Bias-variance tradeoff for linear models

If $Y_i = X_i^T w^* + \epsilon_i$ and $\epsilon_i \sim \mathcal{N}(0,\sigma^2)$

$$\mathbf{y} = \mathbf{X}w^* + \epsilon$$

$$\widehat{w}_{\text{MLE}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} =$$

$$=$$

$$\eta(x) = \mathbb{E}_{Y|X}[Y \,|\, X = x] =$$

$$\hat{f}_{\mathcal{D}}(x) = x^T \widehat{w}_{\text{MLE}} =$$

Bias-variance tradeoff for linear models

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$$\mathbf{y} = \mathbf{X}w^* + \epsilon$$

$$\widehat{w}_{\text{MLE}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{X}w^* + \epsilon)$$

$$= w^* + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon$$

$$\eta(x) = \mathbb{E}_{Y|X}[Y \,|\, X = x] = x^T w^*$$

$$\hat{f}_{\mathcal{D}}(x) = x^T \widehat{w}_{\text{MLE}} = x^T w^* + x^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon$$

$\mathbb{E}[(x_i^T w^* + \epsilon - x_i^T w^*)^2]$

- Irreducible error: $\mathbb{E}_{X,Y}[(Y - \eta(x))^2 \,|\, X = x] =$ $= \mathbb{E}[\epsilon^2] = \sigma^2$
- Bias squared: $\left(\eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]\right)^2 =$ $\mathbb{E}[(x^T(X^TX)^{-1}X^T\epsilon)]$
  (is independent of the sample size!)

Bias-variance tradeoff for linear models

If $Y_i = X_i^T w^* + \epsilon_i$ and $\epsilon_i \sim \mathcal{N}(0,\sigma^2)$

$$\widehat{w}_{\text{MLE}} = w^* + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon$$

$$\eta(x) = x^T w^*$$

$$\hat{f}_{\mathcal{D}}(x) = x^T w^* + x^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon$$

- Variance: $\mathbb{E}_{\mathcal{D}}\left[\left(\hat{f}_{\mathcal{D}}(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]\right)^2\right] =$

$$a^2 = a a^T \text{ when } a \text{ is scalar}$$

$$\left(x^T (X^T X)^{-1} X^T \epsilon\right)^2$$

$$x^T (X^T X)^{-1} X^T \epsilon \left(x^T (X^T X)^{-1} X^T \epsilon\right)^T$$

$$x^T (X^T X)^{-1} X^T \epsilon \epsilon^T X (X^T X)^{-T} x$$

Cexp

$$x^T (X^T X)^{-1} X^T E(\epsilon \epsilon^T) X (X^T X)^{-T} x$$

$$\sigma^2 \cdot x^T (X^T X)^{-T} \cdot x$$

Bias-variance tradeoff for linear models

If $Y_i = X_i^T w^* + \epsilon_i$ and $\epsilon_i \sim \mathcal{N}(0,\sigma^2)$

$$\widehat{w}_{\text{MLE}} = w^* + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon$$

$$\eta(x) = x^T w^*$$

$$\hat{f}_{\mathcal{D}}(x) = x^T w^* + x^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon$$

- Variance: $\mathbb{E}_{\mathcal{D}}\Big[\big(\hat{f}_{\mathcal{D}}(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]\big)^2\Big] = \mathbb{E}_{\mathcal{D}}[x^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon\epsilon^T\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}x]$

$$= \sigma^2\,\mathbb{E}_{\mathcal{D}}[x^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}x]$$

