# Problem Solutions

Chapter 4

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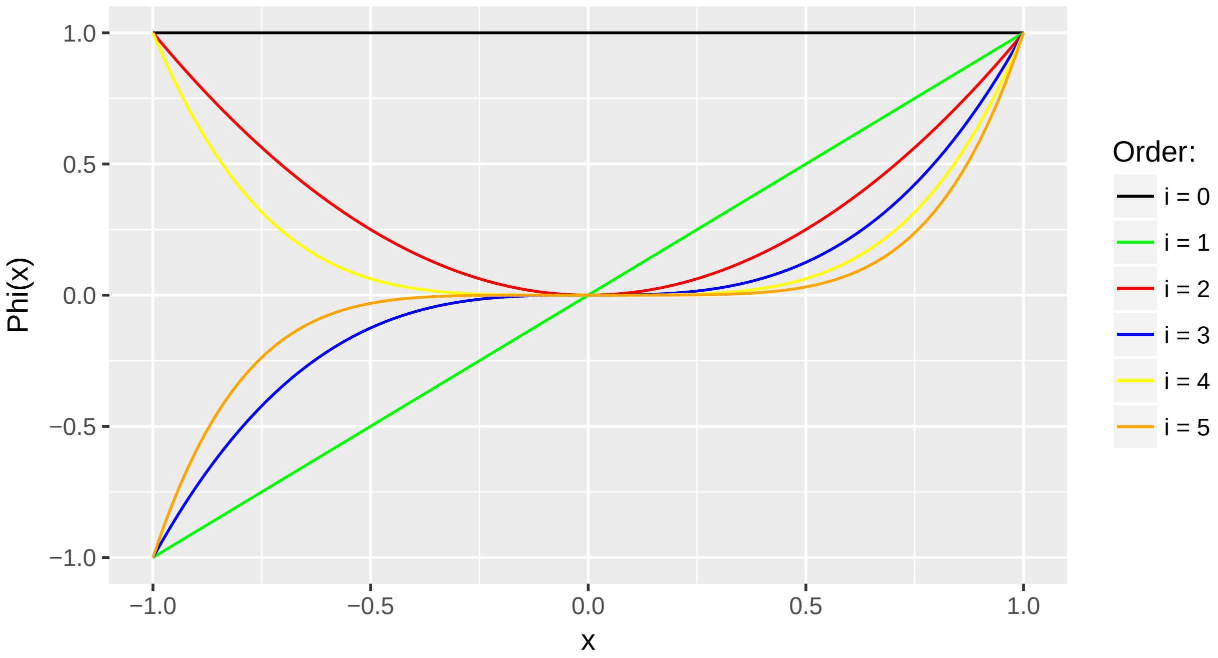
## Problem 4.1

Below we plot the monomials of order $i$, $\phi_i(x) = x^i$.



It is easy to see that as the order $i$ increases, so does the complexity of the curve (in the sense that it is able to fit more complex target functions).

## Problem 4.2

We may write

$$\begin{aligned} h(x) &= \begin{pmatrix} 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} L_0(x) \\ L_1(x) \\ L_2(x) \end{pmatrix} \\ &= L_0(x) - L_1(x) + L_2(x) \\ &= \frac{3}{2}x^2 - x + \frac{1}{2} \end{aligned}$$

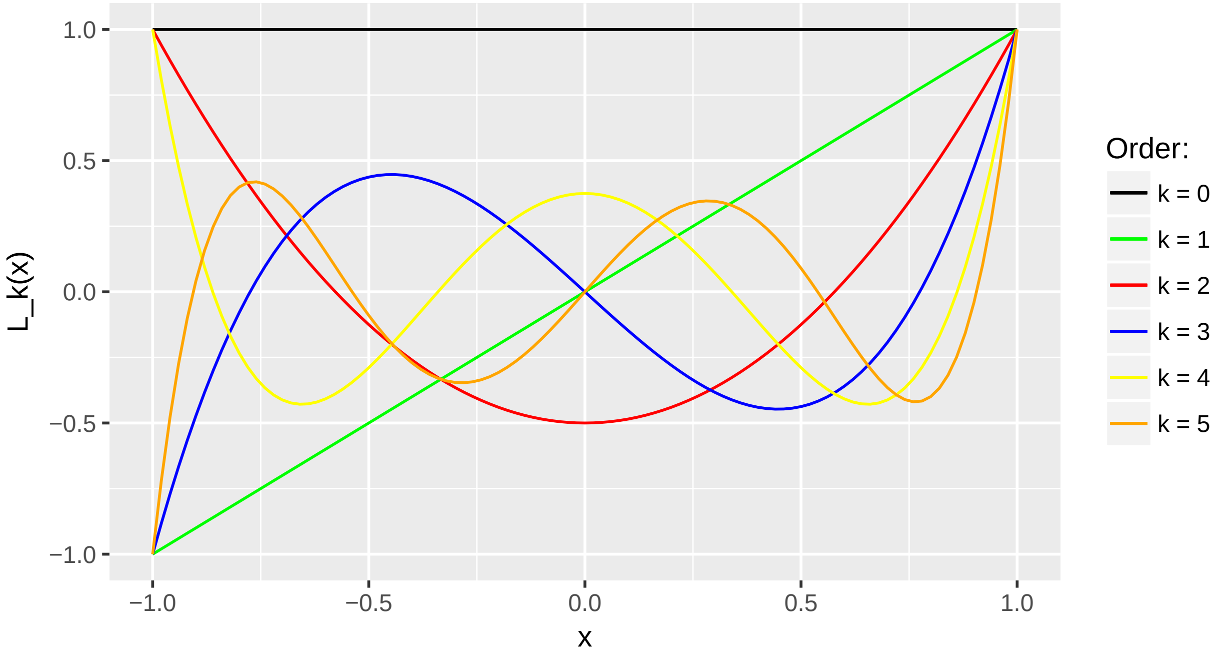
So we get a degree 2 polynomial.

## Problem 4.3

$(a)$ We use the recursive definition of the Legendre polynomials to develop an algorithm to compute $L_k(x)$ given $x$.

```
Legendre <- function(x, k) {
  if (k == 0)
    return(1)
  if (k == 1)
    return(x)
  else
    return(((2 * k - 1) / k) * x * Legendre(x, k - 1) - ((k - 1) / k) * Legendre(x, k - 2))
}
```

Now we plot the first six Legendre polynomials below.



