Solutions Manual to Pattern Recognition and Machine Learning

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1 Introduction

1.1

Let

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

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

then

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

Then,

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

Therefore,

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

where

$$\mathbf{A} = \sum_{n=1}^{N} \boldsymbol{\phi}(x_n) \boldsymbol{\phi}(x_n)^{\mathsf{T}},$$

$$\mathbf{v} = \sum_{n=1}^{N} t_n \boldsymbol{\phi}(x_n).$$
(1.7)

If

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

then

$$A_{mm'} = \sum_{n=1}^{N} x_n^{m+m'},$$

$$v_m = \sum_{n=1}^{N} t_n x_n^m.$$
(1.8)

1.2

Let

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

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

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

If

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

then

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

Then,

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

Therefore,

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

where

$$\mathbf{A} = \sum_{n=1}^{N} \boldsymbol{\phi}(x_n) \boldsymbol{\phi}(x_n)^{\mathsf{T}} + \lambda \mathbf{I},$$

$$\mathbf{v} = \sum_{n=1}^{N} t_n \boldsymbol{\phi}(x_n).$$
(1.15)

If

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

then

$$A_{mm'} = \sum_{n=1}^{N} x_n^{m+m'} + \lambda I_{mm'},$$

$$v_m = \sum_{n=1}^{N} t_n x_n^m.$$
(1.16)

1.3

Let

$$p(a|r) = \frac{3}{10}, p(o|r) = \frac{2}{5}, p(l|r) = \frac{3}{10},$$

$$p(a|b) = \frac{1}{2}, p(o|b) = \frac{1}{2},$$

$$p(a|g) = \frac{3}{10}, p(o|g) = \frac{3}{10}, p(l|g) = \frac{2}{5}.$$

$$(1.17)$$

Let

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

(a)

By the Bayes' theorem,

$$p(a) = p(a|r)p(r) + p(a|b)p(b) + p(a|g)p(g).$$
(1.19)

Therefore,

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

(b)

By the Bayes' thorem,

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

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

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

Therefore,

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

1.4

Let x and y be variables such that

$$x = g(y). (1.24)$$

Let \hat{x} and \hat{y} be the locations of the maximum of p_x and p_y respectively. 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

$$\int p_x(x)dx = \int p_x(g(y)) |g'(y)| dy,$$
(1.27)

we have

$$p_y(y) = p_x(g(y))|g'(y)|.$$
 (1.28)

Taking the derivative and substituting

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

gives

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

Therefore, in general,

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

(b)

$$g(y) = ay + b, (1.32)$$

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

$$\operatorname{var} f(x) = E(f(x) - Ef(x))^{2}.$$
 (1.35)

The right hand side can be written as

$$E((f(x))^{2} - 2f(x) E f(x) + (E f(x))^{2}) = E(f(x))^{2} - (E f(x))^{2}.$$
 (1.36)

Therefore,

$$var f(x) = E(f(x))^{2} - (E f(x))^{2}.$$
 (1.37)

1.6

We have

$$cov(x, y) = E((x - Ex)(y - Ey)).$$
 (1.38)

The right hand side can be written as

$$Exy - E(x Ey) - E(y Ex) + E(Ex Ey) = Exy - Ex Ey.$$
 (1.39)

The right hand side can be written as

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

If x and y are independent, by the definition,

$$f(x,y) = f(x)f(y). (1.41)$$

Then,

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

$$cov(x,y) = 0. (1.43)$$

(a)

Let

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

Then,

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

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

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

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

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

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

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

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

(a)

Let x be a variable such that

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

Then,

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

$$\int_{-\infty}^{\infty} (y+\mu) \exp\left(-\frac{1}{2\sigma^2}y^2\right) dy$$

$$= \int_{-\infty}^{\infty} y \exp\left(-\frac{1}{2\sigma^2}y^2\right) dy + \mu \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}y^2\right) dy.$$
(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,

$$\mathbf{E} x = \mu. \tag{1.59}$$

(b)

By 1.7(b),

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

so that

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

Taking the derivative with respect to σ^2 gives

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

The left hand side can be written as

$$-\frac{1}{2} (\sigma^{2})^{-1} \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^{2}) dx + \frac{1}{2} (\sigma^{2})^{-2} \int_{-\infty}^{\infty} (x-\mu)^{2} \mathcal{N}(x|\mu, \sigma^{2}) dx$$

$$= -\frac{1}{2} (\sigma^{2})^{-1} + \frac{1}{2} (\sigma^{2})^{-2} \operatorname{var} x.$$
(1.63)

Therefore,

$$var x = \sigma^2. (1.64)$$

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

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

Therefore,

$$mode x = \mu. (1.67)$$

(b)

Let \mathbf{x} be a variable such that

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

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

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

Therefore,

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

1.10

(a)

We have

$$E(x+y) = \iint (x+y)p(x,y)dxdy.$$
 (1.71)

The right hand side can be written as

$$\int x \left(\int p(x,y) dy \right) dx + \int y \left(\int p(x,y) dx \right) dy = \int x p(x) dx + \int y p(y) dy.$$
(1.72)

The right hand side can be written as

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

Therefore,

$$E(x+y) = E x + E y. (1.74)$$

(b)

We have

$$var(x+y) = E(x+y - E(x+y))^{2}$$
 (1.75)

The right hand side can be written as

$$E(x - Ex)^{2} + 2E((x - Ex)(y - Ey)) + E(y - Ey)^{2}$$

$$= var x + 2cov(x, y) + var y.$$
(1.76)

By 1.6, if x and y are independent, then

$$cov(x,y) = 0. (1.77)$$

$$var(x+y) = var x + var y. (1.78)$$

Let x_1, \dots, x_N be variables such that

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

Then,

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

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

$$0 = \frac{1}{\sigma^2} \sum_{n=1}^{N} (x_n - \mu),$$

$$0 = -\frac{N}{2\sigma^2} + \frac{1}{2(\sigma^2)^2} \sum_{n=1}^{N} (x_n - \mu)^2.$$
(1.81)

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

$$\mu_{\rm ML} = \frac{1}{N} \sum_{n=1}^{N} x_n,$$

$$\sigma_{\rm ML}^2 = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu_{\rm ML})^2.$$
(1.82)

1.12

(a)

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

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

$$p(x_{n'}) = \mathcal{N}\left(x_{n'}|\mu, \sigma^2\right).$$
(1.83)

Then,

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

By the property

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

we have

$$E x_n^2 = \sigma^2 + \mu^2. (1.86)$$

Therefore,

$$E x_n x_{n'} = \mu^2 + I_{nn'} \sigma^2. (1.87)$$

(b)

Let x_1, \dots, 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

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

Then,

$$E \mu_{ML} = \frac{1}{N} \sum_{n=1}^{N} E x_n.$$
 (1.90)

Therefore,

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

(c)

Let x_1, \dots, 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

$$\sigma_{\rm ML}^2 = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu_{\rm ML})^2.$$
 (1.93)

Then,

$$E \sigma_{ML}^2 = \frac{1}{N} \sum_{n=1}^{N} E (x_n - \mu_{ML})^2.$$
 (1.94)

The right hand side can be writen as

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

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

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

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

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

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

$$-\frac{1}{N^2} \sum_{n=1}^{N} \operatorname{E} x_n^2 - \frac{2}{N^2} \sum_{1 \le n < n' \le N} \operatorname{E} x_n x_{n'}$$

$$= -\frac{1}{N^2} N \left(\mu^2 + \sigma^2 \right) - \frac{2}{N^2} \frac{N(N-1)}{2} \mu^2.$$
(1.98)

The right hand side can be written as

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

Then,

$$E \sigma_{ML}^2 = \mu^2 + \sigma^2 - \mu^2 - \frac{1}{N} \sigma^2.$$
 (1.100)

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

Let x_1, \dots, x_N be variables such that

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

We have

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

The right hand side can be writen as

$$\frac{1}{N^2} \sum_{n=1}^{N} \operatorname{var} x_n = \frac{\sigma^2}{N}.$$
 (1.104)

Therefore,

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

1.14

Let

$$w_{dd'}^{S} = \frac{1}{2}(w_{dd'} + w_{d'd}),$$

$$w_{dd'}^{A} = \frac{1}{2}(w_{dd'} - w_{d'd}).$$
(1.106)

(a)

We have

$$w_{dd'} = w_{dd'}^{S} + w_{dd'}^{A},$$

$$w_{dd'}^{S} = w_{d'd}^{S},$$

$$w_{dd'}^{A} = -w_{d'd}^{A}.$$
(1.107)

(b)

We have

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

The right hand side can be written as

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

Therefore,

$$\sum_{d=1}^{D} \sum_{d'=1}^{D} w_{dd'}^{A} x_{d} x_{d'} = 0.$$
 (1.110)

(c)

We have

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

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

$$\sum_{d=1}^{D} \sum_{d'=1}^{D} w_{dd'}^{S} x_{d} x_{d'} + \sum_{d=1}^{D} \sum_{d'=1}^{D} w_{dd'}^{A} x_{d} x_{d'} = \sum_{d=1}^{D} \sum_{d'=1}^{D} w_{dd'}^{S} x_{d} x_{d'}, \qquad (1.112)$$

Therefore,

$$\sum_{d=1}^{D} \sum_{d'=1}^{D} w_{dd'} x_d x_{d'} = \sum_{d=1}^{D} \sum_{d'=1}^{D} w_{dd'}^{S} x_d x_{d'}.$$
 (1.113)

(d)

Since \mathbf{W}^{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

$$n(1, M) = n(1, M - 1) = 1.$$
 (1.114)

Let us assume that

$$n(D,M) = \sum_{d=1}^{D} n(d, M-1).$$
(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+1th variable. Then,

$$n(D+1,M) = n(D,M) + n(D+1,M-1), (1.116)$$

so that

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

Therefore, the assumption is proved by induction on D.

(b)

We have

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

Let us assume that

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

Then,

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

The right hand side can be written as

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

Therefore, the assumption is proved by induction on D.

(c)

By 1.14(d),

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

Let us assume that

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

By (a),

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

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

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

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

where

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

(b)

By (a),

$$N(D,0) = 1. (1.128)$$

Let us assume that

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

Then,

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

The right hand side can be written as

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

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

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

(c)

By the approximation

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

we have

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

The right hand side can be written as

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

Therefore,

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

(d)

By (b),

$$N(10,3) = 286,$$

 $N(100,3) = 176851,$ (1.137)
 $N(1000,3) = 167668501.$

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

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

$$\prod_{d=1}^{D} \int_{-\infty}^{\infty} \exp(-x_d^2) dx_i = S_D \int_{0}^{\infty} \exp(-r^2) r^{D-1} dr, \qquad (1.147)$$

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

$$s = r^2, (1.148)$$

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,

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

(b)

The volume of the sphere can can be written as

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

Therefore,

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

(c)

By (a) and (b),

$$S_2 = 2\pi,$$
 $V_2 = \pi.$ (1.153)

Similarly,

$$S_3 = 4\pi,$$

$$V_3 = \frac{4}{3}\pi.$$
(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

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

(b)

By (a) and the Stering's formula

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

we have

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

The right hand side can be written as

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

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

where ϕ is the vector of the angular components of the polar coordinate 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

$$(2\pi\sigma^2)^{-\frac{D}{2}} \exp\left(-\frac{r^2}{2\sigma^2}\right) \int_r^{r+\epsilon} \int J dr' d\phi$$

$$= (2\pi\sigma^2)^{-\frac{D}{2}} \exp\left(-\frac{r^2}{2\sigma^2}\right) \int_{r<\|\mathbf{x}\| \le r+\epsilon} d\mathbf{x}.$$
(1.163)

Therefore,

$$\int_{r < \|\mathbf{x}\| \le r + \epsilon} p(\mathbf{x}) d\mathbf{x} \simeq p(r) \epsilon, \qquad (1.164)$$

where

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

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

$$\exp\left((D-1)\ln\left(1+\frac{\epsilon}{\hat{r}}\right) - \frac{2\hat{r}\epsilon + \epsilon^2}{2\sigma^2}\right)$$

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

By the Taylor series

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

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,

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

(d)

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

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

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

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

Therefore,

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

1.21

(a)

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

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

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

(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,

$$p(\mathbf{x}, C_1) > p(\mathbf{x}, C_2) \Rightarrow \mathbf{x} \in C_1,$$

$$p(\mathbf{x}, C_2) > p(\mathbf{x}, C_1) \Rightarrow \mathbf{x} \in C_2.$$
(1.178)

By (a),

$$\int_{\mathcal{R}_{1}} p(\mathbf{x}, \mathcal{C}_{2}) d\mathbf{x} \leq \int_{\mathcal{R}_{1}} \left(p(\mathbf{x}, \mathcal{C}_{1}) p(\mathbf{x}, \mathcal{C}_{2}) \right)^{\frac{1}{2}} d\mathbf{x},
\int_{\mathcal{R}_{2}} p(\mathbf{x}, \mathcal{C}_{1}) d\mathbf{x} \leq \int_{\mathcal{R}_{2}} \left(p(\mathbf{x}, \mathcal{C}_{1}) p(\mathbf{x}, \mathcal{C}_{2}) \right)^{\frac{1}{2}} d\mathbf{x}.$$
(1.179)

Therefore,

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

1.22

Let

$$EL = \sum_{k} \sum_{j} \int_{\mathcal{R}_{j}} L_{kj} p(\mathbf{x}, \mathcal{C}_{k}) d\mathbf{x}.$$
 (1.181)

If

$$L_{ki} = 1 - I_{ki}, (1.182)$$

then the right hand side can be written as

$$\sum_{k} \sum_{j} \int_{\mathcal{R}_{j}} (p(\mathbf{x}, \mathcal{C}_{k}) - p(\mathbf{x}, \mathcal{C}_{j})) d\mathbf{x} = \sum_{j} \int_{\mathcal{R}_{j}} \left(\sum_{k} p(\mathbf{x}, \mathcal{C}_{k}) - p(\mathbf{x}, \mathcal{C}_{j}) \right) d\mathbf{x}.$$
(1.183)

The right hand side can be written as

$$\sum_{i} \int_{\mathcal{R}_{j}} (p(\mathbf{x}) - p(\mathbf{x}, \mathcal{C}_{j})) d\mathbf{x} = 1 - \sum_{i} \int_{\mathcal{R}_{j}} p(\mathbf{x}, \mathcal{C}_{j}) d\mathbf{x}.$$
 (1.184)

Then,

$$EL = 1 - \sum_{j} \int_{\mathcal{R}_{j}} p(\mathcal{C}_{j}|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}.$$
 (1.185)

Therefore, minimising E L reduces to choosing the criterion to maximise the posterior probability $p(C_i|\mathbf{x})$.

1.23

Let

$$EL = \sum_{k} \sum_{j} \int_{\mathcal{R}_{j}} L_{kj} p(\mathbf{x}, \mathcal{C}_{k}) d\mathbf{x}.$$
 (1.186)

The right hand side can be written as

$$\sum_{j} \int_{\mathcal{R}_{j}} \sum_{k} L_{kj} p(\mathbf{x}, \mathcal{C}_{k}) d\mathbf{x} = \sum_{j} \int_{\mathcal{R}_{j}} \left(\sum_{k} L_{kj} p(\mathcal{C}_{k} | \mathbf{x}) \right) p(\mathbf{x}) d\mathbf{x}.$$
 (1.187)

Then,

$$EL = \sum_{j} \int_{\mathcal{R}_{j}} \left(\sum_{k} L_{kj} p(\mathcal{C}_{k} | \mathbf{x}) \right) p(\mathbf{x}) d\mathbf{x}.$$
 (1.188)

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

1.24 (Incomplete)

Let

$$EL = \sum_{k} \sum_{j} \int_{\mathcal{R}_{j}} L_{kj} p(\mathbf{x}, \mathcal{C}_{k}) d\mathbf{x} + \lambda \int_{\forall kp(\mathcal{C}_{k}|\mathbf{x}) < \theta} p(\mathbf{x}) d\mathbf{x}.$$
 (1.189)

1.25

Let

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

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

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

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

Therefore,

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

For a single target variable t, it reduces to

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

1.26

Let

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

The right hand side can be written as

$$\iint \|\mathbf{y}(\mathbf{x}) - \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) + \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}\|^{2} p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}$$

$$= \iint \|\mathbf{y}(\mathbf{x}) - \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\|^{2} p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}$$

$$+ 2 \iint (\mathbf{y}(\mathbf{x}) - \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}))^{\mathsf{T}} (\mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}) p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}$$

$$+ \iint \|\mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}\|^{2} p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}.$$
(1.197)

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

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

The integral of the second term can be written as

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

Since

$$\int E_{\mathbf{t}}(\mathbf{t}|\mathbf{x})p(\mathbf{t}|\mathbf{x})d\mathbf{t} = E_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\frac{\int p(\mathbf{x},\mathbf{t})d\mathbf{t}}{p(\mathbf{x})},$$

$$\int \mathbf{t}p(\mathbf{t}|\mathbf{x})d\mathbf{t} = E_{\mathbf{t}}(\mathbf{t}|\mathbf{x}),$$
(1.200)

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

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

Then,

$$EL(\mathbf{t}, \mathbf{y}(\mathbf{x})) = \int ||\mathbf{y}(\mathbf{x}) - E_{\mathbf{t}}(\mathbf{t}|\mathbf{x})||^{2} p(\mathbf{x}) d\mathbf{x} + \int var_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \quad (1.202)$$

Therefore,

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

1.27 (Incomplete)

(a)

Let

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

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

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

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

(b)

We have

$$EL_1 = \int \left(\int \operatorname{sign}(y(\mathbf{x}) - t) p(t|\mathbf{x}) dt \right) p(\mathbf{x}) d\mathbf{x}.$$
 (1.207)

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

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

Therefore,

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

(c)

We have

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

1.28

(a)

Let us assume that

$$p(x,y) = p(x)p(y) \Rightarrow h(x,y) = h(x) + h(y).$$
 (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,

$$h(p^{n+1}) = h(p^n) + h(p),$$
 (1.214)

so that

$$h(p^{n+1}) = (n+1)h(p).$$
 (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

$$(p \ln p)h'(p) = h(p).$$
 (1.219)

Then,

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

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

where

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

By the Jensen's inequality,

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

Therefore,

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

1.30

Let

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

$$q(x) = \mathcal{N}(x|m, s^2).$$
(1.226)

Then, the Kullback-Leibler divergence is given by

$$KL(p||q) = -\int p(x) \ln \frac{q(x)}{p(x)} dx. \qquad (1.227)$$

The right hand side can be written as

$$-\int_{-\infty}^{\infty} p(x) \ln \frac{(2\pi s^2)^{-\frac{1}{2}} \exp\left(-\frac{(x-m)^2}{2s^2}\right)}{(2\pi\sigma^2)^{-\frac{1}{2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)} dx$$

$$= -\int_{-\infty}^{\infty} p(x) \left(-\frac{1}{2} \ln \frac{s^2}{\sigma^2} - \frac{(x-m)^2}{2s^2} + \frac{(x-\mu)^2}{2\sigma^2}\right) dx.$$
(1.228)

The right hand side can be written as

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

The integral of the second term can be written as

$$\int_{-\infty}^{\infty} (x - \mu + \mu - m)^2 p(x) dx$$

$$= \int_{-\infty}^{\infty} (x - \mu)^2 p(x) dx + 2(\mu - m) \int_{-\infty}^{\infty} (x - \mu) p(x) dx$$

$$+ (\mu - m)^2 \int_{-\infty}^{\infty} p(x) dx.$$
(1.230)

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

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

$$H(\mathbf{x}) = -\int p(\mathbf{x}) \ln p(\mathbf{x}) d\mathbf{x},$$

$$H(\mathbf{y}) = -\int p(\mathbf{y}) \ln p(\mathbf{y}) d\mathbf{y},$$

$$H(\mathbf{x}, \mathbf{y}) = -\int \int p(\mathbf{x}, \mathbf{y}) \ln p(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}.$$
(1.232)

Since

$$H(\mathbf{x}) = -\int \left(\int p(\mathbf{x}, \mathbf{y}) d\mathbf{y}\right) \ln p(\mathbf{x}) d\mathbf{x},$$

$$H(\mathbf{y}) = -\int \left(\int p(\mathbf{x}, \mathbf{y}) d\mathbf{x}\right) \ln p(\mathbf{y}) d\mathbf{y},$$
(1.233)

we have

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

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

The right hand side can be written as

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

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

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

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

where A is a nonsingular matrix. We have

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

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

The right hand side can be written as

$$-\int p_{y}(\mathbf{y}) \ln \left(p_{x} \left(\mathbf{A}^{-1} \mathbf{y} \right) \left| \det \mathbf{A}^{-1} \right| \right) d\mathbf{y}$$

$$= -\int p_{y}(\mathbf{y}) \ln p_{x} \left(\mathbf{A}^{-1} \mathbf{y} \right) d\mathbf{y} + \ln \left| \det \mathbf{A} \right| \int p_{y}(\mathbf{y}) d\mathbf{y}.$$
(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

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

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

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

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

If

$$H(y|x) = 0, (1.249)$$

then

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

Since

$$p(x_k) \ge 0,$$

 $p(y_l|x_k) \ln p(y_l|x_k) \le 0,$ (1.251)

the equation reduces to

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

Then,

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

Since

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

we have

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

1.34

Let x be a variable. We have

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

In order to maximise H(x) with the constratints

$$\int_{-\infty}^{\infty} p(x)dx = 1,$$

$$\int_{-\infty}^{\infty} xp(x)dx = \mu,$$

$$\int_{-\infty}^{\infty} (x - \mu)^2 p(x)dx = \sigma^2,$$
(1.257)

let

$$L(p) = H(x) + \lambda_1 \left(\int_{-\infty}^{\infty} p(x)dx - 1 \right) + \lambda_2 \left(\int_{-\infty}^{\infty} x p(x)dx - \mu \right)$$

$$+ \lambda_3 \left(\int_{-\infty}^{\infty} (x - \mu)^2 p(x)dx - \sigma^2 \right).$$
(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,

$$p(x) = \exp(-1 + \lambda_1 + \lambda_2 x + \lambda_3 (x - \mu)^2),$$
 (1.260)

so that

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

$$c \int_{-\infty}^{\infty} \exp\left(\lambda_3 \left(x - \left(\mu - \frac{\lambda_2}{2\lambda_3}\right)\right)^2\right) dx = 1,$$

$$c \int_{-\infty}^{\infty} x \exp\left(\lambda_3 \left(x - \left(\mu - \frac{\lambda_2}{2\lambda_3}\right)\right)^2\right) dx = \mu,$$

$$c \int_{-\infty}^{\infty} (x - \mu)^2 \exp\left(\lambda_3 \left(x - \left(\mu - \frac{\lambda_2}{2\lambda_3}\right)\right)^2\right) dx = \sigma^2.$$

$$(1.263)$$

By the transformation

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

they can be written as

$$c \int_{-\infty}^{\infty} \exp(-y^{2}) (-\lambda_{3})^{-\frac{1}{2}} dy = 1,$$

$$c \int_{-\infty}^{\infty} \left((-\lambda_{3})^{-\frac{1}{2}} y + \mu - \frac{\lambda_{2}}{2\lambda_{3}} \right) \exp(-y^{2}) (-\lambda_{3})^{-\frac{1}{2}} dy = \mu,$$

$$c \int_{-\infty}^{\infty} \left((-\lambda_{3})^{-\frac{1}{2}} y - \frac{\lambda_{2}}{2\lambda_{3}} \right)^{2} \exp(-y^{2}) (-\lambda_{3})^{-\frac{1}{2}} dy = \sigma^{2}.$$
(1.265)

Since

$$\int_{-\infty}^{\infty} \exp(-y^2) dy = \Gamma\left(\frac{1}{2}\right),$$

$$\int_{-\infty}^{\infty} y \exp(-y^2) dy = 0,$$

$$\int_{-\infty}^{\infty} y^2 \exp(-y^2) dy = \Gamma\left(\frac{3}{2}\right),$$
(1.266)

they can be written as

$$c(-\lambda_3)^{-\frac{1}{2}}\Gamma\left(\frac{1}{2}\right) = 1,$$

$$c\left(\mu - \frac{\lambda_2}{2\lambda_3}\right)(-\lambda_3)^{-\frac{1}{2}}\Gamma\left(\frac{1}{2}\right) = \mu,$$

$$c\left((-\lambda_3)^{-\frac{3}{2}}\Gamma\left(\frac{3}{2}\right) + (-\lambda_3)^{-\frac{1}{2}}\frac{\lambda_2^2}{4\lambda_3^2}\Gamma\left(\frac{1}{2}\right)\right) = \sigma^2.$$

$$(1.267)$$

Then,

$$\lambda_1 = 1 - \frac{1}{2} \ln \left(2\pi \sigma^2 \right),$$

$$\lambda_2 = 0,$$

$$\lambda_3 = -\frac{1}{2\sigma^2}.$$
(1.268)

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

Let x be a variable such that

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

Then,

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

The right hand side can be written as

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

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

Therefore,

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

1.36 (Incomplete)

Let f be a strictly convex function. Then,

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

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

$$f(x) \le \frac{b-x}{b-a}f(a) + \frac{x-a}{b-a}f(b).$$
 (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,

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

Additionally, for x > a,

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

$$f'(c) = \frac{f(b) - f(a)}{b - a},$$

$$f'(y) = \frac{f(x) - f(a)}{x - a}.$$
(1.280)

Then, for x > a, the inequality reduces to

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

1.37

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

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

The right hand side can be written as

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

$$= - \iint p(\mathbf{x}, \mathbf{y}) \ln p(\mathbf{y}|\mathbf{x}) d\mathbf{x} d\mathbf{y} - \int \left(\int p(\mathbf{x}, \mathbf{y}) d\mathbf{y} \right) \ln p(\mathbf{x}) d\mathbf{x}.$$
(1.283)

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

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

1.38

Let f be a strictly convex function. Then,

$$f(\lambda x_1 + (1 - \lambda)x_2) \le \lambda f(x_1) + (1 - \lambda)f(x_2),$$
 (1.285)

where

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

Let us assume that

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

where

$$\sum_{m=1}^{M} \lambda_m = 1,$$

$$\lambda_m \ge 0.$$
(1.288)

Since f is strictly convex,

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

where

$$\sum_{m=1}^{M+1} \lambda_m = 1,$$

$$\lambda_m \ge 0.$$
(1.290)

By the assumption,

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

Then,

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

so that

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

Therefore, the assumption is proved by induction on M.

Let x and y be two binary variables where

$$p(x = 0, y = 0) = \frac{1}{3},$$

$$p(x = 0, y = 1) = \frac{1}{3},$$

$$p(x = 1, y = 0) = 0,$$

$$p(x = 1, y = 1) = \frac{1}{3}.$$
(1.294)

(a)

We have

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

We have

$$p(x = 0) = p(x = 0, y = 0) + p(x = 0, y = 1),$$

$$p(x = 1) = p(x = 1, y = 0) + p(x = 1, y = 1).$$
(1.296)

Then,

$$p(x = 0) = \frac{2}{3},$$

$$p(x = 1) = \frac{1}{3}.$$
(1.297)

Therefore,

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

(b)

We have

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

$$p(y=0) = p(x=0, y=0) + p(x=1, y=0),$$

$$p(y=1) = p(x=0, y=1) + p(x=1, y=1).$$
(1.300)

Then,

$$p(y = 0) = \frac{1}{3},$$

$$p(y = 1) = \frac{2}{3}.$$
(1.301)

Therefore,

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

(c)

We have

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

By the Bayes' theorem,

$$p(y = 0|x = 0) = \frac{p(x = 0, y = 0)}{p(x = 0)},$$

$$p(y = 0|x = 1) = \frac{p(x = 1, y = 0)}{p(x = 1)},$$

$$p(y = 1|x = 0) = \frac{p(x = 0, y = 1)}{p(x = 0)},$$

$$p(y = 1|x = 1) = \frac{p(x = 1, y = 1)}{p(x = 1)}.$$

$$(1.304)$$

Then,

$$p(y = 0|x = 0) = \frac{1}{2},$$

$$p(y = 0|x = 1) = 0,$$

$$p(y = 1|x = 0) = \frac{1}{2},$$

$$p(y = 1|x = 1) = 1.$$
(1.305)

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

(d)

We have

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

By the Bayes' theorem,

$$p(x = 0|y = 0) = \frac{p(x = 0, y = 0)}{p(y = 0)},$$

$$p(x = 0|y = 1) = \frac{p(x = 0, y = 1)}{p(y = 1)},$$

$$p(x = 1|y = 0) = \frac{p(x = 1, y = 0)}{p(y = 0)},$$

$$p(x = 1|y = 1) = \frac{p(x = 1, y = 1)}{p(y = 1)}.$$
(1.308)

Then,

$$p(x = 0|y = 0) = 1,$$

$$p(x = 0|y = 1) = \frac{1}{2},$$

$$p(x = 1|y = 0) = 0,$$

$$p(x = 1|y = 1) = \frac{1}{2}.$$
(1.309)

Therefore,

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

(e)

We have

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

$$H(x, y) = \ln 3.$$
 (1.312)

(f)

We have

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

The right hand side can be written as

$$H(x) + H(y) - H(x, y).$$
 (1.314)

Therefore,

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

1.40

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

$$\sum_{m=1}^{M} \lambda_m = 1,$$

$$\lambda_m \ge 0,$$

$$x_m > 0.$$
(1.316)

By the Jensen's inequality,

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

so that

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

Substituting

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

to the inequality gives

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

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

(a)

We have

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

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

$$- \iint p(\mathbf{x}, \mathbf{y}) \left(\ln p(\mathbf{x}) + \ln \frac{p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} \right) d\mathbf{x} d\mathbf{y}$$

$$= - \iint p(\mathbf{x}, \mathbf{y}) \left(\ln p(\mathbf{x}) - \ln p(\mathbf{x}|\mathbf{y}) \right) d\mathbf{x} d\mathbf{y}.$$
(1.322)

The right hand side can be written as

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

Therefore,

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

(b)

We have

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

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

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

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

2 Probability Distributions

2.1

Let x be a variable such that

$$x \in \{0, 1\},\$$

$$p(x) = \mu^{x} (1 - \mu)^{1 - x}.$$
 (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

$$E x = \sum_{x} xp(x),$$

$$E x^{2} = \sum_{x} x^{2}p(x),$$
(2.4)

Then,

$$E x = \mu,$$

$$E x^2 = \mu.$$
(2.5)

We have

$$\operatorname{var} x = \operatorname{E} x^{2} - (\operatorname{E} x)^{2}.$$
 (2.6)

Therefore,

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

(c)

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

Therefore,

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

2.2

Let x be a variable such that

$$x \in \{-1, 1\},\$$

$$p(x) = \left(\frac{1-\mu}{2}\right)^{\frac{1-x}{2}} \left(\frac{1+\mu}{2}\right)^{\frac{1+x}{2}}.$$
(2.10)

(a)

We have

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

Therefore,

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

(b)

We have

$$E x = \sum_{x} xp(x),$$

$$E x^{2} = \sum_{x} x^{2}p(x).$$
(2.13)

The right hand sides can be written as

$$-\frac{1-\mu}{2} + \frac{1+\mu}{2} = \mu,$$

$$\frac{1-\mu}{2} + \frac{1+\mu}{2} = 1.$$
(2.14)

Then,

$$E x = \mu,$$

$$E x^2 = 1.$$
(2.15)

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

Therefore,

$$var x = 1 - \mu^2. (2.17)$$

(c)

We have

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

Therefore,

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

2.3

(a)

We have

$$\binom{N}{n} = \frac{N!}{n!(N-n)!},$$

$$\binom{N}{n-1} = \frac{N!}{(n-1)!(N-n+1)!}$$
(2.20)

Then,

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

The right hand side can be written as

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

Therefore,

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

(b)

$$1 + x = \sum_{n=0}^{1} {1 \choose n} x^{n}.$$
 (2.24)

Let us assume that

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

Then,

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

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

$$\sum_{n=0}^{N} {N \choose n} x^n + \sum_{n=1}^{N+1} {N \choose n-1} x^n = 1 + x^{N+1} + \sum_{n=1}^{N} {N+1 \choose n} x^n.$$
 (2.27)

Then,

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

Therefore, the assumption is proved by induction on N.

(c)

Let n be a variable such that

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

Then,

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

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

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

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

Let n be a variable such that

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

(a)

We have

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

By 2.3(c),

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

Taking the derivative with respect to μ gives

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

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

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

Since

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

the second term can be written as

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

$$E n = N\mu. (2.40)$$

(b)

By 2.3(c),

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

Taking the second derivative with respect to μ gives

$$\sum_{n=0}^{N} n(n-1) \binom{N}{n} \mu^{n-2} (1-\mu)^{N-n}$$

$$-2 \sum_{n=0}^{N} n(N-n) \binom{N}{n} \mu^{n-1} (1-\mu)^{N-n-1}$$

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

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

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

Since

$$n(N-n)\binom{N}{n} = N(N-1)\binom{N-2}{n-1},$$

$$(N-n)(N-n-1)\binom{N}{n} = N(N-1)\binom{N-2}{n},$$
(2.44)

the second and third terms can be written as

$$-2N(N-1)\sum_{n=1}^{N-1} {N-2 \choose n-1} \mu^{n-1} (1-\mu)^{N-n-1} = -2N(N-1),$$

$$N(N-1)\sum_{n=0}^{N} {N-2 \choose n} \mu^{n} (1-\mu)^{N-n-2} = N(N-1).$$
(2.45)

Then,

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

We have

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

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

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

$$t = x + y, (2.50)$$

the right hand side can be written as

$$\int_{0}^{\infty} x^{a-1} \left(\int_{x}^{\infty} (t-x)^{b-1} \exp(-t) dt \right) dx$$

$$= \int_{0}^{\infty} \left(\int_{0}^{t} x^{a-1} (t-x)^{b-1} dx \right) \exp(-t) dt.$$
(2.51)

By the transformation

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

the right hand side can be written as

$$\int_{0}^{\infty} \left(\int_{0}^{1} (t\mu)^{a-1} t^{b-1} (1-\mu)^{b-1} t d\mu \right) \exp(-t) dt$$

$$= \int_{0}^{1} \mu^{a-1} (1-\mu)^{b-1} d\mu \int_{0}^{\infty} t^{a+b-1} \exp(-t) dt.$$
(2.53)

Then,

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

Therefore,

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

2.6

Let μ be a variable such that

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

(a)

We have

By 2.5,

$$\int_{0}^{1} \mu^{a} (1-\mu)^{b-1} d\mu = \frac{\Gamma(a+1)\Gamma(b)}{\Gamma(a+b+1)},$$

$$\int_{0}^{1} \mu^{a+1} (1-\mu)^{b-1} d\mu = \frac{\Gamma(a+2)\Gamma(b)}{\Gamma(a+b+2)}.$$
(2.58)

Therefore,

$$E \mu = \frac{a}{a+b},$$

$$E \mu^2 = \frac{a(a+1)}{(a+b)(a+b+1)}.$$
(2.59)

(b)

We have

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

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

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

Therefore,

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

(c)

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

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

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

Let m and l be variables such that

$$p(m, l | \mu) = {m+l \choose m} \mu^m (1-\mu)^l,$$

$$p(\mu) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \mu^{a-1} (1-\mu)^{b-1}.$$
(2.65)

By 2.6,

$$E\mu = \frac{a}{a+b}. (2.66)$$

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

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

Then, the maximum likelihood solution for μ is given by

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

By the Bayes' thereorem,

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

Then, by 2.5,

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

The, by 2.6,

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

Therefore,

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

where

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

2.8

Let x and y be variables.

(a)

By the definition,

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

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,

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

(b)

By the definition,

$$\operatorname{var} x = \operatorname{E} (x - \operatorname{E} x)^{2}. \tag{2.77}$$

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

$$E_y\left(E_x\left((x-E_x)^2|y\right)\right) = E_y\left(E_x\left((x-E_x(x|y) + E_x(x|y) - E_x)^2|y\right)\right). \tag{2.78}$$

The right hand side can be written as

$$E_{y} (E_{x} ((x - E_{x}(x|y))^{2}|y)) + 2 E_{y} (((E_{x}(x|y) - E_{x}) E_{x} (x - E_{x}(x|y))|y)) + E_{y} ((E_{x}(x|y) - E_{x})^{2}|y).$$
(2.79)

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

$$2 E_y ((E_x(x|y) - E_x) (E_x(x|y) - E_x(x|y))) = 0.$$
 (2.80)

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

$$E_y (E_x(x|y) - E_y (E_x(x|y)))^2 = var_y (E_x(x|y)).$$
 (2.81)

$$\operatorname{var} x = \operatorname{E}_{y} \left(\operatorname{var}_{x}(x|y) \right) + \operatorname{var}_{y} \left(\operatorname{E}_{x}(x|y) \right). \tag{2.82}$$

2.9 (Incomplete)

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

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

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

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

Under the constraint

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

we have

$$\int_{0}^{c} \prod_{m=1}^{M+1} \mu_{m}^{\alpha_{m}-1} d\mu_{M+1} = \left(\prod_{m=1}^{M-1} \mu_{m}^{\alpha_{m}-1}\right) \int_{0}^{c} \mu_{M+1}^{\alpha_{M+1}-1} \left(c - \mu_{M+1}\right)^{\alpha_{M}-1} d\mu_{M+1},$$
(2.84)

where

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

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

$$\int_{0}^{1} (c\mu'_{M+1})^{\alpha_{M+1}-1} \left(c(1-\mu'_{M+1}) \right)^{\alpha_{M}-1} cd\mu'_{M+1}
= c^{\alpha_{M}+\alpha_{M+1}-1} \int_{0}^{1} {\mu'_{M+1}}^{\alpha_{M+1}-1} (1-\mu'_{M+1})^{\alpha_{M}-1} d\mu'_{M+1}.$$
(2.87)

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

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

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,

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

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

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

The right hand side can be written as

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

Therefore, the assumption is proved by induction on M.

