

Solutions Manual to Pattern Recognition and Machine Learning

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June 15, 2024

1 Introduction

1.1

To minimise

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

setting its derivative to zero gives

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

Substituting

$$y(x_n, \mathbf{w}) = \sum_{j=0}^M w_j x_n^j \quad (1.3)$$

gives

$$0 = \sum_{n=1}^N x_n^i \left(\sum_{j=0}^M w_j x_n^j - t_n \right). \quad (1.4)$$

Therefore,

$$\sum_{j=0}^M A_{ij} w_j = T_i \quad (1.5)$$

where

$$\begin{aligned} A_{ij} &= \sum_{n=1}^N x_n^{i+j}, \\ T_i &= \sum_{n=1}^N x_n^i t_n. \end{aligned} \quad (1.6)$$

1.2

To minimise

$$\tilde{E}(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N (y(x_n, \mathbf{w}) - t_n)^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2, \quad (1.7)$$

setting its derivative to zero gives

$$\mathbf{0} = \sum_{n=1}^N \frac{\partial y(x_n, \mathbf{w})}{\partial \mathbf{w}} (y(x_n, \mathbf{w}) - t_n) + \lambda \mathbf{w}. \quad (1.8)$$

Substituting

$$y(x_n, \mathbf{w}) = \sum_{j=0}^M w_j x_n^j \quad (1.9)$$

gives

$$0 = \sum_{n=1}^N x_n^i \left(\sum_{j=0}^M w_j x_n^j - t_n \right) + \lambda w_i. \quad (1.10)$$

Therefore,

$$\sum_{j=0}^M \tilde{A}_{ij} w_j = T_i \quad (1.11)$$

where

$$\begin{aligned} \tilde{A}_{ij} &= \sum_{n=1}^N x_n^{i+j} + \lambda \delta_{ij}, \\ T_i &= \sum_{n=1}^N x_n^i t_n. \end{aligned} \quad (1.12)$$

1.3

Let a , o and l be the events where an apple, orange and lime are selected respectively. The probability that an apple is selected is given by

$$p(a) = p(a|r)p(r) + p(a|b)p(b) + p(a|g)p(g). \quad (1.13)$$

Substituting $p(a|r) = \frac{3}{10}$, $p(r) = \frac{1}{5}$, $p(a|g) = \frac{1}{2}$, $p(r) = \frac{1}{5}$, $p(a|g) = \frac{3}{10}$ and $p(g) = \frac{3}{5}$ gives

$$p(a) = \frac{17}{50}. \quad (1.14)$$

If an orange is selected, the probability that it came from the green box is given by

$$p(g|o) = \frac{p(g,o)}{p(o)}. \quad (1.15)$$

Here,

$$\begin{aligned} p(g, o) &= p(o|g)p(g), \\ p(o) &= p(o|r)p(r) + p(o|b)p(b) + p(o|g)p(g). \end{aligned} \quad (1.16)$$

Substituting $p(o|r) = \frac{2}{5}$, $p(r) = \frac{1}{5}$, $p(o|b) = \frac{1}{2}$, $p(b) = \frac{1}{5}$, $p(o|g) = \frac{3}{10}$ and $p(g) = \frac{3}{5}$ gives $p(g, o) = \frac{9}{50}$ and $p(o) = \frac{9}{25}$. Therefore,

$$p(g|o) = \frac{1}{2}. \quad (1.17)$$

1.4

Let

$$x = g(y) \quad (1.18)$$

and \hat{x} and \hat{y} be the locations of the maximum of $p_x(x)$ and $p_y(y)$ respectively. Let us assume that there exists $\epsilon > 0$ such that $g'(y) \neq 0$ for $|y - \hat{y}| < \epsilon$. Then, differentiating both sides of the transformation

$$p_y(y) = p_x(g(y)) |g'(y)| \quad (1.19)$$

and substituting $y = \hat{y}$ gives

$$0 = g'(\hat{y})p'_x(g(\hat{y})) + p_x(g(\hat{y}))g''(\hat{y}). \quad (1.20)$$

Therefore, in general,

$$\hat{x} \neq g(\hat{y}). \quad (1.21)$$

Here, let us assume that

$$g(y) = ay + b. \quad (1.22)$$

Then, differentiating both sides of the transformation and substituting $y = \hat{y}$ gives

