1}^{N} t_{nk} + \lambda, \\ 0 &= \sum_{k=1}^{K} \pi_k - 1. \end{aligned} \tag{4.67}$$

Then,

$$\lambda = -\sum_{k=1}^{K} \sum_{n=1}^{N} t_{nk}. \tag{4.68}$$

The right hand side can be written as $-N$. Therefore, the maximum likelihood solution for π_k is given by

$$\pi_k = \frac{N_k}{N}, \tag{4.69}$$

where

$$N_k = \sum_{n=1}^{N} t_{nk}. \tag{4.70}$$

4.10

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables in K dimensions such that

$$p(\mathbf{t}_n, \boldsymbol{\phi}_n) = \prod_{k=1}^{K} \left(p(\boldsymbol{\phi}_n, \mathcal{C}_k)\right)^{t_{nk}}, \tag{4.71}$$

where

$$\sum_{k=1}^{K} p(\mathcal{C}_k) = 1. \tag{4.72}$$

Then,

$$p(\mathbf{T}, \boldsymbol{\Phi}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \left(p(\boldsymbol{\phi}_n, \mathcal{C}_k)\right)^{t_{nk}}. \tag{4.73}$$

If

$$p(\boldsymbol{\phi}_n|\mathcal{C}_k) = \mathcal{N}(\boldsymbol{\phi}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}), \tag{4.74}$$

then, by the Bayes' theorem,

$$\ln p(\mathbf{T}, \boldsymbol{\Phi}) = \sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \left(\ln \mathcal{N}(\boldsymbol{\phi}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}) + \ln p(\mathcal{C}_k)\right). \tag{4.75}$$

The right hand side can be written as

$$\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \left(-\frac{D}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \boldsymbol{\Sigma}) - \frac{1}{2}(\boldsymbol{\phi}_n - \boldsymbol{\mu}_k)^\intercal \boldsymbol{\Sigma}^{-1} (\boldsymbol{\phi}_n - \boldsymbol{\mu}_k) + \ln p(\mathcal{C}_k)\right). \tag{4.76}$$

By 3.21(a), setting the derivatives of $\ln p(\mathbf{T}, \boldsymbol{\Phi})$ with respect to $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}$ to zero gives

$$\begin{aligned} \mathbf{0} &= \frac{1}{2} \sum_{n=1}^{N} t_{nk} \left(\boldsymbol{\Sigma}^{-1} + \left(\boldsymbol{\Sigma}^{-1}\right)^\intercal\right) (\boldsymbol{\phi}_n - \boldsymbol{\mu}_k), \\ \mathbf{O} &= -\frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \left(\left(\boldsymbol{\Sigma}^{-1}\right)^\intercal - \left(\boldsymbol{\Sigma}^{-1}\right)^2 (\boldsymbol{\phi}_n - \boldsymbol{\mu}_k)(\boldsymbol{\phi}_n - \boldsymbol{\mu}_k)^\intercal\right). \end{aligned} \tag{4.77}$$

Therefore, the maximum likelihood solutions for $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}$ are given by

$$\begin{aligned} \boldsymbol{\mu}_k &= \frac{1}{N_k} \sum_{n=1}^{N} t_{nk} \boldsymbol{\phi}_n, \\ \boldsymbol{\Sigma} &= \frac{1}{N} \sum_{k=1}^{K} N_k \mathbf{S}_k, \end{aligned} \tag{4.78}$$

where

$$\begin{aligned} N_k &= \sum_{n=1}^{N} t_{nk}, \\ \mathbf{S}_k &= \frac{1}{N_k} \sum_{n=1}^{N} t_{nk} (\boldsymbol{\phi}_n - \boldsymbol{\mu}_k)(\boldsymbol{\phi}_n - \boldsymbol{\mu}_k)^\intercal. \end{aligned} \tag{4.79}$$

4.11

Let $\boldsymbol{\phi}_1, \cdots, \boldsymbol{\phi}_M$ be variables such that

$$p(\boldsymbol{\phi}_m | \mathcal{C}_k) = \prod_{l=1}^{L} \mu_{kml}^{\phi_{ml}}, \tag{4.80}$$

where

$$\sum_{k=1}^{K} p(\mathcal{C}_k) = 1. \tag{4.81}$$

Then,

$$p(\boldsymbol{\Phi} | \mathcal{C}_k) = \prod_{m=1}^{M} \prod_{l=1}^{L} \mu_{kml}^{\phi_{ml}}. \tag{4.82}$$

By the Bayes' theorem,

$$p(\mathcal{C}_k | \boldsymbol{\Phi}) = \frac{p(\boldsymbol{\Phi} | \mathcal{C}_k) p(\mathcal{C}_k)}{\sum_{k=1}^{K} p(\boldsymbol{\Phi} | \mathcal{C}_k) p(\mathcal{C}_k)}. \tag{4.83}$$

Therefore,

$$p(\mathcal{C}_k | \boldsymbol{\Phi}) = \frac{\exp\left(a_k(\boldsymbol{\Phi})\right)}{\sum_{k=1}^{K} \exp\left(a_k(\boldsymbol{\Phi})\right)}, \tag{4.84}$$

where

$$a_k(\boldsymbol{\Phi}) = \left(\sum_{m=1}^{M} \sum_{l=1}^{L} \phi_{ml} \ln \mu_{kml} \right) + \ln p(\mathcal{C}_k). \tag{4.85}$$

4.12

Let

$$\sigma(a) = \frac{1}{1+\exp(-a)}. \tag{4.86}$$

Then,

$$\frac{d\sigma(a)}{da} = \frac{\exp(-a)}{(1+\exp(-a))^2}. \tag{4.87}$$

The right hand side can be written as

$$\frac{1}{1+\exp(-a)} - \frac{1}{(1+\exp(-a))^2} = \sigma(a) - (\sigma(a))^2. \tag{4.88}$$

Therefore,

$$\frac{d\sigma(a)}{da} = \sigma(a)\left(1-\sigma(a)\right). \tag{4.89}$$

4.13

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} t_n &\in \{0,1\}, \\ p(t_n|\mathbf{w}) &= y_n^{t_n}(1-y_n)^{1-t_n}, \end{aligned} \tag{4.90}$$

where

$$\begin{aligned} y_n &= \sigma\left(\mathbf{w}^\intercal \boldsymbol{\phi}_n\right), \\ \sigma(a) &= \frac{1}{1+\exp(-a)}. \end{aligned} \tag{4.91}$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}). \tag{4.92}$$

The right hand side can be written as

$$-\ln\left(\prod_{n=1}^{N} y_n^{t_n}(1-y_n)^{1-t_n}\right) = -\sum_{n=1}^{N}\left(t_n \ln y_n + (1-t_n)\ln(1-y_n)\right). \tag{4.93}$$

Then, by 4.12,

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N}\left(\frac{t_n}{y_n}y_n(1-y_n)\boldsymbol{\phi}_n - \frac{1-t_n}{1-y_n}y_n(1-y_n)\boldsymbol{\phi}_n\right). \tag{4.94}$$

The right hand side can be written as

$$-\sum_{n=1}^{N}(t_n(1-y_n)\boldsymbol{\phi}_n-(1-t_n)y_n\boldsymbol{\phi}_n)=\sum_{n=1}^{N}(y_n-t_n)\boldsymbol{\phi}_n. \tag{4.95}$$

Therefore,

$$\nabla E(\mathbf{w})=\sum_{n=1}^{N}(y_n-t_n)\boldsymbol{\phi}_n. \tag{4.96}$$

4.14

Let $t_1,\cdots,t_N$ be variables such that

$$\begin{aligned} t_n &\in \{0,1\},\\ p(t_n|\mathbf{w}) &= y_n^{t_n}(1-y_n)^{1-t_n}, \end{aligned} \tag{4.97}$$

where

$$\begin{aligned} y_n &= \sigma\left(\mathbf{w}^\intercal\boldsymbol{\phi}_n\right),\\ \sigma(a) &= \frac{1}{1+\exp(-a)}. \end{aligned} \tag{4.98}$$

Let

$$E(\mathbf{w})=-\ln p(\mathbf{t}|\mathbf{w}). \tag{4.99}$$

By 4.13, setting the derivative with respect to $\mathbf{w}$ to zero gives

$$\mathbf{0}=\sum_{n=1}^{N}\left(y_n-t_n\right)\boldsymbol{\phi}_n. \tag{4.100}$$

If $\boldsymbol{\phi}_1,\cdots,\boldsymbol{\phi}_N$ are linearly independent, then

$$y_n=t_n. \tag{4.101}$$

Then,

$$\sigma\left(\mathbf{w}^\intercal\boldsymbol{\phi}_n\right)=\begin{cases}1, & t_n=1,\\ 0, & \text{otherwise.}\end{cases} \tag{4.102}$$

Threrefore,

$$\mathbf{w}^\intercal\boldsymbol{\phi}_n=\begin{cases}\infty, & t_n=1,\\ -\infty, & \text{otherwise.}\end{cases} \tag{4.103}$$

4.15

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} t_n &\in \{0, 1\}, \\ p(t_n|\mathbf{w}) &= y_n^{t_n}(1 - y_n)^{1-t_n}, \end{aligned} \tag{4.104}$$

where

$$\begin{aligned} y_n &= \sigma\left(\mathbf{w}^\intercal \boldsymbol{\phi}_n\right), \\ \sigma(a) &= \frac{1}{1 + \exp(-a)}. \end{aligned} \tag{4.105}$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}). \tag{4.106}$$

By 4.13,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N}(y_n - t_n)\boldsymbol{\phi}_n. \tag{4.107}$$

Then, by 4.12,

$$\nabla\nabla E(\mathbf{w}) = \sum_{n=1}^{N} y_n(1 - y_n)\boldsymbol{\phi}_n\boldsymbol{\phi}_n^\intercal. \tag{4.108}$$

The right hand side can be written as

$$\mathbf{H} = \boldsymbol{\Phi}^\intercal \mathbf{R}\boldsymbol{\Phi}, \tag{4.109}$$

where

$$R_{nn'} = \begin{cases} y_n(1 - y_n), & n = n', \\ 0, & \text{otherwise.} \end{cases} \tag{4.110}$$

Then,

$$\mathbf{u}^\intercal \mathbf{H}\mathbf{u} = \left(\boldsymbol{\Phi}\mathbf{u}\right)^\intercal \mathbf{R}\left(\boldsymbol{\Phi}\mathbf{u}\right). \tag{4.111}$$

Since

$$y_n(1 - y_n) > 0, \tag{4.112}$$

we have

$$\mathbf{u}^\intercal \mathbf{H}\mathbf{u} > 0. \tag{4.113}$$

Therefore, $\mathbf{H}$ is positive definite. Thus, E is a convex function of $\mathbf{w}$ and it has a unique minimum.

4.16

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} t_n &\in \{0, 1\}, \\ p(t_n = 1|\boldsymbol{\phi}_n) &= \pi_n. \end{aligned} \tag{4.114}$$

Then,

$$p(t_n|\boldsymbol{\phi}_n) = \pi_n^{t_n}(1 - \pi_n)^{1-t_n}. \tag{4.115}$$

Therefore,

$$p(\mathbf{t}|\boldsymbol{\Phi}) = \prod_{n=1}^{N} \pi_n^{t_n}(1 - \pi_n)^{1-t_n}. \tag{4.116}$$

Thus,

$$-\ln p(\mathbf{t}|\boldsymbol{\Phi}) = -\sum_{n=1}^{N} \left(t_n \ln \pi_n + (1 - t_n) \ln(1 - \pi_n)\right). \tag{4.117}$$

4.17

Let

$$y_k = \frac{\exp(a_k)}{\sum_{k=1}^{K} \exp(a_k)}. \tag{4.118}$$

Then,

$$\frac{\partial y_k}{\partial a_k} = \frac{\exp(a_k)}{\sum_{k=1}^{K} \exp(a_k)} - \frac{\exp(2a_k)}{\left(\sum_{k=1}^{K} \exp(a_k)\right)^2}. \tag{4.119}$$

The right hand side can be written as $y_k(1 - y_k)$. If $k \neq k'$, then

$$\frac{\partial y_k}{\partial a_{k'}} = -\frac{\exp(a_k + a_{k'})}{\left(\sum_{k=1}^{K} \exp(a_k)\right)^2}. \tag{4.120}$$

The right hand side can be written as $-y_k y_{k'}$. Therefore,

$$\frac{\partial y_k}{\partial a_{k'}} = y_k(I_{kk'} - y_{k'}). \tag{4.121}$$

4.18

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables such that

$$\begin{aligned} t_{nk} &\in \{0, 1\}, \\ p(\mathbf{t}_n|\mathbf{W}) &= \prod_{k=1}^{K} y_{nk}^{t_{nk}}, \end{aligned} \tag{4.122}$$

where

$$\begin{aligned} y_{nk} &= \frac{\exp(a_{nk})}{\sum_{k=1}^{K} \exp(a_{nk})}, \\ a_{nk} &= \mathbf{w}_k^{\intercal} \boldsymbol{\phi}_n. \end{aligned} \tag{4.123}$$

Then,

$$p(\mathbf{T}|\mathbf{W}) = \prod_{n=1}^{N} \prod_{k=1}^{K} y_{nk}^{t_{nk}}. \tag{4.124}$$

Let

$$E(\mathbf{W}) = -\ln p(\mathbf{T}|\mathbf{W}). \tag{4.125}$$

The right hand side can be written as

$$-\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \ln y_{nk}. \tag{4.126}$$

Then, by 4.17,

$$\nabla_{\mathbf{w}_{k'}} E(\mathbf{W}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} y_{nk}(I_{kk'} - y_{nk'}) \frac{t_{nk}}{y_{nk}} \boldsymbol{\phi}_n. \tag{4.127}$$

The right hand side can be written as

$$-\sum_{n=1}^{N} \left(\sum_{k=1}^{K} (I_{kk'} - y_{nk'}) t_{nk} \right) \boldsymbol{\phi}_n = -\sum_{n=1}^{N} (t_{nk'} - y_{nk'}) \boldsymbol{\phi}_n. \tag{4.128}$$

Therefore,

$$\nabla_{\mathbf{w}_k} E(\mathbf{W}) = \sum_{n=1}^{N} (y_{nk} - t_{nk}) \boldsymbol{\phi}_n. \tag{4.129}$$

4.19

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} t_n &\in \{0, 1\}, \\ p(t_n = 1|a_n) &= \Phi(a_n), \end{aligned} \tag{4.130}$$

where

$$\begin{aligned} \Phi(a) &= \int_{-\infty}^{a} \mathcal{N}(\theta|0, 1)d\theta, \\ a_n &= \mathbf{w}^\mathsf{T}\boldsymbol{\phi}_n. \end{aligned} \tag{4.131}$$

Then,

$$p(t_n|\boldsymbol{\phi}_n) = (\Phi(a_n))^{t_n} (1 - \Phi(a_n))^{1-t_n}. \tag{4.132}$$

Therefore,

$$p(\mathbf{t}|\boldsymbol{\Phi}) = \prod_{n=1}^{N} (\Phi(a_n))^{t_n} (1 - \Phi(a_n))^{1-t_n}. \tag{4.133}$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\boldsymbol{\phi}). \tag{4.134}$$

The right hand side can be written as

$$-\sum_{n=1}^{N} (t_n \ln \Phi(a_n) + (1 - t_n) \ln (1 - \Phi(a_n))). \tag{4.135}$$

Then,

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N} \left(t_n \frac{\mathcal{N}(a_n|0, 1)}{\Phi(a_n)} - (1 - t_n) \frac{\mathcal{N}(a_n|0, 1)}{1 - \Phi(a_n)} \right) \boldsymbol{\phi}_n. \tag{4.136}$$

The right hand side can be written as

$$\begin{aligned} &-\sum_{n=1}^{N} \left(\frac{t_n}{\Phi(a_n)} - \frac{1 - t_n}{1 - \Phi(a_n)} \right) \mathcal{N}(a_n|0, 1)\boldsymbol{\phi}_n \\ =&\sum_{n=1}^{N} \frac{\mathcal{N}(a_n|0, 1)}{\Phi(a_n)(1 - \Phi(a_n))} (\Phi(a_n) - t_n) \boldsymbol{\phi}_n. \end{aligned} \tag{4.137}$$

Therefore,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} \frac{\mathcal{N}(a_n|0,1)}{\Phi(a_n)\left(1-\Phi(a_n)\right)} \left(\Phi(a_n) - t_n\right) \boldsymbol{\phi}_n. \tag{4.138}$$

Then,

$$\begin{aligned}
\nabla\nabla E(\mathbf{w}) = &\sum_{n=1}^{N} \frac{-a_n \mathcal{N}(a_n|0,1)}{\Phi(a_n)\left(1-\Phi(a_n)\right)} \left(\Phi(a_n) - t_n\right) \boldsymbol{\phi}_n \boldsymbol{\phi}_n^\intercal \\
&- \sum_{n=1}^{N} \frac{\left(\mathcal{N}(a_n|0,1)\right)^2}{\left(\Phi(a_n)\right)^2\left(1-\Phi(a_n)\right)} \left(\Phi(a_n) - t_n\right) \boldsymbol{\phi}_n \boldsymbol{\phi}_n^\intercal \\
&+ \sum_{n=1}^{N} \frac{\left(\mathcal{N}(a_n|0,1)\right)^2}{\Phi(a_n)\left(1-\Phi(a_n)\right)^2} \left(\Phi(a_n) - t_n\right) \boldsymbol{\phi}_n \boldsymbol{\phi}_n^\intercal \\
&+ \sum_{n=1}^{N} \frac{\left(\mathcal{N}(a_n|0,1)\right)^2}{\Phi(a_n)\left(1-\Phi(a_n)\right)} \boldsymbol{\phi}_n \boldsymbol{\phi}_n^\intercal.
\end{aligned} \tag{4.139}$$

Therefore,

$$\nabla\nabla E(\mathbf{w}) = \sum_{n=1}^{N} b_n \boldsymbol{\phi}_n \boldsymbol{\phi}_n^\intercal, \tag{4.140}$$

where

$$\begin{aligned}
b_n = &\left(\frac{\mathcal{N}(a_n|0,1)}{\Phi(a_n)\left(1-\Phi(a_n)\right)} \right)^2 \left(\left(\Phi(a_n)\right)^2 - 2t_n\Phi(a_n) + t_n \right) \\
&- \frac{\mathcal{N}(a_n|0,1)}{\Phi(a_n)\left(1-\Phi(a_n)\right)} a_n \left(\Phi(a_n) - t_n\right).
\end{aligned} \tag{4.141}$$

4.20 (Incomplete)

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables such that

$$\begin{aligned}
t_{nk} &\in \{0,1\}, \\
p(\mathbf{t}_n|\mathbf{W}) &= \prod_{k=1}^{K} y_{nk}^{t_{nk}},
\end{aligned} \tag{4.142}$$

where

$$y_{nk} = \frac{\exp(a_{nk})}{\sum_{k=1}^{K} \exp(a_{nk})}, \qquad (4.143)$$
$$a_{nk} = \mathbf{w}_k^\intercal \boldsymbol{\phi}_n.$$

Then,

$$p(\mathbf{T}|\mathbf{W}) = \prod_{n=1}^{N} \prod_{k=1}^{K} y_{nk}^{t_{nk}}. \qquad (4.144)$$

Let

$$E(\mathbf{W}) = -\ln p(\mathbf{T}|\mathbf{W}). \qquad (4.145)$$

By 4.18,

$$\nabla_{\mathbf{w}_k} E(\mathbf{W}) = \sum_{n=1}^{N} (y_{nk} - t_{nk})\, \boldsymbol{\phi}_n. \qquad (4.146)$$

Additionally, by 4.17,

$$\nabla_{\mathbf{w}_k} \nabla_{\mathbf{w}_{k'}} E(\mathbf{W}) = \sum_{n=1}^{N} y_{nk}(I_{kk'} - y_{nk'}) \boldsymbol{\phi}_n \boldsymbol{\phi}_n^\intercal. \qquad (4.147)$$

The right hand side can be written as

$$\mathbf{H}_{kk'} = \boldsymbol{\Phi}^\intercal \mathbf{R}_{kk'} \boldsymbol{\Phi}, \qquad (4.148)$$

where

$$R_{kk'nn'} = \begin{cases} y_{nk}(I_{kk'} - y_{nk'}), & n = n', \\ 0, & \text{otherwise.} \end{cases} \qquad (4.149)$$

Let

$$\mathbf{H} = \begin{bmatrix} \mathbf{H}_{11} & \cdots & \mathbf{H}_{1K} \\ \vdots & \ddots & \vdots \\ \mathbf{H}_{K1} & \cdots & \mathbf{H}_{KK} \end{bmatrix},$$

and

$$\mathbf{u} = \begin{bmatrix} \mathbf{u}_1 \\ \vdots \\ \mathbf{u}_K \end{bmatrix},$$

where $\mathbf{u}_1, \cdots, \mathbf{u}_K$ are vectors in the same dimension as $\mathbf{w}$. Then,

$$\mathbf{u}^\intercal \mathbf{H} \mathbf{u} = \sum_{k=1}^{K} \sum_{k'=1}^{K} \mathbf{u}_k^\intercal \mathbf{H}_{kk'} \mathbf{u}_{k'}, \tag{4.150}$$

Then, the right hand side can be written as

$$\sum_{k=1}^{K} \sum_{k'=1}^{K} \left(\mathbf{\Phi} \mathbf{u}_k\right)^\intercal \mathbf{R}_{kk'} \left(\mathbf{\Phi} \mathbf{u}_{k'}\right). \tag{4.151}$$

4.21

Let

$$\Phi(a) = \int_{-\infty}^{a} \mathcal{N}(\theta|0,1) d\theta. \tag{4.152}$$

The right hand side can be written as

$$\int_{-\infty}^{0} \mathcal{N}(\theta|0,1) d\theta + \int_{0}^{a} \mathcal{N}(\theta|0,1) d\theta = \frac{1}{2} + \frac{1}{\sqrt{2\pi}} \int_{0}^{a} \exp\left(-\frac{\theta^2}{2}\right) d\theta. \tag{4.153}$$

The second term of the right hand side can be written as

$$\frac{1}{\sqrt{2\pi}} \int_{0}^{\frac{a}{\sqrt{2}}} \exp\left(-t^2\right) \sqrt{2} dt = \frac{1}{2} \mathrm{erf}\left(\frac{a}{\sqrt{2}}\right), \tag{4.154}$$

where

$$\mathrm{erf}(a) = \frac{2}{\sqrt{\pi}} \int_{0}^{a} \exp\left(-t^2\right) dt. \tag{4.155}$$

Therefore,

$$\Phi(a) = \frac{1}{2} \left(1 + \mathrm{erf}\left(\frac{a}{\sqrt{2}}\right)\right). \tag{4.156}$$

4.22

Let $\boldsymbol{\theta}$ be a variable in M dimensions. By a Taylor expansion,

$$\ln\left(p(\mathcal{D}|\boldsymbol{\theta}) p(\boldsymbol{\theta})\right) \simeq \ln\left(p(\mathcal{D}|\boldsymbol{\theta}_0) p(\boldsymbol{\theta}_0)\right) + \mathbf{v}(\boldsymbol{\theta}_0)^\intercal (\boldsymbol{\theta} - \boldsymbol{\theta}_0) - \frac{1}{2} (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\intercal \mathbf{A}(\boldsymbol{\theta}_0) (\boldsymbol{\theta} - \boldsymbol{\theta}_0), \tag{4.157}$$

where

$$\begin{aligned}\mathbf{v}(\boldsymbol{\theta}) &= \nabla \ln \left(p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})\right), \\ \mathbf{A}(\boldsymbol{\theta}) &= -\nabla\nabla \ln \left(p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})\right).\end{aligned} \tag{4.158}$$

Let $\boldsymbol{\theta}_{\text{MAP}}$ be a stationary point of $p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})$. Then,

$$\ln \left(p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})\right) \simeq \ln \left(p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}})p(\boldsymbol{\theta}_{\text{MAP}})\right) - \frac{1}{2}(\boldsymbol{\theta}-\boldsymbol{\theta}_{\text{MAP}})^{\intercal}\mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})(\boldsymbol{\theta}-\boldsymbol{\theta}_{\text{MAP}}), \tag{4.159}$$

so that

$$p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta}) \simeq p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}})p(\boldsymbol{\theta}_{\text{MAP}}) \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}})^{\intercal}\mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}})\right). \tag{4.160}$$