$$= \sigma^2\,x^T\mathbb{E}_{\mathcal{D}}[(\mathbf{X}^T\mathbf{X})^{-1}]x$$

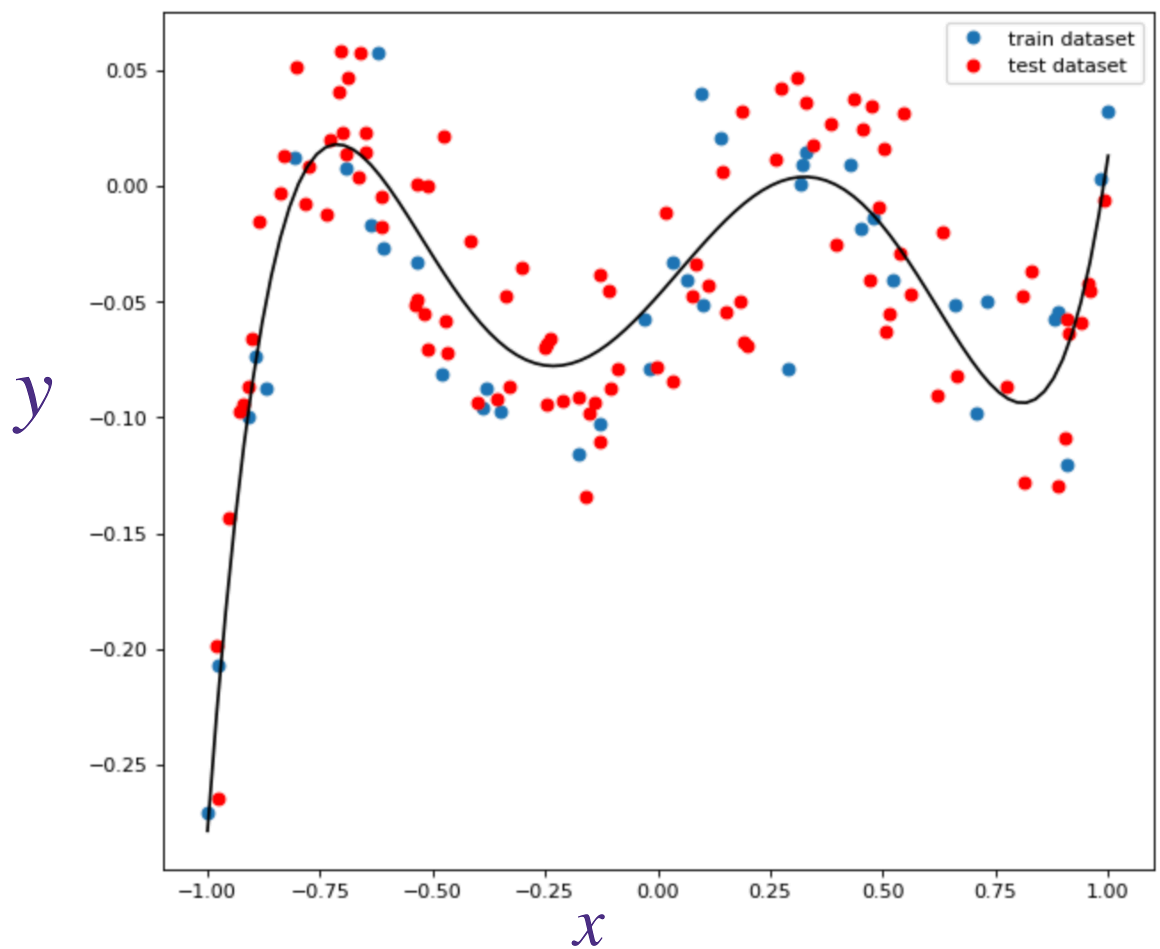
- To analyze this, let's assume that $X_i \sim \mathcal{N}(0,\mathbf{I})$ and number of samples, n, is large enough such that $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$ with high probability and $\mathbb{E}[(\mathbf{X}^T\mathbf{X})^{-1}] \simeq \frac{1}{n}\mathbf{I}$, then
  - Variance is $\dfrac{\sigma^2 x^T x}{n}$, and decreases with increasing sample size n

Regularization

Recap: bias-variance tradeoff

- Consider 100 training examples and 100 test examples i.i.d.drawn from degree-5 polynomial features $x_i \sim \text{Uniform}[-1,1]$, $y_i \sim f_{w*}(x_i) + \epsilon_i$, $\epsilon_i \sim \mathcal{N}(0,\sigma^2)$

$$f_w(x_i) = b^* + w_1^* x_i + w_2^*(x_i)^2 + w_3^*(x_i)^3 + w_4^*(x_i)^4 + w_5^*(x_i)^5$$