$$0 = p'_x(g(\hat{y})). \quad (1.23)$$

Therefore,

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

1.5

By the definition,

$$\text{var} f(x) = E(f(x) - Ef(x))^2. \quad (1.25)$$

The right hand side can be written as

$$E((f(x))^2 - 2f(x)Ef(x) + (Ef(x))^2) = E(f(x))^2 - (Ef(x))^2. \quad (1.26)$$

Therefore,

$$\text{var} f(x) = E(f(x))^2 - (Ef(x))^2. \quad (1.27)$$

1.6

By the definition,

$$\text{cov}(x, y) = E((x - Ex)(y - Ey)). \quad (1.28)$$

The right hand side can be written as

$$Exy - E(xEy) - E(yEx) + E(ExEy) = Exy - ExEy. \quad (1.29)$$

The right hand side can be written as

$$\int xyp(x, y)dxdy - \int xp(x)dx \int yp(y)dy. \quad (1.30)$$

If x and y are independent, by the definition,

$$f(x, y) = f(x)f(y). \quad (1.31)$$

Then,

$$\int xyp(x, y)dxdy = \int p(x)dx \int p(y)dy. \quad (1.32)$$

Therefore,

$$\text{cov}(x, y) = 0. \quad (1.33)$$

1.7

Let

$$I = \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}x^2\right) dx. \quad (1.34)$$

Then

$$I^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}(x^2 + y^2)\right) dx dy. \quad (1.35)$$

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

$$\int_0^{\infty} \int_0^{2\pi} \exp\left(-\frac{1}{2\sigma^2}r^2\right) \begin{vmatrix} \cos \theta & -r \sin \theta \\ \sin \theta & r \cos \theta \end{vmatrix} dr d\theta = 2\pi \int_0^{\infty} \exp\left(-\frac{1}{2\sigma^2}r^2\right) r dr. \quad (1.36)$$

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

$$2\pi\sigma^2 \int_0^{\infty} \exp\left(-\frac{1}{2}s^2\right) s ds = 2\pi\sigma^2 \left[-\exp\left(-\frac{1}{2}s^2\right)\right]_0^{\infty}. \quad (1.37)$$

Therefore,

$$I = (2\pi\sigma^2)^{\frac{1}{2}}. \quad (1.38)$$

By the definition,

$$\mathcal{N}(x|\mu, \sigma^2) = (2\pi\sigma^2)^{-\frac{1}{2}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right). \quad (1.39)$$

Then

$$\int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) dx = (2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right) dx. \quad (1.40)$$

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

$$(2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}t^2\right) dt = (2\pi\sigma^2)^{-\frac{1}{2}} I. \quad (1.41)$$

Therefore,

$$\int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) dx = 1. \quad (1.42)$$

1.8

If x is under the Gaussian distribution with mean μ and variance σ^2 , then

$$\mathbb{E}x = \int_{-\infty}^{\infty} x \mathcal{N}(x|\mu, \sigma^2) dx. \quad (1.43)$$

By the definition, the right hand side can be written as

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

By the transformation $y = x - \mu$, it can be written as

$$(2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} (y + \mu) \exp\left(-\frac{1}{2\sigma^2}y^2\right) dy. \quad (1.45)$$

Since

$$(2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} y \exp\left(-\frac{1}{2\sigma^2}y^2\right) dy = 0, \quad (1.46)$$

and

$$(2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \mu \exp\left(-\frac{1}{2\sigma^2}y^2\right) dy = \mu \int_{-\infty}^{\infty} \mathcal{N}(y|\mu, \sigma^2) dy, \quad (1.47)$$

we have

$$\mathbb{E}x = \mu. \quad (1.48)$$

By the definition,

$$\int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) dx = 1 \quad (1.49)$$

can be written as

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

Differentiating both sides with respect to σ^2 gives

$$\begin{aligned} & (2\pi)^{-\frac{1}{2}} \left(-\frac{1}{2}\right) (\sigma^2)^{-\frac{3}{2}} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right) dx \\ & + (2\pi\sigma^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \frac{1}{2} (\sigma^2)^{-2} (x-\mu)^2 \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right) dx = 0. \end{aligned} \quad (1.51)$$

The left hand side can be written as

$$\begin{aligned} -\frac{1}{2} (\sigma^2)^{-1} \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) dx + \frac{1}{2} (\sigma^2)^{-2} \int_{-\infty}^{\infty} (x - \mu)^2 \mathcal{N}(x|\mu, \sigma^2) dx \\ = -\frac{1}{2} (\sigma^2)^{-1} + \frac{1}{2} (\sigma^2)^{-2} \text{var} x. \end{aligned} \quad (1.52)$$

Therefore,

$$\text{var} x = \sigma^2. \quad (1.53)$$

1.9

By the definition,

$$\mathcal{N}(x|\mu, \sigma^2) = (2\pi\sigma^2)^{-\frac{1}{2}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right). \quad (1.54)$$

Setting its derivative to zero gives

$$0 = (2\pi\sigma^2)^{-\frac{1}{2}} \left(-\frac{1}{\sigma^2}(x - \mu)\right) \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right). \quad (1.55)$$

Therefore, the mode is given by μ .