By marginalisation, integrating both sides with respect to $\boldsymbol{\theta}$ gives

$$p(\mathcal{D}) \simeq p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}})p(\boldsymbol{\theta}_{\text{MAP}}) \int \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}})^{\intercal}\mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}})\right) d\boldsymbol{\theta}. \tag{4.161}$$

The integral of the right hand side can be written as

$$(2\pi)^{\frac{M}{2}} \left(\det \mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})^{-1}\right)^{\frac{1}{2}} = (2\pi)^{\frac{M}{2}} \left(\det \mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})\right)^{-\frac{1}{2}}. \tag{4.162}$$

Therefore,

$$p(\mathcal{D}) \simeq p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}})p(\boldsymbol{\theta}_{\text{MAP}})(2\pi)^{\frac{M}{2}} \left(\det \mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})\right)^{-\frac{1}{2}}, \tag{4.163}$$

so that

$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}}) + \ln p(\boldsymbol{\theta}_{\text{MAP}}) + \frac{M}{2}\ln(2\pi) - \frac{1}{2}\ln \left(\det \mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})\right). \tag{4.164}$$

4.23

Let $\boldsymbol{\theta}$ be a variable in M dimensions. By 4.22,

$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}}) + \ln p(\boldsymbol{\theta}_{\text{MAP}}) + \frac{M}{2}\ln(2\pi) - \frac{1}{2}\ln \left(\det \mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})\right), \tag{4.165}$$

where $\boldsymbol{\theta}_{\text{MAP}}$ is a stationary point of $p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})$ and

$$\mathbf{A}(\boldsymbol{\theta}) = -\nabla\nabla \ln \left(p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})\right). \tag{4.166}$$

If

$$p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}|\mathbf{m}, \mathbf{V}_0), \tag{4.167}$$

then

$$\nabla\nabla \ln p(\theta) = -\mathbf{V}_0^{-1}, \tag{4.168}$$

so that

$$\mathbf{A}(\boldsymbol{\theta}) = \mathbf{H}(\boldsymbol{\theta}) + \mathbf{V}_0^{-1}, \tag{4.169}$$

where

$$\mathbf{H}(\boldsymbol{\theta}) = -\nabla\nabla \ln p(\mathcal{D}|\boldsymbol{\theta}). \tag{4.170}$$

Then, the right hand side of the approximation above can be written as

$$\begin{aligned}
&\ln p(\mathcal{D}|\boldsymbol{\theta}_{\mathrm{MAP}}) - \frac{M}{2}\ln(2\pi) - \frac{1}{2}\ln(\det \mathbf{V}_0) - \frac{1}{2}(\boldsymbol{\theta}_{\mathrm{MAP}} - \mathbf{m}_0)^\intercal \mathbf{V}_0^{-1}(\boldsymbol{\theta}_{\mathrm{MAP}} - \mathbf{m}_0) \\
&+ \frac{M}{2}\ln(2\pi) - \frac{1}{2}\ln\left(\det\left(\mathbf{H}(\boldsymbol{\theta}_{\mathrm{MAP}}) + \mathbf{V}_0^{-1}\right)\right) \\
=& \ln p(\mathcal{D}|\boldsymbol{\theta}_{\mathrm{MAP}}) + \frac{1}{2}\ln\left(\det \mathbf{V}_0^{-1}\right) - \frac{1}{2}(\boldsymbol{\theta}_{\mathrm{MAP}} - \mathbf{m}_0)^\intercal \mathbf{V}_0^{-1}(\boldsymbol{\theta}_{\mathrm{MAP}} - \mathbf{m}_0) \\
&- \frac{1}{2}\ln\left(\det\left(\mathbf{H}(\boldsymbol{\theta}_{\mathrm{MAP}}) + \mathbf{V}_0^{-1}\right)\right).
\end{aligned} \tag{4.171}$$

If $\mathbf{V}_0^{-1}$ can be neglected, the right hand side can be written as

$$\ln p(\mathcal{D}|\boldsymbol{\theta}_{\mathrm{MAP}}) - \frac{1}{2}\ln\left(\det \mathbf{H}(\boldsymbol{\theta}_{\mathrm{MAP}})\right). \tag{4.172}$$

If each data point is independent and identically distributed, then

$$\mathbf{H}(\boldsymbol{\theta}) = N\bar{\mathbf{H}}(\boldsymbol{\theta}), \tag{4.173}$$

where

$$\bar{\mathbf{H}}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{n=1}^{N} \mathbf{H}_n(\boldsymbol{\theta}), \tag{4.174}$$

and $\mathbf{H}_n(\boldsymbol{\theta})$ is the one for each data point. Then,

$$\det \mathbf{H}(\boldsymbol{\theta}_{\mathrm{MAP}}) = N^M \det \bar{\mathbf{H}}(\boldsymbol{\theta}_{\mathrm{MAP}}). \tag{4.175}$$

Threrefore,

$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|\boldsymbol{\theta}_{\mathrm{MAP}}) - \frac{M}{2}\ln N. \tag{4.176}$$

4.24 (Incomplete)

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} t_n &\in \{0, 1\}, \\ p(t_n|\mathbf{w}) &= y_n^{t_n}(1 - y_n)^{1-t_n}, \end{aligned} \tag{4.177}$$

where

$$\begin{aligned} y_n &= \sigma\left(\mathbf{w}^\intercal \boldsymbol{\phi}_n\right), \\ \sigma(a) &= \frac{1}{1 + \exp(-a)}. \end{aligned} \tag{4.178}$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{t})p(\mathbf{t}) = p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \tag{4.179}$$

If

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0), \tag{4.180}$$

then the lograrithm of the right hand side except the terms independent of $\mathbf{w}$ and $\mathbf{t}$ can be written as

$$\sum_{n=1}^{N} \left(t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\right) - \frac{1}{2}(\mathbf{w} - \mathbf{m}_0)^\intercal \mathbf{S}_0^{-1}(\mathbf{w} - \mathbf{m}_0). \tag{4.181}$$

Then, by 4.22,

$$p(\mathbf{w}|\mathbf{t}) \simeq \mathcal{N}(\mathbf{w}|\mathbf{w}_{\mathrm{MAP}}, \mathbf{S}_N)? \tag{4.182}$$

where $\mathbf{w}_{\mathrm{MAP}}$ is the maximum likelihood solution for $p(\mathbf{w})$ and

$$\mathbf{S}_N = -\nabla\nabla \ln p(\mathbf{w}|\mathbf{t}). \tag{4.183}$$

By marginalisation,

$$p(\mathcal{C}_1|\mathbf{t}) = \int p(\mathcal{C}_1|\mathbf{w})p(\mathbf{w}|\mathbf{t})d\mathbf{w}. \tag{4.184}$$

The logarithm of the integrand of the right hand side except the terms independent of $\mathbf{w}$ can be approximated as

$$-\ln\left(1 + \exp\left(-\mathbf{w}^\intercal \boldsymbol{\phi}\right)\right) - \frac{1}{2}(\mathbf{w} - \mathbf{w}_{\mathrm{MAP}})^\intercal \mathbf{S}_N^{-1}(\mathbf{w} - \mathbf{w}_{\mathrm{MAP}}) = \tag{4.185}$$

4.25

Let

$$\begin{aligned}\sigma(a) &= \frac{1}{1+\exp(-a)},\\ \Phi(a) &= \int_{-\infty}^{a} \mathcal{N}(\theta|0,1)d\theta.\end{aligned} \tag{4.186}$$

By 4.12,

$$\frac{d\sigma(a)}{da} = \sigma(a)\left(1-\sigma(a)\right). \tag{4.187}$$

On the other hand, the right hand side can be written as

$$\frac{d\Phi(\lambda a)}{da} = \lambda\mathcal{N}(\lambda a|0,1). \tag{4.188}$$

Let us assume that

$$\left.\frac{d\sigma(a)}{da}\right|_{a=0} = \left.\frac{d\Phi(\lambda a)}{da}\right|_{a=0}. \tag{4.189}$$

Then,

$$\frac{1}{4} = \lambda(2\pi)^{-\frac{1}{2}}. \tag{4.190}$$

Therefore,

$$\lambda^2 = \frac{\pi}{8}. \tag{4.191}$$

4.26

Let

$$I(\mu) = \int \Phi(\lambda a)\mathcal{N}(a|\mu,\sigma^2)da, \tag{4.192}$$

where

$$\Phi(a) = \int_{-\infty}^{a} \mathcal{N}(\theta|0,1)d\theta. \tag{4.193}$$

By the transformation

$$z = \frac{a-\mu}{\sigma}, \tag{4.194}$$

the right hand side can be written as

$$\int \Phi\left(\lambda(\mu+\sigma z)\right)\mathcal{N}(\mu+\sigma z|\mu,\sigma^2)\sigma dz = \int \Phi\left(\lambda(\mu+\sigma z)\right)\mathcal{N}(z|0,1)dz. \tag{4.195}$$

Then,

$$\frac{\partial}{\partial \mu} I(\mu) = \lambda \int \mathcal{N}\left(\lambda(\mu + \sigma z) | 0, 1\right) \mathcal{N}(z|0,1) dz. \tag{4.196}$$

The logarithm of the integrand of the right hand side can be written as

$$\begin{aligned} & -\frac{1}{2}\ln(2\pi) - \frac{\lambda^2(\mu+\sigma z)^2}{2} - \frac{1}{2}\ln(2\pi) - \frac{z^2}{2} \\ =& -\ln(2\pi) - \frac{1+\sigma^2\lambda^2}{2}\left(z + \frac{\mu\sigma\lambda^2}{1+\sigma^2\lambda^2}\right)^2 + \frac{\mu^2\sigma^2\lambda^4}{2\left(1+\sigma^2\lambda^2\right)} - \frac{\mu^2\lambda^2}{2}. \end{aligned} \tag{4.197}$$

The right hand side can be written as

$$\begin{aligned} & -\ln(2\pi) - \frac{1+\sigma^2\lambda^2}{2}\left(z + \frac{\mu\sigma\lambda^2}{1+\sigma^2\lambda^2}\right)^2 - \frac{\mu^2\lambda^2}{2\left(1+\sigma^2\lambda^2\right)} \\ =& -\frac{1}{2}\ln(2\pi) - \frac{1}{2}\ln\left(1+\sigma^2\lambda^2\right)^{-1} - \frac{1+\sigma^2\lambda^2}{2}\left(z + \frac{\mu\sigma\lambda^2}{1+\sigma^2\lambda^2}\right)^2 \\ & -\ln\lambda - \frac{1}{2}\ln(2\pi) - \frac{1}{2}\ln\left(\lambda^{-2}+\sigma^2\right) - \frac{\mu^2}{2\left(\lambda^{-2}+\sigma^2\right)}. \end{aligned} \tag{4.198}$$

Then, the integral can be written as

$$\begin{aligned} & \int \mathcal{N}\left(z| -\frac{\mu\sigma\lambda^2}{1+\sigma^2\lambda^2}, \left(1+\sigma^2\lambda^2\right)^{-1}\right) \frac{1}{\lambda} \mathcal{N}\left(\mu|\, 0, \lambda^{-2}+\sigma^2\right) dz \\ =& \frac{1}{\lambda}\mathcal{N}\left(\mu|\, 0, \lambda^{-2}+\sigma^2\right). \end{aligned} \tag{4.199}$$

Therefore,

$$\frac{\partial}{\partial \mu} I(\mu) = \mathcal{N}\left(\mu|0, \lambda^{-2}+\sigma^2\right). \tag{4.200}$$

Integrating both sides with respect to μ gives

$$I(\mu) = \int_{-\infty}^{\mu} \mathcal{N}\left(m|0, \lambda^{-2}+\sigma^2\right) dm. \tag{4.201}$$

By the transformation

$$m' = \frac{m}{\left(\lambda^{-2}+\sigma^2\right)^{\frac{1}{2}}}, \tag{4.202}$$

the right hand side can be written as

$$\int_{-\infty}^{\frac{\mu}{(\lambda^{-2}+\sigma^2)^{\frac{1}{2}}}} \left(\lambda^{-2}+\sigma^2\right)^{-\frac{1}{2}} \mathcal{N}\left(m'|0,1\right) \left(\lambda^{-2}+\sigma^2\right)^{\frac{1}{2}} dm' = \Phi\left(\frac{\mu}{(\lambda^{-2}+\sigma^2)^{\frac{1}{2}}}\right). \tag{4.203}$$

Therefore,

$$I(\mu) = \Phi\left(\frac{\mu}{(\lambda^{-2}+\sigma^2)^{\frac{1}{2}}}\right). \tag{4.204}$$

5 Neural Networks

5.1

Let

$$y_k(\mathbf{x}, \mathbf{w}) = \sigma\left(\sum_{m=1}^{M} w_{km}^{(2)} \sigma\left(\sum_{d=1}^{D} w_{md}^{(1)} x_d + w_{m0}^{(1)}\right) + w_{k0}^{(2)}\right), \tag{5.1}$$

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}. \tag{5.2}$$

Here,

$$\sigma(a) = \frac{\exp\left(\frac{a}{2}\right)}{\exp\left(\frac{a}{2}\right) + \exp\left(-\frac{a}{2}\right)}. \tag{5.3}$$

The right hand side can be written as

$$\tanh\left(\frac{a}{2}\right) + \sigma(-a) = \tanh\left(\frac{a}{2}\right) + 1 - \sigma(a). \tag{5.4}$$

Therefore,

$$\sigma(a) = \frac{1}{2}\left(1 + \tanh\left(\frac{a}{2}\right)\right). \tag{5.5}$$

Then, the argument of the right hand side can be written as

$$\begin{aligned} &\sum_{m=1}^{M} w_{km}^{(2)} \left(\frac{1}{2}\left(1 + \tanh\left(\frac{1}{2}\left(\sum_{d=1}^{D} w_{md}^{(1)} x_d + w_{m0}^{(1)}\right)\right)\right)\right) + w_{k0}^{(2)} \\ =&\frac{1}{2}\sum_{m=1}^{M} w_{km}^{(2)} \tanh\left(\frac{1}{2}\sum_{d=1}^{D} w_{md}^{(1)} x_d + \frac{1}{2} w_{m0}^{(1)}\right) + \frac{1}{2}\sum_{m=1}^{M} w_{km}^{(2)} + w_{k0}^{(2)}. \end{aligned} \tag{5.6}$$

Therefore,

$$y_k(\mathbf{x}, \mathbf{w}) = \sigma\left(\frac{1}{2}\sum_{m=1}^{M} w_{km}^{(2)} \tanh\left(\frac{1}{2}\sum_{d=1}^{D} w_{md}^{(1)} x_d + \frac{1}{2} w_{m0}^{(1)}\right) + \frac{1}{2}\sum_{m=1}^{M} w_{km}^{(2)} + w_{k0}^{(2)}\right). \tag{5.7}$$

5.2

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables such that

$$p(\mathbf{t}_n|\mathbf{x}_n, \mathbf{w}) = \mathcal{N}\left(\mathbf{t}_n|\mathbf{y}(\mathbf{x}_n, \mathbf{w}), \beta^{-1}\mathbf{I}\right). \tag{5.8}$$

Then, the logarithm of the likelihood except the terms independent of $\mathbf{w}$ can be written as

$$-\frac{1}{2}\sum_{n=1}^{N}(\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w}))^{\intercal}\left(\beta^{-1}\mathbf{I}\right)^{-1}(\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})) = -\frac{\beta}{2}\sum_{n=1}^{N}\|\mathbf{y}(\mathbf{x}_n, \mathbf{w}) - \mathbf{t}_n\|^2. \tag{5.9}$$

Setting the derivative with respect to $\mathbf{w}$ to zero gives

$$\mathbf{0} = -\beta\sum_{n=1}^{N}\frac{\partial\mathbf{y}(\mathbf{x}_n, \mathbf{w})}{\partial\mathbf{w}}(\mathbf{y}(\mathbf{x}_n, \mathbf{w}) - \mathbf{t}_n). \tag{5.10}$$

Let

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\|\mathbf{y}(\mathbf{x}_n, \mathbf{w}) - \mathbf{t}_n\|^2. \tag{5.11}$$

Setting the derivative with respect to $\mathbf{w}$ to zero gives

$$\mathbf{0} = \sum_{n=1}^{N}\frac{\partial\mathbf{y}(\mathbf{x}_n, \mathbf{w})}{\partial\mathbf{w}}(\mathbf{y}(\mathbf{x}_n, \mathbf{w}) - \mathbf{t}_n). \tag{5.12}$$

Therefore, maximising the likelihood is equivalent to minimising $E(\mathbf{w})$.

5.3

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables such that

$$p(\mathbf{t}_n|\mathbf{x}_n, \mathbf{w}) = \mathcal{N}(\mathbf{t}_n|\mathbf{y}(\mathbf{x}_n, \mathbf{w}), \mathbf{\Sigma}). \tag{5.13}$$

Then, the logarithm of the likelihood except the terms independent of $\mathbf{w}$ and $\mathbf{\Sigma}$ can be written as

$$-\frac{1}{2}\ln(\det\mathbf{\Sigma}) - \frac{1}{2}\sum_{n=1}^{N}(\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w}))^{\intercal}\mathbf{\Sigma}^{-1}(\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})). \tag{5.14}$$

Setting the derivatives with respect to $\mathbf{w}$ and $\mathbf{\Sigma}$ to zero gives

$$\begin{aligned}\mathbf{0} &= -\sum_{n=1}^{N} \frac{\partial \mathbf{y}(\mathbf{x}_n, \mathbf{w})}{\partial \mathbf{w}} \mathbf{\Sigma}^{-1} \left(\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})\right), \\ \mathbf{O} &= -\frac{1}{2}\mathbf{\Sigma}^{-1} + \frac{1}{2}\left(\mathbf{\Sigma}^{-1}\right)^2 \sum_{n=1}^{N} \left(\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})\right)\left(\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})\right)^{\mathsf{T}}.\end{aligned} \tag{5.15}$$

Therefore, the maximum likelihood solution for $\mathbf{\Sigma}$ is given by

$$\mathbf{\Sigma} = \sum_{n=1}^{N} \left(\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})\right)\left(\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})\right)^{\mathsf{T}}. \tag{5.16}$$

On the other hand, if $\mathbf{\Sigma}$ is fixed and known, then the maximum likelihood solution for $\mathbf{w}$ is given by minimising

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N} \left(\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})\right)^{\mathsf{T}} \mathbf{\Sigma}^{-1} \left(\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})\right). \tag{5.17}$$

5.4

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} t_n &\in \{0, 1\}, \\ p(t_n = 1|\mathbf{x}_n) &= (1-\epsilon)y_n + \epsilon\left(1 - y_n\right), \end{aligned} \tag{5.18}$$

where

$$y_n = y(\mathbf{x}_n, \mathbf{w}). \tag{5.19}$$

Then,

$$p(t_n|\mathbf{x}_n) = \left((1-\epsilon)y_n + \epsilon\left(1-y_n\right)\right)^{t_n} \left(\epsilon y_n + (1-\epsilon)\left(1-y_n\right)\right)^{1-t_n}. \tag{5.20}$$

Therefore,

$$\begin{aligned} &-\ln\left(\prod_{n=1}^{N} p(t_n|\mathbf{x}_n)\right) \\ &= -\sum_{n=1}^{N} \left(t_n \ln\left((1-\epsilon)y_n + \epsilon(1-y_n)\right) + (1-t_n)\ln\left(\epsilon y_n + (1-\epsilon)(1-y_n)\right)\right). \end{aligned} \tag{5.21}$$

5.5

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables in K dimensions such that

$$\begin{aligned} t_{nk} &\in \{0, 1\}, \\ p(t_{nk} = 1|\mathbf{x}_n) &= y_{nk}, \end{aligned} \tag{5.22}$$

where

$$y_{nk} = y_k(\mathbf{x}_n, \mathbf{w}). \tag{5.23}$$

Then,

$$p(t_{nk}|\mathbf{x}_n) = y_{nk}^{t_{nk}}, \tag{5.24}$$

so that

$$p(\mathbf{t}_n|\mathbf{x}_n) = \prod_{k=1}^{K} y_{nk}^{t_{nk}}. \tag{5.25}$$

Therefore,

$$\ln\left(\prod_{n=1}^{N} p(\mathbf{t}_n|\mathbf{x}_n)\right) = \sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk} \ln y_{nk}. \tag{5.26}$$

5.6

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} t_n &\in \{0, 1\}, \\ p(t_n = 1|\mathbf{x}_n) &= y_n, \end{aligned} \tag{5.27}$$

where

$$y_n = y(\mathbf{x}_n, \mathbf{w}). \tag{5.28}$$

Then,

$$p(t_n|\mathbf{x}_n) = y_n^{t_n}(1 - y_n)^{1-t_n}. \tag{5.29}$$

Let

$$E(\mathbf{w}) = -\ln\left(\prod_{n=1}^{N} p(t_n|\mathbf{x}_n)\right). \tag{5.30}$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \left(t_n \ln y_n + (1 - t_n)\ln(1 - y_n)\right). \tag{5.31}$$

If

$$y_n = \sigma(a_n), \tag{5.32}$$

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}, \tag{5.33}$$

then, by 4.12,

$$\frac{\partial E(\mathbf{w})}{\partial a_n} = -y_n(1 - y_n)\left(\frac{t_n}{y_n} - \frac{1 - t_n}{1 - y_n}\right). \tag{5.34}$$

Therefore,

$$\frac{\partial E(\mathbf{w})}{\partial a_n} = y_n - t_n. \tag{5.35}$$

5.7

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables such that

$$\begin{aligned} t_{nk} &\in \{0, 1\}, \\ p(t_{nk} = 1|\mathbf{x}_n) &= y_{nk}, \end{aligned} \tag{5.36}$$

where

$$\begin{aligned} y_{nk} &= y_k(\mathbf{x}_n, \mathbf{w}), \\ \sum_{k=1}^{K} y_{nk} &= 1. \end{aligned} \tag{5.37}$$

Then,

$$p(\mathbf{t}_n|\mathbf{x}_n) = \prod_{k=1}^{K} y_{nk}^{t_{nk}}. \tag{5.38}$$

Let

$$E(\mathbf{w}) = -\ln\left(\prod_{n=1}^{N} p(\mathbf{t}_n|\mathbf{x}_n)\right). \tag{5.39}$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk} \ln y_{nk}. \tag{5.40}$$

If

$$y_{nk} = \frac{\exp\left(a_k(\mathbf{x}_n, \mathbf{w})\right)}{\sum_{k=1}^{K} \exp\left(a_k(\mathbf{x}_n, \mathbf{w})\right)}, \tag{5.41}$$

then, by 4.17,

$$\frac{\partial E(\mathbf{w})}{\partial a_{k'}} = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk} y_{nk}(I_{kk'} - y_{nk})\frac{1}{y_{nk}}. \tag{5.42}$$

The right hand side can be written as

$$-\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk}(I_{kk'} - y_{nk}) = -\sum_{n=1}^{N}\left(\sum_{k=1}^{K} t_{nk} y_{nk} - t_{nk'}\right). \tag{5.43}$$

Therefore,

$$\frac{\partial E(\mathbf{w})}{\partial a_k} = \sum_{n=1}^{N}(y_{nk} - t_{nk}). \tag{5.44}$$

5.8

Setting the derivative of

$$\tanh a = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)} \tag{5.45}$$

gives

$$\frac{d}{da}\tanh a = 1 - \left(\frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)}\right)^2. \tag{5.46}$$

Therefore,

$$\frac{d}{da}\tanh a = 1 - (\tanh a)^2. \tag{5.47}$$

5.9

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} t_n &\in \{-1, 1\}, \\ p(t_n = 1|\mathbf{x}_n) &= \frac{1 + y_n}{2}, \end{aligned} \tag{5.48}$$

where

$$y_n = y(\mathbf{x}_n, \mathbf{w}). \tag{5.49}$$

Then,

$$p(t_n|\mathbf{x}_n) = \left(\frac{1+y_n}{2}\right)^{\frac{1+t_n}{2}} \left(\frac{1-y_n}{2}\right)^{\frac{1-t_n}{2}}. \tag{5.50}$$

Let

$$E(\mathbf{w}) = -\ln\left(\prod_{n=1}^{N} p(t_n|\mathbf{x}_n)\right). \tag{5.51}$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\left(\frac{1+t_n}{2}\ln\frac{1+y_n}{2} + \frac{1-t_n}{2}\ln\frac{1-y_n}{2}\right). \tag{5.52}$$

The appropriate choice of y is tanh.