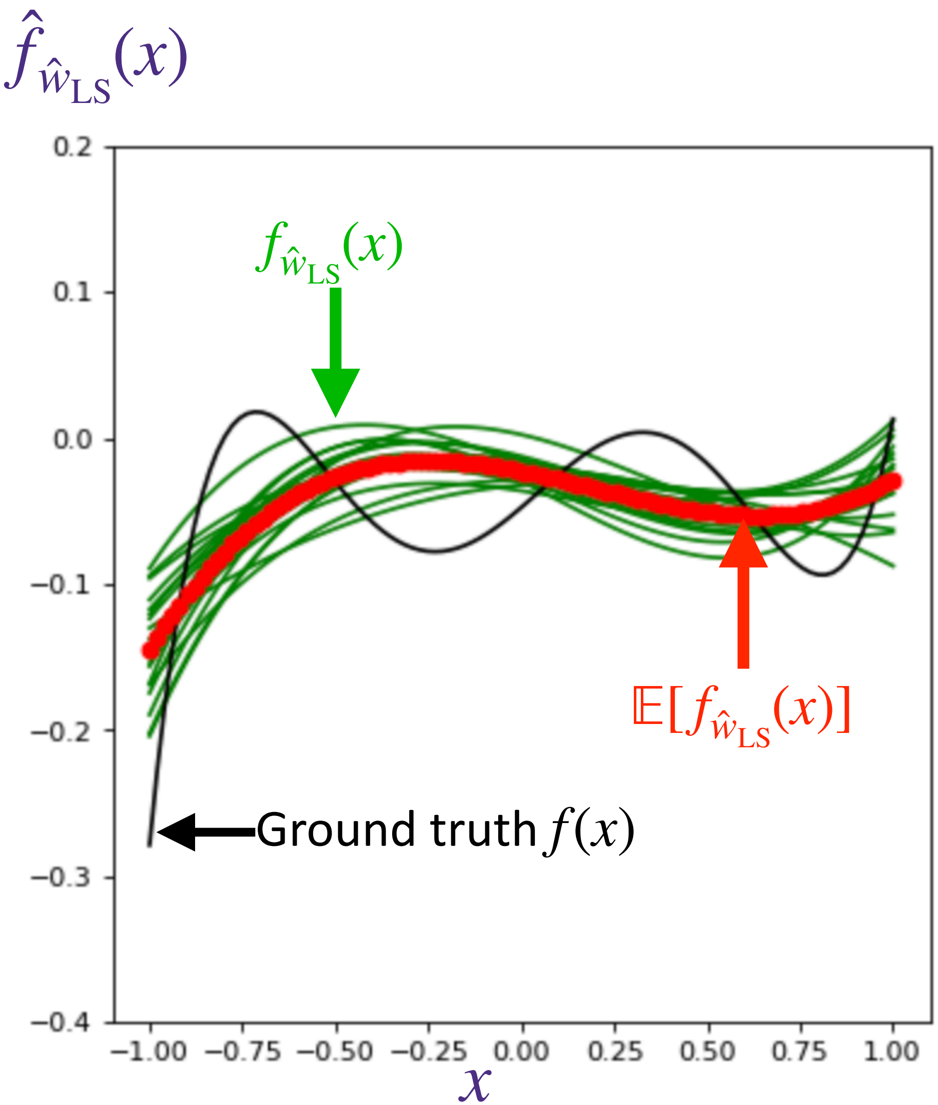


This is a linear model with features

$$h(x_i) = (x_i, (x_i)^2, (x_i)^3, (x_i)^4, (x_i)^5)$$

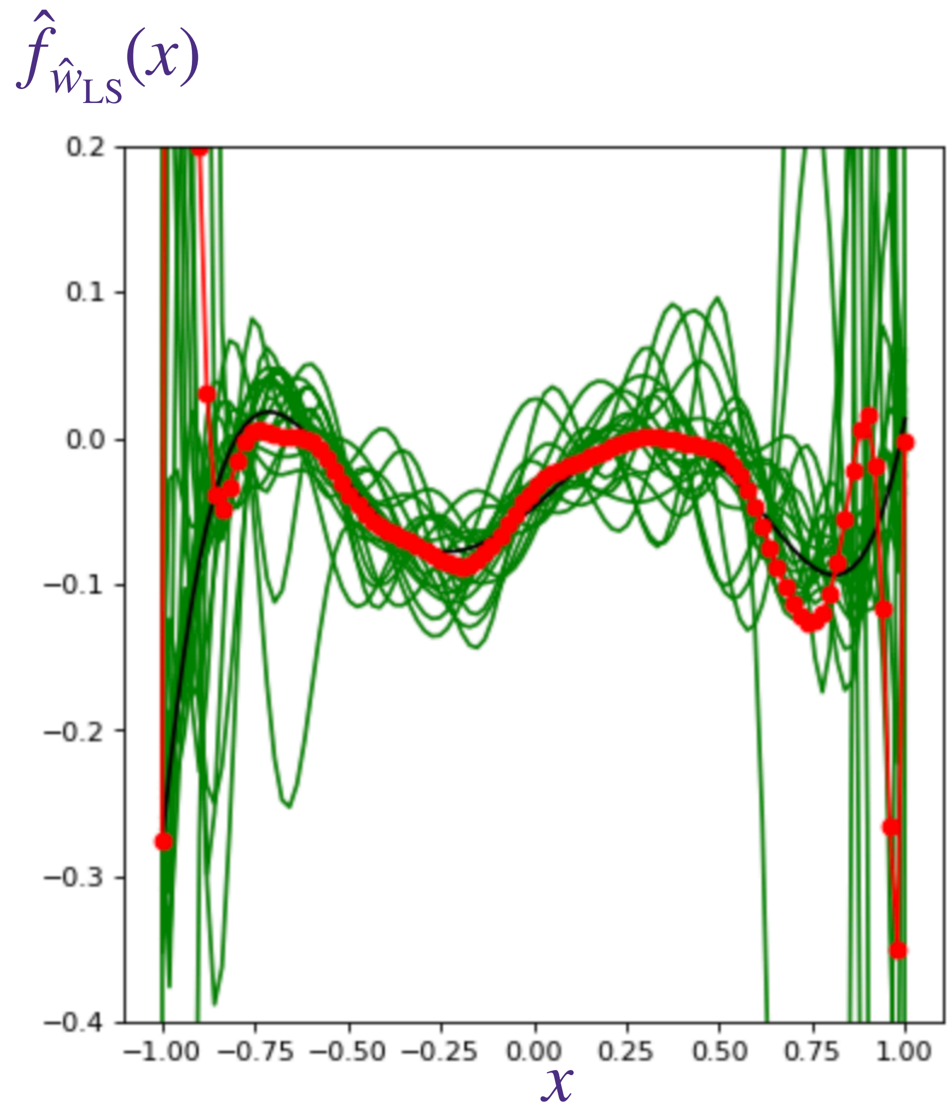
Recap: bias-variance tradeoff

With degree-3 polynomials, we underfit




```
current train error = 0.0036791644380554187
current test error  = 0.0037962529988410953
```

With degree-20 polynomials, we overfit




```
0.00054216863495 68773
0.14210029429557927
```

$$\mathbb{E}_D\left[\left(\hat{f}_D(x) - \mathbb{E}_D\left[\hat{f}_D(x)\right]\right)^2\right]$$

Sensitivity: how to detect overfitting

- For a linear model,
  $y \simeq b + w_1x_1 + w_2x_2 + \cdots + w_dx_d$
  if $|w_j|$ is large then the prediction is sensitive to small changes in x_j
- Large sensitivity leads to overfitting and poor generalization, and equivalently models that overfit tend to have large weights