Similarly, by the definition,

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right). \quad (1.56)$$

Setting its derivative to zero gives

$$\mathbf{0} = -(2\pi)^{-\frac{D}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} (\boldsymbol{\Sigma}^{-1} + (\boldsymbol{\Sigma}^{-1})^\top) (\mathbf{x} - \boldsymbol{\mu}) \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right). \quad (1.57)$$

Therefore, the mode is given by $\boldsymbol{\mu}$.

1.10

By the definition,

$$\mathbb{E}(x + y) = \int \int (x + y) p(x, y) dx dy. \quad (1.58)$$

The right hand side can be written as

$$\int x \left(\int p(x, y) dy \right) dx + \int y \left(\int p(x, y) dx \right) dy = \int xp(x) dx + \int yp(y) dy. \quad (1.59)$$

By the definition, the right hand side can be written as

$$Ex + Ey. \quad (1.60)$$

Therefore,

$$E(x + y) = Ex + Ey. \quad (1.61)$$

Similarly, by the definition,

$$\text{var}(x + y) = E(x + y - E(x + y))^2 \quad (1.62)$$

By the result above and the definition, the right hand side can be written as

$$\begin{aligned} E(x - Ex)^2 + 2E((x - Ex)(y - Ey)) + E(y - Ey)^2 \\ = \text{var}x + 2\text{cov}(x, y) + \text{var}y. \end{aligned} \quad (1.63)$$

If x and y are independent, then

$$\text{cov}(x, y) = 0, \quad (1.64)$$

by 1.6. Therefore,

$$\text{var}(x + y) = \text{var}x + \text{var}y. \quad (1.65)$$

1.11

To maximise

$$\ln p(\mathbf{x}|\mu, \sigma^2) = -\frac{N}{2} \ln(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2, \quad (1.66)$$

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

$$\begin{aligned} 0 &= \frac{1}{\sigma^2} \sum_{n=1}^N (x_n - \mu), \\ 0 &= -\frac{N}{2\sigma^2} + \frac{1}{2(\sigma^2)^2} \sum_{n=1}^N (x_n - \mu)^2. \end{aligned} \quad (1.67)$$

Therefore,

$$\begin{aligned}\mu_{\text{ML}} &= \frac{1}{N} \sum_{n=1}^N x_n, \\ \sigma_{\text{ML}}^2 &= \frac{1}{N} \sum_{n=1}^N (x_n - \mu_{\text{ML}})^2.\end{aligned}\tag{1.68}$$

1.12

If x_m and x_n are independent, then

$$\mathbb{E}x_mx_n = \mathbb{E}x_m\mathbb{E}x_n.\tag{1.69}$$

If they are samples from the Gaussian distribution with mean μ and variance σ^2 , the right hand side is given by μ^2 . On the other hand, by the definition,

$$\mathbb{E}x_n^2 = \text{var}x_n + (\mathbb{E}x_n)^2.\tag{1.70}$$

If x_n is a sample from the Gaussian distribution with mean μ and variance σ^2 , the right hand side is given by $\sigma^2 + \mu^2$. Therefore,

$$\mathbb{E}x_mx_n = \mu^2 + \delta_{mn}\sigma^2.\tag{1.71}$$

Here, since

$$\mu_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N x_n,\tag{1.72}$$

we have

$$\mathbb{E}\mu_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N \mathbb{E}x_n.\tag{1.73}$$

Therefore,

$$\mathbb{E}\mu_{\text{ML}} = \mu.\tag{1.74}$$

Similarly, since

$$\sigma_{\text{ML}}^2 = \frac{1}{N} \sum_{n=1}^N (x_n - \mu_{\text{ML}})^2,\tag{1.75}$$

we have

$$\mathbb{E}\sigma_{\text{ML}}^2 = \frac{1}{N} \sum_{n=1}^N \mathbb{E}(x_n - \mu_{\text{ML}})^2.\tag{1.76}$$

The right hand side can be written as

$$\frac{1}{N} \sum_{n=1}^N \mathbb{E} (x_n^2 - 2\mu_{\text{ML}}x_n + \mu_{\text{ML}}^2) = \frac{1}{N} \sum_{n=1}^N \mathbb{E} x_n^2 - \frac{2}{N} \mathbb{E} \left(\mu_{\text{ML}} \left(\sum_{n=1}^N x_n \right) \right) + \mathbb{E} \mu_{\text{ML}}^2. \quad (1.77)$$

