

Solutions Manual to
Pattern Recognition and Machine Learning

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1 Introduction

1.1

Let

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

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

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

If

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

then

$$\mathbf{0} = \sum_{n=1}^N \boldsymbol{\phi}(x_n) (\mathbf{w}^\top \boldsymbol{\phi}(x_n) - t_n). \quad (1.4)$$

Then,

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

Therefore,

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

where

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

If

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

then

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

1.2

Let

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

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

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

If

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

then

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

Then,

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

Therefore,

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

where

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

If

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

then

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

1.3

Let

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

Let

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

(a)

By the Bayes' theorem,

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

Therefore,

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

(b)

By the Bayes' theorem,

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

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

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

Therefore,

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

1.4

Let x and y be variables such that

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

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

$$|y - \hat{y}| < \epsilon, \quad (1.25)$$

then

$$g'(y) \neq 0. \quad (1.26)$$

(a)

Since

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

we have

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

Taking the derivative and substituting

$$y = \hat{y} \quad (1.29)$$

gives

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

Therefore, in general,

$$\hat{x} \neq g(\hat{y}). \quad (1.31)$$

(b)

By (a), if

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

then

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

Therefore,

$$\hat{x} = g(\hat{y}). \quad (1.34)$$

1.5

We have

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

The right hand side can be written as

$$E((f(x))^2 - 2f(x)E f(x) + (E f(x))^2) = E(f(x))^2 - (E f(x))^2. \quad (1.36)$$

Therefore,

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

1.6

We have

$$\text{cov}(x, y) = E((x - E x)(y - E y)). \quad (1.38)$$

The right hand side can be written as

$$E xy - E(x E y) - E(y E x) + E(E x E y) = E xy - E x E y. \quad (1.39)$$

The right hand side can be written as

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

If x and y are independent, then

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

Then,

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

Therefore,

$$\text{cov}(x, y) = 0. \quad (1.43)$$

1.7

(a)

Let

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

Then,

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

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

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

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

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

Therefore,

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

(b)

We have

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

Then,

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

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

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

By 1.7(a), it can be written as $(2\pi\sigma^2)^{\frac{1}{2}}$. Therefore,

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

1.8

(a)

Let x be a variable such that

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

Then,

$$\mathbb{E} x = \int_{-\infty}^{\infty} x \mathcal{N}(x|\mu, \sigma^2) dx. \quad (1.54)$$

The right hand side can be written as

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

By the transformation

$$y = x - \mu, \quad (1.56)$$

the integral can be written as

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

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

$$\mu (2\pi\sigma^2)^{\frac{1}{2}}. \quad (1.58)$$

Therefore,

$$\mathbb{E} x = \mu. \quad (1.59)$$

(b)

By 1.7(b),

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

so that

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

Taking the derivative with respect to σ^2 gives

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

The left hand side can be written as

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

Therefore,

$$\text{var } x = \sigma^2. \quad (1.64)$$

1.9

(a)

Let x be a variable such that

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

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

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

Therefore,

$$\text{mode } x = \mu. \quad (1.67)$$

(b)

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

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

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

$$\begin{aligned} \mathbf{0} &= - (2\pi)^{-\frac{D}{2}} (\det \boldsymbol{\Sigma})^{-\frac{1}{2}} (\boldsymbol{\Sigma}^{-1} + (\boldsymbol{\Sigma}^{-1})^\top) (\mathbf{x} - \boldsymbol{\mu}) \\ &\quad \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right). \end{aligned} \quad (1.69)$$

Therefore,

$$\text{mode } \mathbf{x} = \boldsymbol{\mu}. \quad (1.70)$$

1.10

(a)

We have

$$\mathbb{E}(x + y) = \iint (x + y) p(x, y) dx dy. \quad (1.71)$$

The right hand side can be written as

$$\begin{aligned} &\int x \left(\int p(x, y) dy \right) dx + \int y \left(\int p(x, y) dx \right) dy \\ &= \int xp(x) dx + \int yp(y) dy. \end{aligned} \quad (1.72)$$

The right hand side can be written as

$$\mathbb{E} x + \mathbb{E} y. \quad (1.73)$$

Therefore,

$$\mathbb{E}(x + y) = \mathbb{E} x + \mathbb{E} y. \quad (1.74)$$

(b)

We have

$$\text{var}(x + y) = \mathbb{E} (x + y - \mathbb{E}(x + y))^2 \quad (1.75)$$

The right hand side can be written as

$$\begin{aligned} & \mathbb{E}(x - \mathbb{E}x)^2 + 2\mathbb{E}((x - \mathbb{E}x)(y - \mathbb{E}y)) + \mathbb{E}(y - \mathbb{E}y)^2 \\ &= \text{var } x + 2 \text{cov}(x, y) + \text{var } y. \end{aligned} \quad (1.76)$$

By 1.6, if x and y are independent, then

$$\text{cov}(x, y) = 0. \quad (1.77)$$

Therefore,

$$\text{var}(x + y) = \text{var } x + \text{var } y. \quad (1.78)$$

1.11

Let x_1, \dots, x_N be variables such that

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

Then,

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

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

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

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

$$\begin{aligned} \mu_{\text{ML}} &= \frac{1}{N} \sum_{n=1}^N x_n, \\ \sigma_{\text{ML}}^2 &= \frac{1}{N} \sum_{n=1}^N (x_n - \mu_{\text{ML}})^2. \end{aligned} \quad (1.82)$$

1.12

(a)

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

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

Then,

$$\mathbb{E} x_n x_{n'} = \mu^2. \quad (1.84)$$

By the property

$$\mathbb{E} x_n^2 = \text{var } x_n + (\mathbb{E} x_n)^2, \quad (1.85)$$

we have

$$\mathbb{E} x_n^2 = \sigma^2 + \mu^2. \quad (1.86)$$

Therefore,

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

(b)

Let x_1, \dots, x_N be independent variables such that

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

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

$$\mu_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N x_n. \quad (1.89)$$

Then,

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

Therefore,

$$\mathbb{E} \mu_{\text{ML}} = \mu. \quad (1.91)$$

(c)

Let x_1, \dots, x_N be independent variables such that

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

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

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

Then,

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

The right hand side can be written as

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

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

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

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

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

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

$$\begin{aligned} & -\frac{1}{N^2} \sum_{n=1}^N \mathbb{E} x_n^2 - \frac{2}{N^2} \sum_{1 \leq n < n' \leq N} \mathbb{E} x_n x_{n'} \\ &= -\frac{1}{N^2} N (\mu^2 + \sigma^2) - \frac{2}{N^2} \frac{N(N-1)}{2} \mu^2. \end{aligned} \quad (1.98)$$

The right hand side can be written as

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

Then,

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

Therefore,

$$\text{E } \sigma_{\text{ML}}^2 = \frac{N-1}{N}\sigma^2. \quad (1.101)$$

1.13

Let x_1, \dots, x_N be variables such that

$$\begin{aligned} \text{E } x_n &= \mu, \\ \text{var } x_n &= \sigma^2. \end{aligned} \quad (1.102)$$

We have

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

The right hand side can be written as

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

Therefore,

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

1.14

Let

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

(a)

We have

$$\begin{aligned} w_{dd'} &= w_{dd'}^S + w_{dd'}^A, \\ w_{dd'}^S &= w_{d'd}^S, \\ w_{dd'}^A &= -w_{d'd}^A. \end{aligned} \quad (1.107)$$

(b)

We have

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

The right hand side can be written as

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

Therefore,

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

(c)

We have

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

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

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

Therefore,

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

(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

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

Let us assume that

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

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

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

so that

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

Therefore, the assumption is proved by induction on D .

(b)

We have

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

Let us assume that

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

Then,

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

The right hand side can be written as

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

Therefore, the assumption is proved by induction on D .

(c)

By 1.14(d),

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

Let us assume that

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

By (a),

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

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

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

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,

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

where

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

(b)

By (a),

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

Let us assume that

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

Then,

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

The right hand side can be written as

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

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

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

(c)

By the approximation

$$n! \simeq n^n \exp(-n), \quad (1.133)$$

we have

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

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,

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

(d)

By (b),

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

1.17

Let

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

(a)

We have

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

The right hand side can be written as

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

Therefore,

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

(b)

We have

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

so that

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

For a positive integer x , let us assume that

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

By (a),

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

so that

$$\Gamma(x+1) = x!. \quad (1.146)$$

Therefore, the assumption is proved by induction on x .

1.18

(a)

Let

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

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

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

the right hand side can be written as

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

Therefore,

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

(b)

The volume of the sphere can be written as

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

Therefore,

$$V_D = \frac{S_D}{D}. \quad (1.152)$$

(c)

By (a) and (b),

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

Similarly,

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

1.19

(a)

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

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

(b)

By (a) and the Stering's formula

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

we have

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

The right hand side can be written as

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

Therefore,

$$\lim_{D \rightarrow \infty} \frac{V_D}{2^D} = 0. \quad (1.159)$$

(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

$$\frac{\sqrt{\sum_{i=1}^D 1^2}}{1} = \sqrt{D}. \quad (1.160)$$

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

1.20

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

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

(a)

We have

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

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

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

Therefore,

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

where

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

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

(b)

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

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

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

$$\hat{r} = \sqrt{D-1}\sigma. \quad (1.167)$$

(c)

We have

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

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

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

By the Taylor series

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

the right hand side can be approximated as

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

Therefore,

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

(d)

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

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

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

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

Therefore,

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

1.21

(a)

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

$$0 \leq a(b-a). \quad (1.176)$$

Therefore,

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

(b)

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

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

By (a),

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

Therefore,

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

1.22

Let

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

where

$$L_{kj} = 1 - I_{kj}. \quad (1.182)$$

The right hand side can be written as

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

The right hand side can be written as

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

Then,

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

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

1.23

Let

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

The right hand side can be written as

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

Then,

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

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

1.24 (Incomplete)

Let

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

1.25

Let

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

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

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

The integral of the right hand side can be written as

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

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

$$\mathbf{0} = p(\mathbf{x}) (\mathbf{y}(\mathbf{x}) - E_t(\mathbf{t} | \mathbf{x})). \quad (1.193)$$

Therefore,

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

For a single target variable t , it reduces to

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

1.26

Let

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

The right hand side can be written as

$$\iint \|\mathbf{y}(\mathbf{x}) - E(\mathbf{t}|\mathbf{x}) + E(\mathbf{t}|\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} dt = I_1 + 2I_2 + I_3, \quad (1.197)$$

where

$$\begin{aligned} I_1 &= \iint \|\mathbf{y}(\mathbf{x}) - E(\mathbf{t}|\mathbf{x})\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} dt, \\ I_2 &= \iint (\mathbf{y}(\mathbf{x}) - E(\mathbf{t}|\mathbf{x}))^\top (E(\mathbf{t}|\mathbf{x}) - \mathbf{t}) p(\mathbf{x}, \mathbf{t}) d\mathbf{x} dt, \\ I_3 &= \iint \|E(\mathbf{t}|\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} dt. \end{aligned} \quad (1.198)$$

The expression of I_1 can be written as

$$\begin{aligned} &\int \|\mathbf{y}(\mathbf{x}) - E(\mathbf{t}|\mathbf{x})\|^2 \left(\int p(\mathbf{x}, \mathbf{t}) dt \right) d\mathbf{x} \\ &= \int \|\mathbf{y}(\mathbf{x}) - E(\mathbf{t}|\mathbf{x})\|^2 p(\mathbf{x}) d\mathbf{x}. \end{aligned} \quad (1.199)$$

The expression of I_2 can be written as

$$\int (\mathbf{y}(\mathbf{x}) - E(\mathbf{t}|\mathbf{x}))^\top \left(\int (E(\mathbf{t}|\mathbf{x}) - \mathbf{t}) p(\mathbf{t}|\mathbf{x}) dt \right) p(\mathbf{x}) d\mathbf{x}. \quad (1.200)$$

We have

$$\int (E(\mathbf{t}|\mathbf{x}) - \mathbf{t}) p(\mathbf{t}|\mathbf{x}) dt = E(\mathbf{t}|\mathbf{x}) \int p(\mathbf{t}|\mathbf{x}) dt - \int t p(\mathbf{t}|\mathbf{x}) dt. \quad (1.201)$$

The right hand side can be written as

$$E(\mathbf{t}|\mathbf{x}) - E(\mathbf{t}|\mathbf{x}) = 0. \quad (1.202)$$

The expression of I_3 can be written as

$$\int \left(\int \|\mathbf{t} - E(\mathbf{t}|\mathbf{x})\|^2 p(\mathbf{t}|\mathbf{x}) dt \right) p(\mathbf{x}) d\mathbf{x} = \int \text{var}(\mathbf{t}|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \quad (1.203)$$

Then,

$$E L(\mathbf{t}, \mathbf{y}(\mathbf{x})) = \int \|\mathbf{y}(\mathbf{x}) - E(\mathbf{t}|\mathbf{x})\|^2 p(\mathbf{x}) d\mathbf{x} + \int \text{var}(\mathbf{t}|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \quad (1.204)$$

Therefore,

$$\underset{\mathbf{y}(\mathbf{x})}{\operatorname{argmin}} E L(\mathbf{t}, \mathbf{y}(\mathbf{x})) = E(\mathbf{t}|\mathbf{x}). \quad (1.205)$$

1.27 (Incomplete)

(a)

Let

$$\mathbb{E} L_q = \iint |y(\mathbf{x}) - t|^q p(\mathbf{x}, t) d\mathbf{x} dt. \quad (1.206)$$

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

$$0 = qp(\mathbf{x}) \int |y(\mathbf{x}) - t|^{q-1} \text{sign}(y(\mathbf{x}) - t) p(t|\mathbf{x}) dt. \quad (1.207)$$

Therefore,

$$\begin{aligned} & \underset{y(\mathbf{x})}{\operatorname{argmin}} \mathbb{E} L_q \\ &= \left\{ y(\mathbf{x}) \mid \int |y(\mathbf{x}) - t|^{q-1} \text{sign}(y(\mathbf{x}) - t) p(t|\mathbf{x}) dt = 0 \right\}. \end{aligned} \quad (1.208)$$

(b)

We have

$$\mathbb{E} L_1 = \int \left(\int \text{sign}(y(\mathbf{x}) - t) p(t|\mathbf{x}) dt \right) p(\mathbf{x}) d\mathbf{x}. \quad (1.209)$$

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

$$\int_{y(\mathbf{x})}^{\infty} p(t|\mathbf{x}) dt - \int_{-\infty}^{y(\mathbf{x})} p(t|\mathbf{x}) dt. \quad (1.210)$$

Therefore,

$$\underset{y(\mathbf{x})}{\operatorname{argmin}} \mathbb{E} L_1 = \text{median}(t|\mathbf{x}). \quad (1.211)$$

(c)

We have

$$\lim_{q \rightarrow 0} \left(\underset{y(\mathbf{x})}{\operatorname{argmin}} \mathbb{E} L_q \right) = \text{mode}(t|\mathbf{x})? \quad (1.212)$$

1.28

(a)

Let us assume that

$$p(x, y) = p(x)p(y) \Rightarrow h(x, y) = h(x) + h(y). \quad (1.213)$$

Then,

$$h(p^2) = 2h(p). \quad (1.214)$$

Let us assume that, for a positive integer n ,

$$h(p^n) = nh(p). \quad (1.215)$$

Then, by the first assumption,

$$h(p^{n+1}) = h(p^n) + h(p), \quad (1.216)$$

so that

$$h(p^{n+1}) = (n+1)h(p). \quad (1.217)$$

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

(b)

For positive integers m and n ,

$$h(p^n) = h(p^{\frac{n}{m}m}). \quad (1.218)$$

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 $mh(p^{\frac{n}{m}})$.

Therefore,

$$h(p^{\frac{n}{m}}) = \frac{n}{m}h(p). \quad (1.219)$$

(c)

By the continuity, for a positive real number a ,

$$h(p^a) = ah(p). \quad (1.220)$$

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

$$(p \ln p)h'(p) = h(p). \quad (1.221)$$

Then,

$$\int \frac{h'(p)}{h(p)} dp = \int \frac{1}{p \ln p} dp + \text{const.} \quad (1.222)$$

Ignoring 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,

$$h(p) \propto \ln p. \quad (1.223)$$

1.29

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

$$H(x) = - \sum_{m=1}^M p(x_m) \ln p(x_m), \quad (1.224)$$

where

$$\sum_{m=1}^M p(x_m) = 1. \quad (1.225)$$

By the Jensen's inequality,

$$\sum_{m=1}^M p(x_m) \ln \frac{1}{p(x_m)} \leq \ln \left(\sum_{m=1}^M 1 \right). \quad (1.226)$$

Therefore,

$$H(x) \leq \ln M. \quad (1.227)$$

1.30

Let

$$\begin{aligned} p(x) &= \mathcal{N}(x|\mu, \sigma^2), \\ q(x) &= \mathcal{N}(x|m, s^2). \end{aligned} \quad (1.228)$$

Then, the Kullback-Leibler divergence is given by

$$\text{KL}(p||q) = - \int p(x) \ln \frac{q(x)}{p(x)} dx. \quad (1.229)$$

The right hand side can be written as

$$\begin{aligned} & - \int_{-\infty}^{\infty} p(x) \ln \frac{(2\pi s^2)^{-\frac{1}{2}} \exp\left(-\frac{(x-m)^2}{2s^2}\right)}{(2\pi\sigma^2)^{-\frac{1}{2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)} dx \\ &= - \int_{-\infty}^{\infty} p(x) \left(-\frac{1}{2} \ln \frac{s^2}{\sigma^2} - \frac{(x-m)^2}{2s^2} + \frac{(x-\mu)^2}{2\sigma^2} \right) dx. \end{aligned} \quad (1.230)$$

The right hand side can be written as

$$\ln \frac{s}{\sigma} \int_{-\infty}^{\infty} p(x) dx + \frac{1}{2s^2} \int_{-\infty}^{\infty} (x-m)^2 p(x) dx - \frac{1}{2\sigma^2} \int_{-\infty}^{\infty} (x-\mu)^2 p(x) dx. \quad (1.231)$$

The integral of the second term can be written as

$$\begin{aligned} & \int_{-\infty}^{\infty} (x - \mu + \mu - m)^2 p(x) dx \\ &= \int_{-\infty}^{\infty} (x - \mu)^2 p(x) dx + 2(\mu - m) \int_{-\infty}^{\infty} (x - \mu) p(x) dx \\ & \quad + (\mu - m)^2 \int_{-\infty}^{\infty} p(x) dx. \end{aligned} \quad (1.232)$$

Therefore,

$$\text{KL}(p||q) = \ln \frac{s}{\sigma} + \frac{\sigma^2 + (\mu - m)^2}{2s^2} - \frac{1}{2}. \quad (1.233)$$

1.31

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

$$\begin{aligned} H(\mathbf{x}) &= - \int p(\mathbf{x}) \ln p(\mathbf{x}) d\mathbf{x}, \\ H(\mathbf{y}) &= - \int p(\mathbf{y}) \ln p(\mathbf{y}) d\mathbf{y}, \\ H(\mathbf{x}, \mathbf{y}) &= - \iint p(\mathbf{x}, \mathbf{y}) \ln p(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}. \end{aligned} \quad (1.234)$$

The expressions of $H(\mathbf{x})$ and $H(\mathbf{y})$ can be written as

$$\begin{aligned} & - \int \left(\int p(\mathbf{x}, \mathbf{y}) d\mathbf{y} \right) \ln p(\mathbf{x}) d\mathbf{x}, \\ & - \int \left(\int p(\mathbf{x}, \mathbf{y}) d\mathbf{x} \right) \ln p(\mathbf{y}) d\mathbf{y}. \end{aligned} \quad (1.235)$$

Then,

$$H(\mathbf{x}) + H(\mathbf{y}) - H(\mathbf{x}, \mathbf{y}) = - \iint p(\mathbf{x}, \mathbf{y}) \ln \left(\frac{p(\mathbf{x})p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} \right) d\mathbf{x}d\mathbf{y}. \quad (1.236)$$

We have

$$\iint p(\mathbf{x}, \mathbf{y}) d\mathbf{x}d\mathbf{y} = 1. \quad (1.237)$$

Then, by the Jensen's inequality,

$$- \iint p(\mathbf{x}, \mathbf{y}) \ln \left(\frac{p(\mathbf{x})p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} \right) d\mathbf{x}d\mathbf{y} \geq - \ln \left(\iint p(\mathbf{x})p(\mathbf{y}) d\mathbf{x}d\mathbf{y} \right). \quad (1.238)$$

The right hand side can be written as

$$- \ln \left(\int p(\mathbf{x}) d\mathbf{x} \int p(\mathbf{y}) d\mathbf{y} \right) = 0. \quad (1.239)$$

Therefore,

$$H(\mathbf{x}, \mathbf{y}) \leq H(\mathbf{x}) + H(\mathbf{y}). \quad (1.240)$$

1.32

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

$$\mathbf{y} = \mathbf{Ax}, \quad (1.241)$$

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

$$\int p_x(\mathbf{x}) d\mathbf{x} = \int p_x(\mathbf{A}^{-1}\mathbf{y}) |\det \mathbf{A}^{-1}| d\mathbf{y}. \quad (1.242)$$

Then,

$$p_y(\mathbf{y}) = p_x(\mathbf{A}^{-1}\mathbf{y}) |\det \mathbf{A}^{-1}|. \quad (1.243)$$

We have

$$H(\mathbf{y}) = - \int p_y(\mathbf{y}) \ln p_y(\mathbf{y}) d\mathbf{y}. \quad (1.244)$$

The right hand side can be written as

$$\begin{aligned} & - \int p_y(\mathbf{y}) \ln (p_x(\mathbf{A}^{-1}\mathbf{y}) |\det \mathbf{A}^{-1}|) d\mathbf{y} \\ &= - \int p_y(\mathbf{y}) \ln p_x(\mathbf{A}^{-1}\mathbf{y}) d\mathbf{y} + \ln |\det \mathbf{A}| \int p_y(\mathbf{y}) d\mathbf{y}. \end{aligned} \quad (1.245)$$

The first term can be written as

$$-\left|\det \mathbf{A}^{-1}\right| \int p_x(\mathbf{A}^{-1} \mathbf{y}) \ln p_x(\mathbf{A}^{-1} \mathbf{y}) d\mathbf{y}. \quad (1.246)$$

By the transformation

$$\mathbf{x} = \mathbf{A}^{-1} \mathbf{y}, \quad (1.247)$$

it can be written as

$$-\int p_x(\mathbf{x}) \ln p_x(\mathbf{x}) d\mathbf{x} = H(\mathbf{x}). \quad (1.248)$$

Therefore,

$$H(\mathbf{y}) = H(\mathbf{x}) + \ln |\det \mathbf{A}|. \quad (1.249)$$

1.33

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

$$H(y|x) = -\sum_{k=1}^K \sum_{l=1}^L p(x_k, y_l) \ln p(y_l|x_k). \quad (1.250)$$

If

$$H(y|x) = 0, \quad (1.251)$$

then

$$0 = -\sum_{k=1}^K p(x_k) \left(\sum_{l=1}^L p(y_l|x_k) \ln p(y_l|x_k) \right). \quad (1.252)$$

We have

$$\begin{aligned} p(x_k) &\geq 0, \\ p(y_l|x_k) \ln p(y_l|x_k) &\leq 0. \end{aligned} \quad (1.253)$$

Then, the equation reduces to

$$p(y_l|x_k) \ln p(y_l|x_k) = 0. \quad (1.254)$$

Then,

$$p(y_l|x_k) = \begin{cases} 1, \\ 0. \end{cases} \quad (1.255)$$

We have

$$\sum_{l=1}^L p(y_l|x_k) = 1. \quad (1.256)$$

Therefore,

$$p(y_l|x_k) = \begin{cases} 1, & \text{if } K = 1, \\ 0, & \text{otherwise.} \end{cases} \quad (1.257)$$

1.34

Let x be a variable. We have

$$H(x) = - \int_{-\infty}^{\infty} p(x) \ln p(x) dx. \quad (1.258)$$

In order to maximise $H(x)$ with the constraints

$$\begin{aligned} \int_{-\infty}^{\infty} p(x) dx &= 1, \\ \int_{-\infty}^{\infty} xp(x) dx &= \mu, \\ \int_{-\infty}^{\infty} (x - \mu)^2 p(x) dx &= \sigma^2, \end{aligned} \quad (1.259)$$

let

$$\begin{aligned} L(p) = H(x) + \lambda_1 &\left(\int_{-\infty}^{\infty} p(x) dx - 1 \right) + \lambda_2 \left(\int_{-\infty}^{\infty} xp(x) dx - \mu \right) \\ &+ \lambda_3 \left(\int_{-\infty}^{\infty} (x - \mu)^2 p(x) dx - \sigma^2 \right). \end{aligned} \quad (1.260)$$

Setting the variation with respect to p to zero gives

$$0 = -\ln p - 1 + \lambda_1 + \lambda_2 x + \lambda_3 (x - \mu)^2. \quad (1.261)$$

Then,

$$p(x) = \exp(-1 + \lambda_1 + \lambda_2 x + \lambda_3 (x - \mu)^2), \quad (1.262)$$

so that

$$p(x) = c \exp(-q(x)), \quad (1.263)$$

where

$$\begin{aligned} c &= \exp \left(-1 + \lambda_1 - \frac{\lambda_2^2}{4\lambda_3} \right), \\ q(x) &= -\lambda_3 \left(x - \left(\mu - \frac{\lambda_2}{2\lambda_3} \right) \right)^2. \end{aligned} \quad (1.264)$$

Substituting it to the constraints gives

$$\begin{aligned} c \int_{-\infty}^{\infty} \exp(-q(x)) dx &= 1, \\ c \int_{-\infty}^{\infty} x \exp(-q(x)) dx &= \mu, \\ c \int_{-\infty}^{\infty} (x - \mu)^2 \exp(-q(x)) dx &= \sigma^2. \end{aligned} \quad (1.265)$$

By the transformation

$$y^2 = q(x), \quad (1.266)$$

they can be written as

$$\begin{aligned} c \int_{-\infty}^{\infty} \exp(-y^2) (-\lambda_3)^{-\frac{1}{2}} dy &= 1, \\ c \int_{-\infty}^{\infty} \left((-\lambda_3)^{-\frac{1}{2}} y + \mu - \frac{\lambda_2}{2\lambda_3} \right) \exp(-y^2) (-\lambda_3)^{-\frac{1}{2}} dy &= \mu, \\ c \int_{-\infty}^{\infty} \left((-\lambda_3)^{-\frac{1}{2}} y - \frac{\lambda_2}{2\lambda_3} \right)^2 \exp(-y^2) (-\lambda_3)^{-\frac{1}{2}} dy &= \sigma^2. \end{aligned} \quad (1.267)$$

We have

$$\begin{aligned} \int_{-\infty}^{\infty} \exp(-y^2) dy &= \Gamma\left(\frac{1}{2}\right), \\ \int_{-\infty}^{\infty} y \exp(-y^2) dy &= 0, \\ \int_{-\infty}^{\infty} y^2 \exp(-y^2) dy &= \Gamma\left(\frac{3}{2}\right), \end{aligned} \quad (1.268)$$

Then,

$$\begin{aligned} c(-\lambda_3)^{-\frac{1}{2}}\Gamma\left(\frac{1}{2}\right) &= 1, \\ c\left(\mu - \frac{\lambda_2}{2\lambda_3}\right)(-\lambda_3)^{-\frac{1}{2}}\Gamma\left(\frac{1}{2}\right) &= \mu, \\ c\left((- \lambda_3)^{-\frac{3}{2}}\Gamma\left(\frac{3}{2}\right) + (-\lambda_3)^{-\frac{1}{2}}\frac{\lambda_2^2}{4\lambda_3^2}\Gamma\left(\frac{1}{2}\right)\right) &= \sigma^2. \end{aligned} \quad (1.269)$$

Then,

$$\begin{aligned} \lambda_1 &= 1 - \frac{1}{2}\ln(2\pi\sigma^2), \\ \lambda_2 &= 0, \\ \lambda_3 &= -\frac{1}{2\sigma^2}. \end{aligned} \quad (1.270)$$

Therefore,

$$p(x) = (2\pi\sigma^2)^{-\frac{1}{2}}\exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right). \quad (1.271)$$

1.35

Let x be a variable such that

$$p(x) = \mathcal{N}(x|\mu, \sigma^2). \quad (1.272)$$

Then,

$$H(x) = -\int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) \ln \mathcal{N}(x|\mu, \sigma^2) dx. \quad (1.273)$$

The right hand side can be written as

$$\begin{aligned} &- \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) \left(-\frac{1}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}(x - \mu)^2 \right) dx \\ &= \frac{1}{2}\ln(2\pi\sigma^2) \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) dx \\ &\quad + \frac{1}{2\sigma^2} \int_{-\infty}^{\infty} (x - \mu)^2 \mathcal{N}(x|\mu, \sigma^2) dx. \end{aligned} \quad (1.274)$$

Therefore,

$$H(x) = \frac{1}{2}(1 + \ln(2\pi\sigma^2)). \quad (1.275)$$

1.36 (Incomplete)

Let f be a strictly convex function. Then,

$$f(\lambda a + (1 - \lambda)b) \leq \lambda f(a) + (1 - \lambda)f(b), \quad (1.276)$$

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

$$x = \lambda a + (1 - \lambda)b. \quad (1.277)$$

Then, the inequality can be written as

$$f(x) \leq \frac{b - x}{b - a} f(a) + \frac{x - a}{b - a} f(b). \quad (1.278)$$

Let

$$g(x) = \frac{b - x}{b - a} f(a) + \frac{x - a}{b - a} f(b) - f(x). \quad (1.279)$$

Then,

$$g(x) \geq 0. \quad (1.280)$$

Additionally, for $x > a$,

$$g(x) = (x - a) \left(\frac{f(b) - f(a)}{b - a} - \frac{f(x) - f(a)}{x - a} \right). \quad (1.281)$$

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

$$\begin{aligned} f'(c) &= \frac{f(b) - f(a)}{b - a}, \\ f'(y) &= \frac{f(x) - f(a)}{x - a}. \end{aligned} \quad (1.282)$$

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

$$f'(y) \leq f'(c). \quad (1.283)$$

1.37

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

$$H(\mathbf{x}, \mathbf{y}) = - \iint p(\mathbf{x}, \mathbf{y}) \ln p(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}. \quad (1.284)$$

The right hand side can be written as

$$\begin{aligned} & - \iint p(\mathbf{x}, \mathbf{y}) (\ln p(\mathbf{y}|\mathbf{x}) + \ln p(\mathbf{x})) d\mathbf{x}d\mathbf{y} \\ &= - \iint p(\mathbf{x}, \mathbf{y}) \ln p(\mathbf{y}|\mathbf{x}) d\mathbf{x}d\mathbf{y} - \int \left(\int p(\mathbf{x}, \mathbf{y}) d\mathbf{y} \right) \ln p(\mathbf{x}) d\mathbf{x}. \end{aligned} \quad (1.285)$$

We have

$$\begin{aligned} H(\mathbf{y}|\mathbf{x}) &= - \iint p(\mathbf{x}, \mathbf{y}) \ln p(\mathbf{y}|\mathbf{x}) d\mathbf{x}d\mathbf{y}, \\ H(\mathbf{x}) &= - \int p(\mathbf{x}) \ln p(\mathbf{x}) d\mathbf{x}. \end{aligned} \quad (1.286)$$

Therefore,

$$H(\mathbf{x}, \mathbf{y}) = H(\mathbf{y}|\mathbf{x}) + H(\mathbf{x}). \quad (1.287)$$

1.38

Let f be a strictly convex function. Then,

$$f(\lambda x_1 + (1 - \lambda)x_2) \leq \lambda f(x_1) + (1 - \lambda)f(x_2), \quad (1.288)$$

where

$$0 \leq \lambda \leq 1. \quad (1.289)$$

Let us assume that

$$f \left(\sum_{m=1}^M \lambda_m x_m \right) \leq \sum_{m=1}^M \lambda_m f(x_m), \quad (1.290)$$

where

$$\begin{aligned} \sum_{m=1}^M \lambda_m &= 1, \\ \lambda_m &\geq 0. \end{aligned} \quad (1.291)$$

We have

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

where

$$\sum_{m=1}^{M+1} \lambda_m = 1, \quad (1.293)$$

$$\lambda_m \geq 0.$$

By the assumption,

$$f\left(\sum_{m=1}^M \frac{\lambda_m}{1 - \lambda_{M+1}} x_m\right) \leq \sum_{m=1}^M \frac{\lambda_m}{1 - \lambda_{M+1}} f(x_m). \quad (1.294)$$

Then,

$$f\left(\sum_{m=1}^{M+1} \lambda_m x_m\right) \leq \lambda_{M+1} f(x_{M+1}) + (1 - \lambda_{M+1}) \sum_{m=1}^M \frac{\lambda_m}{1 - \lambda_{M+1}} f(x_m), \quad (1.295)$$

so that

$$f\left(\sum_{m=1}^{M+1} \lambda_m x_m\right) \leq \sum_{m=1}^{M+1} \lambda_m f(x_m). \quad (1.296)$$

Therefore, the assumption is proved by induction on M .

1.39

Let x and y be two binary variables where

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

(a)

We have

$$H(x) = - \sum_x p(x) \ln p(x). \quad (1.298)$$

We have

$$\begin{aligned} p(x = 0) &= p(x = 0, y = 0) + p(x = 0, y = 1), \\ p(x = 1) &= p(x = 1, y = 0) + p(x = 1, y = 1). \end{aligned} \quad (1.299)$$

Then,

$$\begin{aligned} p(x = 0) &= \frac{2}{3}, \\ p(x = 1) &= \frac{1}{3}. \end{aligned} \quad (1.300)$$

Therefore,

$$H(x) = \ln 3 - \frac{2}{3} \ln 2. \quad (1.301)$$

(b)

We have

$$H(y) = - \sum_y p(y) \ln p(y). \quad (1.302)$$

We have

$$\begin{aligned} p(y = 0) &= p(x = 0, y = 0) + p(x = 1, y = 0), \\ p(y = 1) &= p(x = 0, y = 1) + p(x = 1, y = 1). \end{aligned} \quad (1.303)$$

Then,

$$\begin{aligned} p(y = 0) &= \frac{1}{3}, \\ p(y = 1) &= \frac{2}{3}. \end{aligned} \quad (1.304)$$

Therefore,

$$H(y) = \ln 3 - \frac{2}{3} \ln 2. \quad (1.305)$$

(c)

We have

$$H(y|x) = - \sum_{x,y} p(x, y) \ln p(y|x). \quad (1.306)$$

By the Bayes' theorem,

$$\begin{aligned}
 p(y = 0|x = 0) &= \frac{p(x = 0, y = 0)}{p(x = 0)}, \\
 p(y = 0|x = 1) &= \frac{p(x = 1, y = 0)}{p(x = 1)}, \\
 p(y = 1|x = 0) &= \frac{p(x = 0, y = 1)}{p(x = 0)}, \\
 p(y = 1|x = 1) &= \frac{p(x = 1, y = 1)}{p(x = 1)}. \tag{1.307}
 \end{aligned}$$

Then,

$$\begin{aligned}
 p(y = 0|x = 0) &= \frac{1}{2}, \\
 p(y = 0|x = 1) &= 0, \\
 p(y = 1|x = 0) &= \frac{1}{2}, \\
 p(y = 1|x = 1) &= 1. \tag{1.308}
 \end{aligned}$$

Therefore,

$$H(y|x) = \frac{2}{3} \ln 2. \tag{1.309}$$

(d)

We have

$$H(x|y) = - \sum_{x,y} p(x, y) \ln p(x|y). \tag{1.310}$$

By the Bayes' theorem,

$$\begin{aligned}
 p(x = 0|y = 0) &= \frac{p(x = 0, y = 0)}{p(y = 0)}, \\
 p(x = 0|y = 1) &= \frac{p(x = 0, y = 1)}{p(y = 1)}, \\
 p(x = 1|y = 0) &= \frac{p(x = 1, y = 0)}{p(y = 0)}, \\
 p(x = 1|y = 1) &= \frac{p(x = 1, y = 1)}{p(y = 1)}. \tag{1.311}
 \end{aligned}$$

Then,

$$\begin{aligned} p(x=0|y=0) &= 1, \\ p(x=0|y=1) &= \frac{1}{2}, \\ p(x=1|y=0) &= 0, \\ p(x=1|y=1) &= \frac{1}{2}. \end{aligned} \tag{1.312}$$

Therefore,

$$H(x|y) = \frac{2}{3} \ln 2. \tag{1.313}$$

(e)

We have

$$H(x, y) = - \sum_{x,y} p(x, y) \ln p(x, y). \tag{1.314}$$

Therefore,

$$H(x, y) = \ln 3. \tag{1.315}$$

(f)

We have

$$I(x, y) = - \sum_{x,y} p(x, y) \ln \frac{p(x)p(y)}{p(x, y)}. \tag{1.316}$$

The right hand side can be written as

$$H(x) + H(y) - H(x, y). \tag{1.317}$$

Therefore,

$$I(x, y) = \ln 3 - \frac{4}{3} \ln 2. \tag{1.318}$$

1.40

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

$$\begin{aligned} \sum_{m=1}^M \lambda_m &= 1, \\ \lambda_m &\geq 0, \\ x_m &> 0. \end{aligned} \tag{1.319}$$

By the Jensen's inequality,

$$\sum_{m=1}^M \lambda_m \ln x_m \leq \ln \left(\sum_{m=1}^M \lambda_m x_m \right), \quad (1.320)$$

so that

$$\prod_{m=1}^M x_m^{\lambda_m} \leq \sum_{m=1}^M \lambda_m x_m. \quad (1.321)$$

Substituting

$$\lambda_m = \frac{1}{M} \quad (1.322)$$

to the inequality gives

$$\left(\prod_{m=1}^M x_m \right)^{\frac{1}{M}} \leq \frac{1}{M} \sum_{m=1}^M x_m. \quad (1.323)$$

1.41

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

(a)

We have

$$I(\mathbf{x}, \mathbf{y}) = - \iint p(\mathbf{x}, \mathbf{y}) \ln \left(\frac{p(\mathbf{x})p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} \right) d\mathbf{x}d\mathbf{y}. \quad (1.324)$$

The right hand side can be written as

$$\begin{aligned} & - \iint p(\mathbf{x}, \mathbf{y}) \left(\ln p(\mathbf{x}) + \ln \left(\frac{p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} \right) \right) d\mathbf{x}d\mathbf{y} \\ & = - \iint p(\mathbf{x}, \mathbf{y}) (\ln p(\mathbf{x}) - \ln p(\mathbf{x}|\mathbf{y})) d\mathbf{x}d\mathbf{y}. \end{aligned} \quad (1.325)$$

The right hand side can be written as

$$- \int \left(\int p(\mathbf{x}, \mathbf{y}) d\mathbf{y} \right) \ln p(\mathbf{x}) d\mathbf{x} + \iint p(\mathbf{x}, \mathbf{y}) \ln p(\mathbf{x}|\mathbf{y}) d\mathbf{x}d\mathbf{y}. \quad (1.326)$$

Therefore,

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

(b)

We have

$$I(\mathbf{x}, \mathbf{y}) = I(\mathbf{y}, \mathbf{x}). \quad (1.328)$$

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

$$H(\mathbf{y}) - H(\mathbf{y}|\mathbf{x}). \quad (1.329)$$

Therefore,

$$I(\mathbf{x}, \mathbf{y}) = H(\mathbf{y}) - H(\mathbf{y}|\mathbf{x}). \quad (1.330)$$

2 Probability Distributions

2.1

Let x be a variable such that

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

(a)

We have

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

Therefore,

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

(b)

We have

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

Then,

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

We have

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

Therefore,

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

(c)

We have

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

Therefore,

$$H(x) = -\mu \ln \mu - (1 - \mu) \ln(1 - \mu). \quad (2.9)$$

2.2

Let x be a variable such that

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

(a)

We have

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

Therefore,

$$\sum_x p(x) = 1. \quad (2.12)$$

(b)

We have

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

The right hand sides can be written as

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

Then,

$$\begin{aligned} E x &= \mu, \\ E x^2 &= 1. \end{aligned} \quad (2.15)$$

We have

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

Therefore,

$$\text{var } x = 1 - \mu^2. \quad (2.17)$$

(c)

We have

$$H(x) = - \sum_x p(x|\mu) \ln p(x|\mu). \quad (2.18)$$

Therefore,

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

2.3

(a)

We have

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

Then,

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

The right hand side can be written as

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

Therefore,

$$\binom{N}{n} + \binom{N}{n-1} = \binom{N+1}{n}. \quad (2.23)$$

(b)

We have

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

Let us assume that

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

Then,

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

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

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

Then,

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

Therefore, the assumption is proved by induction on N .

(c)

Let n be a variable such that

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

Then,

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

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

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

Therefore,

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

2.4

Let n be a variable such that

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

(a)

We have

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

By 2.3(c),

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

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

$$\frac{1}{\mu} \sum_{n=0}^N n p(n) = \frac{1}{\mu} \mathbb{E} n. \quad (2.37)$$

Since

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

the second term can be written as

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

Therefore,

$$\mathbb{E} n = N\mu. \quad (2.40)$$

(b)

By 2.3(c),

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

Taking the second derivative with respect to μ gives

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

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

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

Since

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

the second and third terms can be written as

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

Then,

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

We have

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

Therefore,

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

2.5

We have

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

By the transformation

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

the right hand side can be written as

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

By the transformation

$$x = t\mu, \quad (2.52)$$

the right hand side can be written as

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

Then,

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

Therefore,

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

2.6

Let μ be a variable such that

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

(a)

We have

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

By 2.5,

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

Therefore,

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

(b)

We have

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

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

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

Therefore,

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

(c)

We have

$$\ln p(\mu) = \ln \Gamma(a+b) - \ln \Gamma(a) - \ln \Gamma(b) + (a-1) \ln \mu + (b-1) \ln(1-\mu). \quad (2.63)$$

Setting the derivative of $\ln p$ with respect to μ to zero gives

$$0 = \ln \left(\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \right) \left(\frac{a-1}{\mu} - \frac{b-1}{1-\mu} \right). \quad (2.64)$$

Therefore,

$$\text{mode } \mu = \begin{cases} \frac{a-1}{a+b-2}, & \text{if } a \geq 1 \text{ and } b \geq 1, \\ \text{none,} & \text{otherwise.} \end{cases} \quad (2.65)$$

2.7

Let m and l be variables such that

$$\begin{aligned} p(m, l | \mu) &= \binom{m+l}{m} \mu^m (1-\mu)^l, \\ p(\mu) &= \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \mu^{a-1} (1-\mu)^{b-1}. \end{aligned} \quad (2.66)$$

By 2.6,

$$E \mu = \frac{a}{a+b}. \quad (2.67)$$

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

$$0 = \binom{m+l}{m} \mu^m (1-\mu)^l \left(\frac{m}{\mu} + \frac{l}{1-\mu} \right). \quad (2.68)$$

Then, the maximum likelihood solution for μ is given by

$$\mu_{ML} = \frac{m}{m+l}. \quad (2.69)$$

By the Bayes' theorem,

$$p(\mu | m, l) = \frac{p(m, l | \mu) p(\mu)}{p(m, l)}. \quad (2.70)$$

By 2.5, the right hand side can be written as

$$p(\mu | m, l) = \frac{\Gamma(m+l+a+b)}{\Gamma(m+a)\Gamma(l+b)} \mu^{m+a-1} (1-\mu)^{l+b-1}. \quad (2.71)$$

By 2.6,

$$E(\mu | m, l) = \frac{m+a}{m+l+a+b}. \quad (2.72)$$

Therefore,

$$E(\mu | m, l) = \lambda \mu_{ML} + (1-\lambda) E \mu, \quad (2.73)$$

where

$$\lambda = \frac{m+l}{m+l+a+b}. \quad (2.74)$$

2.8

Let x and y be variables.

(a)

We have

$$\mathbb{E} x = \int xp(x)dx. \quad (2.75)$$

The right hand side can be written as

$$\int x \left(\int p(x,y)dy \right) dx = \int \left(\int xp(x|y)dx \right) p(y)dy. \quad (2.76)$$

Therefore,

$$\mathbb{E} x = \mathbb{E} (\mathbb{E}(x|y)). \quad (2.77)$$

(b)

We have

$$\text{var } x = \mathbb{E} (x - \mathbb{E} x)^2. \quad (2.78)$$

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

$$\begin{aligned} & \mathbb{E} (\mathbb{E} ((x - \mathbb{E} x)^2|y)) \\ &= \mathbb{E} (\mathbb{E} ((f(x,y) + g(y))^2|y)), \end{aligned} \quad (2.79)$$

where

$$\begin{aligned} f(x,y) &= x - \mathbb{E}(x|y), \\ g(y) &= \mathbb{E}(x|y) - \mathbb{E} x. \end{aligned} \quad (2.80)$$

The right hand side can be written as $I_1 + 2I_2 + I_3$, where

$$\begin{aligned} I_1 &= \mathbb{E} (\mathbb{E} (f^2(x,y)|y)), \\ I_2 &= \mathbb{E} (\mathbb{E} (f(x,y)g(y)|y)), \\ I_3 &= \mathbb{E} (g^2(y)). \end{aligned} \quad (2.81)$$

We have

$$\text{var}(x|y) = \mathbb{E} (f^2(x,y)|y). \quad (2.82)$$

Then, the expression of I_1 can be written as

$$\mathbb{E} (\text{var}(x|y)). \quad (2.83)$$

We have

$$\mathbb{E}(f(x, y)|y) = 0. \quad (2.84)$$

Then, the expression of I_2 can be written as

$$\mathbb{E}(\mathbb{E}(f(x, y)|y)g(y)) = 0. \quad (2.85)$$

By (a),

$$\mathbb{E}(\mathbb{E}(x|y)) = \mathbb{E}x. \quad (2.86)$$

Then, the expression of I_3 can be written as

$$\text{var}(\mathbb{E}(x|y)). \quad (2.87)$$

Therefore,

$$\text{var } x = \mathbb{E}(\text{var}(x|y)) + \text{var}(\mathbb{E}(x|y)). \quad (2.88)$$

2.9

For a vector μ in 2 dimensions, by 2.5,

$$\int_{\substack{\mu_1+\mu_2=1 \\ \mu_1 \geq 0, \mu_2 \geq 0}} \mu_1^{\alpha_1-1} \mu_2^{\alpha_2-1} d\mu = \frac{\Gamma(\alpha_1)\Gamma(\alpha_2)}{\Gamma(\alpha_1 + \alpha_2)}. \quad (2.89)$$

For a vector μ in K dimensions, let us assume that

$$\int_{\substack{\sum_{k=1}^K \mu_k=1 \\ \mu_k \geq 0}} \prod_{k=1}^K \mu_k^{\alpha_k-1} d\mu = \frac{\prod_{k=1}^K \Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^K \alpha_k)}. \quad (2.90)$$

For a vector μ in $K+1$ dimensions, let

$$\mu' = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_{K-1} \\ \mu_K + \mu_{K+1} \end{bmatrix}. \quad (2.91)$$

Then,

$$\begin{aligned} & \int_{\substack{\sum_{k=1}^{K+1} \mu_k=1 \\ \mu_k \geq 0}} \prod_{k=1}^{K+1} \mu_k^{\alpha_k-1} d\mu \\ &= \int_{\substack{\sum_{k=1}^K \mu'_k=1 \\ \mu'_k \geq 0}} \left(\prod_{k=1}^{K-1} \mu'_k^{\alpha_k-1} \right) I(\mu'_K) d\mu', \end{aligned} \quad (2.92)$$

where

$$I(\mu'_K) = \int_0^{\mu'_K} (\mu'_K - \mu_{K+1})^{\alpha_K-1} \mu_{K+1}^{\alpha_{K+1}-1} d\mu_{K+1}. \quad (2.93)$$

By the transformation

$$x = \frac{\mu_{K+1}}{\mu'_K}, \quad (2.94)$$

the expression of $I(\mu'_K)$ can be written as

$$\begin{aligned} & \int_0^1 (\mu'_K(1-x))^{\alpha_K-1} (\mu'_K x)^{\alpha_{K+1}-1} \mu'_K dx \\ &= \mu'^{\alpha_K+\alpha_{K+1}-1}_K \int_0^1 x^{\alpha_{K+1}-1} (1-x)^{\alpha_K-1} dx. \end{aligned} \quad (2.95)$$

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

$$\frac{\Gamma(\alpha_K)\Gamma(\alpha_{K+1})}{\Gamma(\alpha_K + \alpha_{K+1})}. \quad (2.96)$$

Then,

$$\begin{aligned} & \int_{\sum_{k=1}^{K+1} \mu_k=1 \atop \mu_k \geq 0} \prod_{k=1}^{K+1} \mu_k^{\alpha_k-1} d\boldsymbol{\mu} \\ &= \frac{\Gamma(\alpha_K)\Gamma(\alpha_{K+1})}{\Gamma(\alpha_K + \alpha_{K+1})} \int_{\sum_{k=1}^K \mu'_k=1 \atop \mu'_k \geq 0} \left(\prod_{k=1}^{K-1} \mu'_k^{\alpha_k-1} \right) \mu'^{\alpha_K+\alpha_{K+1}-1}_K d\boldsymbol{\mu}'. \end{aligned} \quad (2.97)$$

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

$$\frac{\left(\prod_{k=1}^{K-1} \Gamma(\alpha_k) \right) \Gamma(\alpha_K + \alpha_{K+1})}{\Gamma(\sum_{k=1}^{K+1} \alpha_k)}. \quad (2.98)$$

Then,

$$\int_{\sum_{k=1}^{K+1} \mu_k=1 \atop \mu_k \geq 0} \prod_{k=1}^{K+1} \mu_k^{\alpha_k-1} d\boldsymbol{\mu} = \frac{\prod_{k=1}^{K+1} \Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^{K+1} \alpha_k)}. \quad (2.99)$$

Therefore, the assumption is proved by induction on K .

