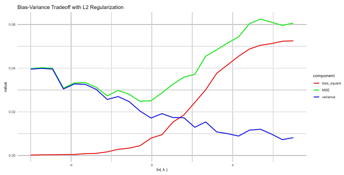
Introduction to Machine Learning

Regularization
Perspectives on Ridge Regression (Deep-Dive)



Learning goals

- Interpretation of $L2$ regularization as row-augmentation
- Interpretation of $L2$ regularization as minimizing risk under feature noise

PERSPECTIVES ON $L2$ REGULARIZATION

We already saw two interpretations of $L2$ regularization.

- We know that it is equivalent to a constrained optimization problem:

$$\hat{\theta}_{\text{ridge}} \quad = \quad \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2 + \lambda \|\boldsymbol{\theta}\|_2^2 = (\mathbf{X}^T\mathbf{X} + \lambda \boldsymbol{I})^{-1}\mathbf{X}^T\mathbf{y}$$

  For some t depending on λ this is equivalent to:

$$\hat{\theta}_{\text{ridge}} \quad = \quad \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2 \text{ s.t. } \|\boldsymbol{\theta}\|_2^2 \leq t$$

- Bayesian interpretation of ridge regression: For additive Gaussian errors $\mathcal{N}(0, \sigma^2)$ and i.i.d. normal priors $\theta_j \sim \mathcal{N}(0, \tau^2)$, the resulting MAP estimate is $\hat{\theta}_{\text{ridge}}$ with $\lambda = \frac{\sigma^2}{\tau^2}$:

$$\hat{\theta}_{\text{MAP}} = \arg\max_{\theta} \log[p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta})p(\boldsymbol{\theta})] = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2 + \frac{\sigma^2}{\tau^2} \|\boldsymbol{\theta}\|_2^2$$

$L2$ AND ROW-AUGMENTATION

We can also recover the ridge estimator by performing least-squares on a **row-augmented** data set: Let $\tilde{\mathbf{X}} := \begin{pmatrix} \mathbf{X} \\ \sqrt{\lambda}\boldsymbol{I}_p \end{pmatrix}$ and $\tilde{\mathbf{y}} := \begin{pmatrix} \mathbf{y} \\ \mathbf{0}_p \end{pmatrix}$.

With the augmented data, the unreg. least-squares solution $\tilde{\boldsymbol{\theta}}$ is:

$$
\begin{aligned}
\tilde{\boldsymbol{\theta}} &= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n+p} \left(y^{\widetilde{(i)}} - \boldsymbol{\theta}^T \mathbf{x}^{\widetilde{(i)}} \right)^2 \\
&= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2 + \sum_{j=1}^{p} \left(0 - \sqrt{\lambda}\theta_j \right)^2 \\
&= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2 + \lambda \|\boldsymbol{\theta}\|_2^2
\end{aligned}
$$

$\Longrightarrow \hat{\theta}_{\text{ridge}}$ is the least-squares solution $\tilde{\boldsymbol{\theta}}$ but using $\tilde{\mathbf{X}}, \tilde{\mathbf{y}}$ instead of $\mathbf{X}, \mathbf{y}$!

This is a sometimes useful “recasting” or “rewriting” for ridge.

$L2$ AND NOISY FEATURES

Now consider perturbed features $\tilde{x}^{(i)} := \mathbf{x}^{(i)} + \boldsymbol{\delta}^{(i)}$ where $\boldsymbol{\delta}^{(i)} \overset{iid}{\sim} (\mathbf{0}, \lambda \boldsymbol{I}_p)$.
We assume no specific distribution. Now minimize risk with L2 loss, we define it slightly different than usual, as here our data $\mathbf{x}^{(i)}$, $y^{(i)}$ are fixed, but we integrate over the random permutations $\boldsymbol{\delta}$:

$$\mathcal{R}(\boldsymbol{\theta}) := \mathbb{E}_{\delta}\Big[\sum_{i=1}^{n}(y^{(i)} - \boldsymbol{\theta}^\top \tilde{\mathbf{x}}^{(i)})^2\Big] = \mathbb{E}_{\delta}\Big[\sum_{i=1}^{n}(y^{(i)} - \boldsymbol{\theta}^\top (\mathbf{x}^{(i)} + \boldsymbol{\delta}^{(i)}))^2\Big] \ \Big| \text{expand}$$

$$\mathcal{R}(\boldsymbol{\theta}) = \mathbb{E}_{\delta}\Big[\sum_{i=1}^{n}\big((y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 - 2\boldsymbol{\theta}^\top \boldsymbol{\delta}^{(i)}(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)}) + \boldsymbol{\theta}^\top \boldsymbol{\delta}^{(i)} \boldsymbol{\delta}^{(i)\top} \boldsymbol{\theta}\big)\Big]$$

By linearity of expectation, $\mathbb{E}_{\delta}[\boldsymbol{\delta}^{(i)}] = \mathbf{0}_p$ and $\mathbb{E}_{\delta}[\boldsymbol{\delta}^{(i)}\boldsymbol{\delta}^{(i)\top}] = \lambda \boldsymbol{I}_p$, this is

$$\begin{aligned}\mathcal{R}(\boldsymbol{\theta}) &= \sum_{i=1}^{n}\big((y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 - 2\boldsymbol{\theta}^\top \mathbb{E}_{\delta}[\boldsymbol{\delta}^{(i)}](y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)}) + \boldsymbol{\theta}^\top \mathbb{E}_{\delta}[\boldsymbol{\delta}^{(i)} \boldsymbol{\delta}^{(i)\top}] \boldsymbol{\theta}\big) \\ &= \sum_{i=1}^{n}(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 + \lambda \|\boldsymbol{\theta}\|_2^2\end{aligned}$$

$\Longrightarrow$ Ridge regression on unperturbed features $\mathbf{x}^{(i)}$ turns out to be the same as minimizing squared loss averaged over feature noise distribution!