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

$$\frac{1}{N} \sum_{n=1}^N (\mu^2 + \sigma^2) = \mu^2 + \sigma^2, \quad (1.78)$$

while the second and third terms can be written as

$$-2\mathbb{E} \mu_{\text{ML}}^2 + \mathbb{E} \mu_{\text{ML}}^2 = -\mathbb{E} \mu_{\text{ML}}^2. \quad (1.79)$$

Here,

$$\mathbb{E} \mu_{\text{ML}}^2 = \mathbb{E} \left(\frac{1}{N} \sum_{n=1}^N x_n \right)^2. \quad (1.80)$$

The right hand side can be written as

$$\frac{1}{N^2} \sum_{n=1}^N \mathbb{E} x_n^2 + \frac{2}{N^2} \sum_{1 \leq m < n \leq N} \mathbb{E} x_m x_n = \frac{1}{N} (\mu^2 + \sigma^2) + \frac{N-1}{N} \mu^2. \quad (1.81)$$

Therefore,

$$\mathbb{E} \mu_{\text{ML}}^2 = \mu^2 + \frac{1}{N} \sigma^2. \quad (1.82)$$

Thus,

$$\mathbb{E} \sigma_{\text{ML}}^2 = \frac{N-1}{N} \sigma^2. \quad (1.83)$$

1.13

It is clear that

$$\mathbb{E} \left(\frac{1}{N} \sum_{n=1}^N (x_n - \mu)^2 \right) = \frac{1}{N} \sum_{n=1}^N \mathbb{E} (x_n - \mu)^2. \quad (1.84)$$

The right hand side can be written as

$$\frac{1}{N} \sum_{n=1}^N \mathbb{E} (x_n^2 - 2\mu x_n + \mu^2) = \frac{1}{N} \sum_{n=1}^N \mathbb{E} x_n^2 - \frac{2\mu}{N} \sum_{n=1}^N \mathbb{E} x_n + \mu^2. \quad (1.85)$$

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

$$\frac{1}{N} \sum_{n=1}^N (\mu^2 + \sigma^2) = \mu^2 + \sigma^2, \quad (1.86)$$

while the second term can be written as

$$-\frac{2\mu}{N} \sum_{n=1}^N \mu = -2\mu^2. \quad (1.87)$$

Therefore,

$$\mathbb{E} \left(\frac{1}{N} \sum_{n=1}^N (x_n - \mu)^2 \right) = \sigma^2. \quad (1.88)$$

1.14

Let

$$\begin{aligned} w_{ij}^S &= \frac{1}{2}(w_{ij} + w_{ji}), \\ w_{ij}^A &= \frac{1}{2}(w_{ij} - w_{ji}). \end{aligned} \quad (1.89)$$

Then

$$\begin{aligned} w_{ij} &= w_{ij}^S + w_{ij}^A, \\ w_{ij}^S &= w_{ji}^S, \\ w_{ij}^A &= -w_{ji}^A. \end{aligned} \quad (1.90)$$

Here,

$$\sum_{i=1}^D \sum_{j=1}^D w_{ij}^A x_i x_j = \frac{1}{2} \sum_{i=1}^D \sum_{j=1}^D (w_{ij} - w_{ji}) x_i x_j. \quad (1.91)$$

The right hand side can be written as

$$\frac{1}{2} \left(\sum_{i=1}^D \sum_{j=1}^D w_{ij} x_i x_j - \sum_{i=1}^D \sum_{j=1}^D w_{ji} x_i x_j \right) = 0. \quad (1.92)$$

Therefore,

$$\sum_{i=1}^D \sum_{j=1}^D w_{ij}^A x_i x_j = 0. \quad (1.93)$$

Additionally,

$$\sum_{i=1}^D \sum_{j=1}^D w_{ij} x_i x_j = \sum_{i=1}^D \sum_{j=1}^D (w_{ij}^S + w_{ij}^A) x_i x_j. \quad (1.94)$$

The right hand side can be written as

$$\sum_{i=1}^D \sum_{j=1}^D w_{ij}^S x_i x_j + \sum_{i=1}^D \sum_{j=1}^D w_{ij}^A x_i x_j = \sum_{i=1}^D \sum_{j=1}^D w_{ij}^S x_i x_j, \quad (1.95)$$

where the result above is used. Therefore,

$$\sum_{i=1}^D \sum_{j=1}^D w_{ij} x_i x_j = \sum_{i=1}^D \sum_{j=1}^D w_{ij}^S x_i x_j. \quad (1.96)$$

Finally, since the matrix w_{ij}^S is $D \times D$ symmetric matrix, its number of independent parameters is $\frac{D(D+1)}{2}$.

