CS 446 / ECE 449 — Homework 4 William Lee (w172)

1. Bias-Variance in Ridge Regression

We have fixed scalar inputs $\{x^{(i)}\}_{i=1}^{N}$ and labels

$$y^{(i)} = w^* x^{(i)} + \varepsilon^{(i)}, \qquad \varepsilon^{(i)} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2),$$

independent of $x^{(i)}$. Ridge regression solves

$$w_D = \arg\min_{w} \frac{1}{N} \sum_{i=1}^{N} (wx^{(i)} - y^{(i)})^2 + \lambda w^2,$$

whose closed form is

$$w_D = \frac{\frac{1}{N} \sum_{i=1}^{N} x^{(i)} y^{(i)}}{\lambda + s^2}, \quad s^2 := \frac{1}{N} \sum_{i=1}^{N} (x^{(i)})^2.$$

(a) Expected label and noise

Conditional mean:

$$\bar{y}(x) = \mathbb{E}[y \mid x] = \mathbb{E}[w^*x + \varepsilon \mid x] = w^*x,$$

since $\mathbb{E}[\varepsilon] = 0$. Therefore

Noise =
$$\frac{1}{N} \sum_{i=1}^{N} \mathbb{E}[(\bar{y}(x^{(i)}) - y^{(i)})^2] = \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}[(\varepsilon^{(i)})^2] = \sigma^2.$$

(b) Mean predictor \bar{w}

$$\frac{1}{N} \sum_{i} x^{(i)} y^{(i)} = \frac{1}{N} \sum_{i} x^{(i)} \left(w^* x^{(i)} + \varepsilon^{(i)} \right) = w^* s^2 + \underbrace{\frac{1}{N} \sum_{i} x^{(i)} \varepsilon^{(i)}}_{\text{mean } 0}.$$

Hence

$$\overline{\bar{w} := \mathbb{E}_D[w_D] = \frac{s^2}{\lambda + s^2} w^*.}$$

(c) Squared bias

Bias² =
$$\frac{1}{N} \sum_{i=1}^{N} (\bar{w} x^{(i)} - w^* x^{(i)})^2 = (w^* - \bar{w})^2 s^2 = (\frac{\lambda}{\lambda + s^2})^2 (w^*)^2 s^2.$$

(d) Variance

From the closed form solution:

$$w_D = \frac{\frac{1}{N} \sum_{i=1}^{N} x^{(i)} y^{(i)}}{\lambda + s^2}$$

Substituting $y^{(i)} = w^* x^{(i)} + \varepsilon^{(i)}$:

$$w_D = \frac{\frac{1}{N} \sum_{i=1}^{N} x^{(i)} (w^* x^{(i)} + \varepsilon^{(i)})}{\lambda + s^2} = \frac{w^* s^2 + \frac{1}{N} \sum_{i=1}^{N} x^{(i)} \varepsilon^{(i)}}{\lambda + s^2}$$

Let $Z := \frac{1}{N} \sum_{i=1}^{N} x^{(i)} \varepsilon^{(i)}$. Then:

$$w_D = \frac{w^* s^2}{\lambda + s^2} + \frac{Z}{\lambda + s^2} = \bar{w} + \frac{Z}{\lambda + s^2}$$

Since $\varepsilon^{(i)} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2)$:

$$\operatorname{Var}(Z) = \operatorname{Var}\left(\frac{1}{N} \sum_{i=1}^{N} x^{(i)} \varepsilon^{(i)}\right) = \frac{1}{N^2} \sum_{i=1}^{N} (x^{(i)})^2 \operatorname{Var}(\varepsilon^{(i)}) = \frac{\sigma^2 s^2}{N}$$

Therefore:

$$Var(w_D) = Var\left(\frac{Z}{\lambda + s^2}\right) = \frac{Var(Z)}{(\lambda + s^2)^2} = \frac{\sigma^2 s^2}{N(\lambda + s^2)^2}$$

The prediction variance is:

