Solution 1: L0 Regularization

- We can show

$$\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \sum_{i=1}^{p} -\hat{\theta}_i\theta_i + \frac{\theta_i^2}{2} + \lambda \mathbb{1}_{|\theta_i|\neq 0}$$

as follows:

$$\begin{aligned}
\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) &= \min_{\boldsymbol{\theta}} \frac{1}{2}\sum_{i=1}^{n}\left(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)}\right)^2 + \lambda \sum_{i=1}^{p} \mathbb{1}_{|\theta_i|\neq 0} \\
&= \min_{\boldsymbol{\theta}} \frac{1}{2}\|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 + \lambda \sum_{i=1}^{p} \mathbb{1}_{|\theta_i|\neq 0} \\
&= \min_{\boldsymbol{\theta}} \frac{1}{2}(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda \sum_{i=1}^{p} \mathbb{1}_{|\theta_i|\neq 0} \\
&= \min_{\boldsymbol{\theta}} \frac{1}{2}\mathbf{y}^\top\mathbf{y} - \mathbf{y}^\top\mathbf{X}\boldsymbol{\theta} + \frac{1}{2}\boldsymbol{\theta}^\top\mathbf{X}^\top\mathbf{X}\boldsymbol{\theta} + \lambda \sum_{i=1}^{p} \mathbb{1}_{|\theta_i|\neq 0} \\
&= \min_{\boldsymbol{\theta}} -\mathbf{y}^\top\mathbf{X}\boldsymbol{\theta} + \frac{1}{2}\boldsymbol{\theta}^\top\mathbf{X}^\top\mathbf{X}\boldsymbol{\theta} + \lambda \sum_{i=1}^{p} \mathbb{1}_{|\theta_i|\neq 0} && (\ \mathbf{y}^\top\mathbf{y} \text{ does not depend on } \boldsymbol{\theta}) \\
&= \min_{\boldsymbol{\theta}} -\mathbf{y}^\top\mathbf{X}\boldsymbol{\theta} + \frac{1}{2}\boldsymbol{\theta}^\top\boldsymbol{\theta} + \lambda \sum_{i=1}^{p} \mathbb{1}_{|\theta_i|\neq 0} && (\text{By assumption } \mathbf{X}^\top\mathbf{X} = \boldsymbol{I}) \\
&= \min_{\boldsymbol{\theta}} -\hat{\boldsymbol{\theta}}^\top\boldsymbol{\theta} + \frac{1}{2}\boldsymbol{\theta}^\top\boldsymbol{\theta} + \lambda \sum_{i=1}^{p} \mathbb{1}_{|\theta_i|\neq 0} \\
& \qquad (\text{By assumption } \mathbf{X}^\top\mathbf{X} = \boldsymbol{I} \text{ so that } \hat{\boldsymbol{\theta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \mathbf{X}^T\mathbf{y}) \\
&= \min_{\boldsymbol{\theta}} \sum_{i=1}^{p} -\hat{\theta}_i\theta_i + \frac{\theta_i^2}{2} + \lambda \mathbb{1}_{|\theta_i|\neq 0} && (\text{Writing out the inner products})
\end{aligned}$$

- Note that the minimization problem on the right-hand side of the previous math display can be written as $\sum_{i=1}^{p} g_i(\theta_i)$, where

$$g_i(\theta) = -\hat{\theta}_i\theta + \frac{\theta^2}{2} + \lambda \mathbb{1}_{|\theta|\neq 0}.$$

The advantage of this representation, if we are interested in finding the $\boldsymbol{\theta}$ with entries $\theta_1, \dots, \theta_p$ minimizing $\mathcal{R}_{\text{reg}}(\boldsymbol{\theta})$, is that we can minimize each g_i separately to obtain the optimal entries.