1.17

By the definition,

$$\Gamma(x) = \int_0^\infty u^{x-1} \exp(-u) du. \quad (1.97)$$

Then

$$\Gamma(x+1) = \int_0^\infty u^x \exp(-u) du. \quad (1.98)$$

The right hand side can be written as

$$[-u^x \exp(-u)]_{u=0}^{u=\infty} + \int_0^\infty x u^{x-1} \exp(-u) du = x \Gamma(x). \quad (1.99)$$

Therefore,

$$\Gamma(x+1) = x \Gamma(x). \quad (1.100)$$

By the definition,

$$\Gamma(1) = \int_0^1 \exp(-u) du. \quad (1.101)$$

The right hand side can be written as

$$[-\exp(-u)]_0^\infty = 1. \quad (1.102)$$

Therefore,

$$\Gamma(1) = 0!. \quad (1.103)$$

For a positive integer x , let us assume that

$$\Gamma(x) = (x-1)!. \quad (1.104)$$

Then,

$$\Gamma(x+1) = x\Gamma(x), \quad (1.105)$$

where the right hand side can be written as

$$x(x-1)! = x!. \quad (1.106)$$

Therefore,

$$\Gamma(x+1) = x!. \quad (1.107)$$

Thus, the assumption is proved by induction on x .

1.18

Let us consider the transformation from Cartesian to polar coordinates

$$\prod_{i=1}^D \int_{-\infty}^{\infty} \exp(-x_i^2) dx_i = S_D \int_0^{\infty} \exp(-r^2) r^{D-1} dr, \quad (1.108)$$

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 $s = r^2$, the right hand side can be written as

$$\frac{S_D}{2} \int_0^{\infty} \exp(-s) s^{\frac{D-1}{2}} s^{-\frac{1}{2}} ds = \frac{S_D}{2} \Gamma\left(\frac{D}{2}\right). \quad (1.109)$$

Therefore,

$$S_D = \frac{2\pi^{\frac{D}{2}}}{\Gamma\left(\frac{D}{2}\right)}. \quad (1.110)$$

Additionally, the volume of the sphere can be written as

$$V_D = S_D \int_0^1 r^{D-1} dr. \quad (1.111)$$

The right hand side can be written as

$$S_D \left[\frac{r^D}{D} \right]_{r=0}^{r=1} = \frac{S_D}{D}. \quad (1.112)$$

Therefore,

$$V_D = \frac{S_D}{D}. \quad (1.113)$$

Finally, the results above reduce to

$$\begin{aligned} S_2 &= \frac{2\pi}{\Gamma(1)}, \\ V_2 &= \frac{S_2}{2}. \end{aligned} \quad (1.114)$$

Therefore,

$$\begin{aligned} S_2 &= 2\pi, \\ V_2 &= \pi. \end{aligned} \quad (1.115)$$

Similarly,

$$\begin{aligned} S_3 &= \frac{2\pi^{\frac{3}{2}}}{\Gamma(\frac{3}{2})}, \\ V_3 &= \frac{S_3}{3}. \end{aligned} \quad (1.116)$$

Therefore,

$$\begin{aligned} S_3 &= 4\pi, \\ V_3 &= \frac{4}{3}\pi. \end{aligned} \quad (1.117)$$

1.19

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

$$\frac{V_D}{2^D} = \frac{\pi^{\frac{D}{2}}}{D 2^{D-1} \Gamma(\frac{D}{2})}, \quad (1.118)$$

by 1.18.

Additionally, by Sterling's formula

$$\Gamma(x+1) \simeq (2\pi)^{\frac{1}{2}} \exp(-x) x^{\frac{x+1}{2}}, \quad (1.119)$$

the ratio can be approximated as

$$\frac{V_D}{2^D} \simeq \frac{\pi^{\frac{D}{2}}}{D 2^{D-1} (2\pi)^{\frac{1}{2}} \exp\left(1 - \frac{D}{2}\right) \left(\frac{D}{2} - 1\right)^{\frac{D}{4}}}. \quad (1.120)$$

The right hand side can be written as

$$\frac{1}{2e(2\pi)^{\frac{1}{2}}} \frac{1}{D} \left(\frac{e^2 \pi^2}{8D - 16} \right)^{\frac{D}{4}}. \quad (1.121)$$