2.10

Let μ be a vector such that

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

Then, by the definition,

$$E \mu_k = \int \mu_k p(\boldsymbol{\mu}) d\boldsymbol{\mu},$$

$$E \mu_k^2 = \int \mu_k^2 p(\boldsymbol{\mu}) d\boldsymbol{\mu},$$

$$E \mu_k \mu_{k'} = \int \mu_k \mu_{k'} p(\boldsymbol{\mu}) d\boldsymbol{\mu}.$$
(2.92)

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

$$\frac{\Gamma\left(\sum_{k=1}^{K} \alpha_{k}\right)}{\prod_{k=1}^{K} \Gamma(\alpha_{k})} \frac{\frac{\Gamma(\alpha_{k}+1)}{\Gamma(\alpha_{k})} \prod_{k=1}^{K} \Gamma(\alpha_{k})}{\Gamma\left(\sum_{k=1}^{K} \alpha_{k}+1\right)} = \frac{\alpha_{k}}{\sum_{k=1}^{K} \alpha_{k}},$$

$$\frac{\Gamma\left(\sum_{k=1}^{K} \alpha_{k}\right)}{\prod_{k=1}^{K} \Gamma(\alpha_{k})} \frac{\frac{\Gamma(\alpha_{k}+2)}{\Gamma(\alpha_{k})} \prod_{k=1}^{K} \Gamma(\alpha_{k})}{\Gamma\left(\sum_{k=1}^{K} \alpha_{k}+2\right)} = \frac{\alpha_{k}(\alpha_{k}+1)}{\sum_{k=1}^{K} \alpha_{k}(\sum_{k=1}^{K} \alpha_{k}+1)}, \quad (2.93)$$

$$\frac{\Gamma\left(\sum_{k=1}^{K} \alpha_{k}\right)}{\prod_{k=1}^{K} \Gamma(\alpha_{k})} \frac{\frac{\Gamma(\alpha_{k}+1)\Gamma(\alpha_{k'}+1)}{\Gamma(\alpha_{k})\Gamma(\alpha_{k'})} \prod_{k=1}^{K} \Gamma(\alpha_{k})}{\Gamma\left(\sum_{k=1}^{K} \alpha_{k}+2\right)} = \frac{\alpha_{k}\alpha_{k'}}{\sum_{k=1}^{K} \alpha_{k}(\sum_{k=1}^{K} \alpha_{k}+1)}.$$

Then,

$$E \mu_k = \frac{\alpha_k}{\sum_{k=1}^K \alpha_k}.$$

$$E \mu_k^2 = \frac{\alpha_k(\alpha_k + 1)}{\sum_{k=1}^K \alpha_k \left(\sum_{k=1}^K \alpha_k + 1\right)},$$

$$E \mu_k \mu_{k'} = \frac{\alpha_k \alpha_{k'}}{\sum_{k=1}^K \alpha_k \left(\sum_{k=1}^K \alpha_k + 1\right)}.$$
(2.94)

Since

$$\operatorname{var} \mu_{k} = \operatorname{E} \mu_{k}^{2} - (\operatorname{E} \mu_{k})^{2}, \operatorname{cov} (\mu_{k}, \mu_{k'}) = \operatorname{E} \mu_{k} \mu_{k'} - \operatorname{E} \mu_{k} \operatorname{E} \mu_{k'},$$
(2.95)

we have

$$\operatorname{var} \mu_{k} = \frac{\alpha_{k} \left(\left(\sum_{k=1}^{K} \alpha_{k} \right) - \alpha_{k} \right)}{\left(\sum_{k=1}^{K} \alpha_{k} \right)^{2} \left(\sum_{k=1}^{K} \alpha_{k} + 1 \right)},$$

$$\operatorname{cov}(\mu_{k}, \mu_{k'}) = -\frac{\alpha_{k} \alpha_{k'}}{\left(\sum_{k=1}^{K} \alpha_{k} \right)^{2} \left(\sum_{k=1}^{K} \alpha_{k} + 1 \right)}.$$
(2.96)

2.11

Let μ be a variable such that

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

Then, by the definition,

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

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

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

where

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

Therefore,

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

2.12

Let x be a variable such that

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

where a < b. Then

$$\int_{a}^{b} p(x)dx = 1. (2.104)$$

Then, by the definition,

$$E x = \frac{1}{b-a} \int_a^b x dx,$$

$$E x^2 = \frac{1}{b-a} \int_a^b x^2 dx.$$
(2.105)

Then,

$$E x = \frac{1}{2}(a+b),$$

$$E x^{2} = \frac{1}{3}(a^{2} + ab + b^{2}).$$
(2.106)

Since

$$var x = E x^2 - (E x)^2, (2.107)$$

we have

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

2.13

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

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

$$q(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mathbf{m}, \mathbf{L}).$$
(2.109)

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

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

Note that

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

The right hand side can be written as

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

Then, the integral can be written as

$$\frac{1}{2} \ln \left| \frac{\det \mathbf{\Sigma}}{\det \mathbf{L}} \right| \int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x}
+ \frac{1}{2} \int (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x}
- \frac{1}{2} \int (\mathbf{x} - \mathbf{m})^{\mathsf{T}} \mathbf{L}^{-1} (\mathbf{x} - \mathbf{m}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x}.$$
(2.113)

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

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

we have

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

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

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

Since

$$(\mathbf{x} - \mathbf{m})^{\mathsf{T}} \mathbf{L}^{-1} (\mathbf{x} - \mathbf{m}) = (\mathbf{x} - \boldsymbol{\mu} + \boldsymbol{\mu} - \mathbf{m})^{\mathsf{T}} \mathbf{L}^{-1} (\mathbf{x} - \boldsymbol{\mu} + \boldsymbol{\mu} - \mathbf{m}), \quad (2.117)$$

the integral of the third term can be written as

$$\int (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{L}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x}$$

$$+ 2(\boldsymbol{\mu} - \mathbf{m})^{\mathsf{T}} \mathbf{L}^{-1} \int (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x}$$

$$+ (\boldsymbol{\mu} - \mathbf{m})^{\mathsf{T}} \mathbf{L}^{-1} (\boldsymbol{\mu} - \mathbf{m}) \int \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x}$$

$$= \operatorname{tr} (\mathbf{L}^{-1} \boldsymbol{\Sigma}) + (\boldsymbol{\mu} - \mathbf{m})^{\mathsf{T}} \mathbf{L}^{-1} (\boldsymbol{\mu} - \mathbf{m}).$$
(2.118)

Therefore,

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

2.14

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

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

In order to maximise H(x) with the constratints

$$\int p(\mathbf{x})d\mathbf{x} = 1,$$

$$\int \mathbf{x}p(\mathbf{x})d\mathbf{x} = \boldsymbol{\mu},$$

$$\int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}}p(\mathbf{x})d\mathbf{x} = \boldsymbol{\Sigma},$$
(2.121)

let

$$L(p) = H(\mathbf{x}) + \lambda \left(\int p(\mathbf{x}) d\mathbf{x} - 1 \right) + \mathbf{l}^{\mathsf{T}} \left(\int \mathbf{x} p(\mathbf{x}) d\mathbf{x} - \boldsymbol{\mu} \right)$$
$$+ \mathbf{m}^{\mathsf{T}} \left(\int (\mathbf{x} - \boldsymbol{\mu}) (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x} - \boldsymbol{\Sigma} \right) \mathbf{m}.$$
(2.122)

Setting the variation with respect to p to zero gives

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

Then,

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

so that

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

where

$$c = \exp(-1 + \lambda - \mathbf{l}^{\mathsf{T}}\mathbf{M}\mathbf{l}),$$

$$\mathbf{M} = -(\mathbf{m}\mathbf{m}^{\mathsf{T}})^{-1}.$$
(2.126)

Substituting it to the constraints and the transformation

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

gives

$$c \int \exp(-\mathbf{y}^{\mathsf{T}} \mathbf{M}^{-1} \mathbf{y}) d\mathbf{y} = 1,$$

$$c \int (\mathbf{y} + \boldsymbol{\mu} + \mathbf{M} \mathbf{l}) \exp(-\mathbf{y}^{\mathsf{T}} \mathbf{M}^{-1} \mathbf{y}) d\mathbf{y} = \boldsymbol{\mu},$$

$$c \int (\mathbf{y} + \mathbf{M} \mathbf{l}) (\mathbf{y} + \mathbf{M} \mathbf{l})^{\mathsf{T}} \exp(-\mathbf{y}^{\mathsf{T}} \mathbf{M}^{-1} \mathbf{y}) d\mathbf{y} = \boldsymbol{\Sigma}.$$
(2.128)

Since

$$\int \exp(-\mathbf{y}^{\mathsf{T}}\mathbf{y}) d\mathbf{y} = \left(\Gamma\left(\frac{1}{2}\right)\right)^{D},$$

$$\int \mathbf{y} \exp(-\mathbf{y}^{\mathsf{T}}\mathbf{y}) d\mathbf{y} = \mathbf{0},$$

$$\int \mathbf{y} \mathbf{y}^{\mathsf{T}} \exp(-\mathbf{y}^{\mathsf{T}}\mathbf{y}) d\mathbf{y} = \Gamma\left(\frac{3}{2}\right) \left(\Gamma\left(\frac{1}{2}\right)\right)^{D-1} \mathbf{I},$$
(2.129)

they can be written as

$$c\left(\Gamma\left(\frac{1}{2}\right)\right)^{D} |\det \mathbf{M}|^{\frac{1}{2}} = 1,$$

$$c(\boldsymbol{\mu} + \mathbf{Ml}) \left(\Gamma\left(\frac{1}{2}\right)\right)^{D} |\det \mathbf{M}|^{\frac{1}{2}} = \boldsymbol{\mu},$$

$$c\left(\Gamma\left(\frac{3}{2}\right) \left(\Gamma\left(\frac{1}{2}\right)\right)^{D-1} \mathbf{M} + \mathbf{Ml}(\mathbf{Ml})^{\mathsf{T}} \left(\Gamma\left(\frac{1}{2}\right)\right)^{D} |\det \mathbf{M}|^{\frac{1}{2}} = \boldsymbol{\Sigma}.$$

$$(2.130)$$

Then,

$$\lambda = 1 - \frac{D}{2} \ln \pi - \frac{1}{2} \ln |\det \mathbf{M}|,$$

$$\mathbf{l} = \mathbf{0},$$

$$\mathbf{M} = 2\Sigma.$$
(2.131)

Therefore,

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

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

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

The right hand side can be written as

$$-\int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) \left(-\frac{D}{2} \ln(2\pi) - \frac{1}{2} \ln|\det \boldsymbol{\Sigma}| - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right) d\mathbf{x}$$

$$= \left(\frac{D}{2} \ln(2\pi) + \frac{1}{2} \ln|\det \boldsymbol{\Sigma}| \right) \int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x}$$

$$+ \frac{1}{2} \int (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x}.$$
(2.135)

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

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

we have

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

Then, the second integral can be written as

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

Therefore,

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

2.16

Let x be a variable such that

$$x = x_1 + x_2, (2.140)$$

where

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

$$\int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu_1 + x_2, \tau_1^{-1}\right) \mathcal{N}\left(x_2|\mu_2, \tau_2^{-1}\right) dx_2$$

$$= \int_{-\infty}^{\infty} \left(\frac{\tau_1}{2\pi}\right)^{\frac{1}{2}} \exp\left(-\frac{\tau_1}{2}(x - \mu_1 - x_2)^2\right) \left(\frac{\tau_2}{2\pi}\right)^{\frac{1}{2}} \exp\left(-\frac{\tau_2}{2}(x_2 - \mu_2)^2\right) dx_2.$$
(2.143)

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

$$-\frac{\tau_1 + \tau_2}{2} \left(x_2 - \frac{\tau_1(x - \mu_1) + \tau_2 \mu_2}{\tau_1 + \tau_2} \right)^2 - \frac{\tau_1}{2} (x - \mu_1)^2 - \frac{\tau_2}{2} \mu_2^2$$

$$+ \frac{\tau_1 + \tau_2}{2} \left(\frac{\tau_1(x - \mu_1) + \tau_2 \mu_2}{\tau_1 + \tau_2} \right)^2$$

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

Then,

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

Therefore, by 1.35,

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

2.17

Let Σ be a matrix and

$$\mathbf{S} = \frac{1}{2} \left(\mathbf{\Sigma}^{-1} + \left(\mathbf{\Sigma}^{-1} \right)^{\mathsf{T}} \right),$$

$$\mathbf{A} = \frac{1}{2} \left(\mathbf{\Sigma}^{-1} - \left(\mathbf{\Sigma}^{-1} \right)^{\mathsf{T}} \right).$$
(2.147)

Then,

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

so that

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

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

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

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

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

Then,

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

Therefore,

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

2.18

(a)

Let Σ be a $D \times D$ real symmetric matrix such that

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

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

$$\overline{\mathbf{u}_d}^{\mathsf{T}} \mathbf{\Sigma} \mathbf{u}_d = \lambda_d, \tag{2.155}$$

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

$$\overline{\mathbf{u}_d}^{\mathsf{T}} \overline{\mathbf{\Sigma}}^{\mathsf{T}} \mathbf{u}_d = \left(\overline{\mathbf{\Sigma}} \overline{\mathbf{u}_d} \right)^{\mathsf{T}} \mathbf{u}_d. \tag{2.156}$$

The right hand side can be written as

$$\overline{\lambda_d} \overline{\mathbf{u}_d}^{\mathsf{T}} \mathbf{u}_d = \overline{\lambda_d}. \tag{2.157}$$

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

(b)

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

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

gives

$$\mathbf{u}_{d'}^{\mathsf{T}} \mathbf{\Sigma} \mathbf{u}_d = \lambda_d \mathbf{u}_{d'}^{\mathsf{T}} \mathbf{u}_d. \tag{2.160}$$

Since Σ is symmetric, the left hand side can be written as

$$\mathbf{u}_{d'}^{\mathsf{T}} \mathbf{\Sigma}^{\mathsf{T}} \mathbf{u}_d = (\mathbf{\Sigma} \mathbf{u}_{d'})^{\mathsf{T}} \mathbf{u}_d. \tag{2.161}$$

The right hand side can be written as $\lambda_{d'} \mathbf{u}_{d'}^{\mathsf{T}} \mathbf{u}_{d}$. Then,

$$\lambda_d \mathbf{u}_{d'}^{\mathsf{T}} \mathbf{u}_d = \lambda_{d'} \mathbf{u}_{d'}^{\mathsf{T}} \mathbf{u}_d. \tag{2.162}$$

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

$$\mathbf{u}_{d'}^{\mathsf{T}}\mathbf{u}_d = 0. \tag{2.163}$$

2.19

Let Σ be a $D \times D$ real symmetric matrix such that

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

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

$$\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_D),
\mathbf{U} = [\mathbf{u}_1 \dots \mathbf{u}_D].$$
(2.165)

Then

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

By 2.18,

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

Then,

$$\Sigma = \mathbf{U}\Lambda\mathbf{U}^{\mathsf{T}}, \Sigma^{-1} = \mathbf{U}\Lambda^{-1}\mathbf{U}^{\mathsf{T}},$$
(2.168)

$$\Sigma = \sum_{d=1}^{D} \lambda_d \mathbf{u}_d \mathbf{u}_d^{\mathsf{T}},$$

$$\Sigma^{-1} = \sum_{d=1}^{D} \frac{1}{\lambda_d} \mathbf{u}_d \mathbf{u}_d^{\mathsf{T}}.$$
(2.169)

Let Σ be a $D \times D$ real symmetric matrix such that

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

where u_1, \dots, u_D are unit vectors. Let

$$\Lambda = \operatorname{diag}(\lambda_1, \cdots, \lambda_D),
\mathbf{U} = [\mathbf{u}_1 \cdots \mathbf{u}_D].$$
(2.171)

By 2.19,

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

where

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

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

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

for any real vector \mathbf{a} is

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

2.21

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

2.22

Let Σ be a $D \times D$ symmetric matrix and

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

Taking the transpose of the both sides gives

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

$$\mathbf{\Lambda}^{\mathsf{T}} = \mathbf{\Lambda}.\tag{2.178}$$

Let Σ be a $D \times D$ real symmetric matrix such that

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

where u_1, \dots, u_D are unit vectors. Let

$$\mathbf{\Lambda}' = \operatorname{diag}\left(\lambda_1^{-\frac{1}{2}}, \cdots, \lambda_D^{-\frac{1}{2}}\right),$$

$$\mathbf{U} = [\mathbf{u}_1 \cdots \mathbf{u}_D].$$
(2.180)

By 2.19,

$$\int_{(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}} \mathbf{\Sigma}^{-1} (\mathbf{x}-\boldsymbol{\mu}) = \Delta} d\mathbf{x} = \int_{(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}} \mathbf{U} \boldsymbol{\Lambda}' \boldsymbol{\Lambda}'^{\mathsf{T}} \mathbf{U}^{\mathsf{T}} (\mathbf{x}-\boldsymbol{\mu}) = \Delta} d\mathbf{x}.$$
 (2.181)

By the transformation

$$\mathbf{y} = \mathbf{\Lambda}'^{\mathsf{T}} \mathbf{U}^{\mathsf{T}} (\mathbf{x} - \boldsymbol{\mu}) \tag{2.182}$$

and the property

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

the right hand side can be written as

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

Therefore,

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

where

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

2.24

Let **A** be a square matrix and **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,

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

$$\mathbf{x} = egin{bmatrix} \mathbf{x}_a \ \mathbf{x}_b \ \mathbf{x}_c \end{bmatrix}, oldsymbol{\mu} = egin{bmatrix} oldsymbol{\mu}_a \ oldsymbol{\mu}_c \end{bmatrix}, oldsymbol{\Sigma} = egin{bmatrix} oldsymbol{\Sigma}_{aa} & oldsymbol{\Sigma}_{ab} & oldsymbol{\Sigma}_{ac} \ oldsymbol{\Sigma}_{ca} & oldsymbol{\Sigma}_{cb} & oldsymbol{\Sigma}_{cc} \end{bmatrix}.$$

Let

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

where

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

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

$$-\frac{1}{2}(\mathbf{x}_{a}-\boldsymbol{\mu}_{a})^{\mathsf{T}}\boldsymbol{\Lambda}_{aa}(\mathbf{x}_{a}-\boldsymbol{\mu}_{a})-\frac{1}{2}(\mathbf{x}_{a}-\boldsymbol{\mu}_{a})^{\mathsf{T}}\boldsymbol{\Lambda}_{ab}(\mathbf{x}_{b}-\boldsymbol{\mu}_{b})$$

$$-\frac{1}{2}(\mathbf{x}_{a}-\boldsymbol{\mu}_{a})^{\mathsf{T}}\boldsymbol{\Lambda}_{ac}(\mathbf{x}_{c}-\boldsymbol{\mu}_{c})-\frac{1}{2}(\mathbf{x}_{b}-\boldsymbol{\mu}_{b})^{\mathsf{T}}\boldsymbol{\Lambda}_{ba}(\mathbf{x}_{a}-\boldsymbol{\mu}_{a})$$

$$-\frac{1}{2}(\mathbf{x}_{c}-\boldsymbol{\mu}_{c})^{\mathsf{T}}\boldsymbol{\Lambda}_{ca}(\mathbf{x}_{a}-\boldsymbol{\mu}_{a}).$$
(2.194)

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

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

where

$$\boldsymbol{\mu}_{a|b,c} = \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ab} (\mathbf{x}_b - \boldsymbol{\mu}_b) - \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ac} (\mathbf{x}_c - \boldsymbol{\mu}_c),$$

$$\boldsymbol{\Sigma}_{a|b,c} = \boldsymbol{\Lambda}_{aa}^{-1}.$$
(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,

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

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

$$-\frac{1}{2} \left(\mathbf{x}_{a} - \boldsymbol{\mu}_{a|b,c} \right)^{\mathsf{T}} \boldsymbol{\Sigma}_{a|b,c}^{-1} \left(\mathbf{x}_{a} - \boldsymbol{\mu}_{a|b,c} \right) - \frac{1}{2} (\mathbf{x}_{c} - \boldsymbol{\mu}_{c})^{\mathsf{T}} \boldsymbol{\Lambda}_{cc} (\mathbf{x}_{c} - \boldsymbol{\mu}_{c})$$

$$= -\frac{1}{2} \mathbf{v}^{\mathsf{T}} \mathbf{M} \mathbf{v},$$
(2.199)

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{x}_{c} - \boldsymbol{\mu}_{c} \\ \mathbf{x}_{a} - \boldsymbol{\mu}_{a} + \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ab} (\mathbf{x}_{b} - \boldsymbol{\mu}_{b}) \end{bmatrix},$$

$$\mathbf{M} = \begin{bmatrix} \boldsymbol{\Lambda}_{cc} + \boldsymbol{\Lambda}_{ac}^{\mathsf{T}} \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ac} & \boldsymbol{\Lambda}_{ac}^{\mathsf{T}} \\ \boldsymbol{\Lambda}_{ac} & \boldsymbol{\Lambda}_{aa} \end{bmatrix}.$$
(2.200)

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{\Lambda}_{cc}^{-1} & -\mathbf{\Lambda}_{cc}^{-1} \mathbf{\Lambda}_{aa}^{\mathsf{T}} \mathbf{\Lambda}_{aa}^{-1} \\ -\mathbf{\Lambda}_{aa}^{-1} \mathbf{\Lambda}_{ac} \mathbf{\Lambda}_{cc}^{-1} & \mathbf{\Lambda}_{aa}^{-1} + \mathbf{\Lambda}_{aa}^{-1} \mathbf{\Lambda}_{ac} \mathbf{\Lambda}_{cc}^{-1} \mathbf{\Lambda}_{ac}^{\mathsf{T}} \mathbf{\Lambda}_{aa}^{-1} \end{bmatrix}.$$
(2.201)

Therefore,

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

where

$$\mu_{a|b} = \mu_a - \Lambda_{aa}^{-1} \Lambda_{ab} \left(\mathbf{x}_b - \mu_b \right),$$

$$\Sigma_{a|b} = \Lambda_{aa}^{-1} + \Lambda_{aa}^{-1} \Lambda_{ac} \Lambda_{cc}^{-1} \Lambda_{ac}^{\mathsf{T}} \Lambda_{aa}^{-1}.$$
(2.203)

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,

$$\begin{bmatrix} -\mathbf{C}^{-1} & \mathbf{D} \\ \mathbf{B} & \mathbf{A} \end{bmatrix}^{-1} = \begin{bmatrix} -\mathbf{N} & \mathbf{N}\mathbf{D}\mathbf{A}^{-1} \\ \mathbf{A}^{-1}\mathbf{B}\mathbf{N} & \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{B}\mathbf{N}\mathbf{D}\mathbf{A}^{-1} \end{bmatrix}, (2.206)$$

where

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

Therefore,

$$\mathbf{M} = \mathbf{A}^{-1} - \mathbf{A}^{-1} \mathbf{B} \mathbf{N} \mathbf{D} \mathbf{A}^{-1}. \tag{2.208}$$

2.27

(a)

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

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

The right hand side can be written as

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

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

(b)

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

$$cov(\mathbf{x} + \mathbf{z}) = \int \int (\mathbf{x} + \mathbf{z} - E(\mathbf{x} + \mathbf{z})) (\mathbf{x} + \mathbf{z} - E(\mathbf{x} + \mathbf{z}))^{\mathsf{T}} p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z}.$$
(2.212)

The right hand side can be written as

$$\int \int (\mathbf{x} - \mathbf{E} \mathbf{x}) (\mathbf{x} - \mathbf{E} \mathbf{x})^{\mathsf{T}} p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z} + \int \int (\mathbf{x} - \mathbf{E} \mathbf{x}) (\mathbf{z} - \mathbf{E} \mathbf{z})^{\mathsf{T}} p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z}
+ \int \int (\mathbf{z} - \mathbf{E} \mathbf{z}) (\mathbf{x} - \mathbf{E} \mathbf{x})^{\mathsf{T}} p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z} + \int \int (\mathbf{z} - \mathbf{E} \mathbf{z}) (\mathbf{z} - \mathbf{E} \mathbf{z})^{\mathsf{T}} p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z}.$$
(2.213)

Each term can be written as

$$\int (\mathbf{x} - \mathbf{E} \, \mathbf{x}) (\mathbf{x} - \mathbf{E} \, \mathbf{x})^{\mathsf{T}} \left(\int p(\mathbf{x}, \mathbf{z}) d\mathbf{z} \right) d\mathbf{x} = \int (\mathbf{x} - \mathbf{E} \, \mathbf{x}) (\mathbf{x} - \mathbf{E} \, \mathbf{x})^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x},$$

$$\int (\mathbf{x} - \mathbf{E} \, \mathbf{x}) p(\mathbf{x}) d\mathbf{x} \int (\mathbf{z} - \mathbf{E} \, \mathbf{z})^{\mathsf{T}} p(\mathbf{z}) d\mathbf{z} = (\mathbf{E} \, \mathbf{x} - \mathbf{E} \, \mathbf{x}) (\mathbf{E} \, \mathbf{z} - \mathbf{E} \, \mathbf{z})^{\mathsf{T}},$$

$$\int (\mathbf{z} - \mathbf{E} \, \mathbf{z}) p(\mathbf{z}) d\mathbf{z} \int (\mathbf{x} - \mathbf{E} \, \mathbf{x})^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x} = (\mathbf{E} \, \mathbf{z} - \mathbf{E} \, \mathbf{z}) (\mathbf{E} \, \mathbf{x} - \mathbf{E} \, \mathbf{x})^{\mathsf{T}},$$

$$\int (\mathbf{z} - \mathbf{E} \, \mathbf{z}) (\mathbf{z} - \mathbf{E} \, \mathbf{z})^{\mathsf{T}} \left(\int p(\mathbf{x}, \mathbf{z}) d\mathbf{x} \right) d\mathbf{z} = \int (\mathbf{z} - \mathbf{E} \, \mathbf{z}) (\mathbf{z} - \mathbf{E} \, \mathbf{z})^{\mathsf{T}} p(\mathbf{z}) d\mathbf{z}.$$

$$(2.214)$$

Therefore,

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

2.28

Let \mathbf{z} be a variable such that

$$\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix},$$

$$\mathbf{E} \mathbf{z} = \begin{bmatrix} \boldsymbol{\mu} \\ \mathbf{A}\boldsymbol{\mu} + \mathbf{b} \end{bmatrix},$$

$$\mathbf{cov} \mathbf{z} = \begin{bmatrix} \boldsymbol{\Lambda}^{-1} & \boldsymbol{\Lambda}^{-1}\mathbf{A}^{\mathsf{T}} \\ \mathbf{A}\boldsymbol{\Lambda}^{-1} & \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\mathsf{T}} \end{bmatrix},$$
(2.216)

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

$$(\cos \mathbf{z})^{-1} = \begin{bmatrix} \mathbf{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A} & -\mathbf{A}^{\mathsf{T}} \mathbf{L} \\ -\mathbf{L} \mathbf{A} & \mathbf{L} \end{bmatrix}.$$

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

$$-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} (\boldsymbol{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A}) (\mathbf{x} - \boldsymbol{\mu}) + \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} \mathbf{L} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b})$$

$$+ \frac{1}{2}(\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b})^{\mathsf{T}} \mathbf{L} \mathbf{A} (\mathbf{x} - \boldsymbol{\mu}) - \frac{1}{2}(\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b})^{\mathsf{T}} \mathbf{L} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b})$$

$$= -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} (\boldsymbol{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A}) (\mathbf{x} - \boldsymbol{\mu}) +$$

$$-\frac{1}{2}(\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b} - \mathbf{A} (\mathbf{x} - \boldsymbol{\mu}))^{\mathsf{T}} \mathbf{L} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b} - \mathbf{A} (\mathbf{x} - \boldsymbol{\mu}))$$

$$+ \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A} (\mathbf{x} - \boldsymbol{\mu}).$$
(2.217)

The right hand side can be written as

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

Therefore,

$$p(\mathbf{x}) = \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}\right),$$

$$p(\mathbf{y}|\mathbf{x}) = \mathcal{N}\left(\mathbf{y}|\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1}\right).$$
(2.219)

2.29

Let

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

By 2.24,

$$\mathbf{R}^{-1} = \begin{bmatrix} \mathbf{\Lambda}^{-1} & \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \\ \mathbf{A}\mathbf{\Lambda}^{-1} & \mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \end{bmatrix}.$$
 (2.221)

2.30

Let

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

Then,

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

2.31

Let y be a variable such that

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

where

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

$$p(\mathbf{z}) = \mathcal{N} \left(\mathbf{z} | \boldsymbol{\mu}_{\mathbf{z}}, \boldsymbol{\Sigma}_{\mathbf{z}} \right).$$
(2.225)

By marginalisation,

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

The right hand side can be written as

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

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

$$-\frac{1}{2}(\mathbf{y} - \mathbf{x} - \boldsymbol{\mu}_{\mathbf{z}})^{\mathsf{T}} \boldsymbol{\Sigma}_{\mathbf{z}}^{-1} (\mathbf{y} - \mathbf{x} - \boldsymbol{\mu}_{\mathbf{z}}) - \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_{\mathbf{x}})^{\mathsf{T}} \boldsymbol{\Sigma}_{\mathbf{x}}^{-1} (\mathbf{x} - \boldsymbol{\mu}_{\mathbf{x}}). \quad (2.228)$$

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

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

where

$$\mathbf{u} = \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix},$$

$$\mathbf{R} = \begin{bmatrix} \mathbf{\Sigma}_{\mathbf{x}}^{-1} + \mathbf{\Sigma}_{\mathbf{z}}^{-1} & -\mathbf{\Sigma}_{\mathbf{z}}^{-1} \\ -\mathbf{\Sigma}_{\mathbf{z}}^{-1} & \mathbf{\Sigma}_{\mathbf{z}}^{-1} \end{bmatrix},$$

$$\mathbf{v} = \begin{bmatrix} \mathbf{\Sigma}_{\mathbf{x}}^{-1} \boldsymbol{\mu}_{\mathbf{x}} - \mathbf{\Sigma}_{\mathbf{z}}^{-1} \boldsymbol{\mu}_{\mathbf{z}} \\ \mathbf{\Sigma}_{\mathbf{z}}^{-1} \boldsymbol{\mu}_{\mathbf{z}} \end{bmatrix},$$
(2.230)

By 2.29 and 2.30,

$$\mathbf{R}^{-1} = \begin{bmatrix} \mathbf{\Sigma}_{\mathbf{x}} & \mathbf{\Sigma}_{\mathbf{x}} \\ \mathbf{\Sigma}_{\mathbf{x}} & \mathbf{\Sigma}_{\mathbf{x}} + \mathbf{\Sigma}_{\mathbf{z}} \end{bmatrix},$$

$$\mathbf{R}^{-1}\mathbf{v} = \begin{bmatrix} \boldsymbol{\mu}_{\mathbf{x}} \\ \boldsymbol{\mu}_{\mathbf{x}} + \boldsymbol{\mu}_{\mathbf{z}} \end{bmatrix}.$$
(2.231)

Therefore,

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

2.32

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

$$p(\mathbf{x}) = \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}\right),$$

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

$$-\frac{1}{2} (\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b})^{\mathsf{T}} \mathbf{L} (\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b}) - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})$$

$$= -\frac{1}{2} (\mathbf{y} - \mathbf{A}(\mathbf{x} - \boldsymbol{\mu}) - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})^{\mathsf{T}} \mathbf{L} (\mathbf{y} - \mathbf{A}(\mathbf{x} - \boldsymbol{\mu}) - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}) \qquad (2.235)$$

$$-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu}).$$

The right hand side can be written as

$$-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} (\boldsymbol{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A}) (\mathbf{x} - \boldsymbol{\mu}) + (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} \mathbf{L} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b})$$

$$-\frac{1}{2} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b})^{\mathsf{T}} \mathbf{L} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b})$$

$$= -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu} - \mathbf{z})^{\mathsf{T}} (\boldsymbol{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A}) (\mathbf{x} - \boldsymbol{\mu} - \mathbf{z}) + \frac{1}{2} \mathbf{z}^{\mathsf{T}} (\boldsymbol{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A}) \mathbf{z}$$

$$-\frac{1}{2} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b})^{\mathsf{T}} \mathbf{L} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b}),$$
(2.236)

where

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

The right hand side can be written as

$$-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu} - \mathbf{z})^{\mathsf{T}} (\boldsymbol{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A}) (\mathbf{x} - \boldsymbol{\mu} - \mathbf{z})$$

$$-\frac{1}{2}(\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b})^{\mathsf{T}} \mathbf{M} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b}),$$
(2.238)

where

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

We have

$$\mu + z = (\Lambda + A^{\mathsf{T}}LA)^{-1} ((\Lambda + A^{\mathsf{T}}LA) \mu + A^{\mathsf{T}}L(y - A\mu - b)).$$
 (2.240)

Then,

$$\mu + \mathbf{z} = (\mathbf{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A})^{-1} (\mathbf{A}^{\mathsf{T}} \mathbf{L} (\mathbf{y} - \mathbf{b}) + \mathbf{\Lambda} \mu).$$
 (2.241)

By 2.26,

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

Then,

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

The right hand side can be written as

$$\mathbf{L} - \mathbf{L} \left(\mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} - \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \left(\mathbf{L}^{-1} + \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \right)^{-1} \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \right) \mathbf{L}$$

$$= \mathbf{L} - \mathbf{L} \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \left(\mathbf{L}^{-1} + \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \right)^{-1} \left(\mathbf{L}^{-1} + \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} - \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \right) \mathbf{L}.$$
(2.244)

The right hand side can be written as

$$\mathbf{L} - \mathbf{L} \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \left(\mathbf{L}^{-1} + \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \right)^{-1}$$

$$= \mathbf{L} \left(\mathbf{L}^{-1} + \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} - \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \right) \left(\mathbf{L}^{-1} + \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \right)^{-1}.$$
(2.245)

Then,

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

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

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

$$p(\mathbf{x}) = \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}\right),$$

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

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

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

$$-\frac{1}{2} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \mathbf{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A} & -\mathbf{A}^{\mathsf{T}} \mathbf{L} \\ -\mathbf{L} \mathbf{A} & \mathbf{L} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} + \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} -\mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{b} + \mathbf{\Lambda} \boldsymbol{\mu} \\ \mathbf{L} \mathbf{b} \end{bmatrix}. \quad (2.251)$$

By 2.24,

$$\begin{bmatrix} \mathbf{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A} & -\mathbf{A}^{\mathsf{T}} \mathbf{L} \\ -\mathbf{L} \mathbf{A} & \mathbf{L} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{\Lambda}^{-1} & \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \\ \mathbf{A} \mathbf{\Lambda}^{-1} & \mathbf{L}^{-1} + \mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathsf{T}} \end{bmatrix}, \quad (2.252)$$

so that

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

Then,

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

By 2.25,

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

We have

$$\mu + (\mathbf{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A})^{-1} \mathbf{A}^{\mathsf{T}} \mathbf{L} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b})$$

$$= (\mathbf{\Lambda} + \mathbf{A}^{\mathsf{T}} \mathbf{L} \mathbf{A})^{-1} (\mathbf{\Lambda} \boldsymbol{\mu} + \mathbf{A}^{\mathsf{T}} \mathbf{L} (\mathbf{y} - \mathbf{b})).$$
(2.256)

Therefore,

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

2.34

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

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

Then,

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

By 3.21(a), setting the derivatives with respect to μ and Σ to zero gives

$$\mathbf{0} = \sum_{n=1}^{N} \left(\mathbf{\Sigma}^{-1} + \left(\mathbf{\Sigma}^{-1} \right)^{\mathsf{T}} \right) (\mathbf{x}_{n} - \boldsymbol{\mu}),$$

$$\mathbf{O} = -\frac{N}{2} \left(\mathbf{\Sigma}^{-1} \right)^{\mathsf{T}} + \frac{1}{2} \left(\mathbf{\Sigma}^{-1} \right)^{2} \sum_{n=1}^{N} (\mathbf{x}_{n} - \boldsymbol{\mu}) (\mathbf{x}_{n} - \boldsymbol{\mu})^{\mathsf{T}}.$$

$$(2.260)$$

Therefore, the maximum likelihood solutions for μ and Σ are given by

$$\boldsymbol{\mu}_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_{n},$$

$$\boldsymbol{\Sigma}_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_{n} - \boldsymbol{\mu}_{\mathrm{ML}}) (\mathbf{x}_{n} - \boldsymbol{\mu}_{\mathrm{ML}})^{\mathsf{T}}.$$
(2.261)

2.35

(a)

Let \mathbf{x} be a variable such that

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

Then,

$$\mathbf{E} \mathbf{x} \mathbf{x}^{\mathsf{T}} = \mathbf{E} (\mathbf{x} - \boldsymbol{\mu} + \boldsymbol{\mu}) (\mathbf{x} - \boldsymbol{\mu} + \boldsymbol{\mu})^{\mathsf{T}}. \tag{2.263}$$

The right hand side can be written as

$$E(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} + \boldsymbol{\mu} E(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} + E(\mathbf{x} - \boldsymbol{\mu})\boldsymbol{\mu}^{\mathsf{T}} + \boldsymbol{\mu}\boldsymbol{\mu}^{\mathsf{T}}. \tag{2.264}$$

Since

$$\begin{aligned}
\mathbf{E} \mathbf{x} &= \boldsymbol{\mu}, \\
\cos \mathbf{x} &= \boldsymbol{\Sigma},
\end{aligned} (2.265)$$

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

$$\mathbf{E} \mathbf{x} \mathbf{x}^{\mathsf{T}} = \mathbf{\Sigma} + \boldsymbol{\mu} \boldsymbol{\mu}^{\mathsf{T}}. \tag{2.266}$$

(b)

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

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

$$p(\mathbf{x}_m) = \mathcal{N}(\mathbf{x}_m | \boldsymbol{\mu}, \boldsymbol{\Sigma}).$$
(2.267)

If $n \neq m$, then

$$\mathbf{E}\,\mathbf{x}_n\mathbf{x}_m^{\mathsf{T}} = \mathbf{E}\,\mathbf{x}_n\,\mathbf{E}\,\mathbf{x}_m^{\mathsf{T}}.\tag{2.268}$$

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

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

(c)

Let $\mathbf{x}_1, \dots, \mathbf{x}_N$ 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 μ and Σ are given by

$$\boldsymbol{\mu}_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_{n},$$

$$\boldsymbol{\Sigma}_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_{n} - \boldsymbol{\mu}_{\mathrm{ML}}) (\mathbf{x}_{n} - \boldsymbol{\mu}_{\mathrm{ML}})^{\mathsf{T}}.$$
(2.271)

Then,

$$E \Sigma_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} E(\mathbf{x}_{n} - \boldsymbol{\mu}_{\mathrm{ML}}) (\mathbf{x}_{n} - \boldsymbol{\mu}_{\mathrm{ML}})^{\mathsf{T}}.$$
 (2.272)

The right hand side can be written as

$$\frac{1}{N} \sum_{n=1}^{N} \mathbf{E} \mathbf{x}_{n} \mathbf{x}_{n}^{\mathsf{T}} - \frac{1}{N^{2}} \sum_{n=1}^{N} \mathbf{E} \left(\sum_{n=1}^{N} \mathbf{x}_{n} \right) \mathbf{x}_{n}^{\mathsf{T}} - \frac{1}{N^{2}} \sum_{n=1}^{N} \mathbf{E} \mathbf{x}_{n} \left(\sum_{n=1}^{N} \mathbf{x}_{n} \right)^{\mathsf{T}} + \frac{1}{N^{3}} \sum_{n=1}^{N} \mathbf{E} \left(\sum_{n=1}^{N} \mathbf{x}_{n} \right) \left(\sum_{n=1}^{N} \mathbf{x}_{n} \right)^{\mathsf{T}}.$$
(2.273)

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

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

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

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

Then,

$$E \Sigma_{ML} = (\Sigma + \mu \mu^{\mathsf{T}}) + 2\left(-\frac{1}{N}\Sigma - \mu \mu^{\mathsf{T}}\right) + \frac{1}{N}\Sigma + \mu \mu^{\mathsf{T}}.$$
 (2.276)

Therefore,

$$E \Sigma_{\rm ML} = \frac{N-1}{N} \Sigma. \tag{2.277}$$

2.36

Let x_1, \dots, 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

$$\sigma_{\rm ML}^{2(N)} = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu)^2.$$
 (2.279)

The right hand side can be written as

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

Then,

$$\sigma_{\rm ML}^{2(N)} = \sigma_{\rm ML}^{2(N-1)} + \frac{1}{N} \left((x_N - \mu)^2 - \sigma_{\rm ML}^{2(N-1)} \right). \tag{2.281}$$

We have

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

Therefore,

$$\sigma_{\rm ML}^{2(N)} = \sigma_{\rm ML}^{2(N-1)} - \frac{2\left(\sigma_{\rm ML}^{2(N-1)}\right)^{2}}{N} \left(\frac{\partial}{\partial \sigma^{2}} \left(-\ln p(x_{N})\right)\right) \bigg|_{\sigma^{2} = \sigma_{\rm ML}^{2(N-1)}}.$$
(2.283)

2.37

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

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

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

$$\Sigma_{\mathrm{ML}}^{(N)} = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_n - \boldsymbol{\mu}) (\mathbf{x}_n - \boldsymbol{\mu})^{\mathsf{T}}.$$
 (2.285)

The right hand side can be written as

$$\frac{1}{N}(\mathbf{x}_N - \boldsymbol{\mu})(\mathbf{x}_N - \boldsymbol{\mu})^{\mathsf{T}} + \frac{1}{N} \sum_{n=1}^{N-1} (\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{x}_n - \boldsymbol{\mu})^{\mathsf{T}}$$

$$= \frac{1}{N} (\mathbf{x}_N - \boldsymbol{\mu})(\mathbf{x}_N - \boldsymbol{\mu})^{\mathsf{T}} + \frac{N-1}{N} \boldsymbol{\Sigma}_{\mathrm{ML}}^{(N-1)}.$$
(2.286)

Then,

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

By 3.21(a), we have

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

Therefore,

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

2.38

Let x_1, \dots, x_N be variables such that

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

$$p(\mu) = \mathcal{N}\left(\mu|\mu_0, \sigma_0^2\right).$$
(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

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

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

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

Then, the first term can be written as

$$-\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu_{\text{ML}} + \mu_{\text{ML}} - \mu)^2$$

$$= -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu_{\text{ML}})^2 - \frac{\mu_{\text{ML}} - \mu}{\sigma^2} \sum_{n=1}^{N} (x_n - \mu_{\text{ML}}) - \frac{N}{2\sigma^2} (\mu_{\text{ML}} - \mu)^2.$$
(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

$$-\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu_{\rm ML})^2 - \frac{N}{2\sigma^2} (\mu_{\rm ML} - \mu)^2 - \frac{1}{2\sigma_0^2} (\mu - \mu_0)^2$$

$$= -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu_{\rm ML})^2 - \frac{1}{2\sigma_N^2} (\mu - \mu_N)^2 + \frac{\mu_N^2}{2\sigma_N^2} - \frac{N\mu_{\rm ML}^2}{2\sigma^2} - \frac{\mu_0^2}{2\sigma_0^2},$$
(2.295)

where

$$\mu_{N} = \frac{N\sigma_{0}^{2}}{N\sigma_{0}^{2} + \sigma^{2}}\mu_{ML} + \frac{\sigma^{2}}{N\sigma_{0}^{2} + \sigma^{2}}\mu_{0},$$

$$\sigma_{N}^{2} = \frac{\sigma^{2}\sigma_{0}^{2}}{N\sigma_{0}^{2} + \sigma^{2}}.$$
(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, \dots, x_N be variables such that

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

$$p(\mu) = \mathcal{N}\left(\mu|\mu_0, \sigma_0^2\right).$$
(2.298)

(a)

By 2.38,

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

where

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

$$\sigma_N^2 = \frac{\sigma^2 \sigma_0^2}{N\sigma_0^2 + \sigma^2}.$$
(2.300)

Then,

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

Therefore,

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

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

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

Therefore,

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

$$p(x_N|\mu)p(\mu|\mathbf{x}_{N-1})p(\mathbf{x}_{N-1}).$$
 (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

$$-\frac{1}{2\sigma_{N-1}^{2}}(\mu-\mu_{N-1})^{2} - \frac{1}{2\sigma^{2}}(x_{N}-\mu)^{2}$$

$$= -\frac{1}{2}\left(\frac{1}{\sigma_{N-1}^{2}} + \frac{1}{\sigma^{2}}\right)\left(\mu - \frac{\frac{1}{\sigma_{N-1}^{2}}}{\frac{1}{\sigma_{N-1}^{2}} + \frac{1}{\sigma^{2}}}\mu_{N-1} - \frac{\frac{1}{\sigma^{2}}}{\frac{1}{\sigma_{N-1}^{2}} + \frac{1}{\sigma^{2}}}x_{N}\right)^{2}$$

$$+\frac{1}{2}\left(\frac{1}{\sigma_{N-1}^{2}} + \frac{1}{\sigma^{2}}\right)\left(\frac{\frac{1}{\sigma_{N-1}^{2}}}{\frac{1}{\sigma_{N-1}^{2}} + \frac{1}{\sigma^{2}}}\mu_{N-1} + \frac{\frac{1}{\sigma^{2}}}{\frac{1}{\sigma_{N-1}^{2}} + \frac{1}{\sigma^{2}}}x_{N}\right)^{2} - \frac{\mu_{N-1}^{2}}{2\sigma_{N-1}^{2}} - \frac{x_{N}^{2}}{2\sigma^{2}}.$$

$$(2.310)$$

Then,

$$\mu_N = \frac{\frac{1}{\sigma_{N-1}^2}}{\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}} \mu_{N-1} + \frac{\frac{1}{\sigma^2}}{\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}} x_N,$$

$$\sigma_N^2 = \frac{1}{\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}}.$$
(2.311)

Therefore,

$$\frac{\mu_N}{\sigma_N^2} = \frac{\mu_{N-1}}{\sigma_{N-1}^2} + \frac{x_N}{\sigma^2},
\frac{1}{\sigma_N^2} = \frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}.$$
(2.312)

2.40

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

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

$$p(\boldsymbol{\mu}) = \mathcal{N}\left(\boldsymbol{\mu}|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0\right).$$
(2.313)

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

$$\boldsymbol{\mu}_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_{n}, \qquad (2.314)$$

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 ${\bf X}$ and ${\boldsymbol \mu}$ can be written as

$$-\frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_{n}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_{n}-\boldsymbol{\mu})-\frac{1}{2}(\boldsymbol{\mu}-\boldsymbol{\mu}_{0})\boldsymbol{\Sigma}_{0}^{-1}(\boldsymbol{\mu}-\boldsymbol{\mu}_{0})^{\mathsf{T}}.$$
 (2.316)

The first term can be written as

$$-\frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}}+\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}}+\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})$$

$$=-\frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}})-(\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}\sum_{n=1}^{N}(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}})$$

$$-\frac{N}{2}(\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu}).$$
(2.317)

The second term of the right hand side is zero. Then, the logarithm except the terms independent of X and μ can be written as

$$-\frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}}) - \frac{N}{2}(\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_{\mathrm{ML}}-\boldsymbol{\mu})$$

$$-\frac{1}{2}(\boldsymbol{\mu}-\boldsymbol{\mu}_{0})\boldsymbol{\Sigma}_{0}^{-1}(\boldsymbol{\mu}-\boldsymbol{\mu}_{0})^{\mathsf{T}}$$

$$=-\frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}}) - \frac{1}{2}(\boldsymbol{\mu}-\boldsymbol{\mu}_{N})^{\mathsf{T}}\boldsymbol{\Sigma}_{N}^{-1}(\boldsymbol{\mu}-\boldsymbol{\mu}_{N})$$

$$+\frac{1}{2}\boldsymbol{\mu}_{N}^{\mathsf{T}}\boldsymbol{\Sigma}_{N}^{-1}\boldsymbol{\mu}_{N} - \frac{N}{2}\boldsymbol{\mu}_{\mathrm{ML}}^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_{\mathrm{ML}},$$

$$(2.318)$$

where

$$\mu_{N} = (N\Sigma^{-1} + \Sigma_{0}^{-1})^{-1} (N\Sigma^{-1}\mu_{ML} + \Sigma_{0}^{-1}\mu_{0}),$$

$$\Sigma_{N} = (N\Sigma^{-1} + \Sigma_{0}^{-1})^{-1}.$$
(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,

$$Gam(\lambda|a,b) = \frac{b^a}{\Gamma(a)} \lambda^{a-1} \exp(-b\lambda). \tag{2.321}$$

Then,

$$\int_0^\infty \operatorname{Gam}(\lambda|a,b)d\lambda = \frac{b^a}{\Gamma(a)} \int_0^\infty \lambda^{a-1} \exp(-b\lambda)d\lambda. \tag{2.322}$$

By the transformation

$$\lambda' = b\lambda, \tag{2.323}$$

the right hand side can be written as

$$\frac{b^a}{\Gamma(a)} \int_0^\infty \left(\frac{\lambda'}{b}\right)^{a-1} \exp(-\lambda') \frac{1}{b} d\lambda' = \frac{1}{\Gamma(a)} \int_0^\infty {\lambda'}^{a-1} \exp(-\lambda') d\lambda'. \quad (2.324)$$

The right hand side can be written as

$$\frac{1}{\Gamma(a)}\Gamma(a) = 1. \tag{2.325}$$

Therefore,

$$\int_0^\infty \operatorname{Gam}(\lambda|a,b)d\lambda = 1. \tag{2.326}$$

2.42

Let λ be a variable such that

$$p(\lambda) = \operatorname{Gam}(\lambda|a, b). \tag{2.327}$$

By the definition,

$$Gam(\lambda|a,b) = \frac{b^a}{\Gamma(a)} \lambda^{a-1} \exp(-b\lambda).$$
 (2.328)

(a)

We have

$$E \lambda = \frac{b^a}{\Gamma(a)} \int_0^\infty \lambda^a \exp\left(-\frac{\lambda}{b}\right) d\lambda. \tag{2.329}$$

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

$$\frac{1}{b\Gamma(a)}\Gamma(a+1) = \frac{a}{b}.$$
(2.332)

$$E\lambda = \frac{a}{b}. (2.333)$$

(b)

We have

$$E \lambda^{2} = \frac{b^{a}}{\Gamma(a)} \int_{0}^{\infty} \lambda^{a+1} \exp\left(-\frac{\lambda}{b}\right) d\lambda. \tag{2.334}$$