2.10

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

$$p(\boldsymbol{\mu}) = \frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \prod_{k=1}^K \mu_k^{\alpha_k-1}. \quad (2.100)$$

We have

$$\begin{aligned} \mathbb{E} \mu_k &= \int \mu_k p(\boldsymbol{\mu}) d\boldsymbol{\mu}, \\ \mathbb{E} \mu_k^2 &= \int \mu_k^2 p(\boldsymbol{\mu}) d\boldsymbol{\mu}, \\ \mathbb{E} \mu_k \mu_{k'} &= \int \mu_k \mu_{k'} p(\boldsymbol{\mu}) d\boldsymbol{\mu}. \end{aligned} \quad (2.101)$$

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

$$\begin{aligned} \frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \frac{\frac{\Gamma(\alpha_k+1)}{\Gamma(\alpha_k)} \prod_{k=1}^K \Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^K \alpha_k + 1)} &= \frac{\alpha_k}{\sum_{k=1}^K \alpha_k}, \\ \frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \frac{\frac{\Gamma(\alpha_k+2)}{\Gamma(\alpha_k)} \prod_{k=1}^K \Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^K \alpha_k + 2)} &= \frac{\alpha_k(\alpha_k + 1)}{\sum_{k=1}^K \alpha_k (\sum_{k=1}^K \alpha_k + 1)}, \quad (2.102) \\ \frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \frac{\frac{\Gamma(\alpha_k+1)\Gamma(\alpha_{k'}+1)}{\Gamma(\alpha_k)\Gamma(\alpha_{k'})} \prod_{k=1}^K \Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^K \alpha_k + 2)} &= \frac{\alpha_k \alpha_{k'}}{\sum_{k=1}^K \alpha_k (\sum_{k=1}^K \alpha_k + 1)}. \end{aligned}$$

Then,

$$\begin{aligned} \mathbb{E} \mu_k &= \frac{\alpha_k}{\sum_{k=1}^K \alpha_k}, \\ \mathbb{E} \mu_k^2 &= \frac{\alpha_k(\alpha_k + 1)}{\sum_{k=1}^K \alpha_k (\sum_{k=1}^K \alpha_k + 1)}, \\ \mathbb{E} \mu_k \mu_{k'} &= \frac{\alpha_k \alpha_{k'}}{\sum_{k=1}^K \alpha_k (\sum_{k=1}^K \alpha_k + 1)}. \end{aligned} \quad (2.103)$$

We have

$$\begin{aligned} \text{var } \mu_k &= \mathbb{E} \mu_k^2 - (\mathbb{E} \mu_k)^2, \\ \text{cov}(\mu_k, \mu_{k'}) &= \mathbb{E} \mu_k \mu_{k'} - \mathbb{E} \mu_k \mathbb{E} \mu_{k'}. \end{aligned} \quad (2.104)$$

Therefore,

$$\begin{aligned}\text{var } \mu_k &= \frac{\alpha_k \left(\left(\sum_{k=1}^K \alpha_k \right) - \alpha_k \right)}{\left(\sum_{k=1}^K \alpha_k \right)^2 \left(\sum_{k=1}^K \alpha_k + 1 \right)}, \\ \text{cov}(\mu_k, \mu_{k'}) &= -\frac{\alpha_k \alpha_{k'}}{\left(\sum_{k=1}^K \alpha_k \right)^2 \left(\sum_{k=1}^K \alpha_k + 1 \right)}.\end{aligned}\quad (2.105)$$

2.11

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

$$p(\boldsymbol{\mu}) = \frac{\Gamma \left(\sum_{k=1}^K \alpha_k \right)}{\prod_{k=1}^K \Gamma(\alpha_k)} \prod_{k=1}^K \mu_k^{\alpha_k - 1}. \quad (2.106)$$

We have

$$\mathbb{E} \ln \mu_k = \int (\ln \mu_k) p(\boldsymbol{\mu}) d\boldsymbol{\mu}. \quad (2.107)$$

We have

$$\frac{\partial}{\partial \alpha_k} p(\boldsymbol{\mu}) = \left(\frac{\Gamma' \left(\sum_{k=1}^K \alpha_k \right)}{\Gamma \left(\sum_{k=1}^K \alpha_k \right)} - \frac{\Gamma'(\alpha_k)}{\Gamma(\alpha_k)} + \ln \mu_k \right) p(\boldsymbol{\mu}). \quad (2.108)$$

Then,

$$\mathbb{E} \ln \mu_k = \frac{\partial}{\partial \alpha_k} \int p(\boldsymbol{\mu}) d\boldsymbol{\mu} + \left(\psi(\alpha_k) - \psi \left(\sum_{k=1}^K \alpha_k \right) \right) \int p(\boldsymbol{\mu}) d\boldsymbol{\mu}, \quad (2.109)$$

where

$$\psi(a) = \frac{d}{da} \ln \Gamma(a). \quad (2.110)$$

Therefore,

$$\mathbb{E} \ln \mu_k = \psi(\alpha_k) - \psi \left(\sum_{k=1}^K \alpha_k \right). \quad (2.111)$$

2.12

Let x be a variable such that

$$p(x) = \frac{1}{b-a}, \quad (2.112)$$

where $a < b$. Then

$$\int_a^b p(x)dx = 1. \quad (2.113)$$

We have

$$\begin{aligned} E x &= \frac{1}{b-a} \int_a^b x dx, \\ E x^2 &= \frac{1}{b-a} \int_a^b x^2 dx. \end{aligned} \quad (2.114)$$

Then,

$$\begin{aligned} E x &= \frac{1}{2}(a+b), \\ E x^2 &= \frac{1}{3}(a^2 + ab + b^2). \end{aligned} \quad (2.115)$$

We have

$$\text{var } x = E x^2 - (E x)^2. \quad (2.116)$$

Therefore,

$$\text{var } x = \frac{1}{12}(b-a)^2. \quad (2.117)$$

2.13

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

$$\begin{aligned} p(\mathbf{x}) &= \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}), \\ q(\mathbf{x}) &= \mathcal{N}(\mathbf{x}|\mathbf{m}, \mathbf{L}). \end{aligned} \quad (2.118)$$

We have

$$\text{KL}(p||q) = - \int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) \ln \frac{\mathcal{N}(\mathbf{x}|\mathbf{m}, \mathbf{L})}{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})} d\mathbf{x}. \quad (2.119)$$

The logarithm in the right hand side can be written as

$$\begin{aligned} &\ln \frac{(2\pi)^{-\frac{D}{2}} |\det \mathbf{L}|^{-\frac{1}{2}} \exp(-\frac{1}{2}(\mathbf{x} - \mathbf{m})^\top \mathbf{L}^{-1}(\mathbf{x} - \mathbf{m}))}{(2\pi)^{-\frac{D}{2}} |\det \boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}))} \\ &= \frac{1}{2} \ln \left| \frac{\det \boldsymbol{\Sigma}}{\det \mathbf{L}} \right| + \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) - \frac{1}{2} (\mathbf{x} - \mathbf{m})^\top \mathbf{L}^{-1}(\mathbf{x} - \mathbf{m}). \end{aligned} \quad (2.120)$$

Then, the integral can be written as

$$\frac{1}{2} \ln \left| \frac{\det \Sigma}{\det L} \right| + \frac{1}{2} I_1 - \frac{1}{2} I_2, \quad (2.121)$$

where

$$\begin{aligned} I_1 &= \int (\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x}, \\ I_2 &= \int (\mathbf{x} - \mathbf{m})^\top \mathbf{L}^{-1} (\mathbf{x} - \mathbf{m}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x}. \end{aligned} \quad (2.122)$$

We have

$$(\mathbf{x} - \mathbf{m})^\top \mathbf{L}^{-1} (\mathbf{x} - \mathbf{m}) = (\mathbf{x} - \boldsymbol{\mu} + \boldsymbol{\mu} - \mathbf{m})^\top \mathbf{L}^{-1} (\mathbf{x} - \boldsymbol{\mu} + \boldsymbol{\mu} - \mathbf{m}). \quad (2.123)$$

Then, the expression of I_2 can be written as

$$\begin{aligned} &\int (\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{L}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x} \\ &+ 2(\boldsymbol{\mu} - \mathbf{m})^\top \mathbf{L}^{-1} \int (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x} \\ &+ (\boldsymbol{\mu} - \mathbf{m})^\top \mathbf{L}^{-1} (\boldsymbol{\mu} - \mathbf{m}) \int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x} \\ &= I'_2 + (\boldsymbol{\mu} - \mathbf{m})^\top \mathbf{L}^{-1} (\boldsymbol{\mu} - \mathbf{m}), \end{aligned} \quad (2.124)$$

where

$$I'_2 = \int (\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{L}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x}. \quad (2.125)$$

We have

$$\int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x} = \Sigma, \quad (2.126)$$

so that

$$\int (\mathbf{x} - \boldsymbol{\mu})^\top (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x} = \text{tr } \Sigma. \quad (2.127)$$

Then,

$$\begin{aligned} I_1 &= \text{tr} (\Sigma^{-1} \Sigma), \\ I'_2 &= \text{tr} (\mathbf{L}^{-1} \Sigma). \end{aligned} \quad (2.128)$$

Therefore,

$$\begin{aligned} &\text{KL}(p||q) \\ &= \frac{1}{2} \left(\ln \left| \frac{\det \mathbf{L}}{\det \Sigma} \right| - D + \text{tr} (\mathbf{L}^{-1} \Sigma) + (\boldsymbol{\mu} - \mathbf{m})^\top \mathbf{L}^{-1} (\boldsymbol{\mu} - \mathbf{m}) \right). \end{aligned} \quad (2.129)$$

2.14

Let \mathbf{x} be a variable in D dimensions. We have

$$H(\mathbf{x}) = - \int p(\mathbf{x}) \ln p(\mathbf{x}) d\mathbf{x}. \quad (2.130)$$

In order to maximise $H(x)$ with the constraints

$$\begin{aligned} \int p(\mathbf{x}) d\mathbf{x} &= 1, \\ \int \mathbf{x} p(\mathbf{x}) d\mathbf{x} &= \boldsymbol{\mu}, \\ \int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top p(\mathbf{x}) d\mathbf{x} &= \boldsymbol{\Sigma}, \end{aligned} \quad (2.131)$$

let

$$\begin{aligned} L(p) &= H(\mathbf{x}) + \lambda \left(\int p(\mathbf{x}) d\mathbf{x} - 1 \right) + \mathbf{l}^\top \left(\int \mathbf{x} p(\mathbf{x}) d\mathbf{x} - \boldsymbol{\mu} \right) \\ &\quad + \mathbf{m}^\top \left(\int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top p(\mathbf{x}) d\mathbf{x} - \boldsymbol{\Sigma} \right) \mathbf{m}. \end{aligned} \quad (2.132)$$

Setting the variation with respect to p to zero gives

$$0 = -\ln p(\mathbf{x}) - 1 + \lambda + \mathbf{l}^\top \mathbf{x} + \|\mathbf{m}^\top(\mathbf{x} - \boldsymbol{\mu})\|^2. \quad (2.133)$$

Then,

$$p(\mathbf{x}) = \exp(-1 + \lambda + \mathbf{l}^\top \mathbf{x} + \|\mathbf{m}^\top(\mathbf{x} - \boldsymbol{\mu})\|^2). \quad (2.134)$$

We have

$$\begin{aligned} &\mathbf{l}^\top \mathbf{x} + \|\mathbf{m}^\top(\mathbf{x} - \boldsymbol{\mu})\|^2 \\ &= -(\mathbf{x} - \boldsymbol{\mu} - \mathbf{M}\mathbf{l})^\top \mathbf{M}^{-1} (\mathbf{x} - \boldsymbol{\mu} - \mathbf{M}\mathbf{l}) + \mathbf{l}^\top \mathbf{M}\mathbf{l} + \mathbf{l}^\top \boldsymbol{\mu}. \end{aligned} \quad (2.135)$$

where

$$\mathbf{M} = -(\mathbf{m}\mathbf{m}^\top)^{-1}. \quad (2.136)$$

Then,

$$p(\mathbf{x}) = c \exp(-(\mathbf{x} - \boldsymbol{\mu} - \mathbf{M}\mathbf{l})^\top \mathbf{M}^{-1} (\mathbf{x} - \boldsymbol{\mu} - \mathbf{M}\mathbf{l})), \quad (2.137)$$

where

$$c = \exp(-1 + \lambda + \mathbf{l}^\top \mathbf{M} \mathbf{l} + \mathbf{l}^\top \boldsymbol{\mu}). \quad (2.138)$$

Substituting it to the constraints and the transformation

$$\mathbf{y} = \mathbf{x} - \boldsymbol{\mu} - \mathbf{M} \mathbf{l} \quad (2.139)$$

gives

$$\begin{aligned} c \int \exp(-\mathbf{y}^\top \mathbf{M}^{-1} \mathbf{y}) d\mathbf{y} &= 1, \\ c \int (\mathbf{y} + \boldsymbol{\mu} + \mathbf{M} \mathbf{l}) \exp(-\mathbf{y}^\top \mathbf{M}^{-1} \mathbf{y}) d\mathbf{y} &= \boldsymbol{\mu}, \\ c \int (\mathbf{y} + \mathbf{M} \mathbf{l}) (\mathbf{y} + \mathbf{M} \mathbf{l})^\top \exp(-\mathbf{y}^\top \mathbf{M}^{-1} \mathbf{y}) d\mathbf{y} &= \Sigma. \end{aligned} \quad (2.140)$$

We have

$$\begin{aligned} \int \exp(-\mathbf{y}^\top \mathbf{y}) d\mathbf{y} &= \left(\Gamma\left(\frac{1}{2}\right) \right)^D, \\ \int \mathbf{y} \exp(-\mathbf{y}^\top \mathbf{y}) d\mathbf{y} &= \mathbf{0}, \\ \int \mathbf{y} \mathbf{y}^\top \exp(-\mathbf{y}^\top \mathbf{y}) d\mathbf{y} &= \Gamma\left(\frac{3}{2}\right) \left(\Gamma\left(\frac{1}{2}\right) \right)^{D-1} \mathbf{I}, \end{aligned} \quad (2.141)$$

so that

$$\begin{aligned} \int \exp(-\mathbf{y}^\top \mathbf{M}^{-1} \mathbf{y}) d\mathbf{y} &= \pi^{\frac{D}{2}} |\det \mathbf{M}|^{\frac{1}{2}}, \\ \int \mathbf{y} \exp(-\mathbf{y}^\top \mathbf{M}^{-1} \mathbf{y}) d\mathbf{y} &= \mathbf{0}, \\ \int \mathbf{y} \mathbf{y}^\top \exp(-\mathbf{y}^\top \mathbf{M}^{-1} \mathbf{y}) d\mathbf{y} &= \frac{1}{2} \pi^{\frac{D}{2}} (\det \mathbf{M})^{\frac{1}{2}} \mathbf{M}. \end{aligned} \quad (2.142)$$

Then,

$$\begin{aligned} c \pi^{\frac{D}{2}} |\det \mathbf{M}|^{\frac{1}{2}} &= 1, \\ c \pi^{\frac{D}{2}} |\det \mathbf{M}|^{\frac{1}{2}} (\boldsymbol{\mu} + \mathbf{M} \mathbf{l}) &= \boldsymbol{\mu}, \\ c \pi^{\frac{D}{2}} |\det \mathbf{M}|^{\frac{1}{2}} \left(\frac{1}{2} \mathbf{M} + \mathbf{M} \mathbf{l} (\mathbf{M} \mathbf{l})^\top \right) &= \Sigma, \end{aligned} \quad (2.143)$$

so that

$$\begin{aligned} c &= (2\pi)^{-\frac{D}{2}} |\det \Sigma|^{-\frac{1}{2}}, \\ \mathbf{l} &= \mathbf{0}, \\ \mathbf{M} &= 2\Sigma. \end{aligned} \quad (2.144)$$

Therefore,

$$p(\mathbf{x}) = (2\pi)^{-\frac{D}{2}} |\det \Sigma|^{-\frac{1}{2}} \exp \left(-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right). \quad (2.145)$$

2.15

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

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma). \quad (2.146)$$

Then, by the definition, the entropy is given by

$$H(\mathbf{x}) = - \int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) \ln \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x}. \quad (2.147)$$

We have

$$\ln \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) = -\frac{D}{2} \ln(2\pi) - \frac{1}{2} \ln |\det \Sigma| - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}). \quad (2.148)$$

Then, the expression of $H(\mathbf{x})$ can be written as

$$\begin{aligned} & \left(\frac{D}{2} \ln(2\pi) + \frac{1}{2} \ln |\det \Sigma| \right) \int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x} \\ & + \frac{1}{2} \int (\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x}. \end{aligned} \quad (2.149)$$

We have

$$\int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x} = \Sigma, \quad (2.150)$$

so that

$$\int (\mathbf{x} - \boldsymbol{\mu})^\top (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x} = \text{tr } \Sigma. \quad (2.151)$$

Then,

$$\int (\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) d\mathbf{x} = \text{tr} (\Sigma^{-1} \Sigma), \quad (2.152)$$

where the right hand side can be written as D . Therefore,

$$H(\mathbf{x}) = \frac{D}{2} (1 + \ln(2\pi)) + \frac{1}{2} \ln |\det \Sigma|. \quad (2.153)$$

2.16

Let x be a variable such that

$$x = x_1 + x_2, \quad (2.154)$$

where

$$\begin{aligned} p(x_1) &= \mathcal{N}(x_1|\mu_1, \tau_1^{-1}), \\ p(x_2) &= \mathcal{N}(x_2|\mu_2, \tau_2^{-1}). \end{aligned} \quad (2.155)$$

By marginalisation,

$$p(x) = \int_{-\infty}^{\infty} p(x|x_2)p(x_2)dx_2. \quad (2.156)$$

The right hand side can be written as

$$\begin{aligned} &\int_{-\infty}^{\infty} \mathcal{N}(x|\mu_1 + x_2, \tau_1^{-1}) \mathcal{N}(x_2|\mu_2, \tau_2^{-1}) dx_2 \\ &= \int_{-\infty}^{\infty} \left(\frac{\tau_1}{2\pi}\right)^{\frac{1}{2}} \exp\left(-\frac{\tau_1}{2}(x - \mu_1 - x_2)^2\right) \left(\frac{\tau_2}{2\pi}\right)^{\frac{1}{2}} \exp\left(-\frac{\tau_2}{2}(x_2 - \mu_2)^2\right) dx_2. \end{aligned} \quad (2.157)$$

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

$$\begin{aligned} &-\frac{\tau_1 + \tau_2}{2} \left(x_2 - \frac{\tau_1(x - \mu_1) + \tau_2\mu_2}{\tau_1 + \tau_2} \right)^2 - \frac{\tau_1}{2}(x - \mu_1)^2 - \frac{\tau_2}{2}\mu_2^2 \\ &+ \frac{\tau_1 + \tau_2}{2} \left(\frac{\tau_1(x - \mu_1) + \tau_2\mu_2}{\tau_1 + \tau_2} \right)^2 \\ &= -\frac{\tau_1 + \tau_2}{2} \left(x_2 - \frac{\tau_1(x - \mu_1) + \tau_2\mu_2}{\tau_1 + \tau_2} \right)^2 - \frac{\tau_1\tau_2}{2(\tau_1 + \tau_2)}(x - \mu_1 - \mu_2)^2. \end{aligned} \quad (2.158)$$

Then,

$$p(x) = \mathcal{N}(x|\mu_1 + \mu_2, \tau_1^{-1} + \tau_2^{-1}). \quad (2.159)$$

Therefore, by 1.35,

$$H(x) = \frac{1}{2} \left(1 + \ln(2\pi) + \ln(\tau_1^{-1} + \tau_2^{-1}) \right). \quad (2.160)$$

2.17

Let Σ be a matrix and

$$\begin{aligned}\mathbf{S} &= \frac{1}{2} (\Sigma^{-1} + (\Sigma^{-1})^\top), \\ \mathbf{A} &= \frac{1}{2} (\Sigma^{-1} - (\Sigma^{-1})^\top).\end{aligned}\tag{2.161}$$

Then,

$$\Sigma^{-1} = \mathbf{S} + \mathbf{A},\tag{2.162}$$

so that

$$(\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) = (\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{S} (\mathbf{x} - \boldsymbol{\mu}) + (\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{A} (\mathbf{x} - \boldsymbol{\mu}).\tag{2.163}$$

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

$$\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top (\Sigma^{-1})^\top (\mathbf{x} - \boldsymbol{\mu}).\tag{2.164}$$

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

$$-\frac{1}{2} (\Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}))^\top (\mathbf{x} - \boldsymbol{\mu}) = -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}).\tag{2.165}$$

Then,

$$(\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{A} (\mathbf{x} - \boldsymbol{\mu}) = 0.\tag{2.166}$$

Therefore,

$$(\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) = (\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{S} (\mathbf{x} - \boldsymbol{\mu}).\tag{2.167}$$

2.18

(a)

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

$$\Sigma \mathbf{u}_d = \lambda_d \mathbf{u}_d,\tag{2.168}$$

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

$$\overline{\mathbf{u}_d}^\top \Sigma \mathbf{u}_d = \lambda_d,\tag{2.169}$$

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

$$\overline{\mathbf{u}_d}^\top \overline{\Sigma}^\top \mathbf{u}_d = (\overline{\Sigma} \overline{\mathbf{u}_d})^\top \mathbf{u}_d. \quad (2.170)$$

The right hand side can be written as

$$\overline{\lambda_d} \overline{\mathbf{u}_d}^\top \mathbf{u}_d = \overline{\lambda_d}. \quad (2.171)$$

Therefore,

$$\lambda_d = \overline{\lambda_d}. \quad (2.172)$$

(b)

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

$$\Sigma \mathbf{u}_d = \lambda_d \mathbf{u}_d \quad (2.173)$$

gives

$$\mathbf{u}'_d^\top \Sigma \mathbf{u}_d = \lambda_d \mathbf{u}'_d^\top \mathbf{u}_d. \quad (2.174)$$

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

$$\mathbf{u}'_d^\top \Sigma^\top \mathbf{u}_d = (\Sigma \mathbf{u}'_d)^\top \mathbf{u}_d. \quad (2.175)$$

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

$$\lambda_d \mathbf{u}'_d^\top \mathbf{u}_d = \lambda_{d'} \mathbf{u}'_d^\top \mathbf{u}_d. \quad (2.176)$$

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

$$\mathbf{u}'_d^\top \mathbf{u}_d = 0. \quad (2.177)$$

2.19

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

$$\Sigma \mathbf{u}_d = \lambda_d \mathbf{u}_d, \quad (2.178)$$

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

$$\begin{aligned} \Lambda &= \text{diag}(\lambda_1, \dots, \lambda_D), \\ \mathbf{U} &= [\mathbf{u}_1 \cdots \mathbf{u}_D]. \end{aligned} \quad (2.179)$$

Then,

$$\Sigma \mathbf{U} = \mathbf{U} \Lambda. \quad (2.180)$$

By 2.18,

$$\mathbf{U}^\top \mathbf{U} = \mathbf{I}. \quad (2.181)$$

Then,

$$\begin{aligned} \Sigma &= \mathbf{U} \Lambda \mathbf{U}^\top, \\ \Sigma^{-1} &= \mathbf{U} \Lambda^{-1} \mathbf{U}^\top, \end{aligned} \quad (2.182)$$

Therefore,

$$\begin{aligned} \Sigma &= \sum_{d=1}^D \lambda_d \mathbf{u}_d \mathbf{u}_d^\top, \\ \Sigma^{-1} &= \sum_{d=1}^D \frac{1}{\lambda_d} \mathbf{u}_d \mathbf{u}_d^\top. \end{aligned} \quad (2.183)$$

2.20

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

$$\Sigma \mathbf{u}_d = \lambda_d \mathbf{u}_d, \quad (2.184)$$

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

$$\begin{aligned} \Lambda &= \text{diag}(\lambda_1, \dots, \lambda_D), \\ \mathbf{U} &= [\mathbf{u}_1 \cdots \mathbf{u}_D]. \end{aligned} \quad (2.185)$$

By 2.19,

$$\mathbf{a}^\top \Sigma \mathbf{a} = \mathbf{b}^\top \Lambda \mathbf{b}, \quad (2.186)$$

where

$$\mathbf{b} = \mathbf{U}^\top \mathbf{a}. \quad (2.187)$$

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

$$\mathbf{a}^\top \Sigma \mathbf{a} > 0 \quad (2.188)$$

for any real vector \mathbf{a} is

$$\lambda_d > 0. \quad (2.189)$$

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

$$\Sigma \Lambda = \mathbf{I}. \quad (2.190)$$

Taking the transpose of the both sides gives

$$\Lambda^\top \Sigma = \mathbf{I}. \quad (2.191)$$

Therefore,

$$\Lambda^\top = \Lambda. \quad (2.192)$$

2.23

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

$$\Sigma \mathbf{u}_d = \lambda_d \mathbf{u}_d, \quad (2.193)$$

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

$$\begin{aligned} \Lambda' &= \text{diag} \left(\lambda_1^{-\frac{1}{2}}, \dots, \lambda_D^{-\frac{1}{2}} \right), \\ \mathbf{U} &= [\mathbf{u}_1 \cdots \mathbf{u}_D]. \end{aligned} \quad (2.194)$$

By 2.19,

$$\int_{(\mathbf{x}-\boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x}-\boldsymbol{\mu}) = \Delta} d\mathbf{x} = \int_{(\mathbf{x}-\boldsymbol{\mu})^\top \mathbf{U} \Lambda' \Lambda'^\top \mathbf{U}^\top (\mathbf{x}-\boldsymbol{\mu}) = \Delta} d\mathbf{x}. \quad (2.195)$$

By the transformation

$$\mathbf{y} = \Lambda'^\top \mathbf{U}^\top (\mathbf{x} - \boldsymbol{\mu}) \quad (2.196)$$

and the property

$$\mathbf{U}^\top \mathbf{U} = \mathbf{I}, \quad (2.197)$$

the right hand side can be written as

$$\int_{\|\mathbf{y}\|^2=\Delta} \left| \det(\mathbf{U}\boldsymbol{\Lambda}'^{-1}) \right| d\mathbf{y} = |\det \boldsymbol{\Sigma}|^{\frac{1}{2}} \int_{\|\mathbf{y}\|^2=\Delta} d\mathbf{y}. \quad (2.198)$$

Therefore,

$$\int_{(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}-\boldsymbol{\mu})=\Delta} d\mathbf{x} = |\det \boldsymbol{\Sigma}|^{\frac{1}{2}} \Delta^D V_D, \quad (2.199)$$

where

$$V_D = \int_{\|\mathbf{x}\|=1} d\mathbf{x}. \quad (2.200)$$

2.24

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

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{BD}^{-1} \\ \mathbf{O} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{A} - \mathbf{BD}^{-1}\mathbf{C} & \mathbf{O} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}. \quad (2.201)$$

The right hand side can be written as

$$\begin{bmatrix} \mathbf{I} & \mathbf{BD}^{-1} \\ \mathbf{O} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{A} - \mathbf{BD}^{-1}\mathbf{C} & \mathbf{O} \\ \mathbf{O} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{O} \\ \mathbf{D}^{-1}\mathbf{C} & \mathbf{I} \end{bmatrix}. \quad (2.202)$$

Then,

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{I} & \mathbf{O} \\ -\mathbf{D}^{-1}\mathbf{C} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{M} & \mathbf{O} \\ \mathbf{O} & \mathbf{D}^{-1} \end{bmatrix} \begin{bmatrix} \mathbf{I} & -\mathbf{BD}^{-1} \\ \mathbf{O} & \mathbf{I} \end{bmatrix}, \quad (2.203)$$

where

$$\mathbf{M} = (\mathbf{A} - \mathbf{BD}^{-1}\mathbf{C})^{-1}. \quad (2.204)$$

Therefore,

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{M} & -\mathbf{BD}^{-1}\mathbf{M} \\ -\mathbf{D}^{-1}\mathbf{CM} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{CMBD}^{-1} \end{bmatrix}. \quad (2.205)$$

2.25

Let \mathbf{x} be a variable such that

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}), \quad (2.206)$$

where

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

Let

$$\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}, \quad (2.207)$$

where

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

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

$$\begin{aligned} & -\frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{aa} (\mathbf{x}_a - \boldsymbol{\mu}_a) - \frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{ab} (\mathbf{x}_b - \boldsymbol{\mu}_b) \\ & - \frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{ac} (\mathbf{x}_c - \boldsymbol{\mu}_c) - \frac{1}{2}(\mathbf{x}_b - \boldsymbol{\mu}_b)^\top \boldsymbol{\Lambda}_{ba} (\mathbf{x}_a - \boldsymbol{\mu}_a) \\ & - \frac{1}{2}(\mathbf{x}_c - \boldsymbol{\mu}_c)^\top \boldsymbol{\Lambda}_{ca} (\mathbf{x}_a - \boldsymbol{\mu}_a). \end{aligned} \quad (2.208)$$

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

$$-\frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_{a|b,c})^\top \boldsymbol{\Sigma}_{a|b,c}^{-1} (\mathbf{x}_a - \boldsymbol{\mu}_{a|b,c}), \quad (2.209)$$

where

$$\begin{aligned} \boldsymbol{\mu}_{a|b,c} &= \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ab} (\mathbf{x}_b - \boldsymbol{\mu}_b) - \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ac} (\mathbf{x}_c - \boldsymbol{\mu}_c), \\ \boldsymbol{\Sigma}_{a|b,c} &= \boldsymbol{\Lambda}_{aa}^{-1}. \end{aligned} \quad (2.210)$$

Then,

$$p(\mathbf{x}_a | \mathbf{x}_b, \mathbf{x}_c) = \mathcal{N}(\mathbf{x}_a | \boldsymbol{\mu}_{a|b,c}, \boldsymbol{\Sigma}_{a|b,c}). \quad (2.211)$$

By marginalisation,

$$p(\mathbf{x}_a | \mathbf{x}_b) = \int p(\mathbf{x}_a | \mathbf{x}_b, \mathbf{x}_c) p(\mathbf{x}_c) d\mathbf{x}_c. \quad (2.212)$$

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

$$\begin{aligned} & -\frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_{a|b,c})^\top \boldsymbol{\Sigma}_{a|b,c}^{-1} (\mathbf{x}_a - \boldsymbol{\mu}_{a|b,c}) - \frac{1}{2}(\mathbf{x}_c - \boldsymbol{\mu}_c)^\top \boldsymbol{\Lambda}_{cc} (\mathbf{x}_c - \boldsymbol{\mu}_c) \\ & = -\frac{1}{2}\mathbf{v}^\top \mathbf{M} \mathbf{v}, \end{aligned} \quad (2.213)$$

where

$$\begin{aligned} \mathbf{v} &= \begin{bmatrix} \mathbf{x}_c - \boldsymbol{\mu}_c \\ \mathbf{x}_a - \boldsymbol{\mu}_a + \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ab} (\mathbf{x}_b - \boldsymbol{\mu}_b) \end{bmatrix}, \\ \mathbf{M} &= \begin{bmatrix} \boldsymbol{\Lambda}_{cc} + \boldsymbol{\Lambda}_{ac}^\top \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ac} & \boldsymbol{\Lambda}_{ac}^\top \\ \boldsymbol{\Lambda}_{ac} & \boldsymbol{\Lambda}_{aa} \end{bmatrix}. \end{aligned} \quad (2.214)$$

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \boldsymbol{\Lambda}_{cc}^{-1} & -\boldsymbol{\Lambda}_{cc}^{-1} \boldsymbol{\Lambda}_{ac}^\top \boldsymbol{\Lambda}_{aa}^{-1} \\ -\boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ac} \boldsymbol{\Lambda}_{cc}^{-1} & \boldsymbol{\Lambda}_{aa}^{-1} + \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ac} \boldsymbol{\Lambda}_{cc}^{-1} \boldsymbol{\Lambda}_{ac}^\top \boldsymbol{\Lambda}_{aa}^{-1} \end{bmatrix}. \quad (2.215)$$

Therefore,

$$p(\mathbf{x}_a | \mathbf{x}_b) = \mathcal{N}(\mathbf{x}_a | \boldsymbol{\mu}_{a|b}, \boldsymbol{\Sigma}_{a|b}), \quad (2.216)$$

where

$$\begin{aligned} \boldsymbol{\mu}_{a|b} &= \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ab} (\mathbf{x}_b - \boldsymbol{\mu}_b), \\ \boldsymbol{\Sigma}_{a|b} &= \boldsymbol{\Lambda}_{aa}^{-1} + \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ac} \boldsymbol{\Lambda}_{cc}^{-1} \boldsymbol{\Lambda}_{ac}^\top \boldsymbol{\Lambda}_{aa}^{-1}. \end{aligned} \quad (2.217)$$

2.26

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

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{D} & -\mathbf{C}^{-1} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{M} & \mathbf{MBC} \\ \mathbf{CDM} & -\mathbf{C} + \mathbf{CDMBC} \end{bmatrix}, \quad (2.218)$$

where

$$\mathbf{M} = (\mathbf{A} + \mathbf{BCD})^{-1}. \quad (2.219)$$

By 2.24,

$$\begin{bmatrix} -\mathbf{C}^{-1} & \mathbf{D} \\ \mathbf{B} & \mathbf{A} \end{bmatrix}^{-1} = \begin{bmatrix} -\mathbf{N} & \mathbf{NDA}^{-1} \\ \mathbf{A}^{-1}\mathbf{BN} & \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{BNDA}^{-1} \end{bmatrix}, \quad (2.220)$$

where

$$\mathbf{N} = (\mathbf{C}^{-1} + \mathbf{DA}^{-1}\mathbf{B})^{-1}. \quad (2.221)$$

Therefore,

$$\mathbf{M} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{BNDA}^{-1}. \quad (2.222)$$

2.27

(a)

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

$$E(\mathbf{x} + \mathbf{z}) = \int \int (\mathbf{x} + \mathbf{z}) p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z}. \quad (2.223)$$

The right hand side can be written as

$$\int \mathbf{x} \left(\int p(\mathbf{x}, \mathbf{z}) d\mathbf{z} \right) d\mathbf{x} + \int \mathbf{z} \left(\int p(\mathbf{x}, \mathbf{z}) d\mathbf{x} \right) d\mathbf{z} = \int \mathbf{x} p(\mathbf{x}) d\mathbf{x} + \int \mathbf{z} p(\mathbf{z}) d\mathbf{z}. \quad (2.224)$$

Therefore,

$$E(\mathbf{x} + \mathbf{z}) = E \mathbf{x} + E \mathbf{z}. \quad (2.225)$$

(b)

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

$$\text{cov}(\mathbf{x} + \mathbf{z}) = \int \int (\mathbf{x} + \mathbf{z} - E(\mathbf{x} + \mathbf{z})) (\mathbf{x} + \mathbf{z} - E(\mathbf{x} + \mathbf{z}))^\top p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z}. \quad (2.226)$$

The right hand side can be written as

$$\begin{aligned} & \int \int (\mathbf{x} - E \mathbf{x}) (\mathbf{x} - E \mathbf{x})^\top p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z} + \int \int (\mathbf{x} - E \mathbf{x}) (\mathbf{z} - E \mathbf{z})^\top p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z} \\ & + \int \int (\mathbf{z} - E \mathbf{z}) (\mathbf{x} - E \mathbf{x})^\top p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z} + \int \int (\mathbf{z} - E \mathbf{z}) (\mathbf{z} - E \mathbf{z})^\top p(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z}. \end{aligned} \quad (2.227)$$

Each term can be written as

$$\begin{aligned} & \int (\mathbf{x} - E \mathbf{x}) (\mathbf{x} - E \mathbf{x})^\top \left(\int p(\mathbf{x}, \mathbf{z}) d\mathbf{z} \right) d\mathbf{x} = \int (\mathbf{x} - E \mathbf{x}) (\mathbf{x} - E \mathbf{x})^\top p(\mathbf{x}) d\mathbf{x}, \\ & \int (\mathbf{x} - E \mathbf{x}) p(\mathbf{x}) d\mathbf{x} \int (\mathbf{z} - E \mathbf{z})^\top p(\mathbf{z}) d\mathbf{z} = (E \mathbf{x} - E \mathbf{x})(E \mathbf{z} - E \mathbf{z})^\top, \\ & \int (\mathbf{z} - E \mathbf{z}) p(\mathbf{z}) d\mathbf{z} \int (\mathbf{x} - E \mathbf{x})^\top p(\mathbf{x}) d\mathbf{x} = (E \mathbf{z} - E \mathbf{z})(E \mathbf{x} - E \mathbf{x})^\top, \\ & \int (\mathbf{z} - E \mathbf{z}) (\mathbf{z} - E \mathbf{z})^\top \left(\int p(\mathbf{x}, \mathbf{z}) d\mathbf{x} \right) d\mathbf{z} = \int (\mathbf{z} - E \mathbf{z}) (\mathbf{z} - E \mathbf{z})^\top p(\mathbf{z}) d\mathbf{z}. \end{aligned} \quad (2.228)$$

Therefore,

$$\text{cov}(\mathbf{x} + \mathbf{z}) = \text{cov} \mathbf{x} + \text{cov} \mathbf{z}. \quad (2.229)$$

2.28

Let \mathbf{z} be a variable such that

$$\begin{aligned} \mathbf{z} &= \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix}, \\ \mathbb{E} \mathbf{z} &= \begin{bmatrix} \boldsymbol{\mu} \\ \mathbf{A}\boldsymbol{\mu} + \mathbf{b} \end{bmatrix}, \\ \text{cov } \mathbf{z} &= \begin{bmatrix} \mathbf{\Lambda}^{-1} & \mathbf{\Lambda}^{-1}\mathbf{A}^\top \\ \mathbf{A}\mathbf{\Lambda}^{-1} & \mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1}\mathbf{A}^\top \end{bmatrix}, \end{aligned} \quad (2.230)$$

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

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

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

$$\begin{aligned} & -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top (\mathbf{\Lambda} + \mathbf{A}^\top \mathbf{L} \mathbf{A}) (\mathbf{x} - \boldsymbol{\mu}) + \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{A}^\top \mathbf{L} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}) \\ & + \frac{1}{2}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})^\top \mathbf{L} \mathbf{A} (\mathbf{x} - \boldsymbol{\mu}) - \frac{1}{2}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})^\top \mathbf{L} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}) \\ & = -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top (\mathbf{\Lambda} + \mathbf{A}^\top \mathbf{L} \mathbf{A}) (\mathbf{x} - \boldsymbol{\mu}) + \\ & -\frac{1}{2}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b} - \mathbf{A}(\mathbf{x} - \boldsymbol{\mu}))^\top \mathbf{L} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b} - \mathbf{A}(\mathbf{x} - \boldsymbol{\mu})) \\ & + \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{A}^\top \mathbf{L} \mathbf{A} (\mathbf{x} - \boldsymbol{\mu}). \end{aligned} \quad (2.231)$$

The right hand side can be written as

$$-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{\Lambda} (\mathbf{x} - \boldsymbol{\mu}) - \frac{1}{2}(\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b})^\top \mathbf{L} (\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b}). \quad (2.232)$$

Therefore,

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

2.29

Let

$$\mathbf{R} = \begin{bmatrix} \Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A} & -\mathbf{A}^\top \mathbf{L} \\ -\mathbf{L} \mathbf{A} & \mathbf{L} \end{bmatrix}. \quad (2.234)$$

By 2.24,

$$\mathbf{R}^{-1} = \begin{bmatrix} \Lambda^{-1} & \Lambda^{-1} \mathbf{A}^\top \\ \mathbf{A} \Lambda^{-1} & \mathbf{L}^{-1} + \mathbf{A} \Lambda^{-1} \mathbf{A}^\top \end{bmatrix}. \quad (2.235)$$

2.30

Let

$$\mathbf{R}^{-1} = \begin{bmatrix} \Lambda^{-1} & \Lambda^{-1} \mathbf{A}^\top \\ \mathbf{A} \Lambda^{-1} & \mathbf{L}^{-1} + \mathbf{A} \Lambda^{-1} \mathbf{A}^\top \end{bmatrix}. \quad (2.236)$$

Then,

$$\mathbf{R}^{-1} \begin{bmatrix} \Lambda \boldsymbol{\mu} - \mathbf{A}^\top \mathbf{L} \mathbf{b} \\ \mathbf{L} \mathbf{b} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\mu} \\ \mathbf{A} \boldsymbol{\mu} + \mathbf{b} \end{bmatrix}. \quad (2.237)$$

2.31

Let \mathbf{y} be a variable such that

$$\mathbf{y} = \mathbf{x} + \mathbf{z}, \quad (2.238)$$

where

$$\begin{aligned} p(\mathbf{x}) &= \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}_x, \Sigma_x), \\ p(\mathbf{z}) &= \mathcal{N}(\mathbf{z} | \boldsymbol{\mu}_z, \Sigma_z). \end{aligned} \quad (2.239)$$

By marginalisation,

$$p(\mathbf{y}) = \int p(\mathbf{y} | \mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \quad (2.240)$$

The right hand side can be written as

$$\int \mathcal{N}(\mathbf{y} | \mathbf{x} + \boldsymbol{\mu}_z, \Sigma_z) \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}_x, \Sigma_x) d\mathbf{x}. \quad (2.241)$$

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

$$-\frac{1}{2} (\mathbf{y} - \mathbf{x} - \boldsymbol{\mu}_z)^\top \Sigma_z^{-1} (\mathbf{y} - \mathbf{x} - \boldsymbol{\mu}_z) - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_x)^\top \Sigma_x^{-1} (\mathbf{x} - \boldsymbol{\mu}_x). \quad (2.242)$$

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

$$-\frac{1}{2}\mathbf{u}^\top \mathbf{R}\mathbf{u} + \mathbf{u}^\top \mathbf{v} = -\frac{1}{2}(\mathbf{u} - \mathbf{R}^{-1}\mathbf{v})^\top \mathbf{R}(\mathbf{u} - \mathbf{R}^{-1}\mathbf{v}) + \frac{1}{2}\mathbf{v}^\top \mathbf{R}^{-1}\mathbf{v}, \quad (2.243)$$

where

$$\begin{aligned} \mathbf{u} &= \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix}, \\ \mathbf{R} &= \begin{bmatrix} \Sigma_{\mathbf{x}}^{-1} + \Sigma_{\mathbf{z}}^{-1} & -\Sigma_{\mathbf{z}}^{-1} \\ -\Sigma_{\mathbf{z}}^{-1} & \Sigma_{\mathbf{z}}^{-1} \end{bmatrix}, \\ \mathbf{v} &= \begin{bmatrix} \Sigma_{\mathbf{x}}^{-1}\boldsymbol{\mu}_{\mathbf{x}} - \Sigma_{\mathbf{z}}^{-1}\boldsymbol{\mu}_{\mathbf{z}} \\ \Sigma_{\mathbf{z}}^{-1}\boldsymbol{\mu}_{\mathbf{z}} \end{bmatrix}, \end{aligned} \quad (2.244)$$

By 2.29 and 2.30,

$$\begin{aligned} \mathbf{R}^{-1} &= \begin{bmatrix} \Sigma_{\mathbf{x}} & \Sigma_{\mathbf{x}} \\ \Sigma_{\mathbf{x}} & \Sigma_{\mathbf{x}} + \Sigma_{\mathbf{z}} \end{bmatrix}, \\ \mathbf{R}^{-1}\mathbf{v} &= \begin{bmatrix} \boldsymbol{\mu}_{\mathbf{x}} \\ \boldsymbol{\mu}_{\mathbf{x}} + \boldsymbol{\mu}_{\mathbf{z}} \end{bmatrix}. \end{aligned} \quad (2.245)$$

Therefore,

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\boldsymbol{\mu}_{\mathbf{x}} + \boldsymbol{\mu}_{\mathbf{z}}, \Sigma_{\mathbf{x}} + \Sigma_{\mathbf{z}}). \quad (2.246)$$

2.32

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

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

By the Bayes' theorem,

$$p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) = p(\mathbf{x}|\mathbf{y})p(\mathbf{y}). \quad (2.248)$$

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

$$\begin{aligned} &-\frac{1}{2}(\mathbf{y} - \mathbf{Ax} - \mathbf{b})^\top \mathbf{L}(\mathbf{y} - \mathbf{Ax} - \mathbf{b}) - \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu}) \\ &= -\frac{1}{2}(\mathbf{y} - \mathbf{A}(\mathbf{x} - \boldsymbol{\mu}) - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})^\top \mathbf{L}(\mathbf{y} - \mathbf{A}(\mathbf{x} - \boldsymbol{\mu}) - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}) \\ &\quad - \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu}). \end{aligned} \quad (2.249)$$

The right hand side can be written as

$$\begin{aligned}
& -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A}) (\mathbf{x} - \boldsymbol{\mu}) + (\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{A}^\top \mathbf{L} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}) \\
& -\frac{1}{2}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})^\top \mathbf{L} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}) \\
= & -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu} - \mathbf{z})^\top (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A}) (\mathbf{x} - \boldsymbol{\mu} - \mathbf{z}) + \frac{1}{2}\mathbf{z}^\top (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A}) \mathbf{z} \\
& -\frac{1}{2}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})^\top \mathbf{L} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}),
\end{aligned} \tag{2.250}$$

where

$$\mathbf{z} = (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{L} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}). \tag{2.251}$$

The right hand side can be written as

$$\begin{aligned}
& -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu} - \mathbf{z})^\top (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A}) (\mathbf{x} - \boldsymbol{\mu} - \mathbf{z}) \\
& -\frac{1}{2}(\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})^\top \mathbf{M} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b}),
\end{aligned} \tag{2.252}$$

where

$$\mathbf{M} = \mathbf{L} - \mathbf{L} \mathbf{A} (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{L}. \tag{2.253}$$

We have

$$\boldsymbol{\mu} + \mathbf{z} = (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1} ((\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A}) \boldsymbol{\mu} + \mathbf{A}^\top \mathbf{L} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu} - \mathbf{b})). \tag{2.254}$$

Then,

$$\boldsymbol{\mu} + \mathbf{z} = (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1} (\mathbf{A}^\top \mathbf{L} (\mathbf{y} - \mathbf{b}) + \Lambda \boldsymbol{\mu}). \tag{2.255}$$

By 2.26,

$$(\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1} = \Lambda^{-1} - \Lambda^{-1} \mathbf{A}^\top (\mathbf{L}^{-1} + \mathbf{A} \Lambda^{-1} \mathbf{A}^\top)^{-1} \mathbf{A} \Lambda^{-1}. \tag{2.256}$$

Then,

$$\mathbf{M} = \mathbf{L} - \mathbf{L} \mathbf{A} \left(\Lambda^{-1} - \Lambda^{-1} \mathbf{A}^\top (\mathbf{L}^{-1} + \mathbf{A} \Lambda^{-1} \mathbf{A}^\top)^{-1} \mathbf{A} \Lambda^{-1} \right) \mathbf{A}^\top \mathbf{L}. \tag{2.257}$$

The right hand side can be written as

$$\begin{aligned}
& \mathbf{L} - \mathbf{L} \left(\mathbf{A} \Lambda^{-1} \mathbf{A}^\top - \mathbf{A} \Lambda^{-1} \mathbf{A}^\top (\mathbf{L}^{-1} + \mathbf{A} \Lambda^{-1} \mathbf{A}^\top)^{-1} \mathbf{A} \Lambda^{-1} \mathbf{A}^\top \right) \mathbf{L} \\
= & \mathbf{L} - \mathbf{L} \mathbf{A} \Lambda^{-1} \mathbf{A}^\top (\mathbf{L}^{-1} + \mathbf{A} \Lambda^{-1} \mathbf{A}^\top)^{-1} (\mathbf{L}^{-1} + \mathbf{A} \Lambda^{-1} \mathbf{A}^\top - \mathbf{A} \Lambda^{-1} \mathbf{A}^\top) \mathbf{L}.
\end{aligned} \tag{2.258}$$

The right hand side can be written as

$$\begin{aligned} & \mathbf{L} - \mathbf{L}\mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^\top (\mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^\top)^{-1} \\ &= \mathbf{L} (\mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^\top - \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^\top) (\mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^\top)^{-1}. \end{aligned} \quad (2.259)$$

Then,

$$\mathbf{M} = (\mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^\top)^{-1}. \quad (2.260)$$

Therefore,

$$\begin{aligned} p(\mathbf{x}|\mathbf{y}) &= \mathcal{N}(\mathbf{x}|(\boldsymbol{\Lambda} + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1} (\mathbf{A}^\top \mathbf{L}(\mathbf{y} - \mathbf{b}) + \boldsymbol{\Lambda} \boldsymbol{\mu}), (\boldsymbol{\Lambda} + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1}), \\ p(\mathbf{y}) &= \mathcal{N}(\mathbf{y}|\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^\top). \end{aligned} \quad (2.261)$$

2.33

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

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

$$\begin{aligned} p(\mathbf{x}) &= \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}), \\ p(\mathbf{y}|\mathbf{x}) &= \mathcal{N}(\mathbf{y}|\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1}). \end{aligned} \quad (2.262)$$

By the Bayes' theorem,

$$p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) = p(\mathbf{x}|\mathbf{y})p(\mathbf{y}). \quad (2.263)$$

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

$$-\frac{1}{2} (\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b})^\top \mathbf{L} (\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b}) - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu}). \quad (2.264)$$

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

$$-\frac{1}{2} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix}^\top \begin{bmatrix} \boldsymbol{\Lambda} + \mathbf{A}^\top \mathbf{L} \mathbf{A} & -\mathbf{A}^\top \mathbf{L} \\ -\mathbf{L} \mathbf{A} & \mathbf{L} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} + \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix}^\top \begin{bmatrix} -\mathbf{A}^\top \mathbf{L} \mathbf{b} + \boldsymbol{\Lambda} \boldsymbol{\mu} \\ \mathbf{L} \mathbf{b} \end{bmatrix}. \quad (2.265)$$

By 2.24,

$$\begin{bmatrix} \Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A} & -\mathbf{A}^\top \mathbf{L} \\ -\mathbf{L} \mathbf{A} & \mathbf{L} \end{bmatrix}^{-1} = \begin{bmatrix} \Lambda^{-1} & \Lambda^{-1} \mathbf{A}^\top \\ \mathbf{A} \Lambda^{-1} & \mathbf{L}^{-1} + \mathbf{A} \Lambda^{-1} \mathbf{A}^\top \end{bmatrix}, \quad (2.266)$$

so that

$$\begin{bmatrix} \Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A} & -\mathbf{A}^\top \mathbf{L} \\ -\mathbf{L} \mathbf{A} & \mathbf{L} \end{bmatrix}^{-1} \begin{bmatrix} -\mathbf{A}^\top \mathbf{L} \mathbf{b} + \Lambda \boldsymbol{\mu} \\ \mathbf{L} \mathbf{b} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\mu} \\ \mathbf{A} \boldsymbol{\mu} + \mathbf{b} \end{bmatrix}. \quad (2.267)$$

Then,

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y} | \mathbf{A} \boldsymbol{\mu} + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A} \Lambda^{-1} \mathbf{A}^\top). \quad (2.268)$$

By 2.25,

$$p(\mathbf{x} | \mathbf{y}) = \mathcal{N}(\mathbf{x} | \boldsymbol{\mu} + (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{L} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b}), (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1}). \quad (2.269)$$

We have

$$\begin{aligned} & \boldsymbol{\mu} + (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{L} (\mathbf{y} - \mathbf{A} \boldsymbol{\mu} - \mathbf{b}) \\ &= (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1} (\Lambda \boldsymbol{\mu} + \mathbf{A}^\top \mathbf{L} (\mathbf{y} - \mathbf{b})). \end{aligned} \quad (2.270)$$

Therefore,

$$p(\mathbf{x} | \mathbf{y}) = \mathcal{N}(\mathbf{x} | (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1} (\Lambda \boldsymbol{\mu} + \mathbf{A}^\top \mathbf{L} (\mathbf{y} - \mathbf{b})), (\Lambda + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1}). \quad (2.271)$$

2.34

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

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Sigma}). \quad (2.272)$$

Then,

$$\ln \left(\prod_{n=1}^N p(\mathbf{x}_n) \right) = -\frac{ND}{2} \ln(2\pi) - \frac{N}{2} \ln |\det \boldsymbol{\Sigma}| - \frac{1}{2} \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu}). \quad (2.273)$$

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

$$\begin{aligned} \mathbf{0} &= \sum_{n=1}^N (\boldsymbol{\Sigma}^{-1} + (\boldsymbol{\Sigma}^{-1})^\top) (\mathbf{x}_n - \boldsymbol{\mu}), \\ \mathbf{O} &= -\frac{N}{2} (\boldsymbol{\Sigma}^{-1})^\top + \frac{1}{2} (\boldsymbol{\Sigma}^{-1})^2 \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{x}_n - \boldsymbol{\mu})^\top. \end{aligned} \quad (2.274)$$

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

$$\begin{aligned}\boldsymbol{\mu}_{\text{ML}} &= \frac{1}{N} \sum_{n=1}^N \mathbf{x}_n, \\ \boldsymbol{\Sigma}_{\text{ML}} &= \frac{1}{N} \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}})(\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}})^\top.\end{aligned}\tag{2.275}$$

2.35

(a)

Let \mathbf{x} be a variable such that

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Sigma}).\tag{2.276}$$

Then,

$$E \mathbf{x} \mathbf{x}^\top = E(\mathbf{x} - \boldsymbol{\mu} + \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu} + \boldsymbol{\mu})^\top.\tag{2.277}$$

The right hand side can be written as

$$E(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top + \boldsymbol{\mu} E(\mathbf{x} - \boldsymbol{\mu})^\top + E(\mathbf{x} - \boldsymbol{\mu})\boldsymbol{\mu}^\top + \boldsymbol{\mu}\boldsymbol{\mu}^\top.\tag{2.278}$$

Since

$$\begin{aligned}E \mathbf{x} &= \boldsymbol{\mu}, \\ \text{cov } \mathbf{x} &= \boldsymbol{\Sigma},\end{aligned}\tag{2.279}$$

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

$$E \mathbf{x} \mathbf{x}^\top = \boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^\top.\tag{2.280}$$

(b)

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

$$\begin{aligned}p(\mathbf{x}_n) &= \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}, \boldsymbol{\Sigma}), \\ p(\mathbf{x}_m) &= \mathcal{N}(\mathbf{x}_m | \boldsymbol{\mu}, \boldsymbol{\Sigma}).\end{aligned}\tag{2.281}$$

If $n \neq m$, then

$$E \mathbf{x}_n \mathbf{x}_m^\top = E \mathbf{x}_n E \mathbf{x}_m^\top.\tag{2.282}$$

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

$$E \mathbf{x}_n \mathbf{x}_m^\top = I_{nm} \boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^\top.\tag{2.283}$$

(c)

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

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

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

$$\begin{aligned} \boldsymbol{\mu}_{\text{ML}} &= \frac{1}{N} \sum_{n=1}^N \mathbf{x}_n, \\ \boldsymbol{\Sigma}_{\text{ML}} &= \frac{1}{N} \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}})(\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}})^T. \end{aligned} \quad (2.285)$$

Then,

$$\mathbb{E} \boldsymbol{\Sigma}_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N \mathbb{E}(\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}})(\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}})^T. \quad (2.286)$$

The right hand side can be written as

$$\begin{aligned} &\frac{1}{N} \sum_{n=1}^N \mathbb{E} \mathbf{x}_n \mathbf{x}_n^T - \frac{1}{N^2} \sum_{n=1}^N \mathbb{E} \left(\sum_{n=1}^N \mathbf{x}_n \right) \mathbf{x}_n^T - \frac{1}{N^2} \sum_{n=1}^N \mathbb{E} \mathbf{x}_n \left(\sum_{n=1}^N \mathbf{x}_n \right)^T \\ &+ \frac{1}{N^3} \sum_{n=1}^N \mathbb{E} \left(\sum_{n=1}^N \mathbf{x}_n \right) \left(\sum_{n=1}^N \mathbf{x}_n \right)^T. \end{aligned} \quad (2.287)$$

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

$$-\frac{1}{N} ((\boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^T) + (N-1)\boldsymbol{\mu}\boldsymbol{\mu}^T) = -\frac{1}{N} \boldsymbol{\Sigma} - \boldsymbol{\mu}\boldsymbol{\mu}^T. \quad (2.288)$$

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

$$\frac{1}{N^2} (N(\boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^T) + N(N-1)\boldsymbol{\mu}\boldsymbol{\mu}^T) = \frac{1}{N} \boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^T. \quad (2.289)$$

Then,

$$\mathbb{E} \boldsymbol{\Sigma}_{\text{ML}} = (\boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^T) + 2 \left(-\frac{1}{N} \boldsymbol{\Sigma} - \boldsymbol{\mu}\boldsymbol{\mu}^T \right) + \frac{1}{N} \boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^T. \quad (2.290)$$

Therefore,

$$\mathbb{E} \boldsymbol{\Sigma}_{\text{ML}} = \frac{N-1}{N} \boldsymbol{\Sigma}. \quad (2.291)$$

2.36

Let x_1, \dots, x_N be variables such that

$$p(x_n) = \mathcal{N}(x_n | \mu, \sigma^2). \quad (2.292)$$

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

$$\sigma_{\text{ML}}^{(N)} = \frac{1}{N} \sum_{n=1}^N (x_n - \mu)^2. \quad (2.293)$$

The right hand side can be written as

$$\frac{1}{N} (x_N - \mu)^2 + \frac{1}{N} \sum_{n=1}^{N-1} (x_n - \mu)^2 = \frac{1}{N} (x_N - \mu)^2 + \frac{N-1}{N} \sigma_{\text{ML}}^{(N-1)}. \quad (2.294)$$

Then,

$$\sigma_{\text{ML}}^{(N)} = \sigma_{\text{ML}}^{(N-1)} + \frac{1}{N} \left((x_N - \mu)^2 - \sigma_{\text{ML}}^{(N-1)} \right). \quad (2.295)$$

We have

$$\frac{\partial}{\partial \sigma^2} (-\ln p(x_n)) = \frac{1}{2\sigma^2} - \frac{1}{2(\sigma^2)^2} (x_n - \mu)^2. \quad (2.296)$$

Therefore,

$$\sigma_{\text{ML}}^{(N)} = \sigma_{\text{ML}}^{(N-1)} - \frac{2 \left(\sigma_{\text{ML}}^{(N-1)} \right)^2}{N} \left(\frac{\partial}{\partial \sigma^2} (-\ln p(x_N)) \right) \Big|_{\sigma^2 = \sigma_{\text{ML}}^{(N-1)}}. \quad (2.297)$$

2.37

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

$$p(\mathbf{x}_n) = \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}, \boldsymbol{\Sigma}). \quad (2.298)$$

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

$$\boldsymbol{\Sigma}_{\text{ML}}^{(N)} = \frac{1}{N} \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{x}_n - \boldsymbol{\mu})^\top. \quad (2.299)$$

The right hand side can be written as

$$\begin{aligned} & \frac{1}{N}(\mathbf{x}_N - \boldsymbol{\mu})(\mathbf{x}_N - \boldsymbol{\mu})^\top + \frac{1}{N} \sum_{n=1}^{N-1} (\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{x}_n - \boldsymbol{\mu})^\top \\ &= \frac{1}{N}(\mathbf{x}_N - \boldsymbol{\mu})(\mathbf{x}_N - \boldsymbol{\mu})^\top + \frac{N-1}{N} \boldsymbol{\Sigma}_{\text{ML}}^{(N-1)}. \end{aligned} \quad (2.300)$$

Then,

$$\boldsymbol{\Sigma}_{\text{ML}}^{(N)} = \boldsymbol{\Sigma}_{\text{ML}}^{(N-1)} + \frac{1}{N} \left((\mathbf{x}_N - \boldsymbol{\mu})(\mathbf{x}_N - \boldsymbol{\mu})^\top - \boldsymbol{\Sigma}_{\text{ML}}^{(N-1)} \right). \quad (2.301)$$

By 3.21??, we have

$$\frac{\partial}{\partial \boldsymbol{\Sigma}} (-\ln p(x_n)) = -\frac{1}{2} (\boldsymbol{\Sigma}^{-1})^\top + \frac{1}{2} (\boldsymbol{\Sigma}^{-1})^2 (\mathbf{x}_N - \boldsymbol{\mu})(\mathbf{x}_N - \boldsymbol{\mu})^\top. \quad (2.302)$$

Therefore,

$$\boldsymbol{\Sigma}_{\text{ML}}^{(N)} = \boldsymbol{\Sigma}_{\text{ML}}^{(N-1)} - \frac{(\boldsymbol{\Sigma}_{\text{ML}}^{(N-1)})^2}{N} \left(\frac{\partial}{\partial \boldsymbol{\Sigma}} (-\ln p(\mathbf{x}_N)) \right) \Big|_{\boldsymbol{\Sigma}=\boldsymbol{\Sigma}_{\text{ML}}^{(N-1)}}. \quad (2.303)$$