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

Finally, 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

$$\frac{\sqrt{\sum_{i=1}^D 1^2}}{1} = \sqrt{D}. \quad (1.122)$$

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

1.20

Integrating both sides of a Gaussian distributino in D dimensions

$$p(\mathbf{x}) = (2\pi\sigma^2)^{-\frac{D}{2}} \exp\left(-\frac{\|\mathbf{x}\|^2}{2\sigma^2}\right) \quad (1.123)$$

from $\|\mathbf{x}\| = r$ to $\|\mathbf{x}\| = r + \epsilon$ gives

$$\int_{r \leq \|\mathbf{x}\| \leq r+\epsilon} p(\mathbf{x}) d\mathbf{x} = \int_r^{r+\epsilon} \int (2\pi\sigma^2)^{-\frac{D}{2}} \exp\left(-\frac{r'^2}{2\sigma^2}\right) J dr' d\phi, \quad (1.124)$$

where ϕ is the vector of the angular components of the polar corrdinate and J is the Jacobian of the transformation from the Cartesian to polar coordinate.

For a sufficiently small ϵ , the right hand side can be approximated as

$$\begin{aligned} & (2\pi\sigma^2)^{-\frac{D}{2}} \exp\left(-\frac{r^2}{2\sigma^2}\right) \int_r^{r+\epsilon} \int J dr' d\phi \\ &= (2\pi\sigma^2)^{-\frac{D}{2}} \exp\left(-\frac{r^2}{2\sigma^2}\right) \int_{r \leq \|\mathbf{x}\| \leq r+\epsilon} d\mathbf{x}. \end{aligned} \quad (1.125)$$

Therefore,

$$\int_{r \leq \|\mathbf{x}\| \leq r+\epsilon} p(\mathbf{x}) d\mathbf{x} \simeq p(r)\epsilon, \quad (1.126)$$

where

$$p(r) = (2\pi\sigma^2)^{-\frac{D}{2}} S_D r^{D-1} \exp\left(-\frac{r^2}{2\sigma^2}\right), \quad (1.127)$$

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

Secondly, to maximise $p(r)$, setting the derivative to zero gives

$$0 = (2\pi\sigma^2)^{-\frac{D}{2}} S_D \left((D-1)r^{D-2} - \frac{r^D}{\sigma^2} \right) \exp\left(-\frac{r^2}{2\sigma^2}\right). \quad (1.128)$$

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

$$\hat{r} = \sqrt{D-1}\sigma. \quad (1.129)$$

Thirdly, by the expression of $p(r)$ above,

$$\frac{p(\hat{r} + \epsilon)}{p(\hat{r})} = \left(\frac{\hat{r} + \epsilon}{\hat{r}} \right)^{D-1} \exp\left(-\frac{2\hat{r}\epsilon + \epsilon^2}{2\sigma^2}\right). \quad (1.130)$$

Using the expression of \hat{r} above, the right hand side can be written as

$$\begin{aligned} & \exp\left((D-1)\ln\left(1 + \frac{\epsilon}{\hat{r}}\right) - \frac{2\hat{r}\epsilon + \epsilon^2}{2\sigma^2}\right) \\ &= \exp\left(\frac{\hat{r}^2}{\sigma^2}\ln\left(1 + \frac{\epsilon}{\hat{r}}\right) - \frac{2\hat{r}\epsilon + \epsilon^2}{2\sigma^2}\right). \end{aligned} \quad (1.131)$$

By the Taylor series

$$\ln(1+x) = x - \frac{1}{2}x^2 + o(x^3), \quad (1.132)$$

the right hand side can be approximated as

$$\exp\left(\frac{\hat{r}^2}{\sigma^2}\left(\frac{\epsilon}{\hat{r}} - \frac{\epsilon^2}{2\hat{r}^2}\right) - \frac{2\hat{r}\epsilon + \epsilon^2}{2\sigma^2}\right) = \exp\left(-\frac{\epsilon^2}{\sigma^2}\right). \quad (1.133)$$

Therefore,

$$p(\hat{r} + \epsilon) \simeq p(\hat{r}) \exp\left(-\frac{\epsilon^2}{\sigma^2}\right). \quad (1.134)$$

Finally, let a vector of length \hat{r} be $\hat{\mathbf{r}}$. Then, by the definition of $p(\mathbf{x})$,

$$\frac{p(\mathbf{0})}{p(\hat{\mathbf{r}})} = \exp\left(\frac{\hat{r}^2}{2\sigma^2}\right). \quad (1.135)$$

Substituting the expression of \hat{r} above, the right hand side can be written as $\exp\left(\frac{D-1}{2}\right)$. Therefore,

$$\frac{p(\mathbf{0})}{p(\hat{\mathbf{r}})} = \exp\left(\frac{D-1}{2}\right). \quad (1.136)$$