5.10

Let

$$\mathbf{H} = \nabla\nabla E(\mathbf{w}), \tag{5.53}$$

where E is a real function of real vectors. Then, $\mathbf{H}$ is a real symmetric matrix. Therefore, by 2.20, $\mathbf{H}$ is positive if and only if its eigenvalues are positive.

5.11

Let $\mathbf{w}$ be a real vector in M dimensions. Let E be a real function of $\mathbf{w}$. Let $\mathbf{w}^*$ be a vector such that

$$\nabla E\left(\mathbf{w}^*\right) = \mathbf{0}. \tag{5.54}$$

Then, by a Taylor expansion,

$$E(\mathbf{w}) \simeq E\left(\mathbf{w}^*\right) + \frac{1}{2}\left(\mathbf{w}-\mathbf{w}^*\right)^{\intercal}\mathbf{H}\left(\mathbf{w}-\mathbf{w}^*\right), \tag{5.55}$$

where

$$\mathbf{H} = \nabla\nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}^*}. \tag{5.56}$$

Let $\mathbf{u}_1, \cdots, \mathbf{u}_M$ be eigenvectors such that

$$\mathbf{H}\mathbf{u}_m = \lambda_m \mathbf{u}_m. \tag{5.57}$$

Note that $\mathbf{H}$ is a real symmetric matrix. Then, by **??**, we have

$$\mathbf{u}_m^\intercal \mathbf{u}_{m'} = I_{mm'}. \tag{5.58}$$

Therefore, there exists $\alpha_1, \cdots, \alpha_M$ such that

$$\mathbf{w} - \mathbf{w}^* = \sum_{m=1}^{M} \alpha_m \mathbf{u}_m. \tag{5.59}$$

Then, the approximation can be written as

$$E(\mathbf{w}) \simeq E\left(\mathbf{w}^*\right) + \frac{1}{2} \sum_{m=1}^{M} \lambda_m \alpha_m^2. \tag{5.60}$$

Therefore, the contours of constant E are ellipses whose axes are aligned with $\mathbf{u}_1, \cdots, \mathbf{u}_M$ with lengths which are proportional to $\lambda_1^{-\frac{1}{2}}, \cdots, \lambda_M^{-\frac{1}{2}}$.

5.12

Let $\mathbf{w}$ be a real vector. Let E be a real function of $\mathbf{w}$. Let $\mathbf{w}^*$ be a vector such that

$$\nabla E\left(\mathbf{w}^*\right) = \mathbf{0}. \tag{5.61}$$

Then, by a Taylor expansion,

$$E(\mathbf{w}) \simeq E\left(\mathbf{w}^*\right) + \frac{1}{2} \left(\mathbf{w} - \mathbf{w}^*\right)^\intercal \mathbf{H} \left(\mathbf{w} - \mathbf{w}^*\right), \tag{5.62}$$

where

$$\mathbf{H} = \nabla\nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}^*}. \tag{5.63}$$

If $\mathbf{H}$ is positive definite, then the second term of the right hand side is positive unless

$$\mathbf{w} = \mathbf{w}^*. \tag{5.64}$$

Therefore, $\mathbf{w}^*$ is a local minimum of the right hand side. On the other hand, if $\mathbf{w}^*$ is a local minimum of the right hand side, then the second term of the right hand side is positive unless

$$\mathbf{w} = \mathbf{w}^*. \tag{5.65}$$

Therefore, $\mathbf{H}$ is positive definite. Thus, the necessary and sufficient condition for $\mathbf{w}^*$ to be a local minimum is that $\mathbf{H}$ be positive definite.

5.13

Let $\mathbf{w}$ be a vector in M dimensions. Let E be a function of $\mathbf{w}$. Then, by a Taylor expansion,

$$E(\mathbf{w}) \simeq E\left(\hat{\mathbf{w}}\right) + \left(\mathbf{w} - \hat{\mathbf{w}}\right)^{\intercal} \mathbf{b} + \frac{1}{2} \left(\mathbf{w} - \hat{\mathbf{w}}\right)^{\intercal} \mathbf{H} \left(\mathbf{w} - \hat{\mathbf{w}}\right), \tag{5.66}$$

where

$$\begin{aligned} \mathbf{b} &= \nabla E(\mathbf{w})|_{\mathbf{w}=\hat{\mathbf{w}}} \,. \\ \mathbf{H} &= \nabla\nabla E(\mathbf{w})|_{\mathbf{w}=\hat{\mathbf{w}}} \,. \end{aligned} \tag{5.67}$$

Since $\mathbf{b}$ is a vector in M dimensions and $\mathbf{H}$ is a $M \times M$ symmetric matrix, the number of independent elements of the right hand side is

$$M + \frac{M(M+1)}{2} = \frac{M(M+3)}{2}. \tag{5.68}$$

5.14

Let w be a variable. Let E_n be a function of w. Then, by a Taylor expansion,

$$\begin{aligned} E_n(w_{mm'} + \epsilon) &= E_n(w_{mm'}) + \left.\frac{\partial E_n}{\partial w}\right|_{w=w_{mm'}} \epsilon + O\left(\epsilon^2\right), \\ E_n(w_{mm'} - \epsilon) &= E_n(w_{mm'}) - \left.\frac{\partial E_n}{\partial w}\right|_{w=w_{mm'}} \epsilon + O\left(\epsilon^2\right). \end{aligned} \tag{5.69}$$

Therefore,

$$\left.\frac{\partial E_n}{\partial w}\right|_{w=w_{mm'}} = \frac{E_n(w_{mm'} + \epsilon) - E_n(w_{mm'} - \epsilon)}{2\epsilon} + O\left(\epsilon^2\right). \tag{5.70}$$

5.15 (Incomplete)

5.16

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be vectors. Let $\mathbf{y}_1, \cdots, \mathbf{y}_N$ be vectors which are dependent on a vector $\mathbf{w}$. Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \|\mathbf{y}_n - \mathbf{t}_n\|^2. \tag{5.71}$$

Then,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (\nabla \mathbf{y}_n)^{\mathsf{T}} (\mathbf{y}_n - \mathbf{t}_n), \tag{5.72}$$

so that

$$\nabla\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (\nabla \operatorname{vec} (\nabla \mathbf{y}_n)^{\mathsf{T}})^{\mathsf{T}} (\mathbf{y}_n - \mathbf{t}_n) + \sum_{n=1}^{N} (\nabla \mathbf{y}_n)^{\mathsf{T}} (\nabla \mathbf{y}_n). \tag{5.73}$$

5.17

Let t be a variable. Let y be a function of a vector $\mathbf{x}$ and a vector $\mathbf{w}$. Let

$$E(\mathbf{w}) = \frac{1}{2} \int \int (y - t)^2 p(\mathbf{x}, t) d\mathbf{x} dt. \tag{5.74}$$

Then,

$$\nabla E(\mathbf{w}) = \int \int (y - t) p(\mathbf{x}, t) \nabla y d\mathbf{x} dt. \tag{5.75}$$

The right hand side can be written as

$$\begin{aligned} &\int y \nabla y \left(\int p(\mathbf{x}, t) dt \right) d\mathbf{x} - \int \nabla y \left(\int t p(t|\mathbf{x}) dt \right) p(\mathbf{x}) d\mathbf{x} \\ &= \int y \nabla y p(\mathbf{x}) d\mathbf{x} - \int \nabla y \, \mathrm{E}(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \end{aligned} \tag{5.76}$$

Then,

$$\nabla\nabla E(\mathbf{w}) = \int \nabla y \, (\nabla y)^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x} + \int y \nabla\nabla y p(\mathbf{x}) d\mathbf{x} - \int \nabla\nabla y \, \mathrm{E}(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \tag{5.77}$$

The second and the third terms of the right hand side can be written as

$$\mathrm{E}\left(y \nabla\nabla y\right) - \mathrm{E}\left(\nabla\nabla y \, \mathrm{E}(t|\mathbf{x})\right) = \mathrm{E}\left(\left(y - \mathrm{E}(t|\mathbf{x})\right) \nabla\nabla y\right). \tag{5.78}$$

Therefore, if

$$y = \mathrm{E}(t|\mathbf{x}), \tag{5.79}$$

then

$$\nabla\nabla E(\mathbf{w}) = \int \nabla y \, (\nabla y)^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x}. \tag{5.80}$$

5.18

Let $t_1, \cdots, t_N$ be variables. Let $y_1, \cdots, y_N$ be variablees such that

$$\begin{aligned} y_n &= \mathbf{w}_n^{(2)\mathsf{T}}\mathbf{z} + \mathbf{w}_n^{(0)\mathsf{T}}\mathbf{x}, \\ z_m &= \tanh\left(\mathbf{w}_m^{(1)\mathsf{T}}\mathbf{x}\right). \end{aligned} \tag{5.81}$$

Let

$$E = \frac{1}{2}\sum_{n=1}^{N}(y_n - t_n)^2. \tag{5.82}$$

Then,

$$\begin{aligned} \frac{\partial E}{\partial \mathbf{w}_n^{(0)}} &= \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial \mathbf{w}_n^{(0)}}, \\ \frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial \mathbf{z}}\frac{\partial \mathbf{z}}{\partial \mathbf{w}_m^{(1)}}, \\ \frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial \mathbf{w}_n^{(2)}}. \end{aligned} \tag{5.83}$$

Therefore,

$$\begin{aligned} \frac{\partial E}{\partial \mathbf{w}_n^{(0)}} &= (y_n - t_n)\mathbf{x}, \\ \frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= (y_n - t_n)\mathbf{A}\mathbf{w}_n^{(2)}, \\ \frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= (y_n - t_n)\mathbf{z}, \end{aligned} \tag{5.84}$$

where

$$A_{mm'} = \left(1 - z_m^2\right)x_{m'}. \tag{5.85}$$

5.19

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} t_n &\in \{0, 1\}, \\ p(t_n|\mathbf{w}) &= y_n^{t_n}(1 - y_n)^{1-t_n}, \end{aligned} \tag{5.86}$$

where

$$\begin{aligned} y_n &= \sigma\left(a_n(\mathbf{w})\right), \\ \sigma(a) &= \frac{1}{1 + \exp(-a)}, \end{aligned} \tag{5.87}$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}). \tag{5.88}$$

The right hand side can be written as

$$-\ln\left(\prod_{n=1}^{N} y_n^{t_n}(1-y_n)^{1-t_n}\right) = -\sum_{n=1}^{N}\left(t_n \ln y_n + (1-t_n)\ln(1-y_n)\right). \tag{5.89}$$

Then, by 4.12,

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N}\left(\frac{t_n}{y_n}y_n(1-y_n)\nabla a_n - \frac{1-t_n}{1-y_n}y_n(1-y_n)\nabla a_n\right). \tag{5.90}$$

The right hand side can be written as

$$-\sum_{n=1}^{N}(t_n(1-y_n)\nabla a_n - (1-t_n)y_n\nabla a_n) = \sum_{n=1}^{N}(y_n - t_n)\nabla a_n. \tag{5.91}$$

Then, by 4.13,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N}(y_n - t_n)\nabla a_n. \tag{5.92}$$

Therefore, by 4.12,

$$\nabla\nabla E(\mathbf{w}) = \sum_{n=1}^{N} y_n(1-y_n)\nabla a_n(\nabla a_n)^{\intercal} + \sum_{n=1}^{N}(y_n - t_n)\nabla\nabla a_n. \tag{5.93}$$

5.20

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables such that

$$\begin{aligned} t_{nk} &\in \{0,1\}, \\ p(t_{nk}=1|\mathbf{x}_n) &= y_{nk}, \end{aligned} \tag{5.94}$$

where

$$\begin{aligned} y_{nk} &= y_k(\mathbf{x}_n, \mathbf{w}), \\ \sum_{k=1}^{K} y_{nk} &= 1. \end{aligned} \tag{5.95}$$

Then,

$$p(\mathbf{t}_n|\mathbf{x}_n) = \prod_{k=1}^{K} y_{nk}^{t_{nk}}. \tag{5.96}$$

Let

$$E(\mathbf{w}) = -\ln\left(\prod_{n=1}^{N} p(\mathbf{t}_n|\mathbf{x}_n)\right). \tag{5.97}$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk}\ln y_{nk}. \tag{5.98}$$

If

$$y_{nk} = \frac{\exp\left(a_k(\mathbf{x}_n, \mathbf{w})\right)}{\sum_{k=1}^{K}\exp\left(a_k(\mathbf{x}_n, \mathbf{w})\right)}, \tag{5.99}$$

then, by 5.7,

$$\frac{\partial E(\mathbf{w})}{\partial a_k} = \sum_{n=1}^{N}(y_{nk} - t_{nk}). \tag{5.100}$$

Then,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N}\sum_{k=1}^{K}(y_{nk} - t_{nk})\nabla a_k. \tag{5.101}$$

Then,

$$\nabla\nabla E(\mathbf{w}) = \sum_{n=1}^{N}\sum_{k=1}^{K} y_{nk}(1 - y_{nk})\nabla a_k\left(\nabla a_k\right)^{\intercal} + \sum_{n=1}^{N}\sum_{k=1}^{K}(y_{nk} - t_{nk})\nabla\nabla a_k. \tag{5.102}$$

5.21 (Incomplete)

5.22

Let $y_1, \cdots, y_N$ be variables such that

$$\begin{aligned} y_n &= {\mathbf{w}_n^{(2)}}^{\intercal}\mathbf{z}, \\ z_m &= h(a_m), \\ a_m &= {\mathbf{w}_m^{(1)}}^{\intercal}\mathbf{x}. \end{aligned} \tag{5.103}$$

Let E be a function of $y_1, \cdots, y_N$. Then,

$$\begin{aligned}\frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial z_m}\frac{\partial z_m}{\partial a_m}\frac{\partial a_m}{\partial \mathbf{w}_m^{(1)}},\\ \frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial \mathbf{w}_n^{(2)}}.\end{aligned} \tag{5.104}$$

Therefore,

$$\begin{aligned}\frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= \frac{\partial E}{\partial y_n} w_{nm}^{(2)} h'(a_m)\mathbf{x},\\ \frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= \frac{\partial E}{\partial y_n}\mathbf{z}.\end{aligned} \tag{5.105}$$

Thus,

$$\begin{aligned}\frac{\partial^2 E}{\partial \mathbf{w}_m^{(1)}\partial \mathbf{w}_{m'}^{(1)}} &= w_{nm}^{(2)}\mathbf{x}\left(\frac{\partial^2 E}{\partial y_n^2} w_{nm'}^{(2)} h'(a_{m'})h'(a_m)\mathbf{x} + \frac{\partial E}{\partial y_n} h''(a_m) I_{mm'}\mathbf{x}\right)^{\mathsf{T}},\\ \frac{\partial^2 E}{\partial \mathbf{w}_m^{(1)}\partial \mathbf{w}_n^{(2)}} &= h'(a_m)\mathbf{x}\left(\frac{\partial^2 E}{\partial y_n^2} w_{nm}^{(2)}\mathbf{z} + \frac{\partial E}{\partial y_n}\mathbf{v}\right)^{\mathsf{T}},\\ \frac{\partial^2 E}{\partial \mathbf{w}_n^{(2)}\partial \mathbf{w}_{n'}^{(2)}} &= \frac{\partial^2 E}{\partial y_n \partial y_{n'}}\mathbf{z}\mathbf{z}^{\mathsf{T}},\end{aligned} \tag{5.106}$$

where

$$v_m = \begin{cases} 1, & m = n,\\ 0 & \text{otherwise.}\end{cases} \tag{5.107}$$

5.23

Let $y_1, \cdots, y_N$ be variables such that

$$\begin{aligned} y_n &= \mathbf{w}_n^{(2)\mathsf{T}}\mathbf{z} + \mathbf{w}_n^{(0)\mathsf{T}}\mathbf{x},\\ z_m &= h(a_m),\\ a_m &= \mathbf{w}_m^{(1)\mathsf{T}}\mathbf{x}.\end{aligned} \tag{5.108}$$

Let E be a function of $y_1, \cdots, y_N$. Then,

$$\begin{aligned}
\frac{\partial E}{\partial \mathbf{w}_n^{(0)}} &= \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial \mathbf{w}_n^{(0)}}, \\
\frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial z_m}\frac{\partial z_m}{\partial a_m}\frac{\partial a_m}{\partial \mathbf{w}_m^{(1)}}, \\
\frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial \mathbf{w}_n^{(2)}}.
\end{aligned} \tag{5.109}$$

Therefore,

$$\begin{aligned}
\frac{\partial E}{\partial \mathbf{w}_n^{(0)}} &= \frac{\partial E}{\partial y_n}\mathbf{x}, \\
\frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= \frac{\partial E}{\partial y_n}w_{nm}^{(2)}h'(a_m)\mathbf{x}, \\
\frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= \frac{\partial E}{\partial y_n}\mathbf{z}.
\end{aligned} \tag{5.110}$$

Thus,

$$\begin{aligned}
\frac{\partial^2 E}{\partial \mathbf{w}_n^{(0)}\partial \mathbf{w}_{n'}^{(0)}} &= \frac{\partial^2 E}{\partial y_n \partial y_{n'}}\mathbf{x}\mathbf{x}^\intercal, \\
\frac{\partial^2 E}{\partial \mathbf{w}_n^{(0)}\partial \mathbf{w}_m^{(1)}} &= \frac{\partial^2 E}{\partial y_n^2}w_{nm}^{(2)}h'(a_m)\mathbf{x}\mathbf{x}^\intercal, \\
\frac{\partial^2 E}{\partial \mathbf{w}_n^{(0)}\partial \mathbf{w}_{n'}^{(2)}} &= \frac{\partial^2 E}{\partial y_n \partial y_{n'}}\mathbf{x}\mathbf{z}^\intercal, \\
\frac{\partial^2 E}{\partial \mathbf{w}_m^{(1)}\partial \mathbf{w}_{m'}^{(1)}} &= w_{nm}^{(2)}\mathbf{x}\left(\frac{\partial^2 E}{\partial y_n^2}w_{nm'}^{(2)}h'(a_{m'})h'(a_m)\mathbf{x} + \frac{\partial E}{\partial y_n}h''(a_m)I_{mm'}\mathbf{x}\right)^\intercal, \\
\frac{\partial^2 E}{\partial \mathbf{w}_m^{(1)}\partial \mathbf{w}_n^{(2)}} &= h'(a_m)\mathbf{x}\left(\frac{\partial^2 E}{\partial y_n^2}w_{nm}^{(2)}\mathbf{z} + \frac{\partial E}{\partial y_n}\mathbf{v}\right)^\intercal, \\
\frac{\partial^2 E}{\partial \mathbf{w}_n^{(2)}\partial \mathbf{w}_{n'}^{(2)}} &= \frac{\partial^2 E}{\partial y_n \partial y_{n'}}\mathbf{z}\mathbf{z}^\intercal,
\end{aligned} \tag{5.111}$$

where

$$v_m = \begin{cases} 1, & m = n, \\ 0 & \text{otherwise.} \end{cases} \tag{5.112}$$

5.24

Let $y_1, \cdots, y_n$ be variables such that

$$\begin{aligned} y_n &= \mathbf{w}_n^\intercal \mathbf{z} + w_{n0}, \\ z_m &= h\left(\mathbf{w}_m^\intercal \mathbf{x} + w_{m0}\right). \end{aligned} \tag{5.113}$$

(a)

Let

$$\tilde{\mathbf{x}} = a\mathbf{x} + b\mathbf{v}, \tag{5.114}$$

where

$$\mathbf{v} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}.$$

Then,

$$z_m = h\left(\frac{1}{a}\mathbf{w}_m^\intercal \left(\tilde{\mathbf{x}} - b\mathbf{v}\right) + w_{m0}\right). \tag{5.115}$$

Therefore,

$$\tilde{z}_m = h\left(\tilde{\mathbf{w}}_m^\intercal \mathbf{x} + \tilde{w}_{m0}\right). \tag{5.116}$$

where

$$\begin{aligned} \tilde{\mathbf{w}}_m &= \frac{1}{a}\mathbf{w}_m, \\ \tilde{w}_{m0} &= w_{m0} - \frac{b}{a}\mathbf{w}_m^\intercal \mathbf{v}. \end{aligned} \tag{5.117}$$

(b)

Let

$$\tilde{y}_n = cy_n + d. \tag{5.118}$$

Then,

$$\frac{\tilde{y}_n - d}{c} = \mathbf{w}_n^\intercal \mathbf{z} + w_{n0}. \tag{5.119}$$

Therefore,

$$\tilde{y}_n = \tilde{\mathbf{w}}_n^\intercal \mathbf{z} + \tilde{w}_{n0}, \tag{5.120}$$

where

$$\begin{aligned} \tilde{\mathbf{w}}_n &= c\mathbf{w}_n, \\ \tilde{w}_{n0} &= cw_{n0} + d. \end{aligned} \tag{5.121}$$

5.25 (Incomplete)

Let E be a quadratic error function such that

$$E(\mathbf{w}) = E_0 + \frac{1}{2}\left(\mathbf{w} - \mathbf{w}^*\right)^\intercal \mathbf{H}\left(\mathbf{w} - \mathbf{w}^*\right), \tag{5.122}$$

where $\mathbf{w}^*$ represents the minimum and $\mathbf{H}$ is a positive definite and constant matrix whose eignevectors and eigenvalues are $\mathbf{u}_1, \cdots, \mathbf{u}_M$ and $\eta_1, \cdots, \eta_M$. Let

$$\begin{aligned} \mathbf{w}^{(\tau)} &= \mathbf{w}^{(\tau-1)} - \rho \nabla E, \\ \mathbf{w}^{(0)} &= \mathbf{0}. \end{aligned} \tag{5.123}$$

(a)

We have

$$\mathbf{w}^{(\tau)} = \mathbf{w}^{(\tau-1)} - \rho \mathbf{H}\left(\mathbf{w}^{(\tau-1)} - \mathbf{w}^*\right), \tag{5.124}$$

so that

$$\mathbf{w}^{(\tau)} = \left(\mathbf{I} - \rho \mathbf{H}\right)\mathbf{w}^{(\tau-1)} + \rho \mathbf{H}\mathbf{w}^*. \tag{5.125}$$

Then,

$$\mathbf{u}_m^\intercal \mathbf{w}^{(\tau)} = \mathbf{u}_m^\intercal \mathbf{w}^{(\tau-1)} - \rho \mathbf{u}_m^\intercal \mathbf{H}\mathbf{w}^{(\tau-1)} + \rho \mathbf{u}_m^\intercal \mathbf{H}\mathbf{w}^*. \tag{5.126}$$

Since $\mathbf{H}$ is symmetric,

$$\mathbf{u}_m^\intercal \mathbf{H}\mathbf{w} = \mathbf{w}^\intercal \mathbf{H}\mathbf{u}_m. \tag{5.127}$$

The right hand side can be written as

$$\eta_m \mathbf{w}^\intercal \mathbf{u}_m = \eta_m w_m, \tag{5.128}$$

where

$$w_m = \mathbf{w}^\intercal \mathbf{u}_m. \tag{5.129}$$

Then,

$$w_m^{(\tau)} = (1 - \rho\eta_m) w_m^{(\tau-1)} + \rho \eta_m w_m^*, \tag{5.130}$$

so that

$$w_m^{(\tau)} - w_m^* = (1 - \rho\eta_m)\left(w_m^{(\tau-1)} - w_m^*\right). \tag{5.131}$$

Therefore,

$$w_m^{(\tau)} = w_m^* - (1 - \rho\eta_m)^\tau \left(w_m^{(0)} - w_m^*\right), \tag{5.132}$$

so that

$$w_m^{(\tau)} = \left(1 - (1 - \rho\eta_m)^\tau\right) w_m^*. \tag{5.133}$$

(b)

