STAT 215A Fall 2023 Week 9

Chengzhong Ye

Announcements

- Lab 3 and homework 3 due next **Monday 10/23 at 11:59pm**
  - Write-up: just answer each question
- Midterm: 10/26
- Practice midterm solutions will be released today
  - We'll go over it on the Tuesday 10/24 lecture
- Happy World Statistics Day!

Lab 3: Stability of K-means + Computability

- Ben-Hur, et al. notes that similarity can be computed in $O(k_1 k_2 n)$
    - This should be your goal (though not required)
- You can do better than the Figure 3 in Ben-Hur
- `foreach`
    - If you're having issues with `foreach`, try `future` or `parallel`
- Remember, no need to push a blinded version
- Make sure your `lab3` folder is well-organized and **only** contains the files I would need to reproduce your results (will be part of your grade)!

Outline for today

- Regularization Pt. 1: Ridge

Regularization Part I: Ridge

Thanks to Tiffany Tang for sharing her slides

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Goal: Evaluate the *error* in estimating an unknown function f by the estimator $\hat{f}$

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Expected prediction error (EPE):

$$\mathbb{E}[y_0 - \hat{f}(x_0)]^2 = \underbrace{\mathrm{Var}(\hat{f}(x_0)) + \mathrm{Bias}^2(\hat{f}(x_0))}_{\textbf{Mean squared error (MSE)}}$$

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"irreducible" error

The Bias-Variance Tradeoff

$$\text{MSE} = \text{Var}(\hat{f}(x_0)) + \text{Bias}^2(\hat{f}(x_0))$$

- **Bias:** On average, how wrong is your prediction?

$$\text{Bias}(\hat{f}(x)) = \mathbb{E}(\hat{f}(x)) - f(x)$$

- **Variance:** If you obtain a new, but similar dataset, how much does this change your predictions?

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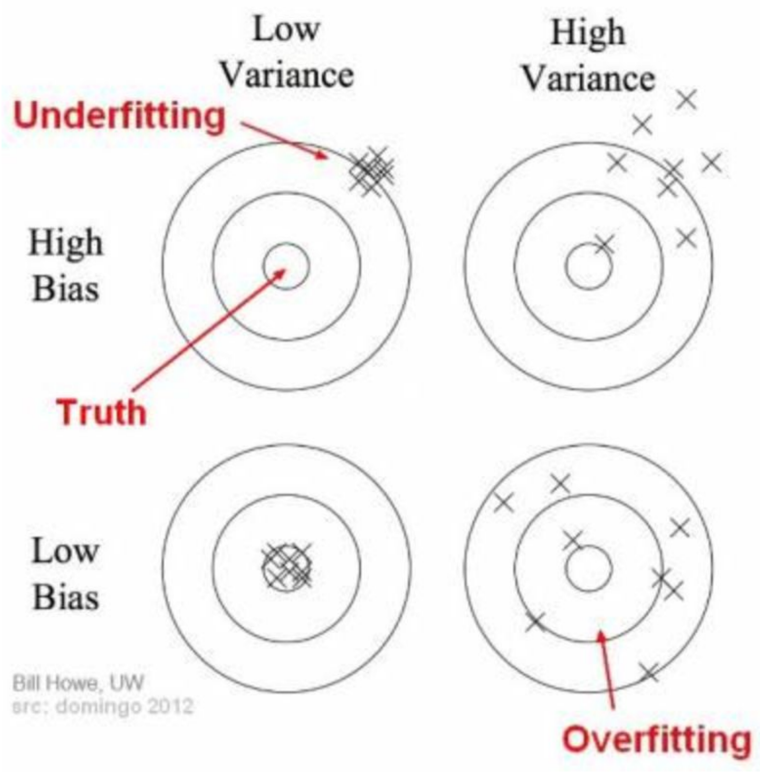