$(b)$ We prove this fact by induction. For $k = 0$, we have $L_0(x) = 1$ which is a monomial of order 0. For $k = 1$, we have $L_1(x) = x$ which is a monomial of order 1. Now we assume that the result is true for all order less than $k + 2$, and we will prove it is still true for order $k + 2$. We will also assume that $k$ is even (the case when it is odd is proved in the same way). We have

$$\begin{aligned} L_{k+2}(x) &= \underbrace{\frac{2k+3}{k+2}}_{=c_1} x \cdot \underbrace{L_{k+1}(x)}_{=a_{k+1}x^{k+1}+a_{k-1}x^{k-1}+\cdots+a_1x} - \underbrace{\frac{k+1}{k+2}}_{=c_0} \cdot \underbrace{L_k(x)}_{=b_kx^k+b_{k-2}x^{k-2}+\cdots+b_0} \\ &= c_1a_{k+1}x^{k+2} + (c_1a_{k-1} - c_0b_k)x^k + \cdots + (c_1a_1 - c_0b_2)x^2 - c_0b_0 \end{aligned}$$

which is actually a linear combination of monomials all of even order with highest order $k + 2$. In this case we obviously have

$$L_k(-x) = (-1)^k L_k(x).$$

$(c)$ Once again we proceed by induction on $k$. For $k = 1$, we have

$$\frac{x^2-1}{1}\underbrace{\frac{dL_1(x)}{dx}}_{=1} = x^2 - 1 = xL_1(x) - L_0(x).$$

Now we assume that the result is true for all order less than $k$, and we prove it is still true for $k$. We have that

$$\begin{aligned}
&\frac{x^2-1}{k}\frac{dL_k(x)}{dx}\\
&= \frac{x^2-1}{k}\left(\frac{2k-1}{k}L_{k-1}(x)+\frac{(2k-1)x}{k}\frac{dL_{k-1}(x)}{dx}-\frac{k-1}{k}\frac{dL_{k-2}(x)}{dx}\right)\\
&= \frac{(x^2-1)(2k-1)}{k^2}L_{k-1}(x)+\frac{(2k-1)(k-1)x}{k^2}\underbrace{\frac{x^2-1}{k-1}\frac{dL_{k-1}(x)}{dx}}_{=xL_{k-1}(x)-L_{k-2}(x)}-\frac{(k-1)(k-2)}{k^2}\underbrace{\frac{x^2-1}{k-2}\frac{dL_{k-2}(x)}{dx}}_{=xL_{k-2}(x)-L_{k-3}(x)}\\
&= \frac{(2k-1)(kx^2-1)}{k^2}L_{k-1}(x)-\frac{(k-1)(3kx-3x)}{k^2}L_{k-2}(x)+\frac{(k-1)(k-2)}{k^2}L_{k-3}(x)\\
&= x\underbrace{\left(\frac{2k-1}{k}xL_{k-1}(x)-\frac{k-1}{k}L_{k-2}(x)\right)}_{=L_k(x)}-\frac{2k-1}{k^2}L_{k-1}(x)-\frac{(k-1)^2}{k^2}\underbrace{\left(\frac{2k-3}{k-1}xL_{k-2}(x)-\frac{k-2}{k-1}L_{k-3}(x)\right)}_{=L_{k-1}(x)}\\
&= xL_k(x)-\frac{(2k-1)+(k-1)^2}{k^2}L_{k-1}(x)\\
&= xL_k(x)-L_{k-1}(x).
\end{aligned}$$

$(d)$ We may write that

$$\begin{aligned}
\frac{d}{dx}\left((x^2-1)\frac{dL_k(x)}{dx}\right) &= \frac{d}{dx}\left(xkL_k(x)-kL_{k-1}(x)\right)\\
&= kL_k(x)+xk\frac{dL_k(x)}{dx}-k\frac{dL_{k-1}(x)}{dx}\\
&= kL_k(x)+\frac{k^2x^2}{x^2-1}L_k(x)-\frac{k^2x}{x^2-1}L_{k-1}(x)-\frac{k(k-1)}{x^2-1}xL_{k-1}(x)+\frac{k(k-1)}{x^2-1}L_{k-2(x)}\\
&= \frac{kx^2-k+k^2x^2}{x^2-1}L_k(x)-\frac{k}{x^2-1}[(2k-1)xL_{k-1}(x)-(k-1)L_{k-2}(x)]\\
&= \frac{kx^2-k+k^2x^2}{x^2-1}L_k(x)-\frac{k^2}{x^2-1}L_k(x)\\
&= \frac{k}{x^2-1}[(x^2-1)+kx^2-k]L_k(x)\\
&= k(k+1)L_k(x).
\end{aligned}$$

$(e)$ We will first consider the case where $l \neq k$. We have that

$$\frac{d}{dx}\left((1-x^2)\frac{dL_k(x)}{dx}\right)+k(k+1)L_k(x)=0$$

and

$$\frac{d}{dx}\left((1-x^2)\frac{dL_l(x)}{dx}\right)+l(l+1)L_l(x)=0,$$

now we multiply the first identity by $L_l(x)$ and the second by $L_k(x)$, if we substract and integrate the two identities obtained, we get

$$\int_{-1}^{1}L_l(x)\frac{d}{dx}\left((1-x^2)\frac{dL_k(x)}{dx}\right)-L_k(x)\frac{d}{dx}\left((1-x^2)\frac{dL_l(x)}{dx}\right)dx+[k(k+1)-l(l+1)]\int_{-1}^{1}L_k(x)L_l(x)dx=0.$$

Using integration by parts for the first integral, we get

$$\left(\underbrace{L_l(x)(1-x^2)\frac{dL_k(x)}{dx}\bigg|_{-1}^{1}}_{=0} - \underbrace{L_k(x)(1-x^2)\frac{dL_l(x)}{dx}\bigg|_{-1}^{1}}_{=0}\right) - \underbrace{\int_{-1}^{1} \frac{dL_l(x)}{dx}(1-x^2)\frac{dL_k(x)}{dx} - \frac{dL_k(x)}{dx}(1-x^2)\frac{dL_l(x)}{dx}dx}_{=0} = 0.$$

Finally, we obtain

$$\int_{-1}^{1} L_k(x)L_l(x)dx = 0.$$

Now, we consider the case where $l = k$. We have that

$$\begin{aligned}
A_k = \int_{-1}^{1} L_k^2(x) &= \frac{2k-1}{k}\int_{-1}^{1} xL_k(x)L_{k-1}(x)dx - \frac{k-1}{k}\underbrace{\int_{-1}^{1} L_k(x)L_{k-2}(x)dx}_{=0} \\
&= \frac{(2k-1)(k+1)}{k(2k+1)}\underbrace{\int_{-1}^{1} L_{k+1}(x)L_{k-1}(x)dx}_{=0} + \frac{(2k-1)k}{k(2k+1)}\int_{-1}^{1} L_{k-1}^2(x)dx \\
&= \frac{2k-1}{2k+1}\int_{-1}^{1} L_{k-1}^2(x)dx.
\end{aligned}$$

Finally, we are able to obtain that

$$\begin{aligned}
A_k &= \frac{2k-1}{2k+1}A_{k-1} \\
&= \frac{2k-1}{2k+1}\cdot\frac{2k-3}{2k-1}A_{k-2} \\
&= \frac{2k-1}{2k+1}\cdot\frac{2k-3}{2k-1}\cdots\frac{3}{5}\frac{1}{3}\underbrace{A_0}_{=2} \\
&= \frac{2}{2k+1}.
\end{aligned}$$

