Solutions for First Course in Machine Learning 2nd Edition by Rogers

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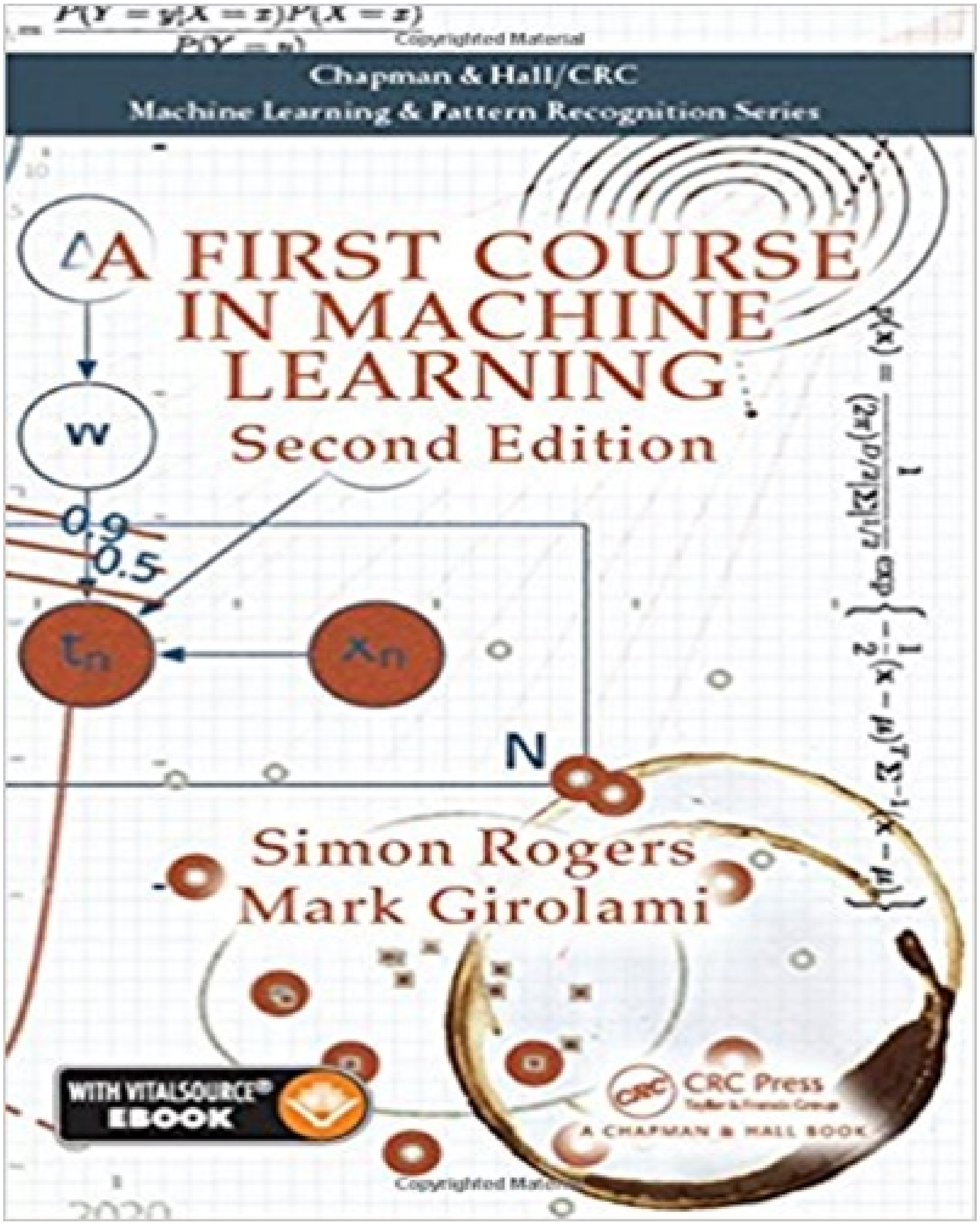

Solutions

Chapter 2

EX 2.1. The errors are real valued and hence a continuous random variable would be more appropriate.