- Consider first the case that $|\hat{\theta}_i| > \sqrt{\lambda}$. Note that

$$\begin{aligned}
g_i(\hat{\theta}_i) &= -\hat{\theta}_i^2 + \frac{\hat{\theta}_i^2}{2} + \lambda && (|\hat{\theta}_i| > \sqrt{\lambda} > 0) \\
&= -\frac{\hat{\theta}_i^2}{2} + \lambda \\
&< -\frac{\lambda}{2}. && (|\hat{\theta}_i| > \sqrt{\lambda} \Rightarrow -\hat{\theta}_i^2 < -\lambda)
\end{aligned}$$

Further, note that $g_i(0) = 0$ and consequently $g_i(\hat{\theta}_i) < g_i(0)$. This means that 0 cannot be the minimizer of

g_i in this case. Next, it holds that for any $\theta \neq 0$ with $sgn(\theta) = sgn(\hat{\theta}_i)$, i.e., $\hat{\theta}_i\theta > 0$, that

$$g_i(\theta) = \underbrace{-\hat{\theta}_i\theta}_{<0} + \underbrace{\frac{\theta^2}{2}}_{=\frac{(-\theta)^2}{2}} + \lambda \mathbb{1}_{|\theta|\neq 0} < \underbrace{\hat{\theta}_i\theta}_{>0} + \frac{(-\theta)^2}{2} + \lambda \mathbb{1}_{|-\theta|\neq 0} = g_i(-\theta),$$

so that for the minimizer of g_i it must hold that it has the same sign as $\hat{\theta}_i$ in this case. Now differentiating g_i (for $\theta > 0$) and setting it to zero implies

$$\begin{aligned} \frac{\partial g_i(\theta)}{\partial \theta} &= -\hat{\theta}_i + \theta \overset{!}{=} 0 \\ \Leftrightarrow \quad \theta &= \hat{\theta}_i. \end{aligned}$$

For sake of completeness, the second derivative is $\frac{\partial^2 g_i(\theta)}{\partial^2 \theta} = 1 > 0$ so that we have indeed a minimum. Thus, for the minimizer θ_i^* of g_i it must hold that $\theta_i^* = \hat{\theta}_i$.

- By taking the constraint of the case into account, we can write $\theta_i^* = \hat{\theta}_i \mathbb{1}_{|\hat{\theta}_i| > \sqrt{\lambda}}$.

- Consider the complementary case, i.e., $|\hat{\theta}_i| \leq \sqrt{\lambda}$. As seen above it holds that $g_i(0) = 0$. Consider the smooth extension of g_i :

$$\tilde{g}_i(\theta) = -\hat{\theta}_i\theta + \frac{\theta^2}{2} + \lambda$$

and note that $\tilde{g}_i$ and g_i are the same for any $\theta \neq 0$, while $\tilde{g}_i$ is smooth on $\mathbb{R}$ and g_i is discontinuous at 0. In particular, it holds that $g_i(\theta) \leq \tilde{g}_i(\theta)$, with equality for any $\theta \neq 0$ and strict inequality for $\theta = 0$. So the minimizer of g_i is either the same as the one for $\tilde{g}_i$ or it is zero. Similarly as above, it holds for any $\theta \neq 0$ with $sgn(\theta) = sgn(\hat{\theta}_i)$, i.e., $\hat{\theta}_i\theta > 0$, that

$$\tilde{g}_i(\theta) = \underbrace{-\hat{\theta}_i\theta}_{<0} + \underbrace{\frac{\theta^2}{2}}_{=\frac{(-\theta)^2}{2}} + \lambda < \underbrace{\hat{\theta}_i\theta}_{>0} + \frac{(-\theta)^2}{2} + \lambda = \tilde{g}_i(-\theta),$$

so that for the minimizer of $\tilde{g}_i$ it must hold that it has the same sign as $\hat{\theta}_i$ in this case. Now differentiating $\tilde{g}_i$ and setting it to zero implies

$$\begin{aligned} \frac{\partial \tilde{g}_i(\theta)}{\partial \theta} &= -\hat{\theta}_i + \theta \overset{!}{=} 0 \\ \Leftrightarrow \quad \theta &= \hat{\theta}_i. \end{aligned}$$

However, if $\hat{\theta}_i \neq 0$ then

$$\begin{aligned} g_i(\hat{\theta}_i) &= -\hat{\theta}_i^2 + \frac{\hat{\theta}_i^2}{2} + \lambda && (\text{If } \hat{\theta}_i \neq 0) \\ &= -\frac{\hat{\theta}_i^2}{2} + \lambda \\ &\geq \frac{\lambda}{2}, && (|\hat{\theta}_i| \leq \sqrt{\lambda} \Rightarrow -\hat{\theta}_i^2 \geq -\lambda) \end{aligned}$$

so that $g_i(\hat{\theta}_i) > 0 = g_i(0)$. Hence, the minimizer θ_i^* of g_i is $\theta_i^* = 0$, which can be written, by taking the constraint of the case into account, as $\theta_i^* = \hat{\theta}_i \mathbb{1}_{|\hat{\theta}_i| > \sqrt{\lambda}}$.