## Problem 4.4

The following code is an implementation of the experimental framework used to study various aspects of overfitting.

```
Legendre2 <- function(x, q) {
  vec <- rep(NA, q + 1)
  for (k in 0:q) {
    vec[k + 1] <- (choose(q, k))^2 * (x - 1)^(q - k) * (x + 1)^k / 2^q
  }

  return(sum(vec))
}

f <- function(x, Qf, aq) {
  Lq <- rep(0, Qf + 1)
  for (k in 0:Qf) {
    Lq[k + 1] <- Legendre2(x, k)
  }

  return(sum(aq * Lq))
}
f <- Vectorize(f, vectorize.args = "x")

experiment <- function(Qf, N, sigma, Ntest) {
  aq <- rnorm(Qf + 1)
  norm <- rep(0, Qf + 1)
  for (q in 0:Qf)
    norm[q + 1] <- 1 / (2 * q + 1)
  norm_fac <- 1 / sqrt(sum(norm))
  aq <- norm_fac * aq

  xn <- runif(N, min = -1, max = 1)
  eps <- rnorm(N)
  yn <- f(xn, Qf, aq) + sigma * eps
  D <- data.frame(x = xn, y = yn)

  y <- D$y
  D2 <- data.frame(x = D$x, x_sq = D$x^2)
  Z2 <- as.matrix(cbind(1, D2))
  Z2_cross <- solve(t(Z2) %*% Z2) %*% t(Z2)
  w2 <- as.vector(Z2_cross %*% y)
  D10 <- data.frame(x = D$x, x_sq = D$x^2, x_cub = D$x^3, x_quad = D$x^4,
                    x_quint = D$x^5, x_six = D$x^6, x_seven = D$x^7,
                    x_eight = D$x^8, x_nine = D$x^9, x_ten = D$x^10)
  Z10 <- as.matrix(cbind(1, D10))
  Z10_cross <- solve(t(Z10) %*% Z10) %*% t(Z10)
  w10 <- as.vector(Z10_cross %*% y)

  x <- runif(Ntest, min = -1, max = 1)
  eps <- rnorm(Ntest)
  y <- f(x, Qf, aq) + sigma * eps
  Dtest <- data.frame(x = x, y = y)
  Eout2 <- mean((as.matrix(cbind(1, Dtest$x, Dtest$x^2)) %*% w2 - Dtest$y)^2)
  Eout10 <- mean((as.matrix(cbind(1, Dtest$x, Dtest$x^2, Dtest$x^3, Dtest$x^4,
                                  Dtest$x^5, Dtest$x^6, Dtest$x^7, Dtest$x^8,
                                  Dtest$x^9, Dtest$x^10)) %*% w10 - Dtest$y)^2)

  return(c(Eout2, Eout10))
}
```

$(a)$ To normalize $f$, we compute $\mathbb{E}_{a,x}[f^2]$ as follows,

$$
\begin{aligned}
\mathbb{E}_{a,x}[f^2] &= \mathbb{E}_x[\mathbb{E}_{a|x}[f^2|x]] \\
&= \mathbb{E}_x[\underbrace{\mathrm{Var}_{a|x}[f]}_{=\sum_q L_q^2(x)\underbrace{\mathrm{Var}_{a|x}[a_q]}_{=1}} + (\underbrace{\mathbb{E}_{a|x}[f]}_{=\sum_q L_q(x)\underbrace{\mathbb{E}_{a|x}[a_q]}_{=0}})^2] \\
&= \sum_{q=0}^{Q_f} \mathbb{E}_x[L_q^2(x)].
\end{aligned}
$$

Moreover, we may write that

$$\mathbb{E}_x[L_q^2(x)] = \frac{1}{2}\int_{-1}^{1} L_q^2(x)dx = \frac{1}{2q+1},$$

with which we can conclude that

$$\mathbb{E}_{a,x}[f^2] = \sum_{q=0}^{Q_f} \frac{1}{2q+1}.$$

This means that, to normalize $f$, we have to multiply each coefficient $a_q$ by the constant factor $1/\sqrt{\sum_q \frac{1}{2q+1}}$. Obviously, if the signal $f$ is normalized to $\mathbb{E}[f^2] = 1$, this implies that the noise level $\sigma^2$ is automatically calibrated to the signal level.

$(b)$ To obtain $g_2$ and $g_{10}$, we first transform the original data $x \in \mathcal{X}$ with a second (resp. tenth) order transformation $z = \Phi_2(x) \in \mathcal{Z}_2$ (resp. $z = \Phi_{10}(x) \in \mathcal{Z}_{10}$). Then, we find the best linear fit for the data in $\mathcal{Z}_2$-space (resp. $\mathcal{Z}_{10}$-space) to find $\tilde{g}_2 = \tilde{w}^T z$ (resp. $\tilde{g}_{10} = \tilde{w}^T z$). And finally, we get the best fit in $\mathcal{X}$-space

$$g_2(x) = \tilde{g}_2(\Phi_2(x)) = \tilde{w}^T\Phi_2(x) \text{ (resp. } g_{10}(x) = \tilde{g}_{10}(\Phi_{10}(x)) = \tilde{w}^T\Phi_{10}(x)).$$

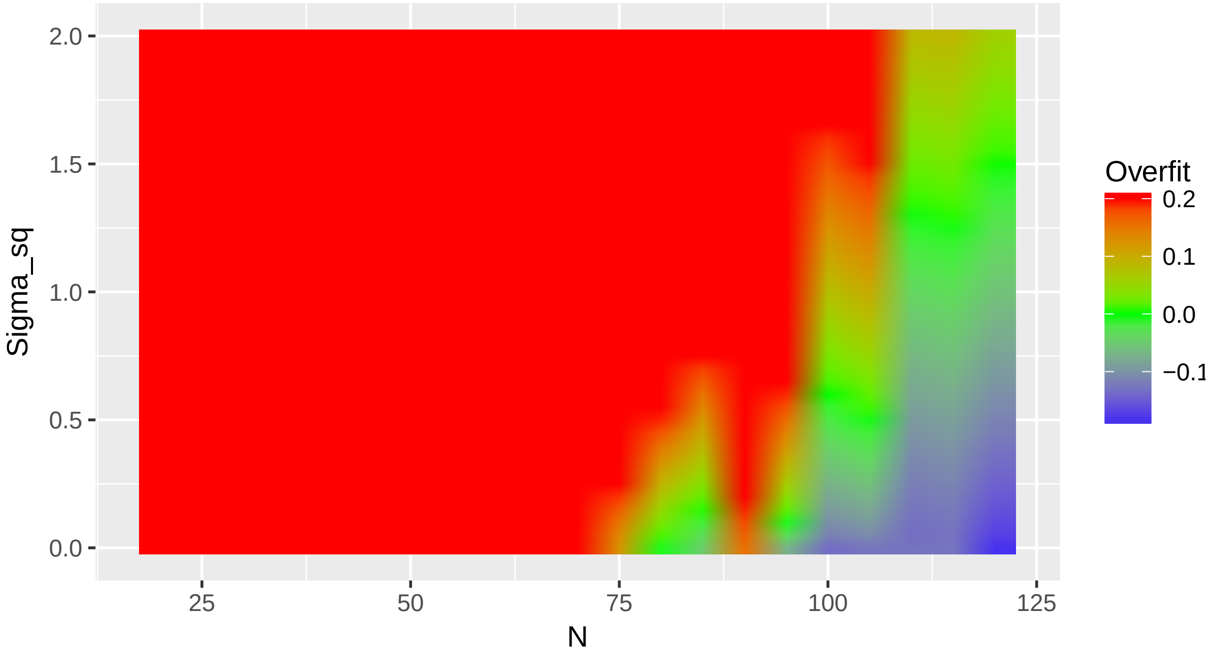
$(c)$ To compute analytically $E_{out}$ for a given $g_{10}$ we have to compute

$$E_{out}(g_{10}) = \mathbb{E}_{x,y}[(g_{10}(x) - y(x))^2] = \mathbb{E}_{x,y}[(g_{10}(x) - f(x) - \sigma\epsilon)^2] = \mathbb{E}_x[\mathbb{E}_{y|x}[(g_{10}(x) - f(x) - \sigma\epsilon)^2|x]].$$

$(d)$ Below we plot the extent of overfitting depending on certain parameters of the learning problem. In the first plot, we fix $Q_f = 20$ to study the stochastic noise.

