1.

1.

The assumption  $X \in \mathbb{R}^{N \times d}$  is a fixed data matrix means the rows  $x_i^{\top}$  (the feature vectors) are not random variables in the probability model. All the randomness in the data-generating process comes only from the noise term  $\vec{\epsilon}$ . The features X are measured without error—i.e., they are "perfect" and are treated as constants. The only uncertainty comes from the outcome  $\vec{y}$ , via the noise term.

So the model is:

$$\vec{y} = X\vec{\theta} + \vec{\epsilon}, \quad \vec{\epsilon} \sim \mathcal{N}(0, \sigma^2 I_N)$$

Here,  $\vec{y}$  is random, but X is treated as deterministic.

Ridge estimator:

$$\begin{aligned} \hat{\vec{\theta}} &= (X^{\top}X + \lambda I_d)^{-1}X^{\top}\vec{y} \\ &= (X^{\top}X + \lambda I_d)^{-1}X^{\top}(X\vec{\theta} + \vec{\epsilon}) \\ &= (X^{\top}X + \lambda I_d)^{-1}X^{\top}X\vec{\theta} + (X^{\top}X + \lambda I_d)^{-1}X^{\top}\vec{\epsilon} \end{aligned}$$

Because X is fixed, all expectations are conditional on X; the only randomness comes from  $\vec{\epsilon}$ . Thus  $\mathbb{E}_{\mathcal{D}}[\hat{\vec{\theta}}] = \mathbb{E}[\hat{\vec{\theta}} \mid X]$ .

$$\begin{split} \mathbb{E}[\hat{\vec{\theta}} \mid X] &= (X^\top X + \lambda I_d)^{-1} X^\top X \vec{\theta} + (X^\top X + \lambda I_d)^{-1} X^\top \mathbb{E}[\vec{\epsilon} \mid X] \\ &= (X^\top X + \lambda I_d)^{-1} X^\top X \vec{\theta} + (X^\top X + \lambda I_d)^{-1} X^\top \cdot 0 \\ &\quad (\text{Since } \vec{\epsilon} \sim \mathcal{N}(0, \sigma^2 I_N) \text{ and is independent of } X, \text{ so } \mathbb{E}[\vec{\epsilon} \mid X] = \mathbb{E}[\vec{\epsilon}] = 0) \\ &= (X^\top X + \lambda I_d)^{-1} X^\top X \vec{\theta} \\ &= (I_d - \lambda (X^\top X + \lambda I_d)^{-1}) \vec{\theta} \\ &\quad (\text{Using } (A + \lambda I_d)^{-1} A = I_d - \lambda (A + \lambda I_d)^{-1} \text{ with } A = X^\top X) \end{split}$$

Therefore

$$\mathbb{E}_{\mathcal{D}}[\hat{\vec{\theta}}] = (I_d - \lambda (X^{\top} X + \lambda I_d)^{-1}) \vec{\theta}$$

2.

No—ridge regression is biased (unless  $\lambda = 0$ ). For  $\hat{\vec{\theta}}$  to be unbiased, we would require

$$\mathbb{E}[\hat{\vec{\theta}}] = \vec{\theta}, \quad \text{for all } \vec{\theta}.$$

But instead we have

$$\mathbb{E}[\hat{\vec{\theta}}] = (I_d - \lambda (X^{\top} X + \lambda I_d)^{-1}) \vec{\theta}.$$

We pay a bias penalty (bias is non-zero) because of the ridge regularization (the  $\ell_2$  penalty), which shrinks coefficient estimates toward zero even when the linear model is correctly specified.

$$\operatorname{Bias}(\hat{\vec{\theta}}) = \mathbb{E}_{\mathcal{D}}[\hat{\vec{\theta}}] - \vec{\theta} = -\lambda (X^{\top}X + \lambda I_d)^{-1}\vec{\theta}.$$

This expression is the parameter bias: it measures the deviation of the expected ridge estimator from the true parameter vector  $\vec{\theta}$ .

