Exercise of Supervised Learning: Regularization Part 1

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Exercise 1: L0 Regularization

Consider the regression learning setting, i.e., $\mathcal{Y} = \mathbb{R}$, and the feature space $\mathcal{X} = \mathbb{R}^p$. Let the hypothesis space be the linear models:

$$\mathcal{H} = \{f(\mathbf{x}) = \boldsymbol{\theta}^T\mathbf{x} \mid \boldsymbol{\theta} \in \mathbb{R}^p\}.$$

Suppose your loss function of interest is the L2 loss $L(y, f(\mathbf{x})) = \frac{1}{2}(y - f(\mathbf{x}))^2$. Consider the L_0-regularized empirical risk of a model $f(\mathbf{x} \mid \boldsymbol{\theta})$:

$$\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + \lambda||\boldsymbol{\theta}||_0 = \frac{1}{2}\sum_{i=1}^{n}(y^{(i)} - \boldsymbol{\theta}^T\mathbf{x}^{(i)})^2 + \lambda\sum_{i=1}^{p}\boldsymbol{I}_{|\theta_i|\neq 0} \qquad \triangleleft\,.$$

Assume that $\mathbf{X}^T\mathbf{X} = \mathbf{I}$, which holds if $\mathbf{X}$ has orthonormal columns. Show that the minimizer $\hat{\theta}_{L0} = (\hat{\theta}_{L0,1}, \dots, \hat{\theta}_{L0,p})^T$ is given by

$$\hat{\theta}_{L0,i} = \hat{\theta}_i\boldsymbol{I}_{\hat{\theta}_i > \sqrt{2\lambda}}, \qquad i = 1, \dots, p,$$

where $\hat{\boldsymbol{\theta}} = (\hat{\theta}_1, \dots, \hat{\theta}_p)^T = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ is the minimizer of the unregularized empirical risk. For this purpose, using the following steps:

Exercise 1 (i)

(i) Derive that

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

Note that θ_i is from the minimizer $\hat{\boldsymbol{\theta}}$ of the unregularized empirical risk :

$$\hat{\boldsymbol{\theta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \mathbf{X}^T\mathbf{y}$$

because we assume that $\mathbf{X}^T\mathbf{X} = \mathbf{I}$.

Solution to Exercise 1 (i)

$$\arg\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \arg\min_{\boldsymbol{\theta}} \frac{1}{2}||\mathbf{X}\boldsymbol{\theta} - \mathbf{y}||_2^2 + \lambda \sum_{i=1}^{p} \boldsymbol{I}_{|\theta_i| \neq 0}$$

Solution to Exercise 1 (i)

$$\begin{aligned}
\arg\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) &= \arg\min_{\boldsymbol{\theta}} \frac{1}{2}||\mathbf{X}\boldsymbol{\theta} - \mathbf{y}||_2^2 + \lambda \sum_{i=1}^{p} \boldsymbol{I}_{|\theta_i| \neq 0} \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2}\mathbf{y}^T\mathbf{y} - \mathbf{y}^T\mathbf{X}\boldsymbol{\theta} + \frac{1}{2}\boldsymbol{\theta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\theta} + \lambda \sum_{i=1}^{p} \boldsymbol{I}_{|\theta_i| \neq 0}
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&= \arg\min_{\boldsymbol{\theta}} -\underbrace{\mathbf{y}^T\mathbf{X}}_{\hat{\boldsymbol{\theta}}^T}\boldsymbol{\theta} + \frac{1}{2}\boldsymbol{\theta}^T\underbrace{\mathbf{X}^T\mathbf{X}}_{=\mathbf{I}}\boldsymbol{\theta} + \lambda \sum_{i=1}^{p} \boldsymbol{I}_{|\theta_i| \neq 0}
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&= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{p} -\hat{\theta}_i\theta_i + \frac{\theta_i^2}{2} + \lambda \sum_{i=1}^{p} \boldsymbol{I}_{|\theta_i| \neq 0} \qquad \triangleleft
\end{aligned}
$$

Exercise 1 (ii)

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

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

What is the advantage of this representation if we seek to find the $\boldsymbol{\theta}$ with entries $\theta_1, \ldots, \theta_p$ minimizing $\mathcal{R}_{\text{reg}}(\boldsymbol{\theta})$?

Solution to Exercise 1 (ii)

Advantage: we can minimize each g_i **separately** to obtain the optimal entries $\theta_1, \ldots, \theta_p$.

Exercise 1 (iii)

(iii) Consider the first case that $|\hat{\theta}_i| > \sqrt{2\lambda}$ and infer that for the minimizer θ_i^* of g_i it must hold that $\theta_i^* = \hat{\theta}_i$.
Hint: Show that $g_i(\theta_i) < 0 = g_i(0)$ and argue that the minimizer must have the same sign as $\hat{\theta}_i$. (**Personally I find this hint is not so useful.**)
In other words, if $|\hat{\theta}_i|$ is larger than the threshold, $\sqrt{2\lambda}$, then the optimal θ_i^* is the consistent between the regularized and un-regularized empirical risk.

