Problem Solutions

Chapter 4

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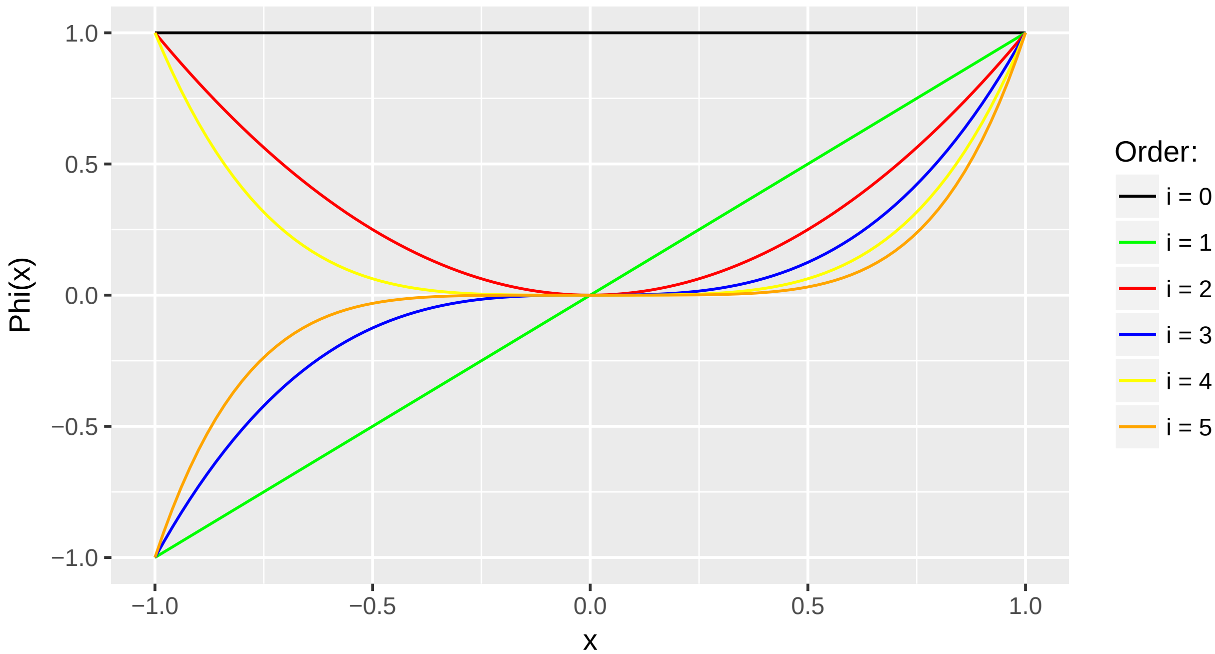
Problem 4.1