By the transformation

$$\lambda' = b\lambda, \tag{2.335}$$

the right hand side can be written as

$$\frac{b^a}{\Gamma(a)} \int_0^\infty \left(\frac{\lambda'}{b}\right)^{a+1} \exp(-\lambda') \frac{1}{b} d\lambda' = \frac{1}{b^2 \Gamma(a)} \int_0^\infty {\lambda'}^{a+1} \exp(-\lambda') d\lambda'. \quad (2.336)$$

The right hand side can be written as

$$\frac{1}{b^2\Gamma(a)}\Gamma(a+2) = \frac{a(a+1)}{b^2}.$$
 (2.337)

Then,

$$E \lambda^2 = \frac{a(a+1)}{b^2}.$$
 (2.338)

We have

$$\operatorname{var} \lambda = \operatorname{E} \lambda^2 - (\operatorname{E} \lambda)^2. \tag{2.339}$$

Therefore,

$$\operatorname{var} \lambda = \frac{a}{b^2}.\tag{2.340}$$

(c)

Setting the derivative of $Gam(\lambda|a,b)$ 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,

$$\operatorname{mode} \lambda = \frac{a-1}{b}.\tag{2.342}$$

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

$$\frac{q}{\Gamma(\frac{1}{q})} \left(2\sigma^2\right)^{-\frac{1}{q}} \int_0^\infty \exp(-x') \left(2\sigma^2\right)^{\frac{1}{q}} \frac{1}{q} x^{\frac{1}{q}-1} dx'$$

$$= \frac{1}{\Gamma(\frac{1}{q})} \int_0^\infty x^{\frac{1}{q}-1} \exp(-x') dx'.$$
(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,

$$p(x|\sigma^2, 2) = \mathcal{N}(x|0, \sigma^2). \tag{2.350}$$

(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 **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 $p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \sigma^2)$ except the terms independent of \mathbf{w} and σ^2 can be written as

$$-\frac{1}{2\sigma^2} \sum_{n=1}^{N} \left| y(\mathbf{x}_n, \mathbf{w}) - t_n \right|^q - \frac{N}{q} \ln\left(2\sigma^2\right). \tag{2.354}$$

2.44

Let x_1, \dots, x_N be variables such that

$$p(x_n|\mu,\tau) = \mathcal{N}\left(x_n|\mu,\tau^{-1}\right),$$

$$p(\mu,\tau) = \mathcal{N}\left(\mu|\mu_0,(\beta\tau)^{-1}\right) \operatorname{Gam}(\tau|a,b).$$
(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

$$\frac{N}{2}\ln\tau - \frac{\tau}{2}\sum_{n=1}^{N}(x_n - \mu)^2 + \frac{1}{2}\ln\tau - \frac{\beta\tau}{2}(\mu - \mu_0)^2 + (a-1)\ln\tau - b\tau$$

$$= \left(a + \frac{N-1}{2}\right)\ln\tau - \frac{\tau}{2}\sum_{n=1}^{N}(x_n - \mu)^2 - \frac{\beta\tau}{2}(\mu - \mu_0)^2 - b\tau.$$
(2.357)

Let

$$\bar{x} = \frac{1}{N} \sum_{n=1}^{N} x_n. \tag{2.358}$$

Then,

$$\sum_{n=1}^{N} (x_n - \mu)^2 = \sum_{n=1}^{N} (x_n - \bar{x} + \bar{x} - \mu)^2.$$
 (2.359)

The right hand side can be written as

$$\sum_{n=1}^{N} (x_n - \bar{x})^2 + 2(\bar{x} - \mu) \sum_{n=1}^{N} (x_n - \bar{x}) + N(\bar{x} - \mu)^2$$

$$= \sum_{n=1}^{N} (x_n - \bar{x})^2 + N(\bar{x} - \mu)^2.$$
(2.360)

Then, the logarithm except the terms independent of \mathbf{x} , μ and τ can be written as

$$\left(a + \frac{N-1}{2}\right) \ln \tau - \frac{N\tau}{2} (\bar{x} - \mu)^2 - \frac{\beta\tau}{2} (\mu - \mu_0)^2 - b\tau - \frac{\tau}{2} \sum_{n=1}^{N} (x_n - \bar{x})^2.$$
(2.361)

The second and third terms can be written as

$$-\frac{N\tau}{2}(\bar{x}-\mu)^2 - \frac{\beta\tau}{2}(\mu-\mu_0)^2$$

$$= -\frac{(N+\beta)\tau}{2}\left(\mu - \frac{N\bar{x}+\beta\mu_0}{N+\beta}\right)^2 + \frac{(N\bar{x}+\beta\mu_0)^2\tau}{2(N+\beta)} - \frac{N\tau}{2}\bar{x}^2 - \frac{\beta\tau}{2}\mu_0^2.$$
(2.362)

The second, third and forth terms on the right hand side can be written as

$$\frac{(N\bar{x} + \beta\mu_0)^2\tau - (N+\beta)N\tau\bar{x}^2 - (N+\beta)\beta\tau\mu_0^2}{2(N+\beta)} = -\frac{N\beta\tau(\bar{x} - \mu_0)^2}{2(N+\beta)}.$$
(2.363)

Then, the logrithm except the terms independent of \mathbf{x} , μ and τ can be written as

$$-\frac{(N+\beta)\tau}{2} \left(\mu - \frac{N\bar{x} + \beta\mu_0}{N+\beta}\right)^2 + \left(a + \frac{N-1}{2}\right) \ln \tau - \left(b + \frac{N\beta(\bar{x} - \mu_0)^2}{2(N+\beta)} + \frac{1}{2} \sum_{n=1}^{N} (x_n - \bar{x})^2\right) \tau.$$
 (2.364)

$$p(\mu, \tau | \mathbf{x}) = \mathcal{N}\left(\mu | \mu_N, \tau_N^{-1}\right) \operatorname{Gam}\left(\tau | a_N, b_N\right), \qquad (2.365)$$

where

$$\mu_{N} = \frac{N\bar{x} + \beta\mu_{0}}{N + \beta},$$

$$\tau_{N} = (N + \beta)\tau,$$

$$a_{N} = a + \frac{N+1}{2},$$

$$b_{N} = b + \frac{N\beta(\bar{x} - \mu_{0})^{2}}{2(N+\beta)} + \frac{1}{2}\sum_{n=1}^{N}(x_{n} - \bar{x})^{2}.$$
(2.366)

2.45

Let $\mathbf{x}_1, \dots, \mathbf{x}_N$ be variables in D dimensions such that

$$p(\mathbf{x}_n|\mathbf{\Lambda}) = \mathcal{N}\left(\mathbf{x}_n|\boldsymbol{\mu}, \mathbf{\Lambda}^{-1}\right),$$

$$p(\mathbf{\Lambda}) = \mathcal{W}(\mathbf{\Lambda}|\mathbf{W}, \nu),$$
(2.367)

where

$$W(\mathbf{\Lambda}|\mathbf{W},\nu) = B(\mathbf{W},\nu)|\det\mathbf{\Lambda}|^{\frac{\nu-D-1}{2}}\exp\left(-\frac{1}{2}\operatorname{tr}\left(\mathbf{W}^{-1}\mathbf{\Lambda}\right)\right). \tag{2.368}$$

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 Λ can be written as

$$-\frac{N}{2}\ln\left|\det\left(\mathbf{\Lambda}^{-1}\right)\right| - \frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_{n} - \boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Lambda}(\mathbf{x}_{n} - \boldsymbol{\mu})$$

$$+\frac{\nu - D - 1}{2}\ln\left|\det\mathbf{\Lambda}\right| - \frac{1}{2}\operatorname{tr}\left(\mathbf{W}^{-1}\boldsymbol{\Lambda}\right)$$

$$=\frac{\nu + N - D - 1}{2}\ln\left|\det\mathbf{\Lambda}\right| - \frac{1}{2}\operatorname{tr}\left(\left(\mathbf{W}^{-1} + \mathbf{S}\right)\boldsymbol{\Lambda}\right),$$
(2.370)

where

$$\mathbf{S} = \sum_{n=1}^{N} (\mathbf{x}_n - \boldsymbol{\mu}) (\mathbf{x}_n - \boldsymbol{\mu})^{\mathsf{T}}.$$
 (2.371)

Then,

$$p(\mathbf{\Lambda}|\mathbf{X}) = \mathcal{W}\left(\mathbf{\Lambda}|\left(\mathbf{W}^{-1} + \mathbf{S}\right)^{-1}, \nu + N\right).$$
 (2.372)

Therefore, W is a conjugate prior distribution of Λ .

2.46

Let x be a variable such that

$$p(x|\tau) = \mathcal{N}\left(x|\mu, \tau^{-1}\right),$$

$$p(\tau) = \operatorname{Gam}(\tau|a, b).$$
(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

$$\int_{0}^{\infty} (2\pi\tau^{-1})^{-\frac{1}{2}} \exp\left(-\frac{\tau}{2}(x-\mu)^{2}\right) \frac{b^{a}}{\Gamma(a)} \tau^{a-1} \exp(-b\tau) d\tau$$

$$= (2\pi)^{-\frac{1}{2}} \frac{b^{a}}{\Gamma(a)} \int_{0}^{\infty} \tau^{a-\frac{1}{2}} \exp\left(-\left(b + \frac{(x-\mu)^{2}}{2}\right)\tau\right) d\tau.$$
(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

$$\int_{0}^{\infty} \left(\frac{\tau'}{b + \frac{(x-\mu)^{2}}{2}} \right)^{a-\frac{1}{2}} \exp(-\tau') \frac{1}{b + \frac{(x-\mu)^{2}}{2}} d\tau'$$

$$= \Gamma \left(a + \frac{1}{2} \right) \left(b + \frac{(x-\mu)^{2}}{2} \right)^{-a-\frac{1}{2}}.$$
(2.377)

Then,

$$p(x) = (2\pi)^{-\frac{1}{2}} \frac{\Gamma(a + \frac{1}{2})}{\Gamma(a)} b^a \left(b + \frac{(x - \mu)^2}{2} \right)^{-a - \frac{1}{2}}.$$
 (2.378)

By the transformation

$$\nu = 2a,$$

$$\lambda = \frac{a}{b},$$
(2.379)

the right hand side can be written as

$$(2\pi)^{-\frac{1}{2}} \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})} \left(\frac{\nu}{2\lambda}\right)^{-\frac{1}{2}} \left(1 + \frac{(x-\mu)^2}{\frac{\nu}{\lambda}}\right)^{-\frac{\nu+1}{2}}$$

$$= \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})} \left(\frac{\lambda}{\pi\nu}\right)^{\frac{1}{2}} \left(1 + \frac{\lambda}{\nu}(x-\mu)^2\right)^{-\frac{\nu+1}{2}}.$$
(2.380)

Therefore,

$$p(x) = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})} \left(\frac{\lambda}{\pi\nu}\right)^{\frac{1}{2}} \left(1 + \frac{\lambda}{\nu}(x-\mu)^2\right)^{-\frac{\nu+1}{2}}.$$
 (2.381)

2.47

Let

$$\operatorname{St}(x|\mu,\lambda,\nu) = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})} \left(\frac{\lambda}{\pi\nu}\right)^{\frac{1}{2}} \left(1 + \frac{\lambda}{\nu}(x-\mu)^2\right)^{-\frac{\nu+1}{2}}.$$
 (2.382)

By the transformation

$$\frac{1}{y} = \frac{\lambda}{\nu} (x - \mu)^2,$$
 (2.383)

the right hand side except the terms independent of x can be written as

$$\left(1 + \frac{1}{y}\right)^{-\frac{\lambda(x-\mu)^2}{2}y - \frac{1}{2}}.$$
(2.384)

By the property

$$\lim_{x \to \infty} \left(1 + \frac{1}{x} \right)^x = e,\tag{2.385}$$

we have

$$\lim_{y \to \infty} \left(1 + \frac{1}{y} \right)^{-\frac{\lambda(x-\mu)^2}{2}y - \frac{1}{2}} = \exp\left(-\frac{\lambda}{2}(x-\mu)^2 \right). \tag{2.386}$$

$$\lim_{\nu \to \infty} \operatorname{St}(x|\mu, \lambda, \nu) = \mathcal{N}(x|\mu, \lambda^{-1}). \tag{2.387}$$

2.48

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

$$p(\mathbf{x}|\eta) = \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, (\eta\boldsymbol{\Lambda})^{-1}\right),$$

$$p(\eta) = \operatorname{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right).$$
(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

$$\int_{0}^{\infty} (2\pi)^{-\frac{D}{2}} \left| \det(\eta \mathbf{\Lambda})^{-1} \right|^{-\frac{1}{2}} \exp\left(-\frac{\eta}{2} (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{\Lambda} (\mathbf{x} - \boldsymbol{\mu})\right) \frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})} \eta^{\frac{\nu}{2} - 1} \exp\left(-\frac{\nu}{2} \eta\right) d\eta$$

$$= (2\pi)^{-\frac{D}{2}} \frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})} \left| \det \mathbf{\Lambda} \right|^{\frac{1}{2}} \int_{0}^{\infty} \eta^{\frac{D+\nu}{2} - 1} \exp\left(-\frac{\nu + (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{\Lambda} (\mathbf{x} - \boldsymbol{\mu})}{2} \eta\right) d\eta.$$
(2.390)

By the transformation

$$\eta' = \frac{\nu + (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})}{2} \eta, \tag{2.391}$$

the integral of the right hand side can be written as

$$\int_{0}^{\infty} \left(\frac{2\eta'}{\nu + (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})} \right)^{\frac{D+\nu}{2} - 1} \exp(-\eta') \frac{2}{\nu + (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})} d\eta'$$

$$= \left(\frac{2}{\nu + (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})} \right)^{\frac{D+\nu}{2}} \int_{0}^{\infty} \eta'^{\frac{D+\nu}{2} - 1} \exp(-\eta') d\eta'.$$
(2.392)

Then,

$$p(\mathbf{x}) = (2\pi)^{-\frac{D}{2}} \frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})} |\det \mathbf{\Lambda}|^{\frac{1}{2}} \left(\frac{2}{\nu + (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{\Lambda} (\mathbf{x} - \boldsymbol{\mu})} \right)^{\frac{D+\nu}{2}} \Gamma\left(\frac{D+\nu}{2}\right). \tag{2.393}$$

The right hand side can be written as

$$(2\pi)^{-\frac{D}{2}} \frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})} |\det \mathbf{\Lambda}|^{\frac{1}{2}} \left(\frac{\nu}{2}\right)^{-\frac{D}{2}} \left(\frac{\nu}{2}\right)^{\frac{D+\nu}{2}} \left(\frac{2}{\nu + (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{\Lambda} (\mathbf{x} - \boldsymbol{\mu})}\right)^{\frac{D+\nu}{2}}$$

$$= (2\pi)^{-\frac{D}{2}} \frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})} |\det \mathbf{\Lambda}|^{\frac{1}{2}} \left(\frac{\nu}{2}\right)^{-\frac{D}{2}} \left(1 + \frac{(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{\Lambda} (\mathbf{x} - \boldsymbol{\mu})}{\nu}\right)^{-\frac{D+\nu}{2}}.$$

$$(2.394)$$

Therefore,

$$p(\mathbf{x}) = \frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})} \frac{|\det \mathbf{\Lambda}|^{\frac{1}{2}}}{(\pi\nu)^{\frac{D}{2}}} \left(1 + \frac{(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{\Lambda} (\mathbf{x} - \boldsymbol{\mu})}{\nu}\right)^{-\frac{D+\nu}{2}}.$$
 (2.395)

2.49

Let \mathbf{x} be a variable such that

$$p(\mathbf{x}) = \text{St}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}, \boldsymbol{\nu}), \tag{2.396}$$

where

$$\operatorname{St}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Lambda},\nu) = \int \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu},(\eta\boldsymbol{\Lambda})^{-1}\right) \operatorname{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta. \tag{2.397}$$

(a)

We have

$$\mathbf{E}\,\mathbf{x} = \int \mathbf{x} \mathrm{St}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}, \nu) d\mathbf{x}. \tag{2.398}$$

The right hand side can be written as

$$\int \mathbf{x} \left(\int \mathcal{N} \left(\mathbf{x} | \boldsymbol{\mu}, (\eta \boldsymbol{\Lambda})^{-1} \right) \operatorname{Gam} \left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2} \right) d\eta \right) d\mathbf{x}$$

$$= \int \left(\int \mathbf{x} \mathcal{N} \left(\mathbf{x} | \boldsymbol{\mu}, (\eta \boldsymbol{\Lambda})^{-1} \right) d\mathbf{x} \right) \operatorname{Gam} \left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2} \right) d\eta.$$
(2.399)

The right hand side can be written as

$$\boldsymbol{\mu} \int \operatorname{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta = \boldsymbol{\mu}. \tag{2.400}$$

Therefore,

$$\mathbf{E}\,\mathbf{x} = \boldsymbol{\mu}.\tag{2.401}$$

(b)

By (a), we have

$$\operatorname{cov} \mathbf{x} = \int (\mathbf{x} - \boldsymbol{\mu}) (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \operatorname{St}(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Lambda}, \nu) d\mathbf{x}. \tag{2.402}$$

The right hand side can be written as

$$\int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \left(\int \mathcal{N} \left(\mathbf{x} | \boldsymbol{\mu}, (\eta \boldsymbol{\Lambda})^{-1} \right) \operatorname{Gam} \left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2} \right) d\eta \right) d\mathbf{x}$$

$$= \int \left(\int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathcal{N} \left(\mathbf{x} | \boldsymbol{\mu}, (\eta \boldsymbol{\Lambda})^{-1} \right) d\mathbf{x} \right) \operatorname{Gam} \left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2} \right) d\eta.$$
(2.403)

The right hand side can be written as

$$\int (\eta \mathbf{\Lambda})^{-1} \operatorname{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta = \frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma\left(\frac{\nu}{2}\right)} \left(\int \eta^{\frac{\nu}{2}-2} \exp\left(-\frac{\nu}{2}\eta\right) d\eta\right) \mathbf{\Lambda}^{-1}.$$
(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,

$$\operatorname{cov} \mathbf{x} = \frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma\left(\frac{\nu}{2}\right)} \left(\frac{2}{\nu}\right)^{\frac{\nu}{2}-1} \Gamma\left(\frac{\nu}{2}-1\right) \mathbf{\Lambda}^{-1}. \tag{2.407}$$

Therefore,

$$\operatorname{cov} \mathbf{x} = \frac{\nu}{\nu - 2} \mathbf{\Lambda}^{-1}. \tag{2.408}$$

(c)

Setting the derivative of $p(\mathbf{x})$ to zero gives

$$\mathbf{0} = -\frac{1}{2} \left(\mathbf{\Lambda} + \mathbf{\Lambda}^{\mathsf{T}} \right) \left(\mathbf{x} - \boldsymbol{\mu} \right) \int \eta \mathcal{N} \left(\mathbf{x} | \boldsymbol{\mu}, (\eta \mathbf{\Lambda})^{-1} \right) \operatorname{Gam} \left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2} \right) d\eta. \quad (2.409)$$

$$mode \mathbf{x} = \boldsymbol{\mu}. \tag{2.410}$$

2.50

Let

$$\operatorname{St}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Lambda},\nu) = \frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})} \frac{(\det \boldsymbol{\Lambda})^{\frac{1}{2}}}{(\pi\nu)^{\frac{D}{2}}} \left(1 + \frac{(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})}{\nu}\right)^{-\frac{D+\nu}{2}}. \quad (2.411)$$

By the transformation

$$y = \frac{\nu}{(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})},$$
 (2.412)

the right hand side except the terms independent of x can be written as

$$\left(1 + \frac{1}{y}\right)^{-\frac{(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})}{2} y - \frac{D}{2}}$$
(2.413)

By the property

$$\lim_{x \to \infty} \left(1 + \frac{1}{x} \right)^x = e,\tag{2.414}$$

we have

$$\lim_{y \to \infty} \left(1 + \frac{1}{y} \right)^{-\frac{(\mathbf{x} - \boldsymbol{\mu})^\mathsf{T} \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})}{2} y - \frac{D}{2}} = \exp\left(-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\mathsf{T} \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu}) \right). \quad (2.415)$$

Therefore,

$$\lim_{\nu \to \infty} \operatorname{St}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}, \nu) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}). \tag{2.416}$$

2.51

(a)

We have

$$\exp(iA)\exp(-iA) = 1. \tag{2.417}$$

The left hand side can be written as

$$(\cos A + i\sin A)(\cos A - i\sin A) = \cos^2 A + \sin^2 A. \tag{2.418}$$

$$\cos^2 A + \sin^2 A = 1. \tag{2.419}$$

(b)

We have

$$\cos(A - B) = \operatorname{Re}\left(\exp\left(i(A - B)\right)\right). \tag{2.420}$$

The right hand side can be written as

$$\operatorname{Re}\left(\exp(iA)\exp(-iB)\right) = \operatorname{Re}\left((\cos A + i\sin A)(\cos B - i\sin B)\right). \quad (2.421)$$

Therefore,

$$\cos(A - B) = \cos A \cos B + \sin A \sin B. \tag{2.422}$$

(c)

We have

$$\sin(A - B) = \text{Im} (\exp(i(A - B))).$$
 (2.423)

The right hand side can be written as

$$\operatorname{Im}\left(\exp(iA)\exp(-iB)\right) = \left((\cos A + i\sin A)(\cos B - i\sin B)\right). \tag{2.424}$$

Therefore,

$$\sin(A - B) = \sin A \cos B - \cos A \sin B. \tag{2.425}$$

2.52

Let

$$f(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp(m\cos(\theta - \theta_0)),$$
 (2.426)

where

$$I_0(m) = \frac{1}{2\pi} \int_0^{2\pi} \exp(m\cos\theta) d\theta.$$
 (2.427)

By the Taylor series

$$\cos \alpha = 1 - \frac{1}{2}\alpha^2 + O\left(\alpha^4\right), \qquad (2.428)$$

the right hand side can be written as

$$\frac{\exp\left(m\left(1 - \frac{1}{2}(\theta - \theta_0)^2 + O\left((\theta - \theta_0)^4\right)\right)\right)}{\int_0^{2\pi} \exp\left(m\left(1 - \frac{1}{2}\theta^2 + O(\theta^4)\right)\right) d\theta}
= \exp\left(-\frac{m}{2}(\theta - \theta_0)^2\right) \frac{\exp\left(mO\left((\theta - \theta_0)^4\right)\right)}{\int_0^{2\pi} \exp\left(m\left(-\frac{1}{2}\theta^2 + O(\theta^4)\right)\right) d\theta}.$$
(2.429)

$$\lim_{m \to \infty} f(\theta | \theta_0, m) = \mathcal{N}\left(\theta | \theta_0, m^{-1}\right). \tag{2.430}$$

2.53

Let

$$\sum_{n=1}^{N} \sin(\theta_n - \theta_0) = 0. \tag{2.431}$$

The left hand side can be written as

$$\sum_{n=1}^{N} (\sin \theta_n \cos \theta_0 - \cos \theta_n \sin \theta_0) = \cos \theta_0 \sum_{n=1}^{N} \sin \theta_n - \sin \theta_0 \sum_{n=1}^{N} \cos \theta_n. \quad (2.432)$$

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

$$f(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp(m\cos(\theta - \theta_0)),$$
 (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 second derivatives with respect to θ to zero gives

$$0 = -m\sin(\theta - \theta_0)f(\theta|\theta_0, m),$$

$$0 = (m^2\sin^2(\theta - \theta_0) - m\cos(\theta - \theta_0))f(\theta|\theta_0, m).$$
(2.436)

Therefore,

$$\underset{\theta}{\operatorname{argmax}} f(\theta|\theta_0, m) = \theta_0,$$

$$\underset{\theta}{\operatorname{argmin}} f(\theta|\theta_0, m) = \theta_0 - \pi \operatorname{sgn}(\theta_0 - \pi).$$
(2.437)

2.55

(a)

Let $\theta_1, \dots, \theta_N$ be variables such that

$$p(\theta_n) = f(\theta_n | \theta_0, m), \tag{2.438}$$

where

$$f(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp\left(m\cos(\theta - \theta_0)\right),$$

$$I_0(m) = \frac{1}{2\pi} \int_0^{2\pi} \exp(m\cos\theta) d\theta.$$
(2.439)

Then,

$$\ln\left(\prod_{n=1}^{N} p(\theta_n | \theta_0, m)\right) = -\frac{N}{2} \ln\left(2\pi I_0(m)\right) + m \sum_{n=1}^{N} \cos(\theta_n - \theta_0).$$
 (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

$$\theta_0^{\text{ML}} = \arctan\left(\frac{\sum_{n=1}^N \sin \theta_n}{\sum_{n=1}^N \cos \theta_n}\right). \tag{2.442}$$

(b)

Let

$$\bar{r}\cos\bar{\theta} = \frac{1}{N} \sum_{n=1}^{N} \cos\theta_n,$$

$$\bar{r}\sin\bar{\theta} = \frac{1}{N} \sum_{n=1}^{N} \sin\theta_n.$$
(2.443)

By (a),
$$\bar{\theta} = \theta_0^{\text{ML}}. \tag{2.444}$$

We have

$$\frac{1}{N} \sum_{n=1}^{N} \cos\left(\theta_n - \theta_0^{\text{ML}}\right) = \left(\frac{1}{N} \sum_{n=1}^{N} \cos\theta_n\right) \cos\theta_0^{\text{ML}} + \left(\frac{1}{N} \sum_{n=1}^{N} \sin\theta_n\right) \sin\theta_0^{\text{ML}}.$$
(2.445)

The right hand side can be written as

$$\bar{r}\cos^2\bar{\theta} + \bar{r}\sin^2\bar{\theta} = \bar{r}.$$
 (2.446)

Therefore,

$$\frac{1}{N} \sum_{n=1}^{N} \cos\left(\theta_n - \theta_0^{\mathrm{ML}}\right) = \bar{r}.$$
 (2.447)

2.56

(a)

Let

Beta
$$(\mu|a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \mu^{a-1} (1-\mu)^{b-1}.$$
 (2.448)

The right hand side can be written as

$$\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \exp((a-1)\ln\mu + (b-1)\ln(1-\mu))$$
 (2.449)

Therefore, the natural parameters are given by

$$\boldsymbol{\eta} = \begin{bmatrix} a-1 \\ b-1 \end{bmatrix}.$$

(b)

Let

$$Gam(\lambda|a,b) = \frac{b^a}{\Gamma(a)} \lambda^{a-1} \exp(-b\lambda). \tag{2.450}$$

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

$$f(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp\left(m\cos(\theta - \theta_0)\right), \qquad (2.452)$$

where

$$I_0(m) = \frac{1}{2\pi} \int_0^{2\pi} \exp(m\cos\theta) d\theta, \qquad (2.453)$$

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,

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}} (\det \boldsymbol{\Sigma})^{-\frac{1}{2}} \exp\left(-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right). \quad (2.455)$$

Therefore,

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = h(\mathbf{x})g(\boldsymbol{\eta}) \exp\left(\boldsymbol{\eta}^{\mathsf{T}}\mathbf{u}(\mathbf{x})\right), \tag{2.456}$$

where

$$h(\mathbf{x}) = (2\pi)^{-\frac{D}{2}},$$

$$g(\boldsymbol{\eta}) = (\det(-2\boldsymbol{\eta}_2))^{-\frac{1}{2}} \exp\left(\frac{1}{4}\boldsymbol{\eta}_1^{\mathsf{T}}\boldsymbol{\eta}_2^{-1}\boldsymbol{\eta}_1\right),$$

$$\boldsymbol{\eta} = \begin{bmatrix} \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} \\ -\frac{1}{2}\boldsymbol{\Sigma}^{-1} \end{bmatrix},$$

$$\mathbf{u}(\mathbf{x}) = \begin{bmatrix} \mathbf{x} \\ \mathbf{x}\mathbf{x}^{\mathsf{T}} \end{bmatrix}.$$

2.58

Let \mathbf{x} be a variable such that

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta}) \exp\left(\boldsymbol{\eta}^{\mathsf{T}}\mathbf{u}(\mathbf{x})\right). \tag{2.457}$$

Then, taking the first derivative of

$$\int p(\mathbf{x}|\boldsymbol{\eta})d\mathbf{x} = 1 \tag{2.458}$$

with respect to η gives

$$\nabla g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp(\boldsymbol{\eta}^{\mathsf{T}} \mathbf{u}(\mathbf{x})) d\mathbf{x} + g(\boldsymbol{\eta}) \int \mathbf{u}(\mathbf{x}) h(\mathbf{x}) \exp(\boldsymbol{\eta}^{\mathsf{T}} \mathbf{u}(\mathbf{x})) d\mathbf{x} = \mathbf{0}.$$
(2.459)

The left hand side can be written as

$$\frac{\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} \int p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} + \int \mathbf{u}(\mathbf{x}) p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} = \frac{\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} + \mathbf{E} \mathbf{u}(\mathbf{x}).$$
(2.460)

Therefore,

$$\mathbf{E}\,\mathbf{u}(\mathbf{x}) = -\frac{\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})}.\tag{2.461}$$

Thus,

$$\mathbf{E}\,\mathbf{u}(\mathbf{x}) = -\nabla \ln g(\boldsymbol{\eta}). \tag{2.462}$$

Taking the second derivative with respect to η gives

$$\nabla \nabla g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp(\boldsymbol{\eta}^{\mathsf{T}} \mathbf{u}(\mathbf{x})) d\mathbf{x} + 2\nabla g(\boldsymbol{\eta}) \int \mathbf{u}(\mathbf{x})^{\mathsf{T}} h(\mathbf{x}) \exp(\boldsymbol{\eta}^{\mathsf{T}} \mathbf{u}(\mathbf{x})) d\mathbf{x}$$
$$+ g(\boldsymbol{\eta}) \int \mathbf{u}(\mathbf{x}) \mathbf{u}(\mathbf{x})^{\mathsf{T}} h(\mathbf{x}) \exp(\boldsymbol{\eta}^{\mathsf{T}} \mathbf{u}(\mathbf{x})) d\mathbf{x} = \mathbf{O}.$$
(2.463)

The left hand side can be written as

$$\frac{\nabla \nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} \int p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} + \frac{2\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} \int \mathbf{u}(\mathbf{x})^{\mathsf{T}} p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} + \int \mathbf{u}(\mathbf{x}) \mathbf{u}(\mathbf{x})^{\mathsf{T}} p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x}
= \frac{\nabla \nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} - 2 \operatorname{E} \mathbf{u}(\mathbf{x}) \operatorname{E} \mathbf{u}(\mathbf{x})^{\mathsf{T}} + \operatorname{E} (\mathbf{u}(\mathbf{x}) \mathbf{u}(\mathbf{x})^{\mathsf{T}}).$$
(2.464)

Therefore,

$$E(\mathbf{u}(\mathbf{x})\mathbf{u}(\mathbf{x})^{\mathsf{T}}) = -\frac{\nabla \nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} + \frac{2\nabla g(\boldsymbol{\eta})(\nabla g(\boldsymbol{\eta}))^{\mathsf{T}}}{g^2(\boldsymbol{\eta})}.$$
 (2.465)

By the definition,

$$\operatorname{cov} \mathbf{u}(\mathbf{x}) = \operatorname{E} (\mathbf{u}(\mathbf{x})\mathbf{u}(\mathbf{x})^{\mathsf{T}}) - \operatorname{E} \mathbf{u}(\mathbf{x})\operatorname{E} \mathbf{u}(\mathbf{x})^{\mathsf{T}}. \tag{2.466}$$

Thus,

$$\operatorname{cov} \mathbf{u}(\mathbf{x}) = -\frac{\nabla \nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} + \frac{\nabla g(\boldsymbol{\eta})(\nabla g(\boldsymbol{\eta}))^{\mathsf{T}}}{g^2(\boldsymbol{\eta})}.$$
 (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

$$\mathbf{x} \in \mathcal{R}_i \Rightarrow p(\mathbf{x}) = h_i,$$
 (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

$$\frac{n_i}{h_i} + \lambda \Delta_i = 0,$$

$$\sum_i h_i \Delta_i - 1 = 0.$$
(2.480)

Then,

$$\lambda = -N,$$

$$h_i = \frac{n_i}{N\Delta_i}.$$
(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 $\mathbf{x}_1, \dots, \mathbf{x}_N$ be observations. Let

$$p(\mathbf{x}) = \frac{K}{NV(\mathbf{x})},\tag{2.482}$$

where

$$V(\mathbf{x}) = \int_{\|\mathbf{x}' - \mathbf{x}\| \le \|\mathbf{x}_{(K)} - \mathbf{x}\|} d\mathbf{x}', \qquad (2.483)$$

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,

$$tanh a = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)}.$$
(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,

$$tanh a = 2\sigma(2a) - 1,$$
(3.3)

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}. (3.4)$$

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

$$w_0 + \sum_{m=1}^{M} w_m \frac{1 + \tanh\left(\frac{x - \mu_m}{2s}\right)}{2} = w_0 + \frac{1}{2} \sum_{m=1}^{M} w_m + \frac{1}{2} \sum_{m=1}^{M} w_m \tanh\left(\frac{x - \mu_m}{2s}\right).$$
(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

$$u_0 = w_0 + \frac{1}{2} \sum_{m=1}^{M} w_m,$$

$$u_m = \frac{1}{2} w_m.$$
(3.8)

3.2 (Incomplete)

Let Φ be an $N \times M$ matarix. Then, for any vector \mathbf{v} in N dimensions,

$$\mathbf{\Phi} \left(\mathbf{\Phi}^{\mathsf{T}}\mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^{\mathsf{T}}\mathbf{v} \tag{3.9}$$

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,

$$(\mathbf{\Phi}^{\mathsf{T}}\mathbf{\Phi})^{-1}\mathbf{\Phi}^{\mathsf{T}}\mathbf{t} \tag{3.10}$$

is an orthogonal projection of ${\bf t}$ onto the space spanned by the columns of ${\bf \Phi}$?

3.3

Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} r_n \left(t_n - \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_n) \right)^2.$$
 (3.11)

The right hand side can be written as

$$\frac{1}{2} \|\mathbf{t}' - \mathbf{\Phi}' \mathbf{w}\|^2, \tag{3.12}$$

where

$$\mathbf{t}' = egin{bmatrix} \sqrt{r_1}t_1 \ dots \ \sqrt{r_N}t_N \end{bmatrix}, \mathbf{\Phi}' = egin{bmatrix} \sqrt{r_1}oldsymbol{\phi}(\mathbf{x}_1)^\intercal \ dots \ \sqrt{r_N}oldsymbol{\phi}(\mathbf{x}_N)^\intercal \end{bmatrix}.$$

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

$$\mathbf{0} = -\mathbf{\Phi}^{\prime\mathsf{T}}(\mathbf{t}^{\prime} - \mathbf{\Phi}^{\prime}\mathbf{w}). \tag{3.13}$$

Therefore,

$$\underset{\mathbf{w}}{\operatorname{argmin}} E(\mathbf{w}) = \left(\mathbf{\Phi}^{\prime \mathsf{T}} \mathbf{\Phi}^{\prime}\right)^{-1} \mathbf{\Phi}^{\prime \mathsf{T}} \mathbf{t}^{\prime}. \tag{3.14}$$

3.4 (Incomplete)

Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} (y(\mathbf{x}_n, \mathbf{w}) - t_n)^2, \qquad (3.15)$$

where

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{m=1}^{M} w_m(x_m + \epsilon_m),$$

$$p(\epsilon_m) = \mathcal{N}\left(\epsilon_m | 0, \sigma^2\right).$$
(3.16)

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

$$\mathbf{0} = \sum_{n=1}^{N} \begin{bmatrix} 1 \\ \mathbf{x}_n + \boldsymbol{\epsilon}_n \end{bmatrix} (y(\mathbf{x}_n, \mathbf{w}) - t_n).$$

The right hand side can be written as

$$\sum_{n=1}^{N} \begin{bmatrix} 1 \\ \mathbf{x}_n \end{bmatrix} (y(\mathbf{x}_n, \mathbf{w}) - t_n) + \sum_{n=1}^{N} \begin{bmatrix} 0 \\ \boldsymbol{\epsilon}_n \end{bmatrix} (y(\mathbf{x}_n, \mathbf{w}) - t_n).$$

3.5

Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} (t_n - \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_n))^2.$$
 (3.17)

Then, the minimisation of $E(\mathbf{w})$ under the constraint

$$\sum_{m=1}^{M} \left| w_m \right|^q \le \eta \tag{3.18}$$

reduces to the minimisation of

$$E(\mathbf{w}) + \lambda \left(\sum_{m=1}^{M} |w_m|^q - \eta \right)$$
 (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 $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables in D dimensions such that

$$p(\mathbf{t}_n|\mathbf{y}_n) = \mathcal{N}\left(\mathbf{t}_n|\mathbf{y}_n, \mathbf{\Sigma}\right), \tag{3.22}$$

where

$$\mathbf{y}_n = \mathbf{W}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_n). \tag{3.23}$$

Then,

$$\ln p(\mathbf{T}|\mathbf{Y}) = -\frac{ND}{2}\ln(2\pi) - \frac{N}{2}\ln(\det \Sigma)$$

$$-\frac{1}{2}\sum_{n=1}^{N} (\mathbf{t}_n - \mathbf{W}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n))^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{t}_n - \mathbf{W}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n)).$$
(3.24)

By 3.21(a), setting the derivatives with respect to **W** and Σ to zero gives

$$\mathbf{O} = -\frac{1}{2} \left(\mathbf{\Sigma}^{-1} + \left(\mathbf{\Sigma}^{-1} \right)^{\mathsf{T}} \right) \sum_{n=1}^{N} \left(\mathbf{t}_{n} - \mathbf{W}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_{n}) \right) \left(\boldsymbol{\phi}(\mathbf{x}_{n}) \right)^{\mathsf{T}},$$

$$\mathbf{O} = -\frac{N}{2} \left(\mathbf{\Sigma}^{-1} \right)^{\mathsf{T}} + \frac{1}{2} \left(\mathbf{\Sigma}^{-1} \right)^{2} \sum_{n=1}^{N} \left(\mathbf{t}_{n} - \mathbf{W}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_{n}) \right) \left(\mathbf{t}_{n} - \mathbf{W}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_{n}) \right)^{\mathsf{T}}.$$

$$(3.25)$$

Therefore, the maximum likelihood solutions for W and Σ are given by

$$\mathbf{W}_{\mathrm{ML}} = (\mathbf{\Phi}^{\mathsf{T}}\mathbf{\Phi})^{-1} \mathbf{\Phi}^{\mathsf{T}}\mathbf{t},$$

$$\mathbf{\Sigma}_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{t}_{n} - \mathbf{W}_{\mathrm{ML}}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_{n})) (\mathbf{t}_{n} - \mathbf{W}_{\mathrm{ML}}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_{n}))^{\mathsf{T}}.$$
(3.26)

3.7

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0).$$
 (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 ${\bf t}$ and ${\bf w}$ can be written as

$$-\frac{\beta}{2} \sum_{n=1}^{N} (t_n - \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_n))^2 - \frac{1}{2} (\mathbf{w} - \mathbf{m}_0)^{\mathsf{T}} \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0)$$

$$= -\frac{\beta}{2} (\mathbf{t} - \boldsymbol{\Phi} \mathbf{w})^{\mathsf{T}} (\mathbf{t} - \boldsymbol{\Phi} \mathbf{w}) - \frac{1}{2} (\mathbf{w} - \mathbf{m}_0)^{\mathsf{T}} \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0),$$
(3.29)

where

$$oldsymbol{\Phi} = egin{bmatrix} oldsymbol{\phi}(\mathbf{x}_1)^\intercal \ dots \ oldsymbol{\phi}(\mathbf{x}_N)^\intercal \end{bmatrix}.$$

The right hand side can be written as

$$-\frac{1}{2} (\mathbf{w} - \mathbf{m}_N)^{\mathsf{T}} \mathbf{S}_N^{-1} (\mathbf{w} - \mathbf{m}_N) + \frac{1}{2} \mathbf{m}_N^{\mathsf{T}} \mathbf{S}_N^{-1} \mathbf{m}_N - \frac{\beta}{2} \mathbf{t}^{\mathsf{T}} \mathbf{t} - \frac{1}{2} \mathbf{m}_0^{\mathsf{T}} \mathbf{S}_0^{-1} \mathbf{m}_0, (3.30)$$

where

$$\mathbf{m}_{N} = \mathbf{S}_{N} \left(\mathbf{S}_{0}^{-1} \mathbf{m}_{0} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{t} \right), \mathbf{S}_{N}^{-1} = \mathbf{S}_{0}^{-1} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi}.$$
(3.31)

Therefore,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N). \tag{3.32}$$

3.8

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0).$$
 (3.33)

Then, by 3.7,

$$p(\mathbf{w}|\mathbf{t}_N) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.34}$$

where

$$\mathbf{m}_{N} = \mathbf{S}_{N} \left(\mathbf{S}_{0}^{-1} \mathbf{m}_{0} + \beta \mathbf{\Phi}_{N}^{\mathsf{T}} \mathbf{t}_{N} \right), \mathbf{S}_{N}^{-1} = \mathbf{S}_{0}^{-1} + \beta \mathbf{\Phi}_{N}^{\mathsf{T}} \mathbf{\Phi}_{N}.$$

$$(3.35)$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{t}_{N+1})p(\mathbf{t}_{N+1}) = p(\mathbf{t}_{N+1}|\mathbf{w})p(\mathbf{w}). \tag{3.36}$$

Since t_{N+1} and \mathbf{t}_N are independent, it can be written as

$$p(\mathbf{w}|\mathbf{t}_{N+1})p(t_{N+1})p(\mathbf{t}_N) = p(t_{N+1}|\mathbf{w})p(\mathbf{t}_N|\mathbf{w})p(\mathbf{w}). \tag{3.37}$$

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

$$p(t_{N+1}|\mathbf{w})p(\mathbf{w}|\mathbf{t}_N)p(\mathbf{t}_N). \tag{3.38}$$

Then,

$$p(\mathbf{w}|\mathbf{t}_{N+1})p(t_{N+1}) = p(\mathbf{w}|\mathbf{t}_N)p(t_{N+1}|\mathbf{w}). \tag{3.39}$$

The logarithm of the right hand side except the terms independent of \mathbf{w} can be written as

$$-\frac{1}{2} (\mathbf{w} - \mathbf{m}_{N})^{\mathsf{T}} \mathbf{S}_{N}^{-1} (\mathbf{w} - \mathbf{m}_{N}) - \frac{\beta}{2} (t_{N+1} - \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_{N+1}))^{2}$$

$$= -\frac{1}{2} (\mathbf{w} - \boldsymbol{\mu}_{N+1})^{\mathsf{T}} \boldsymbol{\Lambda}_{N+1} (\mathbf{w} - \boldsymbol{\mu}_{N+1}) + \frac{1}{2} \boldsymbol{\mu}_{N+1}^{\mathsf{T}} \boldsymbol{\Lambda}_{N+1} \boldsymbol{\mu}_{N+1}$$

$$-\frac{1}{2} \mathbf{m}_{N}^{\mathsf{T}} \mathbf{S}_{N}^{-1} \mathbf{m}_{N} - \frac{\beta}{2} t_{N+1}^{2},$$
(3.40)

where

$$\boldsymbol{\mu}_{N+1} = \boldsymbol{\Lambda}_{N+1}^{-1} \left(\mathbf{S}_N^{-1} \mathbf{m}_N + \beta t_{N+1} \boldsymbol{\phi}(\mathbf{x}_{N+1}) \right), \boldsymbol{\Lambda}_{N+1} = \mathbf{S}_N^{-1} + \beta \boldsymbol{\phi}(\mathbf{x}_{N+1}) \boldsymbol{\phi}(\mathbf{x}_{N+1})^{\mathsf{T}}.$$
(3.41)

Therefore,

$$\mu_{N+1} = \mathbf{m}_{N+1},
\Lambda_{N+1} = \mathbf{S}_{N+1}^{-1}.$$
(3.42)

Thus,

$$p(\mathbf{w}|\mathbf{t}_{N+1}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_{N+1}, \mathbf{S}_{N+1}). \tag{3.43}$$

3.9 (Incomplete)

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0).$$
 (3.44)

