## Exercises

## Introduction to Machine Learning <br> FS 2018

## Series 1, Feb 22, 2018 (Probability and Linear Algebra)

# Institute for Machine Learning 

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## Problem 1 (Linear Regression and Ridge Regression):

Let $D=\left\{\left(\mathbf{x}_{1}, y_{1}\right),\left(\mathbf{x}_{2}, y_{2}\right), \ldots\left(\mathbf{x}_{n}, y_{n}\right)\right\}$ where $\mathbf{x}_{i} \in \mathbb{R}^{d}$ and $y_{i} \in \mathbb{R}$ be the training data that you are given. As you have to predict a continuous variable, one of the simplest possible models is linear regression, i.e. to predict $y$ as $\mathbf{w}^{T} \mathbf{x}$ for some parameter vector $\mathbf{w} \in \mathbb{R}^{d} 1$ We thus suggest minimizing the following loss

$$
\begin{equation*}
\underset{\mathbf{w}}{\operatorname{argmin}} \hat{R}(\mathbf{w})=\underset{\mathbf{w}}{\operatorname{argmin}} \sum_{i=1}^{n}\left(y_{i}-\mathbf{w}^{T} \mathbf{x}_{i}\right)^{2} . \tag{1}
\end{equation*}
$$

Let us introduce the $n \times d$ matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ with the $\mathbf{x}_{i}$ as rows, and the vector $\mathbf{y} \in \mathbb{R}^{n}$ consisting of the scalars $y_{i}$. Then, (1) can be equivalently re-written as

$$
\underset{\mathbf{w}}{\operatorname{argmin}}\|\mathbf{X w}-\mathbf{y}\|^{2} .
$$

We refer to any $\mathbf{w}^{*}$ that attains the above minimum as a solution to the problem.
(a) Show that if $\mathbf{X}^{T} \mathbf{X}$ is invertible, then there is a unique $\mathbf{w}^{*}$ that can be computed as $\mathbf{w}^{*}=\left(\mathbf{X}^{T} \mathbf{X}\right)^{-1} \mathbf{X}^{T} \mathbf{y}$.
(b) Show for $n<d$ that (1) does not admit a unique solution. Intuitively explain why this is the case.
(c) Consider the case $n \geq d$. Under what assumptions on $\mathbf{X}$ does (1) admit a unique solution $\mathbf{w}^{*}$ ? Give an example with $n=3$ and $d=2$ where these assumptions do not hold.

The ridge regression optimization problem with parameter $\lambda>0$ is given by

$$
\begin{equation*}
\underset{\mathbf{w}}{\operatorname{argmin}} \hat{R}_{\text {Ridge }}(\mathbf{w})=\underset{\mathbf{w}}{\operatorname{argmin}}\left[\sum_{i=1}^{n}\left(y_{i}-w^{T} \mathbf{x}_{i}\right)^{2}+\lambda \mathbf{w}^{T} \mathbf{w}\right] . \tag{2}
\end{equation*}
$$

(d) Show that $\hat{R}_{\text {Ridge }}(\mathbf{w})$ is convex with regards to $\mathbf{w}$. You can use the fact that a twice differentiable function is convex if and only if its Hessian $\mathbf{H} \in \mathbb{R}^{d \times d}$ satisfies $\mathbf{w}^{T} \mathbf{H w} \geq 0$ for all $\mathbf{w} \in \mathbb{R}^{d}$ (is positive semi-definite).
(e) Derive the closed form solution $\mathbf{w}_{\text {Ridge }}^{*}=\left(\mathbf{X}^{T} \mathbf{X}+\lambda I_{d}\right)^{-1} \mathbf{X}^{T} \mathbf{y}$ to (2) where $I_{d}$ denotes the identity matrix of size $d \times d$.
(f) Show that (2) admits the unique solution $\mathbf{w}_{\text {Ridge }}^{*}$ for any matrix $\mathbf{X}$. Show that this even holds for the cases in (b) and (c) where (1) does not admit a unique solution $\mathrm{w}^{*}$.
(g) What is the role of the term $\lambda \mathbf{w}^{T} \mathbf{w}$ in $\hat{R}_{\text {Ridge }}(\mathbf{w})$ ? What happens to $\mathbf{w}_{\text {Ridge }}^{*}$ as $\lambda \rightarrow 0$ and $\lambda \rightarrow \infty$ ?