Variance =
$$\frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_D[(w_D x^{(i)} - \bar{w} x^{(i)})^2] = s^2 \text{Var}(w_D) = \boxed{\frac{s^4 \sigma^2}{N(\lambda + s^2)^2}}$$

(e) Behavior as $\lambda \to 0, \infty$

From parts (c) and (d), we have:

$$\operatorname{Bias}^{2} = \left(\frac{\lambda}{\lambda + s^{2}}\right)^{2} (w^{*})^{2} s^{2} \tag{1}$$

$$Variance = \frac{s^4 \sigma^2}{N(\lambda + s^2)^2}$$
 (2)

As $\lambda \to 0$ (no regularization):

- Bias² $\rightarrow \left(\frac{0}{s^2}\right)^2 (w^*)^2 s^2 = 0$ (unbiased estimation)
- Variance $\rightarrow \frac{s^4 \sigma^2}{N s^4} = \frac{\sigma^2}{N}$ (high variance)

As $\lambda \to \infty$ (strong regularization):

- Bias² $\to \left(\frac{\lambda}{\lambda}\right)^2 (w^*)^2 s^2 = (w^*)^2 s^2$ (high bias)
- Variance $\rightarrow \frac{s^4 \sigma^2}{N \lambda^2} = 0$ (low variance)

This demonstrates the classical bias-variance tradeoff: as λ increases, bias increases monotonically while variance decreases monotonically. Since we don't know w^* or the true noise distribution in practice, we use model selection techniques (like cross-validation) to find the optimal λ that balances this tradeoff.

(f) Constraint diameter

Constraint $||w||^2 \le R$ implies $|w_D - \bar{w}| \le |w_D| + |\bar{w}| \le 2\sqrt{R}$, hence $|w_D - \bar{w}|^2 \le 4R$

(g) Variance bound

$$(w_D x^{(i)} - \bar{w} x^{(i)})^2 \le x^{(i)2} |w_D - \bar{w}|^2 \le 4R x^{(i)2}.$$

Averaging and taking expectation gives Variance $\leq 4Rs^2$

2. Optimal Classifier under Squared Loss

Given loss $L(h) = \mathbb{E}_{(x,y),D}[(h(x) - y)^2].$

(a) Optimal predictor

Since we seek an optimal predictor $h_{\text{opt}}(x)$ that is independent of any specific dataset D, we can write the loss as:

$$L(h) = \mathbb{E}_{(x,y) \sim P}[(h(x) - y)^2]$$

Apply the law of total expectation:

$$L(h) = \mathbb{E}_x \left[\mathbb{E}_{y|x} [(h(x) - y)^2] \right]$$

For each fixed x, we need to minimize the inner expectation $\mathbb{E}_{y|x}[(h(x)-y)^2]$. Using the bias-variance decomposition for squared error:

$$\mathbb{E}_{y|x}[(h(x) - y)^{2}] = \text{Var}(y|x) + (h(x) - \mathbb{E}[y|x])^{2}$$

Since Var(y|x) is independent of our choice of h(x), the minimum is achieved when the second term equals zero:

$$h(x) - \mathbb{E}[y|x] = 0$$

Therefore: $h_{\text{opt}}(x) = \mathbb{E}[y|x]$

(b) Minimum achievable error

Substituting the optimal predictor back into the loss function:

$$L_{\min} = \mathbb{E}_x \left[\mathbb{E}_{y|x} [(\mathbb{E}[y|x] - y)^2] \right]$$

Since $\mathbb{E}[y|x]$ is constant with respect to the inner expectation over y|x:

$$L_{\min} = \mathbb{E}_x \left[\mathbb{E}_{y|x} [(y - \mathbb{E}[y|x])^2] \right] = \mathbb{E}_x [\operatorname{Var}(y|x)]$$

Therefore: $L_{\min} = \mathbb{E}_x[\operatorname{Var}(y|x)]$

This represents the **irreducible error** or **Bayes risk** - the fundamental limit on prediction accuracy due to the inherent noise in the relationship between x and y.