1.21

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

$$0 \leq a(b-a). \quad (1.137)$$

Therefore,

$$a \leq (ab)^{\frac{1}{2}}. \quad (1.138)$$

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

$$p(\mathbf{x}, \mathcal{C}_1) > p(\mathbf{x}, \mathcal{C}_2) \Rightarrow \mathbf{x} \in \mathcal{C}_1, \quad (1.139)$$

and

$$p(\mathbf{x}, \mathcal{C}_2) > p(\mathbf{x}, \mathcal{C}_1) \Rightarrow \mathbf{x} \in \mathcal{C}_2. \quad (1.140)$$

Then, using the inequality above,

$$\int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2) d\mathbf{x} \leq \int_{\mathcal{R}_1} (p(\mathbf{x}, \mathcal{C}_1)p(\mathbf{x}, \mathcal{C}_2))^{\frac{1}{2}} d\mathbf{x}, \quad (1.141)$$

and

$$\int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1) d\mathbf{x} \leq \int_{\mathcal{R}_2} (p(\mathbf{x}, \mathcal{C}_1)p(\mathbf{x}, \mathcal{C}_2))^{\frac{1}{2}} d\mathbf{x}. \quad (1.142)$$

Therefore,

$$\int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2) d\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1) d\mathbf{x} \leq \int (p(\mathbf{x}, \mathcal{C}_1)p(\mathbf{x}, \mathcal{C}_2))^{\frac{1}{2}} d\mathbf{x}. \quad (1.143)$$

1.22

Let

$$EL = \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(\mathbf{x}, \mathcal{C}_k) d\mathbf{x}. \quad (1.144)$$

If

$$L_{kj} = 1 - \delta_{kj}, \quad (1.145)$$

then the right hand side can be written as

$$\sum_k \sum_j \int_{\mathcal{R}_j} (p(\mathbf{x}, \mathcal{C}_k) - p(\mathbf{x}, \mathcal{C}_j)) d\mathbf{x} = \sum_j \int_{\mathcal{R}_j} \left(\sum_k p(\mathbf{x}, \mathcal{C}_k) - p(\mathbf{x}, \mathcal{C}_j) \right) d\mathbf{x}. \quad (1.146)$$

The right hand side can be written as

$$\sum_j \int_{\mathcal{R}_j} (p(\mathbf{x}) - p(\mathbf{x}, \mathcal{C}_j)) d\mathbf{x} = 1 - \sum_j \int_{\mathcal{R}_j} p(\mathbf{x}, \mathcal{C}_j) d\mathbf{x}. \quad (1.147)$$

Therefore,

$$EL = 1 - \sum_j \int_{\mathcal{R}_j} p(\mathcal{C}_j | \mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \quad (1.148)$$

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

1.23

Let

$$EL = \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(\mathbf{x}, \mathcal{C}_k) d\mathbf{x}. \quad (1.149)$$

The right hand side can be written as

$$\sum_j \int_{\mathcal{R}_j} \sum_k L_{kj} p(\mathbf{x}, \mathcal{C}_k) d\mathbf{x} = \sum_j \int_{\mathcal{R}_j} \left(\sum_k L_{kj} p(\mathcal{C}_k | \mathbf{x}) \right) p(\mathbf{x}) d\mathbf{x}. \quad (1.150)$$

Therefore,

$$EL = \sum_j \int_{\mathcal{R}_j} \left(\sum_k L_{kj} p(\mathcal{C}_k | \mathbf{x}) \right) p(\mathbf{x}) d\mathbf{x}. \quad (1.151)$$

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

1.25

Let

$$EL(\mathbf{t}, \mathbf{y}(\mathbf{x})) = \int \int \|\mathbf{y}(\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}. \quad (1.152)$$

Then

$$\delta EL(\mathbf{t}, \mathbf{y}(\mathbf{x})) = \int \int (\|\mathbf{y}(\mathbf{x}) + \delta \mathbf{y}(\mathbf{x}) - \mathbf{t}\|^2 - \|\mathbf{y}(\mathbf{x}) - \mathbf{t}\|^2) p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}. \quad (1.153)$$

The right hand side can be written as

$$\int \int (2(\delta \mathbf{y}(\mathbf{x}))^\top (\mathbf{y}(\mathbf{x}) - \mathbf{t}) + (\delta \mathbf{y}(\mathbf{x}))^\top \delta \mathbf{y}(\mathbf{x})) p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}. \quad (1.154)$$

Therefore,

$$\frac{\delta EL(\mathbf{t}, \mathbf{y}(\mathbf{x}))}{\delta \mathbf{y}(\mathbf{x})} = 2 \int (\mathbf{y}(\mathbf{x}) - \mathbf{t} + \delta \mathbf{y}(\mathbf{x})) p(\mathbf{x}, \mathbf{t}) d\mathbf{t}. \quad (1.155)$$