[^0]
## Solution 1:

(a) Note that

$$
\hat{R}(\mathbf{w})=\|\mathbf{X} \mathbf{w}-\mathbf{y}\|^{2}=(\mathbf{X} \mathbf{w}-\mathbf{y})^{T}(\mathbf{X} \mathbf{w}-\mathbf{y})=\mathbf{w}^{T} \mathbf{X}^{T} \mathbf{X} \mathbf{w}-2 \mathbf{w}^{T} \mathbf{X}^{T} \mathbf{y}+\mathbf{y}^{T} \mathbf{y} .
$$

The gradient of this function is equal to (see Lemma 1)

$$
\nabla \hat{R}(\mathbf{w})=2 \mathbf{X}^{T} \mathbf{X} \mathbf{w}-2 \mathbf{X}^{T} \mathbf{y}
$$

Because $\hat{R}(\mathbf{w})$ is convex (formally proven in (d)), its optima are exactly those points that have a zero gradient, i.e. those $\mathbf{w}^{*}$ that satisfy $\mathbf{X}^{T} \mathbf{X} \mathbf{w}^{*}=\mathbf{X}^{T} \mathbf{y}$. Under the given assumption, the unique minimizer is indeed equal to $\mathbf{w}^{*}=\left(\mathbf{X}^{T} \mathbf{X}\right)^{-1} \mathbf{X}^{T} \mathbf{y}$.
(b) Consider the singular value decomposition $\mathbf{X}=\mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^{T}$ where $\mathbf{U}$ is an unitary $n \times n$ matrix, $\mathbf{V}$ is a unitary $d \times d$ matrix and $\boldsymbol{\Sigma}$ is a diagonal $n \times d$ matrix with the singular values of $\mathbf{X}$ on the diagonal. We then have

$$
\underset{\mathbf{w}}{\operatorname{argmin}} \hat{R}(\mathbf{w})=\underset{\mathbf{w}}{\operatorname{argmin}}\left[\mathbf{w}^{T} \mathbf{V} \boldsymbol{\Sigma}^{2} \mathbf{V}^{T} \mathbf{w}-2 \mathbf{y}^{T} \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^{T} \mathbf{w}\right]
$$

Since $\mathbf{V}$ is unitary (and hence it is a bijection), we may rotate $\mathbf{w}$ using $\mathbf{V}$ to $\mathbf{z}=\mathbf{V}^{T} \mathbf{w}$ and formulate the optimization problem in terms of $\mathbf{z}$, i.e.

$$
\underset{\mathbf{z}}{\operatorname{argmin}}\left[\mathbf{z}^{T} \boldsymbol{\Sigma}^{2} \mathbf{z}-2 \mathbf{y}^{T} \mathbf{U} \boldsymbol{\Sigma} \mathbf{z}\right]=\underset{\mathbf{z}}{\operatorname{argmin}} \sum_{i=1}^{d}\left[z_{i}^{2} \sigma_{i}^{2}-2\left(\mathbf{U}^{T} \mathbf{y}\right)_{i} z_{i} \sigma_{i}\right]
$$

where $\sigma_{i}$ is the $i$ entry in the diagonal of $\boldsymbol{\Sigma}$. Note that this problem decomposes into $d$ independent optimization problems of the form

$$
z_{i}=\underset{z}{\operatorname{argmin}}\left[z^{2} \sigma_{i}^{2}-2\left(\mathbf{U}^{T} \mathbf{y}\right)_{i} z \sigma_{i}\right]
$$

for $i=1,2, \ldots, d$. Since each problem is quadratic with positive coefficient and thus convex we may obtain the solution by finding the root of the first derivative. For $i=1,2, \ldots d$ we require that $z_{i}$ satisfies

$$
z_{i} \sigma_{i}^{2}-\left(\mathbf{U}^{t} \mathbf{y}\right)_{i} \sigma_{i}=0
$$