By (a), if

$$|1 - \rho\eta_m| < 1, \tag{5.134}$$

then

$$\lim_{\tau\to\infty} w_m^{(\tau)} = w_m^*. \tag{5.135}$$

(c)

By (a) and a Taylor series

$$(1 - \rho\eta_m)^\tau = 1 - \rho\tau\eta_m + \rho^2\tau^2 O\left(\eta_m^2\right), \tag{5.136}$$

we have

$$w_m^{(\tau)} = \left(\rho\tau\eta_m - \rho^2\tau^2 O\left(\eta_m^2\right)\right) w_m^*, \tag{5.137}$$

so that

$$w_m^{(\tau)} = \rho\tau\eta_m \left(1 - \rho\tau\eta_m O\left(\eta_m\right)\right) w_m^*. \tag{5.138}$$

Therefore,

$$\begin{aligned} w_m^{(\tau)} &\simeq w_m^*, \quad \text{if} \quad \eta_m \gg (\rho\tau)^{-1}? \\ \left|w_m^{(\tau)}\right| &\ll w_m^*, \quad \text{if} \quad \eta_m \ll (\rho\tau)^{-1}. \end{aligned} \tag{5.139}$$

5.26 (Incomplete)

Let

$$\tilde{E} = E + \lambda\Omega, \tag{5.140}$$

where

$$\Omega = \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\left(\frac{\partial y_{nk}}{\partial\xi}\right)^2. \tag{5.141}$$

(a)

We have

$$\frac{\partial y_{nk}}{\partial\xi} = \mathcal{G} y_{nk}, \tag{5.142}$$

where

$$\begin{aligned} \mathcal{G} &= \sum_{d=1}^{D} \tau_d \frac{\partial}{\partial x_d}, \\ \tau_d &= \frac{\partial x_d}{\partial \xi}. \end{aligned} \tag{5.143}$$

Therefore,

$$\Omega = \sum_{n=1}^{N} \Omega_n, \tag{5.144}$$

where

$$\Omega_n = \frac{1}{2} \sum_{k=1}^{K} (\mathcal{G} y_{nk})^2. \tag{5.145}$$

(b)

$$\begin{aligned} \alpha_j &= \mathcal{G} z_j = h'(a_j)\beta_j? \\ \beta_j &= \mathcal{G} a_j = \sum_{d=1}^{D} w_{jd}\alpha_d? \end{aligned} \tag{5.146}$$

5.27

Let

$$\tilde{E} = \frac{1}{2} \iiint \left(y\left(\mathbf{x}+\boldsymbol{\xi}\right) - t\right)^2 p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi}, \tag{5.147}$$

where

$$p(\boldsymbol{\xi}) = \mathcal{N}(\boldsymbol{\xi}|\mathbf{0}, \mathbf{I}). \tag{5.148}$$

By a Taylor series

$$y(\mathbf{x}+\boldsymbol{\xi}) = y(\mathbf{x}) + \boldsymbol{\xi}^\intercal \nabla y(\mathbf{x}) + \frac{1}{2}\boldsymbol{\xi}^\intercal \nabla\nabla y(\mathbf{x})\boldsymbol{\xi} + O\left(\|\boldsymbol{\xi}\|^3\right), \tag{5.149}$$

the integrand can be written as

$$\begin{aligned} &\left(y(\mathbf{x}) - t\right)^2 + 2\left(y(\mathbf{x}) - t\right)\left(\boldsymbol{\xi}^\intercal \nabla y(\mathbf{x}) + \frac{1}{2}\boldsymbol{\xi}^\intercal \nabla\nabla y(\mathbf{x})\boldsymbol{\xi} + O\left(\|\boldsymbol{\xi}\|^3\right)\right) \\ &+ \left(\boldsymbol{\xi}^\intercal \nabla y(\mathbf{x}) + \frac{1}{2}\boldsymbol{\xi}^\intercal \nabla\nabla y(\mathbf{x})\boldsymbol{\xi} + O\left(\|\boldsymbol{\xi}\|^3\right)\right)^2. \end{aligned} \tag{5.150}$$

Omitting the terms of $O(\|\boldsymbol{\xi}\|^3)$, the integral can be approximated as

$$\begin{aligned}
&\iiint (y(\mathbf{x}) - t)^2 \, p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi} \\
&+ 2 \iiint (y(\mathbf{x}) - t) \left(\boldsymbol{\xi}^\mathsf{T} \nabla y(\mathbf{x}) + \frac{1}{2} \boldsymbol{\xi}^\mathsf{T} \nabla \nabla y(\mathbf{x}) \boldsymbol{\xi} \right) p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi} \\
&+ \iiint \left(\boldsymbol{\xi}^\mathsf{T} \nabla y(\mathbf{x}) + \frac{1}{2} \boldsymbol{\xi}^\mathsf{T} \nabla \nabla y(\mathbf{x}) \boldsymbol{\xi} \right)^2 p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi}.
\end{aligned} \tag{5.151}$$

Omitting the terms of $O(\|\boldsymbol{\xi}\|^3)$, the second and third terms can be approximated as

$$\begin{aligned}
&2 \iiint (y(\mathbf{x}) - t) \, \boldsymbol{\xi}^\mathsf{T} \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi} \\
&+ \iiint (y(\mathbf{x}) - t) \, \boldsymbol{\xi}^\mathsf{T} \nabla \nabla y(\mathbf{x}) \boldsymbol{\xi} p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi} \\
&+ \iiint \boldsymbol{\xi}^\mathsf{T} \left(\nabla y(\mathbf{x}) \right) \left(\nabla y(\mathbf{x}) \right)^\mathsf{T} \boldsymbol{\xi} p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi}.
\end{aligned} \tag{5.152}$$

Since

$$\mathrm{E}\, \boldsymbol{\xi} = \mathbf{0}, \tag{5.153}$$

the integral of the first term can be written as

$$\left(\int \boldsymbol{\xi} p(\boldsymbol{\xi}) d\boldsymbol{\xi} \right)^\mathsf{T} \iint (y(\mathbf{x}) - t) \, \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt = \mathbf{0}. \tag{5.154}$$

Since

$$\mathrm{cov}\, \boldsymbol{\xi} = \mathbf{I}, \tag{5.155}$$

The integrals of the second term can be written as

$$\begin{aligned}
&\int \boldsymbol{\xi}^\mathsf{T} \left(\iint (y(\mathbf{x}) - t) \, \nabla \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt \right) \boldsymbol{\xi} p(\boldsymbol{\xi}) d\boldsymbol{\xi} \\
&= \mathrm{tr} \left(\iint (y(\mathbf{x}) - t) \, \nabla \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt \right).
\end{aligned} \tag{5.156}$$

The integral of the right hand side can be written as

$$\begin{aligned}
&\int \left(y(\mathbf{x}) - \int t p(t|\mathbf{x}) dt \right) \nabla \nabla y(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} \\
&= \int (y(\mathbf{x}) - \mathrm{E}(t|\mathbf{x})) \, \nabla \nabla y(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}.
\end{aligned} \tag{5.157}$$

Similarly, the integral of the third term can be written as

$$\begin{aligned}&\int \boldsymbol{\xi}^{\mathsf{T}} \left(\iint (\nabla y(\mathbf{x})) (\nabla y(\mathbf{x}))^{\mathsf{T}} p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt \right) \boldsymbol{\xi} d\boldsymbol{\xi} \\ &= \operatorname{tr} \left(\iint (\nabla y(\mathbf{x})) (\nabla y(\mathbf{x}))^{\mathsf{T}} p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt \right).\end{aligned} \tag{5.158}$$

The integral of the right hand side can be written as

$$\begin{aligned}&\int \left(\int p(t|\mathbf{x}) dt \right) (\nabla y(\mathbf{x})) (\nabla y(\mathbf{x}))^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x} \\ &= \int (\nabla y(\mathbf{x})) (\nabla y(\mathbf{x}))^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x}.\end{aligned} \tag{5.159}$$

If

$$y(\mathbf{x}) = \mathrm{E}(t|\mathbf{x}), \tag{5.160}$$

then

$$\tilde{E} \simeq E + \Omega, \tag{5.161}$$

where

$$\begin{aligned}E &= \frac{1}{2} \iiint (y(\mathbf{x}) - t)^2 p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi}, \\ \Omega &= \frac{1}{2} \operatorname{tr} \left(\int \nabla y(\mathbf{x}) (\nabla y(\mathbf{x}))^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x}. \right).\end{aligned} \tag{5.162}$$

5.28 (Incomplete)

5.29

Let $w_1, \cdots, w_M$ be variables such that

$$p(w_m) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right). \tag{5.163}$$

Let

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w}), \tag{5.164}$$

where

$$\Omega(\mathbf{w}) = -\sum_{m=1}^{M} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right) \right). \tag{5.165}$$

We have

$$\frac{\partial \Omega}{\partial w_m} = -\frac{\sum_{k=1}^{K} \pi_k \frac{w_m - \mu_k}{\sigma_k^2} \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}. \tag{5.166}$$

Therefore,

$$\frac{\partial \tilde{E}}{\partial w_m} = \frac{\partial E}{\partial w_m} - \lambda \sum_{k=1}^{K} \gamma_k(w_m) \frac{w_m - \mu_k}{\sigma_k^2}, \tag{5.167}$$

where

$$\gamma_k(w_m) = \frac{\pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}. \tag{5.168}$$

5.30

Let $w_1, \cdots, w_M$ be variables such that

$$p(w_m) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right). \tag{5.169}$$

Let

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w}), \tag{5.170}$$

where

$$\Omega(\mathbf{w}) = -\sum_{m=1}^{M} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right) \right). \tag{5.171}$$

We have

$$\frac{\partial \Omega}{\partial \mu_k} = -\frac{\sum_{k=1}^{K} \pi_k \frac{w_m - \mu_k}{\sigma_k^2} \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}. \tag{5.172}$$

Therefore,

$$\frac{\partial \tilde{E}}{\partial \mu_k} = -\lambda \sum_{k=1}^{K} \gamma_k(w_m) \frac{w_m - \mu_k}{\sigma_k^2}, \tag{5.173}$$

where

$$\gamma_k(w_m) = \frac{\pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}. \tag{5.174}$$

5.31

Let $w_1, \cdots, w_M$ be variables such that

$$p(w_m) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right). \tag{5.175}$$

Let

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w}), \tag{5.176}$$

where

$$\Omega(\mathbf{w}) = -\sum_{m=1}^{M} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right) \right). \tag{5.177}$$

We have

$$\frac{\partial \Omega}{\partial \sigma_k} = -\frac{\sum_{k=1}^{K} \pi_k \left(-\frac{1}{\sigma_k} + \frac{(w_m - \mu_k)^2}{\sigma_k^3} \right) \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}. \tag{5.178}$$

Therefore,

$$\frac{\partial \tilde{E}}{\partial \sigma_k} = -\lambda \sum_{k=1}^{K} \gamma_k(w_m) \left(-\frac{1}{\sigma_k} + \frac{(w_m - \mu_k)^2}{\sigma_k^3} \right), \tag{5.179}$$

where

$$\gamma_k(w_m) = \frac{\pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}. \tag{5.180}$$

5.32

Let $w_1, \cdots, w_M$ be variables such that

$$p(w_m) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right), \tag{5.181}$$

where

$$\pi_k = \frac{\exp(\eta_k)}{\sum_{k=1}^{K} \exp(\eta_k)}. \tag{5.182}$$

Let

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w}), \tag{5.183}$$

where

$$\Omega(\mathbf{w}) = -\sum_{m=1}^{M} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right) \right). \tag{5.184}$$

(a)

If $k \neq k'$, then

$$\frac{\partial \pi_k}{\partial \eta_{k'}} = -\frac{\exp(\eta_{k'}) \exp(\eta_k)}{(\sum_{k=1}^{K} \exp(\eta_k))^2}. \tag{5.185}$$

We have

$$\frac{\partial \pi_k}{\partial \eta_k} = \frac{\exp(\eta_k)}{\sum_{k=1}^{K} \exp(\eta_k)} - \left(\frac{\exp(\eta_k)}{\sum_{k=1}^{K} \exp(\eta_k)} \right)^2. \tag{5.186}$$

Therefore,

$$\frac{\partial \pi_k}{\partial \eta_{k'}} = I_{kk'} \pi_k - \pi_k \pi_{k'}. \tag{5.187}$$

(b)

We have

$$\frac{\partial \Omega}{\partial \eta_k} = \sum_{k'=1}^{K} \frac{\partial \Omega}{\partial \pi_{k'}} \frac{\partial \pi_{k'}}{\partial \eta_k}. \tag{5.188}$$

We have

$$\frac{\partial \Omega}{\partial \pi_{k'}} = -\frac{\sum_{m=1}^{M} \mathcal{N}\left(w_m | \mu_{k'}, \sigma_{k'}^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}. \tag{5.189}$$

By (a),

$$\frac{\partial \Omega}{\partial \eta_k} = -\sum_{k'=1}^{K} \frac{\sum_{m=1}^{M} \mathcal{N}\left(w_m | \mu_{k'}, \sigma_{k'}^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)} \left(I_{kk'} \pi_k - \pi_k \pi_{k'}\right). \tag{5.190}$$

The right hand side can be written as

$$\begin{aligned} &-\sum_{m=1}^{M} \frac{\pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)} + \pi_k \sum_{m=1}^{M} \frac{\sum_{k'=1}^{K} \pi_{k'} \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)} \\ &= \sum_{m=1}^{M} \left(\pi_k - \frac{\pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)} \right). \end{aligned} \tag{5.191}$$

Therefore,

$$\frac{\partial \tilde{E}}{\partial \eta_k} = \lambda \sum_{m=1}^{M} \left(\pi_k - \gamma_k(w_m)\right), \tag{5.192}$$

where

$$\gamma_k(w_m) = \frac{\pi_k \mathcal{N}\left(w_m|\mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m|\mu_k, \sigma_k^2\right)}. \tag{5.193}$$

5.33

Let (x_1, x_2) be the Cartesian coordinates of the end-effector of a two-link robot arm whose joint angles are θ_1 and θ_2 and whose arm lengths are L_1 and L_2. Let us asuume that the origin of the coordinate system is given by the attachment point of the lower arm. We have

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} L_1 \cos\theta_1 \\ L_1 \sin\theta_1 \end{bmatrix} + \begin{bmatrix} L_2 \cos\left(\theta_2 - (\pi - \theta_1)\right) \\ L_2 \sin\left(\theta_2 - (\pi - \theta_1)\right) \end{bmatrix}. \tag{5.194}$$

The second term of the right hand side can be written as

$$\begin{bmatrix} L_2 \cos\left(\theta_1 + \theta_2 - \pi\right) \\ L_2 \sin\left(\theta_1 + \theta_2 - \pi\right) \end{bmatrix} = \begin{bmatrix} -L_2 \cos(\theta_1 + \theta_2) \\ -L_2 \sin(\theta_1 + \theta_2) \end{bmatrix}. \tag{5.195}$$

Therefore,

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} L_1 \cos\theta_1 - L_2 \cos(\theta_1 + \theta_2) \\ L_1 \sin\theta_1 - L_2 \sin(\theta_1 + \theta_2) \end{bmatrix}. \tag{5.196}$$

5.34

Let

$$E_n(\mathbf{w}) = -\ln\left(\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}\right), \tag{5.197}$$

where

$$\begin{aligned} \pi_k &= \frac{\exp(a_k)}{\sum_{k=1}^{K} \exp(a_k)}, \\ \mathcal{N}_{nk} &= \mathcal{N}\left(\mathbf{t}_n|\boldsymbol{\mu}_k(\mathbf{x}_n, \mathbf{w}), \sigma_k^2(\mathbf{x}_n, \mathbf{w})\mathbf{I}\right). \end{aligned} \tag{5.198}$$

Then,

$$\frac{\partial E_n}{\partial a_k^{\pi}} = \sum_{k'=1}^{K} \frac{\partial E_n}{\partial \pi_{k'}} \frac{\partial \pi_{k'}}{\partial a_k^{\pi}}. \tag{5.199}$$

We have

$$\frac{\partial E_n}{\partial \pi_{k'}} = -\frac{\mathcal{N}_{nk'}}{\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}}. \tag{5.200}$$

By 5.32(a),

$$\frac{\partial \pi_{k'}}{\partial a_k^\pi} = I_{kk'}\pi_{k'} - \pi_k \pi_{k'}. \tag{5.201}$$

Then,

$$\frac{\partial E_n}{\partial a_k^\pi} = -\sum_{k'=1}^{K} \frac{\mathcal{N}_{nk'}}{\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}} (I_{kk'}\pi_{k'} - \pi_k \pi_{k'}). \tag{5.202}$$

The right hand side can be written as

$$\pi_k \frac{\sum_{k'=1}^{K} \pi_{k'} \mathcal{N}_{nk'}}{\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}} - \frac{\pi_k \mathcal{N}_{nk}}{\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}} = \pi_k - \frac{\pi_k \mathcal{N}_{nk}}{\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}}. \tag{5.203}$$

Therefore,

$$\frac{\partial E_n}{\partial a_k^\pi} = \pi_k - \gamma_{nk}, \tag{5.204}$$

where

$$\gamma_{nk} = \frac{\pi_k \mathcal{N}_{nk}}{\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}}. \tag{5.205}$$

5.35

Let

$$E_n(\mathbf{w}) = -\ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk} \right), \tag{5.206}$$

where

$$\begin{aligned} \mathcal{N}_{nk} &= \mathcal{N}\left(\mathbf{t}_n | \boldsymbol{\mu}_k(\mathbf{x}_n, \mathbf{w}), \sigma_k^2(\mathbf{x}_n, \mathbf{w})\mathbf{I}\right), \\ \mu_{km} &= a_{km}^\mu. \end{aligned} \tag{5.207}$$

Then,

$$\frac{\partial E_n}{\partial a_{km}^\mu} = \frac{\partial E_n}{\partial \mathcal{N}_{nk}} \frac{\partial \mathcal{N}_{nk}}{\partial a_{km}^\mu}. \tag{5.208}$$

We have

$$\frac{\partial E_n}{\partial \mathcal{N}_{nk}} = -\frac{\pi_k}{\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}}. \tag{5.209}$$

We have

$$\frac{\partial \mathcal{N}_{nk}}{\partial a_{km}^\mu} = \frac{t_{nm} - \mu_{km}}{\sigma_k^2} \mathcal{N}_{nk}. \tag{5.210}$$

Then,

$$\frac{\partial E_n}{\partial a_{km}^{\mu}} = -\frac{\pi_k}{\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}} \frac{t_{nm} - \mu_{km}}{\sigma_k^2} \mathcal{N}_{nk}. \tag{5.211}$$

Therefore,

$$\frac{\partial E_n}{\partial a_{km}^{\mu}} = \gamma_{nk} \frac{\mu_{km} - t_{nm}}{\sigma_k^2}, \tag{5.212}$$

where

$$\gamma_{nk} = \frac{\pi_k \mathcal{N}_{nk}}{\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}}. \tag{5.213}$$

5.36

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables in M dimensions. Let

$$E_n(\mathbf{w}) = -\ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk} \right), \tag{5.214}$$

where

$$\begin{aligned} \mathcal{N}_{nk} &= \mathcal{N}\left(\mathbf{t}_n | \boldsymbol{\mu}_k(\mathbf{x}_n, \mathbf{w}), \sigma_k^2(\mathbf{x}_n, \mathbf{w})\mathbf{I}\right), \\ \sigma_k &= \exp\left(a_k^{\sigma}\right). \end{aligned} \tag{5.215}$$

Then,

$$\frac{\partial E_n}{\partial a_k^{\sigma}} = \frac{\partial E_n}{\partial \mathcal{N}_{nk}} \frac{\partial \mathcal{N}_{nk}}{\partial a_k^{\sigma}}. \tag{5.216}$$

We have

$$\frac{\partial E_n}{\partial \mathcal{N}_{nk}} = -\frac{\pi_k}{\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}}. \tag{5.217}$$

We have

$$\frac{\partial \mathcal{N}_{nk}}{\partial a_k^{\sigma}} = \frac{\partial \mathcal{N}_{nk}}{\partial \sigma_k} \frac{\partial \sigma_k}{\partial a_k^{\sigma}}. \tag{5.218}$$

The right hand side can be written as

$$\left(-M\sigma_k^{-1} + \frac{\|\mathbf{t}_n - \boldsymbol{\mu}_k\|^2}{\sigma_k^3} \right) \mathcal{N}_{nk} \sigma_k = \left(-M + \frac{\|\mathbf{t}_n - \boldsymbol{\mu}_k\|^2}{\sigma_k^2} \right) \mathcal{N}_{nk}. \tag{5.219}$$

Then,

$$\frac{\partial E_n}{\partial a_k^{\sigma}} = -\frac{\pi_k}{\sum_{k=1}^{K} \pi_k \mathcal{N}_{nk}} \left(-M + \frac{\|\mathbf{t}_n - \boldsymbol{\mu}_k\|^2}{\sigma_k^2} \right) \mathcal{N}_{nk}. \tag{5.220}$$

Therefore,

$$\frac{\partial E_n}{\partial a_k^\sigma} = \gamma_{nk} \left(M - \frac{\|\mathbf{t}_n - \boldsymbol{\mu}_k\|^2}{\sigma_k^2} \right), \tag{5.221}$$

where

$$\gamma_{nk} = \frac{\pi_k \mathcal{N}_{nk}}{\sum_{k=1}^K \pi_k \mathcal{N}_{nk}}. \tag{5.222}$$

5.37

Let $\mathbf{t}$ be a variable such that

$$p(\mathbf{t}|\mathbf{x}) = \sum_{k=1}^K \pi_k(\mathbf{x}) \mathcal{N}\left(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}\right). \tag{5.223}$$

(a)

We have

$$\mathrm{E}(\mathbf{t}|\mathbf{x}) = \int \mathbf{t} p(\mathbf{t}|\mathbf{x}) d\mathbf{t}. \tag{5.224}$$

The right hand side can be written as

$$\sum_{k=1}^K \pi_k(\mathbf{x}) \int \mathbf{t} \mathcal{N}\left(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}\right) d\mathbf{t} = \sum_{k=1}^K \pi_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x}). \tag{5.225}$$

Therefore,

$$\mathrm{E}(\mathbf{t}|\mathbf{x}) = \sum_{k=1}^K \pi_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x}). \tag{5.226}$$

(b)

We have

$$\mathrm{cov}(\mathbf{t}|\mathbf{x}) = \int (\mathbf{t} - \mathrm{E}(\mathbf{t}|\mathbf{x})) (\mathbf{t} - \mathrm{E}(\mathbf{t}|\mathbf{x}))^\intercal p(\mathbf{t}|\mathbf{x}) d\mathbf{t}. \tag{5.227}$$

The right hand side can be written as

$$\begin{aligned}
&\int \mathbf{t}\mathbf{t}^\intercal p(\mathbf{t}|\mathbf{x})d\mathbf{t} - \mathrm{E}(\mathbf{t}|\mathbf{x}) \left(\int \mathbf{t} p(\mathbf{t}|\mathbf{x})d\mathbf{t} \right)^\intercal - \left(\int \mathbf{t} p(\mathbf{t}|\mathbf{x})d\mathbf{t} \right) \mathrm{E}(\mathbf{t}|\mathbf{x})^\intercal \\
&\quad + \mathrm{E}(\mathbf{t}|\mathbf{x})\, \mathrm{E}(\mathbf{t}|\mathbf{x})^\intercal \int p(\mathbf{t}|\mathbf{x})d\mathbf{t} \\
&= \int \mathbf{t}\mathbf{t}^\intercal p(\mathbf{t}|\mathbf{x})d\mathbf{t} - \mathrm{E}(\mathbf{t}|\mathbf{x})\, \mathrm{E}(\mathbf{t}|\mathbf{x})^\intercal.
\end{aligned} \tag{5.228}$$

The first term of the right hand side can be written as

$$\sum_{k=1}^{K} \pi_k(\mathbf{x}) \int \mathbf{t}\mathbf{t}^\intercal \mathcal{N}\left(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}\right) d\mathbf{t}. \tag{5.229}$$