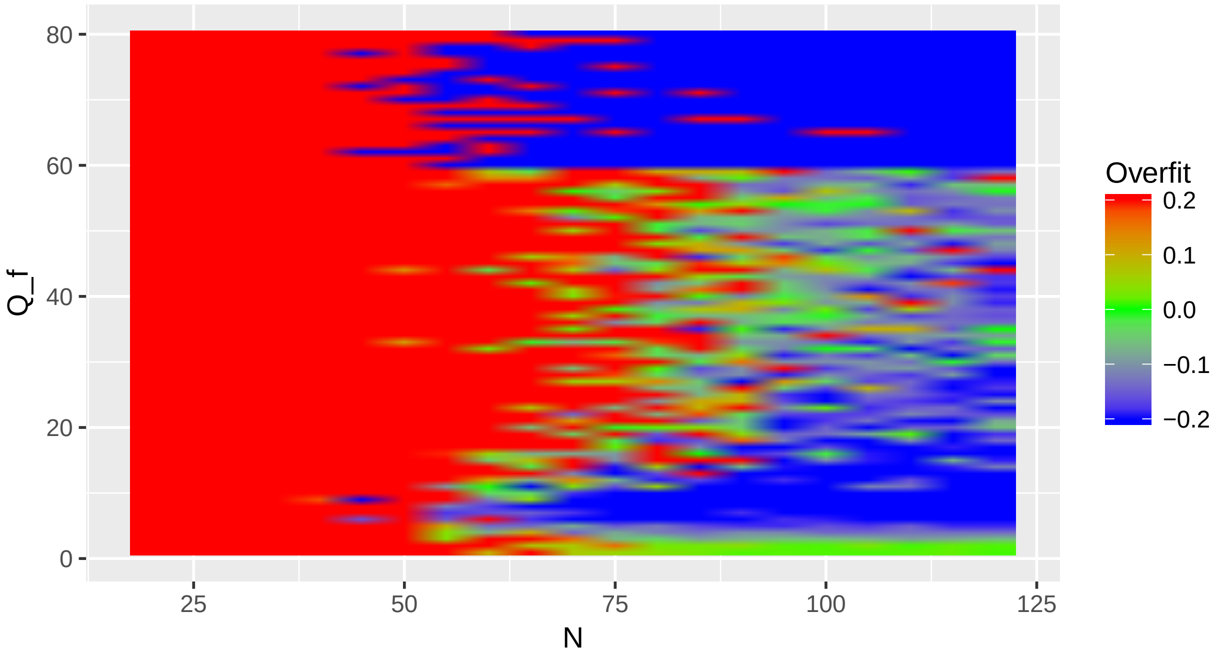
```r
# Grid search with Qf = 20
Nexp <- 1000
grid <- expand.grid(N = seq(20, 120, by = 5), sigma_sq = seq(0, 2, by = 0.05))
E_out_Overfit <- foreach(i = 1:nrow(grid), .combine = "rbind") %dopar% {
                  set.seed(1975)
                  Eout_H2 <- numeric(Nexp)
                  Eout_H10 <- numeric(Nexp)
                  for (n in 1:Nexp) {
                    tmp <- experiment(Qf = 20, grid$N[i], sqrt(grid$sigma[i]), Ntest = 100)
                    Eout_H2[n] <- tmp[1]
                    Eout_H10[n] <- tmp[2]
                  }
                  c(mean(Eout_H2), mean(Eout_H10))
                }
Eout <- cbind(grid, E_out_Overfit)
colnames(Eout) <- c("N", "sigma_sq", "Eout_H2", "Eout_H10")
Eout["Overfit"] <- Eout$Eout_H10 - Eout$Eout_H2
Eout$Overfit <- ifelse(Eout$Overfit > 0.2, 0.2, Eout$Overfit)
```

```
Eout$Overfit <- ifelse(Eout$Overfit < -0.2, -0.2, Eout$Overfit)

ggplot(Eout, aes(N, sigma_sq, fill = Overfit)) + geom_raster(interpolate = TRUE) +
  xlab("N") + ylab("Sigma_sq") +
  scale_fill_gradient2(low = "blue", mid = "green", high = "red")
```



In the second plot, we fix $\sigma^2 = 0.1$ to study the deterministic noise.

```
# grid search with sigma_sq = 0.1
Nexp <- 200
grid <- expand.grid(Qf = seq(1, 80, by = 1), N = seq(20, 120, by = 5))
E_out_Overfit <- foreach(i = 1:nrow(grid), .combine = "rbind") %dopar% {
                  set.seed(1975)
                  Eout_H2 <- numeric(Nexp)
                  Eout_H10 <- numeric(Nexp)
                  for (n in 1:Nexp) {
                    tmp <- experiment(grid$Qf[i], grid$N[i], sqrt(0.1), Ntest = 10)
                    Eout_H2[n] <- tmp[1]
                    Eout_H10[n] <- tmp[2]
                  }
                  c(mean(Eout_H2), mean(Eout_H10))
                }
Eout <- cbind(grid, E_out_Overfit)
colnames(Eout) <- c("Qf", "N", "Eout_H2", "Eout_H10")
Eout["Overfit"] <- Eout$Eout_H10 - Eout$Eout_H2
Eout$Overfit <- ifelse(Eout$Overfit > 0.2, 0.2, Eout$Overfit)
Eout$Overfit <- ifelse(Eout$Overfit < -0.2, -0.2, Eout$Overfit)

ggplot(Eout, aes(N, Qf, fill = Overfit)) + geom_raster(interpolate = TRUE) +
  xlab("N") + ylab("Q_f") +
  scale_fill_gradient2(low = "blue", mid = "green", high = "red")
```



$(e)$ We take the average over many experiments because we want estimates of the expected out-of-sample error for a given learning scenario $(Q_f, N, \sigma)$ using $\mathcal{H}_2$ and $\mathcal{H}_{10}$.

## Problem 4.5

If we consider the following constrained optimization problem

$$\min_w E_{in}(w) \text{ subject to } w^T w \geq C,$$

the theory of Lagrange multipliers tells us that this problem is equivalent to the following unconstrained optimization problem

$$\min_w (E_{in}(w) - \lambda_C' w^T w) \ ; \ \lambda_C' \geq 0.$$

If we let $\lambda_C = -\lambda_C'$, we get that the original constrained optimization problem is equivalent to minimizing the augmented error

$$E_{aug}(w) = E_{in}(w) + \lambda_C w^T w \ ; \ \lambda_C \leq 0.$$

So, we may conclude that the soft order constraint corresponding to this problem is $w^T w \geq C$.