For all $i=1,2, \ldots d$ such that $\sigma_{i} \neq 0$, the solution $z_{i}$ is thus given by

$$
z_{i}=\frac{\left(\mathbf{U}^{t} \mathbf{y}\right)_{i}}{\sigma_{i}}
$$

For the case $n<d$, however, $\mathbf{X}$ has at most rank $n$ as it is a $n \times d$ matrix and hence at most $n$ of its singular values are nonzero. This means that there is at least one index $j$ such that $\sigma_{j}=0$ and hence any $z_{j} \in \mathbb{R}$ is a solution to the optimization problem. As a result the set of optimal solutions for $\mathbf{z}$ is a linear subspace of at least one dimension. By rotating this subspace back using $\mathbf{V}$, i.e. $\mathbf{w}=\mathbf{V} \mathbf{z}$, it is evident that the optimal solution to the optimization problem in terms of $\mathbf{w}$ is also a linear subspace of at least one dimension and that thus no unique solution exists. Furthermore, since $\mathbf{X}$ has at most rank $n, \mathbf{X}^{T} \mathbf{X}$ is not of full rank (see Lemma 22). As a result $\left(\mathbf{X}^{T} \mathbf{X}\right)^{-1}$ does not exist and $\mathbf{w}^{*}$ is ill-defined.
The intuition behind these results is that the "linear system" $\mathbf{X w} \approx \mathbf{y}$ is underdetermined as there are less data points than parameters that we want to estimate.
(c) We showed in (b) that the optimization problem admits a unique solution only if all the singular values of $\mathbf{X}$ are nonzero. For $n \geq d$, this is the case if and only if $\mathbf{X}$ is of full rank, i.e. all the columns of $\mathbf{X}$ are linearly independent. As an example for a matrix not satisfying these assumptions, any matrix with linearly dependent dependent suffices, e.g.

$$
\mathbf{X}_{\text {degenerate }}=\left(\begin{array}{cc}
1 & -2 \\
0 & 0 \\
-2 & 4
\end{array}\right)
$$

(d) Because convex functions are closed under addition, we will show that each term in the objective is convex, from which the claim will follow. Each data term $\left(y_{i}-\mathbf{w}^{T} \mathbf{x}_{i}\right)^{2}$ has a Hessian $\mathbf{x}_{i} \mathbf{x}_{i}^{T}$, which is positive semi-definite because for any $\mathbf{w} \in \mathbf{R}^{d}$ we have $\mathbf{w}^{T} \mathbf{x}_{i} \mathbf{x}_{i}^{T} \mathbf{w}=\left(\mathbf{x}_{i}^{T} \mathbf{w}_{i}\right)^{2} \geq 0$ (note that $\mathbf{x}_{i}^{T} \mathbf{w}=\mathbf{w}^{T} \mathbf{x}_{i}$ are scalars). The regularizer $\lambda \mathbf{w}^{T} \mathbf{w}$ has the identity matrix $\lambda I_{d}$ as a Hessian, which is also postive semi-definite because for any $\mathbf{w} \in \mathbf{R}^{d}$ we have $\mathbf{w}^{T} \lambda I_{d} \mathbf{w}=\lambda\|\mathbf{w}\|^{2} \geq 0$, and this completes the proof.
(e) The gradient of $\hat{R}_{\text {Ridge }}(\mathbf{w})$ with respect to $\mathbf{w}$ is given by

$$
\nabla \hat{R}_{\text {Ridge }}(\mathbf{w})=2 \mathbf{X}^{T}(\mathbf{X} \mathbf{w}-\mathbf{y})+2 \lambda \mathbf{w} .
$$

Similar to (a), because $\hat{R}_{\text {Ridge }}(\mathbf{w})$ is convex, we only have to find a point $\mathbf{w}_{\text {Ridge }}^{*}$ such that

$$
\nabla \hat{R}_{\text {Ridge }}\left(\mathbf{w}_{\text {Ridge }}^{*}\right)=2 \mathbf{X}^{T}\left(\mathbf{X} \mathbf{w}_{\text {Ridge }}^{*}-\mathbf{y}\right)+2 \lambda \mathbf{w}_{\text {Ridge }}^{*}=0 .
$$