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

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

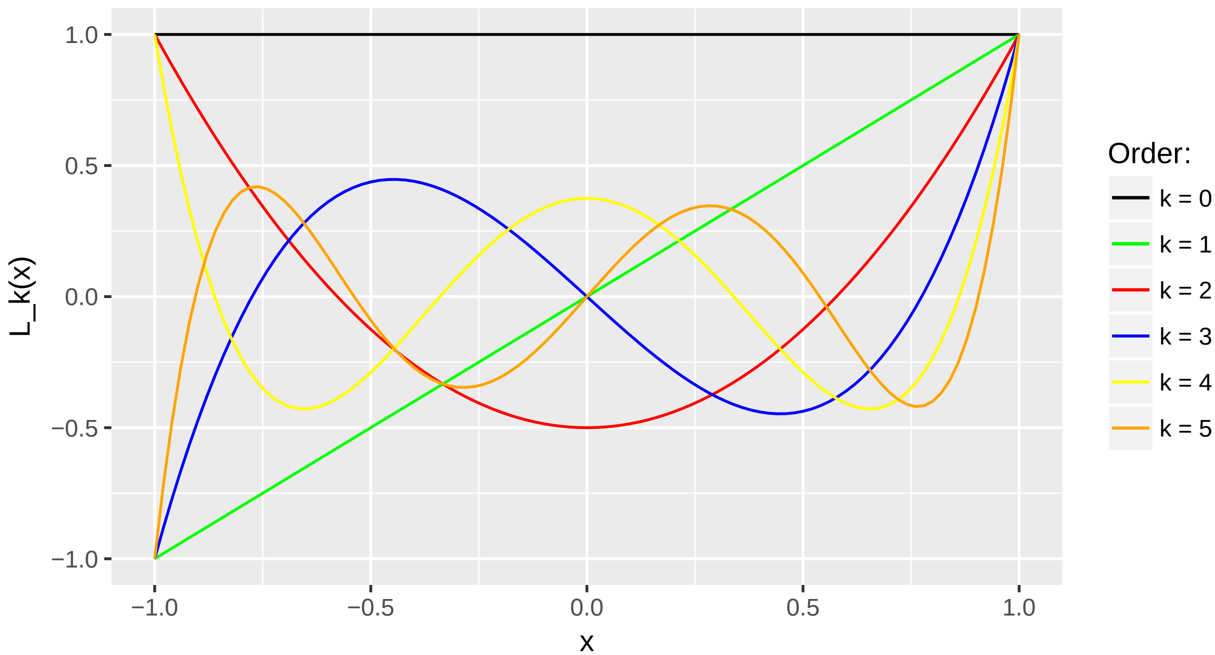
So we get a degree 2 polynomial.

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

$$
\begin{aligned}
L_{k+2}(x) &= \underbrace{\frac{2k+3}{k+2}}_{=c_1} x \cdot \underbrace{L_{k+1}(x)}_{=a_{k+1}x^{k+1}+a_{k-1}x^{k-1}+\cdots+a_1 x} - \underbrace{\frac{k+1}{k+2}}_{=c_0} \cdot \underbrace{L_k(x)}_{=b_k x^k + b_{k-2}x^{k-2}+\cdots+b_0} \\
&= c_1 a_{k+1} x^{k+2} + (c_1 a_{k-1} - c_0 b_k) x^k + \cdots + (c_1 a_1 - c_0 b_2) x^2 - c_0 b_0
\end{aligned}
$$

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

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

(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) {
```

```r
    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 σ^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

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

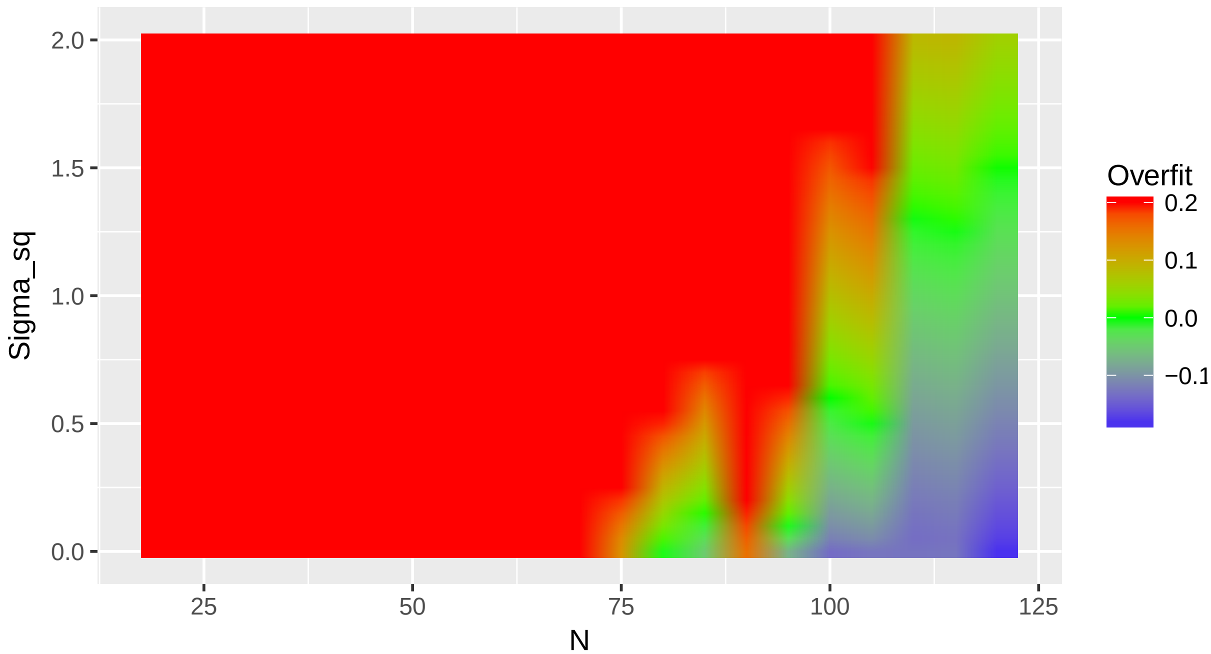
(c) To compute analytically E_{out} for a given g_{10} we have to compute