- Note that b is a constant and hence there is no sensitivity for the offset b

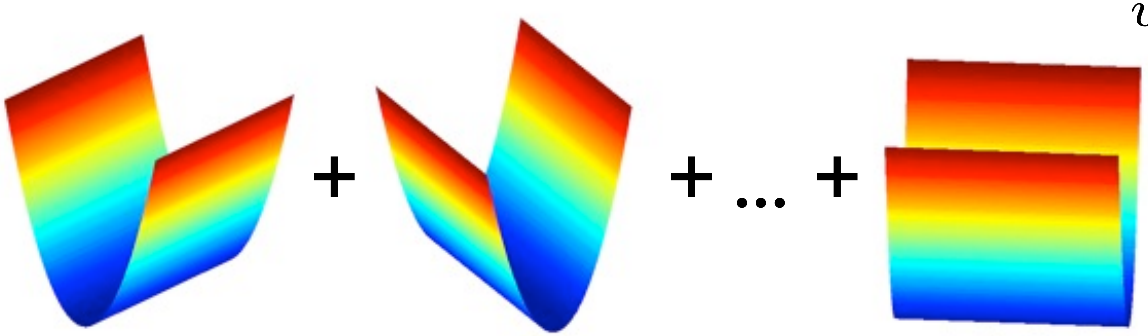
- In **Ridge Regression,** we use a regularizer $||w||_2^2$ to measure and control the sensitivity of the predictor
- And optimize for small loss and small sensitivity, by adding a **regularizer** in the objective (assume no offset for now)

$$\widehat{w}_{ridge} = \arg\min_w \sum_{i=1}^n \left(y_i - x_i^T w\right)^2 + \lambda||w||_2^2$$

Ridge Regression

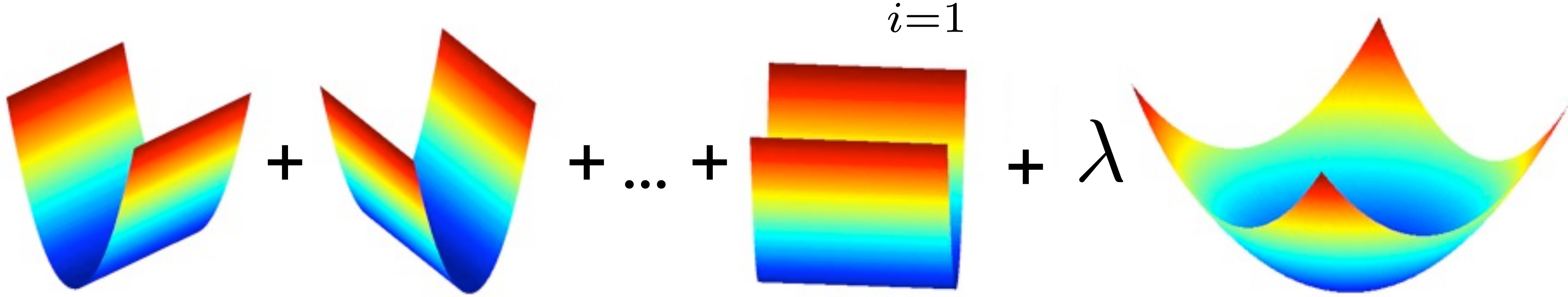
- (Original) Least squares objective:

$$\widehat{w}_{LS} = \arg\min_w \sum_{i=1}^n \left(y_i - x_i^T w\right)^2$$



- Ridge Regression objective:

$$\widehat{w}_{ridge} = \arg\min_w \sum_{i=1}^n \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$