- In summary, we have shown that the minimizer θ_i^* of g_i is $\theta_i^* = \hat{\theta}_i \mathbb{1}_{|\hat{\theta}_i| > \sqrt{\lambda}}$ for any $i = 1, \ldots, p$. Since

$$\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \sum_{i=1}^{p} -\hat{\theta}_i\theta_i + \frac{\theta_i^2}{2} + \lambda \mathbb{1}_{|\theta_i|\neq 0} = \min_{\boldsymbol{\theta}} \sum_{i=1}^{p} g_i(\theta_i),$$

we conclude that $\hat{\theta}_{\text{L0}} = (\hat{\theta}_{\text{L0},1}, \ldots, \hat{\theta}_{\text{L0},p})^\top$ given by

$$\hat{\theta}_{\text{L0},i} = \hat{\theta}_i \mathbb{1}_{|\hat{\theta}_i| > \sqrt{\lambda}}, \quad i = 1, \ldots, p,$$

is the minimizer of the L_0-regularized empirical risk over the linear models.

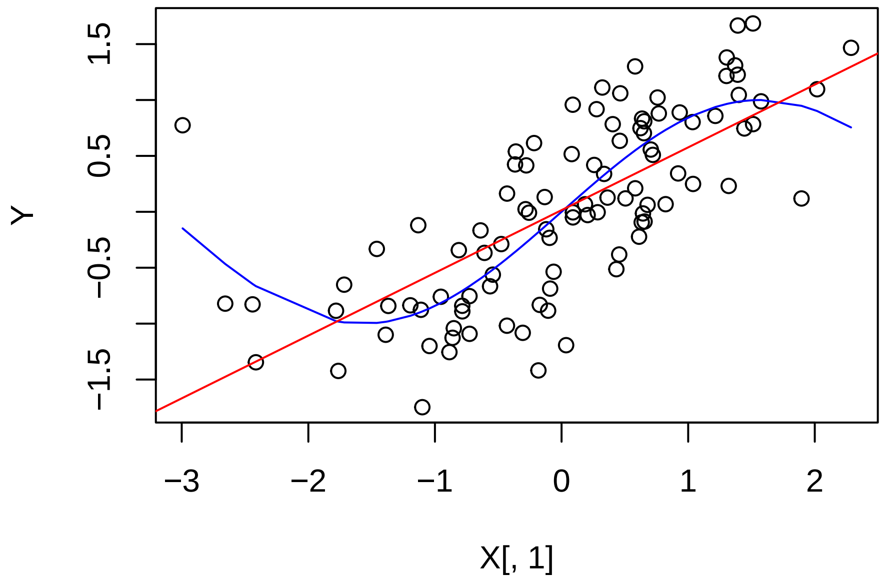
Solution 2: Regularization

(a)
```
set.seed(42)
n = 100
p_add = 100
# create matrix of features
X = matrix(rnorm(n * (p_add + 1)), ncol = p_add + 1)

Y = sin(X[,1]) + rnorm(n, sd = 0.5)
```

(b) Demonstration of

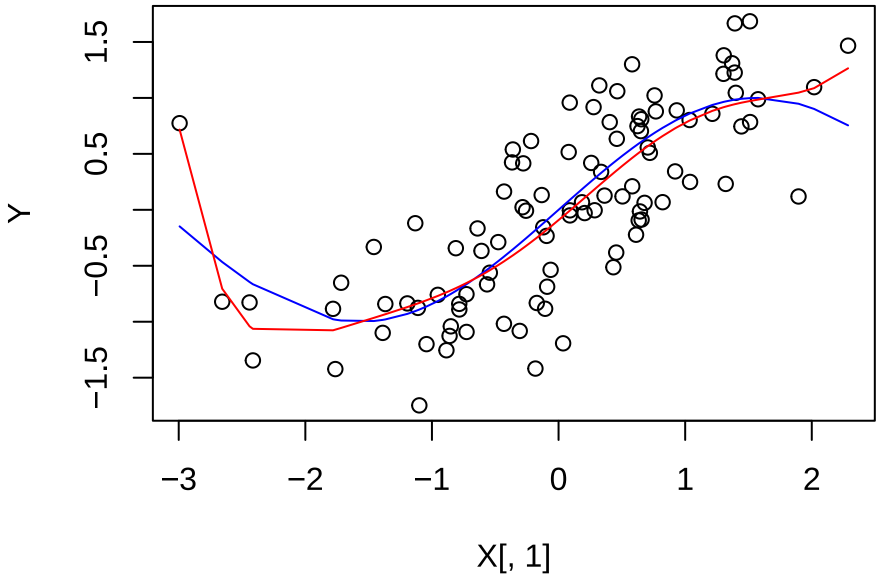
- underfitting:

```
plot(X[,1], Y)
points(sort(X[,1]), sin(sort(X[,1])), type="l", col="blue")
abline(coef(lm(Y ~ X[,1])), col="red")
```