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

(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.

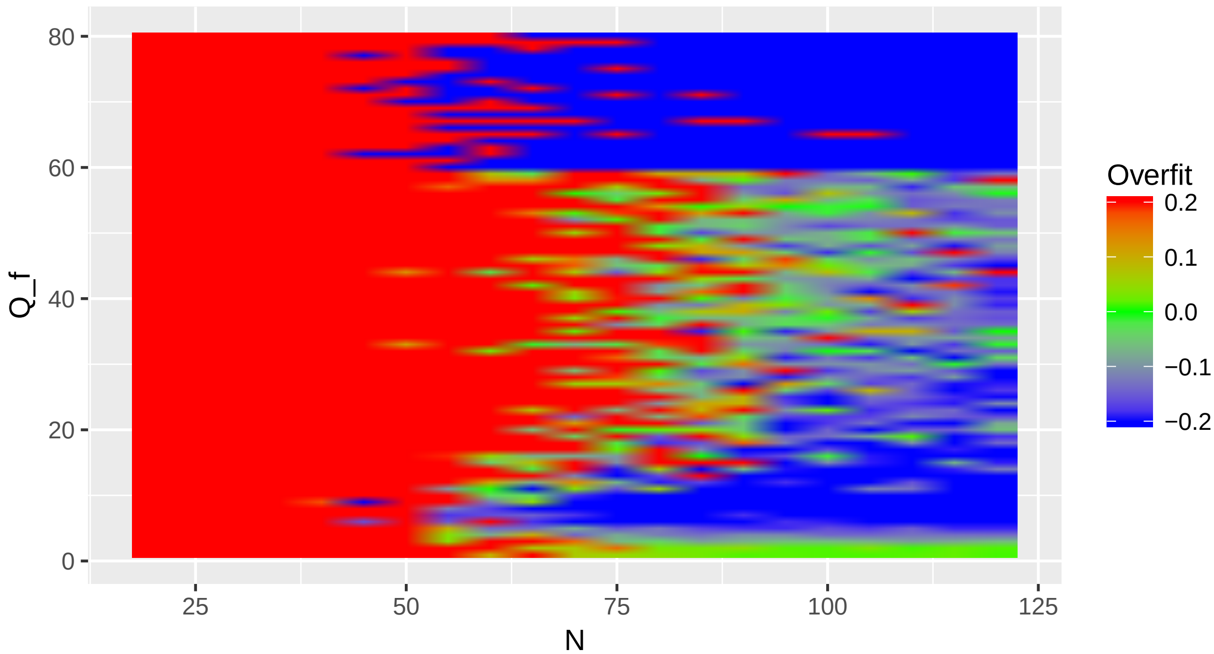
```r
# Grid search with Qf = 20
Nexp <- 1000
grid <- expand.grid(N = seq(20, 120, by = 5), sigma_sq = seq(0, 2, by = 0.05))
E_out_Overfit <- foreach(i = 1:nrow(grid), .combine = "rbind") %dopar% {
                   set.seed(1975)
                   Eout_H2 <- numeric(Nexp)
                   Eout_H10 <- 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)
```

```r
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.

```r
# 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, σ) using $\mathcal{H}_2$ and $\mathcal{H}_{10}$.