Then, by 3.7,

$$p(\mathbf{w}|\mathbf{t}_N) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.45}$$

where

$$\mathbf{m}_{N} = \mathbf{S}_{N} \left(\mathbf{S}_{0}^{-1} \mathbf{m}_{0} + \beta \mathbf{\Phi}_{N}^{\mathsf{T}} \mathbf{t}_{N} \right), \mathbf{S}_{N}^{-1} = \mathbf{S}_{0}^{-1} + \beta \mathbf{\Phi}_{N}^{\mathsf{T}} \mathbf{\Phi}_{N}.$$

$$(3.46)$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{t}_{N+1})p(\mathbf{t}_{N+1}) = p(\mathbf{t}_{N+1}|\mathbf{w})p(\mathbf{w}). \tag{3.47}$$

Since t_{N+1} and \mathbf{t}_N are independent, it can be written as

$$p(\mathbf{w}|\mathbf{t}_{N+1})p(t_{N+1})p(\mathbf{t}_N) = p(t_{N+1}|\mathbf{w})p(\mathbf{t}_N|\mathbf{w})p(\mathbf{w}). \tag{3.48}$$

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

$$p(t_{N+1}|\mathbf{w})p(\mathbf{w}|\mathbf{t}_N)p(\mathbf{t}_N). \tag{3.49}$$

Then,

$$p(\mathbf{w}|\mathbf{t}_{N+1})p(t_{N+1}) = p(\mathbf{w}|\mathbf{t}_N)p(t_{N+1}|\mathbf{w}). \tag{3.50}$$

The logarithm of the right hand side except the terms independent of \mathbf{w} can be written as

$$-\frac{1}{2} \left(\mathbf{w} - \mathbf{m}_N \right)^{\mathsf{T}} \mathbf{S}_N^{-1} \left(\mathbf{w} - \mathbf{m}_N \right) - \frac{\beta}{2} \left(t_{N+1} - \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_{N+1}) \right)^2. \tag{3.51}$$

3.10

Let t be a variable such that

$$p(t|\mathbf{w}) = \mathcal{N}\left(t|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_{0}, \mathbf{S}_{0}).$$
(3.52)

Then, by 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.53}$$

where

$$\mathbf{m}_{N} = \mathbf{S}_{N} \left(\mathbf{S}_{0}^{-1} \mathbf{m}_{0} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{t} \right), \mathbf{S}_{N}^{-1} = \mathbf{S}_{0}^{-1} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi}.$$
 (3.54)

By marginalisation,

$$p(t|\mathbf{t}) = \int p(t|\mathbf{w})p(\mathbf{w}|\mathbf{t})d\mathbf{w}.$$
 (3.55)

The logarithm of the integrand of the right hand side except the terms independent of t and \mathbf{w} can be written as

$$-\frac{\beta}{2} \left(t - \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x})\right)^{2} - \frac{1}{2} (\mathbf{w} - \mathbf{m}_{N})^{\mathsf{T}} \mathbf{S}_{N}^{-1} (\mathbf{w} - \mathbf{m}_{N}). \tag{3.56}$$

It can be written as

$$-\frac{1}{2} \begin{bmatrix} \mathbf{w} \\ t \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \mathbf{S}_N^{-1} + \beta \boldsymbol{\phi}(\mathbf{x}) \boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}} & -\beta \boldsymbol{\phi}(\mathbf{x}) \\ -\beta \boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}} & \beta \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ t \end{bmatrix} + \begin{bmatrix} \mathbf{w} \\ t \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \mathbf{S}_N^{-1} \mathbf{m}_N \\ 0 \end{bmatrix} - \frac{1}{2} \mathbf{m}_N^{\mathsf{T}} \mathbf{S}_N^{-1} \mathbf{m}_N.$$

By 2.24,

$$\begin{bmatrix} \mathbf{S}_N^{-1} + \beta \boldsymbol{\phi}(\mathbf{x}) \boldsymbol{\phi}(\mathbf{x})^\intercal & -\beta \boldsymbol{\phi}(\mathbf{x}) \\ -\beta \boldsymbol{\phi}(\mathbf{x})^\intercal & \beta \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{S}_N & \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}) \\ \boldsymbol{\phi}(\mathbf{x})^\intercal \mathbf{S}_N & \frac{1}{\beta} + \boldsymbol{\phi}(\mathbf{x})^\intercal \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}) \end{bmatrix}.$$

Therefore,

$$\begin{bmatrix} \mathbf{S}_N^{-1} + \beta \boldsymbol{\phi}(\mathbf{x}) \boldsymbol{\phi}(\mathbf{x})^\intercal & \beta \boldsymbol{\phi}(\mathbf{x}) \\ \beta \boldsymbol{\phi}(\mathbf{x})^\intercal & \beta \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{S}_N^{-1} \mathbf{m}_N \\ 0 \end{bmatrix} = \begin{bmatrix} \mathbf{m}_N \\ \mathbf{m}_N^\intercal \boldsymbol{\phi}(\mathbf{x}) \end{bmatrix}.$$

Thus,

$$p(t|\mathbf{t}) = \mathcal{N}\left(t|\mathbf{m}_N^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x})\right), \tag{3.57}$$

where

$$\sigma_N^2(\mathbf{x}) = \frac{1}{\beta} + \boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}} \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}). \tag{3.58}$$

3.11

Let t be a variable such that

$$p(t|\mathbf{w}) = \mathcal{N}\left(t|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_{0}, \mathbf{S}_{0}).$$
(3.59)

Then, by 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N),$$
 (3.60)

where

$$\mathbf{m}_{N} = \mathbf{S}_{N} \left(\mathbf{S}_{0}^{-1} \mathbf{m}_{0} + \beta \mathbf{\Phi}_{N}^{\mathsf{T}} \mathbf{t}_{N} \right), \mathbf{S}_{N}^{-1} = \mathbf{S}_{0}^{-1} + \beta \mathbf{\Phi}_{N}^{\mathsf{T}} \mathbf{\Phi}_{N}.$$

$$(3.61)$$

Then, by 3.10,

$$p(t|\mathbf{t}) = \mathcal{N}\left(t \mid \mathbf{m}_{N}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}), \sigma_{N}^{2}(\mathbf{x})\right), \tag{3.62}$$

where

$$\sigma_N^2(\mathbf{x}) = \frac{1}{\beta} + \boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}} \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}). \tag{3.63}$$

Then,

$$\sigma_N^2(\mathbf{x}) - \sigma_{N+1}^2(\mathbf{x}) = \phi(\mathbf{x})^{\mathsf{T}} \left(\mathbf{S}_N - \mathbf{S}_{N+1} \right) \phi(\mathbf{x}). \tag{3.64}$$

By the expression of \mathbf{S}_N above,

$$\mathbf{S}_{N+1} = \left(\mathbf{S}_N^{-1} + \beta \phi(\mathbf{x}_{N+1}) \phi(\mathbf{x}_{N+1})^{\mathsf{T}}\right)^{-1}.$$
 (3.65)

By the identity

$$\left(\mathbf{M} + \mathbf{v}\mathbf{v}^{\mathsf{T}}\right)^{-1} = \mathbf{M}^{-1} - \frac{\left(\mathbf{M}^{-1}\mathbf{v}\right)\left(\mathbf{v}^{\mathsf{T}}\mathbf{M}^{-1}\right)}{1 + \mathbf{v}^{\mathsf{T}}\mathbf{M}^{-1}\mathbf{v}},\tag{3.66}$$

the right hand side can be written as

$$\mathbf{S}_{N} - \frac{\beta \left(\mathbf{S}_{N} \boldsymbol{\phi}(\mathbf{x}_{N+1})\right) \left(\boldsymbol{\phi}(\mathbf{x}_{N+1})^{\mathsf{T}} \mathbf{S}_{N}\right)}{1 + \beta \boldsymbol{\phi}(\mathbf{x}_{N+1}) \mathbf{S}_{N} \boldsymbol{\phi}(\mathbf{x}_{N+1})^{\mathsf{T}}}.$$
(3.67)

Therefore,

$$\phi(\mathbf{x})^{\mathsf{T}}(\mathbf{S}_{N} - \mathbf{S}_{N+1})\phi(\mathbf{x}) = \frac{\beta \left(\phi(\mathbf{x})^{\mathsf{T}} \mathbf{S}_{N} \phi(\mathbf{x}_{N+1})\right)^{2}}{1 + \beta \phi(\mathbf{x}_{N+1}) \mathbf{S}_{N} \phi(\mathbf{x}_{N+1})^{\mathsf{T}}}.$$
 (3.68)

Thus,

$$\sigma_{N+1}^2(\mathbf{x}) \le \sigma_N^2(\mathbf{x}). \tag{3.69}$$

3.12

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w},\beta) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n),\beta^{-1}\right),$$

$$p(\mathbf{w},\beta) = \mathcal{N}\left(\mathbf{w}|\mathbf{m}_0,\beta^{-1}\mathbf{S}_0\right)\operatorname{Gam}(\beta|a_0,b_0),$$
(3.70)

where **w** and ϕ are vectors in M dimensions. By the Bayes' theorem,

$$p(\mathbf{w}, \beta | \mathbf{t}) p(\mathbf{t}) = p(\mathbf{t} | \mathbf{w}, \beta) p(\mathbf{w}, \beta). \tag{3.71}$$

The logarithm of the right hand side except the terms independent of \mathbf{t} , \mathbf{w} and β can be written as

$$-\frac{N}{2}\ln\beta^{-1} - \frac{\beta}{2}\sum_{n=1}^{N}(t_n - \mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n))^2 - \frac{M}{2}\ln\beta^{-1} - \frac{\beta}{2}(\mathbf{w} - \mathbf{m}_0)^{\mathsf{T}}\mathbf{S}_0^{-1}(\mathbf{w} - \mathbf{m}_0)$$

$$+ (a_0 - 1)\ln\beta - b_0\beta$$

$$= -\frac{M}{2}\ln\beta - \frac{\beta}{2}\mathbf{w}^{\mathsf{T}}\left(\mathbf{S}_0^{-1} + \mathbf{\Phi}^{\mathsf{T}}\mathbf{\Phi}\right)\mathbf{w} + \beta\mathbf{w}^{\mathsf{T}}\left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \mathbf{\Phi}^{\mathsf{T}}\mathbf{t}\right) - \frac{\beta}{2}\|\mathbf{t}\|^2 - \frac{\beta}{2}\mathbf{m}_0^{\mathsf{T}}\mathbf{S}_0^{-1}\mathbf{m}_0$$

$$+ \left(a_0 + \frac{N}{2} - 1\right)\ln\beta - b_0\beta.$$
(3.72)

The right hand side can be written as

$$-\frac{M}{2}\ln\beta - \frac{\beta}{2}(\mathbf{w} - \mathbf{m}_N)^{\mathsf{T}}\mathbf{S}_N^{-1}(\mathbf{w} - \mathbf{m}_N) + (a_N - 1)\ln\beta - b_N\beta, \quad (3.73)$$

where

$$\mathbf{m}_{N} = \mathbf{S}_{N} \left(\mathbf{S}_{0}^{-1} \mathbf{m}_{0} + \mathbf{\Phi}^{\mathsf{T}} \mathbf{t} \right),$$

$$\mathbf{S}_{N}^{-1} = \mathbf{S}_{0}^{-1} + \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi},$$

$$a_{N} = a_{0} + \frac{N}{2},$$

$$b_{N} = b_{0} + \frac{1}{2} \|\mathbf{t}\|^{2} + \frac{1}{2} \mathbf{m}_{0}^{\mathsf{T}} \mathbf{S}_{0} \mathbf{m}_{0} - \frac{1}{2} \mathbf{m}_{N}^{\mathsf{T}} \mathbf{S}_{N}^{-1} \mathbf{m}_{N}.$$

$$(3.74)$$

Therefore,

$$p(\mathbf{w}, \beta | \mathbf{t}) = \mathcal{N}\left(\mathbf{w} | \mathbf{m}_N, \beta^{-1} \mathbf{S}_N\right) \operatorname{Gam}(\beta | a_N, b_N).$$
 (3.75)

Substituting it to the result of the Bayes' theorem above, we have

$$p(\mathbf{t}) = \frac{\mathcal{N}\left(\mathbf{t}|\mathbf{\Phi}\mathbf{w}, \beta^{-1}\mathbf{I}\right) \mathcal{N}\left(\mathbf{w}|\mathbf{m}_{0}, \beta^{-1}\mathbf{S}_{0}\right) \operatorname{Gam}(\beta|a_{0}, b_{0})}{\mathcal{N}\left(\mathbf{w}|\mathbf{m}_{N}, \beta^{-1}\mathbf{S}_{N}\right) \operatorname{Gam}(\beta|a_{N}, b_{N})}.$$
 (3.76)

The logarithm of the right hand side can be written as

$$-\frac{N}{2}\ln(2\pi) - \frac{N}{2}\ln\beta^{-1} - \frac{\beta}{2}(\mathbf{t} - \mathbf{\Phi}\mathbf{w})^{\mathsf{T}}(\mathbf{t} - \mathbf{\Phi}\mathbf{w})$$

$$-\frac{M}{2}\ln(2\pi) - \frac{M}{2}\ln\beta^{-1} - \frac{1}{2}\det\mathbf{S}_{0} - \frac{\beta}{2}(\mathbf{w} - \mathbf{m}_{0})^{\mathsf{T}}\mathbf{S}_{0}^{-1}(\mathbf{w} - \mathbf{m}_{0})$$

$$+ a_{0}\ln b_{0} - \ln\Gamma(a_{0}) + (a_{0} - 1)\ln\beta - b_{0}\beta$$

$$+ \frac{M}{2}\ln(2\pi) + \frac{M}{2}\ln\beta^{-1} + \frac{1}{2}\det\mathbf{S}_{N} + \frac{\beta}{2}(\mathbf{w} - \mathbf{m}_{N})^{\mathsf{T}}\mathbf{S}_{N}^{-1}(\mathbf{w} - \mathbf{m}_{0})$$

$$- a_{N}\ln b_{N} + \ln\Gamma(a_{N}) - (a_{N} - 1)\ln\beta + b_{N}\beta$$

$$= -\frac{N}{2}\ln(2\pi) - \frac{1}{2}\det\mathbf{S}_{0} + a_{0}\ln b_{0} - \ln\Gamma(a_{0}) + \frac{1}{2}\det\mathbf{S}_{N} - a_{N}\ln b_{N} + \ln\Gamma(a_{N}).$$
(3.77)

Therefore,

$$p(\mathbf{t}) = (2\pi)^{-\frac{N}{2}} \left(\frac{\det \mathbf{S}_N}{\det \mathbf{S}_0} \right)^{\frac{1}{2}} \frac{\Gamma(a_N)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b_N^{a_N}}.$$
 (3.78)

3.13

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w},\beta) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n),\beta^{-1}\right),$$

$$p(\mathbf{w},\beta) = \mathcal{N}\left(\mathbf{w}|\mathbf{m}_0,\beta^{-1}\mathbf{S}_0\right)\operatorname{Gam}(\beta|a_0,b_0),$$
(3.79)

where **w** and ϕ are vectors in M dimensions. Then, by 3.12,

$$p(\mathbf{w}, \beta | \mathbf{t}) = \mathcal{N}(\mathbf{w} | \mathbf{m}_N, \beta^{-1} \mathbf{S}_N) \operatorname{Gam}(\beta | a_N, b_N),$$
 (3.80)

where

$$\mathbf{m}_{N} = \mathbf{S}_{N} \left(\mathbf{S}_{0}^{-1} \mathbf{m}_{0} + \mathbf{\Phi}^{\mathsf{T}} \mathbf{t} \right),$$

$$\mathbf{S}_{N}^{-1} = \mathbf{S}_{0}^{-1} + \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi},$$

$$a_{N} = a_{0} + \frac{N}{2},$$

$$b_{N} = b_{0} + \frac{1}{2} \|\mathbf{t}\|^{2} + \frac{1}{2} \mathbf{m}_{0}^{\mathsf{T}} \mathbf{S}_{0} \mathbf{m}_{0} - \frac{1}{2} \mathbf{m}_{N}^{\mathsf{T}} \mathbf{S}_{N}^{-1} \mathbf{m}_{N}.$$

$$(3.81)$$

By marginalisation,

$$p(t|\mathbf{t}) = \int \int p(t|\mathbf{w}, \beta)p(\mathbf{w}, \beta|\mathbf{t})d\mathbf{w}d\beta.$$
 (3.82)

The right hand side can be written as

$$\int \left(\int \mathcal{N} \left(t | \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}), \beta^{-1} \right) \mathcal{N} \left(\mathbf{w} | \mathbf{m}_{N}, \beta^{-1} \mathbf{S}_{N} \right) d\mathbf{w} \right) \operatorname{Gam}(\beta | a_{N}, b_{N}) d\beta.$$
(3.83)

The logarithm of the integrand with respect to \mathbf{w} except the terms indepndent of \mathbf{w} can be written as

$$-\frac{\beta}{2} \left(t - \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x})\right)^{2} - \frac{\beta}{2} (\mathbf{w} - \mathbf{m}_{N})^{\mathsf{T}} \mathbf{S}_{N}^{-1} (\mathbf{w} - \mathbf{m}_{N}). \tag{3.84}$$

It can be written as

$$-\frac{\beta}{2} \begin{bmatrix} \mathbf{w} \\ t \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \mathbf{S}_N^{-1} + \boldsymbol{\phi}(\mathbf{x}) \boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}} & -\boldsymbol{\phi}(\mathbf{x}) \\ -\boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ t \end{bmatrix} + \beta \begin{bmatrix} \mathbf{w} \\ t \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \mathbf{S}_N^{-1} \mathbf{m}_N \\ 0 \end{bmatrix} - \frac{\beta}{2} \mathbf{m}_N^{\mathsf{T}} \mathbf{S}_N^{-1} \mathbf{m}_N.$$

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,

$$\begin{bmatrix} \mathbf{S}_N^{-1} + \boldsymbol{\phi}(\mathbf{x})\boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}} & -\boldsymbol{\phi}(\mathbf{x}) \\ -\boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}} & 1 \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{S}_N^{-1}\mathbf{m}_N \\ 0 \end{bmatrix} = \begin{bmatrix} \mathbf{m}_N \\ \mathbf{m}_N^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}) \end{bmatrix}.$$

Therefore, the integral with respect to \mathbf{w} can be written as

$$\mathcal{N}\left(t|\mathbf{m}_{N}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}),\beta^{-1}\left(1+\boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}}\mathbf{S}_{N}\boldsymbol{\phi}(\mathbf{x})\right)\right). \tag{3.85}$$

Then, the logarithm of the integrand with respect to β except the terms independent of β can be written as

$$-\frac{1}{2}\ln\beta^{-1} - \frac{\beta}{2\left(1 + \boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}}\mathbf{S}_{N}\boldsymbol{\phi}(\mathbf{x})\right)} \left(t - \mathbf{m}_{N}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x})\right)^{2} + (a_{N} - 1)\ln\beta - b_{N}\beta$$

$$= \left(a_{N} + \frac{1}{2} - 1\right)\ln\beta - \left(b_{N} + \frac{\left(t - \mathbf{m}_{N}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x})\right)^{2}}{2\left(1 + \boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}}\mathbf{S}_{N}\boldsymbol{\phi}(\mathbf{x})\right)}\right)\beta.$$
(3.86)

Therefore, the integral with respect to β except the terms independent of t can be written as

$$\left(b_N + \frac{\left(t - \mathbf{m}_N^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x})\right)^2}{2\left(1 + \boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}} \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})\right)}\right)^{-a_N - \frac{1}{2}}.$$
(3.87)

Thus,

$$p(t|\mathbf{x}, \mathbf{t}) = \operatorname{St}(t|\mu, \lambda, \nu), \tag{3.88}$$

where

$$\mu = \mathbf{m}_{N}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}),$$

$$\lambda = \frac{a_{N}}{b_{N}} (1 + \boldsymbol{\phi}(\mathbf{x})^{\mathsf{T}} \mathbf{S}_{N} \boldsymbol{\phi}(\mathbf{x}))^{-1},$$

$$\nu = 2a_{N}.$$
(3.89)

3.14 (Incomplete)

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}),$$
(3.90)

where **w** and ϕ are vectors in M dimensions. Then, by 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.91}$$

where

$$\mathbf{m}_{N} = \beta \mathbf{S}_{N} \mathbf{\Phi}^{\mathsf{T}} \mathbf{t}, \mathbf{S}_{N}^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi}.$$
 (3.92)

Let

$$y(\mathbf{x}, \mathbf{w}) = \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}). \tag{3.93}$$

Then,

$$y(\mathbf{x}, \mathbf{m}_N) = \sum_{n=1}^{N} k(\mathbf{x}, \mathbf{x}_n) t_n,$$
 (3.94)

where

$$k(\mathbf{x}, \mathbf{x}') = \beta \phi(\mathbf{x})^{\mathsf{T}} \mathbf{S}_N \phi(\mathbf{x}'). \tag{3.95}$$

Let us suppose that $\phi_j(\mathbf{x})$ are linearly independent, N > M and

$$\phi_0(\mathbf{x}) = 1. \tag{3.96}$$

Then, we can construct a new basis set $\psi_i(\mathbf{x})$ such that

$$\mathbf{\Psi}^{\mathsf{T}}\mathbf{\Psi} = \mathbf{I}?\tag{3.97}$$

$$\sum_{n=1}^{N} \psi_j(\mathbf{x}_n) \psi_k(\mathbf{x}_n) = I_{jk}?$$
(3.98)

where

$$oldsymbol{\Psi} = egin{bmatrix} oldsymbol{\psi}(\mathbf{x}_1)^\intercal \ dots \ oldsymbol{\psi}(\mathbf{x}_N)^\intercal \end{bmatrix}$$

and

$$\psi_0(\mathbf{x}) = 1. \tag{3.99}$$

Under the basis set, if $\alpha = 0$, then

$$\mathbf{S}_N^{-1} = \beta \mathbf{I},\tag{3.100}$$

so that

$$k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\psi}(\mathbf{x})^{\mathsf{T}} \boldsymbol{\psi}(\mathbf{x}'). \tag{3.101}$$

Then,

$$\sum_{n=1}^{N} k(\mathbf{x}, \mathbf{x}_n) = \sum_{n=1}^{N} \sum_{j=0}^{M-1} \psi_j(\mathbf{x}) \psi_j(\mathbf{x}_n) = 1?$$
 (3.102)

3.15

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}),$$
(3.103)

where **w** and ϕ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.104}$$

where

$$\mathbf{m}_{N} = \beta \mathbf{S}_{N} \mathbf{\Phi}^{\mathsf{T}} \mathbf{t}, \mathbf{S}_{N}^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi}.$$
 (3.105)

By 3.19,

$$\ln p(\mathbf{t}) = \frac{M}{2} \ln \alpha + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \mathbf{S}_N) - E(\mathbf{m}_N), \quad (3.106)$$

where

$$E(\mathbf{m}_N) = \frac{\beta}{2} \|\mathbf{t} - \mathbf{\Phi} \mathbf{m}_N\|^2 + \frac{\alpha}{2} \mathbf{m}_N^{\mathsf{T}} \mathbf{m}_N.$$
 (3.107)

By 3.22, setting the derivatives of $\ln p(\mathbf{t})$ with respect to α and β to zero gives

$$\alpha = \frac{\gamma}{\mathbf{m}_{N}^{\mathsf{T}} \mathbf{m}_{N}},$$

$$\beta = \frac{N - \gamma}{\|\mathbf{t} - \mathbf{\Phi} \mathbf{m}_{N}\|^{2}},$$
(3.108)

where

$$\gamma = \sum_{m=1}^{M} \frac{\lambda_m}{\alpha + \lambda_m} \tag{3.109}$$

and $\lambda_1, \dots, \lambda_M$ are the eigenvalues of $\beta \Phi^{\dagger} \Phi$. If α and β are set as above, then

$$E(\mathbf{m}_N) = \frac{N}{2}. (3.110)$$

3.16

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}).$$
(3.111)

where **w** and ϕ are vectors in M dimensions. By the Bayes' theorem,

$$p(\mathbf{t}, \mathbf{w}) = p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \tag{3.112}$$

Integrating both sides with respect to w gives

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}.$$
 (3.113)

The logarithm of the integrand of the right hand side except the terms independent of \mathbf{w} can be written as

$$-\frac{\beta}{2} \sum_{n=1}^{N} (t_n - \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_n))^2 - \frac{\alpha}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w} = -\frac{1}{2} \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} & -\beta \mathbf{\Phi}^{\mathsf{T}} \\ -\beta \mathbf{\Phi} & \beta \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}.$$

By 2.24,

$$\begin{bmatrix} \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} & -\beta \mathbf{\Phi}^{\mathsf{T}} \\ -\beta \mathbf{\Phi} & \beta \mathbf{I} \end{bmatrix}^{-1} = \begin{bmatrix} \alpha^{-1} \mathbf{I} & \alpha^{-1} \mathbf{\Phi}^{\mathsf{T}} \\ \alpha^{-1} \mathbf{\Phi} & \alpha^{-1} \mathbf{\Phi} \mathbf{\Phi}^{\mathsf{T}} + \beta^{-1} \mathbf{I} \end{bmatrix}.$$

Therefore,

$$p(\mathbf{t}) = \mathcal{N}\left(\mathbf{t}|\mathbf{0}, \alpha^{-1}\mathbf{\Phi}\mathbf{\Phi}^{\mathsf{T}} + \beta^{-1}\mathbf{I}\right). \tag{3.114}$$

3.17

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}),$$
(3.115)

where **w** and ϕ are vectors in M dimensions. By the Bayes' theorem,

$$p(\mathbf{t}, \mathbf{w}) = p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \tag{3.116}$$

Then,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}.$$
 (3.117)

The logarithm of the integrand of the right hand side can be written as

$$-\frac{N}{2}\ln\left(2\pi\beta^{-1}\right) - \frac{\beta}{2}\sum_{n=1}^{N}\left(t_n - \mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n)\right)^2 - \frac{M}{2}\ln\left(2\pi\right) - \frac{1}{2}\ln\left(\det\left(\alpha^{-1}\mathbf{I}\right)\right) - \frac{\alpha}{2}\mathbf{w}^{\mathsf{T}}\mathbf{w}.$$
(3.118)

Therefore,

$$p(\mathbf{t}) = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}} \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} \int \exp\left(-E(\mathbf{w})\right) d\mathbf{w}, \tag{3.119}$$

where

$$E(\mathbf{w}) = \frac{\beta}{2} \|\mathbf{t} - \mathbf{\Phi}\mathbf{w}\|^2 + \frac{\alpha}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w}.$$
 (3.120)

3.18

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}),$$
(3.121)

where **w** and ϕ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.122}$$

where

$$\mathbf{m}_{N} = \beta \mathbf{S}_{N} \mathbf{\Phi}^{\mathsf{T}} \mathbf{t}, \mathbf{S}_{N}^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi}.$$
 (3.123)

By 3.17,

$$p(\mathbf{t}) = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}} \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} \int \exp\left(-E(\mathbf{w})\right) d\mathbf{w}, \tag{3.124}$$

where

$$E(\mathbf{w}) = \frac{\beta}{2} \|\mathbf{t} - \mathbf{\Phi}\mathbf{w}\|^2 + \frac{\alpha}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w}.$$
 (3.125)

The first term of the definition of $E(\mathbf{w})$ can be written as

$$\frac{\beta}{2} \|\mathbf{t} - \mathbf{\Phi} \mathbf{m}_N - \mathbf{\Phi} (\mathbf{w} - \mathbf{m}_N)\|^2
= \frac{\beta}{2} \|\mathbf{t} - \mathbf{\Phi} \mathbf{m}_N\|^2 - \beta (\mathbf{t} - \mathbf{\Phi} \mathbf{m}_N)^{\mathsf{T}} \mathbf{\Phi} (\mathbf{w} - \mathbf{m}_N) + \frac{\beta}{2} (\mathbf{w} - \mathbf{m}_N)^{\mathsf{T}} \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} (\mathbf{w} - \mathbf{m}_N).$$
(3.126)

Similarly, the second term can be written as

$$\frac{\alpha}{2} (\mathbf{w} - \mathbf{m}_N + \mathbf{m}_N)^{\mathsf{T}} (\mathbf{w} - \mathbf{m}_N + \mathbf{m}_N)
= \frac{\alpha}{2} (\mathbf{w} - \mathbf{m}_N)^{\mathsf{T}} (\mathbf{w} - \mathbf{m}_N) + \alpha \mathbf{m}_N^{\mathsf{T}} (\mathbf{w} - \mathbf{m}_N) + \frac{\alpha}{2} \mathbf{m}_N^{\mathsf{T}} \mathbf{m}_N.$$
(3.127)

Here,

$$-\beta(\mathbf{t} - \mathbf{\Phi}\mathbf{m}_N)^{\mathsf{T}}\mathbf{\Phi}(\mathbf{w} - \mathbf{m}_N) + \alpha\mathbf{m}_N^{\mathsf{T}}(\mathbf{w} - \mathbf{m}_N)$$

= $(-\beta\mathbf{\Phi}^{\mathsf{T}}\mathbf{t} + \beta\mathbf{\Phi}^{\mathsf{T}}\mathbf{\Phi}\mathbf{m}_N + \alpha\mathbf{m}_N)^{\mathsf{T}}(\mathbf{w} - \mathbf{m}_N).$ (3.128)

By the definitions of \mathbf{m}_N and \mathbf{S}_N above, the right hand can be written as

$$\left(-\beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{t} + \mathbf{S}_{N}^{-1} \mathbf{m}_{N}\right)^{\mathsf{T}} (\mathbf{w} - \mathbf{m}_{N}) = 0. \tag{3.129}$$

Therefore,

$$E(\mathbf{w}) = E(\mathbf{m}_N) + \frac{1}{2}(\mathbf{w} - \mathbf{m}_N)^{\mathsf{T}} \mathbf{S}_N^{-1} (\mathbf{w} - \mathbf{m}_N). \tag{3.130}$$

3.19

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}),$$
(3.131)

where **w** and ϕ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.132}$$

where

$$\mathbf{m}_{N} = \beta \mathbf{S}_{N} \mathbf{\Phi}^{\mathsf{T}} \mathbf{t}, \mathbf{S}_{N}^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi}.$$
 (3.133)

By 3.17,

$$p(\mathbf{t}) = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}} \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} \int \exp\left(-E(\mathbf{w})\right) d\mathbf{w}, \tag{3.134}$$

where

$$E(\mathbf{w}) = \frac{\beta}{2} \|\mathbf{t} - \mathbf{\Phi}\mathbf{w}\|^2 + \frac{\alpha}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w}.$$
 (3.135)

By 3.18,

$$E(\mathbf{w}) = E(\mathbf{m}_N) + \frac{1}{2}(\mathbf{w} - \mathbf{m}_N)^{\mathsf{T}} \mathbf{S}_N^{-1} (\mathbf{w} - \mathbf{m}_N). \tag{3.136}$$

Therefore, the integral in the expression above of p(t) can be written as

$$\exp\left(-E(\mathbf{m}_N)\right) \int \exp\left(-\frac{1}{2}(\mathbf{w} - \mathbf{m}_N)^{\mathsf{T}} \mathbf{S}_N^{-1}(\mathbf{w} - \mathbf{m}_N)\right) d\mathbf{w}$$

$$= (2\pi)^{\frac{M}{2}} (\det \mathbf{S}_N)^{\frac{1}{2}} \exp\left(-E(\mathbf{m}_N)\right). \tag{3.137}$$

Thus,

$$\ln p(\mathbf{t}) = \frac{M}{2} \ln \alpha + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \mathbf{S}_N) - E(\mathbf{m}_N). \quad (3.138)$$

3.20

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}),$$
(3.139)

where **w** and ϕ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.140}$$

where

$$\mathbf{m}_{N} = \beta \mathbf{S}_{N} \mathbf{\Phi}^{\mathsf{T}} \mathbf{t}, \mathbf{S}_{N}^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi}.$$
 (3.141)

By 3.19,

$$\ln p(\mathbf{t}) = \frac{M}{2} \ln \alpha + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \mathbf{S}_N) - E(\mathbf{m}_N), \quad (3.142)$$

where

$$E(\mathbf{m}_N) = \frac{\beta}{2} \|\mathbf{t} - \mathbf{\Phi} \mathbf{m}_N\|^2 + \frac{\alpha}{2} \mathbf{m}_N^{\mathsf{T}} \mathbf{m}_N.$$
 (3.143)

Let $\mathbf{u}_1, \dots, \mathbf{u}_M$ be eigenvectors of $\beta \mathbf{\Phi}^{\intercal} \mathbf{\Phi}$ such that

$$\beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} \mathbf{u}_m = \lambda_m \mathbf{u}_m. \tag{3.144}$$

Then,

$$\mathbf{S}_N^{-1}\mathbf{u}_m = (\alpha + \lambda_m)\mathbf{u}_m, \tag{3.145}$$

so that

$$\det \mathbf{S}_N = \prod_{m=1}^M \frac{1}{\alpha + \lambda_m}.$$
 (3.146)

Therefore, setting the derivative of $\ln p(\mathbf{t}|\alpha,\beta)$ with respect to α to zero gives

$$0 = \frac{M}{2\alpha} - \frac{1}{2} \sum_{m=1}^{M} \frac{1}{\alpha + \lambda_m} - \frac{1}{2} \mathbf{m}_N^{\mathsf{T}} \mathbf{m}_N. \tag{3.147}$$

Multiplying both sides by 2α gives

$$\alpha \mathbf{m}_{N}^{\mathsf{T}} \mathbf{m}_{N} = M - \sum_{m=1}^{M} \frac{\alpha}{\alpha + \lambda_{m}}.$$
 (3.148)

The right hand side can be written as

$$\sum_{m=1}^{M} \left(1 - \frac{\alpha}{\alpha + \lambda_m} \right) = \sum_{m=1}^{M} \frac{\lambda_i}{\alpha + \lambda_m}.$$
 (3.149)

Thus,

$$\alpha = \frac{\gamma}{\mathbf{m}_N^{\mathsf{T}} \mathbf{m}_N},\tag{3.150}$$

where

$$\gamma = \sum_{m=1}^{M} \frac{\lambda_i}{\alpha + \lambda_m}.$$
 (3.151)

3.21

(a)

Let Σ be a $M \times M$ real symmetric matrix such that

$$\Sigma \mathbf{u}_m = \lambda_m \mathbf{u}_m, \tag{3.152}$$

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

$$\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_M),
\mathbf{U} = [\mathbf{u}_1 \cdots \mathbf{u}_M].$$
(3.153)

By 2.19,

$$\Sigma = \mathbf{U}\Lambda\mathbf{U}^{\mathsf{T}},$$

$$\mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{I}.$$
(3.154)

Therefore,

$$\det \mathbf{\Sigma} = \prod_{m=1}^{M} \lambda_m, \tag{3.155}$$

so that

$$\ln(\det \mathbf{\Sigma}) = \sum_{m=1}^{M} \ln \lambda_i. \tag{3.156}$$

Then,

$$\frac{\partial}{\partial \alpha} \ln(\det \Sigma) = \sum_{m=1}^{M} \frac{\partial \lambda_m}{\partial \alpha} \frac{1}{\lambda_m}.$$
 (3.157)

Therefore,

$$\frac{\partial}{\partial \alpha} \ln(\det \Sigma) = \operatorname{tr} \left(\Lambda^{-1} \frac{\partial \Lambda}{\partial \alpha} \right). \tag{3.158}$$

The right hand side can be written as

$$\operatorname{tr}\left(\mathbf{U}\boldsymbol{\Lambda}^{-1}\mathbf{U}^{\mathsf{T}}\frac{\partial\mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{\mathsf{T}}}{\partial\alpha}\right) = \operatorname{tr}\left(\boldsymbol{\Sigma}^{-1}\frac{\partial\boldsymbol{\Sigma}}{\partial\alpha}\right). \tag{3.159}$$

Therefore,

$$\frac{\partial}{\partial \alpha} \ln(\det \Sigma) = \operatorname{tr} \left(\Sigma^{-1} \frac{\partial \Sigma}{\partial \alpha} \right). \tag{3.160}$$

(b)

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}),$$
(3.161)

where **w** and ϕ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.162}$$

where

$$\mathbf{m}_{N} = \beta \mathbf{S}_{N} \mathbf{\Phi}^{\mathsf{T}} \mathbf{t}, \mathbf{S}_{N}^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi}.$$
 (3.163)

By 3.19,

$$\ln p(\mathbf{t}) = \frac{M}{2} \ln \alpha + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \mathbf{S}_N) - E(\mathbf{m}_N), \quad (3.164)$$

where

$$E(\mathbf{m}_N) = \frac{\beta}{2} \|\mathbf{t} - \mathbf{\Phi} \mathbf{m}_N\|^2 + \frac{\alpha}{2} \mathbf{m}_N^{\mathsf{T}} \mathbf{m}_N.$$
 (3.165)

By 3.21(a),

$$\frac{\partial}{\partial \alpha} \ln \left(\det \mathbf{S}_N^{-1} \right) = \operatorname{tr} \left(\mathbf{S}_N \right). \tag{3.166}$$

The right hand side can be written as

$$\sum_{m=1}^{M} \frac{1}{\alpha + \lambda_m},\tag{3.167}$$

where $\lambda_1, \dots, \lambda_M$ are eigenvalues of $\beta \Phi^{\dagger} \Phi$. Therefore, setting the derivative of $\ln p(\mathbf{t})$ with respect to α to zero gives

$$0 = \frac{M}{2\alpha} - \frac{1}{2} \sum_{m=1}^{M} \frac{1}{\alpha + \lambda_m} - \frac{1}{2} \mathbf{m}_N^{\mathsf{T}} \mathbf{m}_N, \tag{3.168}$$

Thus,

$$\alpha = \frac{\gamma}{\mathbf{m}_N^{\mathsf{T}} \mathbf{m}_N},\tag{3.169}$$

where

$$\gamma = \sum_{m=1}^{M} \frac{\lambda_m}{\alpha + \lambda_m}.$$
 (3.170)

3.22

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}),$$
(3.171)

where **w** and ϕ are vectors in M dimensions. By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N), \tag{3.172}$$

where

$$\mathbf{m}_{N} = \beta \mathbf{S}_{N} \mathbf{\Phi}^{\mathsf{T}} \mathbf{t}, \mathbf{S}_{N}^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi}.$$
 (3.173)

By 3.19,

$$\ln p(\mathbf{t}) = \frac{M}{2} \ln \alpha + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \mathbf{S}_N) - E(\mathbf{m}_N), \quad (3.174)$$

where

$$E(\mathbf{m}_N) = \frac{\beta}{2} \|\mathbf{t} - \mathbf{\Phi} \mathbf{m}_N\|^2 + \frac{\alpha}{2} \mathbf{m}_N^{\mathsf{T}} \mathbf{m}_N.$$
 (3.175)

By 3.21(a),

$$\frac{\partial}{\partial \beta} \ln \left(\det \mathbf{S}_N^{-1} \right) = \operatorname{tr} \left(\mathbf{S}_N \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} \right). \tag{3.176}$$

Since

$$\mathbf{S}_N \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} = \frac{1}{\beta} \left(\mathbf{I} - \alpha \mathbf{S}_N \right), \tag{3.177}$$

the right hand side can be written as

$$\frac{1}{\beta} \left(M - \alpha \sum_{m=1}^{M} \frac{1}{\alpha + \lambda_m} \right) = \frac{1}{\beta} \sum_{m=1}^{M} \frac{\lambda_m}{\alpha + \lambda_m}, \tag{3.178}$$

where $\lambda_1, \dots, \lambda_M$ are eigenvalues of $\beta \Phi^{\dagger} \Phi$. Therefore, setting the derivative of $\ln p(\mathbf{t})$ with respect to β to zero gives

$$0 = \frac{N}{2\beta} - \frac{1}{2\beta} \sum_{m=1}^{M} \frac{\lambda_i}{\alpha + \lambda_m} - \frac{1}{2} \|\mathbf{t} - \mathbf{\Phi} \mathbf{m}_N\|^2.$$
 (3.179)

Thus,

$$\beta = \frac{N - \gamma}{\left\|\mathbf{t} - \mathbf{\Phi}\mathbf{m}_N\right\|^2},\tag{3.180}$$

where

$$\gamma = \sum_{m=1}^{M} \frac{\lambda_m}{\alpha + \lambda_m}.$$
 (3.181)

3.23

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w},\beta) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n),\beta^{-1}\right),$$

$$p(\mathbf{w},\beta) = \mathcal{N}\left(\mathbf{w}|\mathbf{m}_0,\beta^{-1}\mathbf{S}_0\right)\operatorname{Gam}(\beta|a_0,b_0),$$
(3.182)

where \mathbf{w} and $\boldsymbol{\phi}$ are vectors in M dimensions. By marginalisation,

$$p(\mathbf{t}) = \int \int p(\mathbf{t}|\mathbf{w}, \beta) p(\mathbf{w}, \beta) d\mathbf{w} d\beta.$$
 (3.183)

The right hand side can be written as

$$\int \left(\int \left(\prod_{n=1}^{N} \mathcal{N} \left(t_{n} | \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_{n}), \beta^{-1} \right) \right) \mathcal{N} \left(\mathbf{w} | \mathbf{m}_{0}, \beta^{-1} \mathbf{S}_{0} \right) d\mathbf{w} \right) \operatorname{Gam}(\beta | a_{0}, b_{0}) d\beta.$$
(3.184)

The logarithm of the integrand with respect to \mathbf{w} can be written as

$$-\frac{N}{2}\ln(2\pi) - \frac{N}{2}\ln\beta^{-1} - \frac{\beta}{2}\sum_{n=1}^{N}\left(t_{n} - \mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_{n})\right)^{2}$$

$$-\frac{M}{2}\ln(2\pi) - \frac{1}{2}\ln\det(\beta^{-1}\mathbf{S}_{0}) - \frac{\beta}{2}(\mathbf{w} - \mathbf{m}_{0})^{\mathsf{T}}\mathbf{S}_{0}^{-1}(\mathbf{w} - \mathbf{m}_{0})$$

$$= -\frac{N+M}{2}\ln(2\pi) + \frac{N+M}{2}\ln\beta - \frac{1}{2}\ln(\det\mathbf{S}_{0})$$

$$-\frac{\beta}{2}\mathbf{w}^{\mathsf{T}}\left(\mathbf{S}_{0}^{-1} + \mathbf{\Phi}^{\mathsf{T}}\mathbf{\Phi}\right)\mathbf{w} + \beta\mathbf{w}^{\mathsf{T}}\left(\mathbf{S}_{0}^{-1}\mathbf{m}_{0} + \mathbf{\Phi}^{\mathsf{T}}\mathbf{t}\right) - \frac{\beta}{2}\|\mathbf{t}\|^{2} - \frac{\beta}{2}\mathbf{m}_{0}^{\mathsf{T}}\mathbf{S}_{0}^{-1}\mathbf{m}_{0}.$$
(3.185)

The right hand side can be written as

$$-\frac{N+M}{2}\ln(2\pi) + \frac{N+M}{2}\ln\beta - \frac{1}{2}\ln(\det\mathbf{S}_{0})$$

$$-\frac{\beta}{2}(\mathbf{w} - \mathbf{m}_{N})^{\mathsf{T}}\mathbf{S}_{N}^{-1}(\mathbf{w} - \mathbf{m}_{N}) + \frac{\beta}{2}\mathbf{m}_{N}^{\mathsf{T}}\mathbf{S}_{N}^{-1}\mathbf{m}_{N} - \frac{\beta}{2}\|\mathbf{t}\|^{2} - \frac{\beta}{2}\mathbf{m}_{0}^{\mathsf{T}}\mathbf{S}_{0}^{-1}\mathbf{m}_{0},$$
(3.186)

where

$$\mathbf{m}_{N} = \mathbf{S}_{N} \left(\mathbf{S}_{0}^{-1} \mathbf{m}_{0} + \mathbf{\Phi}^{\mathsf{T}} \mathbf{t} \right), \mathbf{S}_{N}^{-1} = \mathbf{S}_{0}^{-1} + \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi}.$$
 (3.187)

Therefore, the logarithm of the integral with respect to \mathbf{w} can be written as

$$-\frac{N}{2}\ln(2\pi) + \frac{N}{2}\ln\beta - \frac{1}{2}\ln(\det\mathbf{S}_0) + \frac{1}{2}\ln(\det\mathbf{S}_N) + \frac{\beta}{2}\mathbf{m}_N^{\mathsf{T}}\mathbf{S}_N^{-1}\mathbf{m}_N - \frac{\beta}{2}\|\mathbf{t}\|^2 - \frac{\beta}{2}\mathbf{m}_0^{\mathsf{T}}\mathbf{S}_0^{-1}\mathbf{m}_0.$$
(3.188)

Then, the logarithm of the integrand with respect to β can be written as

$$-\frac{N}{2}\ln(2\pi) + \frac{N}{2}\ln\beta - \frac{1}{2}\ln(\det \mathbf{S}_{0}) + \frac{1}{2}\ln(\det \mathbf{S}_{N}) + \frac{\beta}{2}\mathbf{m}_{N}^{\mathsf{T}}\mathbf{S}_{N}^{-1}\mathbf{m}_{N} - \frac{\beta}{2}\|\mathbf{t}\|^{2} - \frac{\beta}{2}\mathbf{m}_{0}^{\mathsf{T}}\mathbf{S}_{0}^{-1}\mathbf{m}_{0} - \ln\Gamma(a_{0}) + a_{0}\ln b_{0} + (a_{0} - 1)\ln\beta - b_{0}\beta$$

$$= -\frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln(\det \mathbf{S}_{0}) + \frac{1}{2}\ln(\det \mathbf{S}_{N}) - \ln\Gamma(a_{0}) + a_{0}\ln b_{0} + (a_{N} - 1)\ln\beta - b_{N}\beta,$$
(3.189)

where

$$a_{N} = a_{0} + \frac{N}{2},$$

$$b_{N} = b_{0} + \frac{\beta}{2} \|\mathbf{t}\|^{2} + \frac{\beta}{2} \mathbf{m}_{0}^{\mathsf{T}} \mathbf{S}_{0}^{-1} \mathbf{m}_{0} - \frac{\beta}{2} \mathbf{m}_{N}^{\mathsf{T}} \mathbf{S}_{N}^{-1} \mathbf{m}_{N}.$$
(3.190)

Therefore, the logarithm of the integral with respect to β can be written as

$$-\frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln(\det \mathbf{S}_0) + \frac{1}{2}\ln(\det \mathbf{S}_N) - \ln\Gamma(a_0) + a_0\ln b_0 + \ln\Gamma(a_N) - a_N\ln b_N.$$
(3.191)

Thus,

$$p(\mathbf{t}) = (2\pi)^{-\frac{N}{2}} \left(\frac{\det \mathbf{S}_N}{\det \mathbf{S}_0} \right)^{\frac{1}{2}} \frac{\Gamma(a_N)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b_N^{a_N}}.$$
 (3.192)

3.24

Refer to 3.12.