EX 2.2. If all outcomes are equally likely, they have the same probability of occurring. Defining Y to be the random variable taking the value shown on a die, we can state the following:

$$P(Y = y) = r,$$

where r is a constant. From the definition of probabilities, we know that:

$$\sum_{y=1}^{6} P(Y = y) = 1.$$

Substituting r into this gives us the following:

$$\sum_{y=1}^{6} r = 1, \; 6r = 1, \; r = 1/6.$$

EX 2.3. (a) Y is a discrete random variable that can take any value from 0 to inf. The probability that $Y \leq 4$ is equal to the sum of all of the probabilities that satisfy $Y \leq 4$, $Y = 0, Y = 1, Y = 2, Y = 3, Y = 4$:

$$P(Y \leq 4) = \sum_{y=0}^{4} P(Y = y).$$

When $\lambda = 5$, we can compute these probabilities as:

$P(Y \leq 4) = 0.0067379 + 0.0336897 + 0.0842243 + 0.1403739 + 0.1754674 = 044049.$

(b) Because Y has to satisfy either $P(Y| \leq 4)$ or $P(Y > 4)$, we know that $P(Y > 4) = 1 - P(Y \leq 4)$:

$$P(Y > 4) = 0.5591.$$

EX 2.4. We require $\mathbf{E}_{p(y)}\left\{sin(y)\right\}$ where $p(y) = \mathcal{U}(a, b)$. The uniform density is given by:

$$p(y) = \begin{cases} \frac{1}{b-a} & a \leq y \leq b \\ 0 & \text{otherwise} \end{cases}$$

The required expectation is given by:

$$\begin{aligned}
\mathbf{E}_{p(y)}\left\{sin(y)\right\} &= \int sin(y)p(y)\ dy \\
&= \int_{y=a}^{b} sin(y)\frac{1}{b-a}\ dy \\
&= \frac{1}{b-a}\left[-\cos(y)\right]_a^b \\
&= \frac{\cos(a)-\cos(b)}{b-a}.
\end{aligned}$$

When $a=0,\ b=1$, this is equal to

$$\mathbf{E}_{p(y)}\left\{sin(y)\right\} = \frac{\cos(0)-\cos(1)}{1} = 0.45970.$$

Code to compute a sample-based approximation below (`sampleexpect.m`):

```
clear all;
close all;
% Compute a sample based approximation to the required expectation
u = rand(10000,1); % Take 10000 samples
su = sin(u);
% Plot how the approximation changes as more samples are used
ns = 10:100:10000;
stages = zeros(size(ns));
for i = 1:length(ns)
    stages(i) = mean(su(1:ns(i)));
end
plot(ns,stages)
% Plot the true value
hold on
plot([0 ns(end)],[0.4597 0.4597],'k--')
```

EX 2.5. The multivariate Gaussian pdf is given by:

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

Setting $\boldsymbol{\Sigma}=\sigma^2\mathbf{I}$ gives:

$$p(\mathbf{w}) = \frac{1}{(2\pi)^{D/2}|\sigma^2\mathbf{I}|^{1/2}}\exp\left\{-\frac{1}{2\sigma^2}(\mathbf{w}-\boldsymbol{\mu})^{\mathsf{T}}\mathbf{I}^{-1}(\mathbf{w}-\boldsymbol{\mu})\right\}.$$

Because it only has elements on the diagonal, the determinant of $\sigma^2\mathbf{I}$ is given by the product of these diagonal elements. As they are all the same, $|\sigma^2\mathbf{I}|^{1/2} = \left(\prod_{d=1}^{D}\sigma^2\right)^{1/2} = (\sigma^2)^{D/2}$. $\mathbf{I}^{-1}=\mathbf{I}$ and multiplying a vector/matrix by $\mathbf{I}$ leaves the matrix/vector unchanged. Therefore, the argument within the expectation can be written as $-\frac{1}{2\sigma^2}(\mathbf{w}-\boldsymbol{\mu})^{\mathsf{T}}(\mathbf{w}-\boldsymbol{\mu})$ and recalling that $\mathbf{b}^{\mathsf{T}}\mathbf{b}=\sum_i b_i^2$, we can rewrite the pdf as:

$$p(\mathbf{w}) = \frac{1}{(2\pi)^{D/2}(\sigma^2)^{D/2}}\exp\left\{-\frac{1}{2\sigma^2}\sum_{d=1}^{D}(w_d-\mu_d)^2\right\}.$$