Note:  $\operatorname{Bias}(\hat{\vec{\theta}}) = 0 \iff \lambda = 0 \text{ or } \vec{\theta} = 0$ . The bias is non-zero for  $\lambda > 0$  and  $\vec{\theta} \neq 0$ .

3.

Let 
$$A := (X^{\top}X + \lambda I_d)^{-1}X^{\top} \in \mathbb{R}^{d \times N}$$
  
Since  $X$  is fixed (deterministic),  $\operatorname{Cov}(\hat{\vec{\theta}}) = \operatorname{Cov}(\hat{\vec{\theta}} \mid X)$ .  
Ridge estimator:

$$\hat{\vec{\theta}} = (X^{\top}X + \lambda I_d)^{-1}X^{\top}\vec{y}$$

$$= (X^{\top}X + \lambda I_d)^{-1}X^{\top}(X\vec{\theta} + \vec{\epsilon})$$

$$= (X^{\top}X + \lambda I_d)^{-1}X^{\top}X\vec{\theta} + (X^{\top}X + \lambda I_d)^{-1}X^{\top}\vec{\epsilon}$$

$$= AX\vec{\theta} + A\vec{\epsilon}$$

Expectation:

$$\mathbb{E}[\hat{\vec{\theta}}] = (X^{\top}X + \lambda I_d)^{-1}X^{\top}X\vec{\theta}$$
$$= AX\vec{\theta}$$

Covariance derivation:

$$\operatorname{Cov}(\hat{\vec{\theta}}) = \mathbb{E}\left[(\hat{\vec{\theta}} - \mathbb{E}[\hat{\vec{\theta}}])(\hat{\vec{\theta}} - \mathbb{E}[\hat{\vec{\theta}}])^{\top}\right] \\
= \mathbb{E}\left[(AX\vec{\theta} + A\vec{\epsilon} - AX\vec{\theta})(AX\vec{\theta} + A\vec{\epsilon} - AX\vec{\theta})^{\top}\right] \\
= \mathbb{E}\left[(A\vec{\epsilon})(A\vec{\epsilon})^{\top}\right] \\
= \mathbb{E}\left[A\vec{\epsilon}\vec{\epsilon}^{\top}A^{\top}\right] \qquad (\operatorname{Using}(AB)^{\top} = B^{\top}A^{\top}) \\
= A\mathbb{E}[\vec{\epsilon}\vec{\epsilon}^{\top}]A^{\top} \\
= A(\sigma^{2}I_{N})A^{\top} \qquad (\operatorname{As}\mathbb{E}[\vec{\epsilon}\vec{\epsilon}^{\top}] = \sigma^{2}I_{N}, \operatorname{since}\vec{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^{2}I_{N})) \\
= \sigma^{2}AA^{\top}$$

Substituting back  $A = (X^{\top}X + \lambda I_d)^{-1}X^{\top}$ :

$$\operatorname{Cov}(\hat{\vec{\theta}}) = \sigma^2 A A^{\top}$$

$$= \sigma^2 (X^{\top} X + \lambda I_d)^{-1} X^{\top} \left[ (X^{\top} X + \lambda I_d)^{-1} X^{\top} \right]^{\top}$$

$$= \sigma^2 (X^{\top} X + \lambda I_d)^{-1} X^{\top} X (X^{\top} X + \lambda I_d)^{-1}$$

$$= \sigma^2 (X^{\top} X + \lambda I_d)^{-1} X^{\top} X (X^{\top} X + \lambda I_d)^{-1}$$

Note:  $X^{\top}X + \lambda I_d$  is symmetric positive definite (for  $\lambda > 0$ ), so  $(X^{\top}X + \lambda I_d)^{-T} = (X^{\top}X + \lambda I_d)^{-1}$ .

4.

We consider the ridge regression setting with training data:

$$\vec{y} = X\vec{\theta} + \vec{\varepsilon}, \qquad \vec{\varepsilon} \sim \mathcal{N}(0, \sigma^2 I_N)$$

where  $X \in \mathbb{R}^{N \times d}$  is fixed (deterministic) and  $\vec{\theta} \in \mathbb{R}^d$  is the true parameter vector.