This is equivalent to

$$
\left(\mathbf{X}^{T} \mathbf{X}+\lambda I_{d}\right) \mathbf{w}_{\text {Ridge }}^{*}=\mathbf{X}^{T} \mathbf{y}
$$

which implies the required result

$$
\mathbf{w}_{\text {Ridge }}^{*}=\left(\mathbf{X}^{T} \mathbf{X}+\lambda I_{d}\right)^{-1} \mathbf{X}^{T} \mathbf{y}
$$

(f) Note that $\mathbf{X}^{T} \mathbf{X}$ is a positive semi-definite matrix ${ }^{2}$ since $\forall \mathbf{w} \in \mathbb{R}^{d}: \mathbf{w}^{T} \mathbf{X}^{T} \mathbf{X} \mathbf{w}=\sum_{i=1}^{n}\left[(\mathbf{X} \mathbf{w})_{i}\right]^{2} \geq 0$, which implies that it has non-negative eigenvalues. But then, $\mathbf{X}^{T} \mathbf{X}+\lambda I_{d}$ has eigenvalues bounded from below by $\lambda>0$, which means that it is invertible and thus the optimum is uniquely defined.

Note. Since $\mathbf{X}^{T} \mathbf{X}$ is symmetric, all of its eigenvalues are real, and it is clear that $\mu$ is an eigenvalue of $\mathbf{X}^{T} \mathbf{X}$ if and only if $\mu+\lambda$ is an eigenvalue of $\mathbf{X}^{T} \mathbf{X}+\lambda I$. Also note that if a linear function is injective, then its kernel is $\{0\}$, meaning that it does not have a zero eigenvalue. The converse is also true.
(g) The term $\lambda \mathbf{w}^{T} \mathbf{w}$ "biases" the solution towards the origin, i.e. there is a quadratic penalty for solutions $\mathbf{w}$ that are far from the origin. The parameter $\lambda$ determines the extend of this effect: As $\lambda \rightarrow 0, \hat{R}_{\text {Ridge }}(\mathbf{w})$ converges to $\hat{R}(\mathbf{w})$. As a result the optimal solution $\mathbf{w}_{\text {Ridge }}^{*}$ approaches the solution of (1). As $\lambda \rightarrow \infty$, only the quadratic penalty $\mathbf{w}^{T} \mathbf{w}$ is relevant and $\mathbf{w}_{\text {Ridge }}^{*}$ hence approaches the null vector $(0,0, \ldots, 0)$.
One can also pose this interesting question: Assume $n<d$ (as the situation discussed in (b)). Then $\mathbf{w}^{*}$ for linear regression is not unique. Denote by $\mathbf{w}_{\lambda}^{*}$ the unique solution to the Ridge regression problem for $\lambda>0$. Does the limit $\lim _{\lambda \rightarrow 0} \mathbf{w}_{\lambda}^{*}$ exist? If yes, because of completeness of $\mathbb{R}^{d}$, the limit point should fall inside the space of solutions to linear regression problem. What is this solution?

[^1]
## Problem 2 (Normal Random Variables):

Let $X$ be a Normal random variable with mean $\mu \in \mathbb{R}$ and variance $\tau^{2}>0$, i.e. $X \sim \mathcal{N}\left(\mu, \tau^{2}\right)$. Recall that the probability density of $X$ is given by

$$
f_{X}(x)=\frac{1}{\sqrt{2 \pi} \tau} e^{-(x-\mu)^{2} / 2 \tau^{2}}, \quad-\infty<x<\infty
$$

Furthermore, the random variable $Y$ given $X=x$ is normally distributed with mean $x$ and variance $\sigma^{2}$, i.e. $\left.Y\right|_{X=x} \sim \mathcal{N}\left(x, \sigma^{2}\right)$.
(a) Derive the marginal distribution of $Y$.
(b) Use Bayes' theorem to derive the conditional distribution of $X$ given $Y=y$.