Where w_d and μ_d are the dth elements of $\mathbf{w}$ and $\boldsymbol{\mu}$ respectively. The exponential of a sum is the same as a product of exponentials. Hence,

$$\begin{aligned} p(\mathbf{w}) &= \frac{1}{(2\pi)^{D/2}(\sigma^2)^{D/2}} \prod_{d=1}^{D} \exp\left\{-\frac{1}{2\sigma^2}(w_d - \mu_d)^2\right\} \\ &= \prod_{d=1}^{D} \frac{1}{(2\pi)^{1/2}\sigma} \exp\left\{-\frac{1}{2\sigma^2}(w_d - \mu_d)^2\right\} \\ &= \prod_{d=1}^{D} p(w_d|\mu_d, \sigma^2), \end{aligned}$$

where $p(w_d|\mu_d, \sigma^2) = \mathcal{N}(\mu_d, \sigma^2)$. Hence, the diagonal covariance is equivalent to assuming that the elements of $\mathbf{w}$ are distributed as independent, univariate Gaussians with mean μ_d and variance σ^2.

EX 2.6. Using the same methods as in the previous exercise, we see that the determinant of the covariance matrix is given by $\prod_{d=1}^{D} \sigma_d^2$ and we have the following:

$$p(\mathbf{w}) = \frac{1}{(2\pi)^{D/2}\left(\prod_{d=1}^{D} \sigma_d^2\right)^{1/2}} \exp\left\{-\frac{1}{2}\sum_{d=1}^{D} \frac{(w_d - \mu_d)^2}{\sigma_d^2}\right\}$$

Changing the sum to a product leaves us with

$$\begin{aligned} p(\mathbf{w}) &= \frac{1}{(2\pi)^{D/2}\left(\prod_{d=1}^{D} \sigma_d^2\right)^{1/2}} \prod_{d=1}^{D} \exp\left\{-\frac{1}{2\sigma_d^2}(w_d - \mu_d)^2\right\} \\ &= \prod_{d=1}^{D} \frac{1}{(2\pi)^{1/2}\sigma_d} \exp\left\{-\frac{1}{2\sigma_d^2}(w_d - \mu_d)^2\right\}. \end{aligned}$$

This is the product of D independent univariate Gaussian densities.

EX 2.7. The Hessian for a general model of our form is given by:

$$-\frac{1}{\sigma^2}\mathbf{X}^\mathsf{T}\mathbf{X}$$

For the linear model, $\mathbf{X}$ is defined as:

$$\mathbf{X} = \left[\begin{array}{cc} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{array}\right]$$

Therefore $-\frac{1}{\sigma^2}\mathbf{X}^\mathsf{T}\mathbf{X}$ is:

$$\mathbf{X}^\mathsf{T}\mathbf{X} = \left[\begin{array}{cc} N & \sum_{n=1}^{N} x_n \\ \sum_{n=1}^{N} x_n & \sum_{n=1}^{N} x_n^2 \end{array}\right]$$

The diagonal elements are $-N/\sigma^2$ and $-(1/sigma^2)\sum_{n=1}^{N} x_n^2$ which are equivalent (they differ only by multiplication with a negative constant) the expressions obtained in Chapter 1.

EX 2.8. We have N values, $x_1, \ldots, x_N$. Assuming that these values came from a Gaussian, we want to find the maximum likelihood estimate of the G and want to find the maximum likelihood estimates of the mean and variance of the Gaussian. The Gaussian pdf is:

$$\frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{1}{2\sigma^2}(x_n - \mu)^2\right\}$$

Assuming the IID assumption, the likelihood of all N points is given by a product over the N objects:

$$\prod_{n=1}^{N} \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{1}{2\sigma^2}(x_n - \mu)^2\right\}.$$

We'll work with the log of the likelihood:

$$\log L = \sum_{n=1}^{N}\left(-\frac{1}{2}\log(2\pi) - \frac{1}{2}\log(\sigma^2) - \frac{1}{2\sigma^2}(x_n - \mu)^2\right)$$

To find the maximum likelihood estimate for μ, we differentiate with respect to μ, equate to zero and solve:

$$\begin{aligned}
\frac{\partial \log L}{\partial \mu} &= \sum_{n=1}^{N} \frac{1}{\sigma^2}(x - \mu) \\
0 &= \frac{1}{\sigma^2}\sum_{n=1}^{N}(x_n - \mu) \\
0 &= \sum_{n=1}^{N} x_n - \sum_{n=1}^{N} \mu \\
&= \sum_{n=1}^{N} x_n - N\mu \\
\mu &= \frac{1}{N}\sum_{n=1}^{N} x_n
\end{aligned}$$