## Problem 4.6

$(a)$ We begin by noting that

$$E_{in}(w_{reg}) = \frac{(w_{reg} - w_{lin})^T Z^T Z (w_{reg} - w_{lin}) + y^T (I - H) y}{N} \geq \frac{y^T (I - H) y}{N} = E_{in}(w_{lin}).$$

Now we suppose that $||w_{reg}|| > ||w_{lin}||$, in this case we may write that

$$E_{aug}(w_{reg}) = E_{in}(w_{reg}) + \lambda ||w_{reg}||^2 > E_{in}(w_{lin}) + \lambda ||w_{lin}||^2 = E_{aug}(w_{lin}),$$

which is not possible since $w_{reg} = \text{argmin}_w E_{aug}(w)$. So, we may conclude that $||w_{reg}|| \leq ||w_{lin}||$.

$(b)$ First, we note that if $v_i$ are eigenvectors with eigenvalues $\lambda_i$ of a matrix $A$, then $Av_i = \lambda_i v_i$, and consequently

$$v_i = \lambda_i A^{-1} v_i \Leftrightarrow A^{-1} v_i = \frac{1}{\lambda_i} v_i \Rightarrow A^{-2} v_i = \frac{1}{\lambda_i^2} v_i,$$

which means that $v_i$ are also eigenvectors of $A^{-2}$ with eigenvalues $1/\lambda_i^2$.

Now, let $v_i$ be the orthogonal eigenvectors of non-zero eigenvalues $\lambda_i$ of $Z^TZ$ (since $Z^TZ$ is invertible and symmetric). We have that

$$||w_{reg}||^2 = y^TZ(Z^TZ+\lambda I)^{-2}Z^Ty = u^T(Z^TZ+\lambda I)^{-2}u,$$

and

$$||w_{lin}||^2 = y^TZ(Z^TZ)^{-2}Z^Ty = u^T(Z^TZ)^{-2}u$$

where $u = Z^Ty$; if we let $V = (v_0, \cdots, v_Q)$ be the orthogonal matrix of eigenvectors, we get

$$V^TZ^TZV = \text{diag}(\lambda_i)$$

and

$$V^T(Z^TZ+\lambda I)V = V^TZ^TZV + \lambda V^TV = \text{diag}(\lambda_i+\lambda).$$

If we expand $u$ in the eigenbasis of $Z^TZ$, we get that $u = \sum_i \alpha_i v_i$ and

$$\begin{aligned}
||w_{reg}||^2 &= \sum_{i,j} \alpha_i\alpha_j v_i^T(Z^TZ+\lambda I)^{-2}v_j \\
&= \sum_{i,j} \alpha_i\alpha_j \frac{1}{(\lambda_i+\lambda)^2} v_i^Tv_j \\
&= \sum_i \frac{\alpha_i^2}{(\lambda_i+\lambda)^2} \\
&\leq \sum_i \frac{\alpha_i^2}{\lambda_i^2} = \sum_{i,j} \alpha_i\alpha_j v_i^T(Z^TZ)^{-2}v_j = ||w_{lin}||^2;
\end{aligned}$$

for the above inequality to be true, we have to note that since $Z^TZ$ is (at least) semi positive definite, its eigenvalues are non-negative.

## Problem 4.7

Here, for our $(N \times d)$ matrix $Z$, we assume that $N > d$, and in this case $U$ is a $(N \times d)$ orthogonal matrix, $D$ is a $(d \times d)$ diagonal matrix and $V$ is a $(d \times d)$ orthogonal matrix. We begin by noting that

$$Z^TZ = V\Gamma U^TU\Gamma V^T = V\Gamma^2V^T.$$

Let us first consider the vector $Hy$, we have

$$\begin{aligned}
Hy &= Z(Z^TZ)^{-1}Z^Ty \\
&= U\Gamma V^T(V^T)^{-1}\Gamma^{-2}V^{-1}V\Gamma U^Ty \\
&= UU^Ty;
\end{aligned}$$

moreover, we also have for $H(\lambda)y$ that

$$\begin{aligned} H(\lambda)y &= Z(Z^TZ+\lambda I)^{-1}Z^Ty \\ &= U\Gamma V^T(V\Gamma^2V^T+\lambda I)^{-1}V\Gamma U^Ty \\ &= U\Gamma V^T[V\underbrace{(\Gamma^2+\lambda I)}_{=\text{diag}(\sigma_i^2+\lambda)}V^T]^{-1}V\Gamma U^Ty \\ &= U\Gamma V^T(V^T)^{-1}\text{diag}\left(\frac{1}{\sigma_i^2+\lambda}\right)V^{-1}V\Gamma U^Ty \\ &= U\text{diag}\left(\frac{\sigma_i^2}{\sigma_i^2+\lambda}\right)U^Ty. \end{aligned}$$

Putting all of the above together, we get

$$(I-H(\lambda))y = (I-H)y+(H-H(\lambda))y = (I-H)y+U\text{diag}\left(1-\frac{\sigma_i^2}{\sigma_i^2+\lambda}\right)U^Ty,$$

and consequently

$$\begin{aligned} &E_{in}(w_{reg}) \\ &= \frac{1}{N}y^T(I-H(\lambda))^2y \\ &= \frac{1}{N}y^T(I-H(\lambda))^T(I-H(\lambda))y \\ &= \frac{1}{N}[y^T(I-H)y+2y^T(I-H)U\text{diag}\left(1-\frac{\sigma_i^2}{\sigma_i^2+\lambda}\right)U^Ty+y^TU\text{diag}\left(1-\frac{\sigma_i^2}{\sigma_i^2+\lambda}\right)U^TU\text{diag}\left(1-\frac{\sigma_i^2}{\sigma_i^2+\lambda}\right)U^Ty] \\ &= \frac{1}{N}[y^T(I-H)y+y^TU\text{diag}\left(1-\frac{\sigma_i^2}{\sigma_i^2+\lambda}\right)^2U^Ty+2y^T\underbrace{(I-H)U}_{=U-HU=U-UU^TU=0}\text{diag}\left(1-\frac{\sigma_i^2}{\sigma_i^2+\lambda}\right)U^Ty \\ &= E_{in}(w_{lin})+\frac{1}{N}\sum_i a_i^2\left(1-\frac{\sigma_i^2}{\sigma_i^2+\lambda}\right)^2. \end{aligned}$$

## Problem 4.8

First, we compute $\nabla E_{aug}(w)$, we immediately have

$$\nabla E_{aug}(w) = \nabla E_{in}(w)+2\lambda w.$$

So the gradient descent update rule becomes

$$w(t+1)\leftarrow w(t)-\eta\nabla E_{aug}(w(t)) = (1-2\eta\lambda)w(t)-\eta\nabla E_{in}(w(t)).$$