Hint: For both tasks derive the density up to a constant factor and use this to identify the distribution.

## Solution 2:

Before starting calculations, it is good to mention that one can easily compute the following integral for $a>0$ by creating complete squares:

$$
\begin{aligned}
\int_{\mathbb{R}} e^{-\left(a x^{2}+2 b x+c\right)} d x & =\int_{\mathbb{R}} \exp \left(-a\left[\left(x+\frac{b}{a}\right)^{2}-\frac{b^{2}-a c}{a^{2}}\right]\right) d x \\
& =\exp \left(\frac{b^{2}-a c}{a}\right) \cdot \int_{\mathbb{R}} \exp \left(-\frac{1}{2} \frac{\left(x+\frac{b}{a}\right)^{2}}{1 / 2 a}\right) d x \\
& =\exp \left(\frac{b^{2}-a c}{a}\right) \sqrt{\pi / a}
\end{aligned}
$$

As a prelude to both (a) and (b) we consider the joint density function $f_{X, Y}(x, y)$ of $X$ and $Y$

$$
f_{X, Y}(x, y)=f_{Y \mid X}(y \mid X=x) f_{X}(x)=\frac{1}{2 \pi \sigma \tau} \exp (-\frac{1}{2} \underbrace{\left[\frac{(x-\mu)^{2}}{\tau^{2}}+\frac{(y-x)^{2}}{\sigma^{2}}\right]}_{(\mathrm{A})})
$$

For brevity, let us define

$$
\begin{aligned}
& a:=\frac{\sigma^{2}+\tau^{2}}{2 \sigma^{2} \tau^{2}} \\
& b:=-\frac{\sigma^{2} \mu+\tau^{2} y}{2 \sigma^{2} \tau^{2}}, \\
& c:=\frac{\sigma^{2} \mu^{2}+\tau^{2} y^{2}}{2 \sigma^{2} \tau^{2}} .
\end{aligned}
$$

Using simple algebraic operations, we obtain that $(\mathrm{A})=a x^{2}+2 b x+c$.
(a) The marginal density of $Y$ is given by

$$
f_{Y}(y)=\int_{\mathbb{R}} f_{X, Y}(x, y) d x=\int_{\mathbb{R}} f_{Y \mid X}(y \mid X=x) f_{X}(x) d x
$$

Using the formula discussed at the beginning of the solution, we can compute this integral by just putting in the values of $a, b$ and $c$ :

$$
\begin{aligned}
f_{Y}(y) & =\int_{\mathbb{R}} f_{X, Y}(x, y) d x \\
& =\int_{\mathbb{R}} \frac{1}{2 \pi \sigma \tau} e^{-\left(a x^{2}+2 b x+c\right)} d x \\
& =\frac{1}{2 \pi \sigma \tau} \exp \left(\frac{b^{2}-a c}{a}\right) \sqrt{\pi / a} \\
& \propto \exp \left(\frac{b^{2}-a c}{a}\right) \quad(a \text { does not depend on } y)
\end{aligned}
$$

Now we try to write $\left(b^{2}-a c\right) / a$ as a complete square:

$$
\begin{aligned}
\frac{b^{2}-a c}{a} & =\frac{1}{a}\left\{\left(\frac{\sigma^{2} \mu+\tau^{2} y}{2 \sigma^{2} \tau^{2}}\right)^{2}-\frac{\left(\sigma^{2}+\tau^{2}\right)\left(\sigma^{2} \mu^{2}+\tau^{2} y^{2}\right)}{\left(2 \sigma^{2} \tau^{2}\right)^{2}}\right\} \\
& =-\frac{1}{a} \cdot \frac{1}{\left(2 \sigma^{2} \tau^{2}\right)^{2}} \cdot\left(\sigma^{2} \tau^{2} y^{2}-2 \tau^{2} \sigma^{2} \mu y+\sigma^{2} \tau^{2} \mu^{2}\right) \\
& =-\frac{1}{a} \cdot \frac{\sigma^{2} \tau^{2}}{\left(2 \sigma^{2} \tau^{2}\right)^{2}} \cdot\left((y-\mu)^{2}+\cdots\right) \\
& =-\frac{1}{2} \frac{1}{\left(\sigma^{2}+\tau^{2}\right)} \cdot\left((y-\mu)^{2}+\cdots\right)
\end{aligned}
$$