To minimise $EL(\mathbf{t}, \mathbf{y}(\mathbf{x}))$, setting the left hand side to zero and assuming that $\delta \mathbf{y}(\mathbf{x})$ is sufficiently small gives

$$\mathbf{0} = \int (\mathbf{y}(\mathbf{x}) - \mathbf{t}) p(\mathbf{x}, \mathbf{t}) d\mathbf{t}. \quad (1.156)$$

The right hand side can be written as

$$\mathbf{y}(\mathbf{x}) \int p(\mathbf{x}, \mathbf{t}) d\mathbf{t} - \int \mathbf{t} p(\mathbf{x}, \mathbf{t}) d\mathbf{t} = p(\mathbf{x}) \left(\mathbf{y}(\mathbf{x}) - \int \mathbf{t} p(\mathbf{t}|\mathbf{x}) d\mathbf{t} \right). \quad (1.157)$$

Thus,

$$\mathbf{y}(\mathbf{x}) = E_{\mathbf{t}}(\mathbf{t}|\mathbf{x}). \quad (1.158)$$

Finally, for a single target variable t , it reduces to

$$\mathbf{y}(\mathbf{x}) = E_t(t|\mathbf{x}). \quad (1.159)$$

1.26

Let

$$EL(\mathbf{t}, \mathbf{y}(\mathbf{x})) = \int \int \|\mathbf{y}(\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}. \quad (1.160)$$

The right hand side can be written as

$$\begin{aligned}
& \int \int \|\mathbf{y}(\mathbf{x}) - \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) + \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t} \\
&= \int \int \|\mathbf{y}(\mathbf{x}) - \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t} \\
&+ 2 \int \int (\mathbf{y}(\mathbf{x}) - \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}))^\top (\mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}) p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t} \\
&+ \int \int \|\mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{x}, \mathbf{t}) d\mathbf{x} d\mathbf{t}.
\end{aligned} \tag{1.161}$$

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

$$\int \|\mathbf{y}(\mathbf{x}) - \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\|^2 \left(\int p(\mathbf{x}, \mathbf{t}) d\mathbf{t} \right) d\mathbf{x} = \int \|\mathbf{y}(\mathbf{x}) - \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\|^2 p(\mathbf{x}) d\mathbf{x}. \tag{1.162}$$

Additionally, the second term can be written as

$$2 \int (\mathbf{y}(\mathbf{x}) - \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}))^\top \left(\int (\mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}) p(\mathbf{t}|\mathbf{x}) d\mathbf{t} \right) p(\mathbf{x}) d\mathbf{x}. \tag{1.163}$$

Since

$$\begin{aligned}
\int \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) p(\mathbf{t}|\mathbf{x}) d\mathbf{t} &= \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) \frac{\int p(\mathbf{x}, \mathbf{t}) d\mathbf{t}}{p(\mathbf{x})}, \\
\int \mathbf{t} p(\mathbf{t}|\mathbf{x}) d\mathbf{t} &= \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}),
\end{aligned} \tag{1.164}$$

the second term is zero. Finally, the third term can be written as

$$\int \left(\int \|\mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) - \mathbf{t}\|^2 p(\mathbf{t}|\mathbf{x}) d\mathbf{t} \right) p(\mathbf{x}) d\mathbf{x} = \int \text{var}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \tag{1.165}$$

Therefore,

$$EL(\mathbf{t}, \mathbf{y}(\mathbf{x})) = \int \|\mathbf{y}(\mathbf{x}) - \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x})\|^2 p(\mathbf{x}) d\mathbf{x} + \int \text{var}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \tag{1.166}$$

Thus, $EL(\mathbf{t}, \mathbf{y}(\mathbf{x}))$ is minimised if

$$\mathbf{y}(\mathbf{x}) = \mathbf{E}_{\mathbf{t}}(\mathbf{t}|\mathbf{x}). \tag{1.167}$$

1.27

Let

$$EL_q = \int \int |y(\mathbf{x}) - t|^q p(\mathbf{x}, t) d\mathbf{x} dt. \quad (1.168)$$

Then

$$\frac{\partial EL_q}{\partial y(\mathbf{x})} = \int q |y(\mathbf{x}) - t|^{q-1} \text{sign}(y(\mathbf{x}) - t) p(t|\mathbf{x}) dt. \quad (1.169)$$

To minimise EL_q , setting the left hand side to zero gives

$$0 = \int |y(\mathbf{x}) - t|^{q-1} \text{sign}(y(\mathbf{x}) - t) p(t|\mathbf{x}) dt. \quad (1.170)$$