Minimizing the Ridge Regression Objective

$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

Matrix

$$\arg\min_{w} (Y - X^T w)^T (Y - X^T w) + \lambda ||w||_2^2$$

$$\nabla_w = 2X^TXw - 2X^Ty + 2\lambda w$$

$$X^Ty = X^TXw + \lambda w$$

$$w = (X^TX + \lambda I)^{-1} X^T y$$

Shrinkage Properties

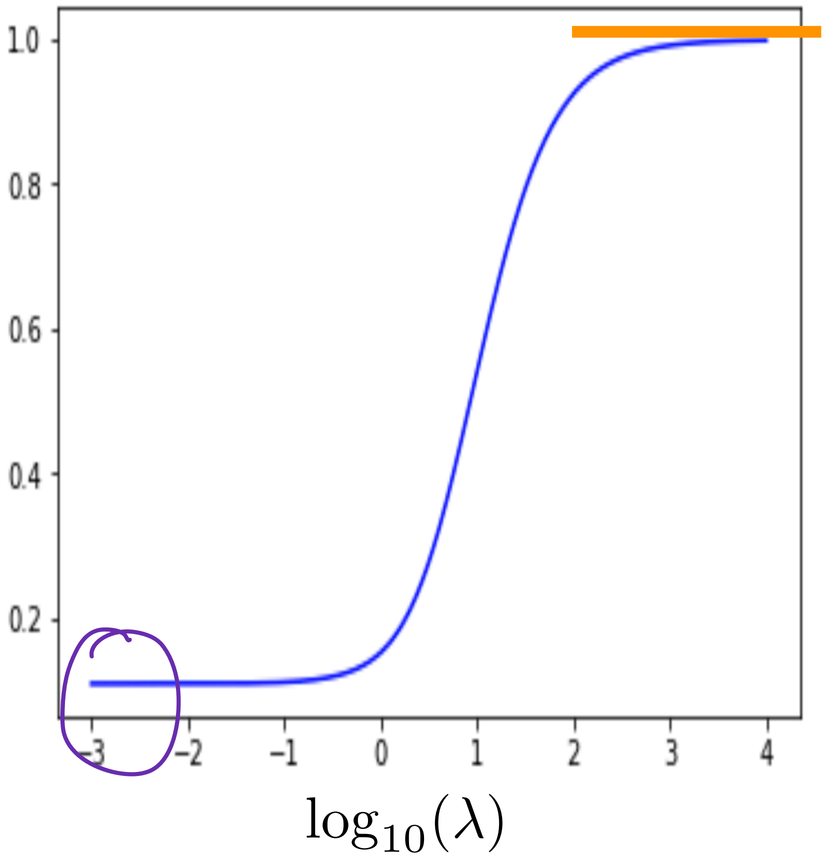
$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

$$= (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

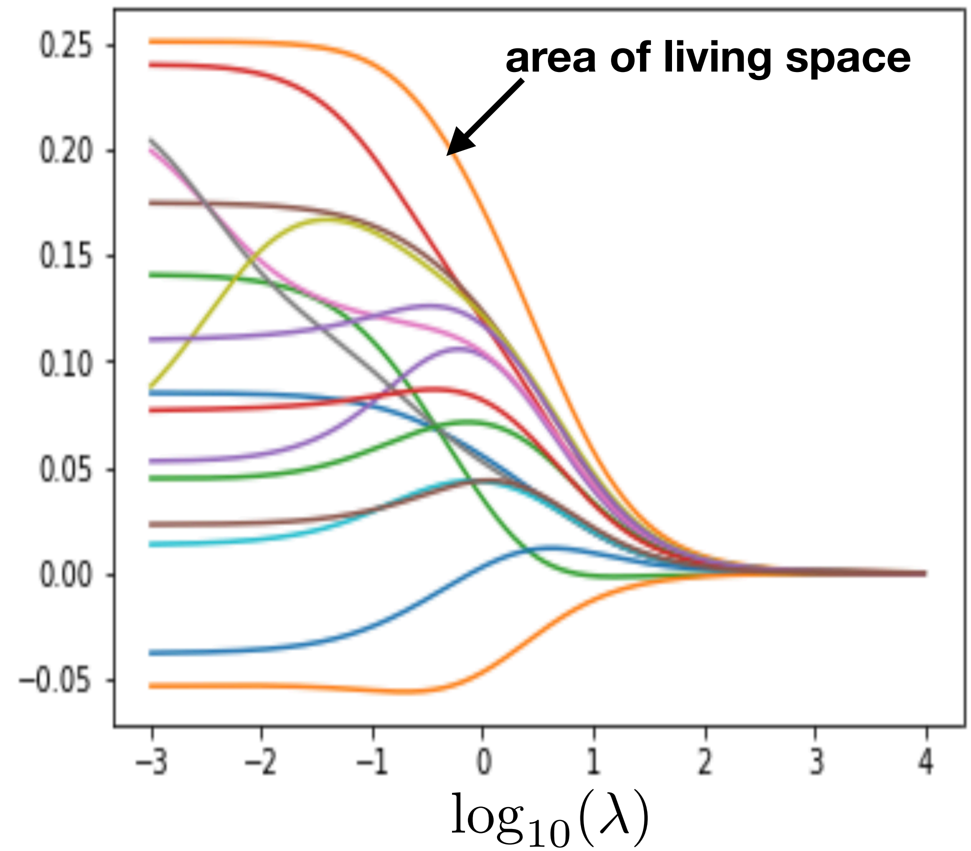
- When $\lambda = 0$, this gives the least squares model
- This defines a family of models hyper-parametrized by λ
- Large λ means more regularization and simpler model
- Small λ means less regularization and more complex model