Similarly, for σ^2,

$$\begin{aligned}
\frac{\partial \log L}{\partial \sigma^2} &= \sum_{n=1}^{N}\left(-\frac{1}{2\sigma^2} + \frac{1}{2(\sigma^2)^2}(x_n - \mu)^2\right) = 0 \\
N\sigma^2 &= \sum_{n=1}^{N}(x_n - \mu)^2 \qquad (2.1) \\
\sigma^2 &= \frac{1}{N}\sum_{n=1}^{N}(x_n - \mu)^2 \qquad (2.2)
\end{aligned}$$

EX 2.9. The Bernoulli distribution is defined as:

$$P(X_n = x|r) = r^x(1-r)^{1-x}$$

where x is either 0 or 1. Using the IID assumption, we have:

$$L = \prod_{n=1}^{N} r^{x_n}(1-r)^{1-x_n}$$

and the log likelihood is:

$$\log L = \sum_{n=1}^{N} x_n \log r + (1-x_n)\log(1-r)$$

Differentiating with respect to r gives us:

$$\begin{aligned}
\frac{\partial \log L}{\partial r} &= \sum_{n=1}^{N}\left(\frac{x_n}{r} - \frac{1-x_n}{1-r}\right) = 0 \\
\sum_{n=1}^{N}\frac{x_n}{r} &= \sum_{n=1}^{N}\frac{1-x_n}{1-r} \\
\sum_{n=1}^{N} x_n - r\sum_{n=1}^{N} x_n &= rN - r\sum_{n=1}^{N} x_n \\
r &= \frac{1}{N}\sum_{n=1}^{N} x_n.
\end{aligned}$$

EX 2.10. The Fisher information is defined as the expectation of the negative second derivative. From the above expression, we can see that the second derivative of the Gaussian likelihood (assuming N observations, $x_1, \ldots, x_N$ is:

$$\frac{\partial^2 \log L}{\partial \mu^2} = -\frac{N}{\sigma^2}.$$

Hence the Fisher information is equal to N/σ^2.

EX 2.11. Starting from the second expression, we have

$$\widehat{\sigma^2} = \frac{1}{N}\left[\sum_{n=1}^{N} t_n^2 - 2\sum_{n=1}^{N} t_n \mathbf{x}_n^{\mathsf{T}}\widehat{\mathbf{w}} + \sum_{n=1}^{N}(\mathbf{x}_n\widehat{\mathbf{w}})^2\right].$$

Concentrating on the final term,

$$\begin{aligned}
\sum_{n=1}^{N} (\mathbf{x}^\mathsf{T}\widehat{\mathbf{w}})^2 &= \sum_{n=1}^{N} \mathbf{x}_n^\mathsf{T}\widehat{\mathbf{w}}\widehat{\mathbf{w}}^\mathsf{T}\mathbf{x}_n \\
&= \mathsf{Tr}(\mathbf{X}\widehat{\mathbf{w}}\widehat{\mathbf{w}}^\mathsf{T}\mathbf{X}^\mathsf{T}) \\
&= \mathsf{Tr}(\mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t}\mathbf{t}^\mathsf{T}\mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}) \\
&= \mathsf{Tr}(\mathbf{X}^\mathsf{T}\mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t}\mathbf{t}^\mathsf{T}\mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}) \\
&= \mathsf{Tr}(\mathbf{X}^\mathsf{T}\mathbf{t}\mathbf{t}^\mathsf{T}\mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}) \\
&= \mathsf{Tr}(\mathbf{t}\mathbf{t}^\mathsf{T}\mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}) \\
&= \mathsf{Tr}(\mathbf{t}^\mathsf{T}\mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t}) \\
&= \mathbf{t}^\mathsf{T}\mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t}) \\
&= \mathbf{t}^\mathsf{T}\mathbf{X}\widehat{\mathbf{w}} \\
&= \sum_{n=1}^{N} t_n \mathbf{x}_n^\mathsf{T}\widehat{\mathbf{w}}.
\end{aligned}$$