## Problem 4.9

$(a)$ Let $\Gamma$ be the following matrix

$$\Gamma = \begin{pmatrix} - & \gamma_1^T & - \\ & \vdots & \\ - & \gamma_k^T & - \end{pmatrix},$$

now we construct a virtual example $(z_i, 0)$ where $z_i = \sqrt{\lambda}\gamma_i$ for $i = 1, \cdots, k$. If $\mathcal{D} = \{(z'_1, y_1), \cdots, (z'_N, y_N)\}$, this means that the matrix for the augmented data is

$$Z_{aug} = \begin{pmatrix} - & z_1'^T & - \\ & \vdots & \\ - & z_N'^T & - \\ \hline - & z_1^T & - \\ & \vdots & \\ - & z_k^T & - \end{pmatrix} = \begin{pmatrix} Z \\ \hline \sqrt{\lambda}\Gamma \end{pmatrix}$$

and

$$y_{aug} = \begin{pmatrix} y_1 \\ \vdots \\ y_N \\ \hline 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} y \\ \hline 0 \end{pmatrix}.$$

$(b)$ If we solve the least squares problem with $Z_{aug}$ and $y_{aug}$, we get

$$\begin{aligned} w_{lin} &= (Z_{aug}^T Z_{aug})^{-1} Z_{aug}^T y_{aug} \\ &= [(Z^T | \sqrt{\lambda}\Gamma^T) \begin{pmatrix} Z \\ \hline \sqrt{\lambda}\Gamma \end{pmatrix}]^{-1} (Z^T | \sqrt{\lambda}\Gamma^T) \begin{pmatrix} y \\ \hline 0 \end{pmatrix} \\ &= (Z^T Z + \lambda \Gamma^T \Gamma)^{-1} Z^T y = w_{reg}. \end{aligned}$$

## Problem 4.10

$(a)$ If $w_{lin}^T \Gamma^T \Gamma w_{lin} \leq C$, then obviously $w_{reg} = w_{lin}$.

$(b)$ If $w_{lin}^T \Gamma^T \Gamma w_{lin} > C$, then we have that $w_{reg}^T \Gamma^T \Gamma w_{reg} = C$ (see the book illustration).

$(c)$ The original constrained problem is equivalent to solving the following unconstrained problem with Lagrange multipliers,

$$\min_w (\underbrace{E_{in}(w) - \lambda_C(-w^T \Gamma^T \Gamma w + C)}_{=L(w,\lambda_C)})$$

where $\lambda_C \geq 0$. We have that

$$\nabla_{w,\lambda_C} L(w, \lambda_C) = (\nabla_w L(w, \lambda_C), \frac{\partial}{\partial \lambda_C} L(w, \lambda_C))$$

where

$$\nabla_w L(w, \lambda_C) = \nabla E_{in}(w) + 2\lambda_C \Gamma^T \Gamma w \text{ and } \frac{\partial}{\partial \lambda_C} L(w, \lambda_C) = w^T \Gamma^T \Gamma w - C.$$

Since $w_{reg}$ is a solution to the original constrained problem, it must also be a solution to the equivalent unconstrained problem, this means that

$$\nabla E_{in}(w_{reg}) + 2\lambda_C \Gamma^T \Gamma w_{reg} = 0 \text{ and } w_{reg}^T \Gamma^T \Gamma w_{reg} - C = 0;$$

if we solve for $\lambda_C$, we get that

$$w_{reg}^T \nabla E_{in}(w_{reg}) + 2\lambda_C \underbrace{w_{reg}^T \Gamma^T \Gamma w_{reg}}_{=C} = 0,$$

and consequently

$$\lambda_C = -\frac{1}{2C} w_{reg}^T \nabla E_{in}(w_{reg}).$$

$(d)$ $(i)$ If $w_{lin}^T \Gamma^T \Gamma w_{lin} \leq C$, we know that $w_{reg} = w_{lin}$, and consequently $\nabla E_{in}(w_{reg}) = 0$, which implies that $\lambda_C = 0$.

$(ii)$ If $w_{lin}^T \Gamma^T \Gamma w_{lin} > C$, let us assume that $\lambda_C = 0$, this means that $w_{reg}$ minimizes

$$E_{in}(w) - \lambda_C(-w^T \Gamma^T \Gamma w + C) = E_{in}(w),$$

so we have $w_{reg} = w_{lin}$ and

$$w_{reg}^T \Gamma^T \Gamma w_{reg} = w_{lin}^T \Gamma^T \Gamma w_{lin} > C,$$

which is not possible since $w_{reg}^T \Gamma^T \Gamma w_{reg} \leq C$ by definition. In conclusion, we have that $\lambda_C > 0$.

$(iii)$ As $w_{lin}^T \Gamma^T \Gamma w_{lin} > C$, we have that $\lambda_C > 0$ which means that $w_{reg}^T \nabla E_{in}(w_{reg}) < 0$. Now, if we compute the derivative relative to $C$, we get

$$\frac{d\lambda_C}{dC} = \frac{1}{2C^2} w_{reg}^T \nabla E_{in}(w_{reg}) < 0.$$

## Problem 4.11

$(a)$ We have immediately

$$w_{lin} = (Z^T Z)^{-1} Z^T y = (Z^T Z)^{-1} Z^T (Z w_f + \epsilon) = w_f + (Z^T Z)^{-1} Z^T \epsilon.$$

And so the average function $\overline{g}$ is given by

$$\begin{aligned}
\overline{g}(x) &= \mathbb{E}_{\mathcal{D}}[g^{\mathcal{D}}(x)] \\
&= \mathbb{E}_{\mathcal{D}}[\Phi(x)^T w_{lin}] \\
&= \Phi(x)^T w_f + \mathbb{E}_{\mathcal{D}}[\Phi(x)^T (Z^T Z)^{-1} Z^T \epsilon]] \\
&= \Phi(x)^T w_f + \mathbb{E}_Z[E_{y|Z}[\Phi(x)^T (Z^T Z)^{-1} Z^T \epsilon | Z]] \\
&= \Phi(x)^T w_f + \mathbb{E}_Z[\Phi(x)^T (Z^T Z)^{-1} Z^T \underbrace{E_{y|Z}[\epsilon | Z]]}_{=\mathbb{E}_\epsilon[\epsilon]=0} \\
&= \Phi(x)^T w_f = f(x),
\end{aligned}$$

which means that

$$\text{bias}(x) = (\overline{g}(x) - f(x))^2 = 0,$$

and consequently bias $= \mathbb{E}_x[\text{bias}(x)] = 0$.