For a fixed test point  $\vec{x}^{(0)} \in \mathbb{R}^d$ , the true response is:

$$y^{(0)} = f(\vec{x}^{(0)}) + \varepsilon^{(0)} = \vec{x}^{(0)\top}\vec{\theta} + \varepsilon^{(0)}, \qquad \varepsilon^{(0)} \sim \mathcal{N}(0, \sigma^2)$$

where  $\varepsilon^{(0)}$  is independent of the training data.

The ridge estimator from training data  $\mathcal{D} = (X, \vec{y})$  is:

$$\hat{\vec{\theta}} = (X^{\top}X + \lambda I_d)^{-1}X^{\top}\vec{y}$$

The prediction at the test point  $\vec{x}^{(0)}$  is:

$$\hat{y}^{(0)} = \vec{x}^{(0)} \, ^{\top} \hat{\vec{\theta}}$$

The EPE at test point  $\vec{x}^{(0)}$  is:

$$\begin{split} \mathrm{EPE}(\vec{x}^{(0)}) &= \mathbb{E}_{\mathcal{D}, y^{(0)}} \left[ \left( y^{(0)} - \hat{y}^{(0)} \right)^2 \right] \\ &= \mathbb{E}_{\mathcal{D}, \varepsilon^{(0)}} \left[ \left( f(\vec{x}^{(0)}) + \varepsilon^{(0)} - \hat{y}^{(0)} \right)^2 \right] \\ &= \mathbb{E}_{\mathcal{D}, \varepsilon^{(0)}} \left[ \left( f(\vec{x}^{(0)}) - \hat{y}^{(0)} + \varepsilon^{(0)} \right)^2 \right] \\ &= \mathbb{E}_{\mathcal{D}, \varepsilon^{(0)}} \left[ \left( f(\vec{x}^{(0)}) - \hat{y}^{(0)} \right)^2 + 2\varepsilon^{(0)} \left( f(\vec{x}^{(0)}) - \hat{y}^{(0)} \right) + \left( \varepsilon^{(0)} \right)^2 \right] \\ &= \mathbb{E}_{\mathcal{D}, \varepsilon^{(0)}} \left[ \left( f(\vec{x}^{(0)}) - \hat{y}^{(0)} \right)^2 \right] + \mathbb{E}_{\mathcal{D}} \left[ f(\vec{x}^{(0)}) - \hat{y}^{(0)} \right] \cdot \mathbb{E}_{\varepsilon^{(0)}} \left[ 2\varepsilon^{(0)} \right] + \mathbb{E}_{\varepsilon^{(0)}} \left[ \left( \varepsilon^{(0)} \right)^2 \right] \\ &= \mathbb{E}_{\mathcal{D}} \left[ \left( f(\vec{x}^{(0)}) - \hat{y}^{(0)} \right)^2 \right] + \sigma^2 \qquad (\mathrm{As} \ \varepsilon^{(0)} \sim \mathcal{N}(0, \sigma^2), \ \mathrm{so} \ \mathbb{E}[\varepsilon^{(0)}] = 0 \ \mathrm{and} \ \mathbb{E}[(\varepsilon^{(0)})^2] = \sigma^2) \\ &= \left( f(\vec{x}^{(0)}) - \mathbb{E}_{\mathcal{D}}[\hat{y}^{(0)}] \right)^2 + \mathrm{Var}_{\mathcal{D}}(\hat{y}^{(0)}) + \sigma^2 \quad (\mathrm{Using} \ \mathbb{E}[(a - Z)^2] = (a - \mathbb{E}[Z])^2 + \mathrm{Var}(Z)) \end{split}$$

Therefore:

$$EPE(\vec{x}^{(0)}) = \sigma^2 + (f(\vec{x}^{(0)}) - \mathbb{E}_{\mathcal{D}}[\hat{y}^{(0)}])^2 + Var_{\mathcal{D}}(\hat{y}^{(0)})$$