2.38

Let x_1, \dots, x_N be variables such that

$$\begin{aligned} p(x_n|\mu) &= \mathcal{N}(x_n|\mu, \sigma^2), \\ p(\mu) &= \mathcal{N}(\mu|\mu_0, \sigma_0^2). \end{aligned} \quad (2.304)$$

By the Bayes' theorem,

$$p(\mu|\mathbf{x})p(\mathbf{x}) = p(\mathbf{x}|\mu)p(\mu). \quad (2.305)$$

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

$$-\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 - \frac{1}{2\sigma_0^2} (\mu - \mu_0)^2. \quad (2.306)$$

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

$$\mu_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N x_n. \quad (2.307)$$

Then, the first term can be written as

$$\begin{aligned} & -\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu_{\text{ML}} + \mu_{\text{ML}} - \mu)^2 \\ &= -\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu_{\text{ML}})^2 - \frac{\mu_{\text{ML}} - \mu}{\sigma^2} \sum_{n=1}^N (x_n - \mu_{\text{ML}}) - \frac{N}{2\sigma^2} (\mu_{\text{ML}} - \mu)^2. \end{aligned} \quad (2.308)$$

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

$$\begin{aligned} & -\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu_{\text{ML}})^2 - \frac{N}{2\sigma^2} (\mu_{\text{ML}} - \mu)^2 - \frac{1}{2\sigma_0^2} (\mu - \mu_0)^2 \\ &= -\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu_{\text{ML}})^2 - \frac{1}{2\sigma_N^2} (\mu - \mu_N)^2 + \frac{\mu_N^2}{2\sigma_N^2} - \frac{N\mu_{\text{ML}}^2}{2\sigma^2} - \frac{\mu_0^2}{2\sigma_0^2}, \end{aligned} \quad (2.309)$$

where

$$\begin{aligned} \mu_N &= \frac{N\sigma_0^2}{N\sigma_0^2 + \sigma^2} \mu_{\text{ML}} + \frac{\sigma^2}{N\sigma_0^2 + \sigma^2} \mu_0, \\ \sigma_N^2 &= \frac{\sigma^2 \sigma_0^2}{N\sigma_0^2 + \sigma^2}. \end{aligned} \quad (2.310)$$

Therefore,

$$p(\mu|\mathbf{x}) = \mathcal{N}(\mu|\mu_N, \sigma_N^2). \quad (2.311)$$

2.39

Let x_1, \dots, x_N be variables such that

$$\begin{aligned} p(x_n|\mu) &= \mathcal{N}(x_n|\mu, \sigma^2), \\ p(\mu) &= \mathcal{N}(\mu|\mu_0, \sigma_0^2). \end{aligned} \quad (2.312)$$

(a)

By 2.38,

$$p(\mu|\mathbf{x}) = \mathcal{N}(\mu|\mu_N, \sigma_N^2), \quad (2.313)$$

where

$$\begin{aligned} \mu_N &= \frac{\sigma_0^2}{N\sigma_0^2 + \sigma^2} \sum_{n=1}^N x_n + \frac{\sigma^2}{N\sigma_0^2 + \sigma^2} \mu_0, \\ \sigma_N^2 &= \frac{\sigma^2 \sigma_0^2}{N\sigma_0^2 + \sigma^2}. \end{aligned} \quad (2.314)$$

Then,

$$\frac{1}{\sigma_N^2} = \frac{(N-1)\sigma_0^2 + \sigma^2}{\sigma^2 \sigma_0^2} + \frac{1}{\sigma^2}. \quad (2.315)$$

Therefore,

$$\frac{1}{\sigma_N^2} = \frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}. \quad (2.316)$$

We have

$$\frac{\mu_N}{\sigma_N^2} = \frac{1}{\sigma^2} \sum_{n=1}^N x_n + \frac{\mu_0}{\sigma_0^2}, \quad (2.317)$$

so that

$$\frac{\mu_{N-1}}{\sigma_{N-1}^2} = \frac{1}{\sigma^2} \sum_{n=1}^{N-1} x_n + \frac{\mu_0}{\sigma_0^2}. \quad (2.318)$$

Therefore,

$$\frac{\mu_N}{\sigma_N^2} = \frac{\mu_{N-1}}{\sigma_{N-1}^2} + \frac{x_N}{\sigma^2}. \quad (2.319)$$

(b)

By the Bayes' theorem,

$$p(\mu|\mathbf{x}_N)p(\mathbf{x}_N) = p(\mathbf{x}_N|\mu)p(\mu). \quad (2.320)$$

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

$$p(\mu|\mathbf{x}_N)p(x_N)p(\mathbf{x}_{N-1}) = p(x_N|\mu)p(\mathbf{x}_{N-1}|\mu)p(\mu). \quad (2.321)$$

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

$$p(x_N|\mu)p(\mu|\mathbf{x}_{N-1})p(\mathbf{x}_{N-1}). \quad (2.322)$$

Then,

$$p(\mu|\mathbf{x}_N)p(x_N) = p(\mu|\mathbf{x}_{N-1})p(x_N|\mu). \quad (2.323)$$

The logarithm of the integrand of the right hand side except the terms independent of μ or x_N can be written as

$$\begin{aligned} & -\frac{1}{2\sigma_{N-1}^2}(\mu - \mu_{N-1})^2 - \frac{1}{2\sigma^2}(x_N - \mu)^2 \\ &= -\frac{1}{2} \left(\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2} \right) \left(\mu - \frac{\frac{1}{\sigma_{N-1}^2}}{\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}} \mu_{N-1} - \frac{\frac{1}{\sigma^2}}{\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}} x_N \right)^2 \\ &+ \frac{1}{2} \left(\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2} \right) \left(\frac{\frac{1}{\sigma_{N-1}^2}}{\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}} \mu_{N-1} + \frac{\frac{1}{\sigma^2}}{\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}} x_N \right)^2 - \frac{\mu_{N-1}^2}{2\sigma_{N-1}^2} - \frac{x_N^2}{2\sigma^2}. \end{aligned} \quad (2.324)$$

Then,

$$\begin{aligned} \mu_N &= \frac{\frac{1}{\sigma_{N-1}^2}}{\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}} \mu_{N-1} + \frac{\frac{1}{\sigma^2}}{\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}} x_N, \\ \sigma_N^2 &= \frac{1}{\frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}}. \end{aligned} \quad (2.325)$$

Therefore,

$$\begin{aligned} \frac{\mu_N}{\sigma_N^2} &= \frac{\mu_{N-1}}{\sigma_{N-1}^2} + \frac{x_N}{\sigma^2}, \\ \frac{1}{\sigma_N^2} &= \frac{1}{\sigma_{N-1}^2} + \frac{1}{\sigma^2}. \end{aligned} \quad (2.326)$$

2.40

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

$$\begin{aligned} p(\mathbf{x}_n|\boldsymbol{\mu}) &= \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}, \boldsymbol{\Sigma}), \\ p(\boldsymbol{\mu}) &= \mathcal{N}(\boldsymbol{\mu}|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0). \end{aligned} \quad (2.327)$$

By 2.34, the maximum likelihood solution for $\boldsymbol{\mu}$ is given by

$$\boldsymbol{\mu}_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N \mathbf{x}_n, \quad (2.328)$$

By the Bayes' theorem,

$$p(\boldsymbol{\mu}|\mathbf{X})p(\mathbf{X}) = p(\mathbf{X}|\boldsymbol{\mu})p(\boldsymbol{\mu}). \quad (2.329)$$

The logarithm of the right hand side except the terms independent of \mathbf{X} and $\boldsymbol{\mu}$ can be written as

$$-\frac{1}{2} \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu}) - \frac{1}{2} (\boldsymbol{\mu} - \boldsymbol{\mu}_0)^\top \boldsymbol{\Sigma}_0^{-1} (\boldsymbol{\mu} - \boldsymbol{\mu}_0). \quad (2.330)$$

The first term can be written as

$$\begin{aligned} & -\frac{1}{2} \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}} + \boldsymbol{\mu}_{\text{ML}} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}} + \boldsymbol{\mu}_{\text{ML}} - \boldsymbol{\mu}) \\ &= -\frac{1}{2} \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}}) - (\boldsymbol{\mu}_{\text{ML}} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}}) \\ & \quad - \frac{N}{2} (\boldsymbol{\mu}_{\text{ML}} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\boldsymbol{\mu}_{\text{ML}} - \boldsymbol{\mu}). \end{aligned} \quad (2.331)$$

The second term of the right hand side is zero. Then, the logarithm except the terms independent of \mathbf{X} and $\boldsymbol{\mu}$ can be written as

$$\begin{aligned} & -\frac{1}{2} \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}}) - \frac{N}{2} (\boldsymbol{\mu}_{\text{ML}} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\boldsymbol{\mu}_{\text{ML}} - \boldsymbol{\mu}) \\ & \quad - \frac{1}{2} (\boldsymbol{\mu} - \boldsymbol{\mu}_0)^\top \boldsymbol{\Sigma}_0^{-1} (\boldsymbol{\mu} - \boldsymbol{\mu}_0) \\ &= -\frac{1}{2} \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu}_{\text{ML}}) - \frac{1}{2} (\boldsymbol{\mu} - \boldsymbol{\mu}_N)^\top \boldsymbol{\Sigma}_N^{-1} (\boldsymbol{\mu} - \boldsymbol{\mu}_N) \\ & \quad + \frac{1}{2} \boldsymbol{\mu}_N^\top \boldsymbol{\Sigma}_N^{-1} \boldsymbol{\mu}_N - \frac{N}{2} \boldsymbol{\mu}_{\text{ML}}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_{\text{ML}}, \end{aligned} \quad (2.332)$$

where

$$\begin{aligned} \boldsymbol{\mu}_N &= (N\boldsymbol{\Sigma}^{-1} + \boldsymbol{\Sigma}_0^{-1})^{-1} (N\boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_{\text{ML}} + \boldsymbol{\Sigma}_0^{-1} \boldsymbol{\mu}_0), \\ \boldsymbol{\Sigma}_N &= (N\boldsymbol{\Sigma}^{-1} + \boldsymbol{\Sigma}_0^{-1})^{-1}. \end{aligned} \quad (2.333)$$

Therefore,

$$p(\boldsymbol{\mu}|\mathbf{X}) = \mathcal{N}(\boldsymbol{\mu}|\boldsymbol{\mu}_N, \boldsymbol{\Sigma}_N). \quad (2.334)$$

2.41

By the definition,

$$\text{Gam}(\lambda|a, b) = \frac{b^a}{\Gamma(a)} \lambda^{a-1} \exp(-b\lambda). \quad (2.335)$$

Then,

$$\int_0^\infty \text{Gam}(\lambda|a, b) d\lambda = \frac{b^a}{\Gamma(a)} \int_0^\infty \lambda^{a-1} \exp(-b\lambda) d\lambda. \quad (2.336)$$

By the transformation

$$\lambda' = b\lambda, \quad (2.337)$$

the right hand side can be written as

$$\frac{b^a}{\Gamma(a)} \int_0^\infty \left(\frac{\lambda'}{b}\right)^{a-1} \exp(-\lambda') \frac{1}{b} d\lambda' = \frac{1}{\Gamma(a)} \int_0^\infty \lambda'^{a-1} \exp(-\lambda') d\lambda'. \quad (2.338)$$

The right hand side can be written as

$$\frac{1}{\Gamma(a)} \Gamma(a) = 1. \quad (2.339)$$

Therefore,

$$\int_0^\infty \text{Gam}(\lambda|a, b) d\lambda = 1. \quad (2.340)$$

2.42

Let λ be a variable such that

$$p(\lambda) = \text{Gam}(\lambda|a, b). \quad (2.341)$$

By the definition,

$$\text{Gam}(\lambda|a, b) = \frac{b^a}{\Gamma(a)} \lambda^{a-1} \exp(-b\lambda). \quad (2.342)$$

(a)

We have

$$E \lambda = \frac{b^a}{\Gamma(a)} \int_0^\infty \lambda^a \exp\left(-\frac{\lambda}{b}\right) d\lambda. \quad (2.343)$$

By the transformation

$$\lambda' = b\lambda, \quad (2.344)$$

the right hand side can be written as

$$\frac{b^a}{\Gamma(a)} \int_0^\infty \left(\frac{\lambda'}{b}\right)^a \exp(-\lambda') \frac{1}{b} d\lambda' = \frac{1}{b\Gamma(a)} \int_0^\infty \lambda'^a \exp(-\lambda') d\lambda'. \quad (2.345)$$

The right hand side can be written as

$$\frac{1}{b\Gamma(a)} \Gamma(a+1) = \frac{a}{b}. \quad (2.346)$$

Therefore,

$$E \lambda = \frac{a}{b}. \quad (2.347)$$

(b)

We have

$$E \lambda^2 = \frac{b^a}{\Gamma(a)} \int_0^\infty \lambda^{a+1} \exp\left(-\frac{\lambda}{b}\right) d\lambda. \quad (2.348)$$

By the transformation

$$\lambda' = b\lambda, \quad (2.349)$$

the right hand side can be written as

$$\frac{b^a}{\Gamma(a)} \int_0^\infty \left(\frac{\lambda'}{b}\right)^{a+1} \exp(-\lambda') \frac{1}{b} d\lambda' = \frac{1}{b^2\Gamma(a)} \int_0^\infty \lambda'^{a+1} \exp(-\lambda') d\lambda'. \quad (2.350)$$

The right hand side can be written as

$$\frac{1}{b^2\Gamma(a)} \Gamma(a+2) = \frac{a(a+1)}{b^2}. \quad (2.351)$$

Then,

$$E \lambda^2 = \frac{a(a+1)}{b^2}. \quad (2.352)$$

We have

$$\text{var } \lambda = E \lambda^2 - (E \lambda)^2. \quad (2.353)$$

Therefore,

$$\text{var } \lambda = \frac{a}{b^2}. \quad (2.354)$$

(c)

Setting the derivative of $\text{Gam}(\lambda|a, b)$ with respect to λ to zero gives

$$0 = \frac{b^a}{\Gamma(a)} \left(\frac{a-1}{\lambda} - b \right) \lambda^{a-1} \exp \left(-\frac{\lambda}{b} \right). \quad (2.355)$$

Therefore,

$$\text{mode } \lambda = \frac{a-1}{b}. \quad (2.356)$$

2.43

Let

$$p(x|\sigma^2, q) = \frac{q}{2\Gamma(\frac{1}{q})} (2\sigma^2)^{-\frac{1}{q}} \exp \left(-\frac{|x|^q}{2\sigma^2} \right). \quad (2.357)$$

(a)

We have

$$\int_{-\infty}^{\infty} p(x|\sigma^2, q) dx = \frac{q}{\Gamma(\frac{1}{q})} (2\sigma^2)^{-\frac{1}{q}} \int_0^{\infty} \exp \left(-\frac{x^q}{2\sigma^2} \right) dx. \quad (2.358)$$

By the transformation

$$x' = \frac{x^q}{2\sigma^2}, \quad (2.359)$$

the right hand side can be written as

$$\begin{aligned} & \frac{q}{\Gamma(\frac{1}{q})} (2\sigma^2)^{-\frac{1}{q}} \int_0^{\infty} \exp(-x') (2\sigma^2)^{\frac{1}{q}} \frac{1}{q} x^{\frac{1}{q}-1} dx' \\ &= \frac{1}{\Gamma(\frac{1}{q})} \int_0^{\infty} x^{\frac{1}{q}-1} \exp(-x') dx'. \end{aligned} \quad (2.360)$$

The right hand side can be written as

$$\frac{1}{\Gamma(\frac{1}{q})} \Gamma\left(\frac{1}{q}\right) = 1. \quad (2.361)$$

Therefore,

$$\int_{-\infty}^{\infty} p(x|\sigma^2, q) dx = 1. \quad (2.362)$$

(b)

We have

$$p(x|\sigma^2, 2) = \frac{1}{\Gamma(\frac{1}{2})} (2\sigma^2)^{-\frac{1}{2}} \exp\left(-\frac{x^2}{2\sigma^2}\right). \quad (2.363)$$

Therefore,

$$p(x|\sigma^2, 2) = \mathcal{N}(x|0, \sigma^2). \quad (2.364)$$

(c)

Let $\mathbf{t} = (t_1, \dots, t_N)^\top$ and $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ such that

$$t_n = y(\mathbf{x}_n, \mathbf{w}) + \epsilon_n, \quad (2.365)$$

where

$$p(\epsilon_n) = p(\epsilon_n|\sigma^2, q). \quad (2.366)$$

Then, the logarithm of $p(\epsilon_n)$ except the terms independent of \mathbf{w} and σ^2 can be written as

$$-\frac{|\epsilon_n|^q}{2\sigma^2} - \frac{1}{q} \ln(2\sigma^2). \quad (2.367)$$

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

$$-\frac{1}{2\sigma^2} \sum_{n=1}^N |\epsilon_n|^q - \frac{N}{q} \ln(2\sigma^2). \quad (2.368)$$

2.44

Let x_1, \dots, x_N be variables such that

$$\begin{aligned} p(x_n|\mu, \tau) &= \mathcal{N}(x_n|\mu, \tau^{-1}), \\ p(\mu, \tau) &= \mathcal{N}(\mu|\mu_0, (\beta\tau)^{-1}) \text{Gam}(\tau|a, b). \end{aligned} \quad (2.369)$$

By the Bayes' theorem,

$$p(\mu, \tau|x)p(x) = p(x|\mu, \tau)p(\mu, \tau). \quad (2.370)$$

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

$$\begin{aligned} &\frac{N}{2} \ln \tau - \frac{\tau}{2} \sum_{n=1}^N (x_n - \mu)^2 + \frac{1}{2} \ln \tau - \frac{\beta\tau}{2} (\mu - \mu_0)^2 + (a - 1) \ln \tau - b\tau \\ &= \left(a + \frac{N-1}{2} \right) \ln \tau - \frac{\tau}{2} \sum_{n=1}^N (x_n - \mu)^2 - \frac{\beta\tau}{2} (\mu - \mu_0)^2 - b\tau. \end{aligned} \quad (2.371)$$

Let

$$\bar{x} = \frac{1}{N} \sum_{n=1}^N x_n. \quad (2.372)$$

Then,

$$\sum_{n=1}^N (x_n - \mu)^2 = \sum_{n=1}^N (x_n - \bar{x} + \bar{x} - \mu)^2. \quad (2.373)$$

The right hand side can be written as

$$\begin{aligned} &\sum_{n=1}^N (x_n - \bar{x})^2 + 2(\bar{x} - \mu) \sum_{n=1}^N (x_n - \bar{x}) + N(\bar{x} - \mu)^2 \\ &= \sum_{n=1}^N (x_n - \bar{x})^2 + N(\bar{x} - \mu)^2. \end{aligned} \quad (2.374)$$

Then, the logarithm except the terms independent of \mathbf{x} , μ and τ can be written as

$$\left(a + \frac{N-1}{2} \right) \ln \tau - \frac{N\tau}{2} (\bar{x} - \mu)^2 - \frac{\beta\tau}{2} (\mu - \mu_0)^2 - b\tau - \frac{\tau}{2} \sum_{n=1}^N (x_n - \bar{x})^2. \quad (2.375)$$

The second and third terms can be written as

$$\begin{aligned} & -\frac{N\tau}{2}(\bar{x} - \mu)^2 - \frac{\beta\tau}{2}(\mu - \mu_0)^2 \\ & = -\frac{(N + \beta)\tau}{2} \left(\mu - \frac{N\bar{x} + \beta\mu_0}{N + \beta} \right)^2 + \frac{(N\bar{x} + \beta\mu_0)^2\tau}{2(N + \beta)} - \frac{N\tau}{2}\bar{x}^2 - \frac{\beta\tau}{2}\mu_0^2. \end{aligned} \quad (2.376)$$

The second, third and forth terms on the right hand side can be written as

$$\frac{(N\bar{x} + \beta\mu_0)^2\tau - (N + \beta)N\tau\bar{x}^2 - (N + \beta)\beta\tau\mu_0^2}{2(N + \beta)} = -\frac{N\beta\tau(\bar{x} - \mu_0)^2}{2(N + \beta)}. \quad (2.377)$$

Then, the logarithm except the terms independent of \mathbf{x} , μ and τ can be written as

$$\begin{aligned} & -\frac{(N + \beta)\tau}{2} \left(\mu - \frac{N\bar{x} + \beta\mu_0}{N + \beta} \right)^2 \\ & + \left(a + \frac{N - 1}{2} \right) \ln \tau - \left(b + \frac{N\beta(\bar{x} - \mu_0)^2}{2(N + \beta)} + \frac{1}{2} \sum_{n=1}^N (x_n - \bar{x})^2 \right) \tau. \end{aligned} \quad (2.378)$$

Therefore,

$$p(\mu, \tau | \mathbf{x}) = \mathcal{N}(\mu | \mu_N, \tau_N^{-1}) \text{Gam}(\tau | a_N, b_N), \quad (2.379)$$

where

$$\begin{aligned} \mu_N &= \frac{N\bar{x} + \beta\mu_0}{N + \beta}, \\ \tau_N &= (N + \beta)\tau, \\ a_N &= a + \frac{N + 1}{2}, \\ b_N &= b + \frac{N\beta(\bar{x} - \mu_0)^2}{2(N + \beta)} + \frac{1}{2} \sum_{n=1}^N (x_n - \bar{x})^2. \end{aligned} \quad (2.380)$$

2.45

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

$$\begin{aligned} p(\mathbf{x}_n | \boldsymbol{\Lambda}) &= \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}), \\ p(\boldsymbol{\Lambda}) &= \mathcal{W}(\boldsymbol{\Lambda} | \mathbf{W}, \nu), \end{aligned} \quad (2.381)$$

where

$$\mathcal{W}(\boldsymbol{\Lambda}|\mathbf{W}, \nu) = B(\mathbf{W}, \nu) |\det \boldsymbol{\Lambda}|^{\frac{\nu-D-1}{2}} \exp\left(-\frac{1}{2} \text{tr}(\mathbf{W}^{-1} \boldsymbol{\Lambda})\right). \quad (2.382)$$

By the Bayes' theorem,

$$p(\boldsymbol{\Lambda}|\mathbf{X})p(\mathbf{X}) = p(\mathbf{X}|\boldsymbol{\Lambda})p(\boldsymbol{\Lambda}). \quad (2.383)$$

The logarithm of the right hand side except the terms independent of $\boldsymbol{\Lambda}$ can be written as

$$\begin{aligned} & -\frac{N}{2} \ln |\det(\boldsymbol{\Lambda}^{-1})| - \frac{1}{2} \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu})^\top \boldsymbol{\Lambda} (\mathbf{x}_n - \boldsymbol{\mu}) \\ & + \frac{\nu - D - 1}{2} \ln |\det \boldsymbol{\Lambda}| - \frac{1}{2} \text{tr}(\mathbf{W}^{-1} \boldsymbol{\Lambda}) \\ & = \frac{\nu + N - D - 1}{2} \ln |\det \boldsymbol{\Lambda}| - \frac{1}{2} \text{tr}((\mathbf{W}^{-1} + \mathbf{S}) \boldsymbol{\Lambda}), \end{aligned} \quad (2.384)$$

where

$$\mathbf{S} = \sum_{n=1}^N (\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{x}_n - \boldsymbol{\mu})^\top. \quad (2.385)$$

Then,

$$p(\boldsymbol{\Lambda}|\mathbf{X}) = \mathcal{W}\left(\boldsymbol{\Lambda} | (\mathbf{W}^{-1} + \mathbf{S})^{-1}, \nu + N\right). \quad (2.386)$$

Therefore, \mathcal{W} is a conjugate prior distribution of $\boldsymbol{\Lambda}$.

2.46

Let x be a variable such that

$$\begin{aligned} p(x|\tau) &= \mathcal{N}(x|\mu, \tau^{-1}), \\ p(\tau) &= \text{Gam}(\tau|a, b). \end{aligned} \quad (2.387)$$

By marginalisation,

$$p(x) = \int_0^\infty p(x|\tau)p(\tau)d\tau. \quad (2.388)$$

The right hand side can be written as

$$\begin{aligned} & \int_0^\infty (2\pi\tau^{-1})^{-\frac{1}{2}} \exp\left(-\frac{\tau}{2}(x-\mu)^2\right) \frac{b^a}{\Gamma(a)} \tau^{a-1} \exp(-b\tau) d\tau \\ &= (2\pi)^{-\frac{1}{2}} \frac{b^a}{\Gamma(a)} \int_0^\infty \tau^{a-\frac{1}{2}} \exp\left(-\left(b + \frac{(x-\mu)^2}{2}\right)\tau\right) d\tau. \end{aligned} \quad (2.389)$$

By the transformation

$$\tau' = \left(b + \frac{(x-\mu)^2}{2}\right)\tau, \quad (2.390)$$

the integral of the right hand side can be written as

$$\begin{aligned} & \int_0^\infty \left(\frac{\tau'}{b + \frac{(x-\mu)^2}{2}}\right)^{a-\frac{1}{2}} \exp(-\tau') \frac{1}{b + \frac{(x-\mu)^2}{2}} d\tau' \\ &= \Gamma\left(a + \frac{1}{2}\right) \left(b + \frac{(x-\mu)^2}{2}\right)^{-a-\frac{1}{2}}. \end{aligned} \quad (2.391)$$

Then,

$$p(x) = (2\pi)^{-\frac{1}{2}} \frac{\Gamma(a + \frac{1}{2})}{\Gamma(a)} b^a \left(b + \frac{(x-\mu)^2}{2}\right)^{-a-\frac{1}{2}}. \quad (2.392)$$

By the transformation

$$\begin{aligned} \nu &= 2a, \\ \lambda &= \frac{a}{b}, \end{aligned} \quad (2.393)$$

the right hand side can be written as

$$\begin{aligned} & (2\pi)^{-\frac{1}{2}} \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})} \left(\frac{\nu}{2\lambda}\right)^{-\frac{1}{2}} \left(1 + \frac{(x-\mu)^2}{\frac{\nu}{\lambda}}\right)^{-\frac{\nu+1}{2}} \\ &= \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})} \left(\frac{\lambda}{\pi\nu}\right)^{\frac{1}{2}} \left(1 + \frac{\lambda}{\nu}(x-\mu)^2\right)^{-\frac{\nu+1}{2}}. \end{aligned} \quad (2.394)$$

Therefore,

$$p(x) = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})} \left(\frac{\lambda}{\pi\nu}\right)^{\frac{1}{2}} \left(1 + \frac{\lambda}{\nu}(x-\mu)^2\right)^{-\frac{\nu+1}{2}}. \quad (2.395)$$

2.47

Let

$$\text{St}(x|\mu, \lambda, \nu) = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})} \left(\frac{\lambda}{\pi\nu} \right)^{\frac{1}{2}} \left(1 + \frac{\lambda}{\nu}(x - \mu)^2 \right)^{-\frac{\nu+1}{2}}. \quad (2.396)$$

By the transformation

$$\frac{1}{y} = \frac{\lambda}{\nu}(x - \mu)^2, \quad (2.397)$$

the right hand side except the terms independent of x can be written as

$$\left(1 + \frac{1}{y} \right)^{-\frac{\lambda(x-\mu)^2}{2} y - \frac{1}{2}}. \quad (2.398)$$

By the property

$$\lim_{x \rightarrow \infty} \left(1 + \frac{1}{x} \right)^x = e, \quad (2.399)$$

we have

$$\lim_{y \rightarrow \infty} \left(1 + \frac{1}{y} \right)^{-\frac{\lambda(x-\mu)^2}{2} y - \frac{1}{2}} = \exp \left(-\frac{\lambda}{2}(x - \mu)^2 \right). \quad (2.400)$$

Therefore,

$$\lim_{\nu \rightarrow \infty} \text{St}(x|\mu, \lambda, \nu) = \mathcal{N}(x|\mu, \lambda^{-1}). \quad (2.401)$$

2.48

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

$$\begin{aligned} p(\mathbf{x}|\eta) &= \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, (\eta\Lambda)^{-1}), \\ p(\eta) &= \text{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right). \end{aligned} \quad (2.402)$$

By marginalisation,

$$p(\mathbf{x}) = \int_0^\infty p(\mathbf{x}|\eta)p(\eta)d\eta. \quad (2.403)$$

The right hand side can be written as

$$\begin{aligned} &\int_0^\infty (2\pi)^{-\frac{D}{2}} |\det(\eta\Lambda)^{-1}|^{-\frac{1}{2}} \exp\left(-\frac{\eta}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \Lambda(\mathbf{x} - \boldsymbol{\mu})\right) \frac{(\frac{\nu}{2})^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})} \eta^{\frac{\nu}{2}-1} \exp\left(-\frac{\nu}{2}\eta\right) d\eta \\ &= (2\pi)^{-\frac{D}{2}} \frac{(\frac{\nu}{2})^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})} |\det \Lambda|^{\frac{1}{2}} \int_0^\infty \eta^{\frac{D+\nu}{2}-1} \exp\left(-\frac{\nu + (\mathbf{x} - \boldsymbol{\mu})^\top \Lambda(\mathbf{x} - \boldsymbol{\mu})}{2}\eta\right) d\eta. \end{aligned} \quad (2.404)$$

By the transformation

$$\eta' = \frac{\nu + (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu})}{2} \eta, \quad (2.405)$$

the integral of the right hand side can be written as

$$\begin{aligned} & \int_0^\infty \left(\frac{2\eta'}{\nu + (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu})} \right)^{\frac{D+\nu}{2}-1} \exp(-\eta') \frac{2}{\nu + (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu})} d\eta' \\ &= \left(\frac{2}{\nu + (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu})} \right)^{\frac{D+\nu}{2}} \int_0^\infty \eta'^{\frac{D+\nu}{2}-1} \exp(-\eta') d\eta'. \end{aligned} \quad (2.406)$$

Then,

$$p(\mathbf{x}) = (2\pi)^{-\frac{D}{2}} \frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma\left(\frac{\nu}{2}\right)} |\det \boldsymbol{\Lambda}|^{\frac{1}{2}} \left(\frac{2}{\nu + (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu})} \right)^{\frac{D+\nu}{2}} \Gamma\left(\frac{D+\nu}{2}\right). \quad (2.407)$$

The right hand side can be written as

$$\begin{aligned} & (2\pi)^{-\frac{D}{2}} \frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})} |\det \boldsymbol{\Lambda}|^{\frac{1}{2}} \left(\frac{\nu}{2}\right)^{-\frac{D}{2}} \left(\frac{\nu}{2}\right)^{\frac{D+\nu}{2}} \left(\frac{2}{\nu + (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu})} \right)^{\frac{D+\nu}{2}} \\ &= (2\pi)^{-\frac{D}{2}} \frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})} |\det \boldsymbol{\Lambda}|^{\frac{1}{2}} \left(\frac{\nu}{2}\right)^{-\frac{D}{2}} \left(1 + \frac{(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu})}{\nu}\right)^{-\frac{D+\nu}{2}}. \end{aligned} \quad (2.408)$$

Therefore,

$$p(\mathbf{x}) = \frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})} \frac{|\det \boldsymbol{\Lambda}|^{\frac{1}{2}}}{(\pi\nu)^{\frac{D}{2}}} \left(1 + \frac{(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda}(\mathbf{x} - \boldsymbol{\mu})}{\nu}\right)^{-\frac{D+\nu}{2}}. \quad (2.409)$$

2.49

Let \mathbf{x} be a variable such that

$$p(\mathbf{x}) = \text{St}(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Lambda}, \nu), \quad (2.410)$$

where

$$\text{St}(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Lambda}, \nu) = \int \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}, (\eta \boldsymbol{\Lambda})^{-1}) \text{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta. \quad (2.411)$$

(a)

We have

$$E \mathbf{x} = \int \mathbf{x} St(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}, \nu) d\mathbf{x}. \quad (2.412)$$

The right hand side can be written as

$$\begin{aligned} & \int \mathbf{x} \left(\int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, (\eta\boldsymbol{\Lambda})^{-1}) \text{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta \right) d\mathbf{x} \\ &= \int \left(\int \mathbf{x} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, (\eta\boldsymbol{\Lambda})^{-1}) d\mathbf{x} \right) \text{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta. \end{aligned} \quad (2.413)$$

The right hand side can be written as

$$\boldsymbol{\mu} \int \text{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta = \boldsymbol{\mu}. \quad (2.414)$$

Therefore,

$$E \mathbf{x} = \boldsymbol{\mu}. \quad (2.415)$$

(b)

By (a), we have

$$\text{cov } \mathbf{x} = \int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top St(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}, \nu) d\mathbf{x}. \quad (2.416)$$

The right hand side can be written as

$$\begin{aligned} & \int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top \left(\int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, (\eta\boldsymbol{\Lambda})^{-1}) \text{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta \right) d\mathbf{x} \\ &= \int \left(\int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, (\eta\boldsymbol{\Lambda})^{-1}) d\mathbf{x} \right) \text{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta. \end{aligned} \quad (2.417)$$

The right hand side can be written as

$$\int (\eta\boldsymbol{\Lambda})^{-1} \text{Gam}\left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2}\right) d\eta = \frac{(\frac{\nu}{2})^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})} \left(\int \eta^{\frac{\nu}{2}-2} \exp\left(-\frac{\nu}{2}\eta\right) d\eta \right) \boldsymbol{\Lambda}^{-1}. \quad (2.418)$$

By the transformation

$$\eta' = \frac{\nu}{2}\eta, \quad (2.419)$$

the integral of the right hand side can be written as

$$\int \left(\frac{2}{\nu} \eta' \right)^{\frac{\nu}{2}-2} \exp(-\eta') \frac{2}{\nu} d\eta' = \left(\frac{2}{\nu} \right)^{\frac{\nu}{2}-1} \Gamma \left(\frac{\nu}{2} - 1 \right). \quad (2.420)$$

Then,

$$\text{cov } \mathbf{x} = \frac{\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}}{\Gamma\left(\frac{\nu}{2}\right)} \left(\frac{2}{\nu} \right)^{\frac{\nu}{2}-1} \Gamma \left(\frac{\nu}{2} - 1 \right) \boldsymbol{\Lambda}^{-1}. \quad (2.421)$$

Therefore,

$$\text{cov } \mathbf{x} = \frac{\nu}{\nu - 2} \boldsymbol{\Lambda}^{-1}. \quad (2.422)$$

(c)

Setting the derivative of $p(\mathbf{x})$ to zero gives

$$\mathbf{0} = -\frac{1}{2} (\boldsymbol{\Lambda} + \boldsymbol{\Lambda}^\top) (\mathbf{x} - \boldsymbol{\mu}) \int \eta \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}, (\eta \boldsymbol{\Lambda})^{-1}) \text{Gam} \left(\eta \mid \frac{\nu}{2}, \frac{\nu}{2} \right) d\eta. \quad (2.423)$$

Therefore,

$$\text{mode } \mathbf{x} = \boldsymbol{\mu}. \quad (2.424)$$

2.50

Let

$$\text{St}(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Lambda}, \nu) = \frac{\Gamma(\frac{D+\nu}{2})}{\Gamma(\frac{\nu}{2})} \frac{(\det \boldsymbol{\Lambda})^{\frac{1}{2}}}{(\pi \nu)^{\frac{D}{2}}} \left(1 + \frac{(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})}{\nu} \right)^{-\frac{D+\nu}{2}}. \quad (2.425)$$

By the transformation

$$y = \frac{\nu}{(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})}, \quad (2.426)$$

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

$$\left(1 + \frac{1}{y} \right)^{-\frac{(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})}{2} y - \frac{D}{2}}. \quad (2.427)$$

By the property

$$\lim_{x \rightarrow \infty} \left(1 + \frac{1}{x} \right)^x = e, \quad (2.428)$$

we have

$$\lim_{y \rightarrow \infty} \left(1 + \frac{1}{y}\right)^{-\frac{(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Lambda} (\mathbf{x}-\boldsymbol{\mu})}{2} y - \frac{D}{2}} = \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})\right). \quad (2.429)$$

Therefore,

$$\lim_{\nu \rightarrow \infty} \text{St}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}, \nu) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}). \quad (2.430)$$

2.51

(a)

We have

$$\exp(iA) \exp(-iA) = 1. \quad (2.431)$$

The left hand side can be written as

$$(\cos A + i \sin A)(\cos A - i \sin A) = \cos^2 A + \sin^2 A. \quad (2.432)$$

Therefore,

$$\cos^2 A + \sin^2 A = 1. \quad (2.433)$$

(b)

We have

$$\cos(A - B) = \text{Re}(\exp(i(A - B))). \quad (2.434)$$

The right hand side can be written as

$$\text{Re}(\exp(iA) \exp(-iB)) = \text{Re}((\cos A + i \sin A)(\cos B - i \sin B)). \quad (2.435)$$

Therefore,

$$\cos(A - B) = \cos A \cos B + \sin A \sin B. \quad (2.436)$$

(c)

We have

$$\sin(A - B) = \text{Im}(\exp(i(A - B))). \quad (2.437)$$

The right hand side can be written as

$$\text{Im}(\exp(iA) \exp(-iB)) = ((\cos A + i \sin A)(\cos B - i \sin B)). \quad (2.438)$$

Therefore,

$$\sin(A - B) = \sin A \cos B - \cos A \sin B. \quad (2.439)$$

2.52

Let

$$f(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp(m \cos(\theta - \theta_0)), \quad (2.440)$$

where

$$I_0(m) = \frac{1}{2\pi} \int_0^{2\pi} \exp(m \cos \theta) d\theta. \quad (2.441)$$

By the Taylor series

$$\cos \alpha = 1 - \frac{1}{2}\alpha^2 + O(\alpha^4), \quad (2.442)$$

the right hand side can be written as

$$\begin{aligned} & \frac{\exp(m(1 - \frac{1}{2}(\theta - \theta_0)^2 + O((\theta - \theta_0)^4)))}{\int_0^{2\pi} \exp(m(1 - \frac{1}{2}\theta^2 + O(\theta^4))) d\theta} \\ &= \exp\left(-\frac{m}{2}(\theta - \theta_0)^2\right) \frac{\exp(mO((\theta - \theta_0)^4))}{\int_0^{2\pi} \exp(m(-\frac{1}{2}\theta^2 + O(\theta^4))) d\theta}. \end{aligned} \quad (2.443)$$

Therefore,

$$\lim_{m \rightarrow \infty} f(\theta|\theta_0, m) = \mathcal{N}(\theta|\theta_0, m^{-1}). \quad (2.444)$$

2.53

Let

$$\sum_{n=1}^N \sin(\theta_n - \theta_0) = 0. \quad (2.445)$$

The left hand side can be written as

$$\sum_{n=1}^N (\sin \theta_n \cos \theta_0 - \cos \theta_n \sin \theta_0) = \cos \theta_0 \sum_{n=1}^N \sin \theta_n - \sin \theta_0 \sum_{n=1}^N \cos \theta_n. \quad (2.446)$$

Therefore,

$$\theta_0 = \arctan \left(\frac{\sum_{n=1}^N \sin \theta_n}{\sum_{n=1}^N \cos \theta_n} \right). \quad (2.447)$$

2.54

Let

$$f(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp(m \cos(\theta - \theta_0)), \quad (2.448)$$

where

$$I_0(m) = \frac{1}{2\pi} \int_0^{2\pi} \exp(m \cos \theta) d\theta. \quad (2.449)$$

Setting the first and second derivatives with respect to θ to zero gives

$$\begin{aligned} 0 &= -m \sin(\theta - \theta_0) f(\theta|\theta_0, m), \\ 0 &= (m^2 \sin^2(\theta - \theta_0) - m \cos(\theta - \theta_0)) f(\theta|\theta_0, m). \end{aligned} \quad (2.450)$$

Therefore,

$$\begin{aligned} \operatorname{argmax}_{\theta} f(\theta|\theta_0, m) &= \theta_0, \\ \operatorname{argmin}_{\theta} f(\theta|\theta_0, m) &= \theta_0 - \pi \operatorname{sgn}(\theta_0 - \pi). \end{aligned} \quad (2.451)$$

2.55

(a)

Let $\theta_1, \dots, \theta_N$ be variables such that

$$p(\theta_n) = f(\theta_n|\theta_0, m), \quad (2.452)$$

where

$$\begin{aligned} f(\theta|\theta_0, m) &= \frac{1}{2\pi I_0(m)} \exp(m \cos(\theta - \theta_0)), \\ I_0(m) &= \frac{1}{2\pi} \int_0^{2\pi} \exp(m \cos \theta) d\theta. \end{aligned} \quad (2.453)$$

Then,

$$\ln \left(\prod_{n=1}^N p(\theta_n|\theta_0, m) \right) = -\frac{N}{2} \ln(2\pi I_0(m)) + m \sum_{n=1}^N \cos(\theta_n - \theta_0). \quad (2.454)$$

Setting the derivative with respect to θ_0 to zero gives

$$0 = m \sum_{n=1}^N \sin(\theta_n - \theta_0). \quad (2.455)$$

Therefore, by 2.53, the maximum likelihood solution for θ_0 is given by

$$\theta_0^{\text{ML}} = \arctan \left(\frac{\sum_{n=1}^N \sin \theta_n}{\sum_{n=1}^N \cos \theta_n} \right). \quad (2.456)$$

(b)

Let

$$\begin{aligned} \bar{r} \cos \bar{\theta} &= \frac{1}{N} \sum_{n=1}^N \cos \theta_n, \\ \bar{r} \sin \bar{\theta} &= \frac{1}{N} \sum_{n=1}^N \sin \theta_n. \end{aligned} \quad (2.457)$$

By (a),

$$\bar{\theta} = \theta_0^{\text{ML}}. \quad (2.458)$$

We have

$$\frac{1}{N} \sum_{n=1}^N \cos (\theta_n - \theta_0^{\text{ML}}) = \left(\frac{1}{N} \sum_{n=1}^N \cos \theta_n \right) \cos \theta_0^{\text{ML}} + \left(\frac{1}{N} \sum_{n=1}^N \sin \theta_n \right) \sin \theta_0^{\text{ML}}. \quad (2.459)$$

The right hand side can be written as

$$\bar{r} \cos^2 \bar{\theta} + \bar{r} \sin^2 \bar{\theta} = \bar{r}. \quad (2.460)$$

Therefore,

$$\frac{1}{N} \sum_{n=1}^N \cos (\theta_n - \theta_0^{\text{ML}}) = \bar{r}. \quad (2.461)$$

2.56

(a)

Let

$$\text{Beta}(\mu|a, b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \mu^{a-1} (1-\mu)^{b-1}. \quad (2.462)$$

The right hand side can be written as

$$\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \exp ((a-1) \ln \mu + (b-1) \ln(1-\mu)) \quad (2.463)$$

Therefore, the natural parameters are given by

$$\boldsymbol{\eta} = \begin{bmatrix} a - 1 \\ b - 1 \end{bmatrix}.$$

(b)

Let

$$\text{Gam}(\lambda|a, b) = \frac{b^a}{\Gamma(a)} \lambda^{a-1} \exp(-b\lambda). \quad (2.464)$$

The right hand side can be written as

$$\frac{b^a}{\Gamma(a)} \exp((a-1)\ln\lambda - b\lambda). \quad (2.465)$$

Therefore, the natural parameters are given by

$$\boldsymbol{\eta} = \begin{bmatrix} a - 1 \\ -b \end{bmatrix}.$$

(c)

Let

$$f(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp(m \cos(\theta - \theta_0)), \quad (2.466)$$

where

$$I_0(m) = \frac{1}{2\pi} \int_0^{2\pi} \exp(m \cos \theta) d\theta, \quad (2.467)$$

the right hand side can be written as

$$\frac{1}{2\pi I_0(m)} \exp(m \cos \theta_0 \cos \theta + m \sin \theta_0 \sin \theta). \quad (2.468)$$

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,

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}} (\det \boldsymbol{\Sigma})^{-\frac{1}{2}} \exp \left(-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right). \quad (2.469)$$

Therefore,

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = h(\mathbf{x})g(\boldsymbol{\eta}) \exp(\boldsymbol{\eta}^\top \mathbf{u}(\mathbf{x})), \quad (2.470)$$

where

$$\begin{aligned} h(\mathbf{x}) &= (2\pi)^{-\frac{D}{2}}, \\ g(\boldsymbol{\eta}) &= (\det(-2\boldsymbol{\eta}_2))^{-\frac{1}{2}} \exp \left(\frac{1}{4} \boldsymbol{\eta}_1^\top \boldsymbol{\eta}_2^{-1} \boldsymbol{\eta}_1 \right), \\ \boldsymbol{\eta} &= \begin{bmatrix} \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu} \\ -\frac{1}{2} \boldsymbol{\Sigma}^{-1} \end{bmatrix}, \\ \mathbf{u}(\mathbf{x}) &= \begin{bmatrix} \mathbf{x} \\ \mathbf{x}\mathbf{x}^\top \end{bmatrix}. \end{aligned}$$

2.58

Let \mathbf{x} be a variable such that

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta}) \exp(\boldsymbol{\eta}^\top \mathbf{u}(\mathbf{x})). \quad (2.471)$$

Then, taking the first derivative of

$$\int p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} = 1 \quad (2.472)$$

with respect to $\boldsymbol{\eta}$ gives

$$\nabla g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp(\boldsymbol{\eta}^\top \mathbf{u}(\mathbf{x})) d\mathbf{x} + g(\boldsymbol{\eta}) \int \mathbf{u}(\mathbf{x}) h(\mathbf{x}) \exp(\boldsymbol{\eta}^\top \mathbf{u}(\mathbf{x})) d\mathbf{x} = \mathbf{0}. \quad (2.473)$$

The left hand side can be written as

$$\frac{\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} \int p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} + \int \mathbf{u}(\mathbf{x}) p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} = \frac{\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} + \mathbf{E} \mathbf{u}(\mathbf{x}). \quad (2.474)$$

Therefore,

$$\mathbf{E} \mathbf{u}(\mathbf{x}) = -\frac{\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})}. \quad (2.475)$$

Thus,

$$E \mathbf{u}(\mathbf{x}) = -\nabla \ln g(\boldsymbol{\eta}). \quad (2.476)$$

Taking the second derivative with respect to $\boldsymbol{\eta}$ gives

$$\begin{aligned} & \nabla \nabla g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp(\boldsymbol{\eta}^\top \mathbf{u}(\mathbf{x})) d\mathbf{x} + 2 \nabla g(\boldsymbol{\eta}) \int \mathbf{u}(\mathbf{x})^\top h(\mathbf{x}) \exp(\boldsymbol{\eta}^\top \mathbf{u}(\mathbf{x})) d\mathbf{x} \\ & + g(\boldsymbol{\eta}) \int \mathbf{u}(\mathbf{x}) \mathbf{u}(\mathbf{x})^\top h(\mathbf{x}) \exp(\boldsymbol{\eta}^\top \mathbf{u}(\mathbf{x})) d\mathbf{x} = \mathbf{O}. \end{aligned} \quad (2.477)$$

The left hand side can be written as

$$\begin{aligned} & \frac{\nabla \nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} \int p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} + \frac{2 \nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} \int \mathbf{u}(\mathbf{x})^\top p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} + \int \mathbf{u}(\mathbf{x}) \mathbf{u}(\mathbf{x})^\top p(\mathbf{x}|\boldsymbol{\eta}) d\mathbf{x} \\ & = \frac{\nabla \nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} - 2 E \mathbf{u}(\mathbf{x}) E \mathbf{u}(\mathbf{x})^\top + E (\mathbf{u}(\mathbf{x}) \mathbf{u}(\mathbf{x})^\top). \end{aligned} \quad (2.478)$$

Therefore,

$$E (\mathbf{u}(\mathbf{x}) \mathbf{u}(\mathbf{x})^\top) = -\frac{\nabla \nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} + \frac{2 \nabla g(\boldsymbol{\eta})(\nabla g(\boldsymbol{\eta}))^\top}{g^2(\boldsymbol{\eta})}. \quad (2.479)$$

By the definition,

$$\text{cov } \mathbf{u}(\mathbf{x}) = E (\mathbf{u}(\mathbf{x}) \mathbf{u}(\mathbf{x})^\top) - E \mathbf{u}(\mathbf{x}) E \mathbf{u}(\mathbf{x})^\top. \quad (2.480)$$

Thus,

$$\text{cov } \mathbf{u}(\mathbf{x}) = -\frac{\nabla \nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} + \frac{\nabla g(\boldsymbol{\eta})(\nabla g(\boldsymbol{\eta}))^\top}{g^2(\boldsymbol{\eta})}. \quad (2.481)$$

Hence,

$$\text{cov } \mathbf{u}(\mathbf{x}) = -\nabla \nabla \ln g(\boldsymbol{\eta}). \quad (2.482)$$

2.59

Let

$$p(x|\sigma) = \frac{1}{\sigma} f\left(\frac{x}{\sigma}\right). \quad (2.483)$$

Then

$$\int p(x|\sigma) dx = \frac{1}{\sigma} \int f\left(\frac{x}{\sigma}\right) dx. \quad (2.484)$$

By the transformation

$$x' = \frac{x}{\sigma}, \quad (2.485)$$

the right hand side can be written as

$$\frac{1}{\sigma} \int f(x') \sigma dx' = \int f(x') dx'. \quad (2.486)$$

Therefore, $p(x|\sigma)$ will be normalised if $f(x)$ is normalised.

2.60

Let \mathbf{x} be a variable such that

$$\mathbf{x} \in \mathcal{R}_i \Rightarrow p(\mathbf{x}) = h_i, \quad (2.487)$$

where

$$\int_{\mathcal{R}_i} d\mathbf{x} = \Delta_i. \quad (2.488)$$

Since

$$\int p(\mathbf{x}) d\mathbf{x} = 1, \quad (2.489)$$

we have

$$\sum_i h_i \Delta_i = 1. \quad (2.490)$$

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

$$\ln \left(\prod_i h_i^{n_i} \right) = \sum_i n_i \ln h_i, \quad (2.491)$$

where

$$\sum_i n_i = N. \quad (2.492)$$

Setting the derivatives of

$$\sum_i n_i \ln h_i + \lambda \left(\sum_i h_i \Delta_i - 1 \right) \quad (2.493)$$

with respect to h_i and λ to zero gives

$$\begin{aligned}\frac{n_i}{h_i} + \lambda\Delta_i &= 0, \\ \sum_i h_i\Delta_i - 1 &= 0.\end{aligned}\tag{2.494}$$

Then,

$$\begin{aligned}\lambda &= -N, \\ h_i &= \frac{n_i}{N\Delta_i}.\end{aligned}\tag{2.495}$$

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

$$p(\mathbf{x}) = \frac{K}{NV(\mathbf{x})},\tag{2.496}$$

where

$$V(\mathbf{x}) = \int_{\|\mathbf{x}' - \mathbf{x}\| \leq \|\mathbf{x}_{(K)} - \mathbf{x}\|} d\mathbf{x}',\tag{2.497}$$

K is a constant and $\mathbf{x}_{(K)}$ is the K th nearest observation from the point \mathbf{x} .

3 Linear Models for Regression

3.1

(a)

We have

$$\tanh a = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)}. \quad (3.1)$$

The right hand side can be written as

$$\frac{1 - \exp(-2a)}{1 + \exp(-2a)} = \frac{2}{1 + \exp(-2a)} - 1. \quad (3.2)$$

Therefore,

$$\tanh a = 2\sigma(2a) - 1, \quad (3.3)$$

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}. \quad (3.4)$$

(b)

Let

$$y(x_n, \mathbf{w}) = w_0 + \sum_{m=1}^M w_m \sigma \left(\frac{x - \mu_m}{s} \right). \quad (3.5)$$

By the result above, the right hand side can be written as

$$\begin{aligned} & w_0 f + \sum_{m=1}^M w_m \frac{1 + \tanh \left(\frac{x - \mu_m}{2s} \right)}{2} \\ &= w_0 + \frac{1}{2} \sum_{m=1}^M w_m + \frac{1}{2} \sum_{m=1}^M w_m \tanh \left(\frac{x - \mu_m}{2s} \right). \end{aligned} \quad (3.6)$$

Therefore, $y(x_n, \mathbf{w})$ is equivalent to

$$y(x_n, \mathbf{u}) = u_0 + \sum_{m=1}^M u_m \tanh \left(\frac{x - \mu_m}{2s} \right), \quad (3.7)$$

where

$$\begin{aligned} u_0 &= w_0 + \frac{1}{2} \sum_{m=1}^M w_m, \\ u_m &= \frac{1}{2} w_m. \end{aligned} \tag{3.8}$$

3.2 (Incomplete)

Let Φ be an $N \times M$ matrix. Then, for any vector \mathbf{v} in N dimensions,

$$\Phi (\Phi^\top \Phi)^{-1} \Phi^\top \mathbf{v} \tag{3.9}$$

is a projection of \mathbf{v} onto the space spanned by the columns of Φ ?

Additionally, for a vector \mathbf{t} in N dimensions,

$$(\Phi^\top \Phi)^{-1} \Phi^\top \mathbf{t} \tag{3.10}$$

is an orthogonal projection of \mathbf{t} onto the space spanned by the columns of Φ ?