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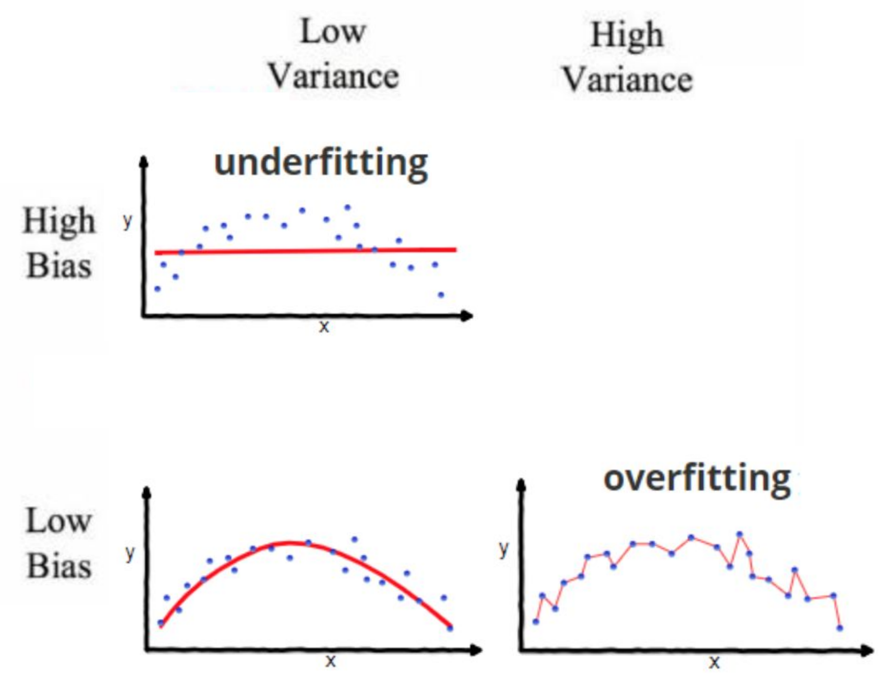