Solution to Exercise 1 (iii)

We start with computing the arg min $g_i(\theta_i) = \frac{\theta_i^2}{2} - \hat{\theta}_i\theta_i + \lambda \boldsymbol{I}_{|\theta_i| \neq 0}$.

- Case 1: $\theta_i = 0$. Then, $g_i(\theta_i) = 0$.
- Case 2: $\theta_i \neq 0$. Then

$$g_i(\theta_i) = \frac{\theta_i^2}{2} - \hat{\theta}_i\theta_i + \lambda,$$

which is a quadratic function, and its minimizer is

$$\theta_i^* = \arg\min_{\theta_i} g_i(\theta_i) = \hat{\theta}_i,$$

and the minimal value of g_i in this case is

$$g_i(\theta_i^*) = -\frac{\hat{\theta}_i^2}{2} + \lambda.$$

Which optimal g_i is smaller? Case 1 or Case 2? It depends on λ. Note that we are given with $|\hat{\theta}_i| > \sqrt{2\lambda}$. So $-\frac{\hat{\theta}_i^2}{2} + \lambda < -\frac{2\lambda}{2} + \lambda = 0$. So the optimal g_i in Case 2 is smaller.
So for the minimizer of g_i it holds that $\theta_i^* = \hat{\theta}_i$.

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We start with computing the arg min $g_i(\theta_i) = \frac{\theta_i^2}{2} - \hat{\theta}_i\theta_i + \lambda \boldsymbol{I}_{|\theta_i| \neq 0}$.

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So for the minimizer of g_i it holds that $\theta_i^* = \hat{\theta}_i$.

Exercise 1 (iv)

(iv) Derive that $\theta_i^* = \hat{\theta}_i \boldsymbol{I}_{|\hat{\theta}_i| > \sqrt{2\lambda}}$, by using (iii) (and also still considering the case $|\hat{\theta}_i| > \sqrt{2\lambda}$).

Solution: In the solution of (iii) we have proven that

$$\theta_i^* = \hat{\theta}_i \quad \text{if} \quad |\hat{\theta}_i| > \sqrt{2\lambda},$$

The optimal θ_i can be written as

$$\theta_i^* = \hat{\theta}_i \cdot 1 = \hat{\theta}_i \boldsymbol{I}_{|\hat{\theta}_i| > \sqrt{2\lambda}}.$$

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Exercise 1 (v)

(v) Consider the complementary case of (iii) and (iv), i.e., $|\hat{\theta}_i| \leq \sqrt{2\lambda}$, and infer that for the minimizer θ_i^* of g_i it must hold that $\theta_i^* = 0$.
Hint: What is $g_i(0)$? Consider $\tilde{g}_i(0) = \hat{\theta}_i\theta + \frac{\theta^2}{2} + \lambda$ which is the smooth extenstion of g_i. What is the relationship between the minimizer of g_i and the minimizer of $\tilde{g}_i$?
(**We do not need this hint in the solution presented in the subsequent slides)**

Solution to Exercise 1 (v)

Similarily, we start with computing arg min $g_i(\theta_i) = \frac{\theta_i^2}{2} - \hat{\theta}_i\theta_i + \lambda \boldsymbol{I}_{|\theta_i| \neq 0}$.

- Case 1: $\theta_i = 0$. Then, $g_i(\theta_i) = 0$.
- Case 2: $\theta_i \neq 0$. Then

$$g_i(\theta_i) = \frac{\theta_i^2}{2} - \hat{\theta}_i\theta_i + \lambda,$$

We have shown that the minimizer in **this case** is $\theta_i^* = \hat{\theta}_i$ and min $g_i(\theta_i^*) = g_i(\hat{\theta}_i) = -\frac{\hat{\theta}_i^2}{2} + \lambda$.

Since we consider the constraint $|\hat{\theta}_i| \leq \sqrt{2\lambda}$. Then in Case 2

$$g_i(\theta_i^*) \geq -\frac{2\lambda}{2} + \lambda = 0.$$

So the minimal g_i in Case 2 is **not smaller** than the minimal g_i in Case 1. **(Plot $g_i(\theta_i)$ vs. θ_i).**
Therefore, combining two cases, for the minimizer θ_i^* of g_i it holds that

$$\theta_i^* = 0.$$

Solution to Exercise 1 (v)

Similarly, we start with computing $\arg\min g_i(\theta_i) = \frac{\theta_i^2}{2} - \hat{\theta}_i\theta_i + \lambda \boldsymbol{I}_{|\theta_i|\neq 0}$.

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$$\theta_i^* = 0.$$

Exercise 2: Regularization

Directly show the standard solution.