The integral of the right hand side can be written as

$$\begin{aligned}
&\int (\mathbf{t} - \boldsymbol{\mu}_k(\mathbf{x}) + \boldsymbol{\mu}_k(\mathbf{x}))\, (\mathbf{t} - \boldsymbol{\mu}_k(\mathbf{x}) + \boldsymbol{\mu}_k(\mathbf{x}))^\intercal \mathcal{N}\left(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}\right) d\mathbf{t} \\
&= \int (\mathbf{t} - \boldsymbol{\mu}_k(\mathbf{x}))\, (\mathbf{t} - \boldsymbol{\mu}_k(\mathbf{x}))^\intercal \mathcal{N}\left(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}\right) d\mathbf{t} \\
&\quad + \boldsymbol{\mu}_k(\mathbf{x}) \left(\int (\mathbf{t} - \boldsymbol{\mu}_k(\mathbf{x})) \mathcal{N}\left(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}\right) d\mathbf{t} \right)^\intercal \\
&\quad + \left(\int (\mathbf{t} - \boldsymbol{\mu}_k(\mathbf{x})) \mathcal{N}\left(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}\right) d\mathbf{t} \right) \boldsymbol{\mu}_k(\mathbf{x})^\intercal \\
&\quad + \boldsymbol{\mu}_k(\mathbf{x})\boldsymbol{\mu}_k(\mathbf{x})^\intercal \int \mathcal{N}\left(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}\right) d\mathbf{t}.
\end{aligned} \tag{5.230}$$

The right hand side can be written as

$$\sigma_k^2(\mathbf{x})\mathbf{I} + \boldsymbol{\mu}_k(\mathbf{x})\boldsymbol{\mu}_k(\mathbf{x})^\intercal. \tag{5.231}$$

Therefore, by (a),

$$\begin{aligned}
\mathrm{cov}(\mathbf{t}|\mathbf{x}) = &\sum_{k=1}^{K} \pi_k(\mathbf{x}) \left(\sigma_k^2(\mathbf{x})\mathbf{I} + \boldsymbol{\mu}_k(\mathbf{x})\boldsymbol{\mu}_k(\mathbf{x})^\intercal \right) \\
&- \left(\sum_{k=1}^{K} \pi_k(\mathbf{x})\boldsymbol{\mu}_k(\mathbf{x}) \right) \left(\sum_{k=1}^{K} \pi_k(\mathbf{x})\boldsymbol{\mu}_k(\mathbf{x}) \right)^\intercal.
\end{aligned} \tag{5.232}$$

5.38

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|y(\mathbf{x},\mathbf{w}),\beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}\left(\mathbf{w}|\mathbf{0},\alpha^{-1}\mathbf{I}\right). \end{aligned} \tag{5.233}$$

By marginalisation,

$$p(t|\mathbf{t}) = \int p(t|\mathbf{w})p(\mathbf{w}|\mathbf{t})d\mathbf{w}. \tag{5.234}$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{t})p(\mathbf{t}) = p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \tag{5.235}$$

The logarithm of the right hand side except the terms independent of $\mathbf{w}$ can be written as $-E(\mathbf{w})$ where

$$E(\mathbf{w}) = \frac{\beta}{2}\sum_{n=1}^{N}\left(t_n - y(\mathbf{x}_n,\mathbf{w})\right)^2 + \frac{\alpha}{2}\mathbf{w}^\intercal\mathbf{w}. \tag{5.236}$$

Let $\mathbf{w}_{\mathrm{MAP}}$ be a stationary point of $p(\mathbf{w}|\mathbf{t})$. Then, we have a Taylor series

$$\begin{aligned} E(\mathbf{w}) =& E(\mathbf{w}_{\mathrm{MAP}}) + \frac{1}{2}(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}})^\intercal\mathbf{A}(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}}) \\ &+ O\left(\|\mathbf{w}-\mathbf{w}_{\mathrm{MAP}}\|^3\right), \end{aligned} \tag{5.237}$$

where

$$\mathbf{A} = \nabla\nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\mathrm{MAP}}}. \tag{5.238}$$

Then,

$$p(\mathbf{w}|\mathbf{t}) \simeq \mathcal{N}\left(\mathbf{w}|\mathbf{w}_{\mathrm{MAP}},\mathbf{A}^{-1}\right). \tag{5.239}$$

By a Taylor series

$$y(\mathbf{x},\mathbf{w}) = y(\mathbf{x},\mathbf{w}_{\mathrm{MAP}}) + \mathbf{g}^\intercal(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}}) + O\left(\|\mathbf{w}-\mathbf{w}_{\mathrm{MAP}}\|^2\right), \tag{5.240}$$

where

$$\mathbf{g} = \nabla_{\mathbf{w}} y(\mathbf{x},\mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\mathrm{MAP}}}, \tag{5.241}$$

we have

$$p(t|\mathbf{w}) \simeq \mathcal{N}\left(t|y(\mathbf{x},\mathbf{w}_{\mathrm{MAP}}) + \mathbf{g}^\intercal(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}}),\beta^{-1}\right). \tag{5.242}$$

Then, the logarithm of the integrand except the terms independent of $\mathbf{w}$ can be approximated as

$$\begin{aligned}
&-\frac{\beta}{2}\left(t-y(\mathbf{x},\mathbf{w}_{\mathrm{MAP}})-\mathbf{g}^{\intercal}(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}})\right)^2-\frac{1}{2}(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}})^{\intercal}\mathbf{A}(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}})\\
=&-\frac{1}{2}\begin{bmatrix}\mathbf{w}-\mathbf{w}_{\mathrm{MAP}}\\ t-y(\mathbf{x},\mathbf{w}_{\mathrm{MAP}})\end{bmatrix}^{\intercal}\begin{bmatrix}\mathbf{A}+\beta\mathbf{g}\mathbf{g}^{\intercal} & -\beta\mathbf{g}\\ -\beta\mathbf{g}^{\intercal} & \beta\end{bmatrix}\begin{bmatrix}\mathbf{w}-\mathbf{w}_{\mathrm{MAP}}\\ t-y(\mathbf{x},\mathbf{w}_{\mathrm{MAP}})\end{bmatrix}.
\end{aligned}\tag{5.243}$$

By 2.24,

$$\begin{bmatrix}\mathbf{A}+\beta\mathbf{g}\mathbf{g}^{\intercal} & -\beta\mathbf{g}\\ -\beta\mathbf{g}^{\intercal} & \beta\end{bmatrix}^{-1}=\begin{bmatrix}\mathbf{A}^{-1} & \mathbf{A}^{-1}\mathbf{g}\\ \mathbf{g}^{\intercal}\mathbf{A}^{-1} & \beta^{-1}+\mathbf{g}^{\intercal}\mathbf{A}^{-1}\mathbf{g}\end{bmatrix}.\tag{5.244}$$

Therefore,

$$p(t|\mathbf{t})\simeq\mathcal{N}\left(t|y(\mathbf{x},\mathbf{w}_{\mathrm{MAP}}),\beta^{-1}+\mathbf{g}^{\intercal}\mathbf{A}^{-1}\mathbf{g}\right).\tag{5.245}$$

5.39

Let $t_1,\cdots,t_N$ be variables such that

$$\begin{aligned}
p(t_n|\mathbf{w})&=\mathcal{N}\left(t_n|y(\mathbf{x},\mathbf{w}),\beta^{-1}\right),\\
p(\mathbf{w})&=\mathcal{N}\left(\mathbf{w}|\mathbf{0},\alpha^{-1}\mathbf{I}\right),
\end{aligned}\tag{5.246}$$

where $\mathbf{w}$ is a vector in M dimensions. By marginalisation,

$$p(\mathbf{t})=\int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}.\tag{5.247}$$

The logarithm of the integrand of the right hand side can be written as

$$\begin{aligned}
&-\frac{N}{2}\ln\left(2\pi\beta^{-1}\right)-\frac{\beta}{2}\sum_{n=1}^{N}\left(t_n-y(\mathbf{x}_n,\mathbf{w})\right)^2\\
&-\frac{M}{2}\ln\left(2\pi\right)-\frac{1}{2}\ln\left(\det\left(\alpha^{-1}\mathbf{I}\right)\right)-\frac{\alpha}{2}\mathbf{w}^{\intercal}\mathbf{w}\\
=&-E(\mathbf{w})-\frac{N+M}{2}\ln(2\pi)+\frac{N}{2}\ln\beta+\frac{M}{2}\ln\alpha,
\end{aligned}\tag{5.248}$$

where

$$E(\mathbf{w})=\frac{\beta}{2}\sum_{n=1}^{N}\left(t_n-y(\mathbf{x}_n,\mathbf{w})\right)^2+\frac{\alpha}{2}\mathbf{w}^{\intercal}\mathbf{w}.\tag{5.249}$$

Let $\mathbf{w}_{\mathrm{MAP}}$ be a stationary point of E. Then, we have a Taylor series

$$\begin{aligned} E(\mathbf{w}) =& E(\mathbf{w}_{\mathrm{MAP}}) + \frac{1}{2}(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}})^{\intercal}\mathbf{A}(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}}) \\ &+ O\left(\|\mathbf{w}-\mathbf{w}_{\mathrm{MAP}}\|^3\right), \end{aligned} \tag{5.250}$$

where

$$\mathbf{A} = \nabla\nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\mathrm{MAP}}}. \tag{5.251}$$

Then, the logarithm of the integrand can be approximated as

$$\begin{aligned} &- E(\mathbf{w}_{\mathrm{MAP}}) - \frac{1}{2}(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}})^{\intercal}\mathbf{A}(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}}) \\ &- \frac{N+M}{2}\ln(2\pi) + \frac{N}{2}\ln\beta + \frac{M}{2}\ln\alpha. \end{aligned} \tag{5.252}$$

Therefore,

$$\ln p(\mathbf{t}) \simeq -E(\mathbf{w}_{\mathrm{MAP}}) - \frac{1}{2}\ln|\det\mathbf{A}| - \frac{N}{2}\ln(2\pi) + \frac{N}{2}\ln\beta + \frac{M}{2}\ln\alpha. \tag{5.253}$$

5.40 (Incomplete)

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables such that

$$\begin{aligned} p(\mathbf{t}_n|\mathbf{w}) &= \prod_{k=1}^{K} y_{nk}^{t_{nk}}, \\ p(\mathbf{w}) &= \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}\right), \end{aligned} \tag{5.254}$$

where

$$\begin{aligned} t_{nk} &\in \{0,1\}, \\ y_{nk} &= y_k(\mathbf{x}_n, \mathbf{w}), \\ \sum_{k=1}^{K} y_{nk} &= 1. \end{aligned} \tag{5.255}$$

By marginalisation,

$$p(\mathbf{t}|\mathbf{T}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w}|\mathbf{T})d\mathbf{w}. \tag{5.256}$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{T})p(\mathbf{T}) = p(\mathbf{T}|\mathbf{w})p(\mathbf{w}). \tag{5.257}$$

The logarithm of the right hand side except the terms independent of $\mathbf{w}$ can be written as $-E(\mathbf{w})$ where

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk} \ln y_{nk} + \frac{\alpha}{2}\mathbf{w}^{\intercal}\mathbf{w}. \tag{5.258}$$

Let $\mathbf{w}_{\mathrm{MAP}}$ be a stationary point of E. Then, we have a Taylor series

$$\begin{aligned} E(\mathbf{w}) =& E(\mathbf{w}_{\mathrm{MAP}}) + \frac{1}{2}(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}})^{\intercal}\mathbf{A}(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}}) \\ &+ O\left(\|(\mathbf{w}-\mathbf{w}_{\mathrm{MAP}})\|^3\right), \end{aligned} \tag{5.259}$$

where

$$\mathbf{A} = \nabla\nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\mathrm{MAP}}}. \tag{5.260}$$

Then,

$$p(\mathbf{w}|\mathbf{T}) \simeq \mathcal{N}\left(\mathbf{w}|\mathbf{w}_{\mathrm{MAP}}, \mathbf{A}^{-1}\right). \tag{5.261}$$

5.41

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables such that

$$\begin{aligned} p(\mathbf{t}_n|\mathbf{w}) &= \prod_{k=1}^{K} y_{nk}^{t_{nk}}, \\ p(\mathbf{w}) &= \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}\right), \end{aligned} \tag{5.262}$$

where

$$\begin{aligned} t_{nk} &\in \{0,1\}, \\ y_{nk} &= y_k(\mathbf{x}_n, \mathbf{w}), \\ \sum_{k=1}^{K} y_{nk} &= 1. \end{aligned} \tag{5.263}$$

By marginalisation,

$$p(\mathbf{T}) = \int p(\mathbf{T}|\mathbf{w})p(\mathbf{w})d\mathbf{w}. \tag{5.264}$$

The logarithm of the integrand of the right hand side can be written as

$$\begin{aligned} &\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk}\ln y_{nk} - \frac{M}{2}\ln(2\pi) - \frac{1}{2}\ln\left(\det\left(\alpha^{-1}\mathbf{I}\right)\right) - \frac{\alpha}{2}\mathbf{w}^{\intercal}\mathbf{w} \\ =& -E(\mathbf{w}) - \frac{M}{2}\ln(2\pi) + \frac{M}{2}\ln\alpha, \end{aligned} \tag{5.265}$$

where

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk} \ln y_{nk} + \frac{\alpha}{2}\mathbf{w}^{\intercal}\mathbf{w}. \tag{5.266}$$

Let $\mathbf{w}_{\mathrm{MAP}}$ be a stationary point of E. Then, we have a Taylor series

$$\begin{aligned} E(\mathbf{w}) =& E(\mathbf{w}_{\mathrm{MAP}}) + \frac{1}{2}(\mathbf{w} - \mathbf{w}_{\mathrm{MAP}})^{\intercal}\mathbf{A}(\mathbf{w} - \mathbf{w}_{\mathrm{MAP}}) \\ &+ O\left(\|(\mathbf{w} - \mathbf{w}_{\mathrm{MAP}})\|^3\right), \end{aligned} \tag{5.267}$$

where

$$\mathbf{A} = \nabla\nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\mathrm{MAP}}}. \tag{5.268}$$

Then, the logarithm of the integrand can be approximated as

$$-E(\mathbf{w}_{\mathrm{MAP}}) - \frac{1}{2}(\mathbf{w} - \mathbf{w}_{\mathrm{MAP}})^{\intercal}\mathbf{A}(\mathbf{w} - \mathbf{w}_{\mathrm{MAP}}) - \frac{M}{2}\ln(2\pi) + \frac{M}{2}\ln\alpha. \tag{5.269}$$

Therefore,

$$\ln p(\mathbf{T}) \simeq -E(\mathbf{w}_{\mathrm{MAP}}) - \frac{1}{2}\ln|\det\mathbf{A}| + \frac{M}{2}\ln\alpha. \tag{5.270}$$

6 Kernel Methods

6.1

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n), 1\right), \\ p(\mathbf{w}) &= \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \lambda^{-1}\mathbf{I}\right). \end{aligned} \tag{6.1}$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{t})p(\mathbf{t}) = p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \tag{6.2}$$

The logarithm of the right hand side except the terms independent of $\mathbf{w}$ can be written as $-E_{\mathbf{w}}(\mathbf{w})$ where

$$E_{\mathbf{w}}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(t_n - \mathbf{w}^\intercal\boldsymbol{\phi}(\mathbf{x}_n)\right)^2 + \frac{\lambda}{2}\mathbf{w}^\intercal\mathbf{w}, \tag{6.3}$$

so that

$$E_{\mathbf{w}}(\mathbf{w}) = \frac{1}{2}\|\mathbf{t} - \boldsymbol{\Phi}\mathbf{w}\|^2 + \frac{\lambda}{2}\mathbf{w}^\intercal\mathbf{w}, \tag{6.4}$$

where

$$\boldsymbol{\Phi} = \begin{bmatrix} \boldsymbol{\phi}(\mathbf{x}_1)^\intercal \\ \vdots \\ \boldsymbol{\phi}(\mathbf{x}_N)^\intercal \end{bmatrix}. \tag{6.5}$$

(a)

Setting the derivative of $E_{\mathbf{w}}$ with respect to $\mathbf{w}$ to zero gives

$$\mathbf{0} = -\boldsymbol{\Phi}^\intercal(\mathbf{t} - \boldsymbol{\Phi}\mathbf{w}) + \lambda\mathbf{w}. \tag{6.6}$$

Let the stationary point of $E_{\mathbf{w}}$ be $\mathbf{w}_{\mathrm{MAP}}$. Then,

$$\mathbf{w}_{\mathrm{MAP}} = \boldsymbol{\Phi}^\intercal\mathbf{a}_{\mathrm{MAP}}, \tag{6.7}$$

where

$$\mathbf{a}_{\mathrm{MAP}} = \frac{1}{\lambda}\left(\mathbf{t} - \boldsymbol{\Phi}\mathbf{w}_{\mathrm{MAP}}\right). \tag{6.8}$$

(b)

Let

$$\mathbf{w} = \mathbf{\Phi}^\intercal \mathbf{a}. \tag{6.9}$$

Then,

$$E_{\mathbf{w}}(\mathbf{w}) = E_{\mathbf{a}}(\mathbf{a}), \tag{6.10}$$

where

$$E_{\mathbf{a}}(\mathbf{a}) = \frac{1}{2}\|\mathbf{t} - \mathbf{\Phi}\mathbf{\Phi}^\intercal \mathbf{a}\|^2 + \frac{\lambda}{2}\mathbf{a}^\intercal \mathbf{\Phi}\mathbf{\Phi}^\intercal \mathbf{a}. \tag{6.11}$$

The right hand side can be written as

$$\frac{1}{2}\|\mathbf{t}\|^2 - \mathbf{t}^\intercal \mathbf{K}\mathbf{a} + \frac{1}{2}\mathbf{a}^\intercal \mathbf{K}\mathbf{K}\mathbf{a} + \frac{\lambda}{2}\mathbf{a}^\intercal \mathbf{K}\mathbf{a}, \tag{6.12}$$

where

$$\mathbf{K} = \mathbf{\Phi}\mathbf{\Phi}^\intercal. \tag{6.13}$$

Setting the derivative of $E_{\mathbf{a}}$ with respect to $\mathbf{a}$ to zero gives

$$\mathbf{0} = -\mathbf{K}\mathbf{t} + \mathbf{K}\mathbf{K}\mathbf{a} + \lambda\mathbf{K}\mathbf{a}. \tag{6.14}$$

Then, the stationary point of $E_{\mathbf{a}}$ is given by

$$\mathbf{a}_{\mathrm{MAP}} = (\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t}. \tag{6.15}$$

(c)

By (a) and (b),

$$\frac{1}{\lambda}\left(\mathbf{t} - \mathbf{\Phi}\mathbf{w}_{\mathrm{MAP}}\right) = (\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t}, \tag{6.16}$$

so that

$$\mathbf{t} - \mathbf{\Phi}\mathbf{w}_{\mathrm{MAP}} = \lambda(\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t}. \tag{6.17}$$

The right hand side can be written as

$$(\mathbf{K} + \lambda\mathbf{I} - \mathbf{K})(\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t} = \mathbf{t} - \mathbf{K}(\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t}. \tag{6.18}$$

Then,

$$\mathbf{\Phi}\mathbf{w}_{\mathrm{MAP}} = \mathbf{K}(\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t}, \tag{6.19}$$

so that

$$\mathbf{\Phi}^\intercal \mathbf{\Phi}\mathbf{w}_{\mathrm{MAP}} = \mathbf{\Phi}^\intercal \mathbf{K}(\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t}. \tag{6.20}$$

By (b),

$$\mathbf{w}_{\text{MAP}} = \boldsymbol{\Phi}^{\intercal}(\mathbf{K} + \boldsymbol{\lambda}\mathbf{I})^{-1}\mathbf{t}, \tag{6.21}$$

so that

$$\lambda\mathbf{w}_{\text{MAP}} = \lambda\boldsymbol{\Phi}^{\intercal}(\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t}. \tag{6.22}$$

Then,

$$(\boldsymbol{\Phi}^{\intercal}\boldsymbol{\Phi} + \lambda\mathbf{I})\,\mathbf{w}_{\text{MAP}} = \boldsymbol{\Phi}^{\intercal}(\mathbf{K} + \lambda\mathbf{I})(\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t}. \tag{6.23}$$

Therefore,

$$\mathbf{w}_{\text{MAP}} = (\boldsymbol{\Phi}^{\intercal}\boldsymbol{\Phi} + \lambda\mathbf{I})^{-1}\,\boldsymbol{\Phi}^{\intercal}\mathbf{t}. \tag{6.24}$$

6.2 (Incomplete)

Let $t_1, \cdots, t_N$ be vaariables such that

$$\begin{aligned} t_n &\in \{-1, 1\}, \\ p(t_n|\mathbf{w}) &= \left(\frac{1+y_n}{2}\right)^{\frac{1+t_n}{2}} \left(\frac{1-y_n}{2}\right)^{\frac{1-t_n}{2}}, \end{aligned} \tag{6.25}$$

where

$$\begin{aligned} y_n &= f\left(\mathbf{w}^{\intercal}\boldsymbol{\phi}_n\right), \\ f(a) &= \begin{cases} 1, & a \geq 0, \\ -1, & \text{otherwise.} \end{cases} \end{aligned} \tag{6.26}$$

Let

$$E(\mathbf{w}) = -\sum_{n\in\mathcal{M}} \mathbf{w}^{\intercal}\boldsymbol{\phi}_n t_n, \tag{6.27}$$

where $\mathcal{M}$ is the set of all misclassification. Setting the derivative of E with respect to $\mathbf{w}$ to zero gives

$$\mathbf{0} = -\sum_{n\in\mathcal{M}} t_n\boldsymbol{\phi}_n. \tag{6.28}$$

6.3

We have

$$\|\mathbf{x} - \mathbf{x}_n\|^2 = \mathbf{x}^{\intercal}\mathbf{x} - 2\mathbf{x}^{\intercal}\mathbf{x}_n + \mathbf{x}_n^{\intercal}\mathbf{x}_n. \tag{6.29}$$

The right hand side can be written as

$$k(\mathbf{x}, \mathbf{x}) - 2k(\mathbf{x}, \mathbf{x}_n) + k(\mathbf{x}_n, \mathbf{x}_n), \tag{6.30}$$

where

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\intercal \mathbf{x}'. \tag{6.31}$$

6.4

Let $\mathbf{A}$ be a 2×2 matrix with positive eigenvalues and with at least one negative element. We have

$$\det(\lambda \mathbf{I} - \mathbf{A}) = (\lambda - A_{11})(\lambda - A_{22}) - A_{12}A_{21}. \tag{6.32}$$

The right hand side can be written as

$$\lambda^2 - (A_{11} + A_{22})\lambda + A_{11}A_{22} - A_{12}A_{21}. \tag{6.33}$$

Then,

$$\begin{aligned} (A_{11} + A_{22})^2 - 4(A_{11}A_{22} - A_{12}A_{21}) > 0, \\ A_{11} + A_{22} > 0, \\ A_{11}A_{22} - A_{12}A_{21} > 0. \end{aligned} \tag{6.34}$$

Therefore, an example is

$$\mathbf{A} = \begin{bmatrix} 2 & 0 \\ -1 & 1 \end{bmatrix}. \tag{6.35}$$

6.5

Let

$$k_1(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}_1(\mathbf{x})^\intercal \boldsymbol{\phi}_1(\mathbf{x}'). \tag{6.36}$$

(a)

Let

$$k(\mathbf{x}, \mathbf{x}') = c k_1(\mathbf{x}, \mathbf{x}'), \tag{6.37}$$

where c is a positive constant. The right hand side can be written as

$$c\boldsymbol{\phi}_1(\mathbf{x})^\intercal \boldsymbol{\phi}_1(\mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^\intercal \boldsymbol{\phi}(\mathbf{x}'), \tag{6.38}$$

where

$$\boldsymbol{\phi} = \sqrt{c}\boldsymbol{\phi}_1. \tag{6.39}$$

Therefore, k is a valid kernel.

(b)

Let

$$k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x})k_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}'). \tag{6.40}$$

The right hand side can be written as

$$f(\mathbf{x})\boldsymbol{\phi}_1(\mathbf{x})^\intercal \boldsymbol{\phi}_1(\mathbf{x}')f(\mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^\intercal \boldsymbol{\phi}(\mathbf{x}'), \tag{6.41}$$

where

$$\boldsymbol{\phi} = f\boldsymbol{\phi}_1. \tag{6.42}$$

Therefore, k is a valid kernel.