Putting everything together yields

$$
f_{Y}(y) \propto \exp \left[-\frac{1}{2} \frac{(y-\mu)^{2}}{\left(\sigma^{2}+\tau^{2}\right)}\right]
$$

meaning that $Y$ has a Gaussian distribution with mean $\mu$ and variance $\sigma^{2}+\tau^{2}$.
(b) The conditional density of $X$ given $Y=y$ is proportional to the joint density function, i.e.

$$
f_{X \mid Y}(x \mid Y=y)=\frac{f_{X, Y}(x, y)}{f_{Y}(y)} \propto f_{X, Y}(x, y)
$$

By the discussion at the beginning of the solution, $f_{X, Y}(x, y) \propto \exp \left(-\left(a x^{2}+2 b x+c\right)\right)$. Since $c$ does not depend on $x$ (and $y$ is considered as fixed/given), we can say :

$$
f_{X \mid Y}(x \mid Y=y) \propto \exp \left(-\frac{1}{2} \frac{\left(x+\frac{b}{a}\right)^{2}}{1 / 2 a}\right)
$$

So the mean would be $-b / a$ and the variance will be $1 / 2 a$. Concretely:

$$
\text { mean }=-\frac{b}{a}=\frac{\sigma^{2} \mu+\tau^{2} y}{\sigma^{2}+\tau^{2}}=\frac{\sigma^{2}}{\sigma^{2}+\tau^{2}} \mu+\frac{\tau^{2}}{\sigma^{2}+\tau^{2}} y
$$

Note that the mean is a convex combination of $\mu$ and the observation $y$. Also

$$
\text { variance }=\frac{1}{2 a}=\frac{\sigma^{2} \tau^{2}}{\sigma^{2}+\tau^{2}}
$$

## Problem 3 (Bivariate Normal Random Variables):

Let $X$ be a bivariate Normal random variable (taking on values in $\mathbb{R}^{2}$ ) with mean $\mu=(1,1)$ and covariance matrix $\Sigma=\left(\begin{array}{ll}3 & 1 \\ 1 & 2\end{array}\right)$. The density of $X$ is then given by

$$
f_{X}(\mathbf{x})=\frac{1}{\sqrt{(2 \pi)^{2} \operatorname{det}(\Sigma)}} \exp \left(-\frac{1}{2}(\mathbf{x}-\mu)^{T} \Sigma^{-1}(\mathbf{x}-\mu)\right)
$$

Find the conditional distribution of $Y=X_{1}+X_{2}$ given $Z=X_{1}-X_{2}=0$.

## Solution 3:

We present two approaches for this exercise:
Approach 1. Note that $Z=0$ implies $X_{1}=X_{2}$. Furthermore by the definition of $Y$, we have $X_{1}=X_{2}=Y / 2$ given $Z=0$. Hence the marginal density of $Y$ given $Z=0$ is proportional to

$$
f_{Y \mid Z}(y \mid Z=0)=\frac{f_{Y, Z}(y, 0)}{f_{Z}(0)} \propto f_{Y, Z}(y, 0) \propto f_{X}\left[\binom{y / 2}{y / 2}\right]
$$

We then have

$$
\begin{aligned}
f_{X}\left[\binom{y / 2}{y / 2}\right] & \propto \exp \left(-\frac{1}{2}\binom{\frac{y}{2}-1}{\frac{y}{2}-1}^{T}\left(\begin{array}{cc}
3 & 1 \\
1 & 2
\end{array}\right)^{-1}\binom{\frac{y}{2}-1}{\frac{y}{2}-1}\right) \\
& =\exp \left(-\frac{1}{2}\binom{\frac{y}{2}-1}{\frac{y}{2}-1}^{T} \frac{1}{5}\left(\begin{array}{cc}
2 & -1 \\
-1 & 3
\end{array}\right)\binom{\frac{y}{2}-1}{\frac{y}{2}-1}\right) \\
& =\exp \left(-\frac{1}{2} \frac{(y-2)^{2}}{\frac{20}{3}}\right)
\end{aligned}
$$