Ridge regression: minimize $\sum_{i=1}^{n}(w^T x_i - y_i)^2 + \lambda\|w\|_2^2$

training MSE $\frac{1}{n}\sum_{i=1}^{n}(y_i - x_i^T \hat{w}_{\text{ridge}}^{(\lambda)})^2$

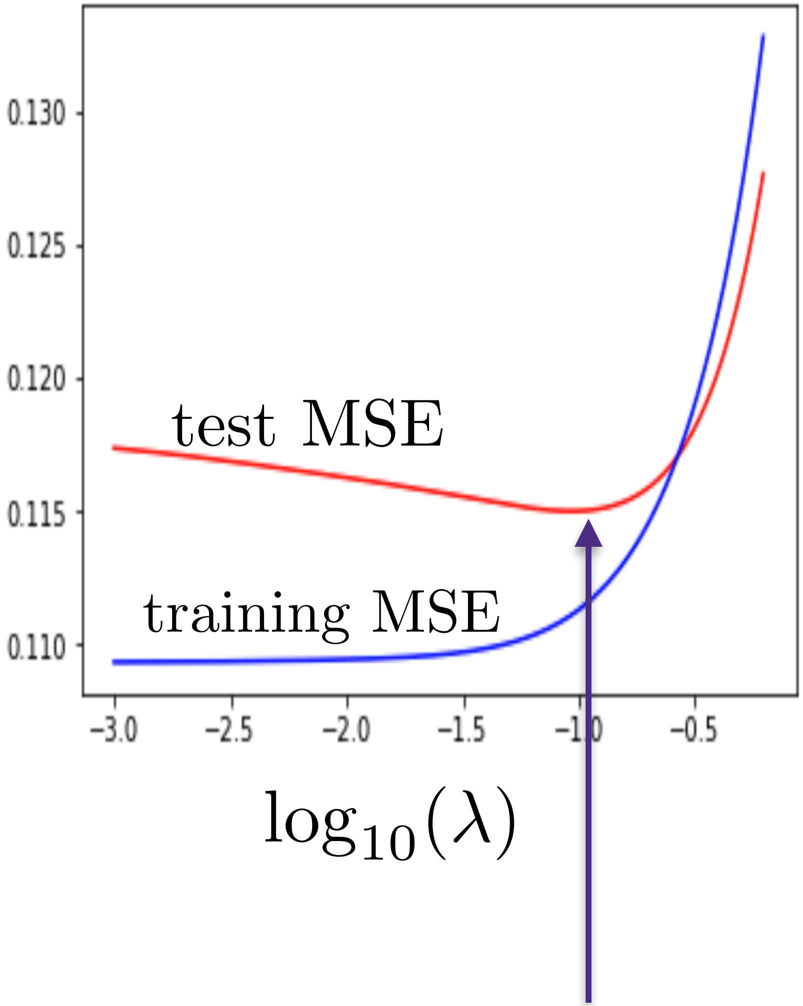


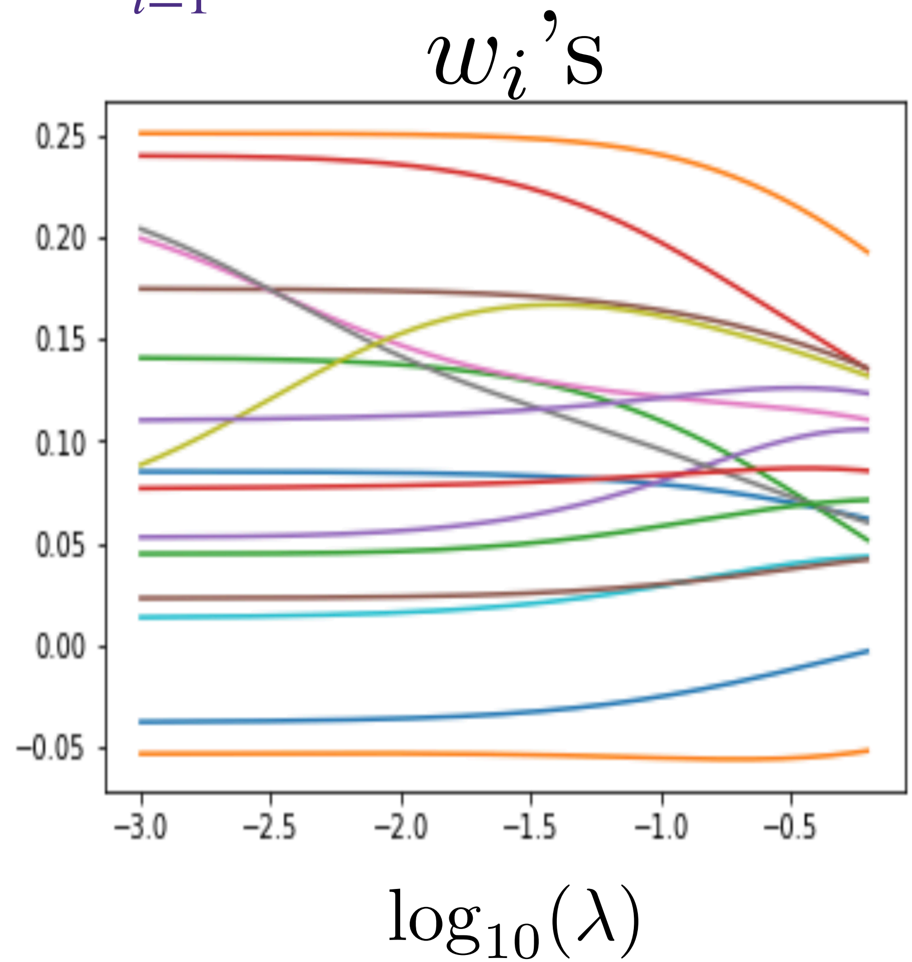
w_i's



- Left plot: leftmost training error is with no regularization: 0.1093
- Left plot: rightmost training error is variance of the training data: 0.9991
- Right plot: called **regularization path**

Ridge regression: minimize $\sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|_2^2$





- this gain in test MSE comes from shrinking w's to get a less sensitive predictor
  (which in turn reduces the variance)

Bias-Variance Properties

- Recall: $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$
- To analyze bias-variance tradeoff, we need to assume probabilistic generative model: $x_i \sim P_X, \;\; \mathbf{y} = \mathbf{X}w + \epsilon, \;\; \epsilon \sim \mathcal{N}(0,\sigma^2\mathbf{I})$
- The true error at a sample with feature x is $\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$

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- The true error at a sample with feature x is

$$\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \mid x]$$

$$= \underbrace{\mathbb{E}_{y|x}[(y - \mathbb{E}[y\mid x])^2 \mid x]}_{\text{Irreducible Error}} + \underbrace{\mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}[y\mid x] - x^T\hat{w}_{\text{ridge}})^2 \mid x]}_{\text{Learning Error}}$$

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$$= \mathbb{E}_{y|x}[(y - x^Tw)^2 \,|\, x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(x^Tw - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