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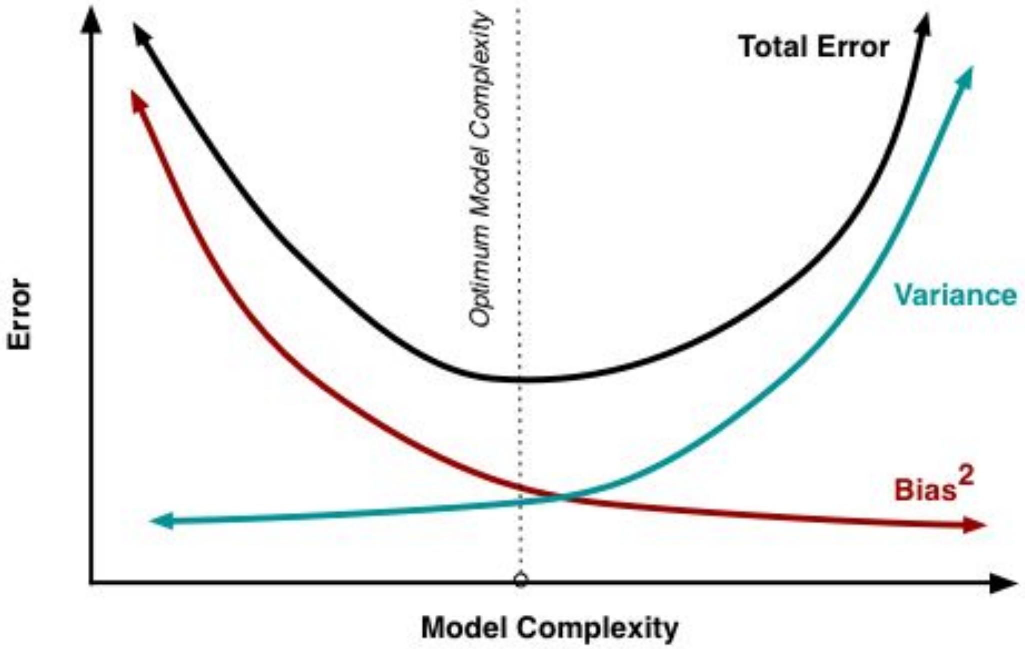
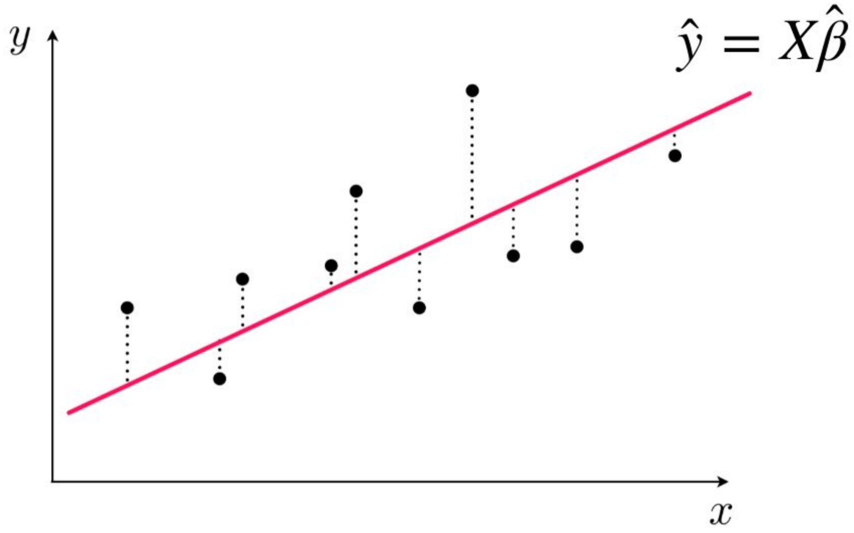
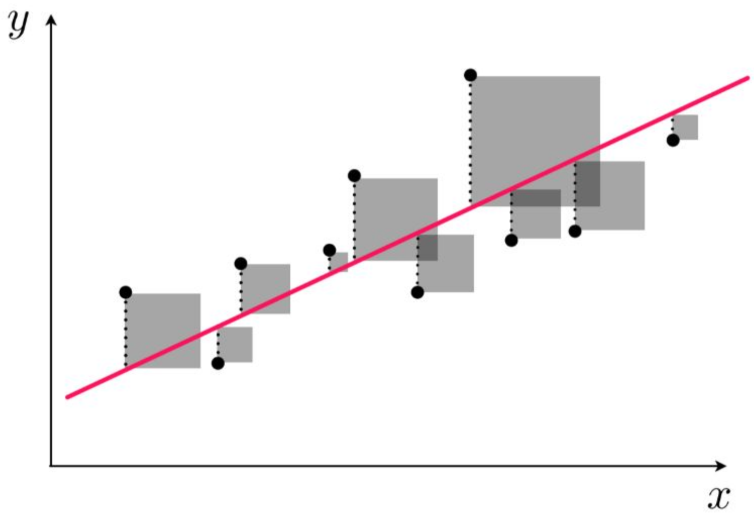


Recall Ordinary Least Squares

$$\hat{\boldsymbol{\beta}}_{OLS} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \; \|\mathbf{y} - \mathbf{X}\,\boldsymbol{\beta}\|_2^2$$

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$





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Advantages

- Simple
- Closed-form solution
- Interpretable (?)
- Under some modeling assumptions, OLS has some desirable properties

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  - $\text{Bias}(\hat{y}_0) = 0$
  - For large n, and assuming $\mathbb{E}(X) = 0$:

EPE = $\mathbb{E}_{x_0} \mathbb{E}(y_0 - \hat{y}_0)^2 \approx \sigma^2 + \sigma^2 (p/n)$

See *The Elements of Statistical Learning*, Section 2.5 for details

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Disadvantages

- No bias (assuming correctly specified), all variance… can lead to overfitting
- When $p > n$:
  - $X^\top X$ singular