For ridge with fixed  $X \in \mathbb{R}^{N \times d}$ :

Let 
$$S = (X^{\top}X + \lambda I_d)^{-1} \in \mathbb{R}^{d \times d}$$
.

$$\mathbb{E}_{\mathcal{D}}[\hat{\vec{\theta}}] = (I_d - \lambda (X^{\top}X + \lambda I_d)^{-1})\vec{\theta}$$
$$= (I_d - \lambda S)\vec{\theta}$$

$$Cov(\hat{\vec{\theta}}) = \sigma^2 (X^\top X + \lambda I_d)^{-1} X^\top X (X^\top X + \lambda I_d)^{-1}$$
$$= \sigma^2 S X^\top X S$$

This gives us:

$$\mathbb{E}[\hat{\vec{\theta}}] = SX^{\top}X\vec{\theta} = (I_d - \lambda S)\vec{\theta}$$
$$Cov(\hat{\vec{\theta}}) = \sigma^2 SX^{\top}XS$$

Irreducible Error:  $\sigma^2$  (noise variance)

Bias: Using prediction space. At test point  $\vec{x}^{(0)}$ , the prediction is  $\hat{y}^{(0)} = \vec{x}^{(0)\top}\hat{\vec{\theta}}$ .

$$\begin{split} \mathbb{E}[\hat{y}^{(0)}] &= \vec{x}^{(0)} \top \mathbb{E}[\hat{\vec{\theta}}] = \vec{x}^{(0)} \top (I_d - \lambda S) \vec{\theta} \\ \text{Bias} &= f(\vec{x}^{(0)}) - \mathbb{E}[\hat{y}^{(0)}] \\ &= \vec{x}^{(0)} \top \vec{\theta} - \vec{x}^{(0)} \top (I_d - \lambda S) \vec{\theta} \\ &= \lambda \vec{x}^{(0)} \top S \vec{\theta} \\ \text{Bias}^2 &= \lambda^2 \vec{\theta}^\top S \vec{x}^{(0)} \vec{x}^{(0)} \top S \vec{\theta} \end{split}$$

Variance: Using  $Var(a^{\top}Z) = a^{\top} Cov(Z)a$  with  $a = \vec{x}^{(0)}$  and  $Z = \hat{\vec{\theta}}$ :

$$Var(\hat{y}^{(0)}) = Var(\vec{x}^{(0)} + \hat{\vec{\theta}}) = \vec{x}^{(0)} Cov(\hat{\vec{\theta}}) \vec{x}^{(0)}$$
$$= \sigma^2 \vec{x}^{(0)} SX^T X S \vec{x}^{(0)}$$

Final decomposition:

$$EPE(\vec{x}^{(0)}) = \sigma^2 + \lambda^2 \vec{\theta}^{\top} S \vec{x}^{(0)} \vec{x}^{(0)} \vec{x}^{(0)} \vec{S} \vec{\theta} + \sigma^2 \vec{x}^{(0)} \vec{S} \vec{X}^{\top} X S \vec{x}^{(0)}$$

Substituting back  $S = (X^{\top}X + \lambda I_d)^{-1}$ :

$$\mathrm{EPE}(\vec{x}^{(0)}) = \sigma^2 + \lambda^2 \vec{\theta}^\top (X^\top X + \lambda I_d)^{-1} \vec{x}^{(0)} \vec{x}^{(0)\top} (X^\top X + \lambda I_d)^{-1} \vec{\theta} + \sigma^2 \vec{x}^{(0)\top} (X^\top X + \lambda I_d)^{-1} X^\top X (X^\top X + \lambda I_d)^{-1} \vec{x}^{(0)}$$

## 2.

## 1.

The assumption  $X \in \mathbb{R}^{N \times d}$  is a fixed data matrix with rank d means the rows  $x_i^{\top}$  (the feature vectors) are not random variables in the probability model. All the randomness in the data-generating process comes only from the noise term  $\vec{\epsilon}$ . The features X are measured without error—i.e., they are "perfect" and are treated as constants. The only uncertainty comes from the outcome  $\vec{y}$ , via the noise term.