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$$= \mathbb{E}_{y|x}[(y - x^T w)^2 \,|\, x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(x^T w - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

$$= \underbrace{\sigma^2}_{\text{Irreduc. Error}} + \underbrace{(x^T w - \mathbb{E}_{\mathcal{D}_{\text{train}}}[x^T\hat{w}_{\text{ridge}} \,|\, x])^2}_{\text{Bias-squared}} + \underbrace{\mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}} \,|\, x] - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]}_{\text{Variance}}$$

Bias-Variance Properties

- Recall: $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$
- To analyze bias-variance tradeoff, we need to assume probabilistic generative model: $x_i \sim P_X, \;\; \mathbf{y} = \mathbf{X}w + \epsilon, \;\; \epsilon \sim \mathcal{N}(0, \sigma^2\mathbf{I})$
- The true error at a sample with feature x is

$$\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

$$= \mathbb{E}_{y|x}[(y - \mathbb{E}[y\,|\,x])^2\,|\,x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}[y\,|\,x] - x^T\hat{w}_{\text{ridge}})^2\,|\,x]$$

$$= \mathbb{E}_{y|x}[(y - x^T w)^2\,|\,x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(x^T w - x^T\hat{w}_{\text{ridge}})^2\,|\,x]$$

$$= \underbrace{\sigma^2}_{\text{Irreduc. Error}} + \underbrace{(x^T w - \mathbb{E}_{\mathcal{D}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x])^2}_{\text{Bias-squared}} + \underbrace{\mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x] - x^T\hat{w}_{\text{ridge}})^2\,|\,x]}_{\text{Variance}}$$