3.3

Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N r_n (t_n - \mathbf{w}^\top \phi_n)^2. \tag{3.11}$$

The right hand side can be written as

$$\frac{1}{2} \|\mathbf{t}' - \Phi' \mathbf{w}\|^2, \tag{3.12}$$

where

$$\mathbf{t}' = \begin{bmatrix} \sqrt{r_1} t_1 \\ \vdots \\ \sqrt{r_N} t_N \end{bmatrix}, \Phi' = \begin{bmatrix} \sqrt{r_1} \phi(\mathbf{x}_1)^\top \\ \vdots \\ \sqrt{r_N} \phi(\mathbf{x}_N)^\top \end{bmatrix}. \tag{3.13}$$

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

$$\mathbf{0} = -\Phi'^\top (\mathbf{t}' - \Phi' \mathbf{w}). \tag{3.14}$$

Therefore,

$$\underset{\mathbf{w}}{\operatorname{argmin}} E(\mathbf{w}) = (\Phi'^\top \Phi')^{-1} \Phi'^\top \mathbf{t}'. \tag{3.15}$$

3.4 (Incomplete)

Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N (y(\mathbf{x}_n, \mathbf{w}) - t_n)^2, \quad (3.16)$$

where

$$\begin{aligned} y(\mathbf{x}, \mathbf{w}) &= w_0 + \sum_{m=1}^M w_m (x_m + \epsilon_m), \\ p(\epsilon_m) &= \mathcal{N}(\epsilon_m | 0, \sigma^2). \end{aligned} \quad (3.17)$$

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

$$\mathbf{0} = \sum_{n=1}^N \begin{bmatrix} 1 \\ \mathbf{x}_n + \boldsymbol{\epsilon}_n \end{bmatrix} (y(\mathbf{x}_n, \mathbf{w}) - t_n). \quad (3.18)$$

The right hand side can be written as

$$\sum_{n=1}^N \begin{bmatrix} 1 \\ \mathbf{x}_n \end{bmatrix} (y(\mathbf{x}_n, \mathbf{w}) - t_n) + \sum_{n=1}^N \begin{bmatrix} 0 \\ \boldsymbol{\epsilon}_n \end{bmatrix} (y(\mathbf{x}_n, \mathbf{w}) - t_n). \quad (3.19)$$

3.5

Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N (t_n - \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}_n))^2. \quad (3.20)$$

Then, the minimisation of $E(\mathbf{w})$ under the constraint

$$\sum_{m=1}^M |w_m|^q \leq \eta \quad (3.21)$$

reduces to the minimisation of

$$E(\mathbf{w}) + \lambda \left(\sum_{m=1}^M |w_m|^q - \eta \right) \quad (3.22)$$

with respect to \mathbf{w} and λ . Then,

$$\eta = \sum_{m=1}^M |w_m^*(\lambda)|^q, \quad (3.23)$$

where

$$\mathbf{w}^*(\lambda) = \operatorname{argmin}_{\mathbf{w}} \left(E(\mathbf{w}) + \lambda \left(\sum_{m=1}^M |w_m|^q - \eta \right) \right). \quad (3.24)$$

3.6

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables in D dimensions such that

$$p(\mathbf{t}_n | \mathbf{y}_n) = \mathcal{N}(\mathbf{t}_n | \mathbf{y}_n, \Sigma), \quad (3.25)$$

where

$$\mathbf{y}_n = \mathbf{W}^\top \boldsymbol{\phi}_n. \quad (3.26)$$

Then,

$$\begin{aligned} \ln p(\mathbf{T} | \mathbf{Y}) &= -\frac{ND}{2} \ln(2\pi) - \frac{N}{2} \ln(\det \Sigma) \\ &\quad - \frac{1}{2} \sum_{n=1}^N (\mathbf{t}_n - \mathbf{W}^\top \boldsymbol{\phi}_n)^\top \Sigma^{-1} (\mathbf{t}_n - \mathbf{W}^\top \boldsymbol{\phi}_n). \end{aligned} \quad (3.27)$$

By 3.21, setting the derivatives with respect to \mathbf{W} and Σ to zero gives

$$\begin{aligned} \mathbf{O} &= -\frac{1}{2} (\Sigma^{-1} + (\Sigma^{-1})^\top) \sum_{n=1}^N (\mathbf{t}_n - \mathbf{W}^\top \boldsymbol{\phi}_n) \boldsymbol{\phi}_n^\top, \\ \mathbf{O} &= -\frac{N}{2} (\Sigma^{-1})^\top + \frac{1}{2} (\Sigma^{-1})^2 \sum_{n=1}^N (\mathbf{t}_n - \mathbf{W}^\top \boldsymbol{\phi}_n) (\mathbf{t}_n - \mathbf{W}^\top \boldsymbol{\phi}_n)^\top. \end{aligned} \quad (3.28)$$

Therefore, the maximum likelihood solutions for \mathbf{W} and Σ are given by

$$\begin{aligned} \mathbf{W}_{\text{ML}} &= (\boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^\top \mathbf{t}, \\ \Sigma_{\text{ML}} &= \frac{1}{N} \sum_{n=1}^N (\mathbf{t}_n - \mathbf{W}_{\text{ML}}^\top \boldsymbol{\phi}_n) (\mathbf{t}_n - \mathbf{W}_{\text{ML}}^\top \boldsymbol{\phi}_n)^\top. \end{aligned} \quad (3.29)$$

3.7

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}) &= \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{m}_0, \mathbf{S}_0). \end{aligned} \quad (3.30)$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{t})p(\mathbf{t}) = p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \quad (3.31)$$

The logarithm of the right hand side except the terms independent of \mathbf{t} and \mathbf{w} can be written as

$$\begin{aligned} & -\frac{\beta}{2} \sum_{n=1}^N (t_n - \mathbf{w}^\top \boldsymbol{\phi}_n)^2 - \frac{1}{2} (\mathbf{w} - \mathbf{m}_0)^\top \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0) \\ & = -\frac{1}{2} \mathbf{v}^\top \mathbf{M} \mathbf{v} + \mathbf{v}^\top \mathbf{u} - \frac{1}{2} \mathbf{m}_0^\top \mathbf{S}_0^{-1} \mathbf{m}_0, \end{aligned} \quad (3.32)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \mathbf{S}_0^{-1} + \beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi} & -\beta \boldsymbol{\Phi}^\top \\ -\beta \boldsymbol{\Phi} & \beta \mathbf{I} \end{bmatrix}, \mathbf{u} = \begin{bmatrix} \mathbf{S}_0^{-1} \mathbf{m}_0 \\ \mathbf{0} \end{bmatrix}. \quad (3.33)$$

Therefore,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{S}), \quad (3.34)$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S} (\mathbf{S}_0^{-1} \mathbf{m}_0 + \beta \boldsymbol{\Phi}^\top \mathbf{t}), \\ \mathbf{S} &= (\mathbf{S}_0^{-1} + \beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1}. \end{aligned} \quad (3.35)$$

3.8

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}(t_n|\mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0). \end{aligned} \quad (3.36)$$

By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{S}), \quad (3.37)$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S} (\mathbf{S}_0^{-1} \mathbf{m}_0 + \beta \boldsymbol{\Phi}^\top \mathbf{t}), \\ \mathbf{S} &= (\mathbf{S}_0^{-1} + \beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1}. \end{aligned} \quad (3.38)$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{t}')p(\mathbf{t}') = p(\mathbf{t}'|\mathbf{w})p(\mathbf{w}), \quad (3.39)$$

where

$$\mathbf{t}' = \begin{bmatrix} \mathbf{t} \\ t_{N+1} \end{bmatrix}. \quad (3.40)$$

Since \mathbf{t} and t_{N+1} are independent, it can be written as

$$p(\mathbf{w}|\mathbf{t}')p(t_{N+1})p(\mathbf{t}) = p(t_{N+1}|\mathbf{w})p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \quad (3.41)$$

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

$$p(t_{N+1}|\mathbf{w})p(\mathbf{w}|\mathbf{t})p(\mathbf{t}). \quad (3.42)$$

Then,

$$p(\mathbf{w}|\mathbf{t}')p(t_{N+1}) = p(\mathbf{w}|\mathbf{t})p(t_{N+1}|\mathbf{w}). \quad (3.43)$$

The logarithm of the right hand side except the terms independent of \mathbf{w} can be written as

$$\begin{aligned} & -\frac{1}{2} (\mathbf{w} - \mathbf{m})^\top \mathbf{S}^{-1} (\mathbf{w} - \mathbf{m}) - \frac{\beta}{2} (t_{N+1} - \mathbf{w}^\top \boldsymbol{\phi}_{N+1})^2 \\ &= -\frac{1}{2} \mathbf{v}^\top \mathbf{M} \mathbf{v} + \mathbf{v}^\top \mathbf{u} - \frac{1}{2} \mathbf{m}^\top \mathbf{S}^{-1} \mathbf{m}, \end{aligned} \quad (3.44)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} \\ t_{N+1} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \mathbf{S}^{-1} + \beta \boldsymbol{\phi}_{N+1} \boldsymbol{\phi}_{N+1}^\top & -\beta \boldsymbol{\phi}_{N+1} \\ -\beta \boldsymbol{\phi}_{N+1}^\top & \beta \end{bmatrix}, \mathbf{u} = \begin{bmatrix} \mathbf{S}^{-1} \mathbf{m} \\ 0 \end{bmatrix}. \quad (3.45)$$

Then,

$$p(\mathbf{w}|\mathbf{t}') = \mathcal{N}(\mathbf{w}|\mathbf{m}', \mathbf{S}'), \quad (3.46)$$

where

$$\begin{aligned} \mathbf{m}' &= \mathbf{S}' (\mathbf{S}^{-1} \mathbf{m} + \beta t_{N+1} \boldsymbol{\phi}_{N+1}), \\ \mathbf{S}' &= (\mathbf{S}^{-1} + \beta \boldsymbol{\phi}_{N+1} \boldsymbol{\phi}_{N+1}^\top)^{-1}. \end{aligned} \quad (3.47)$$

We have

$$\begin{aligned} \mathbf{S}^{-1} \mathbf{m} + \beta t_{N+1} \boldsymbol{\phi}_{N+1} &= \mathbf{S}_0^{-1} \mathbf{m}_0 + \beta \boldsymbol{\Phi}'^\top \mathbf{t}', \\ \mathbf{S}^{-1} + \beta \boldsymbol{\phi}_{N+1} \boldsymbol{\phi}_{N+1}^\top &= \mathbf{S}_0^{-1} + \beta \boldsymbol{\Phi}'^\top \boldsymbol{\Phi}', \end{aligned} \quad (3.48)$$

where

$$\boldsymbol{\Phi}' = \begin{bmatrix} \boldsymbol{\Phi} \\ \boldsymbol{\phi}_{N+1}^\top \end{bmatrix}. \quad (3.49)$$

Therefore,

$$\begin{aligned} \mathbf{m}' &= \mathbf{S}' (\mathbf{S}_0^{-1} \mathbf{m}_0 + \beta \boldsymbol{\Phi}'^\top \mathbf{t}'), \\ \mathbf{S}' &= (\mathbf{S}_0^{-1} + \beta \boldsymbol{\Phi}'^\top \boldsymbol{\Phi}')^{-1}. \end{aligned} \quad (3.50)$$

3.9

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}(t_n|\mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0). \end{aligned} \quad (3.51)$$

Then, by 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{S}), \quad (3.52)$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S} (\mathbf{S}_0^{-1} \mathbf{m}_0 + \beta \boldsymbol{\Phi}^\top \mathbf{t}), \\ \mathbf{S} &= (\mathbf{S}_0^{-1} + \beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1}. \end{aligned} \quad (3.53)$$

Let

$$\mathbf{t}' = \begin{bmatrix} \mathbf{t} \\ t_{N+1} \end{bmatrix}, \boldsymbol{\Phi}' = \begin{bmatrix} \boldsymbol{\Phi} \\ \boldsymbol{\phi}_{N+1}^\top \end{bmatrix}. \quad (3.54)$$

Then,

$$p(\mathbf{w}|\mathbf{t}') = \mathcal{N}(\mathbf{w}|\mathbf{m}', \mathbf{t}'), \quad (3.55)$$

where

$$\begin{aligned} \mathbf{m}' &= \mathbf{S}' (\mathbf{S}_0^{-1} \mathbf{m}_0 + \beta \boldsymbol{\Phi}'^\top \mathbf{t}'), \\ \mathbf{S}' &= (\mathbf{S}_0^{-1} + \beta \boldsymbol{\Phi}'^\top \boldsymbol{\Phi}')^{-1}. \end{aligned} \quad (3.56)$$

3.10

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}(t_n|\mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0). \end{aligned} \quad (3.57)$$

By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{S}), \quad (3.58)$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S} (\mathbf{S}_0^{-1} \mathbf{m}_0 + \beta \boldsymbol{\Phi}^\top \mathbf{t}), \\ \mathbf{S} &= (\mathbf{S}_0^{-1} + \beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1}. \end{aligned} \quad (3.59)$$

By marginalisation,

$$p(t_{N+1}|\mathbf{t}) = \int p(t_{N+1}|\mathbf{w}) p(\mathbf{w}|\mathbf{t}) d\mathbf{w}. \quad (3.60)$$

The logarithm of the integrand of the right hand side except the terms independent of t_{N+1} and \mathbf{w} can be written as

$$\begin{aligned} & -\frac{\beta}{2}(t_{N+1} - \mathbf{w}^\top \boldsymbol{\phi}_{N+1})^2 - \frac{1}{2}(\mathbf{w} - \mathbf{m})^\top \mathbf{S}^{-1}(\mathbf{w} - \mathbf{m}) \\ & = -\frac{1}{2}\mathbf{v}^\top \mathbf{M}\mathbf{v} + \mathbf{v}^\top \mathbf{u} - \frac{1}{2}\mathbf{m}^\top \mathbf{S}^{-1}\mathbf{m}, \end{aligned} \quad (3.61)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} \\ t_{N+1} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \mathbf{S}^{-1} + \beta\boldsymbol{\phi}_{N+1}\boldsymbol{\phi}_{N+1}^\top & -\beta\boldsymbol{\phi}_{N+1} \\ -\beta\boldsymbol{\phi}_{N+1}^\top & \beta \end{bmatrix}, \mathbf{u} = \begin{bmatrix} \mathbf{S}^{-1}\mathbf{m} \\ 0 \end{bmatrix}. \quad (3.62)$$

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{S} & \mathbf{S}\boldsymbol{\phi}_{N+1} \\ \boldsymbol{\phi}_{N+1}^\top \mathbf{S} & \beta^{-1} + \boldsymbol{\phi}_{N+1}^\top \mathbf{S}\boldsymbol{\phi}_{N+1} \end{bmatrix}. \quad (3.63)$$

Then,

$$\mathbf{M}^{-1}\mathbf{u} = \begin{bmatrix} \mathbf{m} \\ \mathbf{m}^\top \boldsymbol{\phi}_{N+1} \end{bmatrix}. \quad (3.64)$$

Therefore,

$$p(t_{N+1}|\mathbf{t}) = \mathcal{N}(t_{N+1}|\mathbf{m}^\top \boldsymbol{\phi}_{N+1}, \sigma^2(\boldsymbol{\phi}_{N+1})), \quad (3.65)$$

where

$$\sigma^2(\boldsymbol{\phi}) = \beta^{-1} + \boldsymbol{\phi}^\top \mathbf{S} \boldsymbol{\phi}. \quad (3.66)$$

3.11

Let t_1, \dots, t_N be a variable such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}(t_n|\mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0). \end{aligned} \quad (3.67)$$

By 3.7,

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{S}), \quad (3.68)$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S}(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\boldsymbol{\Phi}^\top \mathbf{t}), \\ \mathbf{S} &= (\mathbf{S}_0^{-1} + \beta\boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1}. \end{aligned} \quad (3.69)$$

By 3.10,

$$p(t_{N+1}|\mathbf{t}) = \mathcal{N}(t_{N+1}|\mathbf{m}^\top \boldsymbol{\phi}_{N+1}, \sigma^2(\boldsymbol{\phi}_{N+1})), \quad (3.70)$$

where

$$\sigma^2(\boldsymbol{\phi}) = \beta^{-1} + \boldsymbol{\phi}^\top \mathbf{S} \boldsymbol{\phi}. \quad (3.71)$$

Let

$$\mathbf{t}' = \begin{bmatrix} \mathbf{t} \\ t_{N+1} \end{bmatrix}, \boldsymbol{\Phi} = \begin{bmatrix} \boldsymbol{\Phi} \\ \boldsymbol{\phi}_{N+1}^\top \end{bmatrix}. \quad (3.72)$$

Then,

$$p(t_{N+2} | \mathbf{t}') = \mathcal{N} \left(t_{N+2} | \mathbf{m}'^\top \boldsymbol{\phi}_{N+2}, \sigma'^2(\boldsymbol{\phi}_{N+2}) \right), \quad (3.73)$$

where

$$\begin{aligned} \mathbf{m}' &= \mathbf{S}' (\mathbf{S}_0^{-1} \mathbf{m}_0 + \beta \boldsymbol{\Phi}'^\top \mathbf{t}'), \\ \mathbf{S}' &= (\mathbf{S}_0^{-1} + \beta \boldsymbol{\Phi}'^\top \boldsymbol{\Phi}')^{-1}, \\ \sigma'^2(\boldsymbol{\phi}) &= \beta^{-1} + \boldsymbol{\phi}^\top \mathbf{S}' \boldsymbol{\phi}. \end{aligned} \quad (3.74)$$

We have

$$\sigma^2(\boldsymbol{\phi}) - \sigma'^2(\boldsymbol{\phi}) = \boldsymbol{\phi}^\top (\mathbf{S} - \mathbf{S}') \boldsymbol{\phi}, \quad (3.75)$$

and

$$\mathbf{S}' = (\mathbf{S}^{-1} + \beta \boldsymbol{\phi}_{N+1} \boldsymbol{\phi}_{N+1}^\top)^{-1}. \quad (3.76)$$

By 2.26,

$$\mathbf{S}' = \mathbf{S} - c\beta^2 \mathbf{S} \boldsymbol{\phi}_{N+1} \boldsymbol{\phi}_{N+1}^\top \mathbf{S}, \quad (3.77)$$

where

$$c = (\beta + \beta^2 \boldsymbol{\phi}_{N+1}^\top \mathbf{S} \boldsymbol{\phi}_{N+1})^{-1}. \quad (3.78)$$

Then,

$$\sigma^2(\boldsymbol{\phi}) - \sigma'^2(\boldsymbol{\phi}) = c\beta^2 (\boldsymbol{\phi}^\top \mathbf{S} \boldsymbol{\phi}_{N+1})^2. \quad (3.79)$$

Therefore,

$$\sigma^2(\boldsymbol{\phi}) \geq \sigma'^2(\boldsymbol{\phi}). \quad (3.80)$$

3.12

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}, \beta) &= \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}, \beta) &= \mathcal{N}(\mathbf{w} | \mathbf{m}_0, \beta^{-1} \mathbf{S}_0) \text{Gam}(\beta | a_0, b_0), \end{aligned} \quad (3.81)$$

where \mathbf{w} is a vector in M dimensions.

(a)

By the Bayes' theorem,

$$p(\mathbf{w}, \beta | \mathbf{t}) p(\mathbf{t}) = p(\mathbf{t} | \mathbf{w}, \beta) p(\mathbf{w}, \beta). \quad (3.82)$$

The logarithm of the right hand side except the terms independent of \mathbf{t} , \mathbf{w} and β can be written as

$$\begin{aligned} & -\frac{N}{2} \ln \beta^{-1} - \frac{\beta}{2} \sum_{n=1}^N (t_n - \mathbf{w}^\top \boldsymbol{\phi}_n)^2 \\ & - \frac{M}{2} \ln \beta^{-1} - \frac{\beta}{2} (\mathbf{w} - \mathbf{m}_0)^\top \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0) + (a_0 - 1) \ln \beta - b_0 \beta. \end{aligned} \quad (3.83)$$

We have

$$\begin{aligned} & -\frac{\beta}{2} \sum_{n=1}^N (t_n - \mathbf{w}^\top \boldsymbol{\phi}_n)^2 - \frac{\beta}{2} (\mathbf{w} - \mathbf{m}_0)^\top \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0) \\ & = -\frac{\beta}{2} \mathbf{v}^\top \mathbf{M} \mathbf{v} + \beta \mathbf{v}^\top \mathbf{u} - \frac{\beta}{2} \mathbf{m}_0^\top \mathbf{S}_0^{-1} \mathbf{m}_0, \end{aligned} \quad (3.84)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \mathbf{S}_0^{-1} + \boldsymbol{\Phi}^\top \boldsymbol{\Phi} & -\boldsymbol{\Phi}^\top \\ -\boldsymbol{\Phi} & \mathbf{I} \end{bmatrix}, \mathbf{u} = \begin{bmatrix} \mathbf{S}_0^{-1} \mathbf{m}_0 \\ \mathbf{0} \end{bmatrix}. \quad (3.85)$$

The right hand side can be written as

$$-\frac{\beta}{2} (\mathbf{w} - \mathbf{m})^\top \mathbf{S}^{-1} (\mathbf{w} - \mathbf{m}) + \frac{\beta}{2} \mathbf{m}^\top \mathbf{S}^{-1} \mathbf{m} - \frac{\beta}{2} \mathbf{m}_0^\top \mathbf{S}_0^{-1} \mathbf{m}_0, \quad (3.86)$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S} (\mathbf{S}_0^{-1} \mathbf{m}_0 + \boldsymbol{\Phi}^\top \mathbf{t}), \\ \mathbf{S} &= (\mathbf{S}_0^{-1} + \boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1}. \end{aligned} \quad (3.87)$$

Therefore,

$$p(\mathbf{w}, \beta | \mathbf{t}) = \mathcal{N}(\mathbf{w} | \mathbf{m}, \beta^{-1} \mathbf{S}) \text{Gam}(\beta | a, b), \quad (3.88)$$

where

$$\begin{aligned} a &= a_0 + \frac{N}{2}, \\ b &= b_0 + \frac{1}{2} \|\mathbf{t}\|^2 + \frac{1}{2} \mathbf{m}_0^\top \mathbf{S}_0^{-1} \mathbf{m}_0 - \frac{1}{2} \mathbf{m}^\top \mathbf{S}^{-1} \mathbf{m}. \end{aligned} \quad (3.89)$$

(b)

By the expression of the Bayes' theorem in (a),

$$p(\mathbf{t}) = \frac{\mathcal{N}(\mathbf{t}|\Phi\mathbf{w}, \beta^{-1}\mathbf{I}) \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \beta^{-1}\mathbf{S}_0) \text{Gam}(\beta|a_0, b_0)}{\mathcal{N}(\mathbf{w}|\mathbf{m}, \beta^{-1}\mathbf{S}) \text{Gam}(\beta|a, b)}. \quad (3.90)$$

The logarithm of the right hand side can be written as

$$\begin{aligned} & -\frac{N}{2} \ln(2\pi) - \frac{N}{2} \ln \beta^{-1} - \frac{\beta}{2} \|\mathbf{t} - \Phi\mathbf{w}\|^2 \\ & - \frac{M}{2} \ln(2\pi) - \frac{M}{2} \ln \beta^{-1} - \frac{1}{2} \det \mathbf{S}_0 - \frac{\beta}{2} (\mathbf{w} - \mathbf{m}_0)^\top \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0) \\ & + a_0 \ln b_0 - \ln \Gamma(a_0) + (a_0 - 1) \ln \beta - b_0 \beta \\ & + \frac{M}{2} \ln(2\pi) + \frac{M}{2} \ln \beta^{-1} + \frac{1}{2} \det \mathbf{S} + \frac{\beta}{2} (\mathbf{w} - \mathbf{m})^\top \mathbf{S}^{-1} (\mathbf{w} - \mathbf{m}) \\ & - a \ln b + \ln \Gamma(a) - (a - 1) \ln \beta + b \beta \end{aligned} \quad (3.91)$$

$$\begin{aligned} & = -\frac{N}{2} \ln(2\pi) - \frac{N}{2} \ln \beta^{-1} - \frac{\beta}{2} \|\mathbf{t} - \Phi\mathbf{w}\|^2 \\ & - \frac{1}{2} \det \mathbf{S}_0 - \frac{\beta}{2} (\mathbf{w} - \mathbf{m}_0)^\top \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0) + a_0 \ln b_0 - \ln \Gamma(a_0) \\ & + \frac{1}{2} \det \mathbf{S} + \frac{\beta}{2} (\mathbf{w} - \mathbf{m})^\top \mathbf{S}^{-1} (\mathbf{w} - \mathbf{m}) - a \ln b + \ln \Gamma(a) \\ & - (a - a_0) \ln \beta + (b - b_0) \beta. \end{aligned}$$

The right hand side can be written as

$$\begin{aligned} & -\frac{N}{2} \ln(2\pi) - \frac{1}{2} \det \mathbf{S}_0 + a_0 \ln b_0 - \ln \Gamma(a_0) \\ & + \frac{1}{2} \det \mathbf{S} - a \ln b + \ln \Gamma(a). \end{aligned} \quad (3.92)$$

Therefore,

$$p(\mathbf{t}) = (2\pi)^{-\frac{N}{2}} \left(\frac{\det \mathbf{S}}{\det \mathbf{S}_0} \right)^{\frac{1}{2}} \frac{\Gamma(a)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b^a}. \quad (3.93)$$

3.13

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}, \beta) &= \mathcal{N}(t_n|\mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}, \beta) &= \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \beta^{-1}\mathbf{S}_0) \text{Gam}(\beta|a_0, b_0), \end{aligned} \quad (3.94)$$

where \mathbf{w} and $\boldsymbol{\phi}$ are vectors in M dimensions. By marginalisation,

$$p(t_{N+1}|\mathbf{t}) = \iint p(t_{N+1}|\mathbf{w}, \beta) p(\mathbf{w}, \beta|\mathbf{t}) d\mathbf{w} d\beta. \quad (3.95)$$

By 3.12(a),

$$p(\mathbf{w}, \beta|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}, \beta^{-1}\mathbf{S}) \text{Gam}(\beta|a, b), \quad (3.96)$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S} (\mathbf{S}_0^{-1} \mathbf{m}_0 + \boldsymbol{\Phi}^\top \mathbf{t}), \\ \mathbf{S} &= (\mathbf{S}_0^{-1} + \boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1}, \\ a &= a_0 + \frac{N}{2}, \\ b &= b_0 + \frac{1}{2} \|\mathbf{t}\|^2 + \frac{1}{2} \mathbf{m}_0^\top \mathbf{S}_0 \mathbf{m}_0 - \frac{1}{2} \mathbf{m}^\top \mathbf{S}^{-1} \mathbf{m}. \end{aligned} \quad (3.97)$$

Then, the integral can be written as

$$\int \left(\int \mathcal{N}(t_{N+1}|\mathbf{w}^\top \boldsymbol{\phi}_{N+1}, \beta^{-1}) \mathcal{N}(\mathbf{w}|\mathbf{m}, \beta^{-1}\mathbf{S}) d\mathbf{w} \right) \text{Gam}(\beta|a, b) d\beta. \quad (3.98)$$

The logarithm of the integrand with respect to \mathbf{w} except the terms indepndent of \mathbf{w} can be written as

$$\begin{aligned} &- \frac{\beta}{2} (t_{N+1} - \mathbf{w}^\top \boldsymbol{\phi}_{N+1})^2 - \frac{\beta}{2} (\mathbf{w} - \mathbf{m})^\top \mathbf{S}^{-1} (\mathbf{w} - \mathbf{m}) \\ &= -\frac{\beta}{2} \mathbf{v}^\top \mathbf{M} \mathbf{v} + \beta \mathbf{v}^\top \mathbf{u} - \frac{\beta}{2} \mathbf{m}^\top \mathbf{S}^{-1} \mathbf{m}, \end{aligned} \quad (3.99)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} \\ t_{N+1} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \mathbf{S}^{-1} + \boldsymbol{\phi}_{N+1} \boldsymbol{\phi}_{N+1}^\top & -\boldsymbol{\phi}_{N+1} \\ -\boldsymbol{\phi}_{N+1}^\top & 1 \end{bmatrix}, \mathbf{u} = \begin{bmatrix} \mathbf{S}^{-1} \mathbf{m} \\ 0 \end{bmatrix}. \quad (3.100)$$

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{S} & \mathbf{S} \boldsymbol{\phi}_{N+1} \\ \boldsymbol{\phi}_{N+1}^\top \mathbf{S} & 1 + \boldsymbol{\phi}_{N+1}^\top \mathbf{S} \boldsymbol{\phi}_{N+1} \end{bmatrix}. \quad (3.101)$$

Then,

$$\mathbf{M}^{-1} \mathbf{u} = \begin{bmatrix} \mathbf{m} \\ \mathbf{m}^\top \boldsymbol{\phi}_{N+1} \end{bmatrix}. \quad (3.102)$$

Then, the integral with respect to \mathbf{w} can be written as

$$\mathcal{N}(t_{N+1}|\mathbf{m}^\top \boldsymbol{\phi}_{N+1}, \beta^{-1} (1 + \boldsymbol{\phi}_{N+1}^\top \mathbf{S} \boldsymbol{\phi}_{N+1})). \quad (3.103)$$

Then, the logarithm of the integrand with respect to β except the terms independent of β can be written as

$$\begin{aligned} & -\frac{1}{2} \ln \beta^{-1} - \frac{\beta}{2(1 + \boldsymbol{\phi}_{N+1}^\top \mathbf{S} \boldsymbol{\phi}_{N+1})} (t_{N+1} - \mathbf{m}^\top \boldsymbol{\phi}_{N+1})^2 \\ & + (a-1) \ln \beta - b\beta \\ & = \left(a + \frac{1}{2} - 1 \right) \ln \beta - \left(b + \frac{(t_{N+1} - \mathbf{m}^\top \boldsymbol{\phi}_{N+1})^2}{2(1 + \boldsymbol{\phi}_{N+1}^\top \mathbf{S} \boldsymbol{\phi}_{N+1})} \right) \beta. \end{aligned} \quad (3.104)$$

Then, the integral with respect to β except the terms independent of t_{N+1} can be written as

$$\left(b + \frac{(t_{N+1} - \mathbf{m}^\top \boldsymbol{\phi}_{N+1})^2}{2(1 + \boldsymbol{\phi}_{N+1}^\top \mathbf{S} \boldsymbol{\phi}_{N+1})} \right)^{-a-\frac{1}{2}}. \quad (3.105)$$

Therefore,

$$p(t_{N+1} | \mathbf{t}) = \text{St}(t_{N+1} | \mu, \lambda, \nu), \quad (3.106)$$

where

$$\begin{aligned} \mu &= \mathbf{m}^\top \boldsymbol{\phi}_{N+1}, \\ \lambda &= \frac{a}{b} (1 + \boldsymbol{\phi}_{N+1}^\top \mathbf{S} \boldsymbol{\phi}_{N+1})^{-1}, \\ \nu &= 2a. \end{aligned} \quad (3.107)$$

3.14 (Incomplete)

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}) &= \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{0}, \alpha^{-1} \mathbf{I}), \end{aligned} \quad (3.108)$$

where \mathbf{w} is a vector in M dimensions.

(a)

By 3.7,

$$p(\mathbf{w} | \mathbf{t}) = \mathcal{N}(\mathbf{w} | \mathbf{m}, \mathbf{S}), \quad (3.109)$$

where

$$\begin{aligned} \mathbf{m} &= \beta \mathbf{S} \boldsymbol{\Phi}^\top \mathbf{t}, \\ \mathbf{S} &= (\alpha \mathbf{I} + \beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1}. \end{aligned} \quad (3.110)$$

Let

$$y(\phi, \mathbf{w}) = \mathbf{w}^\top \phi. \quad (3.111)$$

Then,

$$y(\phi, \mathbf{m}) = \beta \phi^\top \mathbf{S} \Phi^\top \mathbf{t}. \quad (3.112)$$

The right hand side can be written as

$$\sum_{n=1}^N k(\phi, \phi_n) t_n, \quad (3.113)$$

where

$$k(\phi, \phi') = \beta \phi^\top \mathbf{S} \phi'. \quad (3.114)$$

Let us suppose that ϕ_1, \dots, ϕ_M are linearly independent, $N > M$ and

$$\phi_1 = 1. \quad (3.115)$$

Then, we can construct a new basis set ψ_1, \dots, ψ_M such that

$$\Psi^\top \Psi = \mathbf{I}? \quad (3.116)$$

where

$$\psi_1 = 1. \quad (3.117)$$

(b)

3.15

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}) &= \mathcal{N}(t_n | \mathbf{w}^\top \phi_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{0}, \alpha^{-1} \mathbf{I}), \end{aligned} \quad (3.118)$$

where \mathbf{w} is a vector in M dimensions. By 3.7,

$$p(\mathbf{w} | \mathbf{t}) = \mathcal{N}(\mathbf{w} | \mathbf{m}, \mathbf{S}), \quad (3.119)$$

where

$$\begin{aligned} \mathbf{m} &= \beta \mathbf{S} \Phi^\top \mathbf{t}, \\ \mathbf{S} &= (\alpha \mathbf{I} + \beta \Phi^\top \Phi)^{-1}. \end{aligned} \quad (3.120)$$

By 3.19,

$$\ln p(\mathbf{t}) = \frac{M}{2} \ln \alpha + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \mathbf{S}) - E(\mathbf{m}), \quad (3.121)$$

where

$$E(\mathbf{m}) = \frac{\beta}{2} \|\mathbf{t} - \Phi \mathbf{m}\|^2 + \frac{\alpha}{2} \mathbf{m}^\top \mathbf{m}. \quad (3.122)$$

By 3.22, setting the derivatives of $\ln p(\mathbf{t})$ with respect to α and β to zero gives

$$\begin{aligned} \alpha &= \frac{\gamma}{\mathbf{m}^\top \mathbf{m}}, \\ \beta &= \frac{N - \gamma}{\|\mathbf{t} - \Phi \mathbf{m}\|^2}, \end{aligned} \quad (3.123)$$

where

$$\gamma = \sum_{m=1}^M \frac{\lambda_m}{\alpha + \lambda_m}, \quad (3.124)$$

and $\lambda_1, \dots, \lambda_M$ are the eigenvalues of $\beta \Phi^\top \Phi$. If α and β are set as above, then

$$E(\mathbf{m}) = \frac{N}{2}. \quad (3.125)$$

3.16

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}) &= \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{0}, \alpha^{-1} \mathbf{I}), \end{aligned} \quad (3.126)$$

where \mathbf{w} is a vector in M dimensions. By marginalisation,

$$p(\mathbf{t}) = \int p(\mathbf{t} | \mathbf{w}) p(\mathbf{w}) d\mathbf{w}. \quad (3.127)$$

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

$$-\frac{\beta}{2} \sum_{n=1}^N (t_n - \mathbf{w}^\top \boldsymbol{\phi}_n)^2 - \frac{\alpha}{2} \mathbf{w}^\top \mathbf{w} = -\frac{1}{2} \mathbf{v}^\top \mathbf{M} \mathbf{v}, \quad (3.128)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \alpha\mathbf{I} + \beta\Phi^\top\Phi & -\beta\Phi^\top \\ -\beta\Phi & \beta\mathbf{I} \end{bmatrix}. \quad (3.129)$$

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \alpha^{-1}\mathbf{I} & \alpha^{-1}\Phi^\top \\ \alpha^{-1}\Phi & \alpha^{-1}\Phi\Phi^\top + \beta^{-1}\mathbf{I} \end{bmatrix}. \quad (3.130)$$

Therefore,

$$p(\mathbf{t}) = \mathcal{N}(\mathbf{t}|\mathbf{0}, \alpha^{-1}\Phi\Phi^\top + \beta^{-1}\mathbf{I}). \quad (3.131)$$

3.17

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}(t_n|\mathbf{w}^\top\phi_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \quad (3.132)$$

where \mathbf{w} is a vector in M dimensions. By marginalisation,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}. \quad (3.133)$$

The logarithm of the integrand of the right hand side can be written as

$$\begin{aligned} &- \frac{N}{2} \ln(2\pi\beta^{-1}) - \frac{\beta}{2} \sum_{n=1}^N (t_n - \mathbf{w}^\top\phi_n)^2 \\ &- \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln(\det(\alpha^{-1}\mathbf{I})) - \frac{\alpha}{2} \|\mathbf{w}\|^2. \end{aligned} \quad (3.134)$$

Therefore,

$$p(\mathbf{t}) = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}} \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} \int \exp(-E(\mathbf{w})) d\mathbf{w}, \quad (3.135)$$

where

$$E(\mathbf{w}) = \frac{\beta}{2} \|\mathbf{t} - \Phi\mathbf{w}\|^2 + \frac{\alpha}{2} \|\mathbf{w}\|^2. \quad (3.136)$$

3.18

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}(t_n|\mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \quad (3.137)$$

where \mathbf{w} is a vector in M dimensions. By 3.17,

$$p(\mathbf{t}) = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}} \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} \int \exp(-E(\mathbf{w})) d\mathbf{w}, \quad (3.138)$$

where

$$E(\mathbf{w}) = \frac{\beta}{2}\|\mathbf{t} - \boldsymbol{\Phi}\mathbf{w}\|^2 + \frac{\alpha}{2}\|\mathbf{w}\|^2. \quad (3.139)$$

We have

$$\begin{aligned} \nabla E(\mathbf{w}) &= \mathbf{S}^{-1}(\mathbf{w} - \mathbf{m}), \\ \nabla \nabla E(\mathbf{w}) &= \mathbf{S}^{-1}. \end{aligned} \quad (3.140)$$

where

$$\begin{aligned} \mathbf{m} &= \beta \mathbf{S} \boldsymbol{\Phi}^\top \mathbf{t}, \\ \mathbf{S}^{-1} &= \beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \alpha \mathbf{I}. \end{aligned} \quad (3.141)$$

Then,

$$E(\mathbf{w}) = E(\mathbf{m}) + \frac{1}{2}(\mathbf{w} - \mathbf{m})^\top \mathbf{S}^{-1}(\mathbf{w} - \mathbf{m}). \quad (3.142)$$

3.19

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}(t_n|\mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \quad (3.143)$$

where \mathbf{w} is a vector in M dimensions. By 3.17,

$$p(\mathbf{t}) = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}} \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} \int \exp(-E(\mathbf{w})) d\mathbf{w}, \quad (3.144)$$

where

$$E(\mathbf{w}) = \frac{\beta}{2}\|\mathbf{t} - \boldsymbol{\Phi}\mathbf{w}\|^2 + \frac{\alpha}{2}\|\mathbf{w}\|^2. \quad (3.145)$$

By 3.18,

$$E(\mathbf{w}) = E(\mathbf{m}) + \frac{1}{2}(\mathbf{w} - \mathbf{m})^\top \mathbf{S}^{-1}(\mathbf{w} - \mathbf{m}), \quad (3.146)$$

where

$$\begin{aligned} \mathbf{m} &= \beta \mathbf{S} \Phi^\top \mathbf{t}, \\ \mathbf{S}^{-1} &= \beta \Phi^\top \Phi + \alpha \mathbf{I}. \end{aligned} \quad (3.147)$$

Therefore, the integral in the expression above of $p(\mathbf{t})$ can be written as

$$\begin{aligned} &\exp(-E(\mathbf{m})) \int \exp\left(-\frac{1}{2}(\mathbf{w} - \mathbf{m})^\top \mathbf{S}^{-1}(\mathbf{w} - \mathbf{m})\right) d\mathbf{w} \\ &= (2\pi)^{\frac{M}{2}} (\det \mathbf{S})^{\frac{1}{2}} \exp(-E(\mathbf{m})). \end{aligned} \quad (3.148)$$

Thus,

$$\ln p(\mathbf{t}) = \frac{M}{2} \ln \alpha + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \mathbf{S}) - E(\mathbf{m}). \quad (3.149)$$

3.20

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}) &= \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{0}, \alpha^{-1} \mathbf{I}), \end{aligned} \quad (3.150)$$

where \mathbf{w} is a vector in M dimensions. By 3.19,

$$\ln p(\mathbf{t}) = \frac{M}{2} \ln \alpha + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \mathbf{S}) - E(\mathbf{m}), \quad (3.151)$$

where

$$E(\mathbf{w}) = \frac{\beta}{2} \|\mathbf{t} - \Phi \mathbf{w}\|^2 + \frac{\alpha}{2} \|\mathbf{w}\|^2, \quad (3.152)$$

and

$$\begin{aligned} \mathbf{m} &= \beta \mathbf{S} \Phi^\top \mathbf{t}, \\ \mathbf{S}^{-1} &= \beta \Phi^\top \Phi + \alpha \mathbf{I}. \end{aligned} \quad (3.153)$$

By 3.21, setting the derivatives of $\ln p(\mathbf{t})$ with respect to α and β to zero gives

$$\begin{aligned} 0 &= \frac{M}{2\alpha} + \frac{1}{2} \text{tr} \left(\mathbf{S}^{-1} \frac{\partial \mathbf{S}}{\partial \alpha} \right) - \frac{1}{2} \|\mathbf{m}\|^2, \\ 0 &= \frac{N}{2\beta} + \frac{1}{2} \text{tr} \left(\mathbf{S}^{-1} \frac{\partial \mathbf{S}}{\partial \beta} \right) - \frac{1}{2} \|\mathbf{t} - \Phi \mathbf{m}\|^2. \end{aligned} \quad (3.154)$$

We have

$$\begin{aligned}\mathbf{O} &= \frac{\partial \mathbf{S}^{-1} \mathbf{S}}{\partial \alpha}, \\ \mathbf{O} &= \frac{\partial \mathbf{S}^{-1} \mathbf{S}}{\partial \beta}.\end{aligned}\tag{3.155}$$

The right hand side can be written as

$$\begin{aligned}\mathbf{S}^{-1} \frac{\partial \mathbf{S}}{\partial \alpha} + \mathbf{S} \frac{\partial \mathbf{S}^{-1}}{\partial \alpha} &= \mathbf{S}^{-1} \frac{\partial \mathbf{S}}{\partial \alpha} + \mathbf{S}, \\ \mathbf{S}^{-1} \frac{\partial \mathbf{S}}{\partial \beta} + \mathbf{S} \frac{\partial \mathbf{S}^{-1}}{\partial \beta} &= \mathbf{S}^{-1} \frac{\partial \mathbf{S}}{\partial \beta} + \mathbf{S} \Phi^\top \Phi.\end{aligned}\tag{3.156}$$

Then,

$$\begin{aligned}\mathbf{S}^{-1} \frac{\partial \mathbf{S}}{\partial \alpha} &= -\mathbf{S}, \\ \mathbf{S}^{-1} \frac{\partial \mathbf{S}}{\partial \beta} &= -\mathbf{S} \Phi^\top \Phi.\end{aligned}\tag{3.157}$$

Therefore, the maximum likelihood solutions of $p(\mathbf{t})$ satisfy

$$\begin{aligned}\alpha &= \frac{M}{\|\mathbf{m}\|^2 + \text{tr } \mathbf{S}}, \\ \beta &= \frac{N}{\|\mathbf{t} - \Phi \mathbf{m}\|^2 + \text{tr}(\mathbf{S} \Phi^\top \Phi)}.\end{aligned}\tag{3.158}$$

3.21

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

$$\Sigma \mathbf{u}_m = \lambda_m \mathbf{u}_m,\tag{3.159}$$

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

$$\begin{aligned}\Lambda &= \text{diag}(\lambda_1, \dots, \lambda_M), \\ \mathbf{U} &= [\mathbf{u}_1 \cdots \mathbf{u}_M].\end{aligned}\tag{3.160}$$

By 2.19,

$$\begin{aligned}\Sigma &= \mathbf{U} \Lambda \mathbf{U}^\top, \\ \mathbf{U}^\top \mathbf{U} &= \mathbf{I}.\end{aligned}\tag{3.161}$$

Then,

$$\det \Sigma = \prod_{m=1}^M \lambda_m, \quad (3.162)$$

so that

$$\ln(\det \Sigma) = \sum_{m=1}^M \ln \lambda_m. \quad (3.163)$$

Then,

$$\frac{\partial}{\partial \alpha} \ln(\det \Sigma) = \sum_{m=1}^M \frac{\partial \lambda_m}{\partial \alpha} \frac{1}{\lambda_m}. \quad (3.164)$$

Then,

$$\frac{\partial}{\partial \alpha} \ln(\det \Sigma) = \text{tr} \left(\Lambda^{-1} \frac{\partial \Lambda}{\partial \alpha} \right). \quad (3.165)$$

The right hand side can be written as

$$\text{tr} \left(\mathbf{U} \Lambda^{-1} \mathbf{U}^\top \frac{\partial \mathbf{U} \Lambda \mathbf{U}^\top}{\partial \alpha} \right) = \text{tr} \left(\Sigma^{-1} \frac{\partial \Sigma}{\partial \alpha} \right). \quad (3.166)$$

Therefore,

$$\frac{\partial}{\partial \alpha} \ln(\det \Sigma) = \text{tr} \left(\Sigma^{-1} \frac{\partial \Sigma}{\partial \alpha} \right). \quad (3.167)$$

3.22

Refer to 3.20.

3.23

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}, \beta) &= \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}, \beta) &= \mathcal{N}(\mathbf{w} | \mathbf{m}_0, \beta^{-1} \mathbf{S}_0) \text{Gam}(\beta | a_0, b_0), \end{aligned} \quad (3.168)$$

where \mathbf{w} is a vector in M dimensions. By marginalisation,

$$p(\mathbf{t}) = \iint p(\mathbf{t} | \mathbf{w}, \beta) p(\mathbf{w}, \beta) d\mathbf{w} d\beta. \quad (3.169)$$

The right hand side can be written as

$$\int I(\beta) \text{Gam}(\beta|a_0, b_0) d\beta, \quad (3.170)$$

where

$$I(\beta) = \int \left(\prod_{n=1}^N \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}) \right) \mathcal{N}(\mathbf{w} | \mathbf{m}_0, \beta^{-1} \mathbf{S}_0) d\mathbf{w}. \quad (3.171)$$

The logarithm of the integrand of the expression of $I(\beta)$ can be written as

$$\begin{aligned} & -\frac{N}{2} \ln(2\pi) - \frac{N}{2} \ln \beta^{-1} - \frac{\beta}{2} \sum_{n=1}^N (t_n - \mathbf{w}^\top \boldsymbol{\phi}_n)^2 \\ & - \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln \det(\beta^{-1} \mathbf{S}_0) - \frac{\beta}{2} (\mathbf{w} - \mathbf{m}_0)^\top \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0) \\ & = -\frac{N+M}{2} \ln(2\pi) + \frac{N+M}{2} \ln \beta - \frac{1}{2} \ln(\det \mathbf{S}_0) \\ & - \frac{\beta}{2} \mathbf{v}^\top \mathbf{M} \mathbf{v} + \mathbf{v}^\top \mathbf{u} - \frac{\beta}{2} \mathbf{m}_0^\top \mathbf{S}_0^{-1} \mathbf{m}_0, \end{aligned} \quad (3.172)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \mathbf{S}_0^{-1} + \boldsymbol{\Phi}^\top \boldsymbol{\Phi} & -\boldsymbol{\Phi}^\top \\ -\boldsymbol{\Phi} & \mathbf{I} \end{bmatrix}, \mathbf{u} = \begin{bmatrix} \mathbf{S}_0^{-1} \mathbf{m}_0 \\ \mathbf{0} \end{bmatrix}. \quad (3.173)$$

The right hand side can be written as

$$\begin{aligned} & -\frac{N+M}{2} \ln(2\pi) + \frac{N+M}{2} \ln \beta - \frac{1}{2} \ln(\det \mathbf{S}_0) \\ & - \frac{\beta}{2} \|\mathbf{t}\|^2 - \frac{\beta}{2} (\mathbf{w} - \mathbf{m})^\top \mathbf{S}^{-1} (\mathbf{w} - \mathbf{m}) + \frac{\beta}{2} \mathbf{m}^\top \mathbf{S}^{-1} \mathbf{m} - \frac{\beta}{2} \mathbf{m}_0^\top \mathbf{S}_0^{-1} \mathbf{m}_0, \end{aligned} \quad (3.174)$$

where

$$\begin{aligned} \mathbf{m} &= \mathbf{S} (\mathbf{S}_0^{-1} \mathbf{m}_0 + \boldsymbol{\Phi}^\top \mathbf{t}), \\ \mathbf{S} &= (\mathbf{S}_0^{-1} + \boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1}. \end{aligned} \quad (3.175)$$

Then, the logarithm of $I(\beta)$ can be written as

$$\begin{aligned} & -\frac{N}{2} \ln(2\pi) + \frac{N}{2} \ln \beta - \frac{1}{2} \ln(\det \mathbf{S}_0) + \frac{1}{2} \ln(\det \mathbf{S}) \\ & - \frac{\beta}{2} \|\mathbf{t}\|^2 + \frac{\beta}{2} \mathbf{m}^\top \mathbf{S}^{-1} \mathbf{m} - \frac{\beta}{2} \mathbf{m}_0^\top \mathbf{S}_0^{-1} \mathbf{m}_0. \end{aligned} \quad (3.176)$$

Then, the logarithm of the integrand with respect to β can be written as

$$\begin{aligned}
& -\frac{N}{2} \ln(2\pi) + \frac{N}{2} \ln \beta - \frac{1}{2} \ln(\det \mathbf{S}_0) + \frac{1}{2} \ln(\det \mathbf{S}) \\
& + \frac{\beta}{2} \mathbf{m}^\top \mathbf{S}^{-1} \mathbf{m} - \frac{\beta}{2} \|\mathbf{t}\|^2 - \frac{\beta}{2} \mathbf{m}_0^\top \mathbf{S}_0^{-1} \mathbf{m}_0 \\
& - \ln \Gamma(a_0) + a_0 \ln b_0 + (a_0 - 1) \ln \beta - b_0 \beta \\
= & -\frac{N}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \mathbf{S}_0) + \frac{1}{2} \ln(\det \mathbf{S}) \\
& - \ln \Gamma(a_0) + a_0 \ln b_0 + (a - 1) \ln \beta - b\beta,
\end{aligned} \tag{3.177}$$

where

$$\begin{aligned}
a & = a_0 + \frac{N}{2}, \\
b & = b_0 + \frac{1}{2} \|\mathbf{t}\|^2 + \frac{1}{2} \mathbf{m}_0^\top \mathbf{S}_0^{-1} \mathbf{m}_0 - \frac{1}{2} \mathbf{m}^\top \mathbf{S}^{-1} \mathbf{m}.
\end{aligned} \tag{3.178}$$

Then, the logarithm of the integral with respect to β can be written as

$$\begin{aligned}
& -\frac{N}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \mathbf{S}_0) + \frac{1}{2} \ln(\det \mathbf{S}) \\
& - \ln \Gamma(a_0) + a_0 \ln b_0 + \ln \Gamma(a) - a \ln b.
\end{aligned} \tag{3.179}$$

Therefore,

$$p(\mathbf{t}) = (2\pi)^{-\frac{N}{2}} \left(\frac{\det \mathbf{S}}{\det \mathbf{S}_0} \right)^{\frac{1}{2}} \frac{\Gamma(a)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b^a}. \tag{3.180}$$

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

$$\begin{aligned}\mathbf{x} &= \sum_{m=1}^M \alpha_m \mathbf{x}_m, \\ \mathbf{y} &= \sum_{n=1}^N \beta_n \mathbf{y}_n,\end{aligned}\tag{4.1}$$

where

$$\begin{aligned}\sum_{m=1}^M \alpha_m &= \sum_{n=1}^N \beta_n = 1, \\ \alpha_m &\geq 0, \beta_n \geq 0.\end{aligned}\tag{4.2}$$

Let us assume that $\alpha_1, \dots, \alpha_M$ and β_1, \dots, β_N below are subject to the constraints above.