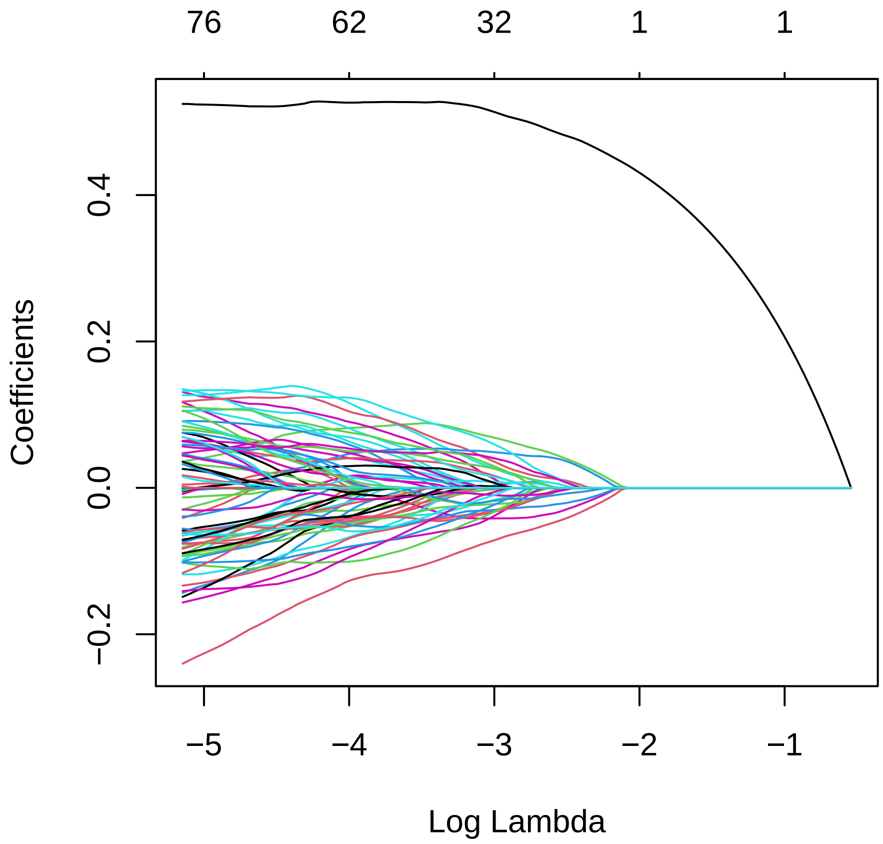
- overfitting:

```
plot(X[,1], Y)
sX1 <- sort(X[,1])
points(sX1, sin(sX1), type="l", col="blue")
points(sX1, fitted(lm(Y ~ X[,1] + I(X[,1]^2) + I(X[,1]^3) +
                        I(X[,1]^4) + I(X[,1]^5) + I(X[,1]^6) +
                        I(X[,1]^7)))[order(X[,1])],
       type="l", col="red")
```