Assume the data was drawn from

$$y = h(\vec{x}) + \epsilon = \vec{\theta}^{\top} \vec{x} + \epsilon, \qquad \epsilon \sim \mathcal{N}(0, \sigma^2).$$

An estimate of  $h(\vec{x})$  is given by

$$\hat{h}(\vec{x}) = \vec{\beta}^{\top} X \vec{x},$$

where the parameter vector  $\vec{\beta} \in \mathbb{R}^N$ .

The cost function is defined as:

$$J(\vec{\beta}) := \sum_{i=1}^{N} (\hat{h}(\vec{x}) - y^{(i)})^{2} + \lambda ||X^{\top} \vec{\beta}||^{2},$$

that is

$$J(\vec{\beta}) := (XX^{\top}\vec{\beta} - \vec{y})^{\top}(XX^{\top}\vec{\beta} - \vec{y}) + \vec{\beta}^{\top}X\lambda X^{\top}\vec{\beta}$$

Let 
$$K := XX^{\top} \in \mathbb{R}^{N \times N}$$

$$\begin{split} J(\vec{\beta}) &= (XX^{\top}\vec{\beta} - \vec{y})^{\top}(XX^{\top}\vec{\beta} - \vec{y}) + \vec{\beta}^{\top}X\lambda X^{\top}\vec{\beta} \\ &= (K\vec{\beta} - \vec{y})^{\top}(K\vec{\beta} - \vec{y}) + \lambda \vec{\beta}^{\top}K\vec{\beta} \\ &= (\vec{\beta}^{\top}K^{\top} - \vec{y}^{\top})(K\vec{\beta} - \vec{y}) + \lambda \vec{\beta}^{\top}K\vec{\beta} \\ &= \vec{\beta}^{\top}K^{\top}K\vec{\beta} - \vec{\beta}^{\top}K^{\top}\vec{y} - \vec{y}^{\top}K\vec{\beta} + \vec{y}^{\top}\vec{y} + \lambda \vec{\beta}^{\top}K\vec{\beta} \end{split}$$

Using  $K = K^{\top}$  (since  $K = XX^{\top}$  is symmetric):

$$\begin{split} J(\vec{\beta}) &= \vec{\beta}^\top K K \vec{\beta} - \vec{\beta}^\top K \vec{y} - \vec{y}^\top K \vec{\beta} + \vec{y}^\top \vec{y} + \lambda \vec{\beta}^\top K \vec{\beta} \\ &= \vec{\beta}^\top K^2 \vec{\beta} - 2 \vec{y}^\top K \vec{\beta} + \vec{y}^\top \vec{y} + \lambda \vec{\beta}^\top K \vec{\beta} \end{split}$$

Taking the gradient with respect to  $\vec{\beta}$ :

$$\nabla_{\beta}J(\vec{\beta}) = \nabla_{\beta} \left[ \vec{\beta}^{\top} K^{2} \vec{\beta} - 2 \vec{y}^{\top} K \vec{\beta} + \vec{y}^{\top} \vec{y} + \lambda \vec{\beta}^{\top} K \vec{\beta} \right]$$

$$= \nabla_{\beta} \left[ \vec{\beta}^{\top} K^{2} \vec{\beta} \right] - \nabla_{\beta} \left[ 2 \vec{y}^{\top} K \vec{\beta} \right] + \nabla_{\beta} \left[ \vec{y}^{\top} \vec{y} \right] + \nabla_{\beta} \left[ \lambda \vec{\beta}^{\top} K \vec{\beta} \right]$$

$$= (K^{2} + (K^{2})^{\top}) \vec{\beta} - 2 K^{\top} \vec{y} + 0 + \lambda (K + K^{\top}) \vec{\beta} \quad (\text{As } \nabla_{\beta} (\vec{\beta}^{\top} A \vec{\beta}) = (A + A^{\top}) \vec{\beta} \text{ and } \nabla_{\beta} (\vec{c}^{\top} \vec{\beta}) = \vec{c})$$