(a)

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,

$$\sum_{m=1}^M \alpha_m (\hat{\mathbf{w}}^\top \mathbf{x}_m + w_0) = \hat{\mathbf{w}}^\top \sum_{m=1}^M \alpha_m \mathbf{x}_m + w_0 \sum_m \alpha_m,\tag{4.4}$$

for any $\hat{\mathbf{w}}$ and w_0 . The right hand side can be written as

$$\hat{\mathbf{w}}^\top \sum_{n=1}^N \beta_n \mathbf{y}_n + w_0 \sum_{n=1}^N \beta_n = \sum_{n=1}^N \beta_n (\hat{\mathbf{w}}^\top \mathbf{y}_n + w_0).\tag{4.5}$$

Therefore, there do not exist $\hat{\mathbf{w}}$ and w_0 such that

$$\begin{aligned}\hat{\mathbf{w}}^\top \mathbf{x}_m + w_0 &> 0, \\ \hat{\mathbf{w}}^\top \mathbf{y}_n + w_0 &< 0.\end{aligned}\tag{4.6}$$

(b)

If there exist $\hat{\mathbf{w}}$ and w_0 such that

$$\begin{aligned}\hat{\mathbf{w}}^\top \mathbf{x}_m + w_0 &> 0, \\ \hat{\mathbf{w}}^\top \mathbf{y}_n + w_0 &< 0,\end{aligned}\tag{4.7}$$

then

$$\begin{aligned}\sum_{m=1}^M \alpha_m (\hat{\mathbf{w}}^\top \mathbf{x}_m + w_0) &> 0, \\ \sum_{n=1}^N \beta_n (\hat{\mathbf{w}}^\top \mathbf{y}_n + w_0) &< 0.\end{aligned}\tag{4.8}$$

The left hand sides can be written as

$$\begin{aligned}\hat{\mathbf{w}}^\top \sum_{m=1}^M \alpha_m \mathbf{x}_m + w_0 \sum_{m=1}^M \alpha_m &= \hat{\mathbf{w}}^\top \sum_{m=1}^M \alpha_m \mathbf{x}_m + w_0, \\ \hat{\mathbf{w}}^\top \sum_{n=1}^N \beta_n \mathbf{y}_n + w_0 \sum_{n=1}^N \beta_n &= \hat{\mathbf{w}}^\top \sum_{n=1}^N \beta_n \mathbf{y}_n + w_0.\end{aligned}\tag{4.9}$$

Then, there do not exist $\alpha_1, \dots, \alpha_M$ and β_1, \dots, β_N such that

$$\sum_{m=1}^M \alpha_m \mathbf{x}_m = \sum_{n=1}^N \beta_n \mathbf{y}_n.\tag{4.10}$$

Therefore, 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

$$E(\tilde{\mathbf{W}}) = \frac{1}{2} \text{tr} \left((\tilde{\mathbf{X}} \tilde{\mathbf{W}} - \mathbf{T})^\top (\tilde{\mathbf{X}} \tilde{\mathbf{W}} - \mathbf{T}) \right),\tag{4.11}$$

where

$$\tilde{\mathbf{X}} = \begin{bmatrix} 1 & \mathbf{x}_1^\top \\ \vdots & \vdots \\ 1 & \mathbf{x}_N^\top \end{bmatrix}, \tilde{\mathbf{W}} = \begin{bmatrix} w_{10} & \cdots & w_{K0} \\ \mathbf{w}_1 & \cdots & \mathbf{w}_K \end{bmatrix}, \mathbf{T} = \begin{bmatrix} \mathbf{t}_1^\top \\ \vdots \\ \mathbf{t}_N^\top \end{bmatrix}.\tag{4.12}$$

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

$$\mathbf{O} = \tilde{\mathbf{X}}^\top (\tilde{\mathbf{X}} \tilde{\mathbf{W}} - \mathbf{T}). \quad (4.13)$$

Therefore,

$$\operatorname{argmin}_{\tilde{\mathbf{W}}} E(\tilde{\mathbf{W}}) = \left(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} \right)^{-1} \tilde{\mathbf{X}}^\top \mathbf{T}. \quad (4.14)$$

Let $\tilde{\mathbf{W}}^*$ denote the least-square solution above. Then,

$$(\tilde{\mathbf{W}}^*)^\top \tilde{\mathbf{x}} - \mathbf{t}_n = \mathbf{T}^\top \tilde{\mathbf{X}} \left(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} \right)^{-1} \tilde{\mathbf{x}} - \mathbf{t}_n, \quad (4.15)$$

where $\tilde{\mathbf{x}}$ is a vector in $M + 1$ dimensions whose first element is 1. The right hand side can be written as

$$\mathbf{T}^\top \left(\tilde{\mathbf{X}} \left(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} \right)^{-1} \tilde{\mathbf{x}} - \mathbf{v}_n \right) = \mathbf{0}? \quad (4.16)$$

where \mathbf{v}_n is a vector in N dimensions whose n th element is 1 and other elements are zero. Therefore,

$$(\tilde{\mathbf{W}}^*)^\top \tilde{\mathbf{x}} - \mathbf{t}_n = \mathbf{0}. \quad (4.17)$$

Thus, if

$$\mathbf{a}^\top \mathbf{t}_n + b = 0, \quad (4.18)$$

then

$$\mathbf{a}^\top (\tilde{\mathbf{W}}^*)^\top \tilde{\mathbf{x}} + b = 0. \quad (4.19)$$

4.3 (Incomplete)

4.4

Let $\mathbf{x}_1, \dots, \mathbf{x}_N$ be variables and let

$$\mathbf{m}_k = \frac{1}{N_k} \sum_{n \in \mathcal{C}_k} \mathbf{x}_n, \quad (4.20)$$

where N_k is the number of \mathbf{x}_n such that n is in \mathcal{C}_k . Setting the derivatives of

$$\mathbf{w}^\top (\mathbf{m}_2 - \mathbf{m}_1) + \lambda (\|\mathbf{w}\|^2 - 1) \quad (4.21)$$

with respect to \mathbf{w} and λ to zero gives

$$\begin{aligned}\mathbf{m}_2 - \mathbf{m}_1 + 2\lambda\mathbf{w} &= \mathbf{0}, \\ \|\mathbf{w}\|^2 - 1 &= 0.\end{aligned}\tag{4.22}$$

Therefore, $\mathbf{w}^\top(\mathbf{m}_2 - \mathbf{m}_1)$ under the constraint

$$\|\mathbf{w}\|^2 = 1\tag{4.23}$$

is maximised if

$$\mathbf{w} \propto \mathbf{m}_2 - \mathbf{m}_1.\tag{4.24}$$

4.5

Let $\mathbf{x}_1, \dots, \mathbf{x}_N$ be variables and let

$$\mathbf{m}_k = \frac{1}{N_k} \sum_{n \in \mathcal{C}_k} \mathbf{x}_n,\tag{4.25}$$

where N_k is the number of \mathbf{x}_n such that n is in \mathcal{C}_k . Let

$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2},\tag{4.26}$$

where

$$\begin{aligned}s_k^2 &= \sum_{n \in \mathcal{C}_k} (y_n - m_k)^2, \\ y_n &= \mathbf{w}^\top \mathbf{x}_n, \\ m_k &= \mathbf{w}^\top \mathbf{m}_k.\end{aligned}\tag{4.27}$$

Then, $J(\mathbf{w})$ can be written as

$$\frac{(\mathbf{w}^\top(\mathbf{m}_2 - \mathbf{m}_1))^2}{\sum_{n \in \mathcal{C}_1} (\mathbf{w}^\top(\mathbf{x}_n - \mathbf{m}_1))^2 + \sum_{n \in \mathcal{C}_2} (\mathbf{w}^\top(\mathbf{x}_n - \mathbf{m}_2))^2} = \frac{\mathbf{w}^\top \mathbf{S}_B \mathbf{w}}{\mathbf{w}^\top \mathbf{S}_W \mathbf{w}},\tag{4.28}$$

where

$$\begin{aligned}\mathbf{S}_B &= (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^\top, \\ \mathbf{S}_W &= \sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^\top + \sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^\top.\end{aligned}\tag{4.29}$$

4.6

Let $\mathbf{x}_1, \dots, \mathbf{x}_N$ be variables and let

$$\mathbf{m}_k = \frac{1}{N_k} \sum_{n \in \mathcal{C}_k} \mathbf{x}_n, \quad (4.30)$$

where N_k is the number of \mathbf{x}_n such that n is in \mathcal{C}_k . Let

$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}, \quad (4.31)$$

where

$$\begin{aligned} s_k^2 &= \sum_{n \in \mathcal{C}_k} (y_n - m_k)^2, \\ y_n &= \mathbf{w}^\top \mathbf{x}_n, \\ m_k &= \mathbf{w}^\top \mathbf{m}_k. \end{aligned} \quad (4.32)$$

By 4.5,

$$J(\mathbf{w}) = \frac{\mathbf{w}^\top \mathbf{S}_B \mathbf{w}}{\mathbf{w}^\top \mathbf{S}_W \mathbf{w}}, \quad (4.33)$$

where

$$\begin{aligned} \mathbf{S}_B &= (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^\top, \\ \mathbf{S}_W &= \sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^\top + \sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^\top. \end{aligned} \quad (4.34)$$

Let

$$E = \frac{1}{2} \sum_{n=1}^N (\mathbf{w}^\top \mathbf{x}_n + w_0 - t_n)^2, \quad (4.35)$$

where

$$t_n = \begin{cases} \frac{N}{N_1}, & n \in \mathcal{C}_1, \\ -\frac{N}{N_2}, & n \in \mathcal{C}_2. \end{cases} \quad (4.36)$$

Setting the derivative with respect to \mathbf{w} and w_0 gives

$$\begin{aligned} 0 &= \sum_{n=1}^N (\mathbf{w}^\top \mathbf{x}_n + w_0 - t_n), \\ \mathbf{0} &= \sum_{n=1}^N (\mathbf{w}^\top \mathbf{x}_n + w_0 - t_n) \mathbf{x}_n. \end{aligned} \quad (4.37)$$

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

$$\mathbf{w}^\top \sum_{n=1}^N \mathbf{x}_n + N w_0 - \sum_{n=1}^N t_n = N (\mathbf{w}^\top \mathbf{m} + w_0), \quad (4.38)$$

where

$$\mathbf{m} = \frac{1}{N} \sum_{n=1}^N \mathbf{x}_n. \quad (4.39)$$

Then,

$$w_0 = -\mathbf{w}^\top \mathbf{m}. \quad (4.40)$$

Then, the right hand side of the second equation above can be written as

$$\begin{aligned} & \sum_{n=1}^N (\mathbf{w}^\top (\mathbf{x}_n - \mathbf{m}) - t_n) \mathbf{x}_n \\ &= \sum_{n \in \mathcal{C}_1} \left(\mathbf{w}^\top (\mathbf{x}_n - \mathbf{m}) - \frac{N}{N_1} \right) \mathbf{x}_n + \sum_{n \in \mathcal{C}_2} \left(\mathbf{w}^\top (\mathbf{x}_n - \mathbf{m}) + \frac{N}{N_2} \right) \mathbf{x}_n. \end{aligned} \quad (4.41)$$

We have

$$\begin{aligned} \mathbf{m} &= \frac{N_1}{N} \mathbf{m}_1 + \frac{N_2}{N} \mathbf{m}_2, \\ \sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1) &= \mathbf{0}. \end{aligned} \quad (4.42)$$

Then, the first term of the right hand side can be written as

$$\begin{aligned} & \sum_{n \in \mathcal{C}_1} \left(\mathbf{w}^\top \left(\mathbf{x}_n - \mathbf{m}_1 + \frac{N_2}{N} (\mathbf{m}_1 - \mathbf{m}_2) \right) - \frac{N}{N_1} \right) (\mathbf{x}_n - \mathbf{m}_1 + \mathbf{m}_1) \\ &= \left(\sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^\top \right) \mathbf{w} + \frac{N_1 N_2}{N} (\mathbf{m}_1 - \mathbf{m}_2) \mathbf{m}_1^\top \mathbf{w} - N \mathbf{m}_1. \end{aligned} \quad (4.43)$$

Similarly, the second term can be written as

$$\left(\sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^\top \right) \mathbf{w} + \frac{N_1 N_2}{N} (\mathbf{m}_2 - \mathbf{m}_1) \mathbf{m}_2^\top \mathbf{w} - N \mathbf{m}_2. \quad (4.44)$$

Then,

$$\begin{aligned} \mathbf{0} &= \left(\sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^\top \right) \mathbf{w} + \frac{N_1 N_2}{N} (\mathbf{m}_1 - \mathbf{m}_2) \mathbf{m}_1^\top \mathbf{w} \\ &\quad - N \mathbf{m}_1 + \left(\sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^\top \right) \mathbf{w} \\ &\quad + \frac{N_1 N_2}{N} (\mathbf{m}_2 - \mathbf{m}_1) \mathbf{m}_2^\top \mathbf{w} - N \mathbf{m}_2. \end{aligned} \quad (4.45)$$

Therefore,

$$\left(\mathbf{S}_W + \frac{N_1 N_2}{N} \mathbf{S}_B \right) \mathbf{w} = N(\mathbf{m}_1 - \mathbf{m}_2). \quad (4.46)$$

4.7

Let

$$\sigma(a) = \frac{1}{1 + \exp(-a)}. \quad (4.47)$$

(a)

We have

$$\sigma(-a) = \frac{1}{1 + \exp(a)}. \quad (4.48)$$

The right hand side can be written as

$$1 - \frac{\exp(a)}{1 + \exp(a)} = 1 - \frac{1}{1 + \exp(-a)}. \quad (4.49)$$

Therefore,

$$\sigma(-a) = 1 - \sigma(a). \quad (4.50)$$

(b)

We have

$$\exp(-a) = \frac{1}{\sigma(a)} - 1. \quad (4.51)$$

Then,

$$a = -\ln \left(\frac{1}{\sigma(a)} - 1 \right). \quad (4.52)$$

Therefore,

$$\sigma^{-1}(y) = \ln \left(\frac{y}{1-y} \right). \quad (4.53)$$

4.8

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

$$p(\mathbf{x}|\mathcal{C}_k) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}), \quad (4.54)$$

where

$$p(\mathcal{C}_1) + p(\mathcal{C}_2) = 1. \quad (4.55)$$

By the Bayes' theorem,

$$p(\mathcal{C}_1|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}. \quad (4.56)$$

The right hand side can be written as

$$\sigma(a) = \frac{1}{1 + \exp(-a)}, \quad (4.57)$$

where

$$a = \ln \left(\frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \right). \quad (4.58)$$

Substituting the expressions above of $p(\mathbf{x}|\mathcal{C}_k)$, we have

$$\begin{aligned} a &= -\frac{D}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \boldsymbol{\Sigma}) - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_1)^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_1) + \ln p(\mathcal{C}_1) \\ &\quad + \frac{D}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \boldsymbol{\Sigma}) + \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_2)^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_2) - \ln p(\mathcal{C}_2). \end{aligned} \quad (4.59)$$

Therefore,

$$p(\mathcal{C}_1|\mathbf{x}) = \sigma(\mathbf{w}^\top \mathbf{x} + w_0), \quad (4.60)$$

where

$$\begin{aligned} \mathbf{w} &= \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2), \\ w_0 &= -\frac{1}{2} \boldsymbol{\mu}_1^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_1 + \frac{1}{2} \boldsymbol{\mu}_2^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_2 + \ln p(\mathcal{C}_1) - \ln p(\mathcal{C}_2). \end{aligned} \quad (4.61)$$

4.9

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables from the standard basis in K dimensions such that

$$p(\mathbf{t}_n, \boldsymbol{\phi}_n) = \prod_{k=1}^K y_{nk}^{t_{nk}}, \quad (4.62)$$

where

$$\begin{aligned} y_{nk} &= p(\boldsymbol{\phi}_n, \mathcal{C}_k), \\ p(\mathcal{C}_k) &= \pi_k, \\ \sum_{k=1}^K \pi_k &= 1. \end{aligned} \quad (4.63)$$

Then,

$$p(\mathbf{T}, \boldsymbol{\Phi}) = \prod_{n=1}^N \prod_{k=1}^K y_{nk}^{t_{nk}}, \quad (4.64)$$

By the Bayes' theorem,

$$y_{nk} = \pi_k p(\boldsymbol{\phi}_n | \mathcal{C}_k). \quad (4.65)$$

Then,

$$\ln p(\mathbf{T}, \boldsymbol{\Phi}) = \sum_{n=1}^N \sum_{k=1}^K t_{nk} (\ln \pi_k + \ln p(\boldsymbol{\phi}_n | \mathcal{C}_k)). \quad (4.66)$$

Setting the derivatives of

$$\ln p(\mathbf{T}, \boldsymbol{\Phi}) + \lambda \left(\sum_{k=1}^K \pi_k - 1 \right) \quad (4.67)$$

with respect to π_k and λ to zero gives

$$\begin{aligned} 0 &= \frac{1}{\pi_k} \sum_{n=1}^N t_{nk} + \lambda, \\ 0 &= \sum_{k=1}^K \pi_k - 1. \end{aligned} \quad (4.68)$$

Then,

$$\lambda = - \sum_{n=1}^N \sum_{k=1}^K t_{nk}. \quad (4.69)$$

Since $\mathbf{t}_1, \dots, \mathbf{t}_N$ are from the standard basis in K dimensions, the right hand side can be written as $-N$. Therefore, the maximum likelihood solution for π_k is given by

$$\pi_{k\text{ML}} = \frac{N_k}{N}, \quad (4.70)$$

where

$$N_k = \sum_{n=1}^N t_{nk}. \quad (4.71)$$

4.10

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables from the standard basis in K dimensions such that

$$p(\mathbf{t}_n, \boldsymbol{\phi}_n) = \prod_{k=1}^K y_{nk}^{t_{nk}}, \quad (4.72)$$

where

$$\begin{aligned} y_{nk} &= p(\boldsymbol{\phi}_n, \mathcal{C}_k), \\ p(\boldsymbol{\phi}_n | \mathcal{C}_k) &= \mathcal{N}(\boldsymbol{\phi}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}), \\ p(\mathcal{C}_k) &= \pi_k, \\ \sum_{k=1}^K \pi_k &= 1. \end{aligned} \quad (4.73)$$

Then,

$$p(\mathbf{T}, \boldsymbol{\Phi}) = \prod_{n=1}^N \prod_{k=1}^K y_{nk}^{t_{nk}}. \quad (4.74)$$

By the Bayes' theorem,

$$y_{nk} = \pi_k \mathcal{N}(\boldsymbol{\phi}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}). \quad (4.75)$$

Then,

$$\ln p(\mathbf{T}, \boldsymbol{\Phi}) = \sum_{n=1}^N \sum_{k=1}^K t_{nk} (\ln \mathcal{N}(\boldsymbol{\phi}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}) + \ln \pi_k). \quad (4.76)$$

The right hand side except the terms independent of $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}$ can be written as

$$\sum_{n=1}^N \sum_{k=1}^K t_{nk} \left(-\frac{1}{2} \ln(\det \boldsymbol{\Sigma}) - \frac{1}{2} (\boldsymbol{\phi}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1} (\boldsymbol{\phi}_n - \boldsymbol{\mu}_k) \right). \quad (4.77)$$

By 3.21??, setting the derivatives with respect to $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}$ to zero gives

$$\begin{aligned}\mathbf{0} &= \frac{1}{2} \sum_{n=1}^N t_{nk} (\boldsymbol{\Sigma}^{-1} + (\boldsymbol{\Sigma}^{-1})^\top) (\boldsymbol{\phi}_n - \boldsymbol{\mu}_k), \\ \mathbf{O} &= -\frac{1}{2} \sum_{n=1}^N \sum_{k=1}^K t_{nk} \left((\boldsymbol{\Sigma}^{-1})^\top - (\boldsymbol{\Sigma}^{-1})^2 (\boldsymbol{\phi}_n - \boldsymbol{\mu}_k)(\boldsymbol{\phi}_n - \boldsymbol{\mu}_k)^\top \right).\end{aligned}\quad (4.78)$$

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

$$\begin{aligned}\boldsymbol{\mu}_{k\text{ML}} &= \frac{1}{N_k} \sum_{n=1}^N t_{nk} \boldsymbol{\phi}_n, \\ \boldsymbol{\Sigma}_{\text{ML}} &= \frac{1}{N} \sum_{k=1}^K N_k \mathbf{S}_k,\end{aligned}\quad (4.79)$$

where

$$\begin{aligned}N_k &= \sum_{n=1}^N t_{nk}, \\ \mathbf{S}_k &= \frac{1}{N_k} \sum_{n=1}^N t_{nk} (\boldsymbol{\phi}_n - \boldsymbol{\mu}_k)(\boldsymbol{\phi}_n - \boldsymbol{\mu}_k)^\top.\end{aligned}\quad (4.80)$$

4.11

Let $\boldsymbol{\phi}$ be a variable in M dimensions whose each component is a binary code with length L such that

$$p(\boldsymbol{\phi}|\mathcal{C}_k) = \prod_{m=1}^M \prod_{l=1}^L \mu_{kml}^{\phi_{ml}}, \quad (4.81)$$

where

$$\sum_{k=1}^K p(\mathcal{C}_k) = 1. \quad (4.82)$$

By the Bayes' theorem,

$$p(\mathcal{C}_k|\boldsymbol{\phi}) = \frac{p(\boldsymbol{\phi}|\mathcal{C}_k)p(\mathcal{C}_k)}{\sum_{k'=1}^K p(\boldsymbol{\phi}|\mathcal{C}_{k'})p(\mathcal{C}_{k'})}. \quad (4.83)$$

Therefore,

$$p(\mathcal{C}_k|\boldsymbol{\phi}) = \frac{\exp(a_k(\boldsymbol{\phi}))}{\sum_{k'=1}^K \exp(a_{k'}(\boldsymbol{\phi}))}, \quad (4.84)$$

where

$$a_k(\boldsymbol{\phi}) = \left(\sum_{m=1}^M \sum_{l=1}^L \phi_{ml} \ln \mu_{kml} \right) + \ln p(\mathcal{C}_k). \quad (4.85)$$

4.12

Let

$$\sigma(a) = \frac{1}{1 + \exp(-a)}. \quad (4.86)$$

Then,

$$\frac{d\sigma(a)}{da} = \frac{\exp(-a)}{(1 + \exp(-a))^2}. \quad (4.87)$$

The right hand side can be written as

$$\frac{1}{1 + \exp(-a)} - \frac{1}{(1 + \exp(-a))^2} = \sigma(a) - (\sigma(a))^2. \quad (4.88)$$

Therefore,

$$\frac{d\sigma(a)}{da} = \sigma(a) (1 - \sigma(a)). \quad (4.89)$$

4.13

Let t_1, \dots, t_N be binary variables such that

$$p(t_n|\mathbf{w}) = y_n^{t_n} (1 - y_n)^{1-t_n}, \quad (4.90)$$

where

$$\begin{aligned} y_n &= \sigma(\mathbf{w}^\top \boldsymbol{\phi}_n), \\ \sigma(a) &= \frac{1}{1 + \exp(-a)}. \end{aligned} \quad (4.91)$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}). \quad (4.92)$$

The right hand side can be written as

$$-\ln \left(\prod_{n=1}^N y_n^{t_n} (1 - y_n)^{1-t_n} \right) = -\sum_{n=1}^N (t_n \ln y_n + (1 - t_n) \ln(1 - y_n)). \quad (4.93)$$

By 4.12,

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^N \left(\frac{t_n}{y_n} y_n (1 - y_n) \boldsymbol{\phi}_n - \frac{1 - t_n}{1 - y_n} y_n (1 - y_n) \boldsymbol{\phi}_n \right). \quad (4.94)$$

The right hand side can be written as

$$-\sum_{n=1}^N (t_n (1 - y_n) \boldsymbol{\phi}_n - (1 - t_n) y_n \boldsymbol{\phi}_n) = \sum_{n=1}^N (y_n - t_n) \boldsymbol{\phi}_n. \quad (4.95)$$

Therefore,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^N (y_n - t_n) \boldsymbol{\phi}_n. \quad (4.96)$$

4.14

Let t_1, \dots, t_N be binary variables such that

$$p(t_n | \mathbf{w}) = y_n^{t_n} (1 - y_n)^{1-t_n}, \quad (4.97)$$

where

$$\begin{aligned} y_n &= \sigma(\mathbf{w}^\top \boldsymbol{\phi}_n), \\ \sigma(a) &= \frac{1}{1 + \exp(-a)}. \end{aligned} \quad (4.98)$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t} | \mathbf{w}). \quad (4.99)$$

By 4.13, setting the derivative with respect to \mathbf{w} to zero gives

$$\mathbf{0} = \sum_{n=1}^N (y_n - t_n) \boldsymbol{\phi}_n. \quad (4.100)$$

If $\boldsymbol{\phi}_1, \dots, \boldsymbol{\phi}_N$ are linearly independent, then

$$y_n = t_n. \quad (4.101)$$

Then,

$$\sigma(\mathbf{w}^\top \boldsymbol{\phi}_n) = \begin{cases} 1, & t_n = 1, \\ 0, & \text{otherwise.} \end{cases} \quad (4.102)$$

Therefore,

$$\mathbf{w}^\top \boldsymbol{\phi}_n = \begin{cases} \infty, & t_n = 1, \\ -\infty, & \text{otherwise.} \end{cases} \quad (4.103)$$

4.15

Let t_1, \dots, t_N be binary variables such that

$$p(t_n | \mathbf{w}) = y_n^{t_n} (1 - y_n)^{1-t_n}, \quad (4.104)$$

where

$$\begin{aligned} y_n &= \sigma(\mathbf{w}^\top \boldsymbol{\phi}_n), \\ \sigma(a) &= \frac{1}{1 + \exp(-a)}. \end{aligned} \quad (4.105)$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t} | \mathbf{w}). \quad (4.106)$$

By 4.13,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^N (y_n - t_n) \boldsymbol{\phi}_n. \quad (4.107)$$

By 4.12,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^N y_n (1 - y_n) \boldsymbol{\phi}_n \boldsymbol{\phi}_n^\top. \quad (4.108)$$

The right hand side can be written as

$$\mathbf{H} = \boldsymbol{\Phi}^\top \mathbf{R} \boldsymbol{\Phi}, \quad (4.109)$$

where

$$R_{nn'} = y_n (1 - y_n) I_{nn'}, \quad (4.110)$$

Then,

$$\mathbf{u}^\top \mathbf{H} \mathbf{u} = \mathbf{v}^\top \mathbf{R} \mathbf{v}, \quad (4.111)$$

where

$$\mathbf{v} = \boldsymbol{\Phi} \mathbf{u}. \quad (4.112)$$

The right hand side can be written as

$$\sum_{n=1}^N \sum_{n'=1}^N v_n y_n (1 - y_n) I_{nn'} v_{n'} = \sum_{n=1}^N y_n (1 - y_n) v_n^2. \quad (4.113)$$

We have

$$y_n (1 - y_n) > 0. \quad (4.114)$$

Then,

$$\mathbf{u}^\top \mathbf{H} \mathbf{u} > 0, \quad (4.115)$$

so that \mathbf{H} is positive definite. Therefore, E is a convex function of \mathbf{w} and it has a unique minimum.

4.16

Let t_1, \dots, t_N be binary variables such that

$$p(t_n = 1 | \boldsymbol{\phi}_n) = \pi_n. \quad (4.116)$$

Then,

$$p(t_n | \boldsymbol{\phi}_n) = \pi_n^{t_n} (1 - \pi_n)^{1-t_n}, \quad (4.117)$$

so that

$$p(\mathbf{t} | \boldsymbol{\Phi}) = \prod_{n=1}^N \pi_n^{t_n} (1 - \pi_n)^{1-t_n}. \quad (4.118)$$

Therefore,

$$-\ln p(\mathbf{t} | \boldsymbol{\Phi}) = -\sum_{n=1}^N (t_n \ln \pi_n + (1 - t_n) \ln(1 - \pi_n)). \quad (4.119)$$

4.17

Let

$$y_k = \frac{\exp(a_k)}{\sum_{k'=1}^K \exp(a_{k'})}. \quad (4.120)$$

Then,

$$\frac{\partial y_k}{\partial a_k} = \frac{\exp(a_k)}{\sum_{k'=1}^K \exp(a_{k'})} - \frac{\exp(2a_k)}{\left(\sum_{k'=1}^K \exp(a_{k'})\right)^2}. \quad (4.121)$$

The right hand side can be written as $y_k(1 - y_k)$. If $k \neq k'$, then

$$\frac{\partial y_k}{\partial a_{k'}} = -\frac{\exp(a_k + a_{k'})}{\left(\sum_{k''=1}^K \exp(a_{k''})\right)^2}. \quad (4.122)$$

The right hand side can be written as $-y_k y_{k'}$. Therefore,

$$\frac{\partial y_k}{\partial a_{k'}} = y_k(I_{kk'} - y_{k'}). \quad (4.123)$$

4.18

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables from the standard basis in K dimensions such that

$$p(\mathbf{t}_n | \mathbf{W}) = \prod_{k=1}^K y_{nk}^{t_{nk}}, \quad (4.124)$$

where

$$\begin{aligned} y_{nk} &= \frac{\exp(a_{nk})}{\sum_{k'=1}^K \exp(a_{nk'})}, \\ a_{nk} &= \mathbf{w}_k^\top \boldsymbol{\phi}_n. \end{aligned} \quad (4.125)$$

Then,

$$p(\mathbf{T} | \mathbf{W}) = \prod_{n=1}^N \prod_{k=1}^K y_{nk}^{t_{nk}}. \quad (4.126)$$

Let

$$E(\mathbf{W}) = -\ln p(\mathbf{T} | \mathbf{W}). \quad (4.127)$$

The right hand side can be written as

$$-\sum_{n=1}^N \sum_{k=1}^K t_{nk} \ln y_{nk}. \quad (4.128)$$

By 4.17,

$$\nabla_{\mathbf{w}_{k'}} E(\mathbf{W}) = -\sum_{n=1}^N \sum_{k=1}^K y_{nk}(I_{kk'} - y_{nk'}) \frac{t_{nk}}{y_{nk}} \boldsymbol{\phi}_n. \quad (4.129)$$

Since $\mathbf{t}_1, \dots, \mathbf{t}_N$ are variables from the standard basis in K dimensions, the right hand side can be written as

$$-\sum_{n=1}^N \left(\sum_{k=1}^K (I_{kk'} - y_{nk'}) t_{nk} \right) \boldsymbol{\phi}_n = -\sum_{n=1}^N (t_{nk'} - y_{nk'}) \boldsymbol{\phi}_n. \quad (4.130)$$

Therefore,

$$\nabla_{\mathbf{w}_k} E(\mathbf{W}) = \sum_{n=1}^N (y_{nk} - t_{nk}) \boldsymbol{\phi}_n. \quad (4.131)$$

4.19

Let t_1, \dots, t_N be binary variables such that

$$p(t_n = 1 | a_n) = \Phi(a_n), \quad (4.132)$$

where

$$\begin{aligned} \Phi(a) &= \int_{-\infty}^a \mathcal{N}(\theta | 0, 1) d\theta, \\ a_n &= \mathbf{w}^\top \boldsymbol{\phi}_n. \end{aligned} \quad (4.133)$$

(a)

We have

$$p(t_n | \boldsymbol{\phi}_n) = (\Phi(a_n))^{t_n} (1 - \Phi(a_n))^{1-t_n}. \quad (4.134)$$

Then,

$$p(\mathbf{t} | \boldsymbol{\Phi}) = \prod_{n=1}^N (\Phi(a_n))^{t_n} (1 - \Phi(a_n))^{1-t_n}. \quad (4.135)$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t} | \boldsymbol{\Phi}). \quad (4.136)$$

The right hand side can be written as

$$-\sum_{n=1}^N (t_n \ln \Phi(a_n) + (1 - t_n) \ln (1 - \Phi(a_n))). \quad (4.137)$$

Then,

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^N \left(t_n \frac{\mathcal{N}(a_n | 0, 1)}{\Phi(a_n)} - (1 - t_n) \frac{\mathcal{N}(a_n | 0, 1)}{1 - \Phi(a_n)} \right) \boldsymbol{\phi}_n. \quad (4.138)$$

The right hand side can be written as

$$\begin{aligned} & - \sum_{n=1}^N \left(\frac{t_n}{\Phi(a_n)} - \frac{1-t_n}{1-\Phi(a_n)} \right) \mathcal{N}(a_n|0,1) \phi_n \\ & = \sum_{n=1}^N \frac{\mathcal{N}(a_n|0,1)}{\Phi(a_n)(1-\Phi(a_n))} (\Phi(a_n) - t_n) \phi_n. \end{aligned} \quad (4.139)$$

Therefore,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^N \frac{\mathcal{N}(a_n|0,1)}{\Phi(a_n)(1-\Phi(a_n))} (\Phi(a_n) - t_n) \phi_n. \quad (4.140)$$

(b)

We have

$$\begin{aligned} \nabla \nabla E(\mathbf{w}) & = \sum_{n=1}^N \frac{-a_n \mathcal{N}(a_n|0,1)}{\Phi(a_n)(1-\Phi(a_n))} (\Phi(a_n) - t_n) \phi_n \phi_n^\top \\ & \quad - \sum_{n=1}^N \frac{(\mathcal{N}(a_n|0,1))^2}{(\Phi(a_n))^2(1-\Phi(a_n))} (\Phi(a_n) - t_n) \phi_n \phi_n^\top \\ & \quad + \sum_{n=1}^N \frac{(\mathcal{N}(a_n|0,1))^2}{\Phi(a_n)(1-\Phi(a_n))^2} (\Phi(a_n) - t_n) \phi_n \phi_n^\top \\ & \quad + \sum_{n=1}^N \frac{(\mathcal{N}(a_n|0,1))^2}{\Phi(a_n)(1-\Phi(a_n))} \phi_n \phi_n^\top. \end{aligned} \quad (4.141)$$

Therefore,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^N b_n \phi_n \phi_n^\top, \quad (4.142)$$

where

$$\begin{aligned} b_n & = \left(\frac{\mathcal{N}(a_n|0,1)}{\Phi(a_n)(1-\Phi(a_n))} \right)^2 ((\Phi(a_n))^2 - 2t_n \Phi(a_n) + t_n) \\ & \quad - \frac{\mathcal{N}(a_n|0,1)}{\Phi(a_n)(1-\Phi(a_n))} a_n (\Phi(a_n) - t_n). \end{aligned} \quad (4.143)$$

4.20

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables from the standard basis in K dimensions such that

$$p(\mathbf{t}_n | \mathbf{W}) = \prod_{k=1}^K y_{nk}^{t_{nk}}, \quad (4.144)$$

where

$$\begin{aligned} y_{nk} &= \frac{\exp(a_{nk})}{\sum_{k'=1}^K \exp(a_{nk'})}, \\ a_{nk} &= \mathbf{w}_k^\top \boldsymbol{\phi}_n. \end{aligned} \quad (4.145)$$

Then,

$$p(\mathbf{T} | \mathbf{W}) = \prod_{n=1}^N \prod_{k=1}^K y_{nk}^{t_{nk}}. \quad (4.146)$$

Let

$$E(\mathbf{W}) = -\ln p(\mathbf{T} | \mathbf{W}). \quad (4.147)$$

By 4.18,

$$\nabla_{\mathbf{w}_k} E(\mathbf{W}) = \sum_{n=1}^N (y_{nk} - t_{nk}) \boldsymbol{\phi}_n. \quad (4.148)$$

By 4.17,

$$\nabla_{\mathbf{w}_k} \nabla_{\mathbf{w}_{k'}} E(\mathbf{W}) = \sum_{n=1}^N y_{nk} (I_{kk'} - y_{nk'}) \boldsymbol{\phi}_n \boldsymbol{\phi}_{n'}^\top. \quad (4.149)$$

The right hand side can be written as

$$\mathbf{H}_{kk'} = \boldsymbol{\Phi}^\top \mathbf{R}_{kk'} \boldsymbol{\Phi}, \quad (4.150)$$

where

$$R_{kk'nn'} = y_{nk}(I_{kk'} - y_{nk'})I_{nn'}. \quad (4.151)$$

Let

$$\mathbf{H} = \begin{bmatrix} \mathbf{H}_{11} & \cdots & \mathbf{H}_{1K} \\ \vdots & \ddots & \vdots \\ \mathbf{H}_{K1} & \cdots & \mathbf{H}_{KK} \end{bmatrix}, \mathbf{u} = \begin{bmatrix} \mathbf{u}_1 \\ \vdots \\ \mathbf{u}_K \end{bmatrix}, \quad (4.152)$$

where $\mathbf{u}_1, \dots, \mathbf{u}_K$ are vectors in the same dimension as \mathbf{w} . Then,

$$\mathbf{u}^\top \mathbf{H} \mathbf{u} = \sum_{k=1}^K \sum_{k'=1}^K \mathbf{v}_k^\top \mathbf{R}_{kk'} \mathbf{v}_{k'}, \quad (4.153)$$

where

$$\mathbf{v}_k = \Phi \mathbf{u}_k. \quad (4.154)$$

The right hand side can be written as

$$\begin{aligned} & \sum_{k=1}^K \sum_{k'=1}^K \sum_{n=1}^N \sum_{n'=1}^N v_{kn} y_{nk} (I_{kk'} - y_{nk'}) I_{nn'} v_{k'n'} \\ &= \sum_{k=1}^K \sum_{k'=1}^K \sum_{n=1}^N v_{kn} y_{nk} (I_{kk'} - y_{nk'}) v_{k'n}. \end{aligned} \quad (4.155)$$

The right hand side can be written as

$$\sum_{n=1}^N \sum_{k=1}^K y_{nk} v_{kn} \left(v_{kn} - \sum_{k'=1}^K y_{nk'} v_{k'n} \right). \quad (4.156)$$

By the Jensen's inequality,

$$\begin{aligned} & \sum_{k=1}^K y_{nk} v_{kn} \left(v_{kn} - \sum_{k'=1}^K y_{nk'} v_{k'n} \right) \\ & \geq \left(\sum_{k=1}^K y_{nk} v_{kn} \right) \left(\sum_{k=1}^K y_{nk} v_{kn} - \sum_{k'=1}^K y_{nk'} v_{k'n} \right), \end{aligned} \quad (4.157)$$

where the right hand side is zero. Then,

$$\mathbf{u}^\top \mathbf{H} \mathbf{u} \geq 0. \quad (4.158)$$

Therefore, \mathbf{H} is positive semidefinite.

4.21

Let

$$\Phi(a) = \int_{-\infty}^a \mathcal{N}(\theta|0, 1) d\theta. \quad (4.159)$$

The right hand side can be written as

$$\int_{-\infty}^0 \mathcal{N}(\theta|0, 1) d\theta + \int_0^a \mathcal{N}(\theta|0, 1) d\theta = \frac{1}{2} + \frac{1}{\sqrt{2\pi}} \int_0^a \exp\left(-\frac{\theta^2}{2}\right) d\theta. \quad (4.160)$$

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

$$\frac{1}{\sqrt{2\pi}} \int_0^{\frac{a}{\sqrt{2}}} \exp(-t^2) \sqrt{2} dt = \frac{1}{2} \operatorname{erf}\left(\frac{a}{\sqrt{2}}\right), \quad (4.161)$$

where

$$\operatorname{erf}(a) = \frac{2}{\sqrt{\pi}} \int_0^a \exp(-t^2) dt. \quad (4.162)$$

Therefore,

$$\Phi(a) = \frac{1}{2} \left(1 + \operatorname{erf}\left(\frac{a}{\sqrt{2}}\right) \right). \quad (4.163)$$

4.22

Let \mathcal{D} be a set of variables dependent on $\boldsymbol{\theta}$ in M dimensions. By marginalisation,

$$p(\mathcal{D}) = \int p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}. \quad (4.164)$$

Let $\boldsymbol{\theta}_{\text{MAP}}$ be a stationary point of $p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})$. Then, we have the Taylor series

$$\begin{aligned} & \ln(p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})) \\ & \simeq \ln(p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}})p(\boldsymbol{\theta}_{\text{MAP}})) - \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}})^T \mathbf{A}(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}}), \end{aligned} \quad (4.165)$$

where

$$\mathbf{A} = -\nabla \nabla \ln(p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta}))|_{\boldsymbol{\theta}=\boldsymbol{\theta}_{\text{MAP}}}. \quad (4.166)$$

Then,

$$\begin{aligned} & \int p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta} \\ & \simeq p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}})p(\boldsymbol{\theta}_{\text{MAP}}) \int \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}})^T \mathbf{A}(\boldsymbol{\theta} - \boldsymbol{\theta}_{\text{MAP}})\right) d\boldsymbol{\theta}. \end{aligned} \quad (4.167)$$

The integral of the right hand side can be written as

$$(2\pi)^{\frac{M}{2}} (\det \mathbf{A}^{-1})^{\frac{1}{2}} = (2\pi)^{\frac{M}{2}} (\det \mathbf{A})^{-\frac{1}{2}}. \quad (4.168)$$

Therefore,

$$p(\mathcal{D}) \simeq p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}})p(\boldsymbol{\theta}_{\text{MAP}})(2\pi)^{\frac{M}{2}} (\det \mathbf{A})^{-\frac{1}{2}}, \quad (4.169)$$

so that

$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}}) + \ln p(\boldsymbol{\theta}_{\text{MAP}}) + \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \mathbf{A}). \quad (4.170)$$

4.23

Let \mathcal{D} be a set of N independent and identically distributed variables dependent on $\boldsymbol{\theta}$ in M dimensions such that

$$p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta} | \mathbf{m}, \mathbf{V}_0). \quad (4.171)$$

By 4.22,

$$\begin{aligned} \ln p(\mathcal{D}) &\simeq \ln p(\mathcal{D} | \boldsymbol{\theta}_{\text{MAP}}) + \ln p(\boldsymbol{\theta}_{\text{MAP}}) + \frac{M}{2} \ln(2\pi) \\ &\quad - \frac{1}{2} \ln (\det (\mathbf{H} + \mathbf{V}_0^{-1})), \end{aligned} \quad (4.172)$$

where $\boldsymbol{\theta}_{\text{MAP}}$ is a stationary point of $p(\mathcal{D} | \boldsymbol{\theta})p(\boldsymbol{\theta})$ and

$$\mathbf{H} = -\nabla \nabla \ln p(\mathcal{D} | \boldsymbol{\theta})|_{\boldsymbol{\theta}=\boldsymbol{\theta}_{\text{MAP}}}. \quad (4.173)$$

The right hand side of the approximation can be written as

$$\begin{aligned} &\ln p(\mathcal{D} | \boldsymbol{\theta}_{\text{MAP}}) - \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \mathbf{V}_0) \\ &- \frac{1}{2} (\boldsymbol{\theta}_{\text{MAP}} - \mathbf{m})^\top \mathbf{V}_0^{-1} (\boldsymbol{\theta}_{\text{MAP}} - \mathbf{m}) + \frac{M}{2} \ln(2\pi) \\ &- \frac{1}{2} \ln (\det (\mathbf{H} + \mathbf{V}_0^{-1})) \\ &= \ln p(\mathcal{D} | \boldsymbol{\theta}_{\text{MAP}}) + \frac{1}{2} \ln (\det \mathbf{V}_0^{-1}) - \frac{1}{2} (\boldsymbol{\theta}_{\text{MAP}} - \mathbf{m})^\top \mathbf{V}_0^{-1} (\boldsymbol{\theta}_{\text{MAP}} - \mathbf{m}) \\ &- \frac{1}{2} \ln (\det (\mathbf{H} + \mathbf{V}_0^{-1})). \end{aligned} \quad (4.174)$$

If \mathbf{V}_0^{-1} can be neglected, the right hand side can be approximated as

$$\ln p(\mathcal{D} | \boldsymbol{\theta}_{\text{MAP}}) - \frac{1}{2} \ln(\det \mathbf{H}). \quad (4.175)$$

Since the elements of \mathcal{D} are independent and identically distributed,

$$\mathbf{H} = N \bar{\mathbf{H}}, \quad (4.176)$$

where

$$\bar{\mathbf{H}} = \frac{1}{N} \sum_{n=1}^N \mathbf{H}_n, \quad (4.177)$$

and $\mathbf{H}_1, \dots, \mathbf{H}_N$ are respectively the one for each element. Then,

$$\det \mathbf{H} = N^M \det \bar{\mathbf{H}}. \quad (4.178)$$

Therefore,

$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|\boldsymbol{\theta}_{\text{MAP}}) - \frac{M}{2} \ln N. \quad (4.179)$$

4.24

Let t_1, \dots, t_N be binary variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= y_n^{t_n} (1-y_n)^{1-t_n}, \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0), \end{aligned} \quad (4.180)$$

where

$$\begin{aligned} y_n &= \sigma(\mathbf{w}^\top \boldsymbol{\phi}_n), \\ \sigma(a) &= \frac{1}{1 + \exp(-a)}. \end{aligned} \quad (4.181)$$

By marginalisation,

$$p(t_{N+1}|\mathbf{t}) = \int p(t_{N+1}|\mathbf{w})p(\mathbf{w}|\mathbf{t})d\mathbf{w}. \quad (4.182)$$

By the Bayes' theorem,

$$p(\mathbf{w}|\mathbf{t})p(\mathbf{t}) = p(\mathbf{t}|\mathbf{w})p(\mathbf{w}). \quad (4.183)$$

The logarithm of the right hand side except the terms independent of \mathbf{w} can be written as $-E(\mathbf{w})$ where

$$\begin{aligned} E(\mathbf{w}) &= \sum_{n=1}^N (t_n \ln y_n + (1-t_n) \ln(1-y_n)) \\ &\quad - \frac{1}{2} (\mathbf{w} - \mathbf{m}_0)^\top \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0). \end{aligned} \quad (4.184)$$

Let \mathbf{w}_{MAP} be a stationary point of E . Then, we have the Taylor series

$$\begin{aligned} E(\mathbf{w}) &= E(\mathbf{w}_{\text{MAP}}) + \frac{1}{2} (\mathbf{w} - \mathbf{w}_{\text{MAP}})^\top \mathbf{A} (\mathbf{w} - \mathbf{w}_{\text{MAP}}) \\ &\quad + O(\|\mathbf{w} - \mathbf{w}_{\text{MAP}}\|^3), \end{aligned} \quad (4.185)$$

where

$$\mathbf{A} = \nabla \nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\text{MAP}}}. \quad (4.186)$$

Then,

$$p(\mathbf{w}|\mathbf{t}) \simeq \mathcal{N}(\mathbf{w}|\mathbf{w}_{\text{MAP}}, \mathbf{A}^{-1}). \quad (4.187)$$

Then,

$$\begin{aligned} & \int p(t_{N+1}|\mathbf{w})p(\mathbf{w}|\mathbf{t})d\mathbf{w} \\ & \simeq \int \sigma(a_{N+1})^{t_{N+1}} (1 - \sigma(a_{N+1}))^{1-t_{N+1}} p(a_{N+1})da_{N+1}, \end{aligned} \quad (4.188)$$

where

$$p(a_{N+1}) = \int \delta(a_{N+1} - \mathbf{w}^\top \boldsymbol{\phi}_{N+1}) \mathcal{N}(\mathbf{w}|\mathbf{w}_{\text{MAP}}, \mathbf{A}^{-1}) d\mathbf{w}, \quad (4.189)$$

and δ is the Dirac delta function. Since t_{N+1} is a binary variable, the right hand side of the approximation can be written as

$$v_{N+1}^{t_{N+1}} (1 - v_{N+1})^{1-t_{N+1}}, \quad (4.190)$$

where

$$v_{N+1} = \int \sigma(a_{N+1})p(a_{N+1})da_{N+1}. \quad (4.191)$$

We have

$$\mathbb{E} a_{N+1} = \int a_{N+1}p(a_{N+1})da_{N+1}. \quad (4.192)$$

The right hand side can be written as

$$\int \mathbf{w}^\top \boldsymbol{\phi}_{N+1} \mathcal{N}(\mathbf{w}|\mathbf{w}_{\text{MAP}}, \mathbf{A}^{-1}) d\mathbf{w} = \mathbf{w}_{\text{MAP}}^\top \boldsymbol{\phi}_{N+1}. \quad (4.193)$$

Then,

$$\text{var } a_{N+1} = \int (a_{N+1} - \mathbf{w}_{\text{MAP}}^\top \boldsymbol{\phi}_{N+1})^2 p(a_{N+1})da_{N+1}. \quad (4.194)$$

The right hand side can be written as

$$\int ((\mathbf{w} - \mathbf{w}_{\text{MAP}})^\top \boldsymbol{\phi}_{N+1})^2 p(a_{N+1})da_{N+1} = \boldsymbol{\phi}_{N+1}^\top \mathbf{A}^{-1} \boldsymbol{\phi}_{N+1}. \quad (4.195)$$

Then,

$$p(a_{N+1}) = \mathcal{N}(a_{N+1} | \mathbf{w}_{\text{MAP}}^\top \boldsymbol{\phi}_{N+1}, \boldsymbol{\phi}_{N+1}^\top \mathbf{A}^{-1} \boldsymbol{\phi}_{N+1}). \quad (4.196)$$

Therefore,

$$p(t_{N+1} | \mathbf{t}) = v_{N+1}^{t_{N+1}} (1 - v_{N+1})^{1-t_{N+1}}, \quad (4.197)$$

where

$$v_{N+1} = \int \sigma(a) \mathcal{N}(a | \mathbf{w}_{\text{MAP}}^\top \boldsymbol{\phi}_{N+1}, \boldsymbol{\phi}_{N+1}^\top \mathbf{A}^{-1} \boldsymbol{\phi}_{N+1}) da. \quad (4.198)$$

4.25

Let λ be a constant such that

$$\left. \frac{d\sigma(a)}{da} \right|_{a=0} = \left. \frac{d\Phi(\lambda a)}{da} \right|_{a=0}, \quad (4.199)$$

where

$$\begin{aligned} \sigma(a) &= \frac{1}{1 + \exp(-a)}, \\ \Phi(a) &= \int_{-\infty}^a \mathcal{N}(\theta | 0, 1) d\theta. \end{aligned} \quad (4.200)$$

By 4.12,

$$\frac{d\sigma(a)}{da} = \sigma(a) (1 - \sigma(a)). \quad (4.201)$$

We have

$$\frac{d\Phi(\lambda a)}{da} = \lambda \mathcal{N}(\lambda a | 0, 1). \quad (4.202)$$

Then,

$$\frac{1}{4} = \lambda (2\pi)^{-\frac{1}{2}}. \quad (4.203)$$

Therefore,

$$\lambda^2 = \frac{\pi}{8}. \quad (4.204)$$

4.26

Let

$$I(\mu) = \int \Phi(\lambda a) \mathcal{N}(a|\mu, \sigma^2) da, \quad (4.205)$$

where

$$\Phi(a) = \int_{-\infty}^a \mathcal{N}(\theta|0, 1) d\theta. \quad (4.206)$$

By the transformation

$$z = \frac{\theta - \mu}{\sigma}, \quad (4.207)$$

the right hand side can be written as

$$\begin{aligned} & \int \Phi(\lambda(\mu + \sigma z)) \mathcal{N}(\mu + \sigma z|\mu, \sigma^2) \sigma dz \\ &= \int \Phi(\lambda(\mu + \sigma z)) \mathcal{N}(z|0, 1) dz. \end{aligned} \quad (4.208)$$

Then,

$$\frac{\partial}{\partial \mu} I(\mu) = \lambda \int \mathcal{N}(\lambda(\mu + \sigma z)|0, 1) \mathcal{N}(z|0, 1) dz. \quad (4.209)$$

The logarithm of the integrand of the right hand side can be written as

$$\begin{aligned} & -\frac{1}{2} \ln(2\pi) - \frac{\lambda^2(\mu + \sigma z)^2}{2} - \frac{1}{2} \ln(2\pi) - \frac{z^2}{2} \\ &= -\ln(2\pi) - \frac{1 + \sigma^2 \lambda^2}{2} \left(z + \frac{\mu \sigma \lambda^2}{1 + \sigma^2 \lambda^2} \right)^2 + \frac{\mu^2 \sigma^2 \lambda^4}{2(1 + \sigma^2 \lambda^2)} - \frac{\mu^2 \lambda^2}{2}. \end{aligned} \quad (4.210)$$

The right hand side can be written as

$$\begin{aligned} & -\ln(2\pi) - \frac{1 + \sigma^2 \lambda^2}{2} \left(z + \frac{\mu \sigma \lambda^2}{1 + \sigma^2 \lambda^2} \right)^2 - \frac{\mu^2 \lambda^2}{2(1 + \sigma^2 \lambda^2)} \\ &= -\frac{1}{2} \ln(2\pi) - \frac{1}{2} \ln(1 + \sigma^2 \lambda^2)^{-1} - \frac{1 + \sigma^2 \lambda^2}{2} \left(z + \frac{\mu \sigma \lambda^2}{1 + \sigma^2 \lambda^2} \right)^2 \\ & \quad - \ln \lambda - \frac{1}{2} \ln(2\pi) - \frac{1}{2} \ln(\lambda^{-2} + \sigma^2) - \frac{\mu^2}{2(\lambda^{-2} + \sigma^2)}. \end{aligned} \quad (4.211)$$

Then, the integral can be written as

$$\begin{aligned} & \frac{1}{\lambda} \mathcal{N}(\mu | 0, \lambda^{-2} + \sigma^2) \int \mathcal{N}\left(z| -\frac{\mu\sigma\lambda^2}{1+\sigma^2\lambda^2}, (1+\sigma^2\lambda^2)^{-1}\right) dz \\ &= \frac{1}{\lambda} \mathcal{N}(\mu | 0, \lambda^{-2} + \sigma^2). \end{aligned} \quad (4.212)$$

Then,

$$\frac{\partial}{\partial \mu} I(\mu) = \mathcal{N}(\mu | 0, \lambda^{-2} + \sigma^2), \quad (4.213)$$

so that

$$I(\mu) = \int_{-\infty}^{\mu} \mathcal{N}(m | 0, \lambda^{-2} + \sigma^2) dm. \quad (4.214)$$

By the transformation

$$m' = (\lambda^{-2} + \sigma^2)^{-\frac{1}{2}} m, \quad (4.215)$$

the right hand side can be written as

$$\begin{aligned} & \int_{-\infty}^{(\lambda^{-2} + \sigma^2)^{-\frac{1}{2}} \mu} (\lambda^{-2} + \sigma^2)^{-\frac{1}{2}} \mathcal{N}(m' | 0, 1) (\lambda^{-2} + \sigma^2)^{\frac{1}{2}} dm' \\ &= \int_{-\infty}^{(\lambda^{-2} + \sigma^2)^{-\frac{1}{2}} \mu} \mathcal{N}(m' | 0, 1) dm'. \end{aligned} \quad (4.216)$$

Therefore,

$$I(\mu) = \Phi\left((\lambda^{-2} + \sigma^2)^{-\frac{1}{2}} \mu\right). \quad (4.217)$$

5 Neural Networks

5.1

Let

$$y_k(\mathbf{x}, \mathbf{w}) = \sigma \left(\sum_{m=1}^M w_{km}^{(2)} \sigma \left(\sum_{d=1}^D w_{md}^{(1)} x_d + w_{m0}^{(1)} \right) + w_{k0}^{(2)} \right), \quad (5.1)$$

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}. \quad (5.2)$$

We have

$$\sigma(a) = \frac{\exp\left(\frac{a}{2}\right)}{\exp\left(\frac{a}{2}\right) + \exp\left(-\frac{a}{2}\right)}. \quad (5.3)$$

The right hand side can be written as

$$\frac{\exp\left(\frac{a}{2}\right) - \exp\left(-\frac{a}{2}\right)}{\exp\left(\frac{a}{2}\right) + \exp\left(-\frac{a}{2}\right)} + \frac{\exp\left(-\frac{a}{2}\right)}{\exp\left(\frac{a}{2}\right) + \exp\left(-\frac{a}{2}\right)} = \tanh\left(\frac{a}{2}\right) + 1 - \sigma(a). \quad (5.4)$$

Then,

$$\sigma(a) = \frac{1}{2} \left(1 + \tanh\left(\frac{a}{2}\right) \right). \quad (5.5)$$

Then, the argument of the expression of $y_k(\mathbf{x}, \mathbf{w})$ can be written as

$$\begin{aligned} & \sum_{m=1}^M w_{km}^{(2)} \left(\frac{1}{2} \left(1 + \tanh\left(\frac{1}{2} \left(\sum_{d=1}^D w_{md}^{(1)} x_d + w_{m0}^{(1)} \right) \right) \right) \right) + w_{k0}^{(2)} \\ &= \frac{1}{2} \sum_{m=1}^M w_{km}^{(2)} \tanh\left(\frac{1}{2} \sum_{d=1}^D w_{md}^{(1)} x_d + \frac{1}{2} w_{m0}^{(1)}\right) + \frac{1}{2} \sum_{m=1}^M w_{km}^{(2)} + w_{k0}^{(2)}. \end{aligned} \quad (5.6)$$

Therefore,

$$\begin{aligned} & y_k(\mathbf{x}, \mathbf{w}) \\ &= \sigma \left(\frac{1}{2} \sum_{m=1}^M w_{km}^{(2)} \tanh\left(\frac{1}{2} \sum_{d=1}^D w_{md}^{(1)} x_d + \frac{1}{2} w_{m0}^{(1)}\right) + \frac{1}{2} \sum_{m=1}^M w_{km}^{(2)} + w_{k0}^{(2)} \right). \end{aligned} \quad (5.7)$$

5.2

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

$$p(\mathbf{t}_n | \mathbf{w}) = \mathcal{N}(\mathbf{t}_n | \mathbf{y}_n, \beta^{-1} \mathbf{I}), \quad (5.8)$$

where

$$\mathbf{y}_n = \mathbf{y}(\mathbf{x}_n, \mathbf{w}). \quad (5.9)$$

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

$$-\frac{\beta}{2} \sum_{n=1}^N \|\mathbf{t}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w})\|^2. \quad (5.10)$$

Therefore, maximising $p(\mathbf{T} | \mathbf{w})$ is equivalent to minimising $E(\mathbf{w})$, where

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \|\mathbf{y}(\mathbf{x}_n, \mathbf{w}) - \mathbf{t}_n\|^2. \quad (5.11)$$

5.3

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

$$p(\mathbf{t}_n | \mathbf{w}) = \mathcal{N}(\mathbf{t}_n | \mathbf{y}_n, \Sigma), \quad (5.12)$$

where

$$\mathbf{y}_n = \mathbf{y}(\mathbf{x}_n, \mathbf{w}). \quad (5.13)$$

(a)

The logarithm of $p(\mathbf{T} | \mathbf{w})$ except the terms independent of \mathbf{w} and Σ can be written as

$$-\frac{1}{2} \ln(\det \Sigma) - \frac{1}{2} \sum_{n=1}^N (\mathbf{t}_n - \mathbf{y}_n)^\top \Sigma^{-1} (\mathbf{t}_n - \mathbf{y}_n). \quad (5.14)$$

Setting the derivatives with respect to \mathbf{w} and Σ to zero gives

$$\begin{aligned} \mathbf{0} &= - \sum_{n=1}^N \frac{\partial \mathbf{y}_n}{\partial \mathbf{w}} \Sigma^{-1} (\mathbf{t}_n - \mathbf{y}_n), \\ \mathbf{O} &= -\frac{1}{2} \Sigma^{-1} + \frac{1}{2} (\Sigma^{-1})^2 \sum_{n=1}^N (\mathbf{t}_n - \mathbf{y}_n) (\mathbf{t}_n - \mathbf{y}_n)^\top. \end{aligned} \quad (5.15)$$

Therefore, the maximum likelihood solution for Σ is given by

$$\Sigma = \sum_{n=1}^N (\mathbf{t}_n - \mathbf{y}_n)(\mathbf{t}_n - \mathbf{y}_n)^\top. \quad (5.16)$$

(b)

If Σ is fixed and known, then the maximum likelihood solution for \mathbf{w} is given by minimising $E(\mathbf{w})$ where

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N (\mathbf{t}_n - \mathbf{y}_n)^\top \Sigma^{-1} (\mathbf{t}_n - \mathbf{y}_n). \quad (5.17)$$

5.4

Let t_1, \dots, t_N be binary variables such that

$$p(t_n = 1 | \mathbf{w}) = (1 - \epsilon)y_n + \epsilon(1 - y_n), \quad (5.18)$$

where

$$y_n = y(\mathbf{x}_n, \mathbf{w}). \quad (5.19)$$

Then,

$$p(t_n | \mathbf{w}) = ((1 - \epsilon)y_n + \epsilon(1 - y_n))^{t_n} (\epsilon y_n + (1 - \epsilon)(1 - y_n))^{1-t_n}. \quad (5.20)$$

Therefore,

$$\begin{aligned} -\ln p(\mathbf{t} | \mathbf{w}) &= - \sum_{n=1}^N t_n \ln ((1 - \epsilon)y_n + \epsilon(1 - y_n)) \\ &\quad - \sum_{n=1}^N (1 - t_n) \ln (\epsilon y_n + (1 - \epsilon)(1 - y_n)). \end{aligned} \quad (5.21)$$

5.5

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables from the standard basis in K dimensions such that

$$p(\mathbf{t}_n | \mathbf{w}) = \prod_{k=1}^K y_{nk}^{t_{nk}}, \quad (5.22)$$

where

$$y_{nk} = y_k(\mathbf{x}_n, \mathbf{w}). \quad (5.23)$$

Therefore,

$$\ln p(\mathbf{T}|\mathbf{w}) = \sum_{n=1}^N \sum_{k=1}^K t_{nk} \ln y_{nk}. \quad (5.24)$$

5.6

Let t_1, \dots, t_N be binary variables such that

$$p(t_n|\mathbf{w}) = y_n^{t_n} (1 - y_n)^{1-t_n}, \quad (5.25)$$

where

$$\begin{aligned} y_n &= \sigma(a_n), \\ \sigma(a) &= \frac{1}{1 + \exp(-a)}, \\ a_n &= a(\mathbf{x}_n, \mathbf{w}). \end{aligned} \quad (5.26)$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}). \quad (5.27)$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^N (t_n \ln y_n + (1 - t_n) \ln(1 - y_n)). \quad (5.28)$$

By 4.12,

$$\frac{\partial E(\mathbf{w})}{\partial a_n} = -y_n(1 - y_n) \left(\frac{t_n}{y_n} - \frac{1 - t_n}{1 - y_n} \right). \quad (5.29)$$

Therefore,

$$\frac{\partial E(\mathbf{w})}{\partial a_n} = y_n - t_n. \quad (5.30)$$

5.7

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables from the standard basis in K dimensions such that

$$p(\mathbf{t}_n|\mathbf{w}) = \prod_{k=1}^K y_{nk}^{t_{nk}}, \quad (5.31)$$

where

$$\begin{aligned} y_{nk} &= y_k(\mathbf{a}_n), \\ y_k(\mathbf{a}) &= \frac{\exp(a_k)}{\sum_{k'=1}^K \exp(a_{k'})}, \\ \mathbf{a}_n &= \mathbf{a}(\mathbf{x}_n, \mathbf{w}). \end{aligned} \tag{5.32}$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{T}|\mathbf{w}). \tag{5.33}$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^N \sum_{k=1}^K t_{nk} \ln y_{nk}. \tag{5.34}$$

Then,

$$\frac{\partial E(\mathbf{w})}{\partial a_{nk'}} = -\sum_{k=1}^K \frac{t_{nk}}{y_{nk}} \frac{\partial y_{nk}}{\partial a_{nk'}}. \tag{5.35}$$

By 4.17,

$$\frac{\partial y_{nk}}{\partial a_{nk'}} = y_{nk}(I_{kk'} - y_{nk'}). \tag{5.36}$$

Then,

$$\frac{\partial E(\mathbf{w})}{\partial a_{nk'}} = \sum_{k=1}^K t_{nk}(y_{nk'} - I_{kk'}). \tag{5.37}$$

The right hand side can be written as

$$y_{nk'} \sum_{k=1}^K t_{nk} - t_{nk'}. \tag{5.38}$$

Since $\mathbf{t}_1, \dots, \mathbf{t}_N$ are from the standard basis in K dimensions,

$$\sum_{k=1}^K t_{nk} = 1. \tag{5.39}$$

Therefore,

$$\frac{\partial E(\mathbf{w})}{\partial a_{nk}} = y_{nk} - t_{nk}. \tag{5.40}$$

5.8

We have

$$\tanh a = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)}. \quad (5.41)$$

Then,

$$\frac{d}{da} \tanh a = 1 - \left(\frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)} \right)^2. \quad (5.42)$$

Therefore,

$$\frac{d}{da} \tanh a = 1 - (\tanh a)^2. \quad (5.43)$$

5.9

Let t_1, \dots, t_N be variables from $\{-1, 1\}$ such that

$$p(t_n | \mathbf{w}) = \left(\frac{1 + y_n}{2} \right)^{\frac{1+t_n}{2}} \left(\frac{1 - y_n}{2} \right)^{\frac{1-t_n}{2}}, \quad (5.44)$$

where

$$\begin{aligned} y_n &= y(\mathbf{x}_n, \mathbf{w}), \\ -1 &\leq y(\mathbf{x}_n, \mathbf{w}) \leq 1. \end{aligned} \quad (5.45)$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t} | \mathbf{w}). \quad (5.46)$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^N \left(\frac{1 + t_n}{2} \ln \frac{1 + y_n}{2} + \frac{1 - t_n}{2} \ln \frac{1 - y_n}{2} \right). \quad (5.47)$$

The appropriate choice of y is \tanh .