6.6

Let

$$k_1(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}_1(\mathbf{x})^\intercal \boldsymbol{\phi}_1(\mathbf{x}'). \tag{6.43}$$

(a)

Let

$$k(\mathbf{x}, \mathbf{x}') = \sum_{j=0}^{J} c_j q_j(\mathbf{x}, \mathbf{x}'), \tag{6.44}$$

where $c_0, \cdots, c_J$ are nonnegative constants and

$$q_j(\mathbf{x}, \mathbf{x}') = \left(k_1(\mathbf{x}, \mathbf{x}')\right)^j. \tag{6.45}$$

We have

$$q_0(\mathbf{x}, \mathbf{x}') = 1. \tag{6.46}$$

Let us asuume that q_j is a valid kernel. Then,

$$q_{j+1}(\mathbf{x}, \mathbf{x}') = q_j(\mathbf{x}, \mathbf{x}')\boldsymbol{\phi}_1(\mathbf{x})^\intercal \boldsymbol{\phi}_1(\mathbf{x}'). \tag{6.47}$$

The right hand side can be written as

$$q_j(\mathbf{x}, \mathbf{x}') \sum_{m=1}^{M} \phi_{1m}(\mathbf{x})\phi_{1m}(\mathbf{x}') = \sum_{m=1}^{M} \phi_{1m}(\mathbf{x}) q_j(\mathbf{x}, \mathbf{x}')\phi_{1m}(\mathbf{x}'). \tag{6.48}$$

By 6.5(b) and 6.7(a), the right hand side is a valid kernel. Then, q_{j+1} is a valid kernel. Then, the assumption is proved by induction on j. Therefore, by 6.5(a) and 6.7(a), k is a valid kernel.

(b)

Let

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right). \tag{6.49}$$

The right hand side can be written as

$$\sum_{j=0}^{\infty} \frac{1}{j!} \left(k_1(\mathbf{x}, \mathbf{x}')\right)^j. \tag{6.50}$$

Therefore, by (a), k is a valid kernel.

6.7

Let

$$\begin{aligned} k_1(\mathbf{x}, \mathbf{x}') &= \boldsymbol{\phi}_1(\mathbf{x})^\intercal \boldsymbol{\phi}_1(\mathbf{x}'), \\ k_2(\mathbf{x}, \mathbf{x}') &= \boldsymbol{\phi}_2(\mathbf{x})^\intercal \boldsymbol{\phi}_2(\mathbf{x}'). \end{aligned} \tag{6.51}$$

(a)

Let

$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}'). \tag{6.52}$$

The right hand side can be written as

$$\boldsymbol{\phi}_1(\mathbf{x})^\intercal \boldsymbol{\phi}_1(\mathbf{x}') + \boldsymbol{\phi}_2(\mathbf{x})^\intercal \boldsymbol{\phi}_2(\mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^\intercal \boldsymbol{\phi}(\mathbf{x}'), \tag{6.53}$$

where

$$\boldsymbol{\phi} = \begin{bmatrix} \boldsymbol{\phi}_1 \\ \boldsymbol{\phi}_2 \end{bmatrix}. \tag{6.54}$$

Therefore, k is a valid kernel.

(b)

Let

$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') k_2(\mathbf{x}, \mathbf{x}'). \tag{6.55}$$

Then,

$$\ln k(\mathbf{x}, \mathbf{x}') = \ln k_1(\mathbf{x}, \mathbf{x}') + \ln k_2(\mathbf{x}, \mathbf{x}'). \tag{6.56}$$

By (a) and 6.6(b), the right hand side is a valid kernel. Then, $\ln k$ is a valid kernel. Therefore, by 6.6(b), k is a valid kernel.

6.8

(a)

Let

$$k(\mathbf{x}, \mathbf{x}') = k_1 \left(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}') \right), \tag{6.57}$$

where k_1 is a valid kernel. Then, k is a valid kernel.

(b)

Let

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\intercal \mathbf{A} \mathbf{x}', \tag{6.58}$$

where $\mathbf{A}$ is a symmetric positive semidefinite matrix. There exists $\mathbf{M}$ such that

$$\mathbf{A} = \mathbf{M}^\intercal \mathbf{M}. \tag{6.59}$$

Then,

$$k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^\intercal \boldsymbol{\phi}(\mathbf{x}'), \tag{6.60}$$

where

$$\boldsymbol{\phi}(\mathbf{x}) = \mathbf{M}\mathbf{x}. \tag{6.61}$$

Therefore, k is a valid kernel.

6.9

Let

$$\begin{aligned} k_a(\mathbf{x}_a, \mathbf{x}'_a) &= \boldsymbol{\phi}_a(\mathbf{x}_a)^\intercal \boldsymbol{\phi}_a(\mathbf{x}'_a), \\ k_b(\mathbf{x}_b, \mathbf{x}'_b) &= \boldsymbol{\phi}_b(\mathbf{x}_b)^\intercal \boldsymbol{\phi}_b(\mathbf{x}'_b). \end{aligned} \tag{6.62}$$

(a)

Let

$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b), \tag{6.63}$$

where

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix}. \tag{6.64}$$

The right hand side can be written as

$$\boldsymbol{\phi}_a(\mathbf{x}_a)^\intercal \boldsymbol{\phi}_a(\mathbf{x}'_a) + \boldsymbol{\phi}_b(\mathbf{x}_b)^\intercal \boldsymbol{\phi}_b(\mathbf{x}'_b) = \boldsymbol{\phi}(\mathbf{x})^\intercal \boldsymbol{\phi}(\mathbf{x}'), \tag{6.65}$$

where

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} \boldsymbol{\phi}_a(\mathbf{x}_a) \\ \boldsymbol{\phi}_b(\mathbf{x}_b) \end{bmatrix}. \tag{6.66}$$

Therefore, k is a valid kernel.

(b)

Let

$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a) k_b(\mathbf{x}_b, \mathbf{x}'_b), \tag{6.67}$$

where

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix}. \tag{6.68}$$

Then,

$$\ln k(\mathbf{x}, \mathbf{x}') = \ln k_a(\mathbf{x}_a, \mathbf{x}'_a) + \ln k_b(\mathbf{x}_b, \mathbf{x}'_b). \tag{6.69}$$

By (a) and 6.6(b), the right hand side is a valid kernel. Then, $\ln k$ is a valid kernel. Therefore, by 6.6(b), k is a valid kernel.

6.10 (Incomplete)

Let

$$k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x}) f(\mathbf{x}'). \tag{6.70}$$

6.11

Let

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right). \tag{6.71}$$

The right hand side can be written as

$$\exp\left(-\frac{\mathbf{x}^\intercal \mathbf{x}}{2\sigma^2}\right) \exp\left(\frac{\mathbf{x}^\intercal \mathbf{x}'}{\sigma^2}\right) \exp\left(-\frac{\mathbf{x}'^\intercal \mathbf{x}'}{2\sigma^2}\right). \tag{6.72}$$

We have

$$\exp\left(\frac{\mathbf{x}^\intercal \mathbf{x}'}{\sigma^2}\right) = \sum_{j=0}^{\infty} q_j(\mathbf{x}, \mathbf{x}'), \tag{6.73}$$

where

$$q_j(\mathbf{x}, \mathbf{x}') = \frac{1}{j!}\left(\frac{\mathbf{x}^\intercal \mathbf{x}'}{\sigma^2}\right)^j. \tag{6.74}$$

By 6.6(a), q_j is a valid kernel. Then, there exists $\boldsymbol{\psi}_j$ such that

$$q_j(\mathbf{x}, \mathbf{x}') = \boldsymbol{\psi}_j(\mathbf{x})^\intercal \boldsymbol{\psi}_j(\mathbf{x}'). \tag{6.75}$$

Then,

$$\exp\left(\frac{\mathbf{x}^\intercal \mathbf{x}'}{\sigma^2}\right) = \sum_{j=0}^{\infty} \boldsymbol{\psi}_j(\mathbf{x})^\intercal \boldsymbol{\psi}_j(\mathbf{x}'). \tag{6.76}$$

The right hand side can be written as $\boldsymbol{\phi}(\mathbf{x})^\intercal \boldsymbol{\phi}(\mathbf{x}')$, where

$$\boldsymbol{\phi} = \begin{bmatrix} \boldsymbol{\psi}_1 \\ \vdots \\ \boldsymbol{\psi}_j \\ \vdots \end{bmatrix}. \tag{6.77}$$

Therefore, k can be written as the inner product of an infinite-dimensional feature vector.

6.12

Let $A_1, \cdots, A_{2^{|D|}}$ are all the subsets of D ordered in the alphabetical order where $|.|$ is the number of elements in $(.)$. Let

$$k(A_m, A_{m'}) = 2^{|A_m \cap A_{m'}|}. \tag{6.78}$$

Let $\boldsymbol{\phi}$ be a vector such that

$$\phi_m(A) = \begin{cases} 1, \text{if } A_m \subseteq A, \\ 0, \text{otherwise.} \end{cases} \tag{6.79}$$

If

$$|A_m \cap A_{m'}| = 0, \tag{6.80}$$

then

$$k(A_m, A_{m'}) = 1. \tag{6.81}$$

The right hand side can be written as

$$\boldsymbol{\phi}(A_m)^\intercal \boldsymbol{\phi}(A_{m'}). \tag{6.82}$$

Let us assume that if

$$|A_m \cap A_{m'}| = n, \tag{6.83}$$

then

$$k(A_m, A_{m'}) = \boldsymbol{\phi}(A_m)^\intercal \boldsymbol{\phi}(A_{m'}). \tag{6.84}$$

Let

$$A_{m''} = A_{m'} \cup \{x\}, \tag{6.85}$$

where x is an element such that

$$x \in A_m - A_{m'}. \tag{6.86}$$

Then,

$$|A_m \cap A_{m''}| = n + 1, \tag{6.87}$$

so that

$$k(A_m, A_{m''}) = 2^{n+1}. \tag{6.88}$$

We have

$$\boldsymbol{\phi}(A_m)^\intercal \boldsymbol{\phi}(A_{m''}) = \boldsymbol{\phi}(A_m)^\intercal \boldsymbol{\phi}(A_{m'}) + \boldsymbol{\phi}(A_m)^\intercal \left(\boldsymbol{\phi}(A_{m''}) - \boldsymbol{\phi}(A_{m'})\right). \tag{6.89}$$

By the assumption, the first term of the right hand side is 2^n. By the assumption, $\boldsymbol{\phi}(A_m)$ and $\boldsymbol{\phi}(A_{m'})$ have a set of 2^n 1s in common. Then, $\boldsymbol{\phi}(A_m)$ and $\boldsymbol{\phi}(A_{m''}) - \boldsymbol{\phi}(A_{m'})$ have another set of 2^n 1s in common. Then, the second term of the right hand side is 2^n. Then,

$$\boldsymbol{\phi}(A_m)^\intercal \boldsymbol{\phi}(A_{m''}) = 2^{n+1}, \tag{6.90}$$

so that

$$k(A_m, A_{m''}) = \boldsymbol{\phi}(A_m)^\intercal \boldsymbol{\phi}(A_{m''}). \tag{6.91}$$

Therefore, the assumption is proved by induction on n.

6.13

Let

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^\intercal \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}'), \tag{6.92}$$

where

$$\begin{aligned} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) &= \nabla_{\boldsymbol{\theta}} \ln p(\mathbf{x}|\boldsymbol{\theta}), \\ \mathbf{F} &= \mathrm{E}_{\mathbf{x}} \left(\mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^\intercal \right). \end{aligned} \tag{6.93}$$

Let

$$k_{\boldsymbol{\psi}}(\mathbf{x}, \mathbf{x}') = \mathbf{g}_{\boldsymbol{\psi}}(\boldsymbol{\theta}, \mathbf{x})^\intercal \mathbf{F}_{\boldsymbol{\psi}}^{-1} \mathbf{g}_{\boldsymbol{\psi}}(\boldsymbol{\theta}, \mathbf{x}'), \tag{6.94}$$

where $\boldsymbol{\psi}$ is invertible and differentiable and

$$\begin{aligned} \mathbf{g}_{\boldsymbol{\psi}}(\boldsymbol{\theta}, \mathbf{x}) &= \nabla_{\boldsymbol{\psi}(\boldsymbol{\theta})} \ln p(\mathbf{x}|\boldsymbol{\theta}), \\ \mathbf{F}_{\boldsymbol{\psi}} &= \mathrm{E}_{\mathbf{x}} \left(\mathbf{g}_{\boldsymbol{\psi}}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}_{\boldsymbol{\psi}}(\boldsymbol{\theta}, \mathbf{x})^\intercal \right). \end{aligned} \tag{6.95}$$

We have

$$\mathbf{g}_{\boldsymbol{\psi}}(\boldsymbol{\theta}, \mathbf{x}) = \frac{\partial \boldsymbol{\theta}}{\partial \boldsymbol{\psi}(\boldsymbol{\theta})} \nabla_{\boldsymbol{\theta}} \ln p(\mathbf{x}|\boldsymbol{\theta}). \tag{6.96}$$

Then,

$$\mathbf{g}_{\boldsymbol{\psi}}(\boldsymbol{\theta}, \mathbf{x}) = \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}). \tag{6.97}$$

We have

$$\mathbf{F}_{\boldsymbol{\psi}} = \int \mathbf{g}_{\boldsymbol{\psi}}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}_{\boldsymbol{\psi}}(\boldsymbol{\theta}, \mathbf{x})^\intercal p(\mathbf{x}) d\mathbf{x}. \tag{6.98}$$

The right hand side can be written as

$$\begin{aligned} &\int \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^\intercal \left(\left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \right)^\intercal p(\mathbf{x}) d\mathbf{x} \\ &= \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \left(\int \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^\intercal p(\mathbf{x}) d\mathbf{x} \right) \left(\left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \right)^\intercal. \end{aligned} \tag{6.99}$$

Then,

$$\mathbf{F}_{\boldsymbol{\psi}} = \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \mathbf{F} \left(\left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \right)^\intercal. \tag{6.100}$$

Then,

$$\begin{aligned} & k_{\boldsymbol{\psi}}(\mathbf{x}, \mathbf{x}') \\ =& \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^{\intercal} \left(\left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \right)^{\intercal} \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{\intercal} \mathbf{F}^{-1} \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right) \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}'). \end{aligned} \tag{6.101}$$

The right hand side can be written as

$$\mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^{\intercal} \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}'). \tag{6.102}$$

Therefore,

$$k_{\boldsymbol{\psi}}(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}'). \tag{6.103}$$

6.14

Let $\mathbf{x}$ be a variable such that

$$p(\mathbf{x}|\boldsymbol{\mu}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{S}). \tag{6.104}$$

Let

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{g}(\boldsymbol{\mu}, \mathbf{x})^{\intercal} \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\mu}, \mathbf{x}'), \tag{6.105}$$

where

$$\begin{aligned} \mathbf{g}(\boldsymbol{\mu}, \mathbf{x}) &= \nabla_{\boldsymbol{\mu}} \ln p(\mathbf{x}|\boldsymbol{\mu}), \\ \mathbf{F} &= \mathrm{E}_{\mathbf{x}} \left(\mathbf{g}(\boldsymbol{\mu}, \mathbf{x}) \mathbf{g}(\boldsymbol{\mu}, \mathbf{x})^{\intercal} \right). \end{aligned} \tag{6.106}$$

We have

$$\mathbf{g}(\boldsymbol{\mu}, \mathbf{x}) = -\mathbf{S}^{-1}(\mathbf{x} - \boldsymbol{\mu}). \tag{6.107}$$

Then,

$$\mathbf{F} = \int \mathbf{S}^{-1}(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^{\intercal} \mathbf{S}^{-1} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{S}) d\mathbf{x}. \tag{6.108}$$

The right hand side can be written as

$$\mathbf{S}^{-1} \left(\int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^{\intercal} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{S}) d\mathbf{x} \right) \mathbf{S}^{-1} = \mathbf{S}^{-1}. \tag{6.109}$$

Then,

$$\mathbf{F} = \mathbf{S}^{-1}, \tag{6.110}$$

so that

$$\mathbf{g}(\boldsymbol{\mu}, \mathbf{x})^{\intercal} \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\mu}, \mathbf{x}') = (\mathbf{x} - \boldsymbol{\mu})^{\intercal} \mathbf{S}^{-1} (\mathbf{x} - \boldsymbol{\mu}). \tag{6.111}$$

Therefore,

$$k(\mathbf{x}, \mathbf{x}') = (\mathbf{x} - \boldsymbol{\mu})^{\intercal} \mathbf{S}^{-1} (\mathbf{x} - \boldsymbol{\mu}). \tag{6.112}$$

6.15

Let k be a positive semidefinite kernel function. Then,

$$k(x,x)k(x',x') - k(x,x')^2 = \det \mathbf{K}, \tag{6.113}$$

where

$$\mathbf{K} = \begin{bmatrix} k(x,x) & k(x,x') \\ k(x,x') & k(x',x') \end{bmatrix}. \tag{6.114}$$

Since $\mathbf{K}$ is positive semidefinite,

$$\det \mathbf{K} \geq 0. \tag{6.115}$$

Therefore,

$$k(x,x')^2 \leq k(x,x)k(x',x'). \tag{6.116}$$

6.16 (Incomplete)

Let

$$J(\mathbf{w}) = f\left(\mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_1), \cdots, \mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_N)\right) + g\left(\mathbf{w}^\intercal \mathbf{w}\right), \tag{6.117}$$

where g is a monotonically increasing function. Setting the derivative with respect to $\mathbf{w}$ to zero gives

$$\mathbf{0} = \sum_{n=1}^{N} \frac{\partial f}{\partial \mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n)} \boldsymbol{\phi}(\mathbf{x}_n) + 2g'\left(\mathbf{w}^\intercal \mathbf{w}\right) \mathbf{w}. \tag{6.118}$$

Therefore,

$$\operatorname*{argmin}_{\mathbf{w}} J(\mathbf{w}) = -\frac{1}{2g'\left(\mathbf{w}^\intercal \mathbf{w}\right)} \sum_{n=1}^{N} \frac{\partial f}{\partial \mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n)} \boldsymbol{\phi}(\mathbf{x}_n). \tag{6.119}$$

6.17

Let

$$E = \frac{1}{2} \sum_{n=1}^{N} \int \left(y(\mathbf{x}_n + \boldsymbol{\xi}) - t_n\right)^2 p(\boldsymbol{\xi}) d\boldsymbol{\xi}. \tag{6.120}$$

By the transformation

$$\mathbf{z} = \mathbf{x}_n + \boldsymbol{\xi}, \tag{6.121}$$

we have

$$E = \frac{1}{2}\sum_{n=1}^{N}\int \left(y(\mathbf{z}) - t_n\right)^2 p(\mathbf{z} - \mathbf{x}_n)d\mathbf{z}. \tag{6.122}$$

Setting the variation with respect to y to zero gives

$$0 = \sum_{n=1}^{N}\left(y(\mathbf{z}) - t_n\right)p(\mathbf{z} - \mathbf{x}_n). \tag{6.123}$$

The right hand side can be written as

$$y(\mathbf{z})\sum_{n=1}^{N} p(\mathbf{z} - \mathbf{x}_n) - \sum_{n=1}^{N} t_n p(\mathbf{z} - \mathbf{x}_n). \tag{6.124}$$

Therefore,

$$y(\mathbf{x}) = \sum_{n=1}^{N} t_n k(\mathbf{x}, \mathbf{x}_n), \tag{6.125}$$

where

$$k(\mathbf{x}, \mathbf{x}_n) = \frac{p(\mathbf{x} - \mathbf{x}_n)}{\sum_{n=1}^{N} p(\mathbf{x} - \mathbf{x}_n)}. \tag{6.126}$$

6.18

Let x be a variable such that

$$p(x, t) = \frac{1}{N}\sum_{n=1}^{N} f(x - x_n, t - t_n), \tag{6.127}$$

where

$$f(x, t) = \mathcal{N}\left(x|0, \sigma^2\right)\mathcal{N}\left(t|0, \sigma^2\right). \tag{6.128}$$

(a)

By the Bayes' theorem,

$$p(t|x) = \frac{p(x, t)}{p(x)}. \tag{6.129}$$

By marginalisation,

$$p(x) = \int p(x, t)dt. \tag{6.130}$$

The right hand side can be written as

$$\begin{aligned}&\frac{1}{N}\sum_{n=1}^{N}\mathcal{N}\left(x-x_n|0,\sigma^2\right)\int\mathcal{N}\left(t-t_n|0,\sigma^2\right)dt\\=&\frac{1}{N}\sum_{n=1}^{N}\mathcal{N}\left(x-x_n|0,\sigma^2\right).\end{aligned}\tag{6.131}$$

Then,

$$p(t|x)=\frac{\frac{1}{N}\sum_{n=1}^{N}\mathcal{N}\left(x-x_n|0,\sigma^2\right)\mathcal{N}\left(t-t_n|0,\sigma^2\right)}{\frac{1}{N}\sum_{n=1}^{N}\mathcal{N}\left(x-x_n|0,\sigma^2\right)}.\tag{6.132}$$

Therefore,

$$p(t|x)=\sum_{n=1}^{N}k(x,x_n)\mathcal{N}\left(t-t_n|0,\sigma^2\right),\tag{6.133}$$

where

$$k(x,x_n)=\frac{\mathcal{N}\left(x-x_n|0,\sigma^2\right)}{\sum_{n=1}^{N}\mathcal{N}\left(x-x_n|0,\sigma^2\right)}.\tag{6.134}$$

(b)

We have

$$\mathrm{E}(t|x)=\int tp(t|x)dt.\tag{6.135}$$

By (a), the right hand side can be written as

$$\sum_{n=1}^{N}k(x,x_n)\int t\mathcal{N}\left(t-t_n|0,\sigma^2\right)dt.\tag{6.136}$$

By the transformation

$$t'=t-t_n,\tag{6.137}$$

the integral can be written as

$$\int(t'+t_n)\mathcal{N}\left(t'|0,\sigma^2\right)dt'=\int t'\mathcal{N}\left(t'|0,\sigma^2\right)dt'+t_n\int\mathcal{N}\left(t'|0,\sigma^2\right)dt'.\tag{6.138}$$

The right hand side can be written as t_n. Therefore,

$$\mathrm{E}(t|x)=\sum_{n=1}^{N}k(x,x_n)t_n.\tag{6.139}$$

(c)

We have

$$\mathrm{var}(t|x) = \int (t - \mathrm{E}(t|x))^2 \, p(t|x) dt. \tag{6.140}$$

By (a) and (b), the right hand side can be written as

$$\sum_{n=1}^{N} k(x, x_n) \int \left(t - \sum_{n=1}^{N} k(x, x_n) t_n \right)^2 \mathcal{N}\left(t - t_n | 0, \sigma^2\right) dt. \tag{6.141}$$

By the transformation

$$t' = t - t_n, \tag{6.142}$$

the integral can be written as

$$\begin{aligned} &\int \left(t' + t_n - \sum_{n=1}^{N} k(x, x_n) t_n \right)^2 \mathcal{N}\left(t' | 0, \sigma^2\right) dt' \\ &= \int t'^2 \mathcal{N}\left(t' | 0, \sigma^2\right) dt' + 2 \left(t_n - \sum_{n=1}^{N} k(x, x_n) t_n \right) \int t' \mathcal{N}\left(t' | 0, \sigma^2\right) dt' \\ &\quad + \left(t_n - \sum_{n=1}^{N} k(x, x_n) t_n \right)^2 \int \mathcal{N}\left(t' | 0, \sigma^2\right) dt'. \end{aligned} \tag{6.143}$$

The right hand side can be written as

$$\sigma^2 + \left(t_n - \sum_{n=1}^{N} k(x, x_n) t_n \right)^2. \tag{6.144}$$

Then,

$$\mathrm{var}(t|x) = \sum_{n=1}^{N} k(x, x_n) \left(\sigma^2 + \left(t_n - \sum_{n'=1}^{N} k(x, x_{n'}) t_{n'} \right)^2 \right). \tag{6.145}$$

Therefore,

$$\mathrm{var}(t|x) = \sigma^2 + \sum_{n=1}^{N} k(x, x_n) \left(t_n - \sum_{n'=1}^{N} k(x, x_{n'}) t_{n'} \right)^2. \tag{6.146}$$