Therefore,

$$\widehat{\sigma^2} = \frac{1}{N}\left[\sum_{n=1}^{N} t_n^2 - \sum_{n=1}^{N} t_n \mathbf{x}_n^\mathsf{T}\widehat{\mathbf{w}}\right].$$

Now, $\sum_{n=1}^{N} t_n^2 = \mathbf{t}^\mathsf{T}\mathbf{t}$ and we already know that $\sum_{n=1}^{N} t_n \mathbf{x}_n \widehat{\mathbf{w}} = \mathbf{t}^\mathsf{T}\mathbf{X}\widehat{\mathbf{w}}$. So,

$$\widehat{\sigma^2} = \frac{1}{N}\left[\mathbf{t}^\mathsf{T}\mathbf{t} - \mathbf{t}^\mathsf{T}\mathbf{X}\widehat{\mathbf{w}}\right],$$

as required.

EX 2.12. Code below (`predvar.m`):

```
clear all;close all;
% Relevant code extracted from predictive_variance_example.m
x = rand(50,1)*10-5;
x = sort(x);
% Compute true function values
f = 5*x.^3 - x.^2 + x;
% Generate some test locations
testx = [min(x):0.2:max(x)]';
% Add some noise
t = f+randn(50,1)*sqrt(1000);
% Remove all training data between -1.5 and 1.5
pos = find(x>-1.5 & x<1.5);
x(pos) = [];
f(pos) = [];
t(pos) = [];

% Choose model order
K = 5;

X = repmat(1,size(x));
testX = repmat(1,size(testx));
```

```
for k = 1:K
    X = [X x.^k];
    testX = [testX testx.^k];
end


w_hat = inv(X'*X)*X'*t;
ss_hat = mean((t - X*w_hat).^2);
pred_va = ss_hat*diag(testX*inv(X'*X)*testX');
% Make a plot
figure(1);hold off
plot(x,t,'b.');
hold on
errorbar(testx,testX*w_hat,pred_va,'r');
```

EX 2.13. The Bernoulli distribution for a binary random variable x is:

$$p(x|\theta) = \theta^x(1-\theta)^{1-x}$$

The Fisher information is defined as the negative expected value of the second derivative of the log density evaluated at some paramater value:

$$\mathcal{F} = -\mathbf{E}_{p(x|\theta)}\left\{ \left. \frac{\partial^2 \log p(x|\theta)}{\partial \theta^2} \right|_{\theta} \right\}$$

Differentiating $\log p(x|\theta)$ twice gives:

$$\begin{aligned} \frac{\partial \log p(x|\theta)}{\partial \theta} &= \frac{x}{\theta} - \frac{1-x}{1-\theta} \\ \frac{\partial^2 \log p(x|\theta)}{\partial \theta^2} &= -\frac{x}{\theta^2} - \frac{1-x}{(1-\theta)^2}. \end{aligned}$$

The Fisher information is therefore:

$$\mathcal{F} = \frac{1}{\theta^2}\mathbf{E}_{p(x|\theta)}\left\{x\right\} + \frac{1}{(1-\theta)^2}\mathbf{E}_{p(x|\theta)}\left\{1-x\right\}.$$

Substituting in the expectations (θ and $1-\theta$ respectively gives:

$$\mathcal{F} = \frac{\theta}{\theta^2} + \frac{1-\theta}{(1-\theta)^2} = \frac{1}{\theta(1-\theta)}$$

EX 2.14. The multivariate Gaussian pdf is given by:

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

Logging and removing terms not including $\boldsymbol{\mu}$:

$$\log p(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) \propto \boldsymbol{\mu}^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}\mathbf{x} - \frac{1}{2}\boldsymbol{\mu}^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}.$$

First and second derivatives are:

$$\begin{aligned}\frac{\partial \log p(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})}{\partial \boldsymbol{\mu}} &= \boldsymbol{\Sigma}^{-1}\mathbf{x} - \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} \\ \frac{\partial^2 \log p(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})}{\partial \boldsymbol{\mu} \partial \boldsymbol{\mu}^\mathsf{T}} &= -\boldsymbol{\Sigma}^{-1}.\end{aligned}$$

Therefore, the Fisher information is:

$$\mathcal{F} = \boldsymbol{\Sigma}^{-1}.$$