5.10

Let

$$\mathbf{H} = \nabla \nabla E(\mathbf{w}), \quad (5.48)$$

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 definite if and only if all of its eigenvalues are positive.

5.11

Let \mathbf{w} be a real vector in M dimensions. We have the Taylor series

$$E(\mathbf{w}) \simeq E(\mathbf{w}^*) + \frac{1}{2} (\mathbf{w} - \mathbf{w}^*)^\top \mathbf{H} (\mathbf{w} - \mathbf{w}^*) + O(\|\mathbf{w} - \mathbf{w}^*\|^3), \quad (5.49)$$

where

$$\begin{aligned} \nabla E(\mathbf{w}^*) &= \mathbf{0}, \\ \mathbf{H} &= \nabla \nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}^*}. \end{aligned} \quad (5.50)$$

Let $\mathbf{u}_1, \dots, \mathbf{u}_M$ be eigenvectors of \mathbf{H} such that

$$\mathbf{H}\mathbf{u}_m = \lambda_m \mathbf{u}_m. \quad (5.51)$$

Then, there exists $\alpha_1, \dots, \alpha_M$ such that

$$\mathbf{w} - \mathbf{w}^* = \sum_{m=1}^M \alpha_m \mathbf{u}_m. \quad (5.52)$$

By 2.19, since \mathbf{H} is a real symmetric matrix,

$$\mathbf{u}_m^\top \mathbf{u}_{m'} = I_{mm'}. \quad (5.53)$$

Then,

$$E(\mathbf{w}) \simeq E(\mathbf{w}^*) + \frac{1}{2} \sum_{m=1}^M \lambda_m \alpha_m^2. \quad (5.54)$$

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 \mathbf{w} be a real vector. We have the Taylor series

$$E(\mathbf{w}) = E(\mathbf{w}^*) + \frac{1}{2} (\mathbf{w} - \mathbf{w}^*)^\top \mathbf{H} (\mathbf{w} - \mathbf{w}^*) + O(\|\mathbf{w} - \mathbf{w}^*\|^3), \quad (5.55)$$

where

$$\begin{aligned} \nabla E(\mathbf{w}^*) &= \mathbf{0}, \\ \mathbf{H} &= \nabla \nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}^*}. \end{aligned} \quad (5.56)$$

If \mathbf{H} is positive definite, then the second term of the right hand side is positive unless

$$\mathbf{w} = \mathbf{w}^*. \quad (5.57)$$

Then, \mathbf{w}^* is a local minimum of E . On the other hand, if \mathbf{w}^* is a local minimum of E , then the second term of the right hand side is positive unless

$$\mathbf{w} = \mathbf{w}^*. \quad (5.58)$$

Then, \mathbf{H} is positive definite. Therefore, the necessary and sufficient condition for \mathbf{w}^* to be a local minimum is that \mathbf{H} is positive definite.

5.13

Let \mathbf{w} be a vector in M dimensions. We have the Taylor series

$$\begin{aligned} E(\mathbf{w}) &= E(\hat{\mathbf{w}}) + (\mathbf{w} - \hat{\mathbf{w}})^\top \mathbf{b} + \frac{1}{2} (\mathbf{w} - \hat{\mathbf{w}})^\top \mathbf{H} (\mathbf{w} - \hat{\mathbf{w}}) \\ &\quad + O(\|\mathbf{w} - \hat{\mathbf{w}}\|^3), \end{aligned} \quad (5.59)$$

where

$$\begin{aligned} \mathbf{b} &= \nabla E(\mathbf{w})|_{\mathbf{w}=\hat{\mathbf{w}}}. \\ \mathbf{H} &= \nabla \nabla E(\mathbf{w})|_{\mathbf{w}=\hat{\mathbf{w}}}. \end{aligned} \quad (5.60)$$

Since \mathbf{b} is a vector in M dimensions and \mathbf{H} is a $M \times M$ symmetric matrix, the number of independent elements of the right hand side is

$$M + \frac{M(M+1)}{2} = \frac{M(M+3)}{2}. \quad (5.61)$$

5.14

Let w be a variable. We have the Taylor series

$$\begin{aligned} E_n(w_{mm'} + \epsilon) &= E_n(w_{mm'}) + \left. \frac{\partial E_n}{\partial w} \right|_{w=w_{mm'}} \epsilon + O(\epsilon^2), \\ E_n(w_{mm'} - \epsilon) &= E_n(w_{mm'}) - \left. \frac{\partial E_n}{\partial w} \right|_{w=w_{mm'}} \epsilon + O(\epsilon^2). \end{aligned} \quad (5.62)$$

Therefore,

$$\left. \frac{\partial E_n}{\partial w} \right|_{w=w_{mm'}} = \frac{E_n(w_{mm'} + \epsilon) - E_n(w_{mm'} - \epsilon)}{2\epsilon} + O(\epsilon^2). \quad (5.63)$$

5.15 (Incomplete)

Let

$$J_{km} = \frac{\partial y_k}{\partial x_m}. \quad (5.64)$$

The right hand side can be written as

$$\sum_{m'=1}^M W_{mm'} \frac{\partial y_k}{\partial a_{m'}}, \quad (5.65)$$

where

$$W_{mm'} = \frac{\partial a_{m'}}{\partial x_m}. \quad (5.66)$$

We have

$$\frac{\partial y_k}{\partial a_{m'}} = \sum_{m''=1}^M \frac{\partial y_k}{\partial a_{m''}} \frac{\partial a_{m''}}{\partial a_{m'}}. \quad (5.67)$$

5.16

Let $\mathbf{y}_1, \dots, \mathbf{y}_N$ be vectors dependent on \mathbf{w} . Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \|\mathbf{y}_n - \mathbf{t}_n\|^2. \quad (5.68)$$

Then,

$$\nabla E(\mathbf{w}) = \sum_{n=1}^N (\nabla \mathbf{y}_n)^\top (\mathbf{y}_n - \mathbf{t}_n). \quad (5.69)$$

Therefore,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^N (\nabla \text{vec}((\nabla \mathbf{y}_n)^\top)^\top (\mathbf{y}_n - \mathbf{t}_n) + \sum_{n=1}^N (\nabla \mathbf{y}_n)^\top (\nabla \mathbf{y}_n)). \quad (5.70)$$

5.17

Let y be a scalar dependent on \mathbf{x} and \mathbf{w} . Let

$$E(\mathbf{w}) = \frac{1}{2} \int \int (y - t)^2 p(\mathbf{x}, t) d\mathbf{x} dt. \quad (5.71)$$

Then,

$$\nabla E(\mathbf{w}) = \int \int (y - t)p(\mathbf{x}, t) \nabla y d\mathbf{x} dt. \quad (5.72)$$

The right hand side can be written as

$$\begin{aligned} & \int y \nabla y \left(\int p(\mathbf{x}, t) dt \right) d\mathbf{x} - \int \nabla y \left(\int t p(t|\mathbf{x}) dt \right) p(\mathbf{x}) d\mathbf{x} \\ &= \int y \nabla y p(\mathbf{x}) d\mathbf{x} - \int \nabla y \mathbb{E}(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \end{aligned} \quad (5.73)$$

Then,

$$\begin{aligned} \nabla \nabla E(\mathbf{w}) &= \int \nabla y (\nabla y)^\top p(\mathbf{x}) d\mathbf{x} + \int y \nabla \nabla y p(\mathbf{x}) d\mathbf{x} \\ &\quad - \int \nabla \nabla y \mathbb{E}(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \end{aligned} \quad (5.74)$$

The second and the third terms of the right hand side can be written as

$$\mathbb{E}(y \nabla \nabla y) - \mathbb{E}(\nabla \nabla y \mathbb{E}(t|\mathbf{x})) = \mathbb{E}((y - \mathbb{E}(t|\mathbf{x})) \nabla \nabla y). \quad (5.75)$$

Therefore, if

$$y = \mathbb{E}(t|\mathbf{x}), \quad (5.76)$$

then

$$\nabla \nabla E(\mathbf{w}) = \int \nabla y (\nabla y)^\top p(\mathbf{x}) d\mathbf{x}. \quad (5.77)$$

5.18

Let y_1, \dots, y_N be scalars such that

$$\begin{aligned} y_n &= \mathbf{w}_n^{(2)\top} \mathbf{z} + \mathbf{w}_n^{(0)\top} \mathbf{x}, \\ z_m &= \tanh(\mathbf{w}_m^{(1)\top} \mathbf{x}). \end{aligned} \quad (5.78)$$

Let

$$E = \frac{1}{2} \sum_{n=1}^N (y_n - t_n)^2. \quad (5.79)$$

Then,

$$\begin{aligned}\frac{\partial E}{\partial \mathbf{w}_n^{(0)}} &= \frac{\partial E}{\partial y_n} \frac{\partial y_n}{\partial \mathbf{w}_n^{(0)}}, \\ \frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= \frac{\partial E}{\partial y_n} \frac{\partial y_n}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{w}_m^{(1)}}, \\ \frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= \frac{\partial E}{\partial y_n} \frac{\partial y_n}{\partial \mathbf{w}_n^{(2)}}.\end{aligned}\tag{5.80}$$

Therefore,

$$\begin{aligned}\frac{\partial E}{\partial \mathbf{w}_n^{(0)}} &= (y_n - t_n) \mathbf{x}, \\ \frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= (y_n - t_n) \mathbf{A} \mathbf{w}_n^{(2)}, \\ \frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= (y_n - t_n) \mathbf{z},\end{aligned}\tag{5.81}$$

where

$$A_{mm'} = (1 - z_m^2) x_{m'}. \tag{5.82}$$

5.19

Let t_1, \dots, t_N be binary variables such that

$$p(t_n | \mathbf{w}) = y_n^{t_n} (1 - y_n)^{1-t_n}, \tag{5.83}$$

where

$$\begin{aligned}y_n &= \sigma(a_n), \\ \sigma(a) &= \frac{1}{1 + \exp(-a)}, \\ a_n &= a(\mathbf{x}_n, \mathbf{w}).\end{aligned}\tag{5.84}$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{t} | \mathbf{w}). \tag{5.85}$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^N (t_n \ln y_n + (1 - t_n) \ln(1 - y_n)). \tag{5.86}$$

Then,

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^N \left(\frac{t_n}{y_n} - \frac{1 - t_n}{1 - y_n} \right) \nabla y_n. \tag{5.87}$$

We have

$$\nabla y_n = \frac{\partial y_n}{\partial a_n} \nabla a_n. \quad (5.88)$$

By 4.12,

$$\frac{\partial y_n}{\partial a_n} = y_n(1 - y_n). \quad (5.89)$$

Then,

$$\nabla y_n = y_n(1 - y_n) \nabla a_n. \quad (5.90)$$

Then,

$$\nabla E(\mathbf{w}) = - \sum_{n=1}^N (t_n(1 - y_n) - (1 - t_n)y_n) \nabla a_n, \quad (5.91)$$

so that

$$\nabla E(\mathbf{w}) = \sum_{n=1}^N (y_n - t_n) \nabla a_n. \quad (5.92)$$

Then,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^N \nabla a_n (\nabla y_n)^\top + \sum_{n=1}^N (y_n - t_n) \nabla \nabla a_n. \quad (5.93)$$

Therefore,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^N y_n(1 - y_n) \nabla a_n (\nabla a_n)^\top + \sum_{n=1}^N (y_n - t_n) \nabla \nabla a_n. \quad (5.94)$$

5.20

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables from the standard basis in K dimensions such that

$$p(\mathbf{t}_n | \mathbf{w}) = \prod_{k=1}^K y_{nk}^{t_{nk}}, \quad (5.95)$$

where

$$\begin{aligned} y_{nk} &= y_k(\mathbf{a}_n), \\ y_k(\mathbf{a}) &= \frac{\exp(a_k)}{\sum_{k'=1}^K \exp(a_{k'})}, \\ \mathbf{a}_n &= \mathbf{a}(\mathbf{x}_n, \mathbf{w}) \end{aligned} \quad (5.96)$$

Let

$$E(\mathbf{w}) = -\ln p(\mathbf{T}|\mathbf{w}). \quad (5.97)$$

Then,

$$E(\mathbf{w}) = -\sum_{n=1}^N \sum_{k=1}^K t_{nk} \ln y_{nk}. \quad (5.98)$$

Then,

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^N \sum_{k=1}^K \frac{t_{nk}}{y_{nk}} \nabla y_{nk}. \quad (5.99)$$

We have

$$\nabla y_{nk} = \sum_{k'=1}^K \frac{\partial y_{nk}}{\partial a_{nk'}} \nabla a_{nk'}. \quad (5.100)$$

By 4.17,

$$\frac{\partial y_{nk}}{\partial a_{nk'}} = y_{nk}(I_{kk'} - y_{nk'}). \quad (5.101)$$

Then,

$$\nabla y_{nk} = y_{nk} \sum_{k'=1}^K (I_{kk'} - y_{nk'}) \nabla a_{nk'}. \quad (5.102)$$

Then,

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^N \sum_{k=1}^K t_{nk} \sum_{k'=1}^K (I_{kk'} - y_{nk'}) \nabla a_{nk}, \quad (5.103)$$

so that

$$\nabla E(\mathbf{w}) = \sum_{n=1}^N \sum_{k=1}^K (y_{nk} - t_{nk}) \nabla a_{nk}. \quad (5.104)$$

Then,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^N \sum_{k=1}^K \nabla a_{nk} (\nabla y_{nk})^\top + \sum_{n=1}^N \sum_{k=1}^K (y_{nk} - t_{nk}) \nabla \nabla a_{nk}. \quad (5.105)$$

Therefore,

$$\begin{aligned} \nabla \nabla E(\mathbf{w}) &= \sum_{n=1}^N \sum_{k=1}^K y_{nk} \nabla a_{nk} \sum_{k'=1}^K (I_{kk'} - y_{nk'}) (\nabla a_{nk'})^\top \\ &\quad + \sum_{n=1}^N \sum_{k=1}^K (y_{nk} - t_{nk}) \nabla \nabla a_{nk}. \end{aligned} \quad (5.106)$$

5.21

Let $\mathbf{y}_1, \dots, \mathbf{y}_N$ be vectors dependent on \mathbf{w} . Let

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \|\mathbf{y}_n - \mathbf{t}_n\|^2. \quad (5.107)$$

By 5.16,

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^N (\nabla \text{vec}(\nabla \mathbf{y}_n)^\top)^\top (\mathbf{y}_n - \mathbf{t}_n) + \mathbf{H}, \quad (5.108)$$

where

$$\mathbf{H} = \sum_{n=1}^N (\nabla \mathbf{y}_n)^\top (\nabla \mathbf{y}_n). \quad (5.109)$$

Let

$$\mathbf{H}' = \sum_{n=1}^{N+1} (\nabla \mathbf{y}_n)^\top (\nabla \mathbf{y}_n). \quad (5.110)$$

Then,

$$\mathbf{H}' = \mathbf{H} + \mathbf{B}^\top \mathbf{B}, \quad (5.111)$$

where

$$\mathbf{B} = \nabla \mathbf{y}_{N+1}. \quad (5.112)$$

Therefore, by 2.26,

$$\mathbf{H}'^{-1} = \mathbf{H}^{-1} - \mathbf{H}^{-1} \mathbf{B}^\top \mathbf{M} \mathbf{B} \mathbf{H}^{-1}, \quad (5.113)$$

where

$$\mathbf{M} = (\mathbf{I} + \mathbf{B} \mathbf{H}^{-1} \mathbf{B}^\top)^{-1}. \quad (5.114)$$

5.22

Let a_1, \dots, a_N be variables such that

$$\begin{aligned} a_n &= \mathbf{w}_n^{(2)\top} \mathbf{z}, \\ z_m &= h(b_m), \\ b_m &= \mathbf{w}_m^{(1)\top} \mathbf{x}. \end{aligned} \quad (5.115)$$

Let E be a function of a_1, \dots, a_N . Then,

$$\begin{aligned}\frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= \sum_{n=1}^N \frac{\partial E}{\partial a_n} \frac{\partial a_n}{\partial z_m} \frac{\partial z_m}{\partial b_m} \frac{\partial b_m}{\partial \mathbf{w}_m^{(1)}}, \\ \frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= \frac{\partial E}{\partial a_n} \frac{\partial a_n}{\partial \mathbf{w}_n^{(2)}}.\end{aligned}\quad (5.116)$$

Then,

$$\begin{aligned}\frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= h'(b_m) \mathbf{x} \sum_{n=1}^N w_{nm}^{(2)} \frac{\partial E}{\partial a_n}, \\ \frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= \frac{\partial E}{\partial a_n} \mathbf{z}.\end{aligned}\quad (5.117)$$

Therefore,

$$\begin{aligned}\frac{\partial^2 E}{\partial \mathbf{w}_m^{(1)} \partial \mathbf{w}_{m'}^{(1)}} &= C_{mm'}^{(11)} \mathbf{x} \mathbf{x}^\top, \\ \frac{\partial^2 E}{\partial \mathbf{w}_m^{(1)} \partial \mathbf{w}_n^{(2)}} &= C_{mn}^{(12)} \mathbf{x} \mathbf{z}^\top + h'(b_m) \frac{\partial E}{\partial a_n} \mathbf{x} \mathbf{v}^\top, \\ \frac{\partial^2 E}{\partial \mathbf{w}_n^{(2)} \partial \mathbf{w}_{n'}^{(2)}} &= C_{nn'}^{(22)} \mathbf{z} \mathbf{z}^\top,\end{aligned}\quad (5.118)$$

where \mathbf{v} is a vector from the standard basis in M dimensions such that

$$v_m = 1, \quad (5.119)$$

and

$$\begin{aligned}C_{mm'}^{(11)} &= h''(b_m) I_{mm'} \sum_{n=1}^N w_{nm}^{(2)} \frac{\partial E}{\partial a_n} \\ &\quad + h'(b_m) h'(b_{m'}) \sum_{n=1}^N w_{nm}^{(2)} \sum_{n'=1}^N w_{n'm'}^{(2)} \frac{\partial^2 E}{\partial y_n \partial a_{n'}}, \\ C_{mn}^{(12)} &= h'(b_m) \sum_{n'=1}^N w_{n'm}^{(2)} \frac{\partial^2 E}{\partial a_n \partial a_{n'}}, \\ C_{nn'}^{(22)} &= \frac{\partial^2 E}{\partial a_n \partial a_{n'}}.\end{aligned}\quad (5.120)$$

5.23

Let a_1, \dots, a_N be variables such that

$$\begin{aligned} a_n &= \mathbf{w}_n^{(2)\top} \mathbf{z} + \mathbf{w}_n^{(0)\top} \mathbf{x}, \\ z_m &= h(b_m), \\ b_m &= \mathbf{w}_m^{(1)\top} \mathbf{x}. \end{aligned} \tag{5.121}$$

Let E be a function of a_1, \dots, a_N . Then,

$$\begin{aligned} \frac{\partial E}{\partial \mathbf{w}_n^{(0)}} &= \frac{\partial E}{\partial a_n} \frac{\partial a_n}{\partial \mathbf{w}_n^{(0)}}, \\ \frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= \sum_{n=1}^N \frac{\partial E}{\partial a_n} \frac{\partial a_n}{\partial z_m} \frac{\partial z_m}{\partial b_m} \frac{\partial b_m}{\partial \mathbf{w}_m^{(1)}}, \\ \frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= \frac{\partial E}{\partial a_n} \frac{\partial a_n}{\partial \mathbf{w}_n^{(2)}}. \end{aligned} \tag{5.122}$$

Then,

$$\begin{aligned} \frac{\partial E}{\partial \mathbf{w}_n^{(0)}} &= \frac{\partial E}{\partial a_n} \mathbf{x}, \\ \frac{\partial E}{\partial \mathbf{w}_m^{(1)}} &= h'(b_m) \mathbf{x} \sum_{n=1}^N w_{nm}^{(2)} \frac{\partial E}{\partial a_n}, \\ \frac{\partial E}{\partial \mathbf{w}_n^{(2)}} &= \frac{\partial E}{\partial a_n} \mathbf{z}. \end{aligned} \tag{5.123}$$

Therefore,

$$\begin{aligned}
\frac{\partial^2 E}{\partial \mathbf{w}_n^{(0)} \partial \mathbf{w}_{n'}^{(0)}} &= C_{nn'}^{(22)} \mathbf{x} \mathbf{x}^\top, \\
\frac{\partial^2 E}{\partial \mathbf{w}_n^{(0)} \partial \mathbf{w}_m^{(1)}} &= C_{nm}^{(12)} \mathbf{x} \mathbf{x}^\top, \\
\frac{\partial^2 E}{\partial \mathbf{w}_n^{(0)} \partial \mathbf{w}_{n'}^{(2)}} &= C_{nn'}^{(22)} \mathbf{x} \mathbf{z}^\top, \\
\frac{\partial^2 E}{\partial \mathbf{w}_m^{(1)} \partial \mathbf{w}_{m'}^{(1)}} &= C_{mm'}^{(11)} \mathbf{x} \mathbf{x}^\top, \\
\frac{\partial^2 E}{\partial \mathbf{w}_m^{(1)} \partial \mathbf{w}_n^{(2)}} &= C_{mn}^{(12)} \mathbf{x} \mathbf{z}^\top + h'(b_m) \frac{\partial E}{\partial a_n} \mathbf{x} \mathbf{v}^\top, \\
\frac{\partial^2 E}{\partial \mathbf{w}_n^{(2)} \partial \mathbf{w}_{n'}^{(2)}} &= C_{nn'}^{(22)} \mathbf{z} \mathbf{z}^\top,
\end{aligned} \tag{5.124}$$

where \mathbf{v} is a vector from the standard basis in M dimensions such that

$$v_m = 1, \tag{5.125}$$

and

$$\begin{aligned}
C_{mm'}^{(11)} &= h''(b_m) I_{mm'} \sum_{n=1}^N w_{nm}^{(2)} \frac{\partial E}{\partial a_n} \\
&\quad + h'(b_m) h'(b_{m'}) \sum_{n=1}^N w_{nm}^{(2)} \sum_{n'=1}^N w_{n'm'}^{(2)} \frac{\partial^2 E}{\partial a_n \partial a_{n'}}, \\
C_{nm}^{(12)} &= h'(b_m) \sum_{n'=1}^N w_{n'm}^{(2)} \frac{\partial^2 E}{\partial a_n \partial a_{n'}}, \\
C_{nn'}^{(22)} &= \frac{\partial^2 E}{\partial a_n \partial a_{n'}}.
\end{aligned} \tag{5.126}$$

5.24

Let y_1, \dots, y_N be variables such that

$$\begin{aligned}
y_n &= \mathbf{w}_n^\top \mathbf{z} + w_{n0}, \\
z_m &= h(\mathbf{w}_m^\top \mathbf{x} + w_{m0}).
\end{aligned} \tag{5.127}$$

(a)

Let

$$\tilde{\mathbf{x}} = a\mathbf{x} + b\mathbf{v}, \quad (5.128)$$

where

$$\mathbf{v} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}.$$

Then,

$$z_m = h \left(\frac{1}{a} \mathbf{w}_m^\top (\tilde{\mathbf{x}} - b\mathbf{v}) + w_{m0} \right). \quad (5.129)$$

Therefore,

$$\tilde{z}_m = h (\tilde{\mathbf{w}}_m^\top \mathbf{x} + \tilde{w}_{m0}), \quad (5.130)$$

where

$$\begin{aligned} \tilde{\mathbf{w}}_m &= \frac{1}{a} \mathbf{w}_m, \\ \tilde{w}_{m0} &= w_{m0} - \frac{b}{a} \mathbf{w}_m^\top \mathbf{v}. \end{aligned} \quad (5.131)$$

(b)

Let

$$\tilde{y}_n = c y_n + d. \quad (5.132)$$

Then,

$$\frac{\tilde{y}_n - d}{c} = \mathbf{w}_n^\top \mathbf{z} + w_{n0}. \quad (5.133)$$

Therefore,

$$\tilde{y}_n = \tilde{\mathbf{w}}_n^\top \mathbf{z} + \tilde{w}_{n0}, \quad (5.134)$$

where

$$\begin{aligned} \tilde{\mathbf{w}}_n &= c \mathbf{w}_n, \\ \tilde{w}_{n0} &= c w_{n0} + d. \end{aligned} \quad (5.135)$$

5.25

Let E be a quadratic error function such that

$$E(\mathbf{w}) = E_0 + \frac{1}{2} (\mathbf{w} - \mathbf{w}^*)^\top \mathbf{H} (\mathbf{w} - \mathbf{w}^*), \quad (5.136)$$

where \mathbf{w}^* represents the minimum and \mathbf{H} is a positive definite and constant matrix whose eigenvectors and eigenvalues are $\mathbf{u}_1, \dots, \mathbf{u}_M$ and η_1, \dots, η_M . Let

$$\begin{aligned} \mathbf{w}^{(\tau)} &= \mathbf{w}^{(\tau-1)} - \rho \nabla E, \\ \mathbf{w}^{(0)} &= \mathbf{0}. \end{aligned} \quad (5.137)$$

(a)

We have

$$\nabla E = \mathbf{H} (\mathbf{w} - \mathbf{w}^*). \quad (5.138)$$

Then,

$$\mathbf{w}^{(\tau)} = \mathbf{w}^{(\tau-1)} - \rho \mathbf{H} (\mathbf{w}^{(\tau-1)} - \mathbf{w}^*). \quad (5.139)$$

so that

$$\mathbf{u}_m^\top \mathbf{w}^{(\tau)} = \mathbf{u}_m^\top \mathbf{w}^{(\tau-1)} - \rho \mathbf{u}_m^\top \mathbf{H} (\mathbf{w}^{(\tau-1)} - \mathbf{w}^*). \quad (5.140)$$

Since \mathbf{H} is symmetric,

$$\mathbf{u}_m^\top \mathbf{H} \mathbf{w} = \mathbf{w}^\top \mathbf{H} \mathbf{u}_m. \quad (5.141)$$

The right hand side can be written as $\eta_m w_m$, where

$$w_m = \mathbf{w}^\top \mathbf{u}_m. \quad (5.142)$$

Then,

$$w_m^{(\tau)} = w_m^{(\tau-1)} - \rho \eta_m (w_m^{(\tau-1)} - w_m^*), \quad (5.143)$$

so that

$$w_m^{(\tau)} - w_m^* = (1 - \rho \eta_m) (w_m^{(\tau-1)} - w_m^*). \quad (5.144)$$

Therefore,

$$w_m^{(\tau)} = w_m^* + (1 - \rho \eta_m)^\tau (w_m^{(0)} - w_m^*), \quad (5.145)$$

so that

$$w_m^{(\tau)} = (1 - (1 - \rho \eta_m)^\tau) w_m^*. \quad (5.146)$$

(b)

By (a), if

$$|1 - \rho\eta_m| < 1, \quad (5.147)$$

then

$$\lim_{\tau \rightarrow \infty} w_m^{(\tau)} = w_m^*. \quad (5.148)$$

(c)

By (a) and the Taylor series

$$(1 - \rho\eta_m)^\tau = 1 - \rho\tau\eta_m + \rho^2\tau^2 O(\eta_m^2), \quad (5.149)$$

we have

$$w_m^{(\tau)} = (\rho\tau\eta_m - \rho^2\tau^2 O(\eta_m^2)) w_m^*, \quad (5.150)$$

so that

$$w_m^{(\tau)} = \rho\tau\eta_m (1 - \rho\tau\eta_m O(\eta_m)) w_m^*. \quad (5.151)$$

Therefore,

$$|w_m^{(\tau)}| \ll |w_m|^*, \quad \text{if } \eta_m \ll (\rho\tau)^{-1}, \quad (5.152)$$

while

$$w_m^{(\tau)} \simeq w_m^*, \quad \text{if } \eta_m \gg (\rho\tau)^{-1}. \quad (5.153)$$

5.26 (Incomplete)

Let

$$\tilde{E} = E + \lambda\Omega, \quad (5.154)$$

where

$$\Omega = \frac{1}{2} \sum_{n=1}^N \sum_{k=1}^K \left(\frac{\partial y_{nk}}{\partial \xi} \right)^2. \quad (5.155)$$

(a)

We have

$$\frac{\partial y_{nk}}{\partial \xi} = \mathcal{G}y_{nk}, \quad (5.156)$$

where

$$\begin{aligned}\mathcal{G} &= \sum_{d=1}^D \tau_d \frac{\partial}{\partial x_d}, \\ \tau_d &= \frac{\partial x_d}{\partial \xi}.\end{aligned}\tag{5.157}$$

Therefore,

$$\Omega = \sum_{n=1}^N \Omega_n,\tag{5.158}$$

where

$$\Omega_n = \frac{1}{2} \sum_{k=1}^K (\mathcal{G} y_{nk})^2.\tag{5.159}$$

(b)

$$\begin{aligned}\alpha_j &= \mathcal{G} z_j = h'(a_j) \beta_j? \\ \beta_j &= \mathcal{G} a_j = \sum_{d=1}^D w_{jd} \alpha_d?\end{aligned}\tag{5.160}$$

5.27

Let

$$\tilde{E} = \frac{1}{2} \iiint (y(\mathbf{x} + \boldsymbol{\xi}) - t)^2 p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi},\tag{5.161}$$

where

$$\begin{aligned}\mathbb{E} \boldsymbol{\xi} &= 0, \\ \text{var } \boldsymbol{\xi} &= \lambda \mathbf{I}.\end{aligned}\tag{5.162}$$

By the Taylor series

$$y(\mathbf{x} + \boldsymbol{\xi}) = y(\mathbf{x}) + \rho(\mathbf{x}, \boldsymbol{\xi}) + O(\|\boldsymbol{\xi}\|^3),\tag{5.163}$$

where

$$\rho(\mathbf{x}, \boldsymbol{\xi}) = \boldsymbol{\xi}^\top \nabla y(\mathbf{x}) + \frac{1}{2} \boldsymbol{\xi}^\top \nabla \nabla y(\mathbf{x}) \boldsymbol{\xi},\tag{5.164}$$

the integrand can be written as

$$\begin{aligned}(y(\mathbf{x}) - t)^2 &+ 2(y(\mathbf{x}) - t)(\rho(\mathbf{x}, \boldsymbol{\xi}) + O(\|\boldsymbol{\xi}\|^3)) \\ &+ (\rho(\mathbf{x}, \boldsymbol{\xi}) + O(\|\boldsymbol{\xi}\|^3))^2.\end{aligned}\tag{5.165}$$

Omitting the terms of $O(\|\boldsymbol{\xi}\|^3)$, the integral can be approximated as

$$2E + 2 \iint (y(\mathbf{x}) - t) \rho(\mathbf{x}, \boldsymbol{\xi}) p(t|\mathbf{x}) p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} dt d\boldsymbol{\xi} \\ + \iint \rho(\mathbf{x}, \boldsymbol{\xi})^2 p(\mathbf{x}) p(\boldsymbol{\xi}) d\mathbf{x} d\boldsymbol{\xi}, \quad (5.166)$$

where

$$E = \frac{1}{2} \iint (y(\mathbf{x}) - t)^2 p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt. \quad (5.167)$$

Omitting the terms of $O(\|\boldsymbol{\xi}\|^3)$, the second and third terms can be approximated as

$$2 \left(\int \boldsymbol{\xi} p(\boldsymbol{\xi}) d\boldsymbol{\xi} \right)^\top \iint (y(\mathbf{x}) - t) \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt \\ + \int \boldsymbol{\xi}^\top \left(\iint (y(\mathbf{x}) - t) \nabla \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt \right) \boldsymbol{\xi} p(\boldsymbol{\xi}) d\boldsymbol{\xi} \\ + \int \boldsymbol{\xi}^\top \left(\int (\nabla y(\mathbf{x})) (\nabla y(\mathbf{x}))^\top p(\mathbf{x}) d\mathbf{x} \right) \boldsymbol{\xi} p(\boldsymbol{\xi}) d\boldsymbol{\xi}. \quad (5.168)$$

Since

$$\mathbb{E} \boldsymbol{\xi} = \mathbf{0}, \quad (5.169)$$

the first term can be written as $\mathbf{0}$. Since

$$\mathbb{E} \boldsymbol{\xi} \boldsymbol{\xi}^\top = \lambda \mathbf{I}, \quad (5.170)$$

The second term can be written as

$$\lambda \operatorname{tr} \left(\iint (y(\mathbf{x}) - t) \nabla \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt \right), \quad (5.171)$$

where the integral can be written as

$$\int \left(y(\mathbf{x}) \int p(t|\mathbf{x}) dt - \int t p(t|\mathbf{x}) dt \right) \nabla \nabla y(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} \\ = \int (y(\mathbf{x}) - \mathbb{E}(t|\mathbf{x})) \nabla \nabla y(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \quad (5.172)$$

Similarly, the third term can be written as $2\lambda\Omega$, where

$$\Omega = \frac{1}{2} \operatorname{tr} \left(\int \nabla y(\mathbf{x}) (\nabla y(\mathbf{x}))^\top p(\mathbf{x}) d\mathbf{x} \right). \quad (5.173)$$

Therefore, if

$$y(\mathbf{x}) = E(t|\mathbf{x}), \quad (5.174)$$

then

$$\tilde{E} \simeq E + \lambda\Omega. \quad (5.175)$$

5.28 (Incomplete)

5.29

Let \mathbf{w} be a variable in M dimensions such that

$$p(w_m) = \sum_{k=1}^K \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2). \quad (5.176)$$

Let

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda\Omega(\mathbf{w}), \quad (5.177)$$

where

$$\Omega(\mathbf{w}) = -\sum_{m=1}^M \ln p(w_m). \quad (5.178)$$

We have

$$\frac{\partial \Omega}{\partial w_m} = \frac{\partial \Omega}{\partial p_m} \frac{\partial p_m}{\partial w_m}, \quad (5.179)$$

where

$$p_m = p(w_m). \quad (5.180)$$

We have

$$\begin{aligned} \frac{\partial \Omega}{\partial p_m} &= -\frac{1}{p_m}, \\ \frac{\partial p_m}{\partial w_m} &= -\sum_{k=1}^K \frac{w_m - \mu_k}{\sigma_k^2} p_{mk}, \end{aligned} \quad (5.181)$$

where

$$p_{mk} = \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2). \quad (5.182)$$

Therefore,

$$\frac{\partial \tilde{E}}{\partial w_m} = \frac{\partial E}{\partial w_m} + \lambda \sum_{k=1}^K \gamma_{mk} \frac{w_m - \mu_k}{\sigma_k^2}, \quad (5.183)$$

where

$$\gamma_{mk} = \frac{p_{mk}}{p_m}. \quad (5.184)$$

5.30

Let \mathbf{w} be a variable in M dimensions such that

$$p(w_m) = \sum_{k=1}^K \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2). \quad (5.185)$$

Let

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w}), \quad (5.186)$$

where

$$\Omega(\mathbf{w}) = - \sum_{m=1}^M \ln p(w_m). \quad (5.187)$$

We have

$$\frac{\partial \Omega}{\partial \mu_k} = \sum_{m=1}^M \frac{\partial \Omega}{\partial p_m} \frac{\partial p_m}{\partial \mu_k}, \quad (5.188)$$

where

$$p_m = p(w_m). \quad (5.189)$$

We have

$$\begin{aligned} \frac{\partial \Omega}{\partial p_m} &= -\frac{1}{p_m}, \\ \frac{\partial p_m}{\partial \mu_k} &= -\frac{\mu_k - w_m}{\sigma_k^2} p_{mk}, \end{aligned} \quad (5.190)$$

where

$$p_{mk} = \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2). \quad (5.191)$$

Therefore,

$$\frac{\partial \tilde{E}}{\partial \mu_k} = \lambda \sum_{m=1}^M \gamma_{mk} \frac{\mu_k - w_m}{\sigma_k^2}, \quad (5.192)$$

where

$$\gamma_{mk} = \frac{p_{mk}}{p_m}. \quad (5.193)$$

5.31

Let \mathbf{w} be a variable in M dimensions such that

$$p(w_m) = \sum_{k=1}^K \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2). \quad (5.194)$$

Let

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w}), \quad (5.195)$$

where

$$\Omega(\mathbf{w}) = - \sum_{m=1}^M \ln p(w_m). \quad (5.196)$$

We have

$$\frac{\partial \Omega}{\partial \sigma_k} = \sum_{m=1}^M \frac{\partial \Omega}{\partial p_m} \frac{\partial p_m}{\partial \sigma_k}, \quad (5.197)$$

where

$$p_m = p(w_m). \quad (5.198)$$

We have

$$\begin{aligned} \frac{\partial \Omega}{\partial p_m} &= -\frac{1}{p_m}, \\ \frac{\partial p_m}{\partial \sigma_k} &= \left(-\frac{1}{\sigma_k} + \frac{(w_m - \mu_k)^2}{\sigma_k^3} \right) p_{mk}, \end{aligned} \quad (5.199)$$

where

$$p_{mk} = \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2). \quad (5.200)$$

Therefore,

$$\frac{\partial \tilde{E}}{\partial \sigma_k} = \lambda \sum_{m=1}^M \gamma_{mk} \left(\frac{1}{\sigma_k} - \frac{(w_m - \mu_k)^2}{\sigma_k^3} \right), \quad (5.201)$$

where

$$\gamma_{mk} = \frac{p_{mk}}{p_m}. \quad (5.202)$$

5.32

Let \mathbf{w} be variable in M dimensions such that

$$p(w_m) = \sum_{k=1}^K \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2), \quad (5.203)$$

where

$$\pi_k = \frac{\exp(\eta_k)}{\sum_{k'=1}^K \exp(\eta_{k'})}. \quad (5.204)$$

Let

$$\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w}), \quad (5.205)$$

where

$$\Omega(\mathbf{w}) = - \sum_{m=1}^M \ln p(w_m). \quad (5.206)$$

(a)

If $k \neq k'$, then

$$\frac{\partial \pi_k}{\partial \eta_{k'}} = -\pi_k \pi_{k'}. \quad (5.207)$$

We have

$$\frac{\partial \pi_k}{\partial \eta_k} = \pi_k - \pi_k^2. \quad (5.208)$$

Therefore,

$$\frac{\partial \pi_k}{\partial \eta_{k'}} = I_{kk'} \pi_k - \pi_k \pi_{k'}. \quad (5.209)$$

(b)

We have

$$\frac{\partial \Omega}{\partial \eta_k} = \sum_{m=1}^M \sum_{k'=1}^K \frac{\partial \Omega}{\partial p_m} \frac{\partial p_m}{\partial \pi_{k'}} \frac{\partial \pi_{k'}}{\partial \eta_k}, \quad (5.210)$$

where

$$p_m = p(w_m). \quad (5.211)$$

We have

$$\begin{aligned}\frac{\partial \Omega}{\partial p_m} &= -\frac{1}{p_m}, \\ \frac{\partial p_m}{\partial \pi_{k'}} &= \frac{p_{mk'}}{\pi_{k'}},\end{aligned}\tag{5.212}$$

where

$$p_{mk} = \pi_k \mathcal{N}(w_m | \mu_k, \sigma_k^2).\tag{5.213}$$

By (a),

$$\frac{\partial \pi_{k'}}{\partial \eta_k} = I_{k'k} \pi_{k'} - \pi_{k'} \pi_{k'}.\tag{5.214}$$

Then,

$$\frac{\partial \Omega}{\partial \eta_k} = - \sum_{m=1}^M \sum_{k'=1}^K \frac{\gamma_{mk'}}{\pi_{k'}} (I_{k'k} \pi_{k'} - \pi_k \pi_{k'}),\tag{5.215}$$

where

$$\gamma_{mk} = \frac{p_{mk}}{p_m}.\tag{5.216}$$

The right hand side can be written as

$$-\sum_{m=1}^M \sum_{k'=1}^K \gamma_{mk'} (I_{k'k} - \pi_k) = \sum_{m=1}^M (\pi_k - \gamma_{mk}).\tag{5.217}$$

Therefore,

$$\frac{\partial \tilde{E}}{\partial \eta_k} = \lambda \sum_{m=1}^M (\pi_k - \gamma_{mk}).\tag{5.218}$$

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

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} L_1 \cos \theta_1 \\ L_1 \sin \theta_1 \end{bmatrix} + \begin{bmatrix} L_2 \cos(\theta_2 - (\pi - \theta_1)) \\ L_2 \sin(\theta_2 - (\pi - \theta_1)) \end{bmatrix}.\tag{5.219}$$

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

$$\begin{bmatrix} L_2 \cos(\theta_1 + \theta_2 - \pi) \\ L_2 \sin(\theta_1 + \theta_2 - \pi) \end{bmatrix} = \begin{bmatrix} -L_2 \cos(\theta_1 + \theta_2) \\ -L_2 \sin(\theta_1 + \theta_2) \end{bmatrix}.\tag{5.220}$$

Therefore,

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} L_1 \cos \theta_1 - L_2 \cos(\theta_1 + \theta_2) \\ L_1 \sin \theta_1 - L_2 \sin(\theta_1 + \theta_2) \end{bmatrix}. \quad (5.221)$$

5.34

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

$$p(\mathbf{t}_n | \mathbf{w}) = \sum_{k=1}^K \pi_k \mathcal{N}_{nk}, \quad (5.222)$$

where

$$\begin{aligned} \pi_k &= \frac{\exp(a_k)}{\sum_{k'=1}^K \exp(a_{k'})}, \\ \mathcal{N}_{nk} &= \mathcal{N}(\mathbf{t}_n | \boldsymbol{\mu}_k(\mathbf{x}_n, \mathbf{w}), \sigma_k^2(\mathbf{x}_n, \mathbf{w}) \mathbf{I}). \end{aligned} \quad (5.223)$$

Let

$$E(\mathbf{w}) = \sum_{n=1}^N E_n(\mathbf{w}), \quad (5.224)$$

where

$$E_n(\mathbf{w}) = -\ln p(\mathbf{t}_n | \mathbf{w}). \quad (5.225)$$

We have

$$\frac{\partial E_n}{\partial a_k} = \sum_{k'=1}^K \frac{\partial E_n}{\partial p_n} \frac{\partial p_n}{\partial \pi_{k'}} \frac{\partial \pi_{k'}}{\partial a_k}, \quad (5.226)$$

where

$$p_n = p(\mathbf{t}_n | \mathbf{w}). \quad (5.227)$$

We have

$$\begin{aligned} \frac{\partial E_n}{\partial p_n} &= -\frac{1}{p_n}, \\ \frac{\partial p_n}{\partial \pi_{k'}} &= \frac{p_{nk'}}{\pi_{k'}}, \end{aligned} \quad (5.228)$$

where

$$p_{nk} = \pi_k \mathcal{N}_{nk}. \quad (5.229)$$

By 5.32(a),

$$\frac{\partial \pi_{k'}}{\partial a_k} = I_{k'k} \pi_{k'} - \pi_k \pi_{k'}. \quad (5.230)$$

Then,

$$\frac{\partial E_n}{\partial a_k} = -\frac{1}{p_n} \sum_{k'=1}^K \frac{p_{nk'}}{\pi_{k'}} (I_{k'k} \pi_{k'} - \pi_k \pi_{k'}). \quad (5.231)$$

The right hand side can be written as

$$-\sum_{k'=1}^K \gamma_{nk'} (I_{kk'} - \pi_k) = \pi_k - \gamma_{nk}, \quad (5.232)$$

where

$$\gamma_{nk} = \frac{p_{nk}}{p_n}, \quad (5.233)$$

Therefore,

$$\frac{\partial E_n}{\partial a_k} = \pi_k - \gamma_{nk}. \quad (5.234)$$

5.35

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

$$p(\mathbf{t}_n | \mathbf{w}) = \sum_{k=1}^K \pi_k \mathcal{N}_{nk}, \quad (5.235)$$

where

$$\mathcal{N}_{nk} = \mathcal{N} (\mathbf{t}_n | \boldsymbol{\mu}_k(\mathbf{x}_n, \mathbf{w}), \sigma_k^2(\mathbf{x}_n, \mathbf{w}) \mathbf{I}). \quad (5.236)$$

Let

$$E(\mathbf{w}) = \sum_{n=1}^N E_n(\mathbf{w}), \quad (5.237)$$

where

$$E_n(\mathbf{w}) = -\ln p(\mathbf{t}_n | \mathbf{w}). \quad (5.238)$$

Then,

$$\frac{\partial E_n}{\partial \boldsymbol{\mu}_k} = \frac{\partial E_n}{\partial p_n} \frac{\partial p_n}{\partial \boldsymbol{\mu}_k}, \quad (5.239)$$

where

$$p_n = p(t_n | \mathbf{w}). \quad (5.240)$$

We have

$$\begin{aligned}\frac{\partial E_n}{\partial p_n} &= -\frac{1}{p_n}, \\ \frac{\partial p_n}{\partial \boldsymbol{\mu}_k} &= -\sigma_k^{-2}(\boldsymbol{\mu}_k - \mathbf{t}_n)p_{nk},\end{aligned}\tag{5.241}$$

where

$$p_{nk} = \pi_k \mathcal{N}_{nk}.\tag{5.242}$$

Therefore,

$$\frac{\partial E_n}{\partial \boldsymbol{\mu}_k} = \gamma_{nk} \sigma_k^{-2}(\boldsymbol{\mu}_k - \mathbf{t}_n),\tag{5.243}$$

where

$$\gamma_{nk} = \frac{p_{nk}}{p_n}.\tag{5.244}$$

5.36

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables in M dimensions such that

$$p(\mathbf{t}_n | \mathbf{w}) = \sum_{k=1}^K \pi_k \mathcal{N}_{nk},\tag{5.245}$$

where

$$\begin{aligned}\mathcal{N}_{nk} &= \mathcal{N}(\mathbf{t}_n | \boldsymbol{\mu}_k(\mathbf{x}_n, \mathbf{w}), \sigma_k^2(\mathbf{x}_n, \mathbf{w})\mathbf{I}), \\ \sigma_k &= \exp(a_k^\sigma).\end{aligned}\tag{5.246}$$

Let

$$E(\mathbf{w}) = \sum_{n=1}^N E_n(\mathbf{w}),\tag{5.247}$$

where

$$E_n(\mathbf{w}) = -\ln p(\mathbf{t}_n | \mathbf{w}).\tag{5.248}$$

Then,

$$\frac{\partial E_n}{\partial a_k^\sigma} = \frac{\partial E_n}{\partial p_n} \frac{\partial p_n}{\partial \sigma_k} \frac{\partial \sigma_k}{\partial a_k^\sigma},\tag{5.249}$$

where

$$p_n = p(\mathbf{t}_n | \mathbf{w}).\tag{5.250}$$

We have

$$\begin{aligned}\frac{\partial E_n}{\partial p_n} &= -\frac{1}{p_n}, \\ \frac{\partial p_n}{\partial \sigma_k} &= \left(-\frac{M}{\sigma_k} + \frac{\|\mathbf{t}_n - \boldsymbol{\mu}_k\|^2}{\sigma_k^3} \right) p_{nk}, \\ \frac{\partial \sigma_k}{\partial a_k^\sigma} &= \sigma_k,\end{aligned}\tag{5.251}$$

where

$$p_{nk} = \pi_k \mathcal{N}_{nk}.\tag{5.252}$$

Therefore,

$$\frac{\partial E_n}{\partial a_k^\sigma} = \gamma_{nk} \left(M - \frac{\|\mathbf{t}_n - \boldsymbol{\mu}_k\|^2}{\sigma_k^2} \right),\tag{5.253}$$

where

$$\gamma_{nk} = \frac{p_{nk}}{p_n}.\tag{5.254}$$

5.37

Let \mathbf{t} be a variable such that

$$p(\mathbf{t}|\mathbf{x}) = \sum_{k=1}^K \pi_k(\mathbf{x}) \mathcal{N}(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x}) \mathbf{I}).\tag{5.255}$$

(a)

We have

$$\mathbb{E}(\mathbf{t}|\mathbf{x}) = \int \mathbf{t} p(\mathbf{t}|\mathbf{x}) d\mathbf{t}.\tag{5.256}$$

The right hand side can be written as

$$\sum_{k=1}^K \pi_k(\mathbf{x}) \int \mathbf{t} \mathcal{N}(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x}) \mathbf{I}) d\mathbf{t} = \sum_{k=1}^K \pi_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x}).\tag{5.257}$$

Therefore,

$$\mathbb{E}(\mathbf{t}|\mathbf{x}) = \sum_{k=1}^K \pi_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x}).\tag{5.258}$$

(b)

We have

$$\text{var}(\mathbf{t}|\mathbf{x}) = \int (\mathbf{t} - E(\mathbf{t}|\mathbf{x})) (\mathbf{t} - E(\mathbf{t}|\mathbf{x}))^\top p(\mathbf{t}|\mathbf{x}) d\mathbf{t}. \quad (5.259)$$

The right hand side can be written as

$$\begin{aligned} & \int \mathbf{t}\mathbf{t}^\top p(\mathbf{t}|\mathbf{x}) d\mathbf{t} - E(\mathbf{t}|\mathbf{x}) \left(\int \mathbf{t}p(\mathbf{t}|\mathbf{x}) d\mathbf{t} \right)^\top \\ & - \left(\int \mathbf{t}p(\mathbf{t}|\mathbf{x}) d\mathbf{t} \right) E(\mathbf{t}|\mathbf{x})^\top + E(\mathbf{t}|\mathbf{x}) E(\mathbf{t}|\mathbf{x})^\top \int p(\mathbf{t}|\mathbf{x}) d\mathbf{t} \\ & = \int \mathbf{t}\mathbf{t}^\top p(\mathbf{t}|\mathbf{x}) d\mathbf{t} - E(\mathbf{t}|\mathbf{x}) E(\mathbf{t}|\mathbf{x})^\top. \end{aligned} \quad (5.260)$$

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

$$\sum_{k=1}^K \pi_k(\mathbf{x}) \int \mathbf{t}\mathbf{t}^\top \mathcal{N}(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}) d\mathbf{t}. \quad (5.261)$$

The integral of the right hand side can be written as

$$\begin{aligned} & \int (\mathbf{t}' + \boldsymbol{\mu}_k(\mathbf{x})) (\mathbf{t}' + \boldsymbol{\mu}_k(\mathbf{x}))^\top \mathcal{N}(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}) d\mathbf{t} \\ & = \int \mathbf{t}'\mathbf{t}'^\top \mathcal{N}(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}) d\mathbf{t} \\ & + \boldsymbol{\mu}_k(\mathbf{x}) \left(\int \mathbf{t}'\mathcal{N}(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}) d\mathbf{t} \right)^\top \\ & + \left(\int \mathbf{t}'\mathcal{N}(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}) d\mathbf{t} \right) \boldsymbol{\mu}_k(\mathbf{x})^\top \\ & + \boldsymbol{\mu}_k(\mathbf{x})\boldsymbol{\mu}_k(\mathbf{x})^\top \int \mathcal{N}(\mathbf{t}|\boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x})\mathbf{I}) d\mathbf{t}, \end{aligned} \quad (5.262)$$

where

$$\mathbf{t}' = \mathbf{t} - \boldsymbol{\mu}_k(\mathbf{x}). \quad (5.263)$$

The right hand side can be written as

$$\begin{aligned}
& \int \mathbf{t}' \mathbf{t}'^\top \mathcal{N}(\mathbf{t}' | \mathbf{0}, \sigma_k^2(\mathbf{x}) \mathbf{I}) d\mathbf{t}' \\
& + \boldsymbol{\mu}_k(\mathbf{x}) \left(\int \mathbf{t}' \mathcal{N}(\mathbf{t}' | \mathbf{0}, \sigma_k^2(\mathbf{x}) \mathbf{I}) d\mathbf{t}' \right)^\top \\
& + \left(\int \mathbf{t}' \mathcal{N}(\mathbf{t}' | \mathbf{0}, \sigma_k^2(\mathbf{x}) \mathbf{I}) d\mathbf{t}' \right) \boldsymbol{\mu}_k(\mathbf{x})^\top \\
& + \boldsymbol{\mu}_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x})^\top \int \mathcal{N}(\mathbf{t} | \boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x}) \mathbf{I}) d\mathbf{t} \\
& = \sigma_k^2(\mathbf{x}) \mathbf{I} + \boldsymbol{\mu}_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x})^\top.
\end{aligned} \tag{5.264}$$