Clearly the conditional distribution of $Y$ given $Z=0$ is hence Normal with mean 2 and variance $\frac{20}{3}$.
Approach 2. We define the random variable $\mathbf{R}$ as

$$
\mathbf{R}=\binom{Y}{Z}=\underbrace{\left(\begin{array}{cc}
1 & 1 \\
1 & -1
\end{array}\right)}_{=\mathbf{A}} \mathbf{X}
$$

By linearity of expectation, the mean $\mu_{\mathbf{R}}$ of $\mathbf{R}$ is

$$
\mathbb{E}[\mathbf{R}]=\mathbf{A} \mathbb{E}[\mathbf{X}]=\mathbf{A} \mu=\binom{2}{0}
$$

The covariance matrix $\boldsymbol{\Sigma}_{\mathbf{R}}$ of $\mathbf{R}$ is given by

$$
\begin{aligned}
\boldsymbol{\Sigma}_{\mathbf{R}} & =\mathbb{E}\left[(\mathbf{R}-\mathbb{E}[\mathbf{R}])(\mathbf{R}-\mathbb{E}[\mathbf{R}])^{T}\right]=\mathbb{E}\left[\mathbf{A}(\mathbf{X}-\mathbb{E}[\mathbf{X}])(\mathbf{X}-\mathbb{E}[\mathbf{X}])^{T} \mathbf{A}^{T}\right] \\
& =\mathbf{A} \mathbb{E}\left[(\mathbf{X}-\mathbb{E}[\mathbf{X}])(\mathbf{X}-\mathbb{E}[\mathbf{X}])^{T}\right] \mathbf{A}^{T}=\mathbf{A} \boldsymbol{\Sigma} \mathbf{A}^{T} \\
& =\left(\begin{array}{cc}
1 & 1 \\
1 & -1
\end{array}\right)\left(\begin{array}{cc}
3 & 1 \\
1 & 2
\end{array}\right)\left(\begin{array}{cc}
1 & 1 \\
1 & -1
\end{array}\right) \\
& =\left(\begin{array}{cc}
4 & 3 \\
2 & -1
\end{array}\right)\left(\begin{array}{cc}
1 & 1 \\
1 & -1
\end{array}\right) \\
& =\left(\begin{array}{cc}
7 & 1 \\
1 & 3
\end{array}\right)
\end{aligned}
$$

Since $\mathbf{X}$ is multivariate Gaussian and $\mathbf{R}$ is an affine transformation of $\mathbf{X}, \mathbf{R}$ is a bivariate Normal random variable with mean $\mu_{\mathbf{R}}$ and covariance matrix $\boldsymbol{\Sigma}_{\mathbf{R}}{ }^{3}$ The conditional density of $Y$ given $Z=0$ is then given by

$$
\begin{aligned}
f_{Y \mid Z}(y \mid Z=0) & =\frac{f_{Y, Z}(y, 0)}{f_{Z}(0)} \propto f_{Y, Z}(y, 0) \\
& \propto \exp \left(-\frac{1}{2}\binom{y-2}{0}^{T}\left(\begin{array}{ll}
7 & 1 \\
1 & 3
\end{array}\right)^{-1}\binom{y-2}{0}\right) \\
& =\exp \left(-\frac{1}{2}\binom{y-2}{0}^{T} \frac{1}{20}\left(\begin{array}{cc}
3 & -1 \\
-1 & 7
\end{array}\right)\binom{y-2}{0}\right) \\
& =\exp \left(-\frac{1}{2} \frac{(y-2)^{2}}{\frac{20}{3}}\right)
\end{aligned}
$$

Clearly the conditional distribution of $Y$ given $Z=0$ is hence Normal with mean 2 and variance $\frac{20}{3}$.