$(b)$ We may write that

$$\begin{aligned}
\text{var}(x) &= \mathbb{E}_{\mathcal{D}}[(g^{\mathcal{D}}(x) - \overline{g}(x))^2] \\
&= \mathbb{E}_{\mathcal{D}}[(g^{\mathcal{D}}(x) - f(x))^2] \\
&= \mathbb{E}_{\mathcal{D}}[(\Phi(x)^T (w_f + (Z^T Z)^{-1} Z^T \epsilon) - \Phi(x)^T w_f)^2] \\
&= \mathbb{E}_{\mathcal{D}}[\underbrace{\epsilon^T Z (Z^T Z)^{-1} \Phi(x) \Phi(x)^T (Z^T Z)^{-1} Z^T \epsilon]}_{=\text{trace}(\Phi(x)\Phi(x)^T (Z^T Z)^{-1} Z^T \epsilon\epsilon^T Z (Z^T Z)^{-1})} \\
&= \text{trace}(\mathbb{E}_Z[\mathbb{E}_{y|Z}[\Phi(x)\Phi(x)^T (Z^T Z)^{-1} Z^T \epsilon\epsilon^T Z (Z^T Z)^{-1} | Z]) \\
&= \text{trace}(\mathbb{E}_Z[\Phi(x)\Phi(x)^T (Z^T Z)^{-1} Z^T \underbrace{\mathbb{E}_{y|Z}[\epsilon\epsilon^T | Z]}_{=\mathbb{E}_\epsilon[\epsilon\epsilon^T]=\sigma^2 I} Z (Z^T Z)^{-1}]) \\
&= \sigma^2 \text{trace}(\mathbb{E}_Z[\Phi(x)\Phi(x)^T (Z^T Z)^{-1}])
\end{aligned}$$

where we have used the cyclic property of the trace. This allows us to write that

$$\begin{aligned}\text{var} &= \mathbb{E}_x[\text{var}(x)]\\ &= \sigma^2\text{trace}(\mathbb{E}_Z[\mathbb{E}_x[\Phi(x)\Phi(x)^T(Z^TZ)^{-1}]])\\ &= \sigma^2\text{trace}(\mathbb{E}_Z[\underbrace{\mathbb{E}_x[\Phi(x)\Phi(x)^T]}_{=\Sigma_\Phi}(Z^TZ)^{-1}])\\ &= \frac{\sigma^2}{N}(\Sigma_\Phi\mathbb{E}_Z[(\frac{1}{N}Z^TZ)^{-1}]).\end{aligned}$$

$(c)$ We know by the law of large numbers that $\frac{1}{N}Z^TZ$ converges in probability to $\Sigma_\Phi$, this implies that $(\frac{1}{N}Z^TZ)^{-1}$ converges in probability to $\Sigma_\Phi^{-1}$. With that in mind, to the first order in $1/N$, we have that

$$\text{var} \approx \frac{\sigma^2}{N}\text{trace}(\Sigma_\Phi\Sigma_\Phi^{-1}) = \frac{\sigma^2(Q+1)}{N}.$$

## Problem 4.12

$(a)$ We may write that

$$\begin{aligned}w_{reg} &= (Z^TZ+\lambda I)^{-1}Z^T(Zw_f+\epsilon)\\ &= (Z^TZ+\lambda I)^{-1}[(Z^TZw_f+\lambda w_f)-\lambda w_f]+(Z^TZ+\lambda I)^{-1}Z^T\epsilon\\ &= w_f-\lambda(Z^TZ+\lambda I)^{-1}w_f+(Z^TZ+\lambda I)^{-1}Z^T\epsilon.\end{aligned}$$

$(b)$ The average function $\overline{g}$ is given by

$$\begin{aligned}\overline{g}(x) &= \mathbb{E}_{\mathcal{D}}[g^{\mathcal{D}}(x)]\\ &= \mathbb{E}_{\mathcal{D}}[\Phi(x)^Tw_{reg}]\\ &= \mathbb{E}_{\mathcal{D}}[\Phi(x)^T(w_f-\lambda(Z^TZ+\lambda I)^{-1}w_f+(Z^TZ+\lambda I)^{-1}Z^T\epsilon)]\\ &= \mathbb{E}_Z[\Phi(x)^Tw_f-\lambda\Phi(x)^T(Z^TZ+\lambda I)^{-1}w_f+\Phi(x)^T(Z^TZ+\lambda I)^{-1}Z^T\underbrace{\mathbb{E}_{y|Z}[\epsilon|Z]]}_{=0}\\ &= \Phi(x)^Tw_f-\lambda\Phi(x)^T\mathbb{E}_Z[(Z^TZ+\lambda I)^{-1}]w_f.\end{aligned}$$

Thus, thanks to the cyclic property of the trace, the bias$(x)$ is equal to

$$\begin{aligned}\text{bias}(x) &= (\overline{g}(x)-f(x))^2\\ &= \lambda^2w_f^T\mathbb{E}_Z[(Z^TZ+\lambda I)^{-1}]\Phi(x)\Phi(x)^T\mathbb{E}_Z[(Z^TZ+\lambda I)^{-1}]w_f\\ &= \lambda^2\text{trace}(\Phi(x)^T\Phi(x)\mathbb{E}_Z[(Z^TZ+\lambda I)^{-1}]w_fw_f^T\mathbb{E}_Z[(Z^TZ+\lambda I)^{-1}]),\end{aligned}$$

consequently, we have that

$$\begin{aligned}
\text{bias} &= \mathbb{E}_x[\text{bias}(x)] \\
&= \lambda^2 \text{trace}(\underbrace{\mathbb{E}_x[\Phi(x)^T\Phi(x)]}_{=I}\mathbb{E}_Z[(Z^TZ+\lambda I)^{-1}]w_f w_f^T \mathbb{E}_Z[(Z^TZ+\lambda I)^{-1}]) \\
&= \lambda^2 \text{trace}(\mathbb{E}_Z[\underbrace{(Z^TZ+\lambda I)^{-1}}_{\approx \frac{1}{N+\lambda}I}]w_f w_f^T \mathbb{E}_Z[\underbrace{(Z^TZ+\lambda I)^{-1}}_{\approx \frac{1}{N+\lambda}I}]) \\
&\approx \frac{\lambda^2}{(N+\lambda)^2} \quad \underbrace{\text{trace}(w_f w_f^T)}_{=\text{trace}(w_f^T w_f)=||w_f||^2} \\
&\approx \frac{\lambda^2}{(N+\lambda)^2}||w_f||^2,
\end{aligned}$$

since $Z^TZ \approx N\Sigma_\Phi = NI$.

Now, if we compute var$(x)$, we get

$$\begin{aligned}
\text{var}(x) &= \mathbb{E}_{\mathcal{D}}[(g^{\mathcal{D}} - \overline{g}(x))^2] \\
&= \mathbb{E}_{\mathcal{D}}[(\lambda\Phi(x)^T(\underbrace{\mathbb{E}_Z[(Z^TZ-\lambda I)^{-1}}_{\approx \frac{1}{N+\lambda}I}] - \underbrace{(Z^TZ-\lambda I)^{-1}}_{\approx \frac{1}{N+\lambda}I})w_f + \Phi(x)^T(Z^TZ+\lambda I)^{-1}Z^T\epsilon)^2] \\
&\approx \mathbb{E}_{\mathcal{D}}[\epsilon^T Z(Z^TZ+\lambda I)^{-1}\Phi(x)\Phi(x)^T(Z^TZ+\lambda I)^{-1}Z^T\epsilon] \\
&\approx \mathbb{E}_Z[\text{trace}(\underbrace{\mathbb{E}_{y|Z}[\epsilon\epsilon^T]}_{=\sigma^2 I}Z(Z^TZ+\lambda I)^{-1}\Phi(x)\Phi(x)^T(Z^TZ+\lambda I)^{-1}Z^T] \\
&\approx \sigma^2\mathbb{E}_Z[\text{trace}(\Phi(x)\Phi(x)^T(Z^TZ+\lambda I)^{-1}Z^TZ(Z^TZ+\lambda I)^{-1})].
\end{aligned}$$