Therefore, by (a),

$$\begin{aligned}
\text{cov}(\mathbf{t} | \mathbf{x}) &= \sum_{k=1}^K \pi_k(\mathbf{x}) (\sigma_k^2(\mathbf{x}) \mathbf{I} + \boldsymbol{\mu}_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x})^\top) \\
& - \left(\sum_{k=1}^K \pi_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x}) \right) \left(\sum_{k=1}^K \pi_k(\mathbf{x}) \boldsymbol{\mu}_k(\mathbf{x}) \right)^\top.
\end{aligned} \tag{5.265}$$

5.38

Let t_1, \dots, t_N be variables such that

$$\begin{aligned}
p(t_n | \mathbf{w}) &= \mathcal{N}(t_n | y(\mathbf{x}_n, \mathbf{w}), \beta^{-1}), \\
p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{0}, \alpha^{-1} \mathbf{I}).
\end{aligned} \tag{5.266}$$

By marginalisation,

$$p(t_{N+1} | \mathbf{t}) = \int p(t_{N+1} | \mathbf{w}) p(\mathbf{w} | \mathbf{t}) d\mathbf{w}. \tag{5.267}$$

By the Bayes' theorem,

$$p(\mathbf{w} | \mathbf{t}) p(\mathbf{t}) = p(\mathbf{t} | \mathbf{w}) p(\mathbf{w}). \tag{5.268}$$

The logarithm of the right hand side except the terms independent of \mathbf{w} can be written as $-E(\mathbf{w})$ where

$$E(\mathbf{w}) = \frac{\beta}{2} \sum_{n=1}^N (t_n - y(\mathbf{x}_n, \mathbf{w}))^2 + \frac{\alpha}{2} \|\mathbf{w}\|^2. \tag{5.269}$$

Let \mathbf{w}_{MAP} be a stationary point of $p(\mathbf{w}|\mathbf{t})$. Then, we have the Taylor series

$$\begin{aligned} E(\mathbf{w}) = & E(\mathbf{w}_{\text{MAP}}) + \frac{1}{2}(\mathbf{w} - \mathbf{w}_{\text{MAP}})^T \mathbf{A}(\mathbf{w} - \mathbf{w}_{\text{MAP}}) \\ & + O(\|\mathbf{w} - \mathbf{w}_{\text{MAP}}\|^3), \end{aligned} \quad (5.270)$$

where

$$\mathbf{A} = \nabla \nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\text{MAP}}}. \quad (5.271)$$

Then,

$$p(\mathbf{w}|\mathbf{t}) \simeq \mathcal{N}(\mathbf{w}|\mathbf{w}_{\text{MAP}}, \mathbf{A}^{-1}). \quad (5.272)$$

By the Taylor series

$$y(\mathbf{x}_{N+1}, \mathbf{w}) = y(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}) + \mathbf{g}^T(\mathbf{w} - \mathbf{w}_{\text{MAP}}) + O(\|\mathbf{w} - \mathbf{w}_{\text{MAP}}\|^2), \quad (5.273)$$

where

$$\mathbf{g} = \nabla_{\mathbf{w}} y(\mathbf{x}_{N+1}, \mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\text{MAP}}}, \quad (5.274)$$

we have

$$p(t_{N+1}|\mathbf{w}) \simeq \mathcal{N}(t_{N+1}|y(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}) + \mathbf{g}^T(\mathbf{w} - \mathbf{w}_{\text{MAP}}), \beta^{-1}). \quad (5.275)$$

Then, the logarithm of the integrand except the terms independent of \mathbf{w} can be approximated as

$$\begin{aligned} & -\frac{\beta}{2} (t_{N+1} - y(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}) - \mathbf{g}^T(\mathbf{w} - \mathbf{w}_{\text{MAP}}))^2 \\ & - \frac{1}{2}(\mathbf{w} - \mathbf{w}_{\text{MAP}})^T \mathbf{A}(\mathbf{w} - \mathbf{w}_{\text{MAP}}) \\ & = -\frac{1}{2}\mathbf{v}^T \mathbf{M} \mathbf{v}, \end{aligned} \quad (5.276)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} - \mathbf{w}_{\text{MAP}} \\ t_{N+1} - y(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}) \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \mathbf{A} + \beta \mathbf{g} \mathbf{g}^T & -\beta \mathbf{g} \\ -\beta \mathbf{g}^T & \beta \end{bmatrix}. \quad (5.277)$$

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{A}^{-1} & \mathbf{A}^{-1} \mathbf{g} \\ \mathbf{g}^T \mathbf{A}^{-1} & \beta^{-1} + \mathbf{g}^T \mathbf{A}^{-1} \mathbf{g} \end{bmatrix}. \quad (5.278)$$

Therefore,

$$p(t_{N+1}|\mathbf{t}) \simeq \mathcal{N}(t_{N+1}|y(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}), \beta^{-1} + \mathbf{g}^T \mathbf{A}^{-1} \mathbf{g}). \quad (5.279)$$

5.39

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}(t_n|y(\mathbf{x}_n, \mathbf{w}), \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}), \end{aligned} \quad (5.280)$$

where \mathbf{w} is in M dimensions. By marginalisation,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}. \quad (5.281)$$

The logarithm of the integrand of the right hand side can be written as

$$\begin{aligned} & -\frac{N}{2} \ln(2\pi\beta^{-1}) - \frac{\beta}{2} \sum_{n=1}^N (t_n - y(\mathbf{x}_n, \mathbf{w}))^2 \\ & - \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln(\det(\alpha^{-1}\mathbf{I})) - \frac{\alpha}{2} \|\mathbf{w}\|^2 \\ & = -E(\mathbf{w}) - \frac{N+M}{2} \ln(2\pi) + \frac{N}{2} \ln \beta + \frac{M}{2} \ln \alpha, \end{aligned} \quad (5.282)$$

where

$$E(\mathbf{w}) = \frac{\beta}{2} \sum_{n=1}^N (t_n - y(\mathbf{x}_n, \mathbf{w}))^2 + \frac{\alpha}{2} \|\mathbf{w}\|^2. \quad (5.283)$$

Let \mathbf{w}_{MAP} be a stationary point of E . Then, we have the Taylor series

$$\begin{aligned} E(\mathbf{w}) &= E(\mathbf{w}_{\text{MAP}}) + \frac{1}{2}(\mathbf{w} - \mathbf{w}_{\text{MAP}})^T \mathbf{A}(\mathbf{w} - \mathbf{w}_{\text{MAP}}) \\ &\quad + O(\|\mathbf{w} - \mathbf{w}_{\text{MAP}}\|^3), \end{aligned} \quad (5.284)$$

where

$$\mathbf{A} = \nabla \nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\text{MAP}}}. \quad (5.285)$$

Then, the logarithm of the integrand can be approximated as

$$\begin{aligned} & -E(\mathbf{w}_{\text{MAP}}) - \frac{1}{2}(\mathbf{w} - \mathbf{w}_{\text{MAP}})^T \mathbf{A}(\mathbf{w} - \mathbf{w}_{\text{MAP}}) \\ & - \frac{N+M}{2} \ln(2\pi) + \frac{N}{2} \ln \beta + \frac{M}{2} \ln \alpha. \end{aligned} \quad (5.286)$$

We have

$$\begin{aligned} & \int \exp \left(-\frac{1}{2}(\mathbf{w} - \mathbf{w}_{\text{MAP}})^T \mathbf{A} (\mathbf{w} - \mathbf{w}_{\text{MAP}}) \right) d\mathbf{w} \\ &= (2\pi)^{\frac{M}{2}} (\det \mathbf{A}^{-1})^{\frac{1}{2}}. \end{aligned} \quad (5.287)$$

Therefore,

$$\ln p(\mathbf{t}) \simeq -E(\mathbf{w}_{\text{MAP}}) - \frac{1}{2} \ln |\det \mathbf{A}| - \frac{N}{2} \ln(2\pi) + \frac{N}{2} \ln \beta + \frac{M}{2} \ln \alpha. \quad (5.288)$$

5.40

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables from the standard basis in K dimensions such that

$$\begin{aligned} p(\mathbf{t}_n | \mathbf{w}) &= \prod_{k=1}^K y_{nk}^{t_{nk}}, \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{0}, \alpha^{-1} \mathbf{I}), \end{aligned} \quad (5.289)$$

where

$$\begin{aligned} y_{nk} &= y_k(\mathbf{a}_n), \\ y_k(\mathbf{a}) &= \frac{\exp(a_k)}{\sum_{k'=1}^K \exp(a_{k'})}, \\ \mathbf{a}_n &= \mathbf{a}(\mathbf{x}_n, \mathbf{w}). \end{aligned} \quad (5.290)$$

By marginalisation,

$$p(\mathbf{t}_{N+1} | \mathbf{T}) = \int p(\mathbf{t}_{N+1} | \mathbf{w}) p(\mathbf{w} | \mathbf{T}) d\mathbf{w}. \quad (5.291)$$

By the Bayes' theorem,

$$p(\mathbf{w} | \mathbf{T}) p(\mathbf{T}) = p(\mathbf{T} | \mathbf{w}) p(\mathbf{w}). \quad (5.292)$$

The logarithm of the right hand side except the terms independent of \mathbf{w} can be written as $-E(\mathbf{w})$ where

$$E(\mathbf{w}) = - \sum_{n=1}^N \sum_{k=1}^K t_{nk} \ln y_{nk} + \frac{\alpha}{2} \|\mathbf{w}\|^2. \quad (5.293)$$

Let \mathbf{w}_{MAP} be a stationary point of E . Then, we have the Taylor series

$$\begin{aligned} E(\mathbf{w}) = & E(\mathbf{w}_{\text{MAP}}) + \frac{1}{2}(\mathbf{w} - \mathbf{w}_{\text{MAP}})^{\top} \mathbf{A}(\mathbf{w} - \mathbf{w}_{\text{MAP}}) \\ & + O(\|\mathbf{w} - \mathbf{w}_{\text{MAP}}\|^3), \end{aligned} \quad (5.294)$$

where

$$\mathbf{A} = \nabla \nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\text{MAP}}}. \quad (5.295)$$

Then,

$$p(\mathbf{w}|\mathbf{T}) \simeq \mathcal{N}(\mathbf{w}|\mathbf{w}_{\text{MAP}}, \mathbf{A}^{-1}). \quad (5.296)$$

We have

$$p(\mathbf{t}_{N+1}|\mathbf{w}) = \prod_{k=1}^K y_{N+1,k}^{t_{N+1,k}}, \quad (5.297)$$

where

$$y_{N+1,k} = y_k(\mathbf{a}(\mathbf{x}_{N+1}, \mathbf{w})). \quad (5.298)$$

We have the Taylor series

$$\begin{aligned} \mathbf{a}(\mathbf{x}_{N+1}, \mathbf{w}) = & \mathbf{a}(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}) + \mathbf{B}(\mathbf{w} - \mathbf{w}_{\text{MAP}}) \\ & + O(\|\mathbf{w} - \mathbf{w}_{\text{MAP}}\|^2), \end{aligned} \quad (5.299)$$

where

$$\mathbf{B} = \nabla_{\mathbf{w}} \mathbf{a}(\mathbf{x}_{N+1}, \mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\text{MAP}}}. \quad (5.300)$$

Then,

$$p(\mathbf{t}_{N+1}|\mathbf{w}) \simeq \int \delta(\mathbf{a}_{N+1} - \mathbf{c}_{N+1}) \left(\prod_{k=1}^K y_k(\mathbf{a}_{N+1})^{t_{N+1,k}} \right) d\mathbf{a}_{N+1}, \quad (5.301)$$

where δ is the Dirac delta function and

$$\mathbf{c}_{N+1} = \mathbf{a}(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}) + \mathbf{B}(\mathbf{w} - \mathbf{w}_{\text{MAP}}). \quad (5.302)$$

Then,

$$\int p(\mathbf{t}_{N+1}|\mathbf{w}) p(\mathbf{w}|\mathbf{T}) d\mathbf{w} \simeq \int \left(\prod_{k=1}^K y_k(\mathbf{a}_{N+1})^{t_{N+1,k}} \right) p(\mathbf{a}_{N+1}) d\mathbf{a}_{N+1}, \quad (5.303)$$

where

$$p(\mathbf{a}_{N+1}) = \int \delta(\mathbf{a}_{N+1} - \mathbf{c}_{N+1}) \mathcal{N}(\mathbf{w} | \mathbf{w}_{\text{MAP}}, \mathbf{A}^{-1}) d\mathbf{w}. \quad (5.304)$$

Since \mathbf{t}_{N+1} is a variable from the standard basis in K dimensions, the right hand side of the approximation can be written as

$$\prod_{k=1}^K \left(\int y_k(\mathbf{a}_{N+1}) p(\mathbf{a}_{N+1}) d\mathbf{a}_{N+1} \right)^{t_{N+1,k}}. \quad (5.305)$$

We have

$$\mathbb{E} \mathbf{a}_{N+1} = \int \mathbf{a}_{N+1} p(\mathbf{a}_{N+1}) d\mathbf{a}_{N+1}. \quad (5.306)$$

The right hand side can be written as

$$\int \mathbf{c}_{N+1} \mathcal{N}(\mathbf{w} | \mathbf{w}_{\text{MAP}}, \mathbf{A}^{-1}) d\mathbf{w} = \mathbf{a}(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}). \quad (5.307)$$

Then,

$$\text{var } \mathbf{a}_{N+1} = \int (\mathbf{a}_{N+1} - \mathbf{a}(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}))^2 p(\mathbf{a}_{N+1}) d\mathbf{a}_{N+1}. \quad (5.308)$$

The right hand side can be written as

$$\int (\mathbf{c}_{N+1} - \mathbf{a}(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}))^2 \mathcal{N}(\mathbf{w} | \mathbf{w}_{\text{MAP}}, \mathbf{A}^{-1}) d\mathbf{w} = \mathbf{B} \mathbf{A}^{-1} \mathbf{B}^\top. \quad (5.309)$$

Then,

$$p(\mathbf{a}_{N+1}) = \mathcal{N}(\mathbf{a}_{N+1} | \mathbf{a}(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}), \mathbf{B} \mathbf{A}^{-1} \mathbf{B}^\top). \quad (5.310)$$

Therefore,

$$p(\mathbf{t}_{N+1} | \mathbf{T}) \simeq \prod_{k=1}^K v_{N+1,k}^{t_{N+1,k}}, \quad (5.311)$$

where

$$v_{N+1,k} = \int y_k(\mathbf{a}) \mathcal{N}(\mathbf{a} | \mathbf{a}(\mathbf{x}_{N+1}, \mathbf{w}_{\text{MAP}}), \mathbf{B} \mathbf{A}^{-1} \mathbf{B}^\top) d\mathbf{a}. \quad (5.312)$$

5.41

Let $\mathbf{t}_1, \dots, \mathbf{t}_N$ be variables from the standard basis in K dimensions such that

$$p(\mathbf{t}_n | \mathbf{w}) = \prod_{k=1}^K y_{nk}^{t_{nk}},$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w} | \mathbf{0}, \alpha^{-1} \mathbf{I}),$$
(5.313)

where \mathbf{w} is in M dimensions and

$$y_{nk} = y_k(\mathbf{x}_n, \mathbf{w}).$$
(5.314)

By marginalisation,

$$p(\mathbf{T}) = \int p(\mathbf{T} | \mathbf{w}) p(\mathbf{w}) d\mathbf{w}.$$
(5.315)

The logarithm of the integrand of the right hand side can be written as

$$\begin{aligned} & \sum_{n=1}^N \sum_{k=1}^K t_{nk} \ln y_{nk} - \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln (\det(\alpha^{-1} \mathbf{I})) - \frac{\alpha}{2} \|\mathbf{w}\|^2 \\ &= -E(\mathbf{w}) - \frac{M}{2} \ln(2\pi) + \frac{M}{2} \ln \alpha, \end{aligned}$$
(5.316)

where

$$E(\mathbf{w}) = - \sum_{n=1}^N \sum_{k=1}^K t_{nk} \ln y_{nk} + \frac{\alpha}{2} \|\mathbf{w}\|^2.$$
(5.317)

Let \mathbf{w}_{MAP} be a stationary point of E . Then, we have the Taylor series

$$\begin{aligned} E(\mathbf{w}) &= E(\mathbf{w}_{\text{MAP}}) + \frac{1}{2} (\mathbf{w} - \mathbf{w}_{\text{MAP}})^T \mathbf{A} (\mathbf{w} - \mathbf{w}_{\text{MAP}}) \\ &\quad + O(\|(\mathbf{w} - \mathbf{w}_{\text{MAP}})\|^3), \end{aligned}$$
(5.318)

where

$$\mathbf{A} = \nabla \nabla E(\mathbf{w})|_{\mathbf{w}=\mathbf{w}_{\text{MAP}}}.$$
(5.319)

Then, the logarithm of the integrand can be approximated as

$$-E(\mathbf{w}_{\text{MAP}}) - \frac{1}{2} (\mathbf{w} - \mathbf{w}_{\text{MAP}})^T \mathbf{A} (\mathbf{w} - \mathbf{w}_{\text{MAP}}) - \frac{M}{2} \ln(2\pi) + \frac{M}{2} \ln \alpha.$$
(5.320)

We have

$$\begin{aligned} & \int \exp \left(-\frac{1}{2}(\mathbf{w} - \mathbf{w}_{\text{MAP}})^T \mathbf{A} (\mathbf{w} - \mathbf{w}_{\text{MAP}}) \right) d\mathbf{w} \\ &= (2\pi)^{\frac{M}{2}} (\det \mathbf{A}^{-1})^{\frac{1}{2}}. \end{aligned} \quad (5.321)$$

Therefore,

$$\ln p(\mathbf{T}) \simeq -E(\mathbf{w}_{\text{MAP}}) - \frac{1}{2} \ln |\det \mathbf{A}| + \frac{M}{2} \ln \alpha. \quad (5.322)$$

6 Kernel Methods

6.1

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}) &= \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, 1), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{0}, \lambda^{-1} \mathbf{I}). \end{aligned} \quad (6.1)$$

By the Bayes' theorem,

$$p(\mathbf{w} | \mathbf{t}) p(\mathbf{t}) = p(\mathbf{t} | \mathbf{w}) p(\mathbf{w}). \quad (6.2)$$

The logarithm of the right hand side except the terms independent of \mathbf{w} can be written as $-E_{\mathbf{w}}(\mathbf{w})$ where

$$E_{\mathbf{w}}(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N (t_n - \mathbf{w}^\top \boldsymbol{\phi}_n)^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2, \quad (6.3)$$

so that

$$E_{\mathbf{w}}(\mathbf{w}) = \frac{1}{2} \|\mathbf{t} - \Phi \mathbf{w}\|^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2. \quad (6.4)$$

(a)

Let \mathbf{w}_{MAP} be a stationary point of $E_{\mathbf{w}}$. Setting the derivative of $E_{\mathbf{w}}$ with respect to \mathbf{w} to zero gives

$$\mathbf{0} = -\Phi^\top (\mathbf{t} - \Phi \mathbf{w}) + \lambda \mathbf{w}. \quad (6.5)$$

Therefore,

$$\mathbf{w}_{\text{MAP}} = \Phi^\top \mathbf{a}_{\text{MAP}}, \quad (6.6)$$

where

$$\mathbf{a}_{\text{MAP}} = \frac{1}{\lambda} (\mathbf{t} - \Phi \mathbf{w}_{\text{MAP}}). \quad (6.7)$$

(b)

Let

$$\mathbf{w} = \Phi^\top \mathbf{a}. \quad (6.8)$$

Then,

$$E_{\mathbf{w}}(\mathbf{w}) = E_{\mathbf{a}}(\mathbf{a}), \quad (6.9)$$

where

$$E_{\mathbf{a}}(\mathbf{a}) = \frac{1}{2} \|\mathbf{t} - \Phi \Phi^T \mathbf{a}\|^2 + \frac{\lambda}{2} \mathbf{a}^T \Phi \Phi^T \mathbf{a}. \quad (6.10)$$

The right hand side can be written as

$$\frac{1}{2} \|\mathbf{t}\|^2 - \mathbf{t}^T \mathbf{K} \mathbf{a} + \frac{1}{2} \mathbf{a}^T \mathbf{K} \mathbf{K} \mathbf{a} + \frac{\lambda}{2} \mathbf{a}^T \mathbf{K} \mathbf{a}, \quad (6.11)$$

where

$$\mathbf{K} = \Phi \Phi^T. \quad (6.12)$$

Let \mathbf{a}_{MAP} be a stationary point of $E_{\mathbf{a}}$. Setting the derivative of $E_{\mathbf{a}}$ with respect to \mathbf{a} to zero gives

$$\mathbf{0} = -\mathbf{K} \mathbf{t} + \mathbf{K} \mathbf{K} \mathbf{a} + \lambda \mathbf{K} \mathbf{a}. \quad (6.13)$$

Therefore,

$$\mathbf{a}_{MAP} = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}. \quad (6.14)$$

(c)

By (a) and (b),

$$\frac{1}{\lambda} (\mathbf{t} - \Phi \mathbf{w}_{MAP}) = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}, \quad (6.15)$$

so that

$$\mathbf{t} - \Phi \mathbf{w}_{MAP} = \mathbf{N} \mathbf{t}, \quad (6.16)$$

where

$$\mathbf{N} = (\mathbf{I} + \lambda^{-1} \mathbf{K})^{-1}. \quad (6.17)$$

By 2.26, the right hand side can be written as

$$\mathbf{I} - \Phi \mathbf{M} \Phi^T, \quad (6.18)$$

where

$$\mathbf{M} = (\lambda \mathbf{I} + \Phi^T \Phi)^{-1}. \quad (6.19)$$

Then,

$$\mathbf{t} - \Phi \mathbf{w}_{MAP} = (\mathbf{I} - \Phi \mathbf{M} \Phi^T) \mathbf{t}, \quad (6.20)$$

so that

$$\Phi (\mathbf{w}_{MAP} - \Phi \mathbf{M} \Phi^T \mathbf{t}) = \mathbf{0}. \quad (6.21)$$

Therefore,

$$\mathbf{w}_{MAP} = \mathbf{M} \Phi^T \mathbf{t}. \quad (6.22)$$

6.2 (Incomplete)

Let t_1, \dots, t_N be variables such that

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

$$p(t_n | \mathbf{w}) = \left(\frac{1 + y_n}{2} \right)^{\frac{1+t_n}{2}} \left(\frac{1 - y_n}{2} \right)^{\frac{1-t_n}{2}}, \quad (6.23)$$

where

$$y_n = f(\mathbf{w}^\top \boldsymbol{\phi}_n),$$

$$f(a) = \begin{cases} 1, & a \geq 0, \\ -1, & \text{otherwise.} \end{cases} \quad (6.24)$$

Let

$$E(\mathbf{w}) = - \sum_{n \in \mathcal{M}} \mathbf{w}^\top \boldsymbol{\phi}_n t_n, \quad (6.25)$$

where \mathcal{M} is the set of all misclassification. We have the Taylor series

$$E(\mathbf{w}^{(\tau)}) = E(\mathbf{w}^{(\tau-1)}) + \mathbf{b}^\top (\mathbf{w}^{(\tau)} - \mathbf{w}^{(\tau-1)}) + O\left(\|\mathbf{w}^{(\tau)} - \mathbf{w}^{(\tau-1)}\|^2\right), \quad (6.26)$$

where

$$\mathbf{b} = - \sum_{n \in \mathcal{M}} t_n \boldsymbol{\phi}_n. \quad (6.27)$$

6.3

We have

$$\|\mathbf{x} - \mathbf{x}_n\|^2 = \|\mathbf{x}\|^2 - 2\mathbf{x}^\top \mathbf{x}_n + \|\mathbf{x}_n\|^2. \quad (6.28)$$

The right hand side can be written as

$$k(\mathbf{x}, \mathbf{x}) - 2k(\mathbf{x}, \mathbf{x}_n) + k(\mathbf{x}_n, \mathbf{x}_n), \quad (6.29)$$

where

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{x}'. \quad (6.30)$$

6.4

Let \mathbf{A} be a 2×2 matrix with positive eigenvalues and with at least one negative element. We have

$$\det(\lambda\mathbf{I} - \mathbf{A}) = (\lambda - A_{11})(\lambda - A_{22}) - A_{12}A_{21}. \quad (6.31)$$

Seeing the left hand side to zero gives

$$0 = \lambda^2 - (A_{11} + A_{22})\lambda + A_{11}A_{22} - A_{12}A_{21}. \quad (6.32)$$

For the equation to have two positive solutions, we have the conditions

$$\begin{aligned} (A_{11} + A_{22})^2 - 4(A_{11}A_{22} - A_{12}A_{21}) &> 0, \\ A_{11} + A_{22} &> 0, \\ A_{11}A_{22} - A_{12}A_{21} &> 0. \end{aligned} \quad (6.33)$$

Therefore, an example of A is given by

$$\begin{bmatrix} 2 & 0 \\ -1 & 1 \end{bmatrix}. \quad (6.34)$$

6.5

Let

$$k_1(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}_1(\mathbf{x})^\top \boldsymbol{\phi}_1(\mathbf{x}'). \quad (6.35)$$

(a)

Let

$$k(\mathbf{x}, \mathbf{x}') = ck_1(\mathbf{x}, \mathbf{x}'), \quad (6.36)$$

where c is a positive constant. The right hand side can be written as

$$c\boldsymbol{\phi}_1(\mathbf{x})^\top \boldsymbol{\phi}_1(\mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^\top \boldsymbol{\phi}(\mathbf{x}'), \quad (6.37)$$

where

$$\boldsymbol{\phi} = \sqrt{c}\boldsymbol{\phi}_1. \quad (6.38)$$

Therefore, k is a valid kernel.

(b)

Let

$$k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x})k_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}'). \quad (6.39)$$

The right hand side can be written as

$$f(\mathbf{x})\phi_1(\mathbf{x})^\top\phi_1(\mathbf{x}')f(\mathbf{x}') = \phi(\mathbf{x})^\top\phi(\mathbf{x}'), \quad (6.40)$$

where

$$\phi = f\phi_1. \quad (6.41)$$

Therefore, k is a valid kernel.

6.6

Let

$$k_1(\mathbf{x}, \mathbf{x}') = \phi_1(\mathbf{x})^\top\phi_1(\mathbf{x}'), \quad (6.42)$$

where ϕ_1 is a vector in M dimensions.

(a)

Let

$$k(\mathbf{x}, \mathbf{x}') = \sum_{j=0}^J c_j q_j(\mathbf{x}, \mathbf{x}'), \quad (6.43)$$

where c_0, \dots, c_J are nonnegative constants and

$$q_j(\mathbf{x}, \mathbf{x}') = (k_1(\mathbf{x}, \mathbf{x}'))^j. \quad (6.44)$$

We have

$$q_0(\mathbf{x}, \mathbf{x}') = 1. \quad (6.45)$$

Let us assume that q_j is a valid kernel. Then,

$$q_{j+1}(\mathbf{x}, \mathbf{x}') = q_j(\mathbf{x}, \mathbf{x}')\phi_1(\mathbf{x})^\top\phi_1(\mathbf{x}'). \quad (6.46)$$

The right hand side can be written as

$$q_j(\mathbf{x}, \mathbf{x}') \sum_{m=1}^M \phi_{1m}(\mathbf{x})\phi_{1m}(\mathbf{x}') = \sum_{m=1}^M \phi_{1m}(\mathbf{x})q_j(\mathbf{x}, \mathbf{x}')\phi_{1m}(\mathbf{x}'). \quad (6.47)$$

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

$$k(\mathbf{x}, \mathbf{x}') = \exp(k_1(\mathbf{x}, \mathbf{x}')). \quad (6.48)$$

The right hand side can be written as

$$\sum_{j=0}^{\infty} \frac{1}{j!} (k_1(\mathbf{x}, \mathbf{x}'))^j. \quad (6.49)$$

Therefore, by (a), k is a valid kernel.

6.7

Let

$$\begin{aligned} k_1(\mathbf{x}, \mathbf{x}') &= \boldsymbol{\phi}_1(\mathbf{x})^\top \boldsymbol{\phi}_1(\mathbf{x}'), \\ k_2(\mathbf{x}, \mathbf{x}') &= \boldsymbol{\phi}_2(\mathbf{x})^\top \boldsymbol{\phi}_2(\mathbf{x}'). \end{aligned} \quad (6.50)$$

(a)

Let

$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}'). \quad (6.51)$$

The right hand side can be written as

$$\boldsymbol{\phi}_1(\mathbf{x})^\top \boldsymbol{\phi}_1(\mathbf{x}') + \boldsymbol{\phi}_2(\mathbf{x})^\top \boldsymbol{\phi}_2(\mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^\top \boldsymbol{\phi}(\mathbf{x}'), \quad (6.52)$$

where

$$\boldsymbol{\phi} = \begin{bmatrix} \boldsymbol{\phi}_1 \\ \boldsymbol{\phi}_2 \end{bmatrix}. \quad (6.53)$$

Therefore, k is a valid kernel.

(b)

Let

$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') k_2(\mathbf{x}, \mathbf{x}'). \quad (6.54)$$

Then,

$$\ln k(\mathbf{x}, \mathbf{x}') = \ln k_1(\mathbf{x}, \mathbf{x}') + \ln k_2(\mathbf{x}, \mathbf{x}'). \quad (6.55)$$

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

$$k(\mathbf{x}, \mathbf{x}') = k_1(\phi(\mathbf{x}), \phi(\mathbf{x}')), \quad (6.56)$$

where k_1 is a valid kernel. Therefore, k is a valid kernel.

(b)

Let

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{A} \mathbf{x}', \quad (6.57)$$

where \mathbf{A} is a symmetric positive semidefinite matrix. Then, there exists \mathbf{M} such that

$$\mathbf{A} = \mathbf{M}^\top \mathbf{M}. \quad (6.58)$$

Then,

$$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^\top \phi(\mathbf{x}'), \quad (6.59)$$

where

$$\phi(\mathbf{x}) = \mathbf{M}\mathbf{x}. \quad (6.60)$$

Therefore, k is a valid kernel.

6.9

Let

$$\begin{aligned} k_a(\mathbf{x}_a, \mathbf{x}'_a) &= \phi_a(\mathbf{x}_a)^\top \phi_a(\mathbf{x}'_a), \\ k_b(\mathbf{x}_b, \mathbf{x}'_b) &= \phi_b(\mathbf{x}_b)^\top \phi_b(\mathbf{x}'_b). \end{aligned} \quad (6.61)$$

(a)

Let

$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b), \quad (6.62)$$

where

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix}. \quad (6.63)$$

The right hand side can be written as

$$\phi_a(\mathbf{x}_a)^\top \phi_a(\mathbf{x}'_a) + \phi_b(\mathbf{x}_b)^\top \phi_b(\mathbf{x}'_b) = \phi(\mathbf{x})^\top \phi(\mathbf{x}'), \quad (6.64)$$

where

$$\phi(\mathbf{x}) = \begin{bmatrix} \phi_a(\mathbf{x}_a) \\ \phi_b(\mathbf{x}_b) \end{bmatrix}. \quad (6.65)$$

Therefore, k is a valid kernel.

(b)

Let

$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a)k_b(\mathbf{x}_b, \mathbf{x}'_b), \quad (6.66)$$

where

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix}. \quad (6.67)$$

Then,

$$\ln k(\mathbf{x}, \mathbf{x}') = \ln k_a(\mathbf{x}_a, \mathbf{x}'_a) + \ln k_b(\mathbf{x}_b, \mathbf{x}'_b). \quad (6.68)$$

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

$$k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x})f(\mathbf{x}'). \quad (6.69)$$

6.11

Let

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right). \quad (6.70)$$

The right hand side can be written as

$$\exp\left(-\frac{\mathbf{x}^\top \mathbf{x}}{2\sigma^2}\right) \exp\left(\frac{\mathbf{x}^\top \mathbf{x}'}{\sigma^2}\right) \exp\left(-\frac{\mathbf{x}'^\top \mathbf{x}'}{2\sigma^2}\right). \quad (6.71)$$

We have

$$\exp\left(\frac{\mathbf{x}^\top \mathbf{x}'}{\sigma^2}\right) = \sum_{j=0}^{\infty} q_j(\mathbf{x}, \mathbf{x}'), \quad (6.72)$$

where

$$q_j(\mathbf{x}, \mathbf{x}') = \frac{1}{j!} \left(\frac{\mathbf{x}^\top \mathbf{x}'}{\sigma^2} \right)^j. \quad (6.73)$$

By 6.6(a), q_j is a valid kernel. Then, there exists ψ_j such that

$$q_j(\mathbf{x}, \mathbf{x}') = \psi_j(\mathbf{x})^\top \psi_j(\mathbf{x}'). \quad (6.74)$$

Then,

$$\exp \left(\frac{\mathbf{x}^\top \mathbf{x}'}{\sigma^2} \right) = \sum_{j=0}^{\infty} \psi_j(\mathbf{x})^\top \psi_j(\mathbf{x}'). \quad (6.75)$$

The right hand side can be written as $\phi(\mathbf{x})^\top \phi(\mathbf{x}')$, where

$$\phi = \begin{bmatrix} \psi_0 \\ \vdots \\ \psi_j \\ \vdots \end{bmatrix}. \quad (6.76)$$

Therefore, k can be written as the inner product of an infinite-dimensional feature vector.

6.12

Let D be a set. Let $A_1, \dots, A_{2^{|D|}}$ be all the subsets of D where $|.|$ is the number of elements in (.). Let

$$k(A_m, A_{m'}) = 2^{|A_m \cap A_{m'}|}. \quad (6.77)$$

Let ϕ be a vector such that

$$\phi_m(A) = \begin{cases} 1, & \text{if } A_m \subseteq A, \\ 0, & \text{otherwise.} \end{cases} \quad (6.78)$$

If

$$|A_m \cap A_{m'}| = 0, \quad (6.79)$$

then

$$k(A_m, A_{m'}) = 1. \quad (6.80)$$

The right hand side can be written as

$$\phi(A_m)^\top \phi(A_{m'}). \quad (6.81)$$

Let us assume that if

$$|A_m \cap A_{m'}| = n, \quad (6.82)$$

then

$$k(A_m, A_{m'}) = \phi(A_m)^\top \phi(A_{m'}). \quad (6.83)$$

Let

$$A_{m''} = A_{m'} \cup \{x\}, \quad (6.84)$$

where x is an element such that

$$x \in A_m - A_{m'}. \quad (6.85)$$

Then,

$$|A_m \cap A_{m''}| = n + 1, \quad (6.86)$$

so that

$$k(A_m, A_{m''}) = 2^{n+1}. \quad (6.87)$$

We have

$$\phi(A_m)^\top \phi(A_{m''}) = \phi(A_m)^\top \phi(A_{m'}) + \phi(A_m)^\top (\phi(A_{m''}) - \phi(A_{m'})). \quad (6.88)$$

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,

$$\phi(A_m)^\top \phi(A_{m''}) = 2^{n+1}, \quad (6.89)$$

so that

$$k(A_m, A_{m''}) = \phi(A_m)^\top \phi(A_{m''}). \quad (6.90)$$

Therefore, the assumption is proved by induction on n .

6.13

Let

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^\top \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}'), \quad (6.91)$$

where

$$\begin{aligned} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) &= \nabla_{\boldsymbol{\theta}} \ln p(\mathbf{x} | \boldsymbol{\theta}), \\ \mathbf{F} &= \mathbb{E}_{\mathbf{x}} (\mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^\top). \end{aligned} \quad (6.92)$$

Let ψ be an invertible and differentiable function of $\boldsymbol{\theta}$. Let

$$k_\psi(\mathbf{x}, \mathbf{x}') = \mathbf{g}_\psi(\boldsymbol{\theta}, \mathbf{x})^\top \mathbf{F}_\psi^{-1} \mathbf{g}_\psi(\boldsymbol{\theta}, \mathbf{x}'), \quad (6.93)$$

where

$$\begin{aligned} \mathbf{g}_\psi(\boldsymbol{\theta}, \mathbf{x}) &= \nabla_{\psi} \ln p(\mathbf{x} | \boldsymbol{\theta}), \\ \mathbf{F}_\psi &= \mathbb{E}_{\mathbf{x}} (\mathbf{g}_\psi(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}_\psi(\boldsymbol{\theta}, \mathbf{x})^\top). \end{aligned} \quad (6.94)$$

We have

$$\mathbf{g}_\psi(\boldsymbol{\theta}, \mathbf{x}) = \frac{\partial \boldsymbol{\theta}}{\partial \psi} \nabla_{\boldsymbol{\theta}} \ln p(\mathbf{x} | \boldsymbol{\theta}). \quad (6.95)$$

Then,

$$\mathbf{g}_\psi(\boldsymbol{\theta}, \mathbf{x}) = \left(\frac{\partial \psi}{\partial \boldsymbol{\theta}} \right)^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}). \quad (6.96)$$

We have

$$\mathbf{F}_\psi = \int \mathbf{g}_\psi(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}_\psi(\boldsymbol{\theta}, \mathbf{x})^\top p(\mathbf{x}) d\mathbf{x}. \quad (6.97)$$

The right hand side can be written as

$$\begin{aligned} &\int \left(\frac{\partial \psi}{\partial \boldsymbol{\theta}} \right)^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^\top \left(\left(\frac{\partial \psi}{\partial \boldsymbol{\theta}} \right)^{-1} \right)^\top p(\mathbf{x}) d\mathbf{x} \\ &= \left(\frac{\partial \psi}{\partial \boldsymbol{\theta}} \right)^{-1} \left(\int \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}) \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^\top p(\mathbf{x}) d\mathbf{x} \right) \left(\left(\frac{\partial \psi}{\partial \boldsymbol{\theta}} \right)^{-1} \right)^\top. \end{aligned} \quad (6.98)$$

Then,

$$\mathbf{F}_\psi = \left(\frac{\partial \psi}{\partial \boldsymbol{\theta}} \right)^{-1} \mathbf{F} \left(\left(\frac{\partial \psi}{\partial \boldsymbol{\theta}} \right)^{-1} \right)^\top. \quad (6.99)$$

Then,

$$\begin{aligned} &k_\psi(\mathbf{x}, \mathbf{x}') \\ &= \mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^\top \left(\left(\frac{\partial \psi}{\partial \boldsymbol{\theta}} \right)^{-1} \right)^\top \left(\frac{\partial \psi}{\partial \boldsymbol{\theta}} \right)^\top \mathbf{F}^{-1} \left(\frac{\partial \psi}{\partial \boldsymbol{\theta}} \right) \left(\frac{\partial \psi}{\partial \boldsymbol{\theta}} \right)^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}'). \end{aligned} \quad (6.100)$$

The right hand side can be written as

$$\mathbf{g}(\boldsymbol{\theta}, \mathbf{x})^\top \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\theta}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}'). \quad (6.101)$$

Therefore,

$$k_{\psi}(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}'). \quad (6.102)$$

6.14

Let \mathbf{x} be a variable such that

$$p(\mathbf{x}|\boldsymbol{\mu}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{S}). \quad (6.103)$$

Let

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{g}(\boldsymbol{\mu}, \mathbf{x})^\top \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\mu}, \mathbf{x}'), \quad (6.104)$$

where

$$\begin{aligned} \mathbf{g}(\boldsymbol{\mu}, \mathbf{x}) &= \nabla_{\boldsymbol{\mu}} \ln p(\mathbf{x}|\boldsymbol{\mu}), \\ \mathbf{F} &= \mathbb{E}_{\mathbf{x}} (\mathbf{g}(\boldsymbol{\mu}, \mathbf{x}) \mathbf{g}(\boldsymbol{\mu}, \mathbf{x})^\top). \end{aligned} \quad (6.105)$$

We have

$$\mathbf{g}(\boldsymbol{\mu}, \mathbf{x}) = -\mathbf{S}^{-1}(\mathbf{x} - \boldsymbol{\mu}). \quad (6.106)$$

Then,

$$\mathbf{F} = \int \mathbf{S}^{-1}(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{S}^{-1} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{S}) d\mathbf{x}. \quad (6.107)$$

The right hand side can be written as

$$\mathbf{S}^{-1} \left(\int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{S}) d\mathbf{x} \right) \mathbf{S}^{-1} = \mathbf{S}^{-1}. \quad (6.108)$$

Then,

$$\mathbf{F} = \mathbf{S}^{-1}, \quad (6.109)$$

so that

$$\mathbf{g}(\boldsymbol{\mu}, \mathbf{x})^\top \mathbf{F}^{-1} \mathbf{g}(\boldsymbol{\mu}, \mathbf{x}') = (\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{S}^{-1} (\mathbf{x} - \boldsymbol{\mu}). \quad (6.110)$$

Therefore,

$$k(\mathbf{x}, \mathbf{x}') = (\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{S}^{-1} (\mathbf{x} - \boldsymbol{\mu}). \quad (6.111)$$

6.15

Let k be a positive definite kernel function. Then,

$$\sum_{n=1}^N \sum_{n'=1}^N c_n c_{n'} k(x_n, x_{n'}) > 0. \quad (6.112)$$

Then,

$$\mathbf{c}^\top \mathbf{K} \mathbf{c} \geq 0, \quad (6.113)$$

where

$$\mathbf{c} = \begin{bmatrix} c \\ c' \end{bmatrix}, \mathbf{K} = \begin{bmatrix} k(x, x) & k(x, x') \\ k(x, x') & k(x', x') \end{bmatrix}. \quad (6.114)$$

Then,

$$\det \mathbf{K} \geq 0. \quad (6.115)$$

Therefore,

$$k(x, x')^2 \leq k(x, x)k(x', x'). \quad (6.116)$$

6.16

Let

$$J(\mathbf{w}) = f(\mathbf{w}^\top \phi(\mathbf{x}_1), \dots, \mathbf{w}^\top \phi(\mathbf{x}_N)) + g(\|\mathbf{w}\|^2), \quad (6.117)$$

where g is a monotonically increasing function. Setting the derivative with respect to \mathbf{w} to zero gives

$$\mathbf{0} = \sum_{n=1}^N (\nabla_n f) \phi(\mathbf{x}_n) + 2g'(\|\mathbf{w}\|^2) \mathbf{w}, \quad (6.118)$$

where ∇_n is the partial derivative with respect to the n th argument. Then,

$$\mathbf{w} = -\frac{1}{2g'(\|\mathbf{w}\|^2)} \sum_{n=1}^N (\nabla_n f) \phi(\mathbf{x}_n). \quad (6.119)$$

Therefore, J is minimised by \mathbf{w} in the form of a linear combination of $\phi(\mathbf{x}_1), \dots, \phi(\mathbf{x}_N)$.

6.17

Let

$$E_{\xi} = \frac{1}{2} \sum_{n=1}^N \int (y(\mathbf{x}_n + \boldsymbol{\xi}) - t_n)^2 p(\boldsymbol{\xi}) d\boldsymbol{\xi}. \quad (6.120)$$

By the transformation

$$\mathbf{z}_n = \mathbf{x}_n + \boldsymbol{\xi}, \quad (6.121)$$

we have

$$E = \frac{1}{2} \sum_{n=1}^N \int (y(\mathbf{z}_n) - t_n)^2 p(\mathbf{z}_n - \mathbf{x}_n) d\mathbf{z}_n. \quad (6.122)$$

Setting the variation with respect to y to zero gives

$$0 = \sum_{n=1}^N \int (y(\mathbf{z}_n) - t_n) p(\mathbf{z}_n - \mathbf{x}_n) \delta y(\mathbf{z}_n) d\mathbf{z}_n. \quad (6.123)$$

Then,

$$\sum_{n=1}^N (y(\mathbf{z}_n) - t_n) p(\mathbf{z}_n - \mathbf{x}_n) = 0, \quad (6.124)$$

so that

$$\sum_{n=1}^N y(\mathbf{z}_n) p(\mathbf{z}_n - \mathbf{x}_n) = \sum_{n=1}^N t_n p(\mathbf{z}_n - \mathbf{x}_n). \quad (6.125)$$

Therefore,

$$y(\mathbf{x}) = \sum_{n=1}^N t_n k(\mathbf{x}, \mathbf{x}_n), \quad (6.126)$$

where

$$k(\mathbf{x}, \mathbf{x}_n) = \frac{p(\mathbf{x} - \mathbf{x}_n)}{\sum_{n=1}^N p(\mathbf{x} - \mathbf{x}_n)}. \quad (6.127)$$

6.18

Let x be a variable such that

$$p(x, t) = \frac{1}{N} \sum_{n=1}^N f(x - x_n, t - t_n), \quad (6.128)$$

where

$$f(x, t) = \mathcal{N}(x|0, \sigma^2) \mathcal{N}(t|0, \sigma^2). \quad (6.129)$$

(a)

By the Bayes' theorem,

$$p(t|x) = \frac{p(x,t)}{p(x)}. \quad (6.130)$$

By marginalisation,

$$p(x) = \int p(x,t)dt. \quad (6.131)$$

The right hand side can be written as

$$\begin{aligned} & \frac{1}{N} \sum_{n=1}^N \mathcal{N}(x - x_n | 0, \sigma^2) \int \mathcal{N}(t - t_n | 0, \sigma^2) dt \\ &= \frac{1}{N} \sum_{n=1}^N \mathcal{N}(x - x_n | 0, \sigma^2). \end{aligned} \quad (6.132)$$

Then,

$$p(t|x) = \frac{\sum_{n=1}^N \mathcal{N}(x - x_n | 0, \sigma^2) \mathcal{N}(t - t_n | 0, \sigma^2)}{\sum_{n=1}^N \mathcal{N}(x - x_n | 0, \sigma^2)}. \quad (6.133)$$

Therefore,

$$p(t|x) = \sum_{n=1}^N k(x, x_n) \mathcal{N}(t - t_n | 0, \sigma^2), \quad (6.134)$$

where

$$k(x, x_n) = \frac{\mathcal{N}(x - x_n | 0, \sigma^2)}{\sum_{n=1}^N \mathcal{N}(x - x_n | 0, \sigma^2)}. \quad (6.135)$$

(b)

We have

$$\mathbb{E}(t|x) = \int tp(t|x)dt. \quad (6.136)$$

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

$$\sum_{n=1}^N k(x, x_n) \int t \mathcal{N}(t - t_n | 0, \sigma^2) dt. \quad (6.137)$$

By the transformation

$$t' = t - t_n, \quad (6.138)$$

the integral can be written as

$$\int (t' + t_n) \mathcal{N}(t'|0, \sigma^2) dt' = \int t' \mathcal{N}(t'|0, \sigma^2) dt' + t_n \int \mathcal{N}(t'|0, \sigma^2) dt'. \quad (6.139)$$

The right hand side can be written as t_n . Therefore,

$$E(t|x) = \sum_{n=1}^N k(x, x_n) t_n. \quad (6.140)$$

(c)

We have

$$\text{var}(t|x) = \int (t - E(t|x))^2 p(t|x) dt. \quad (6.141)$$

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

$$\sum_{n=1}^N k(x, x_n) \int \left(t - \sum_{n=1}^N k(x, x_n) t_n \right)^2 \mathcal{N}(t - t_n|0, \sigma^2) dt. \quad (6.142)$$

By the transformation

$$t' = t - t_n, \quad (6.143)$$

the integral can be written as

$$\begin{aligned} & \int \left(t' + t_n - \sum_{n=1}^N k(x, x_n) t_n \right)^2 \mathcal{N}(t'|0, \sigma^2) dt' \\ &= \int t'^2 \mathcal{N}(t'|0, \sigma^2) dt' + 2 \left(t_n - \sum_{n=1}^N k(x, x_n) t_n \right) \int t' \mathcal{N}(t'|0, \sigma^2) dt' \quad (6.144) \\ &+ \left(t_n - \sum_{n=1}^N k(x, x_n) t_n \right)^2 \int \mathcal{N}(t'|0, \sigma^2) dt'. \end{aligned}$$

The right hand side can be written as

$$\sigma^2 + \left(t_n - \sum_{n=1}^N k(x, x_n) t_n \right)^2. \quad (6.145)$$

Therefore,

$$\text{var}(t|x) = \sum_{n=1}^N k(x, x_n) \left(\sigma^2 + \left(t_n - \sum_{n'=1}^N k(x, x_{n'}) t_{n'} \right)^2 \right), \quad (6.146)$$

so that

$$\text{var}(t|x) = \sigma^2 + \sum_{n=1}^N k(x, x_n) \left(t_n - \sum_{n'=1}^N k(x, x_{n'}) t_{n'} \right)^2. \quad (6.147)$$

6.19

Let

$$E = \frac{1}{2} \sum_{n=1}^N \int (y(\mathbf{x}_n - \boldsymbol{\xi}_n) - t_n)^2 p(\boldsymbol{\xi}_n) d\boldsymbol{\xi}_n. \quad (6.148)$$

By the transformation

$$\mathbf{z}_n = \mathbf{x}_n - \boldsymbol{\xi}_n, \quad (6.149)$$

we have

$$E = \frac{1}{2} \sum_{n=1}^N \int (y(\mathbf{z}_n) - t_n)^2 p(\mathbf{x}_n - \mathbf{z}_n) d\mathbf{z}_n. \quad (6.150)$$

Setting the variation with respect to y to zero gives

$$0 = \sum_{n=1}^N \int (y(\mathbf{z}_n) - t_n) p(\mathbf{x}_n - \mathbf{z}_n) \delta y(\mathbf{z}_n) d\mathbf{z}_n. \quad (6.151)$$

Then,

$$0 = \sum_{n=1}^N (y(\mathbf{z}_n) - t_n) p(\mathbf{x}_n - \mathbf{z}_n), \quad (6.152)$$

so that

$$\sum_{n=1}^N y(\mathbf{z}_n) p(\mathbf{x}_n - \mathbf{z}_n) = \sum_{n=1}^N t_n p(\mathbf{x}_n - \mathbf{z}_n). \quad (6.153)$$

Therefore,

$$y(\mathbf{x}) = \sum_{n=1}^N t_n k(\mathbf{x}, \mathbf{x}_n), \quad (6.154)$$

where

$$k(\mathbf{x}, \mathbf{x}_n) = \frac{p(\mathbf{x}_n - \mathbf{x})}{\sum_{n=1}^N p(\mathbf{x}_n - \mathbf{x})}. \quad (6.155)$$

6.20

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(\mathbf{t}|\mathbf{y}) &= \mathcal{N}(\mathbf{t}|\mathbf{y}, \beta^{-1}\mathbf{I}), \\ p(\mathbf{y}) &= \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}), \end{aligned} \quad (6.156)$$

where

$$K_{nn'} = k(\mathbf{x}_n, \mathbf{x}_{n'}). \quad (6.157)$$

By the Bayes' theorem,

$$p(t_{N+1}|\mathbf{t})p(\mathbf{t}) = p(\mathbf{t}'), \quad (6.158)$$

where

$$\mathbf{t}' = \begin{bmatrix} \mathbf{t} \\ t_{N+1} \end{bmatrix}. \quad (6.159)$$

By marginalisation,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{y})p(\mathbf{y})d\mathbf{y}. \quad (6.160)$$

The logarithm of the integrand of the right hand side except the terms independent of \mathbf{y}_N can be written as

$$-\frac{\beta}{2}(\mathbf{t} - \mathbf{y})^\top(\mathbf{t} - \mathbf{y}) - \frac{1}{2}\mathbf{y}^\top\mathbf{K}^{-1}\mathbf{y} = -\frac{1}{2}\mathbf{v}^\top\mathbf{M}\mathbf{v}, \quad (6.161)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{y} \\ \mathbf{t} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \beta\mathbf{I} + \mathbf{K}^{-1} & -\beta\mathbf{I} \\ -\beta\mathbf{I} & \beta\mathbf{I} \end{bmatrix}. \quad (6.162)$$

By 2.24,

$$\begin{bmatrix} \beta\mathbf{I} + \mathbf{K}^{-1} & -\beta\mathbf{I} \\ -\beta\mathbf{I} & \beta\mathbf{I} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K} + \beta^{-1}\mathbf{I} \end{bmatrix}. \quad (6.163)$$

Then,

$$p(\mathbf{t}) = \mathcal{N}(\mathbf{t}|\mathbf{0}, \mathbf{C}), \quad (6.164)$$

where

$$\mathbf{C} = \mathbf{K} + \beta^{-1}\mathbf{I}. \quad (6.165)$$

Then,

$$p(\mathbf{t}') = \mathcal{N}(\mathbf{t}'|\mathbf{0}, \mathbf{C}'), \quad (6.166)$$

where

$$\mathbf{C}' = \begin{bmatrix} \mathbf{C} & \mathbf{k} \\ \mathbf{k}^\top & c \end{bmatrix}, \quad (6.167)$$

where

$$\begin{aligned} k_n &= k(\mathbf{x}_n, \mathbf{x}_{N+1}), \\ c &= k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}) + \beta^{-1}. \end{aligned} \quad (6.168)$$

By 2.24,

$$\begin{bmatrix} c & \mathbf{k}^\top \\ \mathbf{k} & \mathbf{C} \end{bmatrix}^{-1} = \begin{bmatrix} s^{-1} & -s^{-1}\mathbf{k}^\top\mathbf{C}^{-1} \\ -s^{-1}\mathbf{C}^{-1}\mathbf{k} & \mathbf{C}^{-1} + s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^\top\mathbf{C}^{-1} \end{bmatrix}, \quad (6.169)$$

where

$$s = c - \mathbf{k}^\top\mathbf{C}^{-1}\mathbf{k}. \quad (6.170)$$

Therefore,

$$p(t_{N+1}|\mathbf{t}) = \mathcal{N}(t_{N+1}|m, s), \quad (6.171)$$

where

$$m = \mathbf{k}^\top\mathbf{C}^{-1}\mathbf{t}. \quad (6.172)$$

6.21

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}(t_n|\mathbf{w}^\top\boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{0}, \mathbf{I}). \end{aligned} \quad (6.173)$$

Then,

$$\begin{aligned} p(\mathbf{t}|\mathbf{y}) &= \mathcal{N}(\mathbf{t}|\mathbf{y}, \beta^{-1}\mathbf{I}), \\ p(\mathbf{y}) &= \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}), \end{aligned} \quad (6.174)$$

where

$$\mathbf{K} = \mathbf{\Phi}\mathbf{\Phi}^\top. \quad (6.175)$$

By 6.20,

$$p(t_{N+1}|\mathbf{t}) = \mathcal{N}(t_{N+1}|m, s), \quad (6.176)$$

where

$$\begin{aligned} m &= \mathbf{k}^\top\mathbf{C}^{-1}\mathbf{t}, \\ s &= c - \mathbf{k}^\top\mathbf{C}^{-1}\mathbf{k}, \end{aligned} \quad (6.177)$$

where

$$\begin{aligned}\mathbf{k} &= \Phi\phi_{N+1}, \\ \mathbf{C} &= \mathbf{K} + \beta^{-1}\mathbf{I}, \\ c &= \phi_{N+1}^\top \phi_{N+1} + \beta^{-1}.\end{aligned}\tag{6.178}$$