4 Linear Models for Classification

4.1

Let x_1, \dots, x_M and y_1, \dots, 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

$$\mathbf{x} = \sum_{m=1}^{M} \alpha_m \mathbf{x}_m,$$

$$\mathbf{y} = \sum_{n=1}^{N} \beta_n \mathbf{y}_n,$$
(4.1)

where

$$\sum_{m=1}^{M} \alpha_m = \sum_{n=1}^{N} \beta_n = 1,$$

$$\alpha_m \ge 0, \beta_n \ge 0.$$
(4.2)

Let us assume that $\alpha_1, \dots, \alpha_M$ and β_1, \dots, β_N below are subject to the constraints above.

If the convex hulls intersect, then there exist $\alpha_1, \dots, \alpha_M$ and β_1, \dots, β_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,

$$\sum_{m=1}^{M} \alpha_m \left(\hat{\mathbf{w}}^{\mathsf{T}} \mathbf{x}_m + w_0 \right) = \hat{\mathbf{w}}^{\mathsf{T}} \sum_{m=1}^{M} \alpha_m \mathbf{x}_m + w_0 \sum_m \alpha_m, \tag{4.4}$$

for any $\hat{\mathbf{w}}$ and w_0 . The right hand side can be written as

$$\hat{\mathbf{w}}^{\mathsf{T}} \sum_{n=1}^{N} \beta_n \mathbf{y}_n + w_0 \sum_{n=1}^{N} \beta_n = \sum_{n=1}^{N} \beta_n \left(\hat{\mathbf{w}}^{\mathsf{T}} \mathbf{y}_n + w_0 \right). \tag{4.5}$$

Therefore, there do not exist $\hat{\mathbf{w}}$ and w_0 such that

$$\hat{\mathbf{w}}^{\mathsf{T}} \mathbf{x}_m + w_0 > 0, \hat{\mathbf{w}}^{\mathsf{T}} \mathbf{y}_n + w_0 < 0.$$
 (4.6)

Conversely, if there exist $\hat{\mathbf{w}}$ and w_0 such that

$$\hat{\mathbf{w}}^{\mathsf{T}} \mathbf{x}_m + w_0 > 0, \\ \hat{\mathbf{w}}^{\mathsf{T}} \mathbf{y}_n + w_0 < 0,$$
 (4.7)

then

$$\sum_{m=1}^{M} \alpha_m \left(\hat{\mathbf{w}}^{\mathsf{T}} \mathbf{x}_m + w_0 \right) > 0,$$

$$\sum_{n=1}^{N} \beta_n \left(\hat{\mathbf{w}}^{\mathsf{T}} \mathbf{y}_n + w_0 \right) < 0.$$
(4.8)

The left hand sides can be written as

$$\hat{\mathbf{w}}^{\mathsf{T}} \sum_{m=1}^{M} \alpha_m \mathbf{x}_m + w_0 \sum_{m=1}^{M} \alpha_m = \hat{\mathbf{w}}^{\mathsf{T}} \sum_{m=1}^{M} \alpha_m \mathbf{x}_m + w_0,$$

$$\hat{\mathbf{w}}^{\mathsf{T}} \sum_{n=1}^{N} \beta_n \mathbf{y}_n + w_0 \sum_{n=1}^{N} \beta_n = \hat{\mathbf{w}}^{\mathsf{T}} \sum_{n=1}^{N} \beta_n \mathbf{y}_n + w_0.$$
(4.9)

Therefore, there do not exist $\alpha_1, \dots, \alpha_M$ and β_1, \dots, β_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 $\mathbf{x}_1, \dots, \mathbf{x}_N$ and $\mathbf{w}_1, \dots, \mathbf{w}_K$ are variables in M dimensions and $\mathbf{t}_1, \dots, \mathbf{t}_N$ are ones in K dimensions. Let

$$E(\tilde{\mathbf{W}}) = \frac{1}{2} \operatorname{tr} \left((\tilde{\mathbf{X}} \tilde{\mathbf{W}} - \mathbf{T})^{\mathsf{T}} (\tilde{\mathbf{X}} \tilde{\mathbf{W}} - \mathbf{T}) \right), \tag{4.11}$$

where

$$\tilde{\mathbf{X}} = \begin{bmatrix} 1 & \mathbf{x}_1^{\mathsf{T}} \\ \vdots & \vdots \\ 1 & \mathbf{x}_N^{\mathsf{T}} \end{bmatrix},$$

$$\tilde{\mathbf{W}} = \begin{bmatrix} w_{10} & \cdots & w_{K0} \\ \mathbf{w}_1 & \cdots & \mathbf{w}_K \end{bmatrix}$$

and

$$\mathbf{T} = egin{bmatrix} \mathbf{t}_1^\intercal \ dots \ \mathbf{t}_N^\intercal \end{bmatrix}.$$

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

$$\mathbf{O} = \tilde{\mathbf{X}}^{\mathsf{T}} (\tilde{\mathbf{X}}\tilde{\mathbf{W}} - \mathbf{T}). \tag{4.12}$$

Therefore,

$$\underset{\tilde{\mathbf{W}}}{\operatorname{argmin}} E(\tilde{\mathbf{W}}) = \left(\tilde{\mathbf{X}}^{\mathsf{T}} \tilde{\mathbf{X}}\right)^{-1} \tilde{\mathbf{X}}^{\mathsf{T}} \mathbf{T}. \tag{4.13}$$

Let $\tilde{\mathbf{W}}^*$ denote the least-square solution above. Then,

$$(\tilde{\mathbf{W}}^*)^{\mathsf{T}}\tilde{\mathbf{x}} - \mathbf{t}_n = \mathbf{T}^{\mathsf{T}}\tilde{\mathbf{X}} \left(\tilde{\mathbf{X}}^{\mathsf{T}}\tilde{\mathbf{X}} \right)^{-1} \tilde{\mathbf{x}} - \mathbf{t}_n, \tag{4.14}$$

where $\tilde{\mathbf{x}}$ is a vector in M+1 dimensions whose first element is 1. The right hand side can be written as

$$\mathbf{T}^{\mathsf{T}} \left(\tilde{\mathbf{X}} \left(\tilde{\mathbf{X}}^{\mathsf{T}} \tilde{\mathbf{X}} \right)^{-1} \tilde{\mathbf{x}} - \mathbf{v}_n \right) = \mathbf{0}? \tag{4.15}$$

where \mathbf{v}_n is a vector in N dimensions whose n th element is 1 and other elements are zero. Therefore,

$$(\tilde{\mathbf{W}}^*)^{\mathsf{T}}\tilde{\mathbf{x}} - \mathbf{t}_n = \mathbf{0}. \tag{4.16}$$

Thus, if

$$\mathbf{a}^{\mathsf{T}}\mathbf{t}_n + b = 0,\tag{4.17}$$

then

$$\mathbf{a}^{\mathsf{T}}(\tilde{\mathbf{W}}^*)^{\mathsf{T}}\tilde{\mathbf{x}} + b = 0. \tag{4.18}$$

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

$$\mathbf{w}^{\mathsf{T}}(\mathbf{m}_2 - \mathbf{m}_1) + \lambda \left(\|\mathbf{w}\|^2 - 1 \right) \tag{4.20}$$

with respect to \mathbf{w} and λ to zero gives

$$\mathbf{m}_2 - \mathbf{m}_1 + 2\lambda \mathbf{w} = \mathbf{0},$$

$$\|\mathbf{w}\|^2 - 1 = 0.$$
 (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 $\mathbf{x}_1, \dots, \mathbf{x}_N$ 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 C_k . Let

$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2},\tag{4.25}$$

where

$$s_k^2 = \sum_{n \in \mathcal{C}_k} (y_n - m_k)^2,$$

$$y_n = \mathbf{w}^{\mathsf{T}} \mathbf{x}_n,$$

$$m_k = \mathbf{w}^{\mathsf{T}} \mathbf{m}_k.$$

$$(4.26)$$

Then, $J(\mathbf{w})$ can be written as

$$\frac{\left(\mathbf{w}^{\mathsf{T}}(\mathbf{m}_{2} - \mathbf{m}_{1})\right)^{2}}{\sum_{n \in \mathcal{C}_{1}} \left(\mathbf{w}^{\mathsf{T}}(\mathbf{x}_{n} - \mathbf{m}_{1})\right)^{2} + \sum_{n \in \mathcal{C}_{2}} \left(\mathbf{w}^{\mathsf{T}}(\mathbf{x}_{n} - \mathbf{m}_{2})\right)^{2}} = \frac{\mathbf{w}^{\mathsf{T}} \mathbf{S}_{B} \mathbf{w}}{\mathbf{w}^{\mathsf{T}} \mathbf{S}_{W} \mathbf{w}}, \quad (4.27)$$

where

$$\mathbf{S}_{\mathrm{B}} = (\mathbf{m}_{2} - \mathbf{m}_{1})(\mathbf{m}_{2} - \mathbf{m}_{1})^{\mathsf{T}},$$

$$\mathbf{S}_{\mathrm{W}} = \sum_{n \in \mathcal{C}_{1}} (\mathbf{x}_{n} - \mathbf{m}_{1})(\mathbf{x}_{n} - \mathbf{m}_{1})^{\mathsf{T}} + \sum_{n \in \mathcal{C}_{2}} (\mathbf{x}_{n} - \mathbf{m}_{2})(\mathbf{x}_{n} - \mathbf{m}_{2})^{\mathsf{T}}.$$

$$(4.28)$$

4.6

Let $\mathbf{x}_1, \dots, \mathbf{x}_N$ 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

$$s_k^2 = \sum_{n \in \mathcal{C}_k} (y_n - m_k)^2,$$

$$y_n = \mathbf{w}^{\mathsf{T}} \mathbf{x}_n,$$

$$m_k = \mathbf{w}^{\mathsf{T}} \mathbf{m}_k.$$

$$(4.31)$$

Then, by 4.5,

$$J(\mathbf{w}) = \frac{\mathbf{w}^{\mathsf{T}} \mathbf{S}_{\mathsf{B}} \mathbf{w}}{\mathbf{w}^{\mathsf{T}} \mathbf{S}_{\mathsf{W}} \mathbf{w}},\tag{4.32}$$

where

$$\mathbf{S}_{\mathrm{B}} = (\mathbf{m}_{2} - \mathbf{m}_{1})(\mathbf{m}_{2} - \mathbf{m}_{1})^{\mathsf{T}},$$

$$\mathbf{S}_{\mathrm{W}} = \sum_{n \in \mathcal{C}_{1}} (\mathbf{x}_{n} - \mathbf{m}_{1})(\mathbf{x}_{n} - \mathbf{m}_{1})^{\mathsf{T}} + \sum_{n \in \mathcal{C}_{2}} (\mathbf{x}_{n} - \mathbf{m}_{2})(\mathbf{x}_{n} - \mathbf{m}_{2})^{\mathsf{T}}.$$

$$(4.33)$$

Let

$$E = \frac{1}{2} \sum_{n=1}^{N} (\mathbf{w}^{\mathsf{T}} \mathbf{x}_n + w_0 - t_n)^2, \qquad (4.34)$$

where

$$t_n = \begin{cases} \frac{N}{N_1}, & n \in \mathcal{C}_1, \\ -\frac{N}{N_2}, & n \in \mathcal{C}_2. \end{cases}$$
 (4.35)

Setting the derivative with respect to \mathbf{w} and w_0 gives

$$0 = \sum_{n=1}^{N} (\mathbf{w}^{\mathsf{T}} \mathbf{x}_n + w_0 - t_n),$$

$$\mathbf{0} = \sum_{n=1}^{N} (\mathbf{w}^{\mathsf{T}} \mathbf{x}_n + w_0 - t_n) \mathbf{x}_n.$$

$$(4.36)$$

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

$$\mathbf{w}^{\mathsf{T}} \sum_{n=1}^{N} \mathbf{x}_n + N w_0 - \sum_{n=1}^{N} t_n = N \left(\mathbf{w}^{\mathsf{T}} \mathbf{m} + w_0 \right), \tag{4.37}$$

where

$$\mathbf{m} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n. \tag{4.38}$$

Therefore,

$$w_0 = -\mathbf{w}^{\mathsf{T}}\mathbf{m}.\tag{4.39}$$

Then, the right hand side of the second equation above can be written as

$$\sum_{n=1}^{N} (\mathbf{w}^{\mathsf{T}} (\mathbf{x}_{n} - \mathbf{m}) - t_{n}) \mathbf{x}_{n}$$

$$= \sum_{n \in C_{1}} \left(\mathbf{w}^{\mathsf{T}} (\mathbf{x}_{n} - \mathbf{m}) - \frac{N}{N_{1}} \right) \mathbf{x}_{n} + \sum_{n \in C_{2}} \left(\mathbf{w}^{\mathsf{T}} (\mathbf{x}_{n} - \mathbf{m}) + \frac{N}{N_{2}} \right) \mathbf{x}_{n}.$$
(4.40)

Since

$$\mathbf{m} = \frac{N_1}{N} \mathbf{m}_1 + \frac{N_2}{N} \mathbf{m}_2,$$

$$\sum_{n \in C_1} (\mathbf{x}_n - \mathbf{m}_1) = \mathbf{0},$$
(4.41)

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

$$\sum_{n \in \mathcal{C}_1} \left(\mathbf{w}^{\mathsf{T}} \left(\mathbf{x}_n - \mathbf{m}_1 + \frac{N_2}{N} (\mathbf{m}_1 - \mathbf{m}_2) \right) - \frac{N}{N_1} \right) (\mathbf{x}_n - \mathbf{m}_1 + \mathbf{m}_1)$$

$$= \left(\sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1) (\mathbf{x}_n - \mathbf{m}_1)^{\mathsf{T}} \right) \mathbf{w} + \frac{N_1 N_2}{N} (\mathbf{m}_1 - \mathbf{m}_2) \mathbf{m}_1^{\mathsf{T}} \mathbf{w} - N \mathbf{m}_1.$$
(4.42)

Similarly, the second term can be written as

$$\left(\sum_{n\in\mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^{\mathsf{T}}\right)\mathbf{w} + \frac{N_1 N_2}{N} (\mathbf{m}_2 - \mathbf{m}_1)\mathbf{m}_2^{\mathsf{T}}\mathbf{w} - N\mathbf{m}_2. \quad (4.43)$$

Therefore,

$$\mathbf{0} = \left(\sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^{\mathsf{T}}\right) \mathbf{w} + \frac{N_1 N_2}{N} (\mathbf{m}_1 - \mathbf{m}_2) \mathbf{m}_1^{\mathsf{T}} \mathbf{w} - N \mathbf{m}_1$$
$$+ \left(\sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^{\mathsf{T}}\right) \mathbf{w} + \frac{N_1 N_2}{N} (\mathbf{m}_2 - \mathbf{m}_1) \mathbf{m}_2^{\mathsf{T}} \mathbf{w} - N \mathbf{m}_2.$$

$$(4.44)$$

Thus,

$$\left(\mathbf{S}_{W} + \frac{N_1 N_2}{N} \mathbf{S}_{B}\right) \mathbf{w} = N(\mathbf{m}_1 - \mathbf{m}_2). \tag{4.45}$$

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

$$1 - \frac{\exp(a)}{1 + \exp(a)} = 1 - \frac{1}{1 + \exp(-a)}.$$
 (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,

$$p(C_1|\mathbf{x}) = \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_1)p(C_1) + p(\mathbf{x}|C_2)p(C_2)}.$$
(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

$$a = -\frac{D}{2}\ln(2\pi) - \frac{1}{2}\ln(\det\Sigma) - \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_1)^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_1) + \ln p(\mathcal{C}_1) + \frac{D}{2}\ln(2\pi) + \frac{1}{2}\ln(\det\Sigma) + \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_2)^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_2) - \ln p(\mathcal{C}_2).$$

$$(4.58)$$

Therefore,

$$p(\mathcal{C}_1|\mathbf{x}) = \sigma\left(\mathbf{w}^{\mathsf{T}}\mathbf{x} + w_0\right),\tag{4.59}$$

where

$$\mathbf{w} = \mathbf{\Sigma}^{-1}(\boldsymbol{\mu}_{1} - \boldsymbol{\mu}_{2}),$$

$$w_{0} = -\frac{1}{2}\boldsymbol{\mu}_{1}^{\mathsf{T}}\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_{1} + \frac{1}{2}\boldsymbol{\mu}_{2}^{\mathsf{T}}\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_{2} + \ln p(\mathcal{C}_{1}) - \ln p(\mathcal{C}_{2}).$$
(4.60)

4.9

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables in K dimensions such that

$$p(\mathbf{t}_n, \boldsymbol{\phi}_n) = \prod_{k=1}^K (p(\boldsymbol{\phi}_n, \mathcal{C}_k))^{t_{nk}}, \qquad (4.61)$$

where

$$\sum_{k=1}^{K} p(\mathcal{C}_k) = 1. (4.62)$$

Then,

$$p(\mathbf{T}, \mathbf{\Phi}) = \prod_{n=1}^{N} \prod_{k=1}^{K} (p(\boldsymbol{\phi}_n, \mathcal{C}_k))^{t_{nk}}.$$
 (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

$$\ln p(\mathbf{T}, \mathbf{\Phi}) + \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right)$$
 (4.66)

with respect to π_k and λ to zero gives

$$0 = \frac{1}{\pi_k} \sum_{n=1}^{N} t_{nk} + \lambda,$$

$$0 = \sum_{k=1}^{K} \pi_k - 1.$$
(4.67)

Then,

$$\lambda = -\sum_{k=1}^{K} \sum_{n=1}^{N} t_{nk}.$$
(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

$$N_k = \sum_{n=1}^{N} t_{nk}. (4.70)$$

4.10

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables in K dimensions such that

$$p(\mathbf{t}_n, \boldsymbol{\phi}_n) = \prod_{k=1}^K (p(\boldsymbol{\phi}_n, \mathcal{C}_k))^{t_{nk}}, \qquad (4.71)$$

where

$$\sum_{k=1}^{K} p(\mathcal{C}_k) = 1. (4.72)$$

Then,

$$p(\mathbf{T}, \mathbf{\Phi}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \left(p(\boldsymbol{\phi}_n, \mathcal{C}_k) \right)^{t_{nk}}.$$
 (4.73)

If

$$p(\phi_n|\mathcal{C}_k) = \mathcal{N}(\phi_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}), \tag{4.74}$$

then, by the Bayes' theorem,

$$\ln p(\mathbf{T}, \mathbf{\Phi}) = \sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \left(\ln \mathcal{N}(\boldsymbol{\phi}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}) + \ln p(\mathcal{C}_k) \right). \tag{4.75}$$

The right hand side can be written as

$$\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \left(-\frac{D}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \Sigma) - \frac{1}{2} (\boldsymbol{\phi}_{n} - \boldsymbol{\mu}_{k})^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\boldsymbol{\phi}_{n} - \boldsymbol{\mu}_{k}) + \ln p(\mathcal{C}_{k}) \right). \tag{4.76}$$

By 3.21(a), setting the derivatives of $\ln p(\mathbf{T}, \mathbf{\Phi})$ with respect to $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}$ to zero gives

$$\mathbf{0} = \frac{1}{2} \sum_{n=1}^{N} t_{nk} \left(\mathbf{\Sigma}^{-1} + \left(\mathbf{\Sigma}^{-1} \right)^{\mathsf{T}} \right) (\boldsymbol{\phi}_{n} - \boldsymbol{\mu}_{k}),$$

$$\mathbf{O} = -\frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \left(\left(\mathbf{\Sigma}^{-1} \right)^{\mathsf{T}} - \left(\mathbf{\Sigma}^{-1} \right)^{2} (\boldsymbol{\phi}_{n} - \boldsymbol{\mu}_{k}) (\boldsymbol{\phi}_{n} - \boldsymbol{\mu}_{k})^{\mathsf{T}} \right).$$

$$(4.77)$$

Therefore, the maximum likelihood solutions for μ_k and Σ are given by

$$\mu_k = \frac{1}{N_k} \sum_{n=1}^{N} t_{nk} \phi_n,$$

$$\Sigma = \frac{1}{N} \sum_{k=1}^{K} N_k \mathbf{S}_k,$$
(4.78)

where

$$N_k = \sum_{n=1}^{N} t_{nk},$$

$$\mathbf{S}_k = \frac{1}{N_k} \sum_{n=1}^{N} t_{nk} (\boldsymbol{\phi}_n - \boldsymbol{\mu}_k) (\boldsymbol{\phi}_n - \boldsymbol{\mu}_k)^{\mathsf{T}}.$$

$$(4.79)$$

4.11

Let ϕ_1, \dots, ϕ_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,

$$p(\mathbf{\Phi}|\mathcal{C}_k) = \prod_{m=1}^{M} \prod_{l=1}^{L} \mu_{kml}^{\phi_{ml}}.$$
 (4.82)

By the Bayes' theorem,

$$p(C_k|\mathbf{\Phi}) = \frac{p(\mathbf{\Phi}|C_k)p(C_k)}{\sum_{k=1}^K p(\mathbf{\Phi}|C_k)p(C_k)}.$$
(4.83)

Therefore,

$$p(C_k|\mathbf{\Phi}) = \frac{\exp(a_k(\mathbf{\Phi}))}{\sum_{k=1}^K \exp(a_k(\mathbf{\Phi}))},$$
(4.84)

where

$$a_k(\mathbf{\Phi}) = \left(\sum_{m=1}^M \sum_{l=1}^L \phi_{ml} \ln \mu_{kml}\right) + \ln p(\mathcal{C}_k). \tag{4.85}$$

4.12

Let

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.\tag{4.86}$$

Then,

$$\frac{d\sigma(a)}{da} = \frac{\exp(-a)}{\left(1 + \exp(-a)\right)^2}.$$
(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, \dots, t_N be variables such that

$$t_n \in \{0, 1\},\ p(t_n | \mathbf{w}) = y_n^{t_n} (1 - y_n)^{1 - t_n},$$
(4.90)

where

$$y_n = \sigma(\mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}_n),$$

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$
 (4.91)

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}). \tag{4.92}$$

The right hand side can be written as

$$-\ln\left(\prod_{n=1}^{N} y_n^{t_n} (1 - y_n)^{1 - t_n}\right) = -\sum_{n=1}^{N} \left(t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\right). \quad (4.93)$$

Then, by 4.12,

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N} \left(\frac{t_n}{y_n} y_n (1 - y_n) \phi_n - \frac{1 - t_n}{1 - y_n} y_n (1 - y_n) \phi_n \right). \tag{4.94}$$

The right hand side can be written as

$$-\sum_{n=1}^{N} (t_n(1-y_n)\boldsymbol{\phi}_n - (1-t_n)y_n\boldsymbol{\phi}_n) = \sum_{n=1}^{N} (y_n - t_n)\boldsymbol{\phi}_n.$$
 (4.95)

Therefore,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n) \phi_n. \tag{4.96}$$

4.14

Let t_1, \dots, t_N be variables such that

$$t_n \in \{0, 1\},\ p(t_n | \mathbf{w}) = y_n^{t_n} (1 - y_n)^{1 - t_n},$$
(4.97)

where

$$y_n = \sigma(\mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}_n),$$

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$
 (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

$$\mathbf{0} = \sum_{n=1}^{N} (y_n - t_n) \, \phi_n. \tag{4.100}$$

If ϕ_1, \cdots, ϕ_N are linearly independent, then

$$y_n = t_n. (4.101)$$

Then,

$$\sigma\left(\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}_{n}\right) = \begin{cases} 1, & t_{n} = 1, \\ 0, & \text{otherwise.} \end{cases}$$
 (4.102)

Threrefore,

$$\mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}_n = \begin{cases} \infty, & t_n = 1, \\ -\infty, & \text{otherwise.} \end{cases}$$
 (4.103)

Let t_1, \dots, t_N be variables such that

$$t_n \in \{0, 1\},$$

 $p(t_n | \mathbf{w}) = y_n^{t_n} (1 - y_n)^{1 - t_n},$ (4.104)

where

$$y_n = \sigma(\mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}_n),$$

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$
 (4.105)

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}). \tag{4.106}$$

By 4.13,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n) \phi_n. \tag{4.107}$$

Then, by 4.12,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^{N} y_n (1 - y_n) \phi_n \phi_n^{\mathsf{T}}.$$
 (4.108)

The right hand side can be written as

$$\mathbf{H} = \mathbf{\Phi}^{\mathsf{T}} \mathbf{R} \mathbf{\Phi},\tag{4.109}$$

where

$$R_{nn'} = \begin{cases} y_n(1 - y_n), & n = n', \\ 0, & \text{otherwise.} \end{cases}$$
 (4.110)

Then,

$$\mathbf{u}^{\mathsf{T}}\mathbf{H}\mathbf{u} = (\mathbf{\Phi}\mathbf{u})^{\mathsf{T}}\mathbf{R}(\mathbf{\Phi}\mathbf{u}). \tag{4.111}$$

Since

$$y_n(1-y_n) > 0, (4.112)$$

we have

$$\mathbf{u}^{\mathsf{T}}\mathbf{H}\mathbf{u} > 0. \tag{4.113}$$

Therefore, \mathbf{H} is positive definite. Thus, E is a convex function of \mathbf{w} and it has a unique minimum.

Let t_1, \dots, t_N be variables such that

$$t_n \in \{0, 1\},\ p(t_n = 1 | \phi_n) = \pi_n.$$
 (4.114)

Then,

$$p(t_n|\phi_n) = \pi_n^{t_n} (1 - \pi_n)^{1 - t_n}.$$
(4.115)

Therefore,

$$p(\mathbf{t}|\mathbf{\Phi}) = \prod_{n=1}^{N} \pi_n^{t_n} (1 - \pi_n)^{1 - t_n}.$$
 (4.116)

Thus,

$$-\ln p(\mathbf{t}|\mathbf{\Phi}) = -\sum_{n=1}^{N} (t_n \ln \pi_n + (1 - t_n) \ln(1 - \pi_n)). \tag{4.117}$$

4.17

Let

$$y_k = \frac{\exp(a_k)}{\sum_{k=1}^K \exp(a_k)}.$$
 (4.118)

Then,

$$\frac{\partial y_k}{\partial a_k} = \frac{\exp(a_k)}{\sum_{k=1}^K \exp(a_k)} - \frac{\exp(2a_k)}{\left(\sum_{k=1}^K \exp(a_k)\right)^2}.$$
 (4.119)

The right hand side can be written as $y_k(1-y_k)$. If $k \neq k'$, then

$$\frac{\partial y_k}{\partial a_{k'}} = -\frac{\exp(a_k + a_{k'})}{\left(\sum_{k=1}^K \exp(a_k)\right)^2}.$$
(4.120)

The right hand side can be written as $-y_k y_{k'}$. Therefore,

$$\frac{\partial y_k}{\partial a_{k'}} = y_k (I_{kk'} - y_{k'}). \tag{4.121}$$

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables such that

$$t_{nk} \in \{0, 1\},$$

$$p(\mathbf{t}_n | \mathbf{W}) = \prod_{k=1}^K y_{nk}^{t_{nk}},$$
(4.122)

where

$$y_{nk} = \frac{\exp(a_{nk})}{\sum_{k=1}^{K} \exp(a_{nk})},$$

$$a_{nk} = \mathbf{w}_{1}^{\mathsf{T}} \phi_{n}.$$
(4.123)

Then,

$$p(\mathbf{T}|\mathbf{W}) = \prod_{n=1}^{N} \prod_{k=1}^{K} y_{nk}^{t_{nk}}.$$
 (4.124)

Let

$$E(\mathbf{W}) = -\ln p(\mathbf{T}|\mathbf{W}). \tag{4.125}$$

The right hand side can be written as

$$-\sum_{n=1}^{N}\sum_{k=1}^{K}t_{nk}\ln y_{nk}.$$
(4.126)

Then, by 4.17,

$$\nabla_{\mathbf{w}_{k'}} E(\mathbf{W}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} y_{nk} (I_{kk'} - y_{nk'}) \frac{t_{nk}}{y_{nk}} \phi_n.$$
 (4.127)

The right hand side can be written as

$$-\sum_{n=1}^{N} \left(\sum_{k=1}^{K} (I_{kk'} - y_{nk'}) t_{nk} \right) \phi_n = -\sum_{n=1}^{N} (t_{nk'} - y_{nk'}) \phi_n.$$
 (4.128)

Therefore,

$$\nabla_{\mathbf{w}_k} E(\mathbf{W}) = \sum_{n=1}^N (y_{nk} - t_{nk}) \, \boldsymbol{\phi}_n. \tag{4.129}$$

Let t_1, \dots, t_N be variables such that

$$t_n \in \{0, 1\},\ p(t_n = 1|a_n) = \Phi(a_n),$$
 (4.130)

where

$$\Phi(a) = \int_{-\infty}^{a} \mathcal{N}(\theta|0,1)d\theta,$$

$$a_n = \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}_n.$$
(4.131)

Then,

$$p(t_n|\phi_n) = (\Phi(a_n))^{t_n} (1 - \Phi(a_n))^{1-t_n}.$$
(4.132)

Therefore,

$$p(\mathbf{t}|\mathbf{\Phi}) = \prod_{n=1}^{N} (\Phi(a_n))^{t_n} (1 - \Phi(a_n))^{1-t_n}.$$
 (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,

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N} \left(t_n \frac{\mathcal{N}(a_n|0,1)}{\Phi(a_n)} - (1 - t_n) \frac{\mathcal{N}(a_n|0,1)}{1 - \Phi(a_n)} \right) \phi_n.$$
 (4.136)

The right hand side can be written as

$$-\sum_{n=1}^{N} \left(\frac{t_n}{\Phi(a_n)} - \frac{1 - t_n}{1 - \Phi(a_n)} \right) \mathcal{N}(a_n | 0, 1) \phi_n$$

$$= \sum_{n=1}^{N} \frac{\mathcal{N}(a_n | 0, 1)}{\Phi(a_n) (1 - \Phi(a_n))} \left(\Phi(a_n) - t_n \right) \phi_n.$$
(4.137)

Therefore,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} \frac{\mathcal{N}(a_n|0,1)}{\Phi(a_n) (1 - \Phi(a_n))} (\Phi(a_n) - t_n) \, \phi_n. \tag{4.138}$$

Then,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^{N} \frac{-a_n \mathcal{N}(a_n | 0, 1)}{\Phi(a_n) (1 - \Phi(a_n))} (\Phi(a_n) - t_n) \phi_n \phi_n^{\mathsf{T}}$$

$$- \sum_{n=1}^{N} \frac{(\mathcal{N}(a_n | 0, 1))^2}{(\Phi(a_n))^2 (1 - \Phi(a_n))} (\Phi(a_n) - t_n) \phi_n \phi_n^{\mathsf{T}}$$

$$+ \sum_{n=1}^{N} \frac{(\mathcal{N}(a_n | 0, 1))^2}{\Phi(a_n) (1 - \Phi(a_n))^2} (\Phi(a_n) - t_n) \phi_n \phi_n^{\mathsf{T}}$$

$$+ \sum_{n=1}^{N} \frac{(\mathcal{N}(a_n | 0, 1))^2}{\Phi(a_n) (1 - \Phi(a_n))} \phi_n \phi_n^{\mathsf{T}}.$$
(4.139)

Therefore,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^{N} b_n \phi_n \phi_n^{\mathsf{T}}, \tag{4.140}$$

where

$$b_{n} = \left(\frac{\mathcal{N}(a_{n}|0,1)}{\Phi(a_{n})(1-\Phi(a_{n}))}\right)^{2} ((\Phi(a_{n}))^{2} - 2t_{n}\Phi(a_{n}) + t_{n})$$

$$-\frac{\mathcal{N}(a_{n}|0,1)}{\Phi(a_{n})(1-\Phi(a_{n}))} a_{n} (\Phi(a_{n}) - t_{n}).$$
(4.141)

4.20 (Incomplete)

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables such that

$$t_{nk} \in \{0, 1\},$$

$$p(\mathbf{t}_n | \mathbf{W}) = \prod_{k=1}^{K} y_{nk}^{t_{nk}},$$
(4.142)

where

$$y_{nk} = \frac{\exp(a_{nk})}{\sum_{k=1}^{K} \exp(a_{nk})},$$

$$a_{nk} = \mathbf{w}_{k}^{\mathsf{T}} \boldsymbol{\phi}_{n}.$$

$$(4.143)$$

Then,

$$p(\mathbf{T}|\mathbf{W}) = \prod_{n=1}^{N} \prod_{k=1}^{K} y_{nk}^{t_{nk}}.$$
 (4.144)

Let

$$E(\mathbf{W}) = -\ln p(\mathbf{T}|\mathbf{W}). \tag{4.145}$$

By 4.18,

$$\nabla_{\mathbf{w}_k} E(\mathbf{W}) = \sum_{n=1}^N (y_{nk} - t_{nk}) \, \boldsymbol{\phi}_n. \tag{4.146}$$

Additionally, by 4.17,

$$\nabla_{\mathbf{w}_k} \nabla_{\mathbf{w}_{k'}} E(\mathbf{W}) = \sum_{n=1}^N y_{nk} (I_{kk'} - y_{nk'}) \phi_n \phi_n^{\mathsf{T}}. \tag{4.147}$$

The right hand side can be written as

$$\mathbf{H}_{kk'} = \mathbf{\Phi}^{\mathsf{T}} \mathbf{R}_{kk'} \mathbf{\Phi}, \tag{4.148}$$

where

$$R_{kk'nn'} = \begin{cases} y_{nk}(I_{kk'} - y_{nk'}), & n = n', \\ 0, & \text{otherwise.} \end{cases}$$
 (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,

$$\mathbf{u}^{\mathsf{T}}\mathbf{H}\mathbf{u} = \sum_{k=1}^{K} \sum_{k'=1}^{K} \mathbf{u}_{k}^{\mathsf{T}}\mathbf{H}_{kk'}\mathbf{u}_{k'}, \tag{4.150}$$

Then, the right hand side can be written as

$$\sum_{k=1}^{K} \sum_{k'=1}^{K} (\mathbf{\Phi} \mathbf{u}_k)^{\mathsf{T}} \mathbf{R}_{kk'} (\mathbf{\Phi} \mathbf{u}_{k'}). \tag{4.151}$$

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

$$\int_{-\infty}^{0} \mathcal{N}(\theta|0,1)d\theta + \int_{0}^{a} \mathcal{N}(\theta|0,1)d\theta = \frac{1}{2} + \frac{1}{\sqrt{2\pi}} \int_{0}^{a} \exp\left(-\frac{\theta^{2}}{2}\right) d\theta. \quad (4.153)$$

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

$$\frac{1}{\sqrt{2\pi}} \int_0^{\frac{a}{\sqrt{2}}} \exp\left(-t^2\right) \sqrt{2} dt = \frac{1}{2} \operatorname{erf}\left(\frac{a}{\sqrt{2}}\right), \tag{4.154}$$

where

$$\operatorname{erf}(a) = \frac{2}{\sqrt{\pi}} \int_0^a \exp(-t^2) dt. \tag{4.155}$$

Therefore,

$$\Phi(a) = \frac{1}{2} \left(1 + \operatorname{erf}\left(\frac{a}{\sqrt{2}}\right) \right). \tag{4.156}$$

4.22

Let θ be a variable in M dimensions. By a Taylor expansion,

$$\ln (p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})) \simeq \ln (p(\mathcal{D}|\boldsymbol{\theta}_0)p(\boldsymbol{\theta}_0)) + \mathbf{v}(\boldsymbol{\theta}_0)^{\mathsf{T}}(\boldsymbol{\theta} - \boldsymbol{\theta}_0) - \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^{\mathsf{T}}\mathbf{A}(\boldsymbol{\theta}_0)(\boldsymbol{\theta} - \boldsymbol{\theta}_0),$$
(4.157)

where

$$\mathbf{v}(\boldsymbol{\theta}) = \nabla \ln \left(p(\mathcal{D}|\boldsymbol{\theta}) p(\boldsymbol{\theta}) \right), \mathbf{A}(\boldsymbol{\theta}) = -\nabla \nabla \ln \left(p(\mathcal{D}|\boldsymbol{\theta}) p(\boldsymbol{\theta}) \right).$$
(4.158)

Let $\boldsymbol{\theta}_{\text{MAP}}$ be a stationary point of $p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})$. Then,

$$\ln (p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})) \simeq \ln (p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}})p(\boldsymbol{\theta}_{\text{MAP}})) - \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}})^{\mathsf{T}} \mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}}),$$
(4.159)

so that

$$p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta}) \simeq p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}})p(\boldsymbol{\theta}_{\text{MAP}})\exp\left(-\frac{1}{2}(\boldsymbol{\theta}-\boldsymbol{\theta}_{\text{MAP}})^{\mathsf{T}}\mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})(\boldsymbol{\theta}-\boldsymbol{\theta}_{\text{MAP}})\right). \tag{4.160}$$

By marginalisation, integrating both sides with respect to θ gives

$$p(\mathcal{D}) \simeq p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}})p(\boldsymbol{\theta}_{\text{MAP}}) \int \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}})^{\mathsf{T}} \mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}})\right) d\boldsymbol{\theta}.$$
(4.161)

The integral of the right hand side can be written as

$$(2\pi)^{\frac{M}{2}} \left(\det \mathbf{A}(\boldsymbol{\theta}_{MAP})^{-1} \right)^{\frac{1}{2}} = (2\pi)^{\frac{M}{2}} \left(\det \mathbf{A}(\boldsymbol{\theta}_{MAP}) \right)^{-\frac{1}{2}}.$$
 (4.162)

Therefore,

$$p(\mathcal{D}) \simeq p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}})p(\boldsymbol{\theta}_{\text{MAP}})(2\pi)^{\frac{M}{2}} \left(\det \mathbf{A}(\boldsymbol{\theta}_{\text{MAP}})\right)^{-\frac{1}{2}},$$
 (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

$$\ln p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}}) - \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \mathbf{V}_{0}) - \frac{1}{2} (\boldsymbol{\theta}_{\text{MAP}} - \mathbf{m}_{0})^{\mathsf{T}} \mathbf{V}_{0}^{-1} (\boldsymbol{\theta}_{\text{MAP}} - \mathbf{m}_{0})$$

$$+ \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln\left(\det\left(\mathbf{H}(\boldsymbol{\theta}_{\text{MAP}}) + \mathbf{V}_{0}^{-1}\right)\right)$$

$$= \ln p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}}) + \frac{1}{2} \ln\left(\det\mathbf{V}_{0}^{-1}\right) - \frac{1}{2} (\boldsymbol{\theta}_{\text{MAP}} - \mathbf{m}_{0})^{\mathsf{T}} \mathbf{V}_{0}^{-1} (\boldsymbol{\theta}_{\text{MAP}} - \mathbf{m}_{0})$$

$$- \frac{1}{2} \ln\left(\det\left(\mathbf{H}(\boldsymbol{\theta}_{\text{MAP}}) + \mathbf{V}_{0}^{-1}\right)\right).$$
(4.171)

If \mathbf{V}_0^{-1} can be neglected, the right hand side can be written as

$$\ln p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}}) - \frac{1}{2} \ln \left(\det \mathbf{H}(\boldsymbol{\theta}_{\text{MAP}}) \right). \tag{4.172}$$

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,

$$\det \mathbf{H}(\boldsymbol{\theta}_{\text{MAP}}) = N^M \det \bar{\mathbf{H}}(\boldsymbol{\theta}_{\text{MAP}}). \tag{4.175}$$

Threrefore,

$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}}) - \frac{M}{2} \ln N.$$
 (4.176)

4.24 (Incomplete)

Let t_1, \dots, t_N be variables such that

$$t_n \in \{0, 1\},\ p(t_n | \mathbf{w}) = y_n^{t_n} (1 - y_n)^{1 - t_n},$$
(4.177)

where

$$y_n = \sigma(\mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}_n),$$

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$
 (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 ${\bf w}$ and ${\bf t}$ can be written as

$$\sum_{n=1}^{N} (t_n \ln y_n + (1 - t_n) \ln(1 - y_n)) - \frac{1}{2} (\mathbf{w} - \mathbf{m}_0)^{\mathsf{T}} \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0).$$
 (4.181)

Then, by 4.22,

$$p(\mathbf{w}|\mathbf{t}) \simeq \mathcal{N}(\mathbf{w}|\mathbf{w}_{\text{MAP}}, \mathbf{S}_N)$$
? (4.182)

where \mathbf{w}_{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,

$$p(\mathcal{C}_1|\mathbf{t}) = \int p(\mathcal{C}_1|\mathbf{w})p(\mathbf{w}|\mathbf{t})d\mathbf{w}.$$
 (4.184)

The logarithm of the integrand of the right hand side except the terms independent of \mathbf{w} can be approximated as

$$-\ln\left(1 + \exp\left(-\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}\right)\right) - \frac{1}{2}(\mathbf{w} - \mathbf{w}_{\text{MAP}})^{\mathsf{T}}\mathbf{S}_{N}^{-1}(\mathbf{w} - \mathbf{w}_{\text{MAP}}) = (4.185)$$

Let

$$\sigma(a) = \frac{1}{1 + \exp(-a)},$$

$$\Phi(a) = \int_{-\infty}^{a} \mathcal{N}(\theta|0, 1)d\theta.$$
(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,

$$\frac{1}{4} = \lambda (2\pi)^{-\frac{1}{2}}. (4.190)$$

Therefore,

$$\lambda^2 = \frac{\pi}{8}.\tag{4.191}$$

4.26

Let

$$I(\mu) = \int \Phi(\lambda a) \mathcal{N}(a|\mu, \sigma^2) da, \qquad (4.192)$$

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

$$\int \Phi(\lambda(\mu + \sigma z)) \mathcal{N}(\mu + \sigma z | \mu, \sigma^2) \sigma dz = \int \Phi(\lambda(\mu + \sigma z)) \mathcal{N}(z | 0, 1) dz.$$
(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

$$-\frac{1}{2}\ln(2\pi) - \frac{\lambda^2(\mu + \sigma z)^2}{2} - \frac{1}{2}\ln(2\pi) - \frac{z^2}{2}$$

$$= -\ln(2\pi) - \frac{1 + \sigma^2\lambda^2}{2} \left(z + \frac{\mu\sigma\lambda^2}{1 + \sigma^2\lambda^2}\right)^2 + \frac{\mu^2\sigma^2\lambda^4}{2(1 + \sigma^2\lambda^2)} - \frac{\mu^2\lambda^2}{2}.$$
(4.197)

The right hand side can be written as

$$-\ln(2\pi) - \frac{1+\sigma^2\lambda^2}{2} \left(z + \frac{\mu\sigma\lambda^2}{1+\sigma^2\lambda^2}\right)^2 - \frac{\mu^2\lambda^2}{2(1+\sigma^2\lambda^2)}$$

$$= -\frac{1}{2}\ln(2\pi) - \frac{1}{2}\ln(1+\sigma^2\lambda^2)^{-1} - \frac{1+\sigma^2\lambda^2}{2} \left(z + \frac{\mu\sigma\lambda^2}{1+\sigma^2\lambda^2}\right)^2 - \ln\lambda - \frac{1}{2}\ln(2\pi) - \frac{1}{2}\ln(\lambda^{-2} + \sigma^2) - \frac{\mu^2}{2(\lambda^{-2} + \sigma^2)}.$$
(4.198)

Then, the integral can be written as

$$\int \mathcal{N}\left(z| - \frac{\mu\sigma\lambda^2}{1 + \sigma^2\lambda^2}, \left(1 + \sigma^2\lambda^2\right)^{-1}\right) \frac{1}{\lambda} \mathcal{N}\left(\mu|0, \lambda^{-2} + \sigma^2\right) dz$$

$$= \frac{1}{\lambda} \mathcal{N}\left(\mu|0, \lambda^{-2} + \sigma^2\right).$$
(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

$$I(\mu) = \int_{-\infty}^{\mu} \mathcal{N}(m|0, \lambda^{-2} + \sigma^2) dm.$$
 (4.201)

By the transformation

$$m' = \frac{m}{(\lambda^{-2} + \sigma^2)^{\frac{1}{2}}},\tag{4.202}$$

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,

$$I(\mu) = \Phi\left(\frac{\mu}{(\lambda^{-2} + \sigma^2)^{\frac{1}{2}}}\right).$$
 (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,

$$\sigma(a) = \frac{\exp\left(\frac{a}{2}\right)}{\exp\left(\frac{a}{2}\right) + \exp\left(-\frac{a}{2}\right)}.$$
 (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

$$\sum_{m=1}^{M} w_{km}^{(2)} \left(\frac{1}{2} \left(1 + \tanh \left(\frac{1}{2} \left(\sum_{d=1}^{D} w_{md}^{(1)} x_d + w_{m0}^{(1)} \right) \right) \right) \right) + w_{k0}^{(2)} \\
= \frac{1}{2} \sum_{m=1}^{M} w_{km}^{(2)} \tanh \left(\frac{1}{2} \sum_{d=1}^{D} w_{md}^{(1)} x_d + \frac{1}{2} w_{m0}^{(1)} \right) + \frac{1}{2} \sum_{m=1}^{M} w_{km}^{(2)} + w_{k0}^{(2)}.$$
(5.6)

Therefore,

$$y_k(\mathbf{x}, \mathbf{w}) = \sigma \left(\frac{1}{2} \sum_{m=1}^{M} w_{km}^{(2)} \tanh \left(\frac{1}{2} \sum_{d=1}^{D} w_{md}^{(1)} x_d + \frac{1}{2} w_{m0}^{(1)} \right) + \frac{1}{2} \sum_{m=1}^{M} w_{km}^{(2)} + w_{k0}^{(2)} \right).$$
(5.7)

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ 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

$$-\frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{t}_{n}-\mathbf{y}(\mathbf{x}_{n},\mathbf{w})\right)^{\intercal}\left(\beta^{-1}\mathbf{I}\right)^{-1}\left(\mathbf{t}_{n}-\mathbf{y}(\mathbf{x}_{n},\mathbf{w})\right)=-\frac{\beta}{2}\sum_{n=1}^{N}\|\mathbf{y}(\mathbf{x}_{n},\mathbf{w})-\mathbf{t}_{n}\|^{2}.$$
(5.9)

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

$$\mathbf{0} = -\beta \sum_{n=1}^{N} \frac{\partial \mathbf{y}(\mathbf{x}_{n}, \mathbf{w})}{\partial \mathbf{w}} (\mathbf{y}(\mathbf{x}_{n}, \mathbf{w}) - \mathbf{t}_{n}).$$
 (5.10)

Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \|\mathbf{y}(\mathbf{x}_n, \mathbf{w}) - \mathbf{t}_n\|^2.$$
 (5.11)

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

$$\mathbf{0} = \sum_{n=1}^{N} \frac{\partial \mathbf{y}(\mathbf{x}_{n}, \mathbf{w})}{\partial \mathbf{w}} (\mathbf{y}(\mathbf{x}_{n}, \mathbf{w}) - \mathbf{t}_{n}).$$
 (5.12)

Therefore, maximising the likelihood is equivalent to minimising $E(\mathbf{w})$.