## 1 Supplementary Material

Lemma 1 Let $A \in \mathbb{R}^{n \times n}$ be a real matrix and define $f(\mathbf{x})=\mathbf{x}^{\top} A \mathbf{x}$ to be the quadratic form defined via $A$. Then we have $\nabla f(\mathbf{x})=\left(A+A^{\top}\right) \mathbf{x}$. Moreover, if $A$ is symmetric, then $\nabla f(\mathbf{x})=2 A \mathbf{x}$.

Proof Let us compute the derivative of $f$ at point $\mathbf{x}$. We know

$$
f(\mathbf{x}+\mathbf{h})-f(\mathbf{x})=\mathbf{h}^{\top} A \mathbf{h}+\mathbf{h}^{\top} A \mathbf{x}+\mathbf{x}^{\top} A \mathbf{h}=\left(\mathbf{h}^{\top} A+\mathbf{x}^{\top} A^{\top}+\mathbf{x}^{\top} A\right) \mathbf{h} .
$$

By taking the limit $\|\mathbf{h}\| \rightarrow 0$, the linear operator $\left(\mathbf{x}^{\top} A^{\top}+\mathbf{x}^{\top} A\right)$ would be the derivative. So the gradient would be

$$
\nabla f(\mathbf{x})=\left(A+A^{\top}\right) \mathbf{x}
$$

Lemma 2 Let $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times k}$ be two matrices. Then

$$
\operatorname{rank}(A B) \leq \operatorname{rank}(A)
$$

Proof If we denote the columns of $B$ by $\mathbf{b}_{1}, \ldots, \mathbf{b}_{k}$, then we can write $A B=\left[A \mathbf{b}_{1}, \ldots, A \mathbf{b}_{k}\right]$. Now $A \mathbf{b}_{i}$ is a linear combination of columns of $A$, so the columns of $A B$ are all linear combinations of columns of $A$. It follows that the subspace spanned by the columns of $A B$ is included in the span of columns of $A$. Hence we will have the desired inequality.

[^2]
[^0]:    ${ }^{1}$ Without loss of generality, we assume that both $\mathbf{x}_{i}$ and $y_{i}$ are centered, i.e. they have zero empirical mean. Hence we can neglect the otherwise necessary bias term $b$.

[^1]:    ${ }^{2}$ An equivalent notion for a matrix $A$ being positive semi-definite is that for all $\mathbf{x} \in \mathbb{R}^{n}$ we have $\mathbf{x}^{\top} A \mathbf{x} \geq 0$.

[^2]:    ${ }^{3}$ This result can be easily derived from the characteristic function of the multivariate Normal distribution. $\mathbf{R}$ is bivariate Normal if and only if for any $\mathbf{t} \in \mathbb{R}^{2}$

    $$
    \mathbb{E}\left[e^{i \mathbf{t}^{T} \mathbf{R}}\right]=e^{i \mathbf{t}^{T} \mu_{\mathbf{R}}-\mathbf{t}^{T} \boldsymbol{\Sigma}_{\mathbf{R}} \mathbf{t} / 2}
    $$

    This holds since the corresponding property holds for $\mathbf{X}$ with $\mathbf{s}=\mathbf{t}^{T} \mathbf{A}$, i.e.

    $$
    \mathbb{E}\left[e^{i \mathbf{t}^{T} \mathbf{R}}\right]=\mathbb{E}\left[e^{i \mathbf{t}^{T} \mathbf{A} \mathbf{X}}\right]=\mathbb{E}\left[e^{i \mathbf{s}^{T} \mathbf{X}}\right]=e^{i \mathbf{s}^{T} \mu-\mathbf{s}^{T} \boldsymbol{\Sigma} \mathbf{s} / 2}=e^{i \mathbf{t}^{T} \mathbf{A} \mu-\mathbf{t}^{T} \mathbf{A} \boldsymbol{\Sigma} \mathbf{A}^{T} \mathbf{t} / 2}=e^{i \mathbf{t}^{T} \mu_{\mathbf{R}}-\mathbf{t}^{T} \boldsymbol{\Sigma}_{\mathbf{R}} \mathbf{t} / 2}
    $$