Irreduc. Error Bias-squared Variance

Suppose $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$, then $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T(\mathbf{X}w + \epsilon)$

$$= \frac{n}{n+\lambda}w + \frac{1}{n+\lambda}\mathbf{X}^T\epsilon$$

Bias-Variance Properties

Suppose $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$, then

$$\hat{w}_{\text{ridge}} = \frac{n}{n+\lambda} w + \frac{1}{n+\lambda}\mathbf{X}^T\epsilon$$

- Recall: $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$
- To analyze bias-variance tradeoff, we need to assume probabilistic generative model: $x_i \sim P_X, \;\; \mathbf{y} = \mathbf{X}w + \epsilon, \;\; \epsilon \sim \mathcal{N}(0, \sigma^2\mathbf{I})$
- The true error at a sample with feature x is

$$\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

$$= \mathbb{E}_{y|x}[(y - \mathbb{E}[y|x])^2 \,|\, x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}[y|x] - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

$$= \mathbb{E}_{y|x}[(y - x^Tw)^2 \,|\, x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(x^Tw - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

$$= \sigma^2 + (x^Tw - \mathbb{E}_{\mathcal{D}_{\text{train}}}[x^T\hat{w}_{\text{ridge}} \,|\, x])^2 + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}} \,|\, x] - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

(verify at home)

$$= \sigma^2 + \frac{\lambda^2}{(n+\lambda)^2}(w^Tx)^2 + \frac{\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2$$

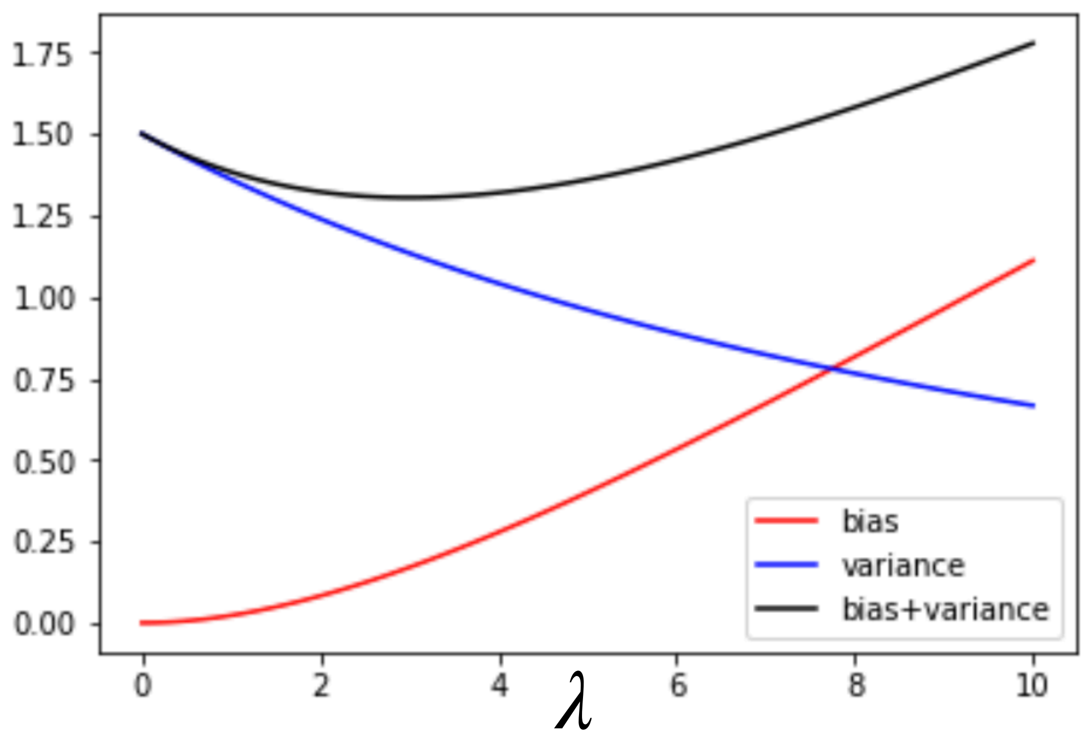
Irreduc. Error — Bias-squared — Variance

Bias-Variance Properties

- Ridge regressor: $\widehat{w}_{ridge} = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$
- True error

$$\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T \hat{w}_{\text{ridge}})^2 \,|\, x] = \sigma^2 + \underbrace{\frac{\lambda^2}{(n+\lambda)^2}(w^T x)^2}_{\text{Bias-squared}} + \underbrace{\frac{\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2}_{\text{Variance}}$$

d=10, n=20, $\sigma^2 = 3.0, \|w\|_2^2 = 10$



as λ →0, $\hat{w}_{\text{ridge}} \to \hat{w}_{\text{LS}}$

as λ →∞ $\hat{w}_{\text{ridge}} \to 0$