5.3

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables such that

$$p(\mathbf{t}_n|\mathbf{x}_n,\mathbf{w}) = \mathcal{N}\left(\mathbf{t}_n|\mathbf{y}(\mathbf{x}_n,\mathbf{w}),\boldsymbol{\Sigma}\right). \tag{5.13}$$

Then, the logarithm of the likelihood except the terms independent of ${\bf w}$ and ${\bf \Sigma}$ can be written as

$$-\frac{1}{2}\ln(\det \mathbf{\Sigma}) - \frac{1}{2}\sum_{n=1}^{N} (\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w}))^{\mathsf{T}} \mathbf{\Sigma}^{-1} (\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})).$$
 (5.14)

Setting the derivatives with respect to \mathbf{w} and Σ to zero gives

$$\mathbf{0} = -\sum_{n=1}^{N} \frac{\partial \mathbf{y}(\mathbf{x}_{n}, \mathbf{w})}{\partial \mathbf{w}} \mathbf{\Sigma}^{-1} \left(\mathbf{t}_{n} - \mathbf{y}(\mathbf{x}_{n}, \mathbf{w}) \right),$$

$$\mathbf{O} = -\frac{1}{2} \mathbf{\Sigma}^{-1} + \frac{1}{2} \left(\mathbf{\Sigma}^{-1} \right)^{2} \sum_{n=1}^{N} \left(\mathbf{t}_{n} - \mathbf{y}(\mathbf{x}_{n}, \mathbf{w}) \right) \left(\mathbf{t}_{n} - \mathbf{y}(\mathbf{x}_{n}, \mathbf{w}) \right)^{\mathsf{T}}.$$
(5.15)

Therefore, the maximum likelihood solution for Σ is given by

$$\Sigma = \sum_{n=1}^{N} (\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})) (\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w}))^{\mathsf{T}}.$$
 (5.16)

On the other hand, if Σ is fixed and known, then the maximum likelihood solution for \mathbf{w} is given by minimising

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} (\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w}))^{\mathsf{T}} \mathbf{\Sigma}^{-1} (\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})).$$
 (5.17)

5.4

Let t_1, \dots, t_N be variables such that

$$t_n \in \{0, 1\},\ p(t_n = 1 | \mathbf{x}_n) = (1 - \epsilon)y_n + \epsilon (1 - y_n),$$
 (5.18)

where

$$y_n = y(\mathbf{x}_n, \mathbf{w}). \tag{5.19}$$

Then,

$$p(t_n|\mathbf{x}_n) = ((1 - \epsilon)y_n + \epsilon (1 - y_n))^{t_n} (\epsilon y_n + (1 - \epsilon) (1 - y_n))^{1 - t_n}.$$
 (5.20)

Therefore,

$$-\ln\left(\prod_{n=1}^{N} p(t_n|\mathbf{x}_n)\right)$$

$$= -\sum_{n=1}^{N} \left(t_n \ln\left((1-\epsilon)y_n + \epsilon(1-y_n)\right) + (1-t_n) \ln\left(\epsilon y_n + (1-\epsilon)(1-y_n)\right)\right).$$
(5.21)

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables in K dimensions such that

$$t_{nk} \in \{0, 1\},\ p(t_{nk} = 1 | \mathbf{x}_n) = y_{nk},$$
 (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

$$p(\mathbf{t}_n|\mathbf{x}_n) = \prod_{k=1}^K y_{nk}^{t_{nk}}.$$
 (5.25)

Therefore,

$$\ln\left(\prod_{n=1}^{N} p(\mathbf{t}_{n}|\mathbf{x}_{n})\right) = \sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \ln y_{nk}.$$
 (5.26)

5.6

Let t_1, \dots, t_N be variables such that

$$t_n \in \{0, 1\},\ p(t_n = 1 | \mathbf{x}_n) = y_n,$$
 (5.27)

where

$$y_n = y(\mathbf{x}_n, \mathbf{w}). \tag{5.28}$$

Then,

$$p(t_n|\mathbf{x}_n) = y_n^{t_n} (1 - y_n)^{1 - t_n}.$$
 (5.29)

Let

$$E(\mathbf{w}) = -\ln\left(\prod_{n=1}^{N} p(t_n|\mathbf{x}_n)\right).$$
 (5.30)

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^{N} (t_n \ln y_n + (1 - t_n) \ln(1 - y_n)).$$
 (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 $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables such that

$$t_{nk} \in \{0, 1\},\$$

$$p(t_{nk} = 1 | \mathbf{x}_n) = y_{nk},$$
(5.36)

where

$$y_{nk} = y_k(\mathbf{x}_n, \mathbf{w}),$$

$$y_{nk} = y_k(\mathbf{x}_n, \mathbf{w}),$$

$$\sum_{k=1}^K y_{nk} = 1.$$
(5.37)

Then,

$$p(\mathbf{t}_n|\mathbf{x}_n) = \prod_{k=1}^K y_{nk}^{t_{nk}}.$$
 (5.38)

Let

$$E(\mathbf{w}) = -\ln\left(\prod_{n=1}^{N} p(\mathbf{t}_n | \mathbf{x}_n)\right). \tag{5.39}$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \ln y_{nk}.$$
 (5.40)

If

$$y_{nk} = \frac{\exp\left(a_k(\mathbf{x}_n, \mathbf{w})\right)}{\sum_{k=1}^K \exp\left(a_k(\mathbf{x}_n, \mathbf{w})\right)},$$
(5.41)

then, by 4.17,

$$\frac{\partial E(\mathbf{w})}{\partial a_{k'}} = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} y_{nk} (I_{kk'} - y_{nk}) \frac{1}{y_{nk}}.$$
 (5.42)

The right hand side can be written as

$$-\sum_{n=1}^{N}\sum_{k=1}^{K}t_{nk}(I_{kk'}-y_{nk}) = -\sum_{n=1}^{N}\left(\sum_{k=1}^{K}t_{nk}y_{nk}-t_{nk'}\right).$$
 (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

$$tanh a = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)}$$
(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, \dots, t_N be variables such that

$$t_n \in \{-1, 1\},\$$

$$p(t_n = 1 | \mathbf{x}_n) = \frac{1 + y_n}{2},$$
(5.48)

where

$$y_n = y(\mathbf{x}_n, \mathbf{w}). \tag{5.49}$$

Then,

$$p(t_n|\mathbf{x}_n) = \left(\frac{1+y_n}{2}\right)^{\frac{1+t_n}{2}} \left(\frac{1-y_n}{2}\right)^{\frac{1-t_n}{2}}.$$
 (5.50)

Let

$$E(\mathbf{w}) = -\ln\left(\prod_{n=1}^{N} p(t_n|\mathbf{x}_n)\right). \tag{5.51}$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \left(\frac{1+t_n}{2} \ln \frac{1+y_n}{2} + \frac{1-t_n}{2} \ln \frac{1-y_n}{2} \right).$$
 (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,

$$E(\mathbf{w}) \simeq E(\mathbf{w}^*) + \frac{1}{2} (\mathbf{w} - \mathbf{w}^*)^{\mathsf{T}} \mathbf{H} (\mathbf{w} - \mathbf{w}^*),$$
 (5.55)

where

$$\mathbf{H} = \left. \nabla \nabla E(\mathbf{w}) \right|_{\mathbf{w} = \mathbf{w}^*}. \tag{5.56}$$

Let $\mathbf{u}_1, \dots, \mathbf{u}_M$ be eigenvectors such that

$$\mathbf{H}\mathbf{u}_m = \lambda_m \mathbf{u}_m. \tag{5.57}$$

Note that **H** is a real symmetric matrix. Then, by ??, we have

$$\mathbf{u}_{m}^{\mathsf{T}}\mathbf{u}_{m'} = I_{mm'}.\tag{5.58}$$

Therefore, there exists $\alpha_1, \dots, \alpha_M$ 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

$$E(\mathbf{w}) \simeq E(\mathbf{w}^*) + \frac{1}{2} \sum_{m=1}^{M} \lambda_m \alpha_m^2.$$
 (5.60)

Therefore, the contours of constant E are ellipses whose axes are aligned with $\mathbf{u}_1, \dots, \mathbf{u}_M$ with lengths which are proportional to $\lambda_1^{-\frac{1}{2}}, \dots, \lambda_M^{-\frac{1}{2}}$.

5.12

Let **w** be a real vector. Let E be a real function of **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,

$$E(\mathbf{w}) \simeq E(\mathbf{w}^*) + \frac{1}{2} (\mathbf{w} - \mathbf{w}^*)^{\mathsf{T}} \mathbf{H} (\mathbf{w} - \mathbf{w}^*),$$
 (5.62)

where

$$\mathbf{H} = \left. \nabla \nabla E(\mathbf{w}) \right|_{\mathbf{w} = \mathbf{w}^*}. \tag{5.63}$$

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.

Let \mathbf{w} be a vector in M dimensions. Let E be a function of \mathbf{w} . Then, by a Taylor expansion,

$$E(\mathbf{w}) \simeq E(\hat{\mathbf{w}}) + (\mathbf{w} - \hat{\mathbf{w}})^{\mathsf{T}} \mathbf{b} + \frac{1}{2} (\mathbf{w} - \hat{\mathbf{w}})^{\mathsf{T}} \mathbf{H} (\mathbf{w} - \hat{\mathbf{w}}),$$
 (5.66)

where

$$\mathbf{b} = \nabla E(\mathbf{w})|_{\mathbf{w} = \hat{\mathbf{w}}}.$$

$$\mathbf{H} = \nabla \nabla E(\mathbf{w})|_{\mathbf{w} = \hat{\mathbf{w}}}.$$
(5.67)

Since **b** is a vector in M dimensions and **H** is a $M \times M$ symmetric matrix, the number of independent elements of the right hand side is

$$M + \frac{M(M+1)}{2} = \frac{M(M+3)}{2}. (5.68)$$

5.14

Let w be a variable. Let E_n be a function of w. Then, by a Taylor expansion,

$$E_{n}(w_{mm'} + \epsilon) = E_{n}(w_{mm'}) + \frac{\partial E_{n}}{\partial w}\Big|_{w=w_{mm'}} \epsilon + O(\epsilon^{2}),$$

$$E_{n}(w_{mm'} - \epsilon) = E_{n}(w_{mm'}) - \frac{\partial E_{n}}{\partial w}\Big|_{w=w_{mm'}} \epsilon + O(\epsilon^{2}).$$
(5.69)

Therefore,

$$\left. \frac{\partial E_n}{\partial w} \right|_{w=w} = \frac{E_n(w_{mm'} + \epsilon) - E_n(w_{mm'} - \epsilon)}{2\epsilon} + O\left(\epsilon^2\right). \tag{5.70}$$

5.15 (Incomplete)

5.16

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be vectors. Let $\mathbf{y}_1, \dots, \mathbf{y}_N$ be vectors which are dependent on a vector \mathbf{w} . Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \|\mathbf{y}_n - \mathbf{t}_n\|^2.$$
 (5.71)

Then,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (\nabla \mathbf{y}_n)^{\mathsf{T}} (\mathbf{y}_n - \mathbf{t}_n), \qquad (5.72)$$

so that

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^{N} (\nabla \operatorname{vec} (\nabla \mathbf{y}_n)^{\mathsf{T}})^{\mathsf{T}} (\mathbf{y}_n - \mathbf{t}_n) + \sum_{n=1}^{N} (\nabla \mathbf{y}_n)^{\mathsf{T}} (\nabla \mathbf{y}_n). \quad (5.73)$$

5.17

Let t be a variable. Let y be a function of a vector \mathbf{x} and a vector \mathbf{w} . Let

$$E(\mathbf{w}) = \frac{1}{2} \int \int (y-t)^2 p(\mathbf{x}, t) d\mathbf{x} dt.$$
 (5.74)

Then,

$$\nabla E(\mathbf{w}) = \int \int (y - t)p(\mathbf{x}, t)\nabla y d\mathbf{x} dt.$$
 (5.75)

The right hand side can be written as

$$\int y \nabla y \left(\int p(\mathbf{x}, t) dt \right) d\mathbf{x} - \int \nabla y \left(\int t p(t|\mathbf{x}) dt \right) p(\mathbf{x}) d\mathbf{x}$$

$$= \int y \nabla y p(\mathbf{x}) d\mathbf{x} - \int \nabla y \, \mathbf{E}(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}.$$
(5.76)

Then,

$$\nabla \nabla E(\mathbf{w}) = \int \nabla y (\nabla y)^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x} + \int y \nabla \nabla y p(\mathbf{x}) d\mathbf{x} - \int \nabla \nabla y E(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}.$$
(5.77)

The second and the third terms of the right hand side can be written as

$$E(y\nabla\nabla y) - E(\nabla\nabla y E(t|\mathbf{x})) = E((y - E(t|\mathbf{x})) \nabla\nabla y).$$
 (5.78)

Therefore, if

$$y = \mathcal{E}(t|\mathbf{x}),\tag{5.79}$$

then

$$\nabla \nabla E(\mathbf{w}) = \int \nabla y (\nabla y)^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x}. \tag{5.80}$$

Let t_1, \dots, t_N be variables. Let y_1, \dots, y_N be variables such that

$$y_n = \mathbf{w}_n^{(2)^{\mathsf{T}}} \mathbf{z} + \mathbf{w}_n^{(0)^{\mathsf{T}}} \mathbf{x},$$

$$z_m = \tanh\left(\mathbf{w}_m^{(1)^{\mathsf{T}}} \mathbf{x}\right).$$
 (5.81)

Let

$$E = \frac{1}{2} \sum_{n=1}^{N} (y_n - t_n)^2.$$
 (5.82)

Then,

$$\frac{\partial E}{\partial \mathbf{w}_{n}^{(0)}} = \frac{\partial E}{\partial y_{n}} \frac{\partial y_{n}}{\partial \mathbf{w}_{n}^{(0)}},$$

$$\frac{\partial E}{\partial \mathbf{w}_{m}^{(1)}} = \frac{\partial E}{\partial y_{n}} \frac{\partial y_{n}}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{w}_{m}^{(1)}},$$

$$\frac{\partial E}{\partial \mathbf{w}_{n}^{(2)}} = \frac{\partial E}{\partial y_{n}} \frac{\partial y_{n}}{\partial \mathbf{w}_{n}^{(2)}}.$$
(5.83)

Therefore,

$$\frac{\partial E}{\partial \mathbf{w}_{n}^{(0)}} = (y_{n} - t_{n})\mathbf{x},$$

$$\frac{\partial E}{\partial \mathbf{w}_{m}^{(1)}} = (y_{n} - t_{n})\mathbf{A}\mathbf{w}_{n}^{(2)},$$

$$\frac{\partial E}{\partial \mathbf{w}_{n}^{(2)}} = (y_{n} - t_{n})\mathbf{z},$$
(5.84)

where

$$A_{mm'} = (1 - z_m^2) x_{m'}. (5.85)$$

5.19

Let t_1, \dots, t_N be variables such that

$$t_n \in \{0, 1\},\ p(t_n | \mathbf{w}) = y_n^{t_n} (1 - y_n)^{1 - t_n},$$
(5.86)

where

$$y_n = \sigma(a_n(\mathbf{w})),$$

$$\sigma(a) = \frac{1}{1 + \exp(-a)},$$
(5.87)

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}). \tag{5.88}$$

The right hand side can be written as

$$-\ln\left(\prod_{n=1}^{N} y_n^{t_n} (1-y_n)^{1-t_n}\right) = -\sum_{n=1}^{N} \left(t_n \ln y_n + (1-t_n) \ln(1-y_n)\right). \quad (5.89)$$

Then, by 4.12,

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N} \left(\frac{t_n}{y_n} y_n (1 - y_n) \nabla a_n - \frac{1 - t_n}{1 - y_n} y_n (1 - y_n) \nabla a_n \right).$$
 (5.90)

The right hand side can be written as

$$-\sum_{n=1}^{N} (t_n(1-y_n)\nabla a_n - (1-t_n)y_n\nabla a_n) = \sum_{n=1}^{N} (y_n - t_n)\nabla a_n.$$
 (5.91)

Then, by 4.13,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n) \nabla a_n.$$
 (5.92)

Therefore, by 4.12,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^{N} y_n (1 - y_n) \nabla a_n (\nabla a_n)^{\mathsf{T}} + \sum_{n=1}^{N} (y_n - t_n) \nabla \nabla a_n.$$
 (5.93)

5.20

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables such that

$$t_{nk} \in \{0, 1\},\ p(t_{nk} = 1 | \mathbf{x}_n) = y_{nk},$$
 (5.94)

where

$$y_{nk} = y_k(\mathbf{x}_n, \mathbf{w}),$$

$$\sum_{k=1}^K y_{nk} = 1.$$
(5.95)

Then,

$$p(\mathbf{t}_n|\mathbf{x}_n) = \prod_{k=1}^K y_{nk}^{t_{nk}}.$$
 (5.96)

Let

$$E(\mathbf{w}) = -\ln\left(\prod_{n=1}^{N} p(\mathbf{t}_n | \mathbf{x}_n)\right). \tag{5.97}$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \ln y_{nk}.$$
 (5.98)

If

$$y_{nk} = \frac{\exp(a_k(\mathbf{x}_n, \mathbf{w}))}{\sum_{k=1}^K \exp(a_k(\mathbf{x}_n, \mathbf{w}))},$$
 (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,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} \sum_{k=1}^{K} (y_{nk} - t_{nk}) \nabla a_k.$$
 (5.101)

Then,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^{N} \sum_{k=1}^{K} y_{nk} (1 - y_{nk}) \nabla a_k (\nabla a_k)^{\mathsf{T}} + \sum_{n=1}^{N} \sum_{k=1}^{K} (y_{nk} - t_{nk}) \nabla \nabla a_k.$$
(5.102)

5.21 (Incomplete)

5.22

Let y_1, \dots, y_N be variables such that

$$y_n = \mathbf{w}_n^{(2)^{\mathsf{T}}} \mathbf{z},$$

$$z_m = h(a_m),$$

$$a_m = \mathbf{w}_m^{(1)^{\mathsf{T}}} \mathbf{x}.$$
(5.103)

Let E be a function of y_1, \dots, y_N . Then,

$$\frac{\partial E}{\partial \mathbf{w}_{m}^{(1)}} = \frac{\partial E}{\partial y_{n}} \frac{\partial y_{n}}{\partial z_{m}} \frac{\partial z_{m}}{\partial a_{m}} \frac{\partial a_{m}}{\partial \mathbf{w}_{m}^{(1)}},$$

$$\frac{\partial E}{\partial \mathbf{w}_{n}^{(2)}} = \frac{\partial E}{\partial y_{n}} \frac{\partial y_{n}}{\partial \mathbf{w}_{n}^{(2)}}.$$
(5.104)

Therefore,

$$\frac{\partial E}{\partial \mathbf{w}_{m}^{(1)}} = \frac{\partial E}{\partial y_{n}} w_{nm}^{(2)} h'(a_{m}) \mathbf{x},
\frac{\partial E}{\partial \mathbf{w}_{n}^{(2)}} = \frac{\partial E}{\partial y_{n}} \mathbf{z}.$$
(5.105)

Thus,

$$\frac{\partial^{2} E}{\partial \mathbf{w}_{m}^{(1)} \partial \mathbf{w}_{m'}^{(1)}} = w_{nm}^{(2)} \mathbf{x} \left(\frac{\partial^{2} E}{\partial y_{n}^{2}} w_{nm'}^{(2)} h'(a_{m'}) h'(a_{m}) \mathbf{x} + \frac{\partial E}{\partial y_{n}} h''(a_{m}) I_{mm'} \mathbf{x} \right)^{\mathsf{T}},$$

$$\frac{\partial^{2} E}{\partial \mathbf{w}_{m}^{(1)} \partial \mathbf{w}_{n}^{(2)}} = h'(a_{m}) \mathbf{x} \left(\frac{\partial^{2} E}{\partial y_{n}^{2}} w_{nm}^{(2)} \mathbf{z} + \frac{\partial E}{\partial y_{n}} \mathbf{v} \right)^{\mathsf{T}},$$

$$\frac{\partial^{2} E}{\partial \mathbf{w}_{n}^{(2)} \partial \mathbf{w}_{n'}^{(2)}} = \frac{\partial^{2} E}{\partial y_{n} \partial y_{n'}} \mathbf{z} \mathbf{z}^{\mathsf{T}},$$
(5.106)

where

$$v_m = \begin{cases} 1, & m = n, \\ 0 & \text{otherwise.} \end{cases}$$
 (5.107)

5.23

Let y_1, \dots, y_N be variables such that

$$y_n = \mathbf{w}_n^{(2)^{\mathsf{T}}} \mathbf{z} + \mathbf{w}_n^{(0)^{\mathsf{T}}} \mathbf{x},$$

$$z_m = h(a_m),$$

$$a_m = \mathbf{w}_m^{(1)^{\mathsf{T}}} \mathbf{x}.$$
(5.108)

Let E be a function of y_1, \dots, y_N . Then,

$$\frac{\partial E}{\partial \mathbf{w}_{n}^{(0)}} = \frac{\partial E}{\partial y_{n}} \frac{\partial y_{n}}{\partial \mathbf{w}_{n}^{(0)}},$$

$$\frac{\partial E}{\partial \mathbf{w}_{m}^{(1)}} = \frac{\partial E}{\partial y_{n}} \frac{\partial y_{n}}{\partial z_{m}} \frac{\partial z_{m}}{\partial a_{m}} \frac{\partial a_{m}}{\partial \mathbf{w}_{m}^{(1)}},$$

$$\frac{\partial E}{\partial \mathbf{w}_{n}^{(2)}} = \frac{\partial E}{\partial y_{n}} \frac{\partial y_{n}}{\partial \mathbf{w}_{n}^{(2)}}.$$
(5.109)

Therefore,

$$\frac{\partial E}{\partial \mathbf{w}_{n}^{(0)}} = \frac{\partial E}{\partial y_{n}} \mathbf{x},$$

$$\frac{\partial E}{\partial \mathbf{w}_{m}^{(1)}} = \frac{\partial E}{\partial y_{n}} w_{nm}^{(2)} h'(a_{m}) \mathbf{x},$$

$$\frac{\partial E}{\partial \mathbf{w}_{n}^{(2)}} = \frac{\partial E}{\partial y_{n}} \mathbf{z}.$$
(5.110)

Thus,

$$\frac{\partial^{2} E}{\partial \mathbf{w}_{n}^{(0)} \partial \mathbf{w}_{n'}^{(0)}} = \frac{\partial^{2} E}{\partial y_{n} \partial y_{n'}} \mathbf{x} \mathbf{x}^{\mathsf{T}},
\frac{\partial^{2} E}{\partial \mathbf{w}_{n}^{(0)} \partial \mathbf{w}_{m}^{(1)}} = \frac{\partial^{2} E}{\partial y_{n}^{2}} w_{nm}^{(2)} h'(a_{m}) \mathbf{x} \mathbf{x}^{\mathsf{T}},
\frac{\partial^{2} E}{\partial \mathbf{w}_{n}^{(0)} \partial \mathbf{w}_{n'}^{(2)}} = \frac{\partial^{2} E}{\partial y_{n} \partial y_{n'}} \mathbf{x} \mathbf{z}^{\mathsf{T}},
\frac{\partial^{2} E}{\partial \mathbf{w}_{m}^{(1)} \partial \mathbf{w}_{m'}^{(1)}} = w_{nm}^{(2)} \mathbf{x} \left(\frac{\partial^{2} E}{\partial y_{n}^{2}} w_{nm'}^{(2)} h'(a_{m'}) h'(a_{m}) \mathbf{x} + \frac{\partial E}{\partial y_{n}} h''(a_{m}) I_{mm'} \mathbf{x} \right)^{\mathsf{T}},
\frac{\partial^{2} E}{\partial \mathbf{w}_{m}^{(1)} \partial \mathbf{w}_{n'}^{(2)}} = h'(a_{m}) \mathbf{x} \left(\frac{\partial^{2} E}{\partial y_{n}^{2}} w_{nm}^{(2)} \mathbf{z} + \frac{\partial E}{\partial y_{n}} \mathbf{v} \right)^{\mathsf{T}},
\frac{\partial^{2} E}{\partial \mathbf{w}_{n}^{(2)} \partial \mathbf{w}_{n'}^{(2)}} = \frac{\partial^{2} E}{\partial y_{n} \partial y_{n'}} \mathbf{z} \mathbf{z}^{\mathsf{T}},$$

$$(5.111)$$

where

$$v_m = \begin{cases} 1, & m = n, \\ 0 & \text{otherwise.} \end{cases}$$
 (5.112)

Let y_1, \dots, y_n be variables such that

$$y_n = \mathbf{w}_n^{\mathsf{T}} \mathbf{z} + w_{n0},$$

$$z_m = h \left(\mathbf{w}_m^{\mathsf{T}} \mathbf{x} + w_{m0} \right).$$
(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,

$$z_m = h\left(\frac{1}{a}\mathbf{w}_m^{\mathsf{T}}\left(\tilde{\mathbf{x}} - b\mathbf{v}\right) + w_{m0}\right). \tag{5.115}$$

Therefore,

$$\tilde{z}_m = h\left(\tilde{\mathbf{w}}_m^{\dagger} \mathbf{x} + \tilde{w}_{m0}\right). \tag{5.116}$$

where

$$\tilde{\mathbf{w}}_{m} = \frac{1}{a} \mathbf{w}_{m},$$

$$\tilde{w}_{m0} = w_{m0} - \frac{b}{a} \mathbf{w}_{m}^{\mathsf{T}} \mathbf{v}.$$
(5.117)

(b)

Let

$$\tilde{y}_n = cy_n + d. (5.118)$$

Then,

$$\frac{\tilde{y}_n - d}{c} = \mathbf{w}_n^{\mathsf{T}} \mathbf{z} + w_{n0}. \tag{5.119}$$

Therefore,

$$\tilde{y}_n = \tilde{\mathbf{w}}_n^{\mathsf{T}} \mathbf{z} + \tilde{w}_{n0}, \tag{5.120}$$

where

$$\tilde{\mathbf{w}}_n = c\mathbf{w}_n,
\tilde{w}_{n0} = cw_{n0} + d.$$
(5.121)

5.25 (Incomplete)

Let E be a quadratic error function such that

$$E(\mathbf{w}) = E_0 + \frac{1}{2} (\mathbf{w} - \mathbf{w}^*)^{\mathsf{T}} \mathbf{H} (\mathbf{w} - \mathbf{w}^*), \qquad (5.122)$$

where \mathbf{w}^* represents the minimum and \mathbf{H} is a positive definite and constant matrix whose eignevectors and eigenvalues are $\mathbf{u}_1, \dots, \mathbf{u}_M$ and η_1, \dots, η_M . Let

$$\mathbf{w}^{(\tau)} = \mathbf{w}^{(\tau-1)} - \rho \nabla E,$$

$$\mathbf{w}^{(0)} = \mathbf{0}.$$
(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

$$\mathbf{w}^{(\tau)} = (\mathbf{I} - \rho \mathbf{H}) \,\mathbf{w}^{(\tau - 1)} + \rho \mathbf{H} \mathbf{w}^*. \tag{5.125}$$

Then,

$$\mathbf{u}_{m}^{\mathsf{T}}\mathbf{w}^{(\tau)} = \mathbf{u}_{m}^{\mathsf{T}}\mathbf{w}^{(\tau-1)} - \rho\mathbf{u}_{m}^{\mathsf{T}}\mathbf{H}\mathbf{w}^{(\tau-1)} + \rho\mathbf{u}_{m}^{\mathsf{T}}\mathbf{H}\mathbf{w}^{*}. \tag{5.126}$$

Since \mathbf{H} is symmetric,

$$\mathbf{u}_{m}^{\mathsf{T}}\mathbf{H}\mathbf{w} = \mathbf{w}^{\mathsf{T}}\mathbf{H}\mathbf{u}_{m}.\tag{5.127}$$

The right hand side can be written as

$$\eta_m \mathbf{w}^{\mathsf{T}} \mathbf{u}_m = \eta_m w_m, \tag{5.128}$$

where

$$w_m = \mathbf{w}^\mathsf{T} \mathbf{u}_m. \tag{5.129}$$

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

$$w_m^{(\tau)} = (1 - (1 - \rho \eta_m)^{\tau}) w_m^*. \tag{5.133}$$

(b)

$$|1 - \rho \eta_m| < 1, (5.134)$$

then

$$\lim_{\tau \to \infty} w_m^{(\tau)} = w_m^*. \tag{5.135}$$

(c)

By (a) and a Taylor series

$$(1 - \rho \eta_m)^{\tau} = 1 - \rho \tau \eta_m + \rho^2 \tau^2 O(\eta_m^2), \qquad (5.136)$$

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

$$w_m^{(\tau)} = \rho \tau \eta_m \left(1 - \rho \tau \eta_m O(\eta_m) \right) w_m^*. \tag{5.138}$$

Therefore,

$$w_m^{(\tau)} \simeq w_m^*, \quad \text{if} \quad \eta_m \gg (\rho \tau)^{-1}?$$

$$\left| w_m^{(\tau)} \right| \ll w_m^*, \quad \text{if} \quad \eta_m \ll (\rho \tau)^{-1}.$$

$$(5.139)$$

5.26 (Incomplete)

Let

$$\tilde{E} = E + \lambda \Omega, \tag{5.140}$$

where

$$\Omega = \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} \left(\frac{\partial y_{nk}}{\partial \xi} \right)^{2}.$$
 (5.141)

(a)

We have

$$\frac{\partial y_{nk}}{\partial \xi} = \mathcal{G}y_{nk},\tag{5.142}$$

where

$$\mathcal{G} = \sum_{d=1}^{D} \tau_d \frac{\partial}{\partial x_d},$$

$$\tau_d = \frac{\partial x_d}{\partial \xi}.$$
(5.143)

Therefore,

$$\Omega = \sum_{n=1}^{N} \Omega_n, \tag{5.144}$$

where

$$\Omega_n = \frac{1}{2} \sum_{k=1}^K (\mathcal{G} y_{nk})^2.$$
 (5.145)

(b)

$$\alpha_j = \mathcal{G}z_j = h'(a_j)\beta_j?$$

$$\beta_j = \mathcal{G}a_j = \sum_{d=1}^D w_{jd}\alpha_d?$$
(5.146)

5.27

Let

$$\tilde{E} = \frac{1}{2} \iiint (y(\mathbf{x} + \boldsymbol{\xi}) - t)^2 p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi},$$
 (5.147)

where

$$p(\boldsymbol{\xi}) = \mathcal{N}(\boldsymbol{\xi}|\mathbf{0}, \mathbf{I}). \tag{5.148}$$

By a Taylor series

$$y(\mathbf{x} + \boldsymbol{\xi}) = y(\mathbf{x}) + \boldsymbol{\xi}^{\mathsf{T}} \nabla y(\mathbf{x}) + \frac{1}{2} \boldsymbol{\xi}^{\mathsf{T}} \nabla \nabla y(\mathbf{x}) \boldsymbol{\xi} + O\left(\|\boldsymbol{\xi}\|^{3}\right), \tag{5.149}$$

the integrand can be written as

$$(y(\mathbf{x}) - t)^{2} + 2(y(\mathbf{x}) - t) \left(\boldsymbol{\xi}^{\mathsf{T}} \nabla y(\mathbf{x}) + \frac{1}{2} \boldsymbol{\xi}^{\mathsf{T}} \nabla \nabla y(\mathbf{x}) \boldsymbol{\xi} + O(\|\boldsymbol{\xi}\|^{3})\right) + \left(\boldsymbol{\xi}^{\mathsf{T}} \nabla y(\mathbf{x}) + \frac{1}{2} \boldsymbol{\xi}^{\mathsf{T}} \nabla \nabla y(\mathbf{x}) \boldsymbol{\xi} + O(\|\boldsymbol{\xi}\|^{3})\right)^{2}.$$
(5.150)

Omitting the terms of $O(\|\boldsymbol{\xi}\|^3)$, the integral can be approximated as

$$\iiint (y(\mathbf{x}) - t)^{2} p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi}
+ 2 \iiint (y(\mathbf{x}) - t) \left(\boldsymbol{\xi}^{\mathsf{T}} \nabla y(\mathbf{x}) + \frac{1}{2} \boldsymbol{\xi}^{\mathsf{T}} \nabla \nabla y(\mathbf{x}) \boldsymbol{\xi}\right) p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi}
+ \iiint \left(\boldsymbol{\xi}^{\mathsf{T}} \nabla y(\mathbf{x}) + \frac{1}{2} \boldsymbol{\xi}^{\mathsf{T}} \nabla \nabla y(\mathbf{x}) \boldsymbol{\xi}\right)^{2} p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi}.$$
(5.151)

Omitting the terms of $O(\|\boldsymbol{\xi}\|^3)$, the second and third terms can be approximated as

$$2 \iiint (y(\mathbf{x}) - t) \boldsymbol{\xi}^{\mathsf{T}} \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi}$$

$$+ \iiint (y(\mathbf{x}) - t) \boldsymbol{\xi}^{\mathsf{T}} \nabla \nabla y(\mathbf{x}) \boldsymbol{\xi} p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi}$$

$$+ \iiint \boldsymbol{\xi}^{\mathsf{T}} (\nabla y(\mathbf{x})) (\nabla y(\mathbf{x}))^{\mathsf{T}} \boldsymbol{\xi} p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi}.$$

$$(5.152)$$

Since

$$\mathbf{E}\,\boldsymbol{\xi} = \mathbf{0},\tag{5.153}$$

the integral of the first term can be written as

$$\left(\int \boldsymbol{\xi} p(\boldsymbol{\xi}) d\boldsymbol{\xi}\right)^{\mathsf{T}} \int \int (y(\mathbf{x}) - t) \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt = \mathbf{0}.$$
 (5.154)

Since

$$cov \boldsymbol{\xi} = \mathbf{I}, \tag{5.155}$$

The integrals of the second term can be written as

$$\int \boldsymbol{\xi}^{\mathsf{T}} \left(\int \int (y(\mathbf{x}) - t) \, \nabla \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt \right) \boldsymbol{\xi} p(\boldsymbol{\xi}) d\boldsymbol{\xi}
= \operatorname{tr} \left(\int \int (y(\mathbf{x}) - t) \, \nabla \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt \right).$$
(5.156)

The integral of the right hand side can be written as

$$\int \left(y(\mathbf{x}) - \int t p(t|\mathbf{x}) dt \right) \nabla \nabla y(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}$$

$$= \int \left(y(\mathbf{x}) - \mathbf{E}(t|\mathbf{x}) \right) \nabla \nabla y(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}.$$
(5.157)

Similarly, the integral of the third term can be written as

$$\int \boldsymbol{\xi}^{\mathsf{T}} \left(\int \int (\nabla y(\mathbf{x})) (\nabla y(\mathbf{x}))^{\mathsf{T}} p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt \right) \boldsymbol{\xi} d\boldsymbol{\xi}
= \operatorname{tr} \left(\int \int (\nabla y(\mathbf{x})) (\nabla y(\mathbf{x}))^{\mathsf{T}} p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt \right).$$
(5.158)

The integral of the right hand side can be written as

$$\int \left(\int p(t|\mathbf{x})dt \right) (\nabla y(\mathbf{x})) (\nabla y(\mathbf{x}))^{\mathsf{T}} p(\mathbf{x})d\mathbf{x}
= \int (\nabla y(\mathbf{x})) (\nabla y(\mathbf{x}))^{\mathsf{T}} p(\mathbf{x})d\mathbf{x}.$$
(5.159)

If

$$y(\mathbf{x}) = \mathbf{E}(t|\mathbf{x}),\tag{5.160}$$

then

$$\tilde{E} \simeq E + \Omega,$$
 (5.161)

where

$$E = \frac{1}{2} \iiint (y(\mathbf{x}) - t)^2 p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi},$$

$$\Omega = \frac{1}{2} \operatorname{tr} \left(\int \nabla y(\mathbf{x}) (\nabla y(\mathbf{x}))^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x}. \right).$$
(5.162)

5.28 (Incomplete)

5.29

Let w_1, \dots, 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

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w}),$$
 (5.164)

where

$$\Omega(\mathbf{w}) = -\sum_{m=1}^{M} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right) \right).$$
 (5.165)

We have

$$\frac{\partial \Omega}{\partial w_m} = -\frac{\sum_{k=1}^K \pi_k \frac{w_m - \mu_k}{\sigma_k^2} \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}{\sum_{k=1}^K \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}.$$
 (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

$$\gamma_k(w_m) = \frac{\pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2)}{\sum_{k=1}^K \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2)}.$$
 (5.168)

5.30

Let w_1, \dots, 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

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w}),$$
 (5.170)

where

$$\Omega(\mathbf{w}) = -\sum_{m=1}^{M} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right) \right).$$
 (5.171)

We have

$$\frac{\partial \Omega}{\partial \mu_k} = -\frac{\sum_{k=1}^K \pi_k \frac{w_m - \mu_k}{\sigma_k^2} \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}{\sum_{k=1}^K \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}.$$
 (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

$$\gamma_k(w_m) = \frac{\pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2)}{\sum_{k=1}^K \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2)}.$$
 (5.174)

5.31

Let w_1, \dots, 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

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w}),$$
 (5.176)

where

$$\Omega(\mathbf{w}) = -\sum_{m=1}^{M} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right) \right).$$
 (5.177)

We have

$$\frac{\partial \Omega}{\partial \sigma_k} = -\frac{\sum_{k=1}^K \pi_k \left(-\frac{1}{\sigma_k} + \frac{(w_m - \mu_k)^2}{\sigma_k^3} \right) \mathcal{N}\left(w_m | \mu_k, \sigma_k^2 \right)}{\sum_{k=1}^K \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2 \right)}.$$
 (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

$$\gamma_k(w_m) = \frac{\pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2)}{\sum_{k=1}^K \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2)}.$$
 (5.180)

5.32

Let w_1, \dots, w_M be variables such that

$$p(w_m) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right), \qquad (5.181)$$

where

$$\pi_k = \frac{\exp(\eta_k)}{\sum_{k=1}^K \exp(\eta_k)}.$$
 (5.182)

Let

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w}),$$
 (5.183)

$$\Omega(\mathbf{w}) = -\sum_{m=1}^{M} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right) \right).$$
 (5.184)

(a)

If $k \neq k'$, then

$$\frac{\partial \pi_k}{\partial \eta_{k'}} = -\frac{\exp(\eta_{k'}) \exp(\eta_k)}{\left(\sum_{k=1}^K \exp(\eta_k)\right)^2}.$$
 (5.185)

We have

$$\frac{\partial \pi_k}{\partial \eta_k} = \frac{\exp(\eta_k)}{\sum_{k=1}^K \exp(\eta_k)} - \left(\frac{\exp(\eta_k)}{\sum_{k=1}^K \exp(\eta_k)}\right)^2.$$
 (5.186)

Therefore,

$$\frac{\partial \pi_k}{\partial \eta_{k'}} = I_{kk'} \pi_k - \pi_k \pi_{k'}. \tag{5.187}$$

(b)