$$= 2 K^{2} \vec{\beta} - 2 K \vec{y} + 2 \lambda K \vec{\beta} \quad (\text{As } K = K^{\top} \Rightarrow K^{2} = (K^{2})^{\top})$$

$$= 2 (K^{2} \vec{\beta} + \lambda K \vec{\beta} - K \vec{y})$$

$$= 2 K (K + \lambda I) \vec{\beta} - 2 K \vec{y}$$

Therefore:

$$\nabla_{\beta}J(\vec{\beta}) = 2K(K + \lambda I)\vec{\beta} - 2K\vec{y}$$
$$\nabla_{\beta}J(\vec{\beta}) = 0$$
$$\Rightarrow 2K(K + \lambda I)\vec{\beta} - 2K\vec{y} = 0$$
$$\Rightarrow K(K + \lambda I)\vec{\beta} = K\vec{y}$$

For any vector  $\vec{v} \in \mathbb{R}^N$ , we have:

$$\vec{v}^{\top} K \vec{v} = \vec{v}^{\top} (X X^{\top}) \vec{v}$$

$$= (\vec{v}^{\top} X) (X^{\top} \vec{v}) \quad (\text{As } (AB)C = A(BC))$$

$$= (X^{\top} \vec{v})^{\top} (X^{\top} \vec{v}) \quad (\text{As } \vec{v}^{\top} X = (X^{\top} \vec{v})^{\top})$$

$$= ||X^{\top} \vec{v}||^2 > 0 \quad (\text{As } ||\vec{u}||^2 = \vec{u}^{\top} \vec{u} > 0)$$

Since  $\vec{v}^{\top}K\vec{v} \geq 0$  for all  $\vec{v} \in \mathbb{R}^N$ , the matrix  $K = XX^{\top}$  is positive semi-definite. For  $\lambda > 0$ , the matrix  $(K + \lambda I)$  is positive definite because:

$$\vec{v}^{\top}(K + \lambda I)\vec{v} = \vec{v}^{\top}K\vec{v} + \lambda ||\vec{v}||^2 > 0$$
 for all  $\vec{v} \neq \vec{0}$ 

Therefore  $(K + \lambda I)$  is invertible.

The solution  $\hat{\vec{\beta}} = (K + \lambda I)^{-1} \vec{y}$  satisfies the optimality condition:

$$K(K + \lambda I)\hat{\vec{\beta}} = K(K + \lambda I)(K + \lambda I)^{-1}\vec{y}$$
$$= K\vec{y}$$

Therefore, the optimal solution that minimizes the cost function is:

$$\hat{\vec{\beta}} = (K + \lambda I)^{-1} \vec{y} = (XX^{\top} + \lambda I)^{-1} \vec{y}$$

## 2.

We want the degrees of freedom:

$$df(\hat{y}) = \frac{1}{\sigma^2} tr(Cov(\hat{y}, y)).$$

From the optimization problem, the solution is

$$\hat{\beta} = (K + \lambda I)^{-1} y, \qquad K = X X^{\top}.$$

Therefore, the fitted values are

$$\hat{y} = K\hat{\beta} = K(K + \lambda I)^{-1}y.$$

This can be written as

$$\hat{y} = Ay, \qquad A := K(K + \lambda I)^{-1}.$$

As  $y = X\theta + \varepsilon$  with  $X\theta$  fixed (non-random), all randomness in y comes from  $\varepsilon$ . Hence

$$Cov(y, y) = Cov(\varepsilon, \varepsilon) = \sigma^2 I.$$

Using  $\hat{y} = Ay$ ,

$$Cov(\hat{y}, y) = Cov(Ay, y) = A Cov(y, y) = A\sigma^2 I.$$

Therefore,

$$df(\hat{y}) = \frac{1}{\sigma^2} tr(A\sigma^2 I) = tr(A).$$

Substituting back  $A = K(K + \lambda I)^{-1}$ :

$$df(\hat{y}) = tr \left( K(K + \lambda I)^{-1} \right)$$