6.19

Let

$$E = \frac{1}{2}\sum_{n=1}^{N}\int \left(y(\mathbf{x}_n - \boldsymbol{\xi}_n) - t_n\right)^2 p(\boldsymbol{\xi}_n)d\boldsymbol{\xi}_n. \tag{6.147}$$

By the transformation

$$\mathbf{z} = \mathbf{x}_n - \boldsymbol{\xi}_n, \tag{6.148}$$

we have

$$E = \frac{1}{2}\sum_{n=1}^{N}\int \left(y(\mathbf{z}) - t_n\right)^2 p(\mathbf{x}_n - \mathbf{z})d\mathbf{z}. \tag{6.149}$$

Setting the variation with respect to y to zero gives

$$0 = \sum_{n=1}^{N}\left(y(\mathbf{z}) - t_n\right) p(\mathbf{x}_n - \mathbf{z}). \tag{6.150}$$

The right hand side can be written as

$$y(\mathbf{z})\sum_{n=1}^{N} p(\mathbf{x}_n - \mathbf{z}) - \sum_{n=1}^{N} t_n p(\mathbf{x}_n - \mathbf{z}). \tag{6.151}$$

Therefore,

$$y(\mathbf{x}) = \sum_{n=1}^{N} t_n k(\mathbf{x}, \mathbf{x}_n), \tag{6.152}$$

where

$$k(\mathbf{x}, \mathbf{x}_n) = \frac{p(\mathbf{x}_n - \mathbf{x})}{\sum_{n=1}^{N} p(\mathbf{x}_n - \mathbf{x})}. \tag{6.153}$$

6.20

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(\mathbf{t}|\mathbf{y}) &= \mathcal{N}\left(\mathbf{t}|\mathbf{y}, \beta^{-1}\mathbf{I}\right), \\ p(\mathbf{y}) &= \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}), \end{aligned} \tag{6.154}$$

where

$$K_{nn'} = k(\mathbf{x}_n, \mathbf{x}_{n'}). \tag{6.155}$$

By the Bayes' theorem,

$$p(t_{N+1}|\mathbf{t})p(\mathbf{t}) = p(\mathbf{t}'), \tag{6.156}$$

where

$$\mathbf{t}' = \begin{bmatrix} \mathbf{t} \\ t_{N+1} \end{bmatrix}. \tag{6.157}$$

By marginalisation,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{y})p(\mathbf{y})d\mathbf{y}. \tag{6.158}$$

The logarighm of the integrand of the right hand side except the terms independent of $\mathbf{y}_N$ can be written as

$$\begin{aligned} &-\frac{\beta}{2}(\mathbf{t}-\mathbf{y})^\intercal(\mathbf{t}-\mathbf{y}) - \frac{1}{2}\mathbf{y}^\intercal\mathbf{K}^{-1}\mathbf{y} \\ =&-\frac{1}{2}\begin{bmatrix}\mathbf{y}\\ \mathbf{t}\end{bmatrix}^\intercal \begin{bmatrix}\beta\mathbf{I}+\mathbf{K}^{-1} & -\beta\mathbf{I} \\ -\beta\mathbf{I} & \beta\mathbf{I}\end{bmatrix}\begin{bmatrix}\mathbf{y}\\ \mathbf{t}\end{bmatrix}. \end{aligned} \tag{6.159}$$

By 2.24,

$$\begin{bmatrix}\beta\mathbf{I}+\mathbf{K}^{-1} & -\beta\mathbf{I} \\ -\beta\mathbf{I} & \beta\mathbf{I}\end{bmatrix}^{-1} = \begin{bmatrix}\mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K}+\beta^{-1}\mathbf{I}\end{bmatrix}. \tag{6.160}$$

Then,

$$p(\mathbf{t}) = \mathcal{N}(\mathbf{t}|\mathbf{0}, \mathbf{C}), \tag{6.161}$$

where

$$\mathbf{C} = \mathbf{K} + \beta^{-1}\mathbf{I}. \tag{6.162}$$

Then,

$$p(\mathbf{t}') = \mathcal{N}(\mathbf{t}'|\mathbf{0}, \mathbf{C}'), \tag{6.163}$$

where

$$\mathbf{C}' = \begin{bmatrix}\mathbf{C} & \mathbf{k} \\ \mathbf{k}^\intercal & c\end{bmatrix}, \tag{6.164}$$

where

$$\begin{aligned} k_n &= k(\mathbf{x}_n, \mathbf{x}_{N+1}), \\ c &= k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}) + \beta^{-1}. \end{aligned} \tag{6.165}$$

By 2.24,

$$\begin{bmatrix}c & \mathbf{k}^\intercal \\ \mathbf{k} & \mathbf{C}\end{bmatrix}^{-1} = \begin{bmatrix}s^{-1} & -s^{-1}\mathbf{k}^\intercal\mathbf{C}^{-1} \\ -s^{-1}\mathbf{C}^{-1}\mathbf{k} & \mathbf{C}^{-1}+s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^\intercal\mathbf{C}^{-1}\end{bmatrix}, \tag{6.166}$$

where

$$s = c - \mathbf{k}^\intercal \mathbf{C}^{-1} \mathbf{k}. \tag{6.167}$$

Therefore,

$$p(t_{N+1}|\mathbf{t}) = \mathcal{N}\left(t_{N+1}|m, s\right), \tag{6.168}$$

where

$$m = \mathbf{k}^\intercal \mathbf{C}^{-1} \mathbf{t}. \tag{6.169}$$

6.21

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(\mathbf{t}|\mathbf{y}) &= \mathcal{N}\left(\mathbf{t}|\mathbf{y}, \beta^{-1}\mathbf{I}\right), \\ p(\mathbf{y}) &= \mathcal{N}\left(\mathbf{y}|\mathbf{0}, \mathbf{\Phi}\mathbf{\Phi}^\intercal\right). \end{aligned} \tag{6.170}$$

By 3.10,

$$p(t_{N+1}|\mathbf{t}) = \mathcal{N}\left(t_{N+1}|m, s\right), \tag{6.171}$$

where

$$\begin{aligned} m &= \beta \boldsymbol{\phi}_{N+1}^\intercal \left(\mathbf{I} + \beta \mathbf{\Phi}^\intercal \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^\intercal \mathbf{t}, \\ s &= \beta^{-1} + \boldsymbol{\phi}_{N+1}^\intercal \left(\mathbf{I} + \beta \mathbf{\Phi}^\intercal \mathbf{\Phi}\right)^{-1} \boldsymbol{\phi}_{N+1}. \end{aligned} \tag{6.172}$$

By 2.26,

$$\left(\mathbf{I} + \beta \mathbf{\Phi}^\intercal \mathbf{\Phi}\right)^{-1} = \mathbf{I} - \mathbf{\Phi}^\intercal \mathbf{C}^{-1} \mathbf{\Phi}, \tag{6.173}$$

where

$$\mathbf{C} = \beta^{-1}\mathbf{I} + \mathbf{\Phi}\mathbf{\Phi}^\intercal. \tag{6.174}$$

Then,

$$m = \beta \boldsymbol{\phi}_{N+1}^\intercal \left(\mathbf{I} - \mathbf{\Phi}^\intercal \mathbf{C}^{-1} \mathbf{\Phi}\right) \mathbf{\Phi}^\intercal \mathbf{t}. \tag{6.175}$$

The right hand side can be written as

$$\beta \left(\boldsymbol{\phi}_{N+1}^\intercal \mathbf{\Phi}^\intercal - \boldsymbol{\phi}_{N+1}^\intercal \mathbf{\Phi}^\intercal \mathbf{C}^{-1} \mathbf{\Phi}\mathbf{\Phi}^\intercal\right) \mathbf{t} = \beta \boldsymbol{\phi}_{N+1}^\intercal \mathbf{\Phi}^\intercal \mathbf{C}^{-1} \left(\mathbf{C} - \mathbf{\Phi}\mathbf{\Phi}^\intercal\right) \mathbf{t}. \tag{6.176}$$

The right hand side can be written as

$$\beta \mathbf{k}^\intercal \mathbf{C}^{-1} \beta^{-1} \mathbf{I} \mathbf{t} = \mathbf{k}^\intercal \mathbf{C}^{-1} \mathbf{t}, \tag{6.177}$$

where

$$\mathbf{k} = \mathbf{\Phi} \boldsymbol{\phi}_{N+1}. \tag{6.178}$$

Similarly,

$$s = \beta^{-1} + \boldsymbol{\phi}_{N+1}^{\intercal} \left(\mathbf{I} - \boldsymbol{\Phi}^{\intercal} \mathbf{C}^{-1} \boldsymbol{\Phi} \right) \boldsymbol{\phi}_{N+1}. \tag{6.179}$$

The right hand side can be written as

$$\beta^{-1} + \boldsymbol{\phi}_{N+1}^{\intercal} \boldsymbol{\phi}_{N+1} - \boldsymbol{\phi}_{N+1}^{\intercal} \boldsymbol{\Phi}^{\intercal} \mathbf{C}^{-1} \boldsymbol{\Phi} \boldsymbol{\phi}_{N+1} = c - \mathbf{k}^{\intercal} \mathbf{C}^{-1} \mathbf{k}, \tag{6.180}$$

where

$$c = \beta^{-1} + \boldsymbol{\phi}_{N+1}^{\intercal} \boldsymbol{\phi}_{N+1}. \tag{6.181}$$

Therefore,

$$\begin{aligned} m &= \mathbf{k}^{\intercal} \mathbf{C}^{-1} \mathbf{t}, \\ s &= c - \mathbf{k}^{\intercal} \mathbf{C}^{-1} \mathbf{k}. \end{aligned} \tag{6.182}$$

6.22

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(\mathbf{t}|\mathbf{y}) &= \mathcal{N}\left(\mathbf{t}|\mathbf{y}, \beta^{-1}\mathbf{I}\right), \\ p(\mathbf{y}) &= \mathcal{N}\left(\mathbf{y}|\mathbf{0}, \mathbf{K}\right), \end{aligned} \tag{6.183}$$

where

$$K_{nn'} = k(\mathbf{x}_n, \mathbf{x}_{n'}). \tag{6.184}$$

(a)

By the Bayes' theorem,

$$p(t_{N+1}, \cdots, t_{N+L}|\mathbf{t}) p(\mathbf{t}) = p(\mathbf{t}'), \tag{6.185}$$

where

$$\mathbf{t}' = \begin{bmatrix} \mathbf{t} \\ t_{N+1} \\ \vdots \\ t_{N+L} \end{bmatrix}. \tag{6.186}$$

By 6.20,

$$p(\mathbf{t}) = \mathcal{N}\left(\mathbf{t}|\mathbf{0}, \mathbf{C}\right), \tag{6.187}$$

where

$$\mathbf{C} = \beta^{-1}\mathbf{I} + \mathbf{K}. \tag{6.188}$$

Let

$$\begin{aligned} K'_{nl} &= k(\mathbf{x}_n, \mathbf{x}_{N+l}), \\ \Gamma_{ll'} &= \beta^{-1} I_{ll'} + k(\mathbf{x}_{N+l}, \mathbf{x}_{N+l'}). \end{aligned} \tag{6.189}$$

Then,

$$p(\mathbf{t}') = \mathcal{N}\left(\mathbf{t}' | \mathbf{0}, \mathbf{C}'\right), \tag{6.190}$$

where

$$\mathbf{C}' = \begin{bmatrix} \mathbf{C} & \mathbf{K}' \\ \mathbf{K}'^{\intercal} & \mathbf{\Gamma} \end{bmatrix}. \tag{6.191}$$

By 2.24,

$$\begin{bmatrix} \mathbf{\Gamma} & \mathbf{K}'^{\intercal} \\ \mathbf{K}' & \mathbf{C} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{S}^{-1} & -\mathbf{S}^{-1}\mathbf{K}'^{\intercal}\mathbf{C}^{-1} \\ -\mathbf{C}^{-1}\mathbf{K}'\mathbf{S}^{-1} & \mathbf{C}^{-1} + \mathbf{C}^{-1}\mathbf{K}'\mathbf{S}^{-1}\mathbf{K}'^{\intercal}\mathbf{C}^{-1} \end{bmatrix}, \tag{6.192}$$

where

$$\mathbf{S} = \mathbf{\Gamma} - \mathbf{K}'^{\intercal}\mathbf{C}^{-1}\mathbf{K}'. \tag{6.193}$$

Therefore,

$$p(t_{N+1}, \cdots, t_{N+L} | \mathbf{t}_N) = \mathcal{N}\left(t_{N+1}, \cdots, t_{N+L} | \mathbf{m}, \mathbf{S}\right), \tag{6.194}$$

where

$$\mathbf{m} = \mathbf{K}'^{\intercal}\mathbf{C}^{-1}\mathbf{t}. \tag{6.195}$$

(b)

Let

$$\begin{aligned} k_n &= k(\mathbf{x}_n, \mathbf{x}_{N+1}), \\ c &= \beta^{-1} + k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}). \end{aligned} \tag{6.196}$$

By (a),

$$p(t_{N+1} | \mathbf{t}) = \mathcal{N}\left(t_{N+1} | m, s\right), \tag{6.197}$$

where

$$\begin{aligned} m &= \mathbf{k}^{\intercal}\mathbf{C}^{-1}\mathbf{t}, \\ s &= c - \mathbf{k}^{\intercal}\mathbf{C}^{-1}\mathbf{k}. \end{aligned} \tag{6.198}$$

6.23

Let $\mathbf{t}_1, \cdots, \mathbf{t}_N$ be variables such that

$$\begin{aligned} p(\mathbf{t}_n|\mathbf{y}_n) &= \mathcal{N}\left(\mathbf{t}_n|\mathbf{y}_n, \beta^{-1}\mathbf{I}\right), \\ p(\mathbf{Y}) &= \mathcal{N}\left(\mathbf{Y}|\mathbf{O}, \mathbf{K}\right), \end{aligned} \tag{6.199}$$

where

$$K_{nn'} = k(\mathbf{x}_n, \mathbf{x}_{n'}). \tag{6.200}$$

By the Bayes' theorem,

$$p(\mathbf{t}_{N+1}|\mathbf{T})p(\mathbf{T}) = p(\mathbf{T}'). \tag{6.201}$$

By marginalisation,

$$p(\mathbf{T}) = \int p(\mathbf{T}|\mathbf{Y})p(\mathbf{Y})d\mathbf{Y}. \tag{6.202}$$

The logarithm of the integrannd of the right hand side except the terms independent of $\mathbf{T}$ and $\mathbf{Y}$ can be written as

$$-\frac{\beta}{2}\sum_{n=1}^{N}\|\mathbf{t}_n - \mathbf{y}_n\|^2 - \frac{1}{2}\operatorname{tr}\left(\mathbf{Y}^\intercal\mathbf{K}^{-1}\mathbf{Y}\right) = -\frac{1}{2}\operatorname{tr}\mathbf{M}, \tag{6.203}$$

where

$$\mathbf{M} = \begin{bmatrix}\mathbf{Y}\\ \mathbf{T}\end{bmatrix}^\intercal \begin{bmatrix}\beta\mathbf{I} + \mathbf{K}^{-1} & -\beta\mathbf{I}\\ -\beta\mathbf{I} & \beta\mathbf{I}\end{bmatrix}\begin{bmatrix}\mathbf{Y}\\ \mathbf{T}\end{bmatrix}. \tag{6.204}$$

By 2.24,

$$\begin{bmatrix}\beta\mathbf{I} + \mathbf{K}^{-1} & -\beta\mathbf{I}\\ -\beta\mathbf{I} & \beta\mathbf{I}\end{bmatrix}^{-1} = \begin{bmatrix}\mathbf{K} & \mathbf{K}\\ \mathbf{K} & \beta^{-1}\mathbf{I} + \mathbf{K}\end{bmatrix}. \tag{6.205}$$

Then,

$$p(\mathbf{T}) = \mathcal{N}\left(\mathbf{T}|\mathbf{O}, \mathbf{C}\right), \tag{6.206}$$

where

$$\mathbf{C} = \beta^{-1}\mathbf{I} + \mathbf{K}. \tag{6.207}$$

Then,

$$p(\mathbf{T}') = \mathcal{N}\left(\mathbf{T}'|\mathbf{O}, \mathbf{C}'\right), \tag{6.208}$$

where

$$\mathbf{C}' = \begin{bmatrix}\mathbf{C} & \mathbf{k}\\ \mathbf{k}^\intercal & c\end{bmatrix}, \tag{6.209}$$

where

$$\begin{aligned} k_n &= k(\mathbf{x}_n, \mathbf{x}_{N+1}), \\ c &= \beta^{-1} + k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}). \end{aligned} \tag{6.210}$$

By 2.24,

$$\begin{bmatrix} c & \mathbf{k}^\intercal \\ \mathbf{k} & \mathbf{C} \end{bmatrix}^{-1} = \begin{bmatrix} s^{-1} & -s^{-1}\mathbf{k}^\intercal\mathbf{C}^{-1} \\ -s^{-1}\mathbf{C}^{-1}\mathbf{k} & \mathbf{C}^{-1} + s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^\intercal\mathbf{C}^{-1} \end{bmatrix}, \tag{6.211}$$

where

$$s = c - \mathbf{k}^\intercal\mathbf{C}^{-1}\mathbf{k}. \tag{6.212}$$

Therefore,

$$p(\mathbf{t}_{N+1}|\mathbf{T}) = \mathcal{N}\left(\mathbf{t}_{N+1}|\mathbf{m}, s\mathbf{I}\right), \tag{6.213}$$

where

$$\mathbf{m} = \mathbf{T}^\intercal\mathbf{C}^{-1}\mathbf{k}. \tag{6.214}$$

6.24

(a)

Let $\mathbf{M}$ be a $D \times D$ diagonal matrix such that $0 < M_{dd} < 1$. For any vector $\mathbf{v}$ in D dimensions,

$$\mathbf{v}^\intercal\mathbf{M}\mathbf{v} = \sum_{d=1}^{D}\sum_{d'=1}^{D} v_d M_{dd'} v_{d'}. \tag{6.215}$$

The right hand side can be written as

$$\sum_{d=1}^{D} M_{dd} v_d^2 > 0. \tag{6.216}$$

Therefore, $\mathbf{M}$ is positive definite.

(b)

Let $\mathbf{M}_1$ and $\mathbf{M}_2$ be $D \times D$ positive definite matrices. Then, for any vector $\mathbf{v}$ in D dimensions,

$$\begin{aligned} \mathbf{v}^\intercal\mathbf{M}_1\mathbf{v} > 0, \\ \mathbf{v}^\intercal\mathbf{M}_2\mathbf{v} > 0. \end{aligned} \tag{6.217}$$

Then,

$$\mathbf{v}^\intercal(\mathbf{M}_1 + \mathbf{M}_2)\mathbf{v} > 0. \tag{6.218}$$

Therefore, $\mathbf{M}_1 + \mathbf{M}_2$ is positive definite.

6.25

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|a_n) &= \sigma(a_n)^{t_n} \left(1 - \sigma(a_n)\right)^{1-t_n}, \\ p(\mathbf{a}) &= \mathcal{N}\left(\mathbf{a}|\mathbf{0}, \mathbf{C}\right), \end{aligned} \tag{6.219}$$

where

$$\begin{aligned} \sigma(a) &= \frac{1}{1 + \exp(-a)}, \\ C_{nn'} &= k(\mathbf{x}_n, \mathbf{x}_{n'}) + \nu I_{nn'}. \end{aligned} \tag{6.220}$$

(a)

By the Bayes' theorem,

$$p(\mathbf{a}|\mathbf{t})p(\mathbf{t}) = p(\mathbf{t}|\mathbf{a})p(\mathbf{a}). \tag{6.221}$$

The logarithm of the right hand side except the terms independent of $\mathbf{t}$ and $\mathbf{a}$ can be written as

$$\Psi(\mathbf{a}) = \sum_{n=1}^{N} \left(t_n \ln \sigma(a_n) + (1 - t_n) \ln\left(1 - \sigma(a_n)\right)\right) - \frac{1}{2}\mathbf{a}^\intercal \mathbf{C}^{-1}\mathbf{a}. \tag{6.222}$$

In order to maximise $p(\mathbf{a}|\mathbf{t})$ with respect to $\mathbf{a}$, Ψ needs to be maximised. We have

$$\frac{d}{da}\sigma(a) = \sigma(a)\left(1 - \sigma(a)\right). \tag{6.223}$$

Then,

$$\left(\nabla\Psi(\mathbf{a})\right)_n = \left(t_n\left(1 - \sigma(a_n)\right) - (1 - t_n)\sigma(a_n)\right) - \left(\mathbf{C}^{-1}\mathbf{a}\right)_n, \tag{6.224}$$

so that

$$\nabla\Psi(\mathbf{a}) = \mathbf{t} - \boldsymbol{\sigma} - \mathbf{C}^{-1}\mathbf{a}, \tag{6.225}$$

where

$$\sigma_n = \sigma(a_n). \tag{6.226}$$

Since $\boldsymbol{\sigma}$ non-linearly depends on $\mathbf{a}$, the Taylor series

$$\nabla\Psi(\mathbf{a}^{\text{new}}) = \nabla\Psi(\mathbf{a}) + \nabla\nabla\Psi(\mathbf{a})\left(\mathbf{a}^{\text{new}} - \mathbf{a}\right) + O\left(\|\mathbf{a} - \mathbf{a}^{\text{new}}\|^2\right). \tag{6.227}$$

is used to iteratively find $\mathbf{a}$ which maximises Ψ. Setting the left hand side to zero and neglecting the second order term of the right hand side gives

$$\mathbf{0} = \nabla\Psi(\mathbf{a}) + \nabla\nabla\Psi(\mathbf{a})\left(\mathbf{a}^{\text{new}} - \mathbf{a}\right). \tag{6.228}$$

Then,

$$\mathbf{a}^{\text{new}} = \mathbf{a} - \left(\nabla\nabla\Psi(\mathbf{a})\right)^{-1}\nabla\Psi(\mathbf{a}). \tag{6.229}$$

We have

$$\nabla\nabla\Psi(\mathbf{a}) = -\mathbf{W} - \mathbf{C}^{-1}, \tag{6.230}$$

where

$$W_{nn'} = \sigma(a_n)\left(1 - \sigma(a_n)\right) I_{nn'}. \tag{6.231}$$

Then, the right hand side can be written as

$$\mathbf{a}^{\text{new}} = \mathbf{a} + \left(\mathbf{W} + \mathbf{C}^{-1}\right)^{-1}\left(\mathbf{t} - \boldsymbol{\sigma} - \mathbf{C}^{-1}\mathbf{a}\right). \tag{6.232}$$

The right hand side can be written as

$$\begin{aligned} &\left(\mathbf{W} + \mathbf{C}^{-1}\right)^{-1}\left(\left(\mathbf{W} + \mathbf{C}^{-1}\right)\mathbf{a} + \mathbf{t} - \boldsymbol{\sigma} - \mathbf{C}^{-1}\mathbf{a}\right) \\ =&\mathbf{C}\left(\mathbf{WC} + \mathbf{I}\right)^{-1}\left(\mathbf{Wa} + \mathbf{t} - \boldsymbol{\sigma}\right). \end{aligned} \tag{6.233}$$

Therefore,

$$\mathbf{a}^{\text{new}} = \mathbf{C}\left(\mathbf{WC} + \mathbf{I}\right)^{-1}\left(\mathbf{Wa} + \mathbf{t} - \boldsymbol{\sigma}\right). \tag{6.234}$$

(b)

Let $\mathbf{a}_{\text{MAP}}$ be a stationary point of $p(\mathbf{a}|\mathbf{t})$ which is found by the iterative process given in (a). We have the Taylor series

$$\begin{aligned} \Psi(\mathbf{a}) =&\Psi(\mathbf{a}_{\text{MAP}}) + \nabla\Psi(\mathbf{a}_{\text{MAP}})(\mathbf{a} - \mathbf{a}_{\text{MAP}}) \\ &+ \frac{1}{2}(\mathbf{a} - \mathbf{a}_{\text{MAP}})^{\intercal}\nabla\nabla\Psi(\mathbf{a}_{\text{MAP}})(\mathbf{a} - \mathbf{a}_{\text{MAP}}) + O\left(\|\mathbf{a} - \mathbf{a}_{\text{MAP}}\|^3\right). \end{aligned} \tag{6.235}$$