By 2.26,

$$\mathbf{C}^{-1} = \beta\mathbf{I} - \beta^2\Phi\mathbf{S}\Phi^\top,\tag{6.179}$$

where

$$\mathbf{S} = (\mathbf{I} + \beta\Phi^\top\Phi)^{-1}.\tag{6.180}$$

Then,

$$\begin{aligned}m &= \phi_{N+1}^\top \Phi^\top (\beta\mathbf{I} - \beta^2\Phi\mathbf{S}\Phi^\top) \mathbf{t}, \\ s &= \beta^{-1} + \phi_{N+1}^\top \phi_{N+1} - \phi_{N+1}^\top \Phi^\top (\beta\mathbf{I} - \beta^2\Phi\mathbf{S}\Phi^\top) \Phi\phi_{N+1}.\end{aligned}\tag{6.181}$$

We have

$$\beta\Phi^\top\Phi = \mathbf{S}^{-1} - \mathbf{I}.\tag{6.182}$$

Then,

$$\begin{aligned}m &= \beta\phi_{N+1}^\top (\mathbf{I} - (\mathbf{S}^{-1} - \mathbf{I})\mathbf{S}) \Phi^\top \mathbf{t}, \\ s &= \beta^{-1} + \phi_{N+1}^\top (\mathbf{I} - (\mathbf{S}^{-1} - \mathbf{I}) + (\mathbf{S}^{-1} - \mathbf{I})\mathbf{S}(\mathbf{S}^{-1} - \mathbf{I})) \phi_{N+1}.\end{aligned}\tag{6.183}$$

Therefore,

$$\begin{aligned}m &= \beta\phi_{N+1}^\top \mathbf{S}\Phi^\top \mathbf{t}, \\ s &= \beta^{-1} + \phi_{N+1}^\top \mathbf{S}\phi_{N+1}.\end{aligned}\tag{6.184}$$

6.22

Let t_1, \dots, t_N be variables such that

$$\begin{aligned}p(\mathbf{t}|\mathbf{y}) &= \mathcal{N}(\mathbf{t}|\mathbf{y}, \beta^{-1}\mathbf{I}), \\ p(\mathbf{y}) &= \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}),\end{aligned}\tag{6.185}$$

where

$$K_{nn'} = k(\mathbf{x}_n, \mathbf{x}_{n'}).\tag{6.186}$$

(a)

By the Bayes' theorem,

$$p(t_{N+1}, \dots, t_{N+L} | \mathbf{t}) p(\mathbf{t}) = p(\mathbf{t}'), \quad (6.187)$$

where

$$\mathbf{t}' = \begin{bmatrix} \mathbf{t} \\ t_{N+1} \\ \vdots \\ t_{N+L} \end{bmatrix}. \quad (6.188)$$

By 6.20,

$$p(\mathbf{t}) = \mathcal{N}(\mathbf{t} | \mathbf{0}, \mathbf{C}), \quad (6.189)$$

where

$$\mathbf{C} = \beta^{-1} \mathbf{I} + \mathbf{K}. \quad (6.190)$$

Let \mathbf{K}' and $\mathbf{\Gamma}$ be matrices where

$$\begin{aligned} K'_{nl} &= k(\mathbf{x}_n, \mathbf{x}_{N+l}), \\ \Gamma_{ll'} &= \beta^{-1} I_{ll'} + k(\mathbf{x}_{N+l}, \mathbf{x}_{N+l'}). \end{aligned} \quad (6.191)$$

Then,

$$p(\mathbf{t}') = \mathcal{N}(\mathbf{t}' | \mathbf{0}, \mathbf{C}'), \quad (6.192)$$

where

$$\mathbf{C}' = \begin{bmatrix} \mathbf{C} & \mathbf{K}' \\ \mathbf{K}'^\top & \mathbf{\Gamma} \end{bmatrix}. \quad (6.193)$$

By 2.24,

$$\begin{bmatrix} \mathbf{\Gamma} & \mathbf{K}'^\top \\ \mathbf{K}' & \mathbf{C} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{S}^{-1} & -\mathbf{S}^{-1} \mathbf{K}'^\top \mathbf{C}^{-1} \\ -\mathbf{C}^{-1} \mathbf{K}' \mathbf{S}^{-1} & \mathbf{C}^{-1} + \mathbf{C}^{-1} \mathbf{K}' \mathbf{S}^{-1} \mathbf{K}'^\top \mathbf{C}^{-1} \end{bmatrix}, \quad (6.194)$$

where

$$\mathbf{S} = \mathbf{\Gamma} - \mathbf{K}'^\top \mathbf{C}^{-1} \mathbf{K}'. \quad (6.195)$$

Therefore,

$$p(t_{N+1}, \dots, t_{N+L} | \mathbf{t}_N) = \mathcal{N}(t_{N+1}, \dots, t_{N+L} | \mathbf{m}, \mathbf{S}), \quad (6.196)$$

where

$$\mathbf{m} = \mathbf{K}'^\top \mathbf{C}^{-1} \mathbf{t}. \quad (6.197)$$

(b)

By (a),

$$p(t_{N+1}|\mathbf{t}) = \mathcal{N}(t_{N+1}|m, s), \quad (6.198)$$

where

$$\begin{aligned} m &= \mathbf{k}^\top \mathbf{C}^{-1} \mathbf{t}, \\ s &= c - \mathbf{k}^\top \mathbf{C}^{-1} \mathbf{k}, \end{aligned} \quad (6.199)$$

and

$$\begin{aligned} k_n &= k(\mathbf{x}_n, \mathbf{x}_{N+1}), \\ c &= \beta^{-1} + k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}). \end{aligned} \quad (6.200)$$

6.23

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

$$\begin{aligned} p(\mathbf{t}_n | \mathbf{y}_n) &= \mathcal{N}(\mathbf{t}_n | \mathbf{y}_n, \beta^{-1} \mathbf{I}), \\ p(\mathbf{Y}) &= \mathcal{N}(\mathbf{Y} | \mathbf{O}, \mathbf{K}), \end{aligned} \quad (6.201)$$

where

$$K_{nn'} = k(\mathbf{x}_n, \mathbf{x}_{n'}). \quad (6.202)$$

By the Bayes' theorem,

$$p(\mathbf{t}_{N+1} | \mathbf{T}) p(\mathbf{T}) = p(\mathbf{T}'). \quad (6.203)$$

By marginalisation,

$$p(\mathbf{T}) = \int p(\mathbf{T} | \mathbf{Y}) p(\mathbf{Y}) d\mathbf{Y}. \quad (6.204)$$

The logarithm of the integrand of the right hand side except the terms independent of \mathbf{T} and \mathbf{Y} can be written as

$$-\frac{\beta}{2} \sum_{n=1}^N \|\mathbf{t}_n - \mathbf{y}_n\|^2 - \frac{1}{2} \text{tr}(\mathbf{Y}^\top \mathbf{K}^{-1} \mathbf{Y}) = -\frac{1}{2} \text{tr} \mathbf{M}, \quad (6.205)$$

where

$$\mathbf{M} = \begin{bmatrix} \mathbf{Y} \\ \mathbf{T} \end{bmatrix}^\top \begin{bmatrix} \beta \mathbf{I} + \mathbf{K}^{-1} & -\beta \mathbf{I} \\ -\beta \mathbf{I} & \beta \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{Y} \\ \mathbf{T} \end{bmatrix}. \quad (6.206)$$

By 2.24,

$$\begin{bmatrix} \beta \mathbf{I} + \mathbf{K}^{-1} & -\beta \mathbf{I} \\ -\beta \mathbf{I} & \beta \mathbf{I} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \beta^{-1} \mathbf{I} + \mathbf{K} \end{bmatrix}. \quad (6.207)$$

Then,

$$p(\mathbf{T}) = \mathcal{N}(\mathbf{T} | \mathbf{O}, \mathbf{C}), \quad (6.208)$$

where

$$\mathbf{C} = \beta^{-1}\mathbf{I} + \mathbf{K}. \quad (6.209)$$

Then,

$$p(\mathbf{T}') = \mathcal{N}(\mathbf{T}' | \mathbf{O}, \mathbf{C}'), \quad (6.210)$$

where

$$\mathbf{C}' = \begin{bmatrix} \mathbf{C} & \mathbf{k} \\ \mathbf{k}^\top & c \end{bmatrix}, \quad (6.211)$$

and

$$\begin{aligned} k_n &= k(\mathbf{x}_n, \mathbf{x}_{N+1}), \\ c &= \beta^{-1} + k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}). \end{aligned} \quad (6.212)$$

By 2.24,

$$\begin{bmatrix} c & \mathbf{k}^\top \\ \mathbf{k} & \mathbf{C} \end{bmatrix}^{-1} = \begin{bmatrix} s^{-1} & -s^{-1}\mathbf{k}^\top\mathbf{C}^{-1} \\ -s^{-1}\mathbf{C}^{-1}\mathbf{k} & \mathbf{C}^{-1} + s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^\top\mathbf{C}^{-1} \end{bmatrix}, \quad (6.213)$$

where

$$s = c - \mathbf{k}^\top\mathbf{C}^{-1}\mathbf{k}. \quad (6.214)$$

Therefore,

$$p(\mathbf{t}_{N+1} | \mathbf{T}) = \mathcal{N}(\mathbf{t}_{N+1} | \mathbf{m}, s\mathbf{I}), \quad (6.215)$$

where

$$\mathbf{m} = \mathbf{T}^\top\mathbf{C}^{-1}\mathbf{k}. \quad (6.216)$$

6.24

(a)

Let \mathbf{M} be a $D \times D$ diagonal matrix such that $0 < M_{dd} < 1$. For any vector \mathbf{v} in D dimensions,

$$\mathbf{v}^\top \mathbf{M} \mathbf{v} = \sum_{d=1}^D \sum_{d'=1}^D v_d M_{dd'} v_{d'}. \quad (6.217)$$

The right hand side can be written as

$$\sum_{d=1}^D M_{dd} v_d^2 > 0. \quad (6.218)$$

Therefore, \mathbf{M} is positive definite.

(b)

Let \mathbf{M}_1 and \mathbf{M}_2 be $D \times D$ positive definite matrices. Then, for any vector \mathbf{v} in D dimensions,

$$\begin{aligned}\mathbf{v}^\top \mathbf{M}_1 \mathbf{v} &> 0, \\ \mathbf{v}^\top \mathbf{M}_2 \mathbf{v} &> 0.\end{aligned}\tag{6.219}$$

Then,

$$\mathbf{v}^\top (\mathbf{M}_1 + \mathbf{M}_2) \mathbf{v} > 0.\tag{6.220}$$

Therefore, $\mathbf{M}_1 + \mathbf{M}_2$ is positive definite.

6.25

Let t_1, \dots, t_N be variables such that

$$\begin{aligned}p(t_n | a_n) &= \sigma(a_n)^{t_n} (1 - \sigma(a_n))^{1-t_n}, \\ p(\mathbf{a}) &= \mathcal{N}(\mathbf{a} | \mathbf{0}, \mathbf{C}),\end{aligned}\tag{6.221}$$

where

$$\begin{aligned}\sigma(a) &= \frac{1}{1 + \exp(-a)}, \\ C_{nn'} &= k(\mathbf{x}_n, \mathbf{x}_{n'}) + \nu I_{nn'}.\end{aligned}\tag{6.222}$$

(a)

By the Bayes' theorem,

$$p(\mathbf{a} | \mathbf{t}) p(\mathbf{t}) = p(\mathbf{t} | \mathbf{a}) p(\mathbf{a}).\tag{6.223}$$

The logarithm of the right hand side except the terms independent of \mathbf{t} and \mathbf{a} can be written as

$$\Psi(\mathbf{a}) = \sum_{n=1}^N (t_n \ln \sigma(a_n) + (1 - t_n) \ln (1 - \sigma(a_n))) - \frac{1}{2} \mathbf{a}^\top \mathbf{C}^{-1} \mathbf{a}.\tag{6.224}$$

In order to maximise $p(\mathbf{a} | \mathbf{t})$ with respect to \mathbf{a} , Ψ needs to be maximised. We have

$$\frac{d}{da} \sigma(a) = \sigma(a) (1 - \sigma(a)).\tag{6.225}$$

Then,

$$(\nabla \Psi(\mathbf{a}))_n = (t_n(1 - \sigma(a_n)) - (1 - t_n)\sigma(a_n)) - (\mathbf{C}^{-1}\mathbf{a})_n, \quad (6.226)$$

so that

$$\nabla \Psi(\mathbf{a}) = \mathbf{t} - \boldsymbol{\sigma} - \mathbf{C}^{-1}\mathbf{a}, \quad (6.227)$$

where

$$\sigma_n = \sigma(a_n). \quad (6.228)$$

Since $\boldsymbol{\sigma}$ non-linearly depends on \mathbf{a} , the Taylor series

$$\nabla \Psi(\mathbf{a}^{\text{new}}) = \nabla \Psi(\mathbf{a}) + \nabla \nabla \Psi(\mathbf{a}) (\mathbf{a}^{\text{new}} - \mathbf{a}) + O(\|\mathbf{a} - \mathbf{a}^{\text{new}}\|^2). \quad (6.229)$$

is used to iteratively find \mathbf{a} which maximises Ψ . Setting the left hand side to zero and omitting the second order term of the right hand side gives

$$\mathbf{0} = \nabla \Psi(\mathbf{a}) + \nabla \nabla \Psi(\mathbf{a}) (\mathbf{a}^{\text{new}} - \mathbf{a}). \quad (6.230)$$

Then,

$$\mathbf{a}^{\text{new}} = \mathbf{a} - (\nabla \nabla \Psi(\mathbf{a}))^{-1} \nabla \Psi(\mathbf{a}). \quad (6.231)$$

We have

$$\nabla \nabla \Psi(\mathbf{a}) = -\mathbf{W} - \mathbf{C}^{-1}, \quad (6.232)$$

where

$$W_{nn'} = \sigma(a_n)(1 - \sigma(a_n)) I_{nn'}. \quad (6.233)$$

Then,

$$\mathbf{a}^{\text{new}} = \mathbf{a} + (\mathbf{W} + \mathbf{C}^{-1})^{-1} (\mathbf{t} - \boldsymbol{\sigma} - \mathbf{C}^{-1}\mathbf{a}). \quad (6.234)$$

The right hand side can be written as

$$\begin{aligned} & (\mathbf{W} + \mathbf{C}^{-1})^{-1} ((\mathbf{W} + \mathbf{C}^{-1})\mathbf{a} + \mathbf{t} - \boldsymbol{\sigma} - \mathbf{C}^{-1}\mathbf{a}) \\ &= \mathbf{C}(\mathbf{W}\mathbf{C} + \mathbf{I})^{-1}(\mathbf{W}\mathbf{a} + \mathbf{t} - \boldsymbol{\sigma}). \end{aligned} \quad (6.235)$$

Therefore,

$$\mathbf{a}^{\text{new}} = \mathbf{C}(\mathbf{W}\mathbf{C} + \mathbf{I})^{-1}(\mathbf{W}\mathbf{a} + \mathbf{t} - \boldsymbol{\sigma}). \quad (6.236)$$

(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

$$\begin{aligned}\Psi(\mathbf{a}) &= \Psi(\mathbf{a}_{\text{MAP}}) + \nabla\Psi(\mathbf{a}_{\text{MAP}})(\mathbf{a} - \mathbf{a}_{\text{MAP}}) \\ &\quad + \frac{1}{2}(\mathbf{a} - \mathbf{a}_{\text{MAP}})^T \nabla \nabla \Psi(\mathbf{a}_{\text{MAP}})(\mathbf{a} - \mathbf{a}_{\text{MAP}}) \\ &\quad + O\left(\|\mathbf{a} - \mathbf{a}_{\text{MAP}}\|^3\right).\end{aligned}\quad (6.237)$$

Then,

$$\Psi(\mathbf{a}) \simeq \Psi(\mathbf{a}_{\text{MAP}}) - \frac{1}{2}(\mathbf{a} - \mathbf{a}_{\text{MAP}})^T \mathbf{H}(\mathbf{a} - \mathbf{a}_{\text{MAP}}), \quad (6.238)$$

where

$$\mathbf{H} = \mathbf{W} \Big|_{\mathbf{a}=\mathbf{a}_{\text{MAP}}} + \mathbf{C}^{-1}. \quad (6.239)$$

Therefore,

$$p(\mathbf{a}|\mathbf{t}) \simeq \mathcal{N}(\mathbf{a}|\mathbf{a}_{\text{MAP}}, \mathbf{H}^{-1}). \quad (6.240)$$

(c)

By (a),

$$\mathbf{a}_{\text{MAP}} = \mathbf{C}(\mathbf{W}\mathbf{C} + \mathbf{I})^{-1}(\mathbf{W}\mathbf{a}_{\text{MAP}} + \mathbf{t} - \boldsymbol{\sigma}). \quad (6.241)$$

Then,

$$(\mathbf{W}\mathbf{C} + \mathbf{I})\mathbf{C}^{-1}\mathbf{a}_{\text{MAP}} = \mathbf{W}\mathbf{a}_{\text{MAP}} + \mathbf{t} - \boldsymbol{\sigma}. \quad (6.242)$$

Therefore,

$$\mathbf{a}_{\text{MAP}} = \mathbf{C}(\mathbf{t} - \boldsymbol{\sigma}). \quad (6.243)$$

6.26

Let t_1, \dots, t_N be variables such that

$$\begin{aligned}p(t_n|a_n) &= \sigma(a_n)^{t_n} (1 - \sigma(a_n))^{1-t_n}, \\ p(\mathbf{a}) &= \mathcal{N}(\mathbf{a}|\mathbf{0}, \mathbf{C}),\end{aligned}\quad (6.244)$$

where

$$\begin{aligned}\sigma(a) &= \frac{1}{1 + \exp(-a)}, \\ C_{nn'} &= k(\mathbf{x}_n, \mathbf{x}_{n'}) + \nu I_{nn'}.\end{aligned}\quad (6.245)$$

By marginalisation,

$$p(a_{N+1}|\mathbf{t}) = \int p(a_{N+1}|\mathbf{a})p(\mathbf{a}|\mathbf{t})d\mathbf{a}. \quad (6.246)$$

We have

$$p(\mathbf{a}') = \mathcal{N}(\mathbf{a}'|\mathbf{0}, \mathbf{C}'), \quad (6.247)$$

where

$$\mathbf{a}' = \begin{bmatrix} \mathbf{a} \\ a_{N+1} \end{bmatrix}, \mathbf{C}' = \begin{bmatrix} \mathbf{C} & \mathbf{k} \\ \mathbf{k}^\top & c \end{bmatrix}, \quad (6.248)$$

and

$$\begin{aligned} k_n &= k(\mathbf{x}_n, \mathbf{x}_{N+1}), \\ c &= k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}) + \nu. \end{aligned} \quad (6.249)$$

By 2.24,

$$\begin{bmatrix} c & \mathbf{k}^\top \\ \mathbf{k} & \mathbf{C} \end{bmatrix}^{-1} = \begin{bmatrix} s^{-1} & -s^{-1}\mathbf{k}^\top \mathbf{C}^{-1} \\ -s^{-1}\mathbf{C}^{-1}\mathbf{k} & \mathbf{C}^{-1} + s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^\top \mathbf{C}^{-1} \end{bmatrix}, \quad (6.250)$$

where

$$s = c - \mathbf{k}^\top \mathbf{C}^{-1} \mathbf{k}. \quad (6.251)$$

Then,

$$p(a_{N+1}|\mathbf{a}) = \mathcal{N}(a_{N+1}|m, s), \quad (6.252)$$

where

$$m = \mathbf{k}^\top \mathbf{C}^{-1} \mathbf{a}. \quad (6.253)$$

By 6.25(b),

$$p(\mathbf{a}|\mathbf{t}) \simeq \mathcal{N}(\mathbf{a}|\mathbf{a}_{\text{MAP}}, \mathbf{H}^{-1}), \quad (6.254)$$

where \mathbf{a}_{MAP} is a stationary point of $p(\mathbf{a}|\mathbf{t})$ and

$$\begin{aligned} \mathbf{H} &= \mathbf{W} |_{\mathbf{a}=\mathbf{a}_{\text{MAP}}} + \mathbf{C}^{-1}, \\ W_{nn'} &= \sigma(a_n)(1 - \sigma(a_n)) I_{nn'}. \end{aligned} \quad (6.255)$$

Then, the logarithm of the integrand except the terms independent of \mathbf{t} and \mathbf{a} can be approximated as

$$\begin{aligned} &- \frac{1}{2s} (a_{N+1} - m)^2 - \frac{1}{2} (\mathbf{a} - \mathbf{a}_{\text{MAP}})^\top \mathbf{H} (\mathbf{a} - \mathbf{a}_{\text{MAP}}) \\ &= -\frac{1}{2} \mathbf{a}'^\top \mathbf{M} \mathbf{a}' + \mathbf{a}'^\top \mathbf{v} - \frac{1}{2} \mathbf{a}_{\text{MAP}}^\top \mathbf{H} \mathbf{a}_{\text{MAP}}. \end{aligned} \quad (6.256)$$

where

$$\mathbf{M} = \begin{bmatrix} \mathbf{H} + s^{-1}\mathbf{C}^{-1}\mathbf{k}\mathbf{k}^\top\mathbf{C}^{-1} & -s^{-1}\mathbf{C}^{-1}\mathbf{k} \\ -s^{-1}\mathbf{k}^\top\mathbf{C}^{-1} & s^{-1} \end{bmatrix}, \mathbf{v} = \begin{bmatrix} \mathbf{H}\mathbf{a}_{\text{MAP}} \\ 0 \end{bmatrix}. \quad (6.257)$$

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{H}^{-1} & \mathbf{H}^{-1}\mathbf{C}^{-1}\mathbf{k} \\ \mathbf{k}^\top\mathbf{C}^{-1}\mathbf{H}^{-1} & s + \mathbf{k}^\top\mathbf{C}^{-1}\mathbf{H}^{-1}\mathbf{C}^{-1}\mathbf{k} \end{bmatrix}, \quad (6.258)$$

so that

$$\mathbf{M}^{-1}\mathbf{v} = \begin{bmatrix} \mathbf{a}_{\text{MAP}} \\ \mathbf{k}^\top\mathbf{C}^{-1}\mathbf{a}_{\text{MAP}} \end{bmatrix}. \quad (6.259)$$

Then,

$$p(a_{N+1}|\mathbf{t}) \simeq \mathcal{N}(a_{N+1}|\mu, \sigma^2), \quad (6.260)$$

where

$$\begin{aligned} \mu &= \mathbf{k}^\top\mathbf{C}^{-1}\mathbf{a}_{\text{MAP}}, \\ \sigma^2 &= s + \mathbf{k}^\top\mathbf{C}^{-1}\mathbf{H}^{-1}\mathbf{C}^{-1}\mathbf{k}. \end{aligned} \quad (6.261)$$

By 6.25(c),

$$\mathbf{a}_{\text{MAP}} = \mathbf{C}(\mathbf{t} - \boldsymbol{\sigma}), \quad (6.262)$$

where

$$\sigma_n = \sigma(a_n). \quad (6.263)$$

Therefore,

$$\begin{aligned} \mu &= \mathbf{k}^\top(\mathbf{t} - \boldsymbol{\sigma}), \\ \sigma^2 &= c - \mathbf{k}^\top\mathbf{C}^{-1}(\mathbf{C} - \mathbf{H}^{-1})\mathbf{C}^{-1}\mathbf{k}. \end{aligned} \quad (6.264)$$

6.27 (Incomplete)

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|a_n) &= \sigma(a_n)^{t_n} (1 - \sigma(a_n))^{1-t_n}, \\ p(\mathbf{a}|\boldsymbol{\theta}) &= \mathcal{N}(\mathbf{a}|\mathbf{0}, \mathbf{C}), \end{aligned} \quad (6.265)$$

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)} \quad (6.266)$$

and \mathbf{C} is dependent on $\boldsymbol{\theta}$ with M dimensions.

(a)

By marginalisation,

$$p(\mathbf{t}|\boldsymbol{\theta}) = \int p(\mathbf{t}|\mathbf{a})p(\mathbf{a}|\boldsymbol{\theta})d\mathbf{a}. \quad (6.267)$$

Let \mathbf{a}_{MAP} be a stationary point of $p(\mathbf{a}|\mathbf{t})$ and

$$\Psi(\mathbf{a}) = \ln p(\mathbf{t}|\mathbf{a}) + \ln p(\mathbf{a}|\boldsymbol{\theta}). \quad (6.268)$$

By 6.25(b),

$$\Psi(\mathbf{a}) \simeq \Psi(\mathbf{a}_{\text{MAP}}) - \frac{1}{2} (\mathbf{a} - \mathbf{a}_{\text{MAP}})^T \mathbf{H} (\mathbf{a} - \mathbf{a}_{\text{MAP}}), \quad (6.269)$$

where

$$\begin{aligned} \mathbf{H} &= \mathbf{W} |_{\mathbf{a}=\mathbf{a}_{\text{MAP}}} + \mathbf{C}^{-1}, \\ W_{nn'} &= \sigma(a_n)(1 - \sigma(a_n)) I_{nn'}. \end{aligned} \quad (6.270)$$

Therefore,

$$\ln p(\mathbf{t}|\boldsymbol{\theta}) \simeq \Psi(\mathbf{a}_{\text{MAP}}) + \frac{N}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \mathbf{H}). \quad (6.271)$$

(b)

We have

$$\frac{\partial \Psi(\mathbf{a}_{\text{MAP}})}{\partial \theta_m} = \sum_{n=1}^N \sum_{n'=1}^N \frac{\partial \Psi(\mathbf{a}_{\text{MAP}})}{\partial C_{nn'}} \frac{\partial C_{nn'}}{\partial \theta_m}. \quad (6.272)$$

The right hand side can be written as

$$\frac{1}{2} \text{tr} \left(\mathbf{a}_{\text{MAP}} \mathbf{a}_{\text{MAP}}^T (\mathbf{C}^{-1})^2 \frac{\partial \mathbf{C}}{\partial \theta_m} \right). \quad (6.273)$$

We have

$$\frac{\partial \ln(\det \mathbf{H})}{\partial \theta_m} = \sum_{n=1}^N \sum_{n'=1}^N \frac{\partial \ln(\det \mathbf{H})}{\partial H_{nn'}} \frac{\partial H_{nn'}}{\partial \theta_m}. \quad (6.274)$$

By 3.21??, the right hand side can be written as

$$\text{tr} \left(\mathbf{H}^{-1} \frac{\partial \mathbf{C}^{-1}}{\partial \theta_m} \right). \quad (6.275)$$

Therefore,

$$\frac{\partial \ln p(\mathbf{t}|\boldsymbol{\theta})}{\partial \theta_m} \simeq \frac{1}{2} \text{tr} \left(\mathbf{a}_{\text{MAP}} \mathbf{a}_{\text{MAP}}^T (\mathbf{C}^{-1})^2 \frac{\partial \mathbf{C}}{\partial \theta_m} - \mathbf{H}^{-1} \frac{\partial \mathbf{C}^{-1}}{\partial \theta_m} \right). \quad (6.276)$$

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

$$t_n (\mathbf{w}^\top \phi(\mathbf{x}_n) + b) \geq \gamma, \quad (7.1)$$

for $\gamma > 0$, let

$$L = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^N a_n (t_n (\mathbf{w}^\top \phi(\mathbf{x}_n) + b) - \gamma). \quad (7.2)$$

Setting the derivatives of L with respect to \mathbf{w} and b to zero gives

$$\begin{aligned} \mathbf{0} &= \mathbf{w} - \sum_{n=1}^N a_n t_n \phi(\mathbf{x}_n), \\ 0 &= - \sum_{n=1}^N a_n t_n. \end{aligned} \quad (7.3)$$

Therefore,

$$\begin{aligned} \mathbf{w} &= \sum_{n=1}^N a_n t_n \phi(\mathbf{x}_n), \\ 0 &= \sum_{n=1}^N a_n t_n, \end{aligned} \quad (7.4)$$

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

$$\begin{aligned} t_n &\in \{-1, 1\}, \\ p(t_n|y_n) &= \sigma(y_n)^{\frac{1+t_n}{2}} (1 - \sigma(y_n))^{\frac{1-t_n}{2}}, \end{aligned} \quad (7.5)$$

where

$$\begin{aligned} \sigma(a) &= \frac{1}{1 + \exp(-a)}, \\ y_n &= \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}_n) + b. \end{aligned} \quad (7.6)$$

We have

$$1 - \sigma(a) = \sigma(-a). \quad (7.7)$$

Then,

$$p(t_n|y_n) = \sigma(y_n t_n). \quad (7.8)$$

Then,

$$p(\mathbf{t}|\mathbf{y}) = \prod_{n=1}^N \sigma(y_n t_n), \quad (7.9)$$

so that

$$-\ln p(\mathbf{t}|\mathbf{y}) = -\sum_{n=1}^N \ln \sigma(y_n t_n). \quad (7.10)$$

Therefore,

$$-\ln p(\mathbf{t}|\mathbf{y}) = \sum_{n=1}^N \ln (1 + \exp(-y_n t_n)). \quad (7.11)$$

7.7

Let t_1, \dots, t_N be variables. Let

$$E = C \sum_{n=1}^N E_\epsilon(y_n - t_n) + \frac{1}{2} \|\mathbf{w}\|^2, \quad (7.12)$$

where $\epsilon > 0$ and

$$E_\epsilon(a) = \begin{cases} 0, & |a| < \epsilon, \\ |a| - \epsilon, & \text{otherwise,} \end{cases} \quad (7.13)$$

$$y_n = \mathbf{w}^\top \phi(\mathbf{x}_n) + b.$$

In order to minimise E under the constraints

$$\begin{aligned} t_n &\leq y_n + \epsilon + \xi_n, \\ t_n &\geq y_n - \epsilon - \hat{\xi}_n, \end{aligned} \quad (7.14)$$

where $\xi_n \geq 0$ and $\hat{\xi}_n \geq 0$, let us minimise

$$\begin{aligned} L = & C \sum_{n=1}^N (\xi_n + \hat{\xi}_n) + \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^N (\mu_n \xi_n + \hat{\mu}_n \hat{\xi}_n) \\ & - \sum_{n=1}^N a_n (\epsilon + \xi_n + y_n - t_n) - \sum_{n=1}^N \hat{a}_n (\epsilon + \hat{\xi}_n - y_n + t_n). \end{aligned} \quad (7.15)$$

Setting the derivatives of L with respect to \mathbf{w} , b , ξ_n and $\hat{\xi}_n$ to zero gives

$$\begin{aligned} \mathbf{0} &= \mathbf{w} - \sum_{n=1}^N a_n \phi(\mathbf{x}_n) + \sum_{n=1}^N \hat{a}_n \phi(\mathbf{x}_n), \\ 0 &= - \sum_{n=1}^N a_n + \sum_{n=1}^N \hat{a}_n, \\ 0 &= C - \mu_n - a_n, \\ 0 &= C - \hat{\mu}_n - \hat{a}_n. \end{aligned} \quad (7.16)$$

Then, L can be written as

$$\begin{aligned} & \sum_{n=1}^N ((\mu_n + a_n) \xi_n + (\hat{\mu}_n + \hat{a}_n) \hat{\xi}_n) + \frac{1}{2} \left\| \sum_{n=1}^N (\hat{a}_n - a_n) \phi(\mathbf{x}_n) \right\|^2 \\ & - \sum_{n=1}^N (\mu_n \xi_n + \hat{\mu}_n \hat{\xi}_n) - \sum_{n=1}^N a_n (\epsilon + \xi_n + y_n - t_n) \\ & - \sum_{n=1}^N \hat{a}_n (\epsilon + \hat{\xi}_n - y_n + t_n). \end{aligned} \quad (7.17)$$

Therefore, minimising L is equivalent to maximising

$$\begin{aligned}\tilde{L} = & -\frac{1}{2} \sum_{n=1}^N \sum_{n'=1}^N (\hat{a}_n - a_n)(\hat{a}_{n'} - a_{n'}) k(\mathbf{x}_n, \mathbf{x}_{n'}) \\ & + \epsilon \sum_{n=1}^N (a_n + \hat{a}_n) + \sum_{n=1}^N (a_n - \hat{a}_n)(y_n - t_n),\end{aligned}\tag{7.18}$$

where

$$k(\mathbf{x}_n, \mathbf{x}_{n'}) = \phi(\mathbf{x}_n)^\top \phi(\mathbf{x}_{n'}).\tag{7.19}$$

7.8 (Incomplete)

Let t_1, \dots, t_N be variables. Let

$$E = C \sum_{n=1}^N E_\epsilon(y_n - t_n) + \frac{1}{2} \|\mathbf{w}\|^2,\tag{7.20}$$

where $\epsilon > 0$ and

$$\begin{aligned}E_\epsilon(a) &= \begin{cases} 0, & |a| < \epsilon, \\ |a| - \epsilon, & \text{otherwise,} \end{cases} \\ y_n &= \mathbf{w}^\top \phi(\mathbf{x}_n) + b.\end{aligned}\tag{7.21}$$

(a)

In order to minimise E under the constraints

$$t_n \leq y_n + \epsilon + \xi_n,\tag{7.22}$$

where $\xi_n \geq 0$, let us minimise

$$L = C \sum_{n=1}^N \xi_n + \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^N \mu_n \xi_n - \sum_{n=1}^N a_n (\epsilon + \xi_n + y_n - t_n).\tag{7.23}$$

Setting the derivatives of L with respect to \mathbf{w} , b and ξ_n to zero gives

$$\begin{aligned}\mathbf{0} &= \mathbf{w} - \sum_{n=1}^N a_n \phi(\mathbf{x}_n), \\ 0 &= -\sum_{n=1}^N a_n, \\ 0 &= C - \mu_n - a_n.\end{aligned}\tag{7.24}$$

Then, L can be written as

$$\begin{aligned} & \sum_{n=1}^N (\mu_n + a_n) \xi_n + \frac{1}{2} \left\| \sum_{n=1}^N a_n \boldsymbol{\phi}(\mathbf{x}_n) \right\|^2 - \sum_{n=1}^N \mu_n \xi_n \\ & - \sum_{n=1}^N a_n (\epsilon + \xi_n + y_n - t_n). \end{aligned} \quad (7.25)$$

Therefore, minimising L is equivalent to maximising

$$\tilde{L} = -\frac{1}{2} \sum_{n=1}^N \sum_{n'=1}^N a_n a_{n'} k(\mathbf{x}_n, \mathbf{x}_{n'}) + \sum_{n=1}^N a_n (y_n - t_n), \quad (7.26)$$

where

$$k(\mathbf{x}_n, \mathbf{x}_{n'}) = \boldsymbol{\phi}(\mathbf{x}_n)^\top \boldsymbol{\phi}(\mathbf{x}_{n'}). \quad (7.27)$$

7.9

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}) &= \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{0}, \mathbf{A}^{-1}). \end{aligned} \quad (7.28)$$

By the Bayes' theorem,

$$p(\mathbf{w} | \mathbf{t}) p(\mathbf{t}) = p(\mathbf{t} | \mathbf{w}) p(\mathbf{w}). \quad (7.29)$$

The logarithm of the right hand side except the terms independent of \mathbf{t} and \mathbf{w} can be written as

$$-\frac{\beta}{2} \sum_{n=1}^N \|t_n - \mathbf{w}^\top \boldsymbol{\phi}_n\|^2 - \frac{1}{2} \mathbf{w}^\top \mathbf{A} \mathbf{w} = -\frac{1}{2} \mathbf{v}^\top \mathbf{M} \mathbf{v}, \quad (7.30)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \mathbf{A} & -\beta \boldsymbol{\Phi}^\top \\ -\beta \boldsymbol{\Phi} & \beta \mathbf{I} \end{bmatrix}. \quad (7.31)$$

Therefore,

$$p(\mathbf{w} | \mathbf{t}) = \mathcal{N}(\mathbf{w} | \mathbf{m}, \mathbf{S}), \quad (7.32)$$

where

$$\begin{aligned} \mathbf{m} &= \beta \mathbf{S} \boldsymbol{\Phi}^\top \mathbf{t}, \\ \mathbf{S} &= (\beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \mathbf{A})^{-1}. \end{aligned} \quad (7.33)$$

7.10

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}) &= \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{0}, \mathbf{A}^{-1}). \end{aligned} \quad (7.34)$$

By marginalisation,

$$p(\mathbf{t}) = \int p(\mathbf{t} | \mathbf{w}) p(\mathbf{w}) d\mathbf{w}. \quad (7.35)$$

The logarithm of the integrand of the right hand side except the terms independent of \mathbf{t} and \mathbf{w} can be written as

$$-\frac{\beta}{2} \sum_{n=1}^N \|t_n - \mathbf{w}^\top \boldsymbol{\phi}_n\|^2 - \frac{1}{2} \mathbf{w}^\top \mathbf{A} \mathbf{w} = -\frac{1}{2} \mathbf{v}^\top \mathbf{M} \mathbf{v}, \quad (7.36)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \mathbf{S}^{-1} & -\beta \boldsymbol{\Phi}^\top \\ -\beta \boldsymbol{\Phi} & \beta \mathbf{I} \end{bmatrix}, \quad (7.37)$$

and

$$\mathbf{S}^{-1} = \beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \mathbf{A}. \quad (7.38)$$

The right hand side can be written as

$$-\frac{1}{2} \mathbf{u}^\top \mathbf{S}^{-1} \mathbf{u} - \frac{1}{2} \mathbf{t}^\top \mathbf{N} \mathbf{t}, \quad (7.39)$$

where

$$\begin{aligned} \mathbf{u} &= \mathbf{w} - \beta \mathbf{S} \boldsymbol{\Phi}^\top \mathbf{t}, \\ \mathbf{N} &= \beta \mathbf{I} - \beta^2 \boldsymbol{\Phi} \mathbf{S} \boldsymbol{\Phi}^\top. \end{aligned} \quad (7.40)$$

By 2.26,

$$\mathbf{N}^{-1} = \beta^{-1} \mathbf{I} + \boldsymbol{\Phi} \mathbf{A}^{-1} \boldsymbol{\Phi}^\top. \quad (7.41)$$

Therefore,

$$p(\mathbf{t}) = \mathcal{N}(\mathbf{t} | \mathbf{0}, \beta^{-1} \mathbf{I} + \boldsymbol{\Phi} \mathbf{A}^{-1} \boldsymbol{\Phi}^\top). \quad (7.42)$$

7.11

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}(t_n|\mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{A}^{-1}). \end{aligned} \quad (7.43)$$

By marginalisation,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}. \quad (7.44)$$

The logarithm of the integrand of the right hand side except the terms independent of \mathbf{t} and \mathbf{w} can be written as

$$-\frac{\beta}{2} \sum_{n=1}^N \|t_n - \mathbf{w}^\top \boldsymbol{\phi}_n\|^2 - \frac{1}{2}\mathbf{w}^\top \mathbf{A}\mathbf{w} = -\frac{1}{2}\mathbf{v}^\top \mathbf{M}\mathbf{v}, \quad (7.45)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} \\ \mathbf{t} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \beta\boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \mathbf{A} & -\beta\boldsymbol{\Phi}^\top \\ -\beta\boldsymbol{\Phi} & \beta\mathbf{I} \end{bmatrix}. \quad (7.46)$$

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{A}^{-1} & \mathbf{A}^{-1}\boldsymbol{\Phi}^\top \\ \boldsymbol{\Phi}\mathbf{A}^{-1} & \beta^{-1}\mathbf{I} + \boldsymbol{\Phi}\mathbf{A}^{-1}\boldsymbol{\Phi}^\top \end{bmatrix}. \quad (7.47)$$

Therefore,

$$p(\mathbf{t}) = \mathcal{N}(\mathbf{t}|\mathbf{0}, \beta^{-1}\mathbf{I} + \boldsymbol{\Phi}\mathbf{A}^{-1}\boldsymbol{\Phi}^\top). \quad (7.48)$$

7.12

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n|\mathbf{w}) &= \mathcal{N}(t_n|\mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{A}^{-1}), \end{aligned} \quad (7.49)$$

where

$$\mathbf{A} = \text{diag}(\alpha_m). \quad (7.50)$$

By marginalisation,

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}. \quad (7.51)$$

The logarithm of the integrand of the right hand side can be written as

$$\begin{aligned}
& -\frac{N}{2} \ln(2\pi\beta^{-1}) - \frac{\beta}{2} \sum_{n=1}^N \|t_n - \mathbf{w}^\top \boldsymbol{\phi}_n\|^2 \\
& - \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \mathbf{A}^{-1}) - \frac{1}{2} \mathbf{w}^\top \mathbf{A} \mathbf{w} \\
& = -\frac{N}{2} \ln(2\pi\beta^{-1}) - \frac{M}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \mathbf{A}) - E(\mathbf{w}),
\end{aligned} \tag{7.52}$$

where

$$E(\mathbf{w}) = \frac{\beta}{2} \|\mathbf{t} - \boldsymbol{\Phi} \mathbf{w}\|^2 + \frac{1}{2} \mathbf{w}^\top \mathbf{A} \mathbf{w}. \tag{7.53}$$

Then,

$$p(\mathbf{t}) = (2\pi\beta^{-1})^{-\frac{N}{2}} (2\pi)^{-\frac{M}{2}} (\det \mathbf{A})^{\frac{1}{2}} \int \exp(-E(\mathbf{w})) d\mathbf{w}. \tag{7.54}$$

We have

$$\begin{aligned}
\nabla E(\mathbf{w}) &= \boldsymbol{\Sigma}^{-1}(\mathbf{w} - \boldsymbol{\mu}), \\
\nabla \nabla E(\mathbf{w}) &= \boldsymbol{\Sigma}^{-1}.
\end{aligned} \tag{7.55}$$

where

$$\begin{aligned}
\boldsymbol{\mu} &= \beta \boldsymbol{\Sigma} \boldsymbol{\Phi}^\top \mathbf{t}, \\
\boldsymbol{\Sigma}^{-1} &= \beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \alpha \mathbf{I}.
\end{aligned} \tag{7.56}$$

Then,

$$E(\mathbf{w}) = E(\boldsymbol{\mu}) + \frac{1}{2} (\mathbf{w} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{w} - \boldsymbol{\mu}), \tag{7.57}$$

so that

$$\int \exp(-E(\mathbf{w})) d\mathbf{w} = (2\pi)^{\frac{M}{2}} (\det \boldsymbol{\Sigma})^{\frac{1}{2}} \exp(-E(\boldsymbol{\mu})). \tag{7.58}$$

Then,

$$\ln p(\mathbf{t}) = -\frac{N}{2} \ln(2\pi\beta^{-1}) + \frac{1}{2} \ln(\det \mathbf{A}) + \frac{1}{2} \ln(\det \boldsymbol{\Sigma}) - E(\boldsymbol{\mu}). \tag{7.59}$$

By 3.21, setting the derivatives of $\ln p(\mathbf{t})$ with respect to α_m and β to zero gives

$$\begin{aligned}
0 &= \frac{1}{2\alpha_m} + \frac{1}{2} \text{tr} \left(\boldsymbol{\Sigma}^{-1} \frac{\partial \boldsymbol{\Sigma}}{\partial \alpha_m} \right) - \frac{\mu_m^2}{2}, \\
0 &= \frac{N}{2\beta} + \frac{1}{2} \text{tr} \left(\boldsymbol{\Sigma}^{-1} \frac{\partial \boldsymbol{\Sigma}}{\partial \beta} \right) - \frac{\|\mathbf{t} - \boldsymbol{\Phi} \boldsymbol{\mu}\|^2}{2}.
\end{aligned} \tag{7.60}$$

We have

$$\begin{aligned}\mathbf{O} &= \frac{\partial \Sigma^{-1} \Sigma}{\partial \alpha_m}, \\ \mathbf{O} &= \frac{\partial \Sigma^{-1} \Sigma}{\partial \beta}.\end{aligned}\tag{7.61}$$

The right hand side can be written as

$$\begin{aligned}\Sigma^{-1} \frac{\partial \Sigma}{\partial \alpha_m} + \Sigma \frac{\partial \Sigma^{-1}}{\partial \alpha_m} &= \Sigma^{-1} \frac{\partial \Sigma}{\partial \alpha_m} + \Sigma, \\ \Sigma^{-1} \frac{\partial \Sigma}{\partial \beta} + \Sigma \frac{\partial \Sigma^{-1}}{\partial \beta} &= \Sigma^{-1} \frac{\partial \Sigma}{\partial \beta} + \Sigma \Phi^\top \Phi.\end{aligned}\tag{7.62}$$

Then,

$$\begin{aligned}\Sigma^{-1} \frac{\partial \Sigma}{\partial \alpha_m} &= -\Sigma, \\ \Sigma^{-1} \frac{\partial \Sigma}{\partial \beta} &= -\Sigma \Phi^\top \Phi.\end{aligned}\tag{7.63}$$

Therefore, the maximum likelihood solutions of $p(\mathbf{t})$ satisfy

$$\begin{aligned}\alpha_m &= \frac{1}{\mu_m^2 + \text{tr } \Sigma}, \\ \beta &= \frac{N}{\|\mathbf{t} - \Phi \boldsymbol{\mu}\|^2 + \text{tr}(\Sigma \Phi^\top \Phi)}.\end{aligned}\tag{7.64}$$

7.13 (Incomplete)

Let t_1, \dots, t_N be variables such that

$$\begin{aligned}p(t_n | \mathbf{w}, \beta) &= \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{0}, \mathbf{A}^{-1}), \\ p(\beta) &= \text{Gam}(\beta | a_0, b_0),\end{aligned}\tag{7.65}$$

where

$$\mathbf{A} = \text{diag}(\alpha_m).\tag{7.66}$$

By marginalisation,

$$p(\mathbf{t}) = \iint p(\mathbf{t} | \mathbf{w}, \beta) p(\mathbf{w}) p(\beta) d\mathbf{w} d\beta.\tag{7.67}$$

The logarithm of the integrand of the right hand side can be written as

$$\begin{aligned}
& -\frac{N}{2} \ln(2\pi\beta^{-1}) - \frac{\beta}{2} \sum_{n=1}^N \|t_n - \mathbf{w}^\top \boldsymbol{\phi}_n\|^2 \\
& - \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln(\det \mathbf{A}^{-1}) - \frac{1}{2} \mathbf{w}^\top \mathbf{A} \mathbf{w} \\
& + a_0 \ln b_0 - \ln \Gamma(a_0) + (a_0 - 1) \ln \beta - b_0 \beta \\
& = -\frac{N+M}{2} \ln(2\pi) + \frac{1}{2} \ln(\det \mathbf{A}) + a_0 \ln b_0 - \ln \Gamma(a_0) \\
& - E(\mathbf{w}, \beta) + G(\beta),
\end{aligned} \tag{7.68}$$

where

$$\begin{aligned}
E(\mathbf{w}, \beta) &= \frac{\beta}{2} \|\mathbf{t} - \boldsymbol{\Phi} \mathbf{w}\|^2 + \frac{1}{2} \mathbf{w}^\top \mathbf{A} \mathbf{w}, \\
G(\beta) &= (a-1) \ln \beta - b_0 \beta,
\end{aligned} \tag{7.69}$$

and

$$a = a_0 + \frac{N}{2}. \tag{7.70}$$

Then,

$$p(\mathbf{t}) = (2\pi)^{-\frac{N+M}{2}} (\det \mathbf{A})^{\frac{1}{2}} \frac{b_0^{a_0}}{\Gamma(a_0)} \int I(\beta) \exp(-G(\beta)) d\beta, \tag{7.71}$$

where

$$I(\beta) = \int \exp(-E(\mathbf{w}, \beta)) d\mathbf{w}. \tag{7.72}$$

We have

$$\begin{aligned}
\nabla_{\mathbf{w}} E(\mathbf{w}, \beta) &= \boldsymbol{\Sigma}^{-1}(\mathbf{w} - \boldsymbol{\mu}), \\
\nabla_{\mathbf{w}} \nabla_{\mathbf{w}} E(\mathbf{w}, \beta) &= \boldsymbol{\Sigma}^{-1}.
\end{aligned} \tag{7.73}$$

where

$$\begin{aligned}
\boldsymbol{\mu} &= \beta \boldsymbol{\Sigma} \boldsymbol{\Phi}^\top \mathbf{t}, \\
\boldsymbol{\Sigma}^{-1} &= \beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \alpha \mathbf{I}.
\end{aligned} \tag{7.74}$$

Then,

$$E(\mathbf{w}, \beta) = E(\boldsymbol{\mu}, \beta) + \frac{1}{2} (\mathbf{w} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{w} - \boldsymbol{\mu}), \tag{7.75}$$

so that

$$I(\beta) = (2\pi)^{\frac{M}{2}} (\det \boldsymbol{\Sigma})^{\frac{1}{2}} \exp(-E(\boldsymbol{\mu}, \beta)). \tag{7.76}$$

Then,

$$p(\mathbf{t}) = (2\pi)^{-\frac{N}{2}} (\det \mathbf{A})^{\frac{1}{2}} \frac{b_0^{a_0}}{\Gamma(a_0)} \int (\det \Sigma)^{\frac{1}{2}} \exp(-E(\boldsymbol{\mu}, \beta) + G(\beta)) d\beta. \quad (7.77)$$

The integral can be written as

$$\int (\det \Sigma)^{\frac{1}{2}} \exp(-E(\boldsymbol{\mu}, \beta) + G(\beta)) d\beta = . \quad (7.78)$$

Then,

$$\ln p(\mathbf{t}) = . \quad (7.79)$$

By 3.21, setting the derivatives of $\ln p(\mathbf{t})$ with respect to α_m and β to zero gives

$$\begin{aligned} 0 &= \frac{1}{2\alpha_m} + \frac{1}{2} \text{tr} \left(\Sigma^{-1} \frac{\partial \Sigma}{\partial \alpha_m} \right) - \frac{\mu_m^2}{2}, \\ 0 &= \frac{N}{2\beta} + \frac{1}{2} \text{tr} \left(\Sigma^{-1} \frac{\partial \Sigma}{\partial \beta} \right) - \frac{\|\mathbf{t} - \Phi \boldsymbol{\mu}\|^2}{2}. \end{aligned} \quad (7.80)$$

We have

$$\begin{aligned} \mathbf{O} &= \frac{\partial \Sigma^{-1} \Sigma}{\partial \alpha_m}, \\ \mathbf{O} &= \frac{\partial \Sigma^{-1} \Sigma}{\partial \beta}. \end{aligned} \quad (7.81)$$

The right hand side can be written as

$$\begin{aligned} \Sigma^{-1} \frac{\partial \Sigma}{\partial \alpha_m} + \Sigma \frac{\partial \Sigma^{-1}}{\partial \alpha_m} &= \Sigma^{-1} \frac{\partial \Sigma}{\partial \alpha_m} + \Sigma, \\ \Sigma^{-1} \frac{\partial \Sigma}{\partial \beta} + \Sigma \frac{\partial \Sigma^{-1}}{\partial \beta} &= \Sigma^{-1} \frac{\partial \Sigma}{\partial \beta} + \Sigma \Phi^\top \Phi. \end{aligned} \quad (7.82)$$

Then,

$$\begin{aligned} \Sigma^{-1} \frac{\partial \Sigma}{\partial \alpha_m} &= -\Sigma, \\ \Sigma^{-1} \frac{\partial \Sigma}{\partial \beta} &= -\Sigma \Phi^\top \Phi. \end{aligned} \quad (7.83)$$

Therefore, the maximum likelihood solutions of $p(\mathbf{t})$ satisfy

$$\begin{aligned} \alpha_m &= \frac{1}{\mu_m^2 + \text{tr } \Sigma}, \\ \beta &= \frac{N}{\|\mathbf{t} - \Phi \boldsymbol{\mu}\|^2 + \text{tr}(\Sigma \Phi^\top \Phi)}. \end{aligned} \quad (7.84)$$

7.14

Let t_1, \dots, t_N be variables such that

$$\begin{aligned} p(t_n | \mathbf{w}) &= \mathcal{N}(t_n | \mathbf{w}^\top \boldsymbol{\phi}_n, \beta^{-1}), \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w} | \mathbf{0}, \mathbf{A}^{-1}). \end{aligned} \quad (7.85)$$

By marginalisation,

$$p(t_{N+1} | \mathbf{t}) = \int p(t_{N+1} | \mathbf{w}) p(\mathbf{w} | \mathbf{t}) d\mathbf{w}. \quad (7.86)$$

By 7.9,

$$p(\mathbf{w} | \mathbf{t}) = \mathcal{N}(\mathbf{w} | \mathbf{m}, \mathbf{S}), \quad (7.87)$$

where

$$\begin{aligned} \mathbf{m} &= \beta \mathbf{S} \boldsymbol{\Phi}^\top \mathbf{t}, \\ \mathbf{S} &= (\beta \boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \mathbf{A})^{-1}. \end{aligned} \quad (7.88)$$

Then, the logarithm of the integrand except the terms independent of \mathbf{w} can be written as

$$\begin{aligned} & -\frac{\beta}{2} (t_{N+1} - \mathbf{w}^\top \boldsymbol{\phi}_{N+1})^2 - \frac{1}{2} (\mathbf{w} - \mathbf{m})^\top \mathbf{S}^{-1} (\mathbf{w} - \mathbf{m}) \\ &= -\frac{1}{2} \mathbf{v}^\top \mathbf{M} \mathbf{v} + \mathbf{v}^\top \mathbf{u} - \frac{1}{2} \mathbf{m}^\top \mathbf{S}^{-1} \mathbf{m}, \end{aligned} \quad (7.89)$$

where

$$\mathbf{v} = \begin{bmatrix} \mathbf{w} \\ t_{N+1} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} \mathbf{S}^{-1} + \beta \boldsymbol{\phi}_{N+1} \boldsymbol{\phi}_{N+1}^\top & -\beta \boldsymbol{\phi}_{N+1} \\ -\beta \boldsymbol{\phi}_{N+1}^\top & \beta \end{bmatrix}, \mathbf{u} = \begin{bmatrix} \mathbf{S}^{-1} \mathbf{m} \\ 0 \end{bmatrix}. \quad (7.90)$$

By 2.24,

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{S} & \mathbf{S} \boldsymbol{\phi}_{N+1} \\ \boldsymbol{\phi}_{N+1}^\top \mathbf{S} & \beta^{-1} + \boldsymbol{\phi}_{N+1}^\top \mathbf{S} \boldsymbol{\phi}_{N+1} \end{bmatrix}, \quad (7.91)$$

so that

$$\mathbf{M}^{-1} \mathbf{u} = \begin{bmatrix} \mathbf{m} \\ \mathbf{m}^\top \boldsymbol{\phi}_{N+1} \end{bmatrix}. \quad (7.92)$$

Therefore,

$$p(t_{N+1} | \mathbf{t}) = \mathcal{N}(t_{N+1} | \mathbf{m}^\top \boldsymbol{\phi}_{N+1}, \beta^{-1} + \boldsymbol{\phi}_{N+1}^\top \mathbf{S} \boldsymbol{\phi}_{N+1}). \quad (7.93)$$