We have

$$\frac{\partial \Omega}{\partial \eta_k} = \sum_{k'=1}^K \frac{\partial \Omega}{\partial \pi_{k'}} \frac{\partial \pi_{k'}}{\partial \eta_k}.$$
 (5.188)

We have

$$\frac{\partial \Omega}{\partial \pi_{k'}} = -\frac{\sum_{m=1}^{M} \mathcal{N}\left(w_m | \mu_{k'}, \sigma_{k'}^2\right)}{\sum_{k=1}^{K} \pi_k \mathcal{N}\left(w_m | \mu_k, \sigma_k^2\right)}.$$
 (5.189)

By (a),

$$\frac{\partial \Omega}{\partial \eta_k} = -\sum_{k'=1}^K \frac{\sum_{m=1}^M \mathcal{N}(w_m | \mu_{k'}, \sigma_{k'}^2)}{\sum_{k=1}^K \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2)} (I_{kk'} \pi_k - \pi_k \pi_{k'}).$$
 (5.190)

The right hand side can be written as

$$-\sum_{m=1}^{M} \frac{\pi_{k} \mathcal{N}\left(w_{m} | \mu_{k}, \sigma_{k}^{2}\right)}{\sum_{k=1}^{K} \pi_{k} \mathcal{N}\left(w_{m} | \mu_{k}, \sigma_{k}^{2}\right)} + \pi_{k} \sum_{m=1}^{M} \frac{\sum_{k'=1}^{K} \pi_{k'} \mathcal{N}\left(w_{m} | \mu_{k}, \sigma_{k}^{2}\right)}{\sum_{k=1}^{K} \pi_{k} \mathcal{N}\left(w_{m} | \mu_{k}, \sigma_{k}^{2}\right)}$$

$$= \sum_{m=1}^{M} \left(\pi_{k} - \frac{\pi_{k} \mathcal{N}\left(w_{m} | \mu_{k}, \sigma_{k}^{2}\right)}{\sum_{k=1}^{K} \pi_{k} \mathcal{N}\left(w_{m} | \mu_{k}, \sigma_{k}^{2}\right)}\right).$$
(5.191)

Therefore,

$$\frac{\partial \tilde{E}}{\partial \eta_k} = \lambda \sum_{m=1}^{M} (\pi_k - \gamma_k(w_m)), \qquad (5.192)$$

where

$$\gamma_k(w_m) = \frac{\pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2)}{\sum_{k=1}^K \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2)}.$$
 (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 assume that the origin of the coordinate system is given by the attachment point of the lower arm. We have

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} L_1 \cos \theta_1 \\ L_1 \sin \theta_1 \end{bmatrix} + \begin{bmatrix} L_2 \cos (\theta_2 - (\pi - \theta_1)) \\ L_2 \sin (\theta_2 - (\pi - \theta_1)) \end{bmatrix}.$$
 (5.194)

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

$$\begin{bmatrix} L_2 \cos (\theta_1 + \theta_2 - \pi) \\ L_2 \sin (\theta_1 + \theta_2 - \pi) \end{bmatrix} = \begin{bmatrix} -L_2 \cos(\theta_1 + \theta_2) \\ -L_2 \sin(\theta_1 + \theta_2) \end{bmatrix}.$$
 (5.195)

Therefore,

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} L_1 \cos \theta_1 - L_2 \cos(\theta_1 + \theta_2) \\ L_1 \sin \theta_1 - L_2 \sin(\theta_1 + \theta_2) \end{bmatrix}.$$
 (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

$$\pi_k = \frac{\exp(a_k)}{\sum_{k=1}^K \exp(a_k)},$$

$$\mathcal{N}_{nk} = \mathcal{N}\left(\mathbf{t}_n | \boldsymbol{\mu}_k(\mathbf{x}_n, \mathbf{w}), \sigma_k^2(\mathbf{x}_n, \mathbf{w})\mathbf{I}\right).$$
(5.198)

Then,

$$\frac{\partial E_n}{\partial a_k^{\pi}} = \sum_{k'=1}^K \frac{\partial E_n}{\partial \pi_{k'}} \frac{\partial \pi_{k'}}{\partial a_k^{\pi}}.$$
 (5.199)

We have

$$\frac{\partial E_n}{\partial \pi_{k'}} = -\frac{\mathcal{N}_{nk'}}{\sum_{k=1}^K \pi_k \mathcal{N}_{nk}}.$$
 (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

$$\pi_k \frac{\sum_{k'=1}^K \pi_{k'} \mathcal{N}_{nk'}}{\sum_{k=1}^K \pi_k \mathcal{N}_{nk}} - \frac{\pi_k \mathcal{N}_{nk}}{\sum_{k=1}^K \pi_k \mathcal{N}_{nk}} = \pi_k - \frac{\pi_k \mathcal{N}_{nk}}{\sum_{k=1}^K \pi_k \mathcal{N}_{nk}}.$$
 (5.203)

Therefore,

$$\frac{\partial E_n}{\partial a_k^{\pi}} = \pi_k - \gamma_{nk},\tag{5.204}$$

where

$$\gamma_{nk} = \frac{\pi_k \mathcal{N}_{nk}}{\sum_{k=1}^K \pi_k \mathcal{N}_{nk}}.$$
 (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

$$\mathcal{N}_{nk} = \mathcal{N}\left(\mathbf{t}_n | \boldsymbol{\mu}_k(\mathbf{x}_n, \mathbf{w}), \sigma_k^2(\mathbf{x}_n, \mathbf{w})\mathbf{I}\right),$$

$$\mu_{km} = a_{km}^{\mu}.$$
(5.207)

Then,

$$\frac{\partial E_n}{\partial a_{km}^{\mu}} = \frac{\partial E_n}{\partial \mathcal{N}_{nk}} \frac{\partial \mathcal{N}_{nk}}{\partial a_{km}^{\mu}}.$$
 (5.208)

We have

$$\frac{\partial E_n}{\partial \mathcal{N}_{nk}} = -\frac{\pi_k}{\sum_{k=1}^K \pi_k \mathcal{N}_{nk}}.$$
 (5.209)

We have

$$\frac{\partial \mathcal{N}_{nk}}{\partial a_{km}^{\mu}} = \frac{t_{nm} - \mu_{km}}{\sigma_k^2} \mathcal{N}_{nk}.$$
 (5.210)

Then,

$$\frac{\partial E_n}{\partial a_{km}^{\mu}} = -\frac{\pi_k}{\sum_{k=1}^K \pi_k \mathcal{N}_{nk}} \frac{t_{nm} - \mu_{km}}{\sigma_k^2} \mathcal{N}_{nk}.$$
 (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

$$\gamma_{nk} = \frac{\pi_k \mathcal{N}_{nk}}{\sum_{k=1}^K \pi_k \mathcal{N}_{nk}}.$$
 (5.213)

5.36

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ 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

$$\mathcal{N}_{nk} = \mathcal{N} \left(\mathbf{t}_n | \boldsymbol{\mu}_k(\mathbf{x}_n, \mathbf{w}), \sigma_k^2(\mathbf{x}_n, \mathbf{w}) \mathbf{I} \right),$$

$$\sigma_k = \exp\left(a_k^{\sigma}\right).$$
(5.215)

Then,

$$\frac{\partial E_n}{\partial a_k^\sigma} = \frac{\partial E_n}{\partial \mathcal{N}_{nk}} \frac{\partial \mathcal{N}_{nk}}{\partial a_k^\sigma}.$$
 (5.216)

We have

$$\frac{\partial E_n}{\partial \mathcal{N}_{nk}} = -\frac{\pi_k}{\sum_{k=1}^K \pi_k \mathcal{N}_{nk}}.$$
 (5.217)

We have

$$\frac{\partial \mathcal{N}_{nk}}{\partial a_k^{\sigma}} = \frac{\partial \mathcal{N}_{nk}}{\partial \sigma_k} \frac{\partial \sigma_k}{\partial a_k^{\sigma}}.$$
 (5.218)

The right hand side can be written as

$$\left(-M\sigma_k^{-1} + \frac{\|\mathbf{t}_n - \boldsymbol{\mu}_k\|^2}{\sigma_k^3}\right) \mathcal{N}_{nk} \sigma_k = \left(-M + \frac{\|\mathbf{t}_n - \boldsymbol{\mu}_k\|^2}{\sigma_k^2}\right) \mathcal{N}_{nk}.$$
(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

$$\gamma_{nk} = \frac{\pi_k \mathcal{N}_{nk}}{\sum_{k=1}^K \pi_k \mathcal{N}_{nk}}.$$
 (5.222)

5.37

Let \mathbf{t} be a variable such that

$$p(\mathbf{t}|\mathbf{x}) = \sum_{k=1}^{K} \pi_k(\mathbf{x}) \mathcal{N}\left(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}\right).$$
 (5.223)

(a)

We have

$$E(\mathbf{t}|\mathbf{x}) = \int \mathbf{t}p(\mathbf{t}|\mathbf{x})d\mathbf{t}.$$
 (5.224)

The right hand side can be written as

$$\sum_{k=1}^{K} \pi_k(\mathbf{x}) \int \mathbf{t} \mathcal{N} \left(\mathbf{t} | \boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x}) \mathbf{I} \right) d\mathbf{t} = \sum_{k=1}^{K} \pi_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x}).$$
 (5.225)

Therefore,

$$E(\mathbf{t}|\mathbf{x}) = \sum_{k=1}^{K} \pi_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x}). \tag{5.226}$$

(b)

We have

$$cov(\mathbf{t}|\mathbf{x}) = \int (\mathbf{t} - E(\mathbf{t}|\mathbf{x})) (\mathbf{t} - E(\mathbf{t}|\mathbf{x}))^{\mathsf{T}} p(\mathbf{t}|\mathbf{x}) d\mathbf{t}.$$
 (5.227)

The right hand side can be written as

$$\int \mathbf{t} \mathbf{t}^{\mathsf{T}} p(\mathbf{t}|\mathbf{x}) d\mathbf{t} - \mathbf{E}(\mathbf{t}|\mathbf{x}) \left(\int \mathbf{t} p(\mathbf{t}|\mathbf{x}) d\mathbf{t} \right)^{\mathsf{T}} - \left(\int \mathbf{t} p(\mathbf{t}|\mathbf{x}) d\mathbf{t} \right) \mathbf{E}(\mathbf{t}|\mathbf{x})^{\mathsf{T}}
+ \mathbf{E}(\mathbf{t}|\mathbf{x}) \mathbf{E}(\mathbf{t}|\mathbf{x})^{\mathsf{T}} \int p(\mathbf{t}|\mathbf{x}) d\mathbf{t}
= \int \mathbf{t} \mathbf{t}^{\mathsf{T}} p(\mathbf{t}|\mathbf{x}) d\mathbf{t} - \mathbf{E}(\mathbf{t}|\mathbf{x}) \mathbf{E}(\mathbf{t}|\mathbf{x})^{\mathsf{T}}.$$
(5.228)

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

$$\sum_{k=1}^{K} \pi_k(\mathbf{x}) \int \mathbf{t} \mathbf{t}^{\mathsf{T}} \mathcal{N}\left(\mathbf{t} | \boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x}) \mathbf{I}\right) d\mathbf{t}. \tag{5.229}$$

The integral of the right hand side can be written as

$$\int (\mathbf{t} - \boldsymbol{\mu}_{k}(\mathbf{x}) + \boldsymbol{\mu}_{k}(\mathbf{x})) (\mathbf{t} - \boldsymbol{\mu}_{k}(\mathbf{x}) + \boldsymbol{\mu}_{k}(\mathbf{x}))^{\mathsf{T}} \mathcal{N} (\mathbf{t} | \boldsymbol{\mu}_{k}(\mathbf{x}), \sigma_{k}^{2}(\mathbf{x}) \mathbf{I}) d\mathbf{t}$$

$$= \int (\mathbf{t} - \boldsymbol{\mu}_{k}(\mathbf{x})) (\mathbf{t} - \boldsymbol{\mu}_{k}(\mathbf{x}))^{\mathsf{T}} \mathcal{N} (\mathbf{t} | \boldsymbol{\mu}_{k}(\mathbf{x}), \sigma_{k}^{2}(\mathbf{x}) \mathbf{I}) d\mathbf{t}$$

$$+ \boldsymbol{\mu}_{k}(\mathbf{x}) \left(\int (\mathbf{t} - \boldsymbol{\mu}_{k}(\mathbf{x})) \mathcal{N} (\mathbf{t} | \boldsymbol{\mu}_{k}(\mathbf{x}), \sigma_{k}^{2}(\mathbf{x}) \mathbf{I}) d\mathbf{t} \right)^{\mathsf{T}}$$

$$+ \left(\int (\mathbf{t} - \boldsymbol{\mu}_{k}(\mathbf{x})) \mathcal{N} (\mathbf{t} | \boldsymbol{\mu}_{k}(\mathbf{x}), \sigma_{k}^{2}(\mathbf{x}) \mathbf{I}) d\mathbf{t} \right) \boldsymbol{\mu}_{k}(\mathbf{x})^{\mathsf{T}}$$

$$+ \boldsymbol{\mu}_{k}(\mathbf{x}) \boldsymbol{\mu}_{k}(\mathbf{x})^{\mathsf{T}} \int \mathcal{N} (\mathbf{t} | \boldsymbol{\mu}_{k}(\mathbf{x}), \sigma_{k}^{2}(\mathbf{x}) \mathbf{I}) d\mathbf{t}.$$
(5.230)

The right hand side can be written as

$$\sigma_k^2(\mathbf{x})\mathbf{I} + \boldsymbol{\mu}_k(\mathbf{x})\boldsymbol{\mu}_k(\mathbf{x})^{\mathsf{T}}.$$
 (5.231)

Therefore, by (a),

$$cov(\mathbf{t}|\mathbf{x}) = \sum_{k=1}^{K} \pi_k(\mathbf{x}) \left(\sigma_k^2(\mathbf{x}) \mathbf{I} + \boldsymbol{\mu}_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x})^{\mathsf{T}} \right) - \left(\sum_{k=1}^{K} \pi_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x}) \right) \left(\sum_{k=1}^{K} \pi_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x}) \right)^{\mathsf{T}}.$$
 (5.232)

5.38

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|y(\mathbf{x}, \mathbf{w}), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}\right).$$
(5.233)

By marginalisation,

$$p(t|\mathbf{t}) = \int p(t|\mathbf{w})p(\mathbf{w}|\mathbf{t})d\mathbf{w}.$$
 (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

$$E(\mathbf{w}) = \frac{\beta}{2} \sum_{n=1}^{N} (t_n - y(\mathbf{x}_n, \mathbf{w}))^2 + \frac{\alpha}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w}.$$
 (5.236)

Let \mathbf{w}_{MAP} be a stationary point of $p(\mathbf{w}|\mathbf{t})$. Then, we have a Taylor series

$$E(\mathbf{w}) = E(\mathbf{w}_{\text{MAP}}) + \frac{1}{2} (\mathbf{w} - \mathbf{w}_{\text{MAP}})^{\mathsf{T}} \mathbf{A} (\mathbf{w} - \mathbf{w}_{\text{MAP}}) + O(\|\mathbf{w} - \mathbf{w}_{\text{MAP}}\|^{3}),$$
(5.237)

where

$$\mathbf{A} = \left. \nabla \nabla E(\mathbf{w}) \right|_{\mathbf{w} = \mathbf{w}_{\text{MAP}}}. \tag{5.238}$$

Then,

$$p(\mathbf{w}|\mathbf{t}) \simeq \mathcal{N}\left(\mathbf{w}|\mathbf{w}_{\text{MAP}}, \mathbf{A}^{-1}\right).$$
 (5.239)

By a Taylor series

$$y(\mathbf{x}, \mathbf{w}) = y(\mathbf{x}, \mathbf{w}_{MAP}) + \mathbf{g}^{\mathsf{T}}(\mathbf{w} - \mathbf{w}_{MAP}) + O(\|\mathbf{w} - \mathbf{w}_{MAP}\|^{2}),$$
 (5.240)

where

$$\mathbf{g} = \left. \nabla_{\mathbf{w}} y(\mathbf{x}, \mathbf{w}) \right|_{\mathbf{w} = \mathbf{w}_{\text{MAP}}},\tag{5.241}$$

we have

$$p(t|\mathbf{w}) \simeq \mathcal{N}\left(t|y(\mathbf{x}, \mathbf{w}_{\text{MAP}}) + \mathbf{g}^{\mathsf{T}}(\mathbf{w} - \mathbf{w}_{\text{MAP}}), \beta^{-1}\right).$$
 (5.242)

Then, the logarithm of the integrand except the terms independent of \mathbf{w} can be approximated as

$$-\frac{\beta}{2} (t - y(\mathbf{x}, \mathbf{w}_{\text{MAP}}) - \mathbf{g}^{\mathsf{T}} (\mathbf{w} - \mathbf{w}_{\text{MAP}}))^{2} - \frac{1}{2} (\mathbf{w} - \mathbf{w}_{\text{MAP}})^{\mathsf{T}} \mathbf{A} (\mathbf{w} - \mathbf{w}_{\text{MAP}})$$

$$= -\frac{1}{2} \begin{bmatrix} \mathbf{w} - \mathbf{w}_{\text{MAP}} \\ t - y(\mathbf{x}, \mathbf{w}_{\text{MAP}}) \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \mathbf{A} + \beta \mathbf{g} \mathbf{g}^{\mathsf{T}} & -\beta \mathbf{g} \\ -\beta \mathbf{g}^{\mathsf{T}} & \beta \end{bmatrix} \begin{bmatrix} \mathbf{w} - \mathbf{w}_{\text{MAP}} \\ t - y(\mathbf{x}, \mathbf{w}_{\text{MAP}}) \end{bmatrix}.$$
(5.243)

By 2.24,

$$\begin{bmatrix} \mathbf{A} + \beta \mathbf{g} \mathbf{g}^{\mathsf{T}} & -\beta \mathbf{g} \\ -\beta \mathbf{g}^{\mathsf{T}} & \beta \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{A}^{-1} & \mathbf{A}^{-1} \mathbf{g} \\ \mathbf{g}^{\mathsf{T}} \mathbf{A}^{-1} & \beta^{-1} + \mathbf{g}^{\mathsf{T}} \mathbf{A}^{-1} \mathbf{g} \end{bmatrix}. \tag{5.244}$$

Therefore,

$$p(t|\mathbf{t}) \simeq \mathcal{N}\left(t|y(\mathbf{x}, \mathbf{w}_{\text{MAP}}), \beta^{-1} + \mathbf{g}^{\mathsf{T}}\mathbf{A}^{-1}\mathbf{g}\right).$$
 (5.245)

5.39

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|y(\mathbf{x}, \mathbf{w}), \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}\right),$$
 (5.246)

where \mathbf{w} is a vector in M dimensions. By marginalisation,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}.$$
 (5.247)

The logarithm of the integrand of the right hand side can be written as

$$-\frac{N}{2}\ln\left(2\pi\beta^{-1}\right) - \frac{\beta}{2}\sum_{n=1}^{N}\left(t_{n} - y(\mathbf{x}_{n}, \mathbf{w})\right)^{2}$$

$$-\frac{M}{2}\ln\left(2\pi\right) - \frac{1}{2}\ln\left(\det\left(\alpha^{-1}\mathbf{I}\right)\right) - \frac{\alpha}{2}\mathbf{w}^{\mathsf{T}}\mathbf{w}$$

$$= -E(\mathbf{w}) - \frac{N+M}{2}\ln(2\pi) + \frac{N}{2}\ln\beta + \frac{M}{2}\ln\alpha,$$

$$(5.248)$$

$$E(\mathbf{w}) = \frac{\beta}{2} \sum_{n=1}^{N} (t_n - y(\mathbf{x}_n, \mathbf{w}))^2 + \frac{\alpha}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w}.$$
 (5.249)

Let \mathbf{w}_{MAP} be a stationary point of E. Then, we have a Taylor series

$$E(\mathbf{w}) = E(\mathbf{w}_{\text{MAP}}) + \frac{1}{2} (\mathbf{w} - \mathbf{w}_{\text{MAP}})^{\mathsf{T}} \mathbf{A} (\mathbf{w} - \mathbf{w}_{\text{MAP}}) + O(\|\mathbf{w} - \mathbf{w}_{\text{MAP}}\|^{3}),$$
(5.250)

where

$$\mathbf{A} = \left. \nabla \nabla E(\mathbf{w}) \right|_{\mathbf{w} = \mathbf{w}_{\text{MAR}}}. \tag{5.251}$$

Then, the logarithm of the integrand can be approximated as

$$-E(\mathbf{w}_{\text{MAP}}) - \frac{1}{2}(\mathbf{w} - \mathbf{w}_{\text{MAP}})^{\mathsf{T}} \mathbf{A}(\mathbf{w} - \mathbf{w}_{\text{MAP}})$$
$$-\frac{N+M}{2} \ln(2\pi) + \frac{N}{2} \ln\beta + \frac{M}{2} \ln\alpha.$$
(5.252)

Therefore,

$$\ln p(\mathbf{t}) \simeq -E(\mathbf{w}_{\text{MAP}}) - \frac{1}{2} \ln |\det \mathbf{A}| - \frac{N}{2} \ln(2\pi) + \frac{N}{2} \ln \beta + \frac{M}{2} \ln \alpha.$$
 (5.253)

5.40 (Incomplete)

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables such that

$$p(\mathbf{t}_n|\mathbf{w}) = \prod_{k=1}^K y_{nk}^{t_{nk}},$$

$$p(\mathbf{w}) = \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}\right),$$
(5.254)

where

$$t_{nk} \in \{0, 1\},$$

$$y_{nk} = y_k(\mathbf{x}_n, \mathbf{w}),$$

$$\sum_{k=1}^{K} y_{nk} = 1.$$

$$(5.255)$$

By marginalisation,

$$p(\mathbf{t}|\mathbf{T}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w}|\mathbf{T})d\mathbf{w}.$$
 (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

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \ln y_{nk} + \frac{\alpha}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w}.$$
 (5.258)

Let \mathbf{w}_{MAP} be a stationary point of E. Then, we have a Taylor series

$$E(\mathbf{w}) = E(\mathbf{w}_{\text{MAP}}) + \frac{1}{2} (\mathbf{w} - \mathbf{w}_{\text{MAP}})^{\mathsf{T}} \mathbf{A} (\mathbf{w} - \mathbf{w}_{\text{MAP}}) + O(\|(\mathbf{w} - \mathbf{w}_{\text{MAP}})\|^{3}),$$
(5.259)

where

$$\mathbf{A} = \left. \nabla \nabla E(\mathbf{w}) \right|_{\mathbf{w} = \mathbf{w}_{\text{MAP}}}. \tag{5.260}$$

Then,

$$p(\mathbf{w}|\mathbf{T}) \simeq \mathcal{N}\left(\mathbf{w}|\mathbf{w}_{\text{MAP}}, \mathbf{A}^{-1}\right).$$
 (5.261)

5.41

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables such that

$$p(\mathbf{t}_n|\mathbf{w}) = \prod_{k=1}^K y_{nk}^{t_{nk}},$$

$$p(\mathbf{w}) = \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}\right),$$
(5.262)

where

$$t_{nk} \in \{0, 1\},$$

$$y_{nk} = y_k(\mathbf{x}_n, \mathbf{w}),$$

$$\sum_{k=1}^{K} y_{nk} = 1.$$

$$(5.263)$$

By marginalisation,

$$p(\mathbf{T}) = \int p(\mathbf{T}|\mathbf{w})p(\mathbf{w})d\mathbf{w}.$$
 (5.264)

The logarithm of the integrand of the right hand side can be written as

$$\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \ln y_{nk} - \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln\left(\det\left(\alpha^{-1}\mathbf{I}\right)\right) - \frac{\alpha}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w}$$

$$= -E(\mathbf{w}) - \frac{M}{2} \ln(2\pi) + \frac{M}{2} \ln \alpha,$$
(5.265)

where

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \ln y_{nk} + \frac{\alpha}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w}.$$
 (5.266)

Let \mathbf{w}_{MAP} be a stationary point of E. Then, we have a Taylor series

$$E(\mathbf{w}) = E(\mathbf{w}_{\text{MAP}}) + \frac{1}{2} (\mathbf{w} - \mathbf{w}_{\text{MAP}})^{\mathsf{T}} \mathbf{A} (\mathbf{w} - \mathbf{w}_{\text{MAP}}) + O(\|(\mathbf{w} - \mathbf{w}_{\text{MAP}})\|^{3}),$$
(5.267)

where

$$\mathbf{A} = \left. \nabla \nabla E(\mathbf{w}) \right|_{\mathbf{w} = \mathbf{w}_{\text{MAP}}}. \tag{5.268}$$

Then, the logarithm of the integrand can be approximated as

$$-E(\mathbf{w}_{\text{MAP}}) - \frac{1}{2}(\mathbf{w} - \mathbf{w}_{\text{MAP}})^{\mathsf{T}}\mathbf{A}(\mathbf{w} - \mathbf{w}_{\text{MAP}}) - \frac{M}{2}\ln(2\pi) + \frac{M}{2}\ln\alpha. \quad (5.269)$$

Therefore,

$$\ln p(\mathbf{T}) \simeq -E(\mathbf{w}_{\text{MAP}}) - \frac{1}{2} \ln |\det \mathbf{A}| + \frac{M}{2} \ln \alpha.$$
 (5.270)

6 Kernel Methods

6.1

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n), 1),$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \lambda^{-1}\mathbf{I}).$$
(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

$$E_{\mathbf{w}}(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} (t_n - \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_n))^2 + \frac{\lambda}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w},$$
(6.3)

so that

$$E_{\mathbf{w}}(\mathbf{w}) = \frac{1}{2} \|\mathbf{t} - \mathbf{\Phi}\mathbf{w}\|^2 + \frac{\lambda}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w}, \tag{6.4}$$

where

$$\mathbf{\Phi} = \begin{bmatrix} \boldsymbol{\phi}(\mathbf{x}_1)^{\mathsf{T}} \\ \vdots \\ \boldsymbol{\phi}(\mathbf{x}_N)^{\mathsf{T}} \end{bmatrix}. \tag{6.5}$$

(a)

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

$$\mathbf{0} = -\mathbf{\Phi}^{\mathsf{T}}(\mathbf{t} - \mathbf{\Phi}\mathbf{w}) + \lambda\mathbf{w}. \tag{6.6}$$

Let the stationary point of $E_{\mathbf{w}}$ be \mathbf{w}_{MAP} . Then,

$$\mathbf{w}_{\text{MAP}} = \mathbf{\Phi}^{\mathsf{T}} \mathbf{a}_{\text{MAP}},\tag{6.7}$$

$$\mathbf{a}_{\text{MAP}} = \frac{1}{\lambda} \left(\mathbf{t} - \mathbf{\Phi} \mathbf{w}_{\text{MAP}} \right). \tag{6.8}$$

(b)

Let

$$\mathbf{w} = \mathbf{\Phi}^{\mathsf{T}} \mathbf{a}.\tag{6.9}$$

Then,

$$E_{\mathbf{w}}(\mathbf{w}) = E_{\mathbf{a}}(\mathbf{a}),\tag{6.10}$$

where

$$E_{\mathbf{a}}(\mathbf{a}) = \frac{1}{2} \|\mathbf{t} - \mathbf{\Phi} \mathbf{\Phi}^{\mathsf{T}} \mathbf{a}\|^{2} + \frac{\lambda}{2} \mathbf{a}^{\mathsf{T}} \mathbf{\Phi} \mathbf{\Phi}^{\mathsf{T}} \mathbf{a}. \tag{6.11}$$

The right hand side can be written as

$$\frac{1}{2} \|\mathbf{t}\|^2 - \mathbf{t}^{\mathsf{T}} \mathbf{K} \mathbf{a} + \frac{1}{2} \mathbf{a}^{\mathsf{T}} \mathbf{K} \mathbf{K} \mathbf{a} + \frac{\lambda}{2} \mathbf{a}^{\mathsf{T}} \mathbf{K} \mathbf{a}, \tag{6.12}$$

where

$$\mathbf{K} = \mathbf{\Phi} \mathbf{\Phi}^{\mathsf{T}}.\tag{6.13}$$

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

$$\mathbf{a}_{\text{MAP}} = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}. \tag{6.15}$$

(c)

By (a) and (b),

$$\frac{1}{\lambda} \left(\mathbf{t} - \mathbf{\Phi} \mathbf{w}_{\text{MAP}} \right) = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}, \tag{6.16}$$

so that

$$\mathbf{t} - \mathbf{\Phi} \mathbf{w}_{\text{MAP}} = \lambda (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}. \tag{6.17}$$

The right hand side can be written as

$$(\mathbf{K} + \lambda \mathbf{I} - \mathbf{K})(\mathbf{K} + \lambda \mathbf{I})^{-1}\mathbf{t} = \mathbf{t} - \mathbf{K}(\mathbf{K} + \lambda \mathbf{I})^{-1}\mathbf{t}.$$
 (6.18)

Then,

$$\mathbf{\Phi w}_{\text{MAP}} = \mathbf{K}(\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}, \tag{6.19}$$

so that

$$\mathbf{\Phi}^{\mathsf{T}}\mathbf{\Phi}\mathbf{w}_{\mathrm{MAP}} = \mathbf{\Phi}^{\mathsf{T}}\mathbf{K}(\mathbf{K} + \lambda \mathbf{I})^{-1}\mathbf{t}.$$
 (6.20)

$$\mathbf{w}_{\text{MAP}} = \mathbf{\Phi}^{\mathsf{T}} (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}, \tag{6.21}$$

so that

$$\lambda \mathbf{w}_{\text{MAP}} = \lambda \mathbf{\Phi}^{\mathsf{T}} (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}. \tag{6.22}$$

Then,

$$(\mathbf{\Phi}^{\mathsf{T}}\mathbf{\Phi} + \lambda \mathbf{I})\mathbf{w}_{\mathrm{MAP}} = \mathbf{\Phi}^{\mathsf{T}}(\mathbf{K} + \lambda \mathbf{I})(\mathbf{K} + \lambda \mathbf{I})^{-1}\mathbf{t}.$$
 (6.23)

Therefore,

$$\mathbf{w}_{\text{MAP}} = (\mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} + \lambda \mathbf{I})^{-1} \mathbf{\Phi}^{\mathsf{T}} \mathbf{t}. \tag{6.24}$$

6.2 (Incomplete)

Let t_1, \dots, t_N be vaariables such that

$$t_n \in \{-1, 1\},\$$

$$p(t_n | \mathbf{w}) = \left(\frac{1 + y_n}{2}\right)^{\frac{1 + t_n}{2}} \left(\frac{1 - y_n}{2}\right)^{\frac{1 - t_n}{2}},$$
(6.25)

where

$$y_n = f(\mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}_n),$$

$$f(a) = \begin{cases} 1, & a \ge 0, \\ -1, & \text{otherwise.} \end{cases}$$
(6.26)

Let

$$E(\mathbf{w}) = -\sum_{n \in \mathcal{M}} \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}_n t_n, \tag{6.27}$$

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

$$\|\mathbf{x} - \mathbf{x}_n\|^2 = \mathbf{x}^\mathsf{T} \mathbf{x} - 2\mathbf{x}^\mathsf{T} \mathbf{x}_n + \mathbf{x}_n^\mathsf{T} \mathbf{x}_n. \tag{6.29}$$

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

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^{\mathsf{T}} \mathbf{x}'. \tag{6.31}$$

6.4

Let **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,

$$(A_{11} + A_{22})^{2} - 4(A_{11}A_{22} - A_{12}A_{21}) > 0,$$

$$A_{11} + A_{22} > 0,$$

$$A_{11}A_{22} - A_{12}A_{21} > 0.$$
(6.34)

Therefore, an example is

$$\mathbf{A} = \begin{bmatrix} 2 & 0 \\ -1 & 1 \end{bmatrix}. \tag{6.35}$$

6.5

Let

$$k_1(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}_1(\mathbf{x})^{\mathsf{T}} \boldsymbol{\phi}_1(\mathbf{x}'). \tag{6.36}$$

(a)

Let

$$k(\mathbf{x}, \mathbf{x}') = ck_1(\mathbf{x}, \mathbf{x}'), \tag{6.37}$$

where c is a positive constant. The right hand side can be written as

$$c\phi_1(\mathbf{x})^{\mathsf{T}}\phi_1(\mathbf{x}') = \phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{x}'), \tag{6.38}$$

where

$$\phi = \sqrt{c}\phi_1. \tag{6.39}$$

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

$$f(\mathbf{x})\phi_1(\mathbf{x})^{\mathsf{T}}\phi_1(\mathbf{x}')f(\mathbf{x}') = \phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{x}'), \tag{6.41}$$

where

$$\phi = f\phi_1. \tag{6.42}$$

Therefore, k is a valid kernel.

6.6

Let

$$k_1(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}_1(\mathbf{x})^{\mathsf{T}} \boldsymbol{\phi}_1(\mathbf{x}'). \tag{6.43}$$

(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, \dots, c_J are nonnegative constants and

$$q_j(\mathbf{x}, \mathbf{x}') = (k_1(\mathbf{x}, \mathbf{x}'))^j. \tag{6.45}$$

We have

$$q_0(\mathbf{x}, \mathbf{x}') = 1. \tag{6.46}$$

Let us assume that q_j is a valid kernel. Then,

$$q_{j+1}(\mathbf{x}, \mathbf{x}') = q_j(\mathbf{x}, \mathbf{x}')\phi_1(\mathbf{x})^{\mathsf{T}}\phi_1(\mathbf{x}'). \tag{6.47}$$

The right hand side can be written as

$$q_j(\mathbf{x}, \mathbf{x}') \sum_{m=1}^M \phi_{1m}(\mathbf{x}) \phi_{1m}(\mathbf{x}') = \sum_{m=1}^M \phi_{1m}(\mathbf{x}) q_j(\mathbf{x}, \mathbf{x}') \phi_{1m}(\mathbf{x}').$$
 (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

$$k_1(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}_1(\mathbf{x})^{\mathsf{T}} \boldsymbol{\phi}_1(\mathbf{x}'), k_2(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}_2(\mathbf{x})^{\mathsf{T}} \boldsymbol{\phi}_2(\mathbf{x}').$$
(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

$$\phi_1(\mathbf{x})^{\mathsf{T}}\phi_1(\mathbf{x}') + \phi_2(\mathbf{x})^{\mathsf{T}}\phi_2(\mathbf{x}') = \phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{x}'), \tag{6.53}$$

where

$$\phi = \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}. \tag{6.54}$$

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

$$k(\mathbf{x}, \mathbf{x}') = k_1(\phi(\mathbf{x}), \phi(\mathbf{x}')), \qquad (6.57)$$

where k_1 is a valid kernel. Then, k is a valid kernel.

(b)

Let

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^{\mathsf{T}} \mathbf{A} \mathbf{x}',\tag{6.58}$$

where \mathbf{A} is a symmetric positive semidefinite matrix. There exists \mathbf{M} such that

$$\mathbf{A} = \mathbf{M}^{\mathsf{T}} \mathbf{M}.\tag{6.59}$$

Then,

$$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^{\mathsf{T}} \phi(\mathbf{x}'), \tag{6.60}$$

where

$$\phi(\mathbf{x}) = \mathbf{M}\mathbf{x}.\tag{6.61}$$

Therefore, k is a valid kernel.

6.9

Let

$$k_a(\mathbf{x}_a, \mathbf{x}_a') = \boldsymbol{\phi}_a(\mathbf{x}_a)^{\mathsf{T}} \boldsymbol{\phi}_a(\mathbf{x}_a'), k_b(\mathbf{x}_b, \mathbf{x}_b') = \boldsymbol{\phi}_b(\mathbf{x}_b)^{\mathsf{T}} \boldsymbol{\phi}_b(\mathbf{x}_b').$$
(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

$$\phi_a(\mathbf{x}_a)^{\mathsf{T}}\phi_a(\mathbf{x}_a') + \phi_b(\mathbf{x}_b)^{\mathsf{T}}\phi_b(\mathbf{x}_b') = \phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{x}'), \tag{6.65}$$

where

$$\phi(\mathbf{x}) = \begin{bmatrix} \phi_a(\mathbf{x}_a) \\ \phi_b(\mathbf{x}_b) \end{bmatrix}. \tag{6.66}$$

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

$$\exp\left(-\frac{\mathbf{x}^{\mathsf{T}}\mathbf{x}}{2\sigma^{2}}\right)\exp\left(\frac{\mathbf{x}^{\mathsf{T}}\mathbf{x}'}{\sigma^{2}}\right)\exp\left(-\frac{\mathbf{x}'^{\mathsf{T}}\mathbf{x}'}{2\sigma^{2}}\right). \tag{6.72}$$

We have

$$\exp\left(\frac{\mathbf{x}^{\mathsf{T}}\mathbf{x}'}{\sigma^2}\right) = \sum_{j=0}^{\infty} q_j(\mathbf{x}, \mathbf{x}'), \tag{6.73}$$

where

$$q_j(\mathbf{x}, \mathbf{x}') = \frac{1}{j!} \left(\frac{\mathbf{x}^\mathsf{T} \mathbf{x}'}{\sigma^2} \right)^j. \tag{6.74}$$

By 6.6(a), q_j is a valid kernel. Then, there exists ψ_j such that

$$q_j(\mathbf{x}, \mathbf{x}') = \boldsymbol{\psi}_j(\mathbf{x})^{\mathsf{T}} \boldsymbol{\psi}_j(\mathbf{x}'). \tag{6.75}$$

Then,

$$\exp\left(\frac{\mathbf{x}^{\mathsf{T}}\mathbf{x}'}{\sigma^2}\right) = \sum_{j=0}^{\infty} \boldsymbol{\psi}_j(\mathbf{x})^{\mathsf{T}} \boldsymbol{\psi}_j(\mathbf{x}'). \tag{6.76}$$

The right hand side can be written as $\phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{x}')$, 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 $A_1, \dots, A_{2^{|D|}}$ are all the subsets of D ordered in the alphabetical order where |.| is the number of elements in (.). Let

$$k(A_m, A_{m'}) = 2^{|A_m \cap A_{m'}|}. (6.78)$$

Let ϕ be a vector such that

$$\phi_m(A) = \begin{cases} 1, & \text{if } A_m \subseteq A, \\ 0, & \text{otherwise.} \end{cases}$$
 (6.79)

If

$$|A_m \cap A_{m'}| = 0, (6.80)$$

then

$$k(A_m, A_{m'}) = 1. (6.81)$$

The right hand side can be written as

$$\boldsymbol{\phi}(A_m)^{\mathsf{T}} \boldsymbol{\phi}(A_{m'}). \tag{6.82}$$

Let us assume that if

$$|A_m \cap A_{m'}| = n, \tag{6.83}$$

then

$$k(A_m, A_{m'}) = \boldsymbol{\phi}(A_m)^{\mathsf{T}} \boldsymbol{\phi}(A_{m'}). \tag{6.84}$$

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,

$$|A_m \cap A_{m''}| = n + 1, (6.87)$$

so that

$$k(A_m, A_{m''}) = 2^{n+1}. (6.88)$$

We have

$$\phi(A_m)^{\mathsf{T}}\phi(A_{m''}) = \phi(A_m)^{\mathsf{T}}\phi(A_{m'}) + \phi(A_m)^{\mathsf{T}}(\phi(A_{m''}) - \phi(A_{m'})). \quad (6.89)$$

By the assumption, the first term of the right hand side is 2^n . By the assumption, $\phi(A_m)$ and $\phi(A_{m'})$ have a set of 2^n 1s in common. Then, $\phi(A_m)$ and $\phi(A_{m''}) - \phi(A_{m'})$ have another set of 2^n 1s in common. Then, the second term of the right hand side is 2^n . Then,

$$\phi(A_m)^{\mathsf{T}}\phi(A_{m''}) = 2^{n+1},$$
 (6.90)

so that

$$k(A_m, A_{m''}) = \phi(A_m)^{\mathsf{T}} \phi(A_{m''}).$$
 (6.91)

Therefore, the assumption is proved by induction on n.