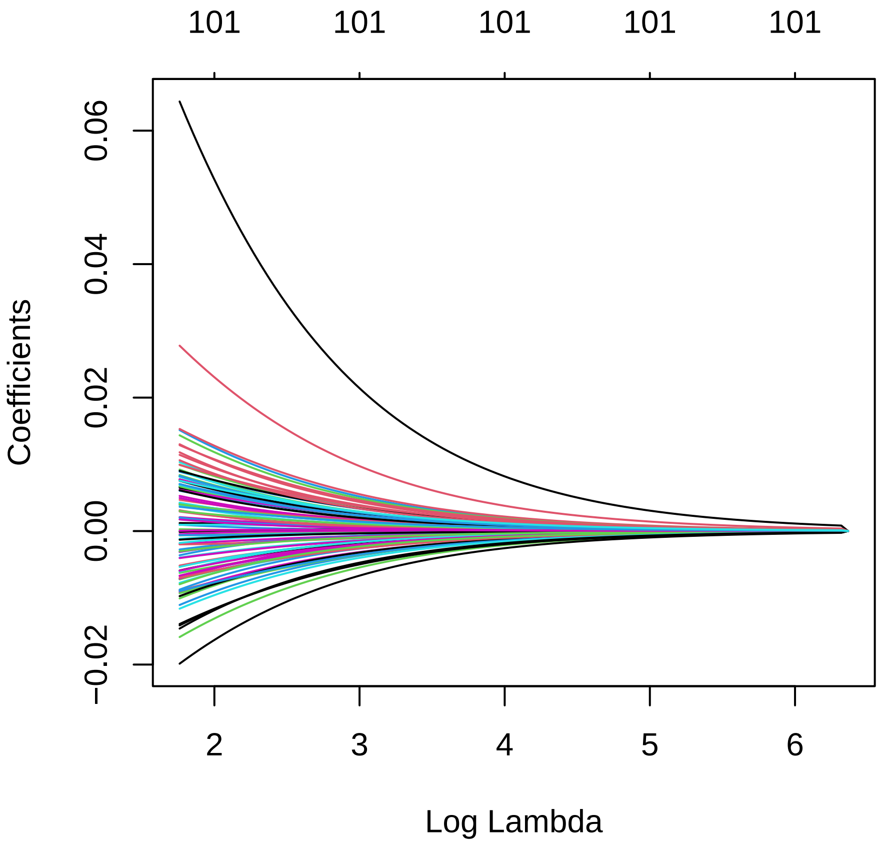
- $L1$ penalty:

```
library(glmnet)

## Warning:  Paket 'glmnet' wurde unter R Version 4.1.3 erstellt

plot(glmnet(X, Y), xvar = "lambda")
```



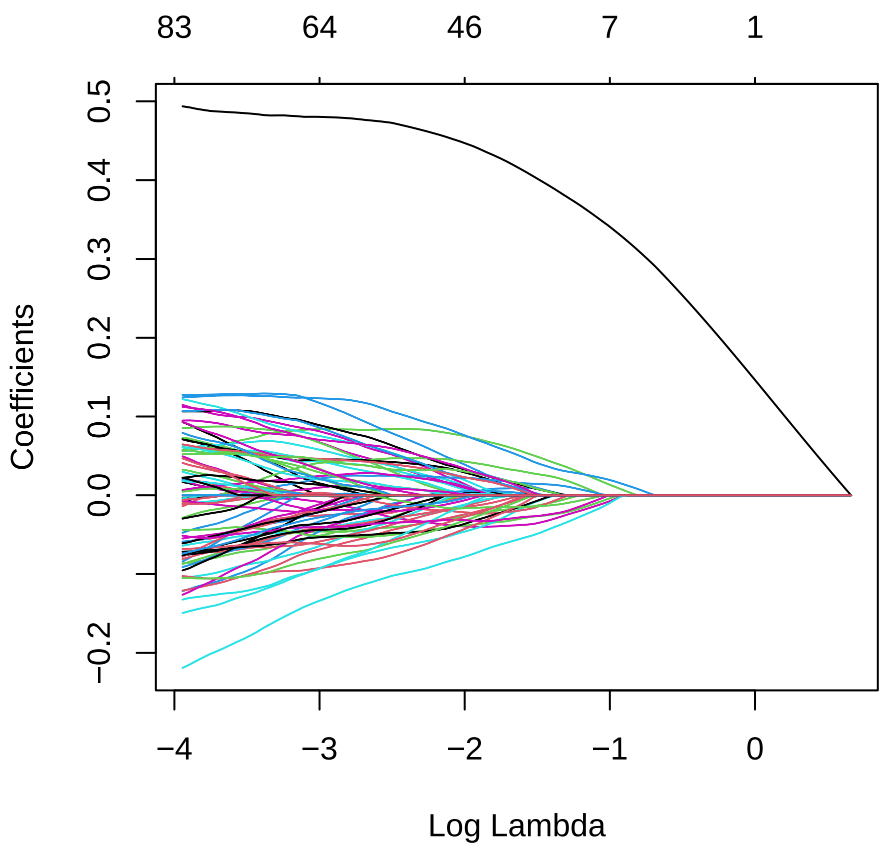
- $L2$ penalty

```
plot(glmnet(X, Y, alpha = 0), xvar = "lambda")
```