Then,

$$\Psi(\mathbf{a}) \simeq \Psi(\mathbf{a}_{\text{MAP}}) - \frac{1}{2}(\mathbf{a} - \mathbf{a}_{\text{MAP}})^{\intercal}\mathbf{H}(\mathbf{a} - \mathbf{a}_{\text{MAP}}), \tag{6.236}$$

where

$$\mathbf{H} = \mathbf{W}\,|_{\mathbf{a}=\mathbf{a}_{\text{MAP}}} + \mathbf{C}^{-1}. \tag{6.237}$$

Therefore,

$$p(\mathbf{a}|\mathbf{t}) \simeq \mathcal{N}\left(\mathbf{a}|\mathbf{a}_{\text{MAP}}, \mathbf{H}^{-1}\right). \tag{6.238}$$

(c)

By (a),

$$\mathbf{a}_{\mathrm{MAP}} = \mathbf{C}\left(\mathbf{WC} + \mathbf{I}\right)^{-1}\left(\mathbf{W}\mathbf{a}_{\mathrm{MAP}} + \mathbf{t} - \boldsymbol{\sigma}\right). \tag{6.239}$$

Then,

$$\left(\mathbf{WC} + \mathbf{I}\right)\mathbf{C}^{-1}\mathbf{a}_{\mathrm{MAP}} = \mathbf{W}\mathbf{a}_{\mathrm{MAP}} + \mathbf{t} - \boldsymbol{\sigma}. \tag{6.240}$$

Therefore,

$$\mathbf{a}_{\mathrm{MAP}} = \mathbf{C}(\mathbf{t} - \boldsymbol{\sigma}). \tag{6.241}$$

6.26

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|a_n) &= \sigma(a_n)^{t_n}\left(1 - \sigma(a_n)\right)^{1-t_n}, \\ p(\mathbf{a}) &= \mathcal{N}\left(\mathbf{a}|\mathbf{0}, \mathbf{C}\right), \end{aligned} \tag{6.242}$$

where

$$\begin{aligned} \sigma(a) &= \frac{1}{1 + \exp(-a)}, \\ C_{nn'} &= k(\mathbf{x}_n, \mathbf{x}_{n'}) + \nu I_{nn'}. \end{aligned} \tag{6.243}$$

By marginalisation,

$$p(a_{N+1}|\mathbf{t}) = \int p(a_{N+1}|\mathbf{a})p(\mathbf{a}|\mathbf{t})d\mathbf{a}. \tag{6.244}$$

Let

$$\begin{aligned} \mathbf{a}' &= \begin{bmatrix} \mathbf{a} \\ a_{N+1} \end{bmatrix}, \\ k_n &= k(\mathbf{x}_n, \mathbf{x}_{N+1}), \\ c &= k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}) + \nu. \end{aligned} \tag{6.245}$$

Then,

$$p(\mathbf{a}') = \mathcal{N}\left(\mathbf{a}'|\mathbf{0}, \mathbf{C}'\right), \tag{6.246}$$

where

$$\mathbf{C}' = \begin{bmatrix} \mathbf{C} & \mathbf{k} \\ \mathbf{k}^\intercal & c \end{bmatrix}. \tag{6.247}$$

By 2.24,

$$\begin{bmatrix} c & \mathbf{k}^\intercal \\ \mathbf{k} & \mathbf{C} \end{bmatrix}^{-1} = \begin{bmatrix} s^{-1} & -s^{-1}\mathbf{k}^\intercal\mathbf{C}^{-1} \\ -s^{-1}\mathbf{C}^{-1}\mathbf{k} & \mathbf{C}^{-1} + s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^\intercal\mathbf{C}^{-1} \end{bmatrix}, \tag{6.248}$$

where

$$s = c - \mathbf{k}^\intercal \mathbf{C}^{-1} \mathbf{k}. \tag{6.249}$$

Then,

$$p(a_{N+1}|\mathbf{a}) = \mathcal{N}\left(a_{N+1}|m, s\right), \tag{6.250}$$

where

$$m = \mathbf{k}^\intercal \mathbf{C}^{-1} \mathbf{a}. \tag{6.251}$$

By 6.25(b),

$$p(\mathbf{a}|\mathbf{t}) \simeq \mathcal{N}\left(\mathbf{a}|\mathbf{a}_{\mathrm{MAP}}, \mathbf{H}^{-1}\right), \tag{6.252}$$

where $\mathbf{a}_{\mathrm{MAP}}$ is a stationary point of $p(\mathbf{a}|\mathbf{t})$ and

$$\begin{aligned} \mathbf{H} &= \mathbf{W}\,|_{\mathbf{a}=\mathbf{a}_{\mathrm{MAP}}} + \mathbf{C}^{-1}, \\ W_{nn'} &= \sigma(a_n)\left(1 - \sigma(a_n)\right) I_{nn'}. \end{aligned} \tag{6.253}$$

Then, the logarithm of the integrand except the terms independent of $\mathbf{t}$ and $\mathbf{a}$ can be approximated as

$$\begin{aligned} &-\frac{1}{2s}\left(a_{N+1} - m\right)^2 - \frac{1}{2}\left(\mathbf{a} - \mathbf{a}_{\mathrm{MAP}}\right)^\intercal \mathbf{H}\left(\mathbf{a} - \mathbf{a}_{\mathrm{MAP}}\right) \\ =& -\frac{1}{2}\mathbf{a}'^\intercal \mathbf{M}\mathbf{a}' + \mathbf{a}'^\intercal \mathbf{v} - \frac{1}{2}\mathbf{a}_{\mathrm{MAP}}^\intercal \mathbf{H}\mathbf{a}_{\mathrm{MAP}}. \end{aligned} \tag{6.254}$$

where

$$\begin{aligned} \mathbf{M} &= \begin{bmatrix} \mathbf{H} + s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^\intercal \mathbf{C}^{-1} & -s^{-1}\mathbf{C}^{-1}\mathbf{k} \\ -s^{-1}\mathbf{k}^\intercal \mathbf{C}^{-1} & s^{-1} \end{bmatrix}, \\ \mathbf{v} &= \begin{bmatrix} \mathbf{H}\mathbf{a}_{\mathrm{MAP}} \\ 0 \end{bmatrix}. \end{aligned} \tag{6.255}$$

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{H}^{-1} & \mathbf{H}^{-1}\mathbf{C}^{-1}\mathbf{k} \\ \mathbf{k}^\intercal \mathbf{C}^{-1}\mathbf{H}^{-1} & s + \mathbf{k}^\intercal \mathbf{C}^{-1}\mathbf{H}^{-1}\mathbf{C}^{-1}\mathbf{k} \end{bmatrix}, \tag{6.256}$$

so that

$$\mathbf{M}^{-1}\mathbf{v} = \begin{bmatrix} \mathbf{a}_{\mathrm{MAP}} \\ \mathbf{k}^\intercal \mathbf{C}^{-1}\mathbf{a}_{\mathrm{MAP}} \end{bmatrix}. \tag{6.257}$$

Then,

$$p(a_{N+1}|\mathbf{t}) \simeq \mathcal{N}\left(a_{N+1}|\mu, \sigma^2\right), \tag{6.258}$$

where

$$\begin{aligned} \mu &= \mathbf{k}^\intercal \mathbf{C}^{-1}\mathbf{a}_{\mathrm{MAP}}, \\ \sigma^2 &= s + \mathbf{k}^\intercal \mathbf{C}^{-1}\mathbf{H}^{-1}\mathbf{C}^{-1}\mathbf{k}. \end{aligned} \tag{6.259}$$

By 6.25(c),

$$\mathbf{a}_{\text{MAP}} = \mathbf{C}(\mathbf{t} - \boldsymbol{\sigma}), \tag{6.260}$$

where

$$\sigma_n = \sigma(a_n). \tag{6.261}$$

Therefore,

$$\begin{aligned} \mu &= \mathbf{k}^\intercal(\mathbf{t} - \boldsymbol{\sigma}), \\ \sigma^2 &= c - \mathbf{k}^\intercal \mathbf{C}^{-1} \left(\mathbf{C} - \mathbf{H}^{-1}\right) \mathbf{C}^{-1}\mathbf{k}. \end{aligned} \tag{6.262}$$

6.27 (Incomplete)

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|a_n) &= \sigma(a_n)^{t_n} \left(1 - \sigma(a_n)\right)^{1-t_n}, \\ p(\mathbf{a}|\boldsymbol{\theta}) &= \mathcal{N}\left(\mathbf{a}|\mathbf{0}, \mathbf{C}\right), \end{aligned} \tag{6.263}$$

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)} \tag{6.264}$$

and $\mathbf{C}$ is dependent on $\boldsymbol{\theta}$ with M dimensions.

(a)

By marginalisation,

$$p(\mathbf{t}|\boldsymbol{\theta}) = \int p(\mathbf{t}|\mathbf{a}) p(\mathbf{a}|\boldsymbol{\theta}) d\mathbf{a}. \tag{6.265}$$

Let $\mathbf{a}_{\text{MAP}}$ be a stationary point of $p(\mathbf{a}|\mathbf{t})$ and

$$\Psi(\mathbf{a}) = \ln p(\mathbf{t}|\mathbf{a}) + \ln p(\mathbf{a}|\boldsymbol{\theta}). \tag{6.266}$$

By 6.25(b),

$$\Psi(\mathbf{a}) \simeq \Psi(\mathbf{a}_{\text{MAP}}) - \frac{1}{2} \left(\mathbf{a} - \mathbf{a}_{\text{MAP}}\right)^\intercal \mathbf{H} \left(\mathbf{a} - \mathbf{a}_{\text{MAP}}\right), \tag{6.267}$$

where

$$\begin{aligned} \mathbf{H} &= \mathbf{W} \left|_{\mathbf{a}=\mathbf{a}_{\text{MAP}}} + \mathbf{C}^{-1}, \right. \\ W_{nn'} &= \sigma(a_n) \left(1 - \sigma(a_n)\right) I_{nn'}. \end{aligned} \tag{6.268}$$

Therefore,

$$\ln p(\mathbf{t}|\boldsymbol{\theta}) \simeq \Psi(\mathbf{a}_{\text{MAP}}) + \frac{N}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \mathbf{H}). \tag{6.269}$$

(b)

We have

$$\frac{\partial \Psi(\mathbf{a}_{\mathrm{MAP}})}{\partial \theta_m} = \sum_{n=1}^{N} \sum_{n'=1}^{N} \frac{\partial \Psi(\mathbf{a}_{\mathrm{MAP}})}{\partial C_{nn'}} \frac{\partial C_{nn'}}{\partial \theta_m}. \tag{6.270}$$

The right hand side can be written as

$$\frac{1}{2} \operatorname{tr} \left(\mathbf{a}_{\mathrm{MAP}} \mathbf{a}_{\mathrm{MAP}}^{\intercal} \left(\mathbf{C}^{-1} \right)^2 \frac{\partial \mathbf{C}}{\partial \theta_m} \right). \tag{6.271}$$

We have

$$\frac{\partial \ln(\det \mathbf{H})}{\partial \theta_m} = \sum_{n=1}^{N} \sum_{n'=1}^{N} \frac{\partial \ln(\det \mathbf{H})}{\partial H_{nn'}} \frac{\partial H_{nn'}}{\partial \theta_m}. \tag{6.272}$$

By 3.21(a), the right hand side can be written as

$$\operatorname{tr} \left(\mathbf{H}^{-1} \frac{\partial \mathbf{C}^{-1}}{\partial \theta_m} \right). \tag{6.273}$$

Therefore,

$$\frac{\partial \ln p(\mathbf{t}|\boldsymbol{\theta})}{\partial \theta_m} \simeq \frac{1}{2} \operatorname{tr} \left(\mathbf{a}_{\mathrm{MAP}} \mathbf{a}_{\mathrm{MAP}}^{\intercal} \left(\mathbf{C}^{-1} \right)^2 \frac{\partial \mathbf{C}}{\partial \theta_m} - \mathbf{H}^{-1} \frac{\partial \mathbf{C}^{-1}}{\partial \theta_m} \right). \tag{6.274}$$

7 Sparse Kernel Machines

7.1 (Incomplete)

7.2

Let $t_1, \cdots, t_N$ be variables. In order to minimise $\|\mathbf{w}\|^2$ under the constraint

$$t_n \left(\mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n) + b\right) \geq \gamma, \tag{7.1}$$

for $\gamma > 0$, let

$$L = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n \left(t_n \left(\mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n) + b\right) - \gamma\right). \tag{7.2}$$

Setting the derivatives of L with respect to $\mathbf{w}$ and b to zero gives

$$\begin{aligned} \mathbf{0} &= \mathbf{w} - \sum_{n=1}^{N} a_n t_n \boldsymbol{\phi}(\mathbf{x}_n), \\ 0 &= -\sum_{n=1}^{N} a_n t_n. \end{aligned} \tag{7.3}$$

Therefore,

$$\begin{aligned} \mathbf{w} &= \sum_{n=1}^{N} a_n t_n \boldsymbol{\phi}(\mathbf{x}_n), \\ 0 &= \sum_{n=1}^{N} a_n t_n, \end{aligned} \tag{7.4}$$

which is independent of γ.

7.3 (Incomplete)

7.4 (Incomplete)

7.5 (Incomplete)

7.6

Let $t_1, \cdots, t_N$ be a variable such that

$$\begin{aligned} t_n &\in \{-1, 1\}, \\ p(t_n|y_n) &= \sigma(y_n)^{\frac{1+t_n}{2}} \left(1 - \sigma(y_n)\right)^{\frac{1-t_n}{2}}, \end{aligned} \tag{7.5}$$

where

$$\begin{aligned} \sigma(a) &= \frac{1}{1 + \exp(-a)}, \\ y_n &= \mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n) + b. \end{aligned} \tag{7.6}$$

We have

$$1 - \sigma(a) = \sigma(-a). \tag{7.7}$$

Then,

$$p(t_n|y_n) = \sigma(y_n t_n). \tag{7.8}$$

Then,

$$p(\mathbf{t}|\mathbf{y}) = \prod_{n=1}^{N} \sigma(y_n t_n), \tag{7.9}$$

so that

$$-\ln p(\mathbf{t}|\mathbf{y}) = -\sum_{n=1}^{N} \ln \sigma(y_n t_n). \tag{7.10}$$

Therefore,

$$-\ln p(\mathbf{t}|\mathbf{y}) = \sum_{n=1}^{N} \ln\left(1 + \exp(-y_n t_n)\right). \tag{7.11}$$

7.7

Let $t_1, \cdots, t_N$ be vaariables. Let

$$E = C \sum_{n=1}^{N} E_\epsilon(y_n - t_n) + \frac{1}{2}\|\mathbf{w}\|^2, \tag{7.12}$$

where $\epsilon > 0$ and

$$E_\epsilon(a) = \begin{cases} 0, & |a| < \epsilon, \\ |a| - \epsilon, & \text{otherwise}, \end{cases} \tag{7.13}$$
$$y_n = \mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n) + b.$$

In order to minimise E under the constraints

$$\begin{aligned} t_n &\leq y_n + \epsilon + \xi_n, \\ t_n &\geq y_n - \epsilon - \hat{\xi}_n, \end{aligned} \tag{7.14}$$

where $\xi_n \geq 0$ and $\hat{\xi}_n \geq 0$, let us minimise

$$\begin{aligned} L =& C \sum_{n=1}^{N} (\xi_n + \hat{\xi}_n) + \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} \left(\mu_n \xi_n + \hat{\mu}_n \hat{\xi}_n\right) \\ & - \sum_{n=1}^{N} a_n (\epsilon + \xi_n + y_n - t_n) - \sum_{n=1}^{N} \hat{a}_n (\epsilon + \hat{\xi}_n - y_n + t_n). \end{aligned} \tag{7.15}$$

Setting the derivatives of L with respect to $\mathbf{w}$, b, ξ_n and $\hat{\xi}_n$ to zero gives

$$\begin{aligned} \mathbf{0} &= \mathbf{w} - \sum_{n=1}^{N} a_n \boldsymbol{\phi}(\mathbf{x}_n) + \sum_{n=1}^{N} \hat{a}_n \boldsymbol{\phi}(\mathbf{x}_n), \\ 0 &= -\sum_{n=1}^{N} a_n + \sum_{n=1}^{N} \hat{a}_n, \\ 0 &= C - \mu_n - a_n, \\ 0 &= C - \hat{\mu}_n - \hat{a}_n. \end{aligned} \tag{7.16}$$

Then, L can be written as

$$\begin{aligned} & \sum_{n=1}^{N} \left((\mu_n + a_n)\xi_n + (\hat{\mu}_n + \hat{a}_n)\hat{\xi}_n\right) + \frac{1}{2}\left\|\sum_{n=1}^{N} (\hat{a}_n - a_n)\boldsymbol{\phi}(\mathbf{x}_n)\right\|^2 \\ & - \sum_{n=1}^{N} \left(\mu_n \xi_n + \hat{\mu}_n \hat{\xi}_n\right) - \sum_{n=1}^{N} a_n (\epsilon + \xi_n + y_n - t_n) \\ & - \sum_{n=1}^{N} \hat{a}_n (\epsilon + \hat{\xi}_n - y_n + t_n). \end{aligned} \tag{7.17}$$

Therefore, minimising L is equilvalent to maximising

$$\begin{aligned}\tilde{L} = &-\frac{1}{2}\sum_{n=1}^{N}\sum_{n'=1}^{N}(\hat{a}_n - a_n)(\hat{a}_{n'} - a_{n'})k(\mathbf{x}_n, \mathbf{x}_{n'}) \\ &+ \epsilon\sum_{n=1}^{N}(a_n + \hat{a}_n) + \sum_{n=1}^{N}(a_n - \hat{a}_n)(y_n - t_n),\end{aligned} \tag{7.18}$$

where

$$k(\mathbf{x}_n, \mathbf{x}_{n'}) = \boldsymbol{\phi}(\mathbf{x}_n)^\intercal \boldsymbol{\phi}(\mathbf{x}_{n'}). \tag{7.19}$$

7.8 (Incomplete)

Let $t_1, \cdots, t_N$ be vaariables. Let

$$E = C\sum_{n=1}^{N} E_\epsilon(y_n - t_n) + \frac{1}{2}\|\mathbf{w}\|^2, \tag{7.20}$$

where $\epsilon > 0$ and

$$\begin{aligned}E_\epsilon(a) &= \begin{cases} 0, & |a| < \epsilon, \\ |a| - \epsilon, & \text{otherwise}, \end{cases} \\ y_n &= \mathbf{w}^\intercal \boldsymbol{\phi}(\mathbf{x}_n) + b.\end{aligned} \tag{7.21}$$

(a)

In order to minimise E under the constraints

$$t_n \leq y_n + \epsilon + \xi_n, \tag{7.22}$$

where $\xi_n \geq 0$, let us minimise

$$L = C\sum_{n=1}^{N}\xi_n + \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N}\mu_n\xi_n - \sum_{n=1}^{N}a_n(\epsilon + \xi_n + y_n - t_n). \tag{7.23}$$

Setting the derivatives of L with respect to $\mathbf{w}$, b and ξ_n to zero gives

$$\begin{aligned}\mathbf{0} &= \mathbf{w} - \sum_{n=1}^{N} a_n \boldsymbol{\phi}(\mathbf{x}_n), \\ 0 &= -\sum_{n=1}^{N} a_n, \\ 0 &= C - \mu_n - a_n.\end{aligned} \tag{7.24}$$

Then, L can be written as

$$\begin{aligned}&\sum_{n=1}^{N}(\mu_n + a_n)\xi_n + \frac{1}{2}\left\|\sum_{n=1}^{N} a_n \boldsymbol{\phi}(\mathbf{x}_n)\right\|^2 - \sum_{n=1}^{N}\mu_n\xi_n \\ &- \sum_{n=1}^{N} a_n(\epsilon + \xi_n + y_n - t_n).\end{aligned} \tag{7.25}$$

Therefore, minimising L is equilvalent to maximising

$$\tilde{L} = -\frac{1}{2}\sum_{n=1}^{N}\sum_{n'=1}^{N} a_n a_{n'} k(\mathbf{x}_n, \mathbf{x}_{n'}) + \sum_{n=1}^{N} a_n(y_n - t_n), \tag{7.26}$$

where

$$k(\mathbf{x}_n, \mathbf{x}_{n'}) = \boldsymbol{\phi}(\mathbf{x}_n)^\intercal \boldsymbol{\phi}(\mathbf{x}_{n'}). \tag{7.27}$$

7.9

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned}p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}_n, \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \mathbf{A}^{-1}\right).\end{aligned} \tag{7.28}$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{t})p(\mathbf{t}) = p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \tag{7.29}$$

The logarithm of the right hand side except the terms independent of $\mathbf{t}$ and $\mathbf{w}$ can be written as

$$\begin{aligned}&-\frac{\beta}{2}\sum_{n=1}^{N}\|t_n - \mathbf{w}^\intercal\boldsymbol{\phi}_n\|^2 - \frac{1}{2}\mathbf{w}^\intercal\mathbf{A}\mathbf{w} \\ =&-\frac{1}{2}\begin{bmatrix}\mathbf{w}\\ \mathbf{t}\end{bmatrix}^\intercal\begin{bmatrix}\beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi} + \mathbf{A} & -\beta\boldsymbol{\Phi}^\intercal \\ -\beta\boldsymbol{\Phi} & \beta\mathbf{I}\end{bmatrix}\begin{bmatrix}\mathbf{w}\\ \mathbf{t}\end{bmatrix}.\end{aligned} \tag{7.30}$$

Therefore,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}\left(\mathbf{w}|\mathbf{m}, \mathbf{S}\right), \tag{7.31}$$

where

$$\begin{aligned}\mathbf{m} &= \beta\mathbf{S}\boldsymbol{\Phi}^\intercal\mathbf{t}, \\ \mathbf{S} &= \left(\beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi} + \mathbf{A}\right)^{-1}.\end{aligned} \tag{7.32}$$

7.10

Let $t_1, \cdots, t_N$ be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}\left(t_n|\mathbf{w}^\intercal\boldsymbol{\phi}_n, \beta^{-1}\right), \\ p(\mathbf{w}) &= \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \mathbf{A}^{-1}\right). \end{aligned} \tag{7.33}$$

By marginalisation,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}. \tag{7.34}$$

The logarithm of the integrand of the right hand side except the terms independent of $\mathbf{t}$ and $\mathbf{w}$ can be written as

$$\begin{aligned} &-\frac{\beta}{2}\sum_{n=1}^{N}\|t_n - \mathbf{w}^\intercal\boldsymbol{\phi}_n\|^2 - \frac{1}{2}\mathbf{w}^\intercal\mathbf{A}\mathbf{w} \\ =&-\frac{1}{2}\begin{bmatrix}\mathbf{w}\\ \mathbf{t}\end{bmatrix}^\intercal\begin{bmatrix}\beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi} + \mathbf{A} & -\beta\boldsymbol{\Phi}^\intercal \\ -\beta\boldsymbol{\Phi} & \beta\mathbf{I}\end{bmatrix}\begin{bmatrix}\mathbf{w}\\ \mathbf{t}\end{bmatrix}. \end{aligned} \tag{7.35}$$

By 2.24,

$$\begin{bmatrix}\beta\boldsymbol{\Phi}^\intercal\boldsymbol{\Phi} + \mathbf{A} & -\beta\boldsymbol{\Phi}^\intercal \\ -\beta\boldsymbol{\Phi} & \beta\mathbf{I}\end{bmatrix}^{-1} = \begin{bmatrix}\mathbf{A}^{-1} & \mathbf{A}^{-1}\boldsymbol{\Phi}^\intercal \\ \boldsymbol{\Phi}\mathbf{A}^{-1} & \beta^{-1}\mathbf{I} + \boldsymbol{\Phi}\mathbf{A}^{-1}\boldsymbol{\Phi}^\intercal\end{bmatrix}. \tag{7.36}$$

Therefore,

$$p(\mathbf{t}) = \mathcal{N}\left(\mathbf{t}|\mathbf{0}, \beta^{-1}\mathbf{I} + \boldsymbol{\Phi}\mathbf{A}^{-1}\boldsymbol{\Phi}^\intercal\right). \tag{7.37}$$