6.13

Let

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^{\mathsf{T}} \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}'),$$
 (6.92)

where

$$\mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) = \nabla_{\boldsymbol{\theta}} \ln p(\mathbf{x}|\boldsymbol{\theta}),$$

$$\mathbf{F} = \mathbf{E}_{\mathbf{x}} \left(\mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^{\mathsf{T}} \right).$$
(6.93)

Let

$$k_{\psi}(\mathbf{x}, \mathbf{x}') = \mathbf{g}_{\psi}(\boldsymbol{\theta}, \mathbf{x})^{\mathsf{T}} \mathbf{F}_{\psi}^{-1} \mathbf{g}_{\psi}(\boldsymbol{\theta}, \mathbf{x}'),$$
 (6.94)

where ψ is invertible and differentiable and

$$\mathbf{g}_{\psi}(\boldsymbol{\theta}, \mathbf{x}) = \nabla_{\psi(\boldsymbol{\theta})} \ln p(\mathbf{x}|\boldsymbol{\theta}),$$

$$\mathbf{F}_{\psi} = \mathbf{E}_{\mathbf{x}} \left(\mathbf{g}_{\psi}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}_{\psi}(\boldsymbol{\theta}, \mathbf{x})^{\mathsf{T}} \right).$$
(6.95)

We have

$$\mathbf{g}_{\psi}(\boldsymbol{\theta}, \mathbf{x}) = \frac{\partial \boldsymbol{\theta}}{\partial \psi(\boldsymbol{\theta})} \nabla_{\boldsymbol{\theta}} \ln p(\mathbf{x}|\boldsymbol{\theta}). \tag{6.96}$$

Then,

$$\mathbf{g}_{\psi}(\boldsymbol{\theta}, \mathbf{x}) = \left(\frac{\partial \psi(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right)^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}). \tag{6.97}$$

We have

$$\mathbf{F}_{\psi} = \int \mathbf{g}_{\psi}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}_{\psi}(\boldsymbol{\theta}, \mathbf{x})^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x}. \tag{6.98}$$

The right hand side can be written as

$$\int \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right)^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^{\mathsf{T}} \left(\left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right)^{-1}\right)^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x}$$

$$= \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right)^{-1} \left(\int \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^{\mathsf{T}} p(\mathbf{x}) d\mathbf{x}\right) \left(\left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right)^{-1}\right)^{\mathsf{T}}.$$
(6.99)

Then,

$$\mathbf{F}_{\psi} = \left(\frac{\partial \psi(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right)^{-1} \mathbf{F} \left(\left(\frac{\partial \psi(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right)^{-1}\right)^{\mathsf{T}}.$$
 (6.100)

Then,

$$k_{\psi}(\mathbf{x}, \mathbf{x}')$$

$$= \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^{\mathsf{T}} \left(\left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \right)^{\mathsf{T}} \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{\mathsf{T}} \mathbf{F}^{-1} \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right) \left(\frac{\partial \boldsymbol{\psi}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}').$$
(6.101)

The right hand side can be written as

$$\mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^{\mathsf{T}} \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}'). \tag{6.102}$$

Therefore,

$$k_{\psi}(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}'). \tag{6.103}$$

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

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{g}(\boldsymbol{\mu}, \mathbf{x})^{\mathsf{T}} \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\mu}, \mathbf{x}'), \tag{6.105}$$

where

$$\mathbf{g}(\boldsymbol{\mu}, \mathbf{x}) = \nabla_{\boldsymbol{\mu}} \ln p(\mathbf{x}|\boldsymbol{\mu}),$$

$$\mathbf{F} = \mathbf{E}_{\mathbf{x}} \left(\mathbf{g}(\boldsymbol{\mu}, \mathbf{x}) \mathbf{g}(\boldsymbol{\mu}, \mathbf{x})^{\mathsf{T}} \right).$$
 (6.106)

We have

$$\mathbf{g}(\boldsymbol{\mu}, \mathbf{x}) = -\mathbf{S}^{-1}(\mathbf{x} - \boldsymbol{\mu}). \tag{6.107}$$

Then,

$$\mathbf{F} = \int \mathbf{S}^{-1} (\mathbf{x} - \boldsymbol{\mu}) (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{S}^{-1} \mathcal{N} (\mathbf{x} | \boldsymbol{\mu}, \mathbf{S}) d\mathbf{x}. \tag{6.108}$$

The right hand side can be written as

$$\mathbf{S}^{-1} \left(\int (\mathbf{x} - \boldsymbol{\mu}) (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}, \mathbf{S}) d\mathbf{x} \right) \mathbf{S}^{-1} = \mathbf{S}^{-1}.$$
 (6.109)

Then,

$$\mathbf{F} = \mathbf{S}^{-1},\tag{6.110}$$

so that

$$\mathbf{g}(\boldsymbol{\mu}, \mathbf{x})^{\mathsf{T}} \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\mu}, \mathbf{x}') = (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{S}^{-1} (\mathbf{x} - \boldsymbol{\mu}). \tag{6.111}$$

Therefore,

$$k(\mathbf{x}, \mathbf{x}') = (\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{S}^{-1} (\mathbf{x} - \boldsymbol{\mu}). \tag{6.112}$$

6.15

Let k be a positive semidefinite kernel function. Then,

$$k(x,x)k(x',x') - k(x,x')^2 = \det \mathbf{K},$$
 (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,

$$\det \mathbf{K} \ge 0. \tag{6.115}$$

Therefore,

$$k(x, x')^2 \le k(x, x)k(x', x').$$
 (6.116)

6.16 (Incomplete)

Let

$$J(\mathbf{w}) = f(\mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_1), \cdots, \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_N)) + g(\mathbf{w}^{\mathsf{T}} \mathbf{w}), \qquad (6.117)$$

where g is a monotonically increasing function. Setting the derivative with respect to \mathbf{w} to zero gives

$$\mathbf{0} = \sum_{n=1}^{N} \frac{\partial f}{\partial \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_n)} \boldsymbol{\phi}(\mathbf{x}_n) + 2g'(\mathbf{w}^{\mathsf{T}} \mathbf{w}) \mathbf{w}. \tag{6.118}$$

Therefore,

$$\underset{\mathbf{w}}{\operatorname{argmin}} J(\mathbf{w}) = -\frac{1}{2g'(\mathbf{w}^{\mathsf{T}}\mathbf{w})} \sum_{n=1}^{N} \frac{\partial f}{\partial \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_n)} \boldsymbol{\phi}(\mathbf{x}_n). \tag{6.119}$$

6.17

Let

$$E = \frac{1}{2} \sum_{n=1}^{N} \int (y(\mathbf{x}_n + \boldsymbol{\xi}) - t_n)^2 p(\boldsymbol{\xi}) d\boldsymbol{\xi}.$$
 (6.120)

By the transformation

$$\mathbf{z} = \mathbf{x}_n + \boldsymbol{\xi},\tag{6.121}$$

we have

$$E = \frac{1}{2} \sum_{n=1}^{N} \int (y(\mathbf{z}) - t_n)^2 p(\mathbf{z} - \mathbf{x}_n) d\mathbf{z}.$$
 (6.122)

Setting the variation with respect to y to zero gives

$$0 = \sum_{n=1}^{N} (y(\mathbf{z}) - t_n) p(\mathbf{z} - \mathbf{x}_n).$$

$$(6.123)$$

The right hand side can be written as

$$y(\mathbf{z}) \sum_{n=1}^{N} p(\mathbf{z} - \mathbf{x}_n) - \sum_{n=1}^{N} t_n p(\mathbf{z} - \mathbf{x}_n).$$
 (6.124)

Therefore,

$$y(\mathbf{x}) = \sum_{n=1}^{N} t_n k(\mathbf{x}, \mathbf{x}_n), \tag{6.125}$$

where

$$k(\mathbf{x}, \mathbf{x}_n) = \frac{p(\mathbf{x} - \mathbf{x}_n)}{\sum_{n=1}^{N} p(\mathbf{x} - \mathbf{x}_n)}.$$
 (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

$$f(x,t) = \mathcal{N}(x|0,\sigma^2) \mathcal{N}(t|0,\sigma^2).$$
 (6.128)

(a)

By the Bayes' theorem,

$$p(t|x) = \frac{p(x,t)}{p(x)}. (6.129)$$

By marginalisation,

$$p(x) = \int p(x,t)dt. \tag{6.130}$$

The right hand side can be written as

$$\frac{1}{N} \sum_{n=1}^{N} \mathcal{N}\left(x - x_n | 0, \sigma^2\right) \int \mathcal{N}\left(t - t_n | 0, \sigma^2\right) dt$$

$$= \frac{1}{N} \sum_{n=1}^{N} \mathcal{N}\left(x - x_n | 0, \sigma^2\right).$$
(6.131)

Then,

$$p(t|x) = \frac{\frac{1}{N} \sum_{n=1}^{N} \mathcal{N}(x - x_n | 0, \sigma^2) \mathcal{N}(t - t_n | 0, \sigma^2)}{\frac{1}{N} \sum_{n=1}^{N} \mathcal{N}(x - x_n | 0, \sigma^2)}.$$
 (6.132)

Therefore,

$$p(t|x) = \sum_{n=1}^{N} k(x, x_n) \mathcal{N} (t - t_n | 0, \sigma^2), \qquad (6.133)$$

where

$$k(x, x_n) = \frac{\mathcal{N}(x - x_n | 0, \sigma^2)}{\sum_{n=1}^{N} \mathcal{N}(x - x_n | 0, \sigma^2)}.$$
 (6.134)

(b)

We have

$$E(t|x) = \int tp(t|x)dt.$$
 (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

$$\int (t'+t_n)\mathcal{N}\left(t'|0,\sigma^2\right)dt' = \int t'\mathcal{N}\left(t'|0,\sigma^2\right)dt' + t_n \int \mathcal{N}\left(t'|0,\sigma^2\right)dt'. \quad (6.138)$$

The right hand side can be written as t_n . Therefore,

$$E(t|x) = \sum_{n=1}^{N} k(x, x_n) t_n.$$
 (6.139)

(c)

We have

$$var(t|x) = \int (t - E(t|x))^2 p(t|x)dt.$$
 (6.140)

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

$$\sum_{n=1}^{N} k(x, x_n) \int \left(t - \sum_{n=1}^{N} k(x, x_n) t_n \right)^2 \mathcal{N} \left(t - t_n | 0, \sigma^2 \right) dt.$$
 (6.141)

By the transformation

$$t' = t - t_n, \tag{6.142}$$

the integral can be written as

$$\int \left(t' + t_n - \sum_{n=1}^{N} k(x, x_n) t_n \right)^2 \mathcal{N} \left(t' | 0, \sigma^2 \right) dt'
= \int t'^2 \mathcal{N} \left(t' | 0, \sigma^2 \right) dt' + 2 \left(t_n - \sum_{n=1}^{N} k(x, x_n) t_n \right) \int t' \mathcal{N} \left(t' | 0, \sigma^2 \right) dt' \quad (6.143)
+ \left(t_n - \sum_{n=1}^{N} k(x, x_n) t_n \right)^2 \int \mathcal{N} \left(t' | 0, \sigma^2 \right) dt'.$$

The right hand side can be written as

$$\sigma^{2} + \left(t_{n} - \sum_{n=1}^{N} k(x, x_{n})t_{n}\right)^{2}.$$
 (6.144)

Then,

$$var(t|x) = \sum_{n=1}^{N} k(x, x_n) \left(\sigma^2 + \left(t_n - \sum_{n'=1}^{N} k(x, x_{n'}) t_{n'} \right)^2 \right).$$
 (6.145)

Therefore,

$$\operatorname{var}(t|x) = \sigma^2 + \sum_{n=1}^{N} k(x, x_n) \left(t_n - \sum_{n'=1}^{N} k(x, x_{n'}) t_{n'} \right)^2.$$
 (6.146)

6.19

Let

$$E = \frac{1}{2} \sum_{n=1}^{N} \int (y(\mathbf{x}_n - \boldsymbol{\xi}_n) - t_n)^2 p(\boldsymbol{\xi}_n) d\boldsymbol{\xi}_n.$$
 (6.147)

By the transformation

$$\mathbf{z} = \mathbf{x}_n - \boldsymbol{\xi}_n,\tag{6.148}$$

we have

$$E = \frac{1}{2} \sum_{n=1}^{N} \int (y(\mathbf{z}) - t_n)^2 p(\mathbf{x}_n - \mathbf{z}) d\mathbf{z}.$$
 (6.149)

Setting the variation with respect to y to zero gives

$$0 = \sum_{n=1}^{N} (y(\mathbf{z}) - t_n) p(\mathbf{x}_n - \mathbf{z}).$$

$$(6.150)$$

The right hand side can be written as

$$y(\mathbf{z})\sum_{n=1}^{N}p(\mathbf{x}_{n}-\mathbf{z})-\sum_{n=1}^{N}t_{n}p(\mathbf{x}_{n}-\mathbf{z}).$$
(6.151)

Therefore,

$$y(\mathbf{x}) = \sum_{n=1}^{N} t_n k(\mathbf{x}, \mathbf{x}_n), \qquad (6.152)$$

where

$$k(\mathbf{x}, \mathbf{x}_n) = \frac{p(\mathbf{x}_n - \mathbf{x})}{\sum_{n=1}^{N} p(\mathbf{x}_n - \mathbf{x})}.$$
(6.153)

6.20

Let t_1, \dots, t_N be variables such that

$$p(\mathbf{t}|\mathbf{y}) = \mathcal{N}\left(\mathbf{t}|\mathbf{y}, \beta^{-1}\mathbf{I}\right),$$

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}),$$
(6.154)

$$K_{nn'} = k(\mathbf{x}_n, \mathbf{x}_{n'}). \tag{6.155}$$

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,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{y})p(\mathbf{y})d\mathbf{y}.$$
 (6.158)

The logarighm of the integrand of the right hand side except the terms independent of \mathbf{y}_N can be written as

$$-\frac{\beta}{2}(\mathbf{t} - \mathbf{y})^{\mathsf{T}}(\mathbf{t} - \mathbf{y}) - \frac{1}{2}\mathbf{y}^{\mathsf{T}}\mathbf{K}^{-1}\mathbf{y}$$

$$= -\frac{1}{2}\begin{bmatrix} \mathbf{y} \\ \mathbf{t} \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \beta \mathbf{I} + \mathbf{K}^{-1} & -\beta \mathbf{I} \\ -\beta \mathbf{I} & \beta \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{t} \end{bmatrix}.$$
(6.159)

By 2.24,

$$\begin{bmatrix} \beta \mathbf{I} + \mathbf{K}^{-1} & -\beta \mathbf{I} \\ -\beta \mathbf{I} & \beta \mathbf{I} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K} + \beta^{-1} \mathbf{I} \end{bmatrix}.$$
 (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,

$$p(\mathbf{t}') = \mathcal{N}\left(\mathbf{t}'|\mathbf{0}, \mathbf{C}'\right), \tag{6.163}$$

where

$$\mathbf{C}' = \begin{bmatrix} \mathbf{C} & \mathbf{k} \\ \mathbf{k}^{\mathsf{T}} & c \end{bmatrix}, \tag{6.164}$$

where

$$k_n = k(\mathbf{x}_n, \mathbf{x}_{N+1}),$$

 $c = k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}) + \beta^{-1}.$ (6.165)

By 2.24,

$$\begin{bmatrix} c & \mathbf{k}^{\mathsf{T}} \\ \mathbf{k} & \mathbf{C} \end{bmatrix}^{-1} = \begin{bmatrix} s^{-1} & -s^{-1}\mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1} \\ -s^{-1}\mathbf{C}^{-1}\mathbf{k} & \mathbf{C}^{-1} + s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1} \end{bmatrix}, \tag{6.166}$$

where

$$s = c - \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{k}. \tag{6.167}$$

Therefore,

$$p(t_{N+1}|\mathbf{t}) = \mathcal{N}(t_{N+1}|m,s),$$
 (6.168)

where

$$m = \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{t}. \tag{6.169}$$

6.21

Let t_1, \dots, t_N be variables such that

$$p(\mathbf{t}|\mathbf{y}) = \mathcal{N}\left(\mathbf{t}|\mathbf{y}, \beta^{-1}\mathbf{I}\right),$$

$$p(\mathbf{y}) = \mathcal{N}\left(\mathbf{y}|\mathbf{0}, \mathbf{\Phi}\mathbf{\Phi}^{\mathsf{T}}\right).$$
(6.170)

By 3.10,

$$p(t_{N+1}|\mathbf{t}) = \mathcal{N}(t_{N+1}|m,s),$$
 (6.171)

where

$$m = \beta \boldsymbol{\phi}_{N+1}^{\mathsf{T}} \left(\mathbf{I} + \beta \boldsymbol{\Phi}^{\mathsf{T}} \boldsymbol{\Phi} \right)^{-1} \boldsymbol{\Phi}^{\mathsf{T}} \mathbf{t},$$

$$s = \beta^{-1} + \boldsymbol{\phi}_{N+1}^{\mathsf{T}} \left(\mathbf{I} + \beta \boldsymbol{\Phi}^{\mathsf{T}} \boldsymbol{\Phi} \right)^{-1} \boldsymbol{\phi}_{N+1}.$$
(6.172)

By 2.26,

$$(\mathbf{I} + \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi})^{-1} = \mathbf{I} - \mathbf{\Phi}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{\Phi}, \tag{6.173}$$

where

$$\mathbf{C} = \beta^{-1} \mathbf{I} + \mathbf{\Phi} \mathbf{\Phi}^{\mathsf{T}}.\tag{6.174}$$

Then,

$$m = \beta \boldsymbol{\phi}_{N+1}^{\mathsf{T}} \left(\mathbf{I} - \boldsymbol{\Phi}^{\mathsf{T}} \mathbf{C}^{-1} \boldsymbol{\Phi} \right) \boldsymbol{\Phi}^{\mathsf{T}} \mathbf{t}. \tag{6.175}$$

The right hand side can be written as

$$\beta \left(\boldsymbol{\phi}_{N+1}^{\mathsf{T}} \boldsymbol{\Phi}^{\mathsf{T}} - \boldsymbol{\phi}_{N+1}^{\mathsf{T}} \boldsymbol{\Phi}^{\mathsf{T}} \mathbf{C}^{-1} \boldsymbol{\Phi} \boldsymbol{\Phi}^{\mathsf{T}} \right) \mathbf{t} = \beta \boldsymbol{\phi}_{N+1}^{\mathsf{T}} \boldsymbol{\Phi}^{\mathsf{T}} \mathbf{C}^{-1} \left(\mathbf{C} - \boldsymbol{\Phi} \boldsymbol{\Phi}^{\mathsf{T}} \right) \mathbf{t}. \quad (6.176)$$

The right hand side can be written as

$$\beta \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \beta^{-1} \mathbf{I} \mathbf{t} = \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{t}, \tag{6.177}$$

$$\mathbf{k} = \mathbf{\Phi} \phi_{N+1}. \tag{6.178}$$

Similarly,

$$s = \beta^{-1} + \boldsymbol{\phi}_{N+1}^{\mathsf{T}} \left(\mathbf{I} - \boldsymbol{\Phi}^{\mathsf{T}} \mathbf{C}^{-1} \boldsymbol{\Phi} \right) \boldsymbol{\phi}_{N+1}. \tag{6.179}$$

The right hand side can be written as

$$\beta^{-1} + \phi_{N+1}^{\mathsf{T}} \phi_{N+1} - \phi_{N+1}^{\mathsf{T}} \Phi^{\mathsf{T}} \mathbf{C}^{-1} \Phi \phi_{N+1} = c - \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{k}, \tag{6.180}$$

where

$$c = \beta^{-1} + \phi_{N+1}^{\mathsf{T}} \phi_{N+1}. \tag{6.181}$$

Therefore,

$$m = \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{t},$$

$$s = c - \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{k}.$$
(6.182)

6.22

Let t_1, \dots, t_N be variables such that

$$p(\mathbf{t}|\mathbf{y}) = \mathcal{N}\left(\mathbf{t}|\mathbf{y}, \beta^{-1}\mathbf{I}\right),$$

$$p(\mathbf{y}) = \mathcal{N}\left(\mathbf{y}|\mathbf{0}, \mathbf{K}\right),$$
(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,

$$p(\mathbf{t}) = \mathcal{N}\left(\mathbf{t}|\mathbf{0}, \mathbf{C}\right),\tag{6.187}$$

$$\mathbf{C} = \beta^{-1} \mathbf{I} + \mathbf{K}. \tag{6.188}$$

Let

$$K'_{nl} = k(\mathbf{x}_n, \mathbf{x}_{N+l}),$$

$$\Gamma_{ll'} = \beta^{-1} I_{ll'} + k(\mathbf{x}_{N+l}, \mathbf{x}_{N+l'}).$$
(6.189)

Then,

$$p(\mathbf{t}') = \mathcal{N}\left(\mathbf{t}'|\mathbf{0}, \mathbf{C}'\right),\tag{6.190}$$

where

$$\mathbf{C}' = \begin{bmatrix} \mathbf{C} & \mathbf{K}' \\ \mathbf{K}'^{\mathsf{T}} & \mathbf{\Gamma} \end{bmatrix}. \tag{6.191}$$

By 2.24,

$$\begin{bmatrix} \mathbf{\Gamma} & \mathbf{K}'^{\mathsf{T}} \\ \mathbf{K}' & \mathbf{C} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{S}^{-1} & -\mathbf{S}^{-1}\mathbf{K}'^{\mathsf{T}}\mathbf{C}^{-1} \\ -\mathbf{C}^{-1}\mathbf{K}'\mathbf{S}^{-1} & \mathbf{C}^{-1} + \mathbf{C}^{-1}\mathbf{K}'\mathbf{S}^{-1}\mathbf{K}'^{\mathsf{T}}\mathbf{C}^{-1} \end{bmatrix}, \quad (6.192)$$

where

$$\mathbf{S} = \mathbf{\Gamma} - \mathbf{K}'^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{K}'. \tag{6.193}$$

Therefore,

$$p(t_{N+1}, \dots, t_{N+L} | \mathbf{t}_N) = \mathcal{N}(t_{N+1}, \dots, t_{N+L} | \mathbf{m}, \mathbf{S}),$$
 (6.194)

where

$$\mathbf{m} = \mathbf{K}^{\prime \mathsf{T}} \mathbf{C}^{-1} \mathbf{t}. \tag{6.195}$$

(b)

Let

$$k_n = k(\mathbf{x}_n, \mathbf{x}_{N+1}),$$

 $c = \beta^{-1} + k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}).$ (6.196)

By (a),

$$p(t_{N+1}|\mathbf{t}) = \mathcal{N}(t_{N+1}|m,s),$$
 (6.197)

$$m = \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{t},$$

$$s = c - \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{k}.$$
(6.198)

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables such that

$$p(\mathbf{t}_n|\mathbf{y}_n) = \mathcal{N}\left(\mathbf{t}_n|\mathbf{y}_n, \beta^{-1}\mathbf{I}\right),$$

$$p(\mathbf{Y}) = \mathcal{N}\left(\mathbf{Y}|\mathbf{O}, \mathbf{K}\right),$$
(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,

$$p(\mathbf{T}) = \int p(\mathbf{T}|\mathbf{Y})p(\mathbf{Y})d\mathbf{Y}.$$
 (6.202)

The logarithm of the integrannd of the right hand side except the terms independent of T and Y can be written as

$$-\frac{\beta}{2} \sum_{n=1}^{N} \|\mathbf{t}_n - \mathbf{y}_n\|^2 - \frac{1}{2} \operatorname{tr} \left(\mathbf{Y}^{\mathsf{T}} \mathbf{K}^{-1} \mathbf{Y} \right) = -\frac{1}{2} \operatorname{tr} \mathbf{M}, \tag{6.203}$$

where

$$\mathbf{M} = \begin{bmatrix} \mathbf{Y} \\ \mathbf{T} \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \beta \mathbf{I} + \mathbf{K}^{-1} & -\beta \mathbf{I} \\ -\beta \mathbf{I} & \beta \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{Y} \\ \mathbf{T} \end{bmatrix}. \tag{6.204}$$

By 2.24,

$$\begin{bmatrix} \beta \mathbf{I} + \mathbf{K}^{-1} & -\beta \mathbf{I} \\ -\beta \mathbf{I} & \beta \mathbf{I} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \beta^{-1} \mathbf{I} + \mathbf{K} \end{bmatrix}.$$
 (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,

$$p(\mathbf{T}') = \mathcal{N}(\mathbf{T}'|\mathbf{O}, \mathbf{C}'), \qquad (6.208)$$

$$\mathbf{C}' = \begin{bmatrix} \mathbf{C} & \mathbf{k} \\ \mathbf{k}^{\mathsf{T}} & c \end{bmatrix}, \tag{6.209}$$

where

$$k_n = k(\mathbf{x}_n, \mathbf{x}_{N+1}),$$

 $c = \beta^{-1} + k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}).$ (6.210)

By 2.24,

$$\begin{bmatrix} c & \mathbf{k}^{\mathsf{T}} \\ \mathbf{k} & \mathbf{C} \end{bmatrix}^{-1} = \begin{bmatrix} s^{-1} & -s^{-1}\mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1} \\ -s^{-1}\mathbf{C}^{-1}\mathbf{k} & \mathbf{C}^{-1} + s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1} \end{bmatrix}, \tag{6.211}$$

where

$$s = c - \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{k}. \tag{6.212}$$

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

$$\mathbf{m} = \mathbf{T}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{k}. \tag{6.214}$$

6.24

(a)

Let **M** be a $D \times D$ diagonal matrix such that $0 < M_{dd} < 1$. For any vector **v** in D dimensions,

$$\mathbf{v}^{\mathsf{T}} \mathbf{M} \mathbf{v} = \sum_{d=1}^{D} \sum_{d'=1}^{D} v_d M_{dd'} v_{d'}.$$
 (6.215)

The right hand side can be written as

$$\sum_{d=1}^{D} M_{dd} v_d^2 > 0. (6.216)$$

Therefore, 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,

$$\mathbf{v}^{\mathsf{T}}\mathbf{M}_{1}\mathbf{v} > 0,$$

$$\mathbf{v}^{\mathsf{T}}\mathbf{M}_{2}\mathbf{v} > 0.$$
 (6.217)

Then,

$$\mathbf{v}^{\mathsf{T}}(\mathbf{M}_1 + \mathbf{M}_2)\mathbf{v} > 0. \tag{6.218}$$

Therefore, $\mathbf{M}_1 + \mathbf{M}_2$ is positive definite.

6.25

Let t_1, \dots, t_N be variables such that

$$p(t_n|a_n) = \sigma(a_n)^{t_n} (1 - \sigma(a_n))^{1 - t_n},$$

$$p(\mathbf{a}) = \mathcal{N}(\mathbf{a}|\mathbf{0}, \mathbf{C}),$$
(6.219)

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)},$$

$$C_{nn'} = k(\mathbf{x}_n, \mathbf{x}_{n'}) + \nu I_{nn'}.$$
(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 ${\bf t}$ and ${\bf a}$ can be written as

$$\Psi(\mathbf{a}) = \sum_{n=1}^{N} (t_n \ln \sigma(a_n) + (1 - t_n) \ln (1 - \sigma(a_n))) - \frac{1}{2} \mathbf{a}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{a}.$$
 (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,

$$(\nabla \Psi(\mathbf{a}))_n = (t_n (1 - \sigma(a_n)) - (1 - t_n)\sigma(a_n)) - (\mathbf{C}^{-1}\mathbf{a})_n,$$
 (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 σ non-linearly depends on \mathbf{a} , the Taylor series

$$\nabla \Psi(\mathbf{a}^{\text{new}}) = \nabla \Psi(\mathbf{a}) + \nabla \nabla \Psi(\mathbf{a}) \left(\mathbf{a}^{\text{new}} - \mathbf{a}\right) + O\left(\|\mathbf{a} - \mathbf{a}^{\text{new}}\|^{2}\right). \quad (6.227)$$

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,

$$\mathbf{a}^{\text{new}} = \mathbf{a} - (\nabla \nabla \Psi(\mathbf{a}))^{-1} \nabla \Psi(\mathbf{a}). \tag{6.229}$$

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

$$(\mathbf{W} + \mathbf{C}^{-1})^{-1} ((\mathbf{W} + \mathbf{C}^{-1}) \mathbf{a} + \mathbf{t} - \boldsymbol{\sigma} - \mathbf{C}^{-1} \mathbf{a})$$

$$= \mathbf{C} (\mathbf{W} \mathbf{C} + \mathbf{I})^{-1} (\mathbf{W} \mathbf{a} + \mathbf{t} - \boldsymbol{\sigma}).$$
(6.233)

Therefore,

$$\mathbf{a}^{\text{new}} = \mathbf{C} \left(\mathbf{W} \mathbf{C} + \mathbf{I} \right)^{-1} \left(\mathbf{W} \mathbf{a} + \mathbf{t} - \boldsymbol{\sigma} \right). \tag{6.234}$$

(b)

Let \mathbf{a}_{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

$$\begin{split} \Psi(\mathbf{a}) = & \Psi(\mathbf{a}_{MAP}) + \nabla \Psi(\mathbf{a}_{MAP})(\mathbf{a} - \mathbf{a}_{MAP}) \\ & + \frac{1}{2}(\mathbf{a} - \mathbf{a}_{MAP})^{\intercal} \nabla \nabla \Psi(\mathbf{a}_{MAP})(\mathbf{a} - \mathbf{a}_{MAP}) + O\left(\|\mathbf{a} - \mathbf{a}_{MAP}\|^{3}\right). \end{split} \tag{6.235}$$

Then,

$$\Psi(\mathbf{a}) \simeq \Psi(\mathbf{a}_{MAP}) - \frac{1}{2}(\mathbf{a} - \mathbf{a}_{MAP})^{\mathsf{T}}\mathbf{H}(\mathbf{a} - \mathbf{a}_{MAP}),$$
 (6.236)

where

$$\mathbf{H} = \mathbf{W} \mid_{\mathbf{a} = \mathbf{a}_{\text{MAP}}} + \mathbf{C}^{-1}. \tag{6.237}$$

Therefore,

$$p(\mathbf{a}|\mathbf{t}) \simeq \mathcal{N}\left(\mathbf{a}|\mathbf{a}_{\text{MAP}}, \mathbf{H}^{-1}\right).$$
 (6.238)

(c)

By (a),

$$\mathbf{a}_{\text{MAP}} = \mathbf{C} \left(\mathbf{WC} + \mathbf{I} \right)^{-1} \left(\mathbf{W} \mathbf{a}_{\text{MAP}} + \mathbf{t} - \boldsymbol{\sigma} \right). \tag{6.239}$$

Then,

$$(\mathbf{WC} + \mathbf{I}) \mathbf{C}^{-1} \mathbf{a}_{MAP} = \mathbf{W} \mathbf{a}_{MAP} + \mathbf{t} - \boldsymbol{\sigma}. \tag{6.240}$$

Therefore,

$$\mathbf{a}_{\text{MAP}} = \mathbf{C}(\mathbf{t} - \boldsymbol{\sigma}). \tag{6.241}$$

6.26

Let t_1, \dots, t_N be variables such that

$$p(t_n|a_n) = \sigma(a_n)^{t_n} (1 - \sigma(a_n))^{1 - t_n},$$

$$p(\mathbf{a}) = \mathcal{N}(\mathbf{a}|\mathbf{0}, \mathbf{C}),$$
(6.242)

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)},$$

$$C_{nn'} = k(\mathbf{x}_n, \mathbf{x}_{n'}) + \nu I_{nn'}.$$
(6.243)

By marginalisation,

$$p(a_{N+1}|\mathbf{t}) = \int p(a_{N+1}|\mathbf{a})p(\mathbf{a}|\mathbf{t})d\mathbf{a}.$$
 (6.244)

Let

$$\mathbf{a}' = \begin{bmatrix} \mathbf{a} \\ a_{N+1} \end{bmatrix},$$

$$k_n = k(\mathbf{x}_n, \mathbf{x}_{N+1}),$$

$$c = k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}) + \nu.$$
(6.245)

Then,

$$p(\mathbf{a}') = \mathcal{N}(\mathbf{a}'|\mathbf{0}, \mathbf{C}'),$$
 (6.246)

where

$$\mathbf{C}' = \begin{bmatrix} \mathbf{C} & \mathbf{k} \\ \mathbf{k}^{\mathsf{T}} & c \end{bmatrix}. \tag{6.247}$$

By 2.24,

$$\begin{bmatrix} c & \mathbf{k}^{\mathsf{T}} \\ \mathbf{k} & \mathbf{C} \end{bmatrix}^{-1} = \begin{bmatrix} s^{-1} & -s^{-1}\mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1} \\ -s^{-1}\mathbf{C}^{-1}\mathbf{k} & \mathbf{C}^{-1} + s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1} \end{bmatrix}, \tag{6.248}$$

where

$$s = c - \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{k}. \tag{6.249}$$

Then,

$$p(a_{N+1}|\mathbf{a}) = \mathcal{N}(a_{N+1}|m,s),$$
 (6.250)

where

$$m = \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{a}. \tag{6.251}$$

By 6.25(b),

$$p(\mathbf{a}|\mathbf{t}) \simeq \mathcal{N}\left(\mathbf{a}|\mathbf{a}_{\text{MAP}}, \mathbf{H}^{-1}\right),$$
 (6.252)

where \mathbf{a}_{MAP} is a stationary point of $p(\mathbf{a}|\mathbf{t})$ and

$$\mathbf{H} = \mathbf{W} \mid_{\mathbf{a} = \mathbf{a}_{\text{MAP}}} + \mathbf{C}^{-1},$$

$$W_{nn'} = \sigma(a_n) \left(1 - \sigma(a_n)\right) I_{nn'}.$$
(6.253)

Then, the logarithm of the integrand except the terms independent of ${\bf t}$ and ${\bf a}$ can be approximated as

$$-\frac{1}{2s} (a_{N+1} - m)^{2} - \frac{1}{2} (\mathbf{a} - \mathbf{a}_{MAP})^{\mathsf{T}} \mathbf{H} (\mathbf{a} - \mathbf{a}_{MAP})$$

$$= -\frac{1}{2} \mathbf{a}'^{\mathsf{T}} \mathbf{M} \mathbf{a}' + \mathbf{a}'^{\mathsf{T}} \mathbf{v} - \frac{1}{2} \mathbf{a}_{MAP}^{\mathsf{T}} \mathbf{H} \mathbf{a}_{MAP}.$$
(6.254)

where

$$\mathbf{M} = \begin{bmatrix} \mathbf{H} + s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1} & -s^{-1}\mathbf{C}^{-1}\mathbf{k} \\ -s^{-1}\mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1} & s^{-1} \end{bmatrix},$$

$$\mathbf{v} = \begin{bmatrix} \mathbf{H}\mathbf{a}_{\text{MAP}} \\ 0 \end{bmatrix}.$$
(6.255)

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{H}^{-1} & \mathbf{H}^{-1}\mathbf{C}^{-1}\mathbf{k} \\ \mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1}\mathbf{H}^{-1} & s + \mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1}\mathbf{H}^{-1}\mathbf{C}^{-1}\mathbf{k} \end{bmatrix}, \tag{6.256}$$

so that

$$\mathbf{M}^{-1}\mathbf{v} = \begin{bmatrix} \mathbf{a}_{\text{MAP}} \\ \mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1}\mathbf{a}_{\text{MAP}} \end{bmatrix}. \tag{6.257}$$

Then,

$$p(a_{N+1}|\mathbf{t}) \simeq \mathcal{N}\left(a_{N+1}|\mu,\sigma^2\right),$$
 (6.258)

$$\mu = \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{a}_{\text{MAP}},$$

$$\sigma^{2} = s + \mathbf{k}^{\mathsf{T}} \mathbf{C}^{-1} \mathbf{H}^{-1} \mathbf{C}^{-1} \mathbf{k}.$$
(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,

$$\mu = \mathbf{k}^{\mathsf{T}}(\mathbf{t} - \boldsymbol{\sigma}),$$

$$\sigma^{2} = c - \mathbf{k}^{\mathsf{T}}\mathbf{C}^{-1}(\mathbf{C} - \mathbf{H}^{-1})\mathbf{C}^{-1}\mathbf{k}.$$
(6.262)

6.27 (Incomplete)

Let t_1, \dots, t_N be variables such that

$$p(t_n|a_n) = \sigma(a_n)^{t_n} (1 - \sigma(a_n))^{1 - t_n},$$

$$p(\mathbf{a}|\boldsymbol{\theta}) = \mathcal{N}(\mathbf{a}|\mathbf{0}, \mathbf{C}),$$
(6.263)

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)} \tag{6.264}$$

and ${\bf C}$ is dependent on ${\boldsymbol \theta}$ with M dimensions.

(a)

By marginalisation,

$$p(\mathbf{t}|\boldsymbol{\theta}) = \int p(\mathbf{t}|\mathbf{a})p(\mathbf{a}|\boldsymbol{\theta})d\mathbf{a}.$$
 (6.265)

Let \mathbf{a}_{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),

$$\Psi(\mathbf{a}) \simeq \Psi(\mathbf{a}_{\text{MAP}}) - \frac{1}{2} (\mathbf{a} - \mathbf{a}_{\text{MAP}})^{\mathsf{T}} \mathbf{H} (\mathbf{a} - \mathbf{a}_{\text{MAP}}),$$
 (6.267)

where

$$\mathbf{H} = \mathbf{W} \mid_{\mathbf{a} = \mathbf{a}_{\text{MAP}}} + \mathbf{C}^{-1},$$

$$W_{nn'} = \sigma(a_n) (1 - \sigma(a_n)) I_{nn'}.$$
(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

$$\frac{\partial \Psi(\mathbf{a}_{\text{MAP}})}{\partial \theta_m} = \sum_{n=1}^{N} \sum_{n'=1}^{N} \frac{\partial \Psi(\mathbf{a}_{\text{MAP}})}{\partial C_{nn'}} \frac{\partial C_{nn'}}{\partial \theta_m}.$$
 (6.270)

The right hand side can be written as

$$\frac{1}{2} \operatorname{tr} \left(\mathbf{a}_{\text{MAP}} \mathbf{a}_{\text{MAP}}^{\mathsf{T}} \left(\mathbf{C}^{-1} \right)^{2} \frac{\partial \mathbf{C}}{\partial \theta_{m}} \right). \tag{6.271}$$

We have

$$\frac{\partial \ln(\det \mathbf{H})}{\partial \theta_m} = \sum_{n=1}^{N} \sum_{n'=1}^{N} \frac{\partial \ln(\det \mathbf{H})}{\partial H_{nn'}} \frac{\partial H_{nn'}}{\partial \theta_m}.$$
 (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,

$$\frac{\partial \ln p(\mathbf{t}|\boldsymbol{\theta})}{\partial \theta_m} \simeq \frac{1}{2} \operatorname{tr} \left(\mathbf{a}_{\text{MAP}} \mathbf{a}_{\text{MAP}}^{\mathsf{T}} \left(\mathbf{C}^{-1} \right)^2 \frac{\partial \mathbf{C}}{\partial \theta_m} - \mathbf{H}^{-1} \frac{\partial \mathbf{C}^{-1}}{\partial \theta_m} \right). \tag{6.274}$$

7 Sparse Kernel Machines

7.1 (Incomplete)

7.2

Let t_1, \dots, t_N be variables. In order to minimise $\|\mathbf{w}\|^2$ under the constraint

$$t_n\left(\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}_n) + b\right) \ge \gamma,$$
 (7.1)

for $\gamma > 0$, let

$$L = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n \left(t_n \left(\mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_n) + b \right) - \gamma \right). \tag{7.2}$$

Setting the derivatives of L with respect to \mathbf{w} and b to zero gives

$$\mathbf{0} = \mathbf{w} - \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n),$$

$$0 = -\sum_{n=1}^{N} a_n t_n.$$
(7.3)

Therefore,

$$\mathbf{w} = \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n),$$

$$0 = \sum_{n=1}^{N} a_n t_n,$$
(7.4)

which is independent of γ .

- 7.3 (Incomplete)
- 7.4 (Incomplete)
- 7.5 (Incomplete)

7.6

Let t_1, \dots, t_N be a variable such that

$$t_n \in \{-1, 1\},\ p(t_n|y_n) = \sigma(y_n)^{\frac{1+t_n}{2}} \left(1 - \sigma(y_n)\right)^{\frac{1-t_n}{2}},$$
(7.5)

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)},$$

$$y_n = \mathbf{w}^{\mathsf{T}} \phi(\mathbf{x}_n) + b.$$
(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, \dots, t_N be vaariables. Let

$$E = C \sum_{n=1}^{N} E_{\epsilon}(y_n - t_n) + \frac{1}{2} \|\mathbf{w}\|^2,$$
 (7.12)

where $\epsilon > 0$ and

$$E_{\epsilon}(a) = \begin{cases} 0, & |a| < \epsilon, \\ |a| - \epsilon, & \text{otherwise,} \end{cases}$$

$$y_n = \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_n) + b.$$
(7.13)

In order to minimise E under the constraints

$$t_n \le y_n + \epsilon + \xi_n,$$

$$t_n > y_n - \epsilon - \hat{\xi}_n,$$
(7.14)

where $\xi_n \geq 0$ and $\hat{\xi}_n \geq 0$, let us minimise

$$L = C \sum_{n=1}^{N} (\xi_n + \hat{\xi}_n) + \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^{N} \left(\mu_n \xi_n + \hat{\mu}_n \hat{\xi}_n \right) - \sum_{n=1}^{N} a_n (\epsilon + \xi_n + y_n - t_n) - \sum_{n=1}^{N} \hat{a}_n (\epsilon + \hat{\xi}_n - y_n + t_n).$$
(7.15)

Setting the derivatives of L with respect to \mathbf{w} , b, ξ_n and $\hat{\xi}_n$ to zero gives

$$\mathbf{0} = \mathbf{w} - \sum_{n=1}^{N} a_n \phi(\mathbf{x}_n) + \sum_{n=1}^{N} \hat{a}_n \phi(\mathbf{x}_n),$$

$$0 = -\sum_{n=1}^{N} a_n + \sum_{n=1}^{N} \hat{a}_n,$$

$$0 = C - \mu_n - a_n,$$

$$0 = C - \hat{\mu}_n - \hat{a}_n.$$
(7.16)

Then, L can be written as

$$\sum_{n=1}^{N} \left((\mu_n + a_n) \xi_n + (\hat{\mu}_n + \hat{a}_n) \hat{\xi}_n \right) + \frac{1}{2} \left\| \sum_{n=1}^{N} (\hat{a}_n - a_n) \phi(\mathbf{x}_n) \right\|^2 - \sum_{n=1}^{N} \left(\mu_n \xi_n + \hat{\mu}_n \hat{\xi}_n \right) - \sum_{n=1}^{N} a_n (\epsilon + \xi_n + y_n - t_n)$$

$$- \sum_{n=1}^{N} \hat{a}_n (\epsilon + \hat{\xi}_n - y_n + t_n).$$
(7.17)

Therefore, minimising L is equilvalent to maximising

$$\tilde{L} = -\frac{1}{2} \sum_{n=1}^{N} \sum_{n'=1}^{N} (\hat{a}_n - a_n)(\hat{a}_{n'} - a_{n'}) k(\mathbf{x}_n, \mathbf{x}_{n'})$$

$$+ \epsilon \sum_{n=1}^{N} (a_n + \hat{a}_n) + \sum_{n=1}^{N} (a_n - \hat{a}_n) (y_n - t_n),$$
(7.18)

where

$$k(\mathbf{x}_n, \mathbf{x}_{n'}) = \phi(\mathbf{x}_n)^{\mathsf{T}} \phi(\mathbf{x}_{n'}). \tag{7.19}$$

7.8 (Incomplete)

Let t_1, \dots, t_N be vaariables. Let

$$E = C \sum_{n=1}^{N} E_{\epsilon}(y_n - t_n) + \frac{1}{2} \|\mathbf{w}\|^2,$$
 (7.20)

where $\epsilon > 0$ and

$$E_{\epsilon}(a) = \begin{cases} 0, & |a| < \epsilon, \\ |a| - \epsilon, & \text{otherwise,} \end{cases}$$

$$y_n = \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_n) + b.$$
(7.21)

(a)

In order to minimise E under the constraints

$$t_n \le y_n + \epsilon + \xi_n, \tag{7.22}$$

where $\xi_n \geq 0$, let us minimise

$$L = C \sum_{n=1}^{N} \xi_n + \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^{N} \mu_n \xi_n - \sum_{n=1}^{N} a_n (\epsilon + \xi_n + y_n - t_n).$$
 (7.23)

Setting the derivatives of L with respect to \mathbf{w} , b and ξ_n to zero gives

$$\mathbf{0} = \mathbf{w} - \sum_{n=1}^{N} a_n \boldsymbol{\phi}(\mathbf{x}_n),$$

$$0 = -\sum_{n=1}^{N} a_n,$$

$$0 = C - \mu_n - a_n.$$

$$(7.24)$$

Then, L can be written as

$$\sum_{n=1}^{N} (\mu_n + a_n) \xi_n + \frac{1}{2} \left\| \sum_{n=1}^{N} a_n \phi(\mathbf{x}_n) \right\|^2 - \sum_{n=1}^{N} \mu_n \xi_n - \sum_{n=1}^{N} a_n (\epsilon + \xi_n + y_n - t_n).$$
(7.25)

Therefore, minimising L is equilvalent to maximising

$$\tilde{L} = -\frac{1}{2} \sum_{n=1}^{N} \sum_{n'=1}^{N} a_n a_{n'} k(\mathbf{x}_n, \mathbf{x}_{n'}) + \sum_{n=1}^{N} a_n (y_n - t_n),$$
 (7.26)

where

$$k(\mathbf{x}_n, \mathbf{x}_{n'}) = \boldsymbol{\phi}(\mathbf{x}_n)^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_{n'}). \tag{7.27}$$

7.9

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}_n, \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \mathbf{A}^{-1}\right).$$
 (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 ${\bf t}$ and ${\bf w}$ can be written as

$$-\frac{\beta}{2} \sum_{n=1}^{N} \|t_n - \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}_n\|^2 - \frac{1}{2} \mathbf{w}^{\mathsf{T}} \mathbf{A} \mathbf{w}$$

$$= -\frac{1}{2} \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} + \mathbf{A} & -\beta \mathbf{\Phi}^{\mathsf{T}} \\ -\beta \mathbf{\Phi} & \beta \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}.$$
(7.30)

Therefore,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{S}), \qquad (7.31)$$

$$\mathbf{m} = \beta \mathbf{S} \mathbf{\Phi}^{\mathsf{T}} \mathbf{t}, \mathbf{S} = (\beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} + \mathbf{A})^{-1}.$$
 (7.32)

7.10

Let t_1, \dots, t_N be variables such that

$$p(t_n|\mathbf{w}) = \mathcal{N}\left(t_n|\mathbf{w}^{\mathsf{T}}\boldsymbol{\phi}_n, \beta^{-1}\right),$$

$$p(\mathbf{w}) = \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \mathbf{A}^{-1}\right).$$
 (7.33)

By marginalisation,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}.$$
 (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

$$-\frac{\beta}{2} \sum_{n=1}^{N} \|t_n - \mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}_n\|^2 - \frac{1}{2} \mathbf{w}^{\mathsf{T}} \mathbf{A} \mathbf{w}$$

$$= -\frac{1}{2} \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \beta \boldsymbol{\Phi}^{\mathsf{T}} \boldsymbol{\Phi} + \mathbf{A} & -\beta \boldsymbol{\Phi}^{\mathsf{T}} \\ -\beta \boldsymbol{\Phi} & \beta \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}.$$
(7.35)

By 2.24,

$$\begin{bmatrix} \beta \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} + \mathbf{A} & -\beta \mathbf{\Phi}^{\mathsf{T}} \\ -\beta \mathbf{\Phi} & \beta \mathbf{I} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{A}^{-1} & \mathbf{A}^{-1} \mathbf{\Phi}^{\mathsf{T}} \\ \mathbf{\Phi} \mathbf{A}^{-1} & \beta^{-1} \mathbf{I} + \mathbf{\Phi} \mathbf{A}^{-1} \mathbf{\Phi}^{\mathsf{T}} \end{bmatrix}. \tag{7.36}$$

Therefore,

$$p(\mathbf{t}) = \mathcal{N}\left(\mathbf{t}|\mathbf{0}, \beta^{-1}\mathbf{I} + \mathbf{\Phi}\mathbf{A}^{-1}\mathbf{\Phi}^{\mathsf{T}}\right). \tag{7.37}$$