- elastic net regularization:

```
plot(glmnet(X, Y, alpha = 0.3), xvar = "lambda")
```

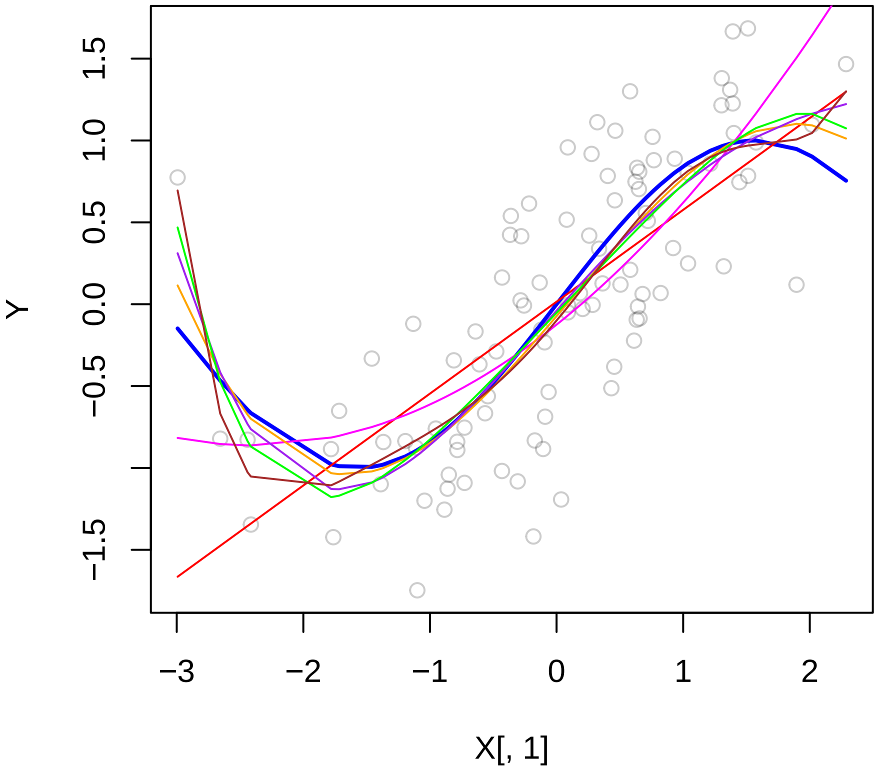


- the underdetermined problem:

```
try(ls_estimator <- solve(crossprod(X), crossprod(X,Y)))

## Error in solve.default(crossprod(X), crossprod(X, Y)) :
##   System ist für den Rechner singulär: reziproke Konditionszahl = 5.84511e-18
```

- the bias-variance trade-off:

```
plot(X[,1], Y, col=rgb(0,0,0,0.2))
sX1 <- sort(X[,1])
points(sX1, sin(sX1), type="l", col="blue", lwd=2)
points(sX1, fitted(lm(Y ~ X[,1]))[order(X[,1])],
       type="l", col="red")
points(sX1, fitted(lm(Y ~ X[,1] + I(X[,1]^2)))[order(X[,1])],
       type="l", col="magenta")
points(sX1, fitted(lm(Y ~ X[,1] + I(X[,1]^2) + I(X[,1]^3)))[order(X[,1])],
       type="l", col="orange")
points(sX1, fitted(lm(Y ~ X[,1] + I(X[,1]^2) + I(X[,1]^3) +
                        I(X[,1]^4)))[order(X[,1])],
       type="l", col="purple")
points(sX1, fitted(lm(Y ~ X[,1] + I(X[,1]^2) + I(X[,1]^3) +
                        I(X[,1]^4) + I(X[,1]^5)))[order(X[,1])],
       type="l", col="green")
points(sX1, fitted(lm(Y ~ X[,1] + I(X[,1]^2) + I(X[,1]^3) +
                        I(X[,1]^4) + I(X[,1]^5) + I(X[,1]^6)))[order(X[,1])],
       type="l", col="brown")
```



Y
X[, 1]
−1.5
−0.5
0.0
0.5
1.0
1.5
−3
−2
−1
0
1
2