And finally we get the variance below,

$$\begin{aligned}
\text{var} &= \mathbb{E}_x[\text{var}(x)] \\
&\approx \sigma^2\mathbb{E}_Z[\text{trace}(\underbrace{\mathbb{E}_x[\Phi(x)\Phi(x)^T]}_{=I}(Z^TZ+\lambda I)^{-1}Z^TZ(Z^TZ+\lambda I)^{-1})] \\
&\approx \sigma^2\mathbb{E}_Z[\text{trace}(\underbrace{I}_{\approx \frac{1}{N}Z^TZ}(Z^TZ+\lambda I)^{-1}Z^TZ(Z^TZ+\lambda I)^{-1})] \\
&\approx \frac{\sigma^2}{N}\mathbb{E}_Z[\text{trace}(Z(Z^TZ+\lambda I)^{-1}Z^TZ(Z^TZ+\lambda I)^{-1}Z^T)] \\
&\approx \frac{\sigma^2}{N}\mathbb{E}_Z[\text{trace}(H(\lambda)^2)].
\end{aligned}$$

## Problem 4.13

$(a)$ When $\lambda = 0$, we have $H(0) = Z(Z^TZ)^{-1}Z^T$ and $H(0)^2 = Z(Z^TZ)^{-1}Z^TZ(Z^TZ)^{-1}Z^T = H(0)$, which means that

$$\text{trace}(H(0)) = \text{trace}(H(0)^2) = \text{trace}(Z^TZ(Z^TZ)^{-1}) = \text{trace}(I_{\tilde{d}+1}) = \tilde{d}+1.$$

So, for $(i)$, we get

$$d_{eff}(0) = 2(\tilde{d}+1) - (\tilde{d}+1) = \tilde{d}+1,$$

for $(ii)$, we get

$$d_{eff}(0)=\tilde{d}+1,$$

and for $(iii)$, we get

$$d_{eff}(0)=\tilde{d}+1.$$

$(b)$ Here again, for our $(N\times(\tilde{d}+1))$ matrix $Z$, we assume that $N>(\tilde{d}+1)$, and in this case $Z=U\Gamma V^T$ where $U$ is a $(N\times(\tilde{d}+1))$ orthogonal matrix, $D$ is a $((\tilde{d}+1)\times(\tilde{d}+1))$ diagonal matrix and $V$ is a $((\tilde{d}+1)\times(\tilde{d}+1))$ orthogonal matrix. From Problem 4.7, we know that

$$Z^TZ=V\Gamma^2V^T \text{ and } H(\lambda)=U\text{diag}\left(\frac{\sigma_i^2}{\sigma_i^2+\lambda}\right)U^T;$$

we begin by considering $(ii)$, in this case we have

$$0\leq d_{eff}=\text{trace}(H(\lambda))=\text{trace}(U^TU\text{diag}\left(\frac{\sigma_i^2}{\sigma_i^2+\lambda}\right))=\sum_{i=0}^{\tilde{d}}\frac{\sigma_i^2}{\sigma_i^2+\lambda}\leq\sum_{i=0}^{\tilde{d}}1=\tilde{d}+1$$

by the cyclic property of the trace. Obviously, if $\lambda$ increases, $d_{eff}$ decreases. Now, we consider $(iii)$, here we have

$$0\leq d_{eff}=\text{trace}(H(\lambda)^2)=\text{trace}(U^TU\text{diag}\left(\frac{\sigma_i^4}{(\sigma_i^2+\lambda)^2}\right))=\sum_{i=0}^{\tilde{d}}\frac{\sigma_i^4}{(\sigma_i^2+\lambda)^2}\leq\sum_{i=0}^{\tilde{d}}1=\tilde{d}+1;$$

here also, if $\lambda$ increases $d_{eff}$ decreases. Finally, we consider $(i)$, and we get

$$0\leq d_{eff}=2\sum_{i=0}^{\tilde{d}}\frac{\sigma_i^2}{\sigma_i^2+\lambda}-\sum_{i=0}^{\tilde{d}}\frac{\sigma_i^4}{(\sigma_i^2+\lambda)^2}=\sum_{i=0}^{\tilde{d}}\frac{\sigma_i^4+2\sigma_i^2\lambda}{(\sigma_i^2+\lambda)^2}\leq\sum_{i=0}^{\tilde{d}}1=\tilde{d}+1;$$

and here again, if $\lambda$ increases, then $d_{eff}$ increases.

## Problem 4.14

We know from Problem 4.7 that

$$\begin{aligned}
E_{in}(w_{reg}) &= \frac{1}{N}y^T(I-H(\lambda))^2y\\
&= \frac{1}{N}(f^T+\epsilon^T)(I-H(\lambda))^2(f+\epsilon)\\
&= \frac{1}{N}[f^T(I-H(\lambda))^2f+2f^T(I-H(\lambda))^2\epsilon+\epsilon^T(I-H(\lambda))^2\epsilon].
\end{aligned}$$

Now, if we compute the expectation of $E_{in}(w_{reg})$ relative to $\epsilon$, we get

$$\begin{aligned}
\mathbb{E}_\epsilon[E_{in}(w_{reg})] &= \frac{1}{N}[f^T(I-H(\lambda))^2f+2f^T(I-H(\lambda))^2\underbrace{\mathbb{E}_\epsilon[\epsilon]}_{=0}+\mathbb{E}_\epsilon[\epsilon^T(I-H(\lambda))^2\epsilon]]\\
&= \frac{1}{N}[f^T(I-H(\lambda))^2f+\mathbb{E}_\epsilon[\text{trace}(\epsilon\epsilon^T(I-H(\lambda))^2)]]\\
&= \frac{1}{N}[f^T(I-H(\lambda))^2f+\text{trace}(\underbrace{\mathbb{E}_\epsilon[\epsilon\epsilon^T]}_{=\text{diag}(\sigma^2)}(I-H(\lambda))^2)]\\
&= \frac{1}{N}f^T(I-H(\lambda))^2f+\frac{\sigma^2}{N}\text{trace}((I-H(\lambda))^2);
\end{aligned}$$

moreover, we also have that

$$\text{trace}((I-H(\lambda))^2) = \underbrace{\text{trace}(I_N)}_{=N} - 2\text{trace}(H(\lambda)) + \text{trace}(H(\lambda)^2) = N - d_{eff}(\lambda),$$

with which we conclude that

$$\mathbb{E}_\epsilon[E_{in}(w_{reg})] = \frac{1}{N} f^T (I - H(\lambda))^2 f + \sigma^2 \left(1 - \frac{d_{eff}(\lambda)}{N}\right).$$

$(a)$ The term involving $\sigma^2$ should be $\sigma^2 d_{eff}/N$.

$(b)$ It is clear that, if $d_{eff}$ increases, the expected in-sample error $\mathbb{E}_\epsilon[E_{in}(w_{reg})]$ decreases, which is exactly the behaviour exhibited by the number of parameters in the simpler case of linear regression. That explains why $d_{eff}$ is seen as an effective number of parameters in this more complex case.