A possible solution

$$\text{MSE} = \text{Var}(\hat{f}(x_0)) + \text{Bias}^2(\hat{f}(x_0))$$

- We could try to sacrifice some of the bias to reduce the variance
- One way to reduce the variance of your predictions is to restrict the parameter space in the optimization $\underset{\boldsymbol{\beta}}{\operatorname{argmin}} \; \|\mathbf{y} - \mathbf{X}\,\boldsymbol{\beta}\|_2^2$
- In the linear setting, this motivates regularized linear regression methods such as ridge, Lasso, and elastic net

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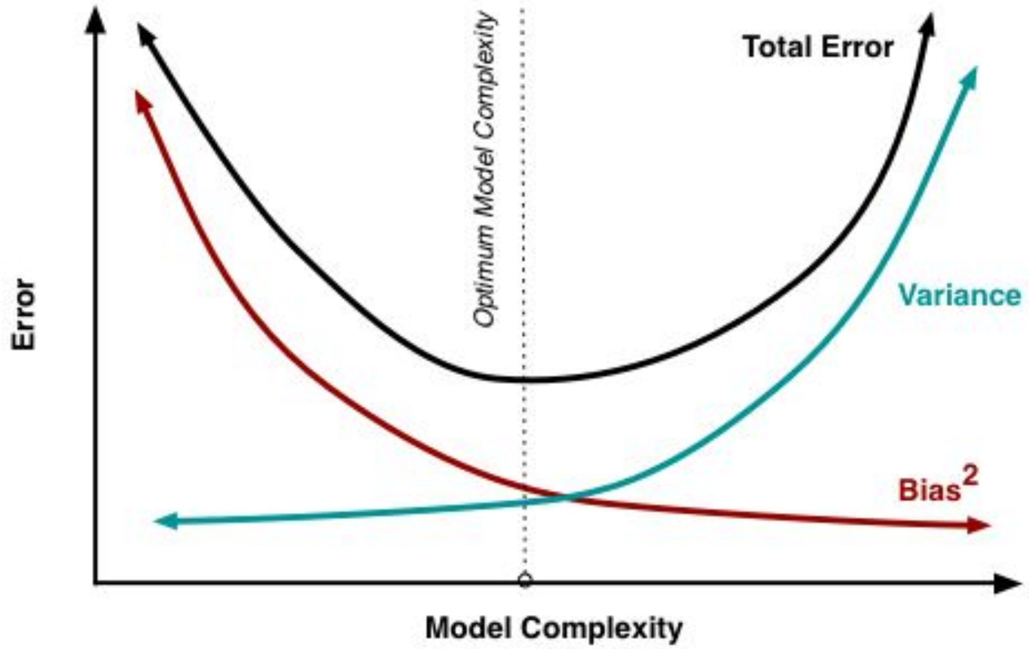

Ridge regression

$$\hat{\boldsymbol{\beta}}^r = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \underbrace{||\, \mathbf{y} - \mathbf{X}\,\boldsymbol{\beta}\,||_2^2}_{\text{Loss function}} \quad \text{subject to} \quad \overbrace{||\,\boldsymbol{\beta}\,||_2^2 \leq \tau}^{\text{constraint}}$$

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- $\lambda \to 0 \implies \hat{\beta}^r \to \text{OLS}$
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- Usually try to find an intermediate value that provides some shrinkage
- Can choose λ via CV

Why ridge?

$$\hat{\boldsymbol{\beta}}^r = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \; ||\,\mathbf{y} - \mathbf{X}\,\boldsymbol{\beta}\,||_2^2 + \lambda||\,\boldsymbol{\beta}\,||_2^2$$

1. The solution exists and is unique even when $p > n$ (unlike OLS)

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   - Exercise: show this

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2. Assume the setup from before: $y = X\beta + \varepsilon$, $\mathbb{E}(\varepsilon) = 0$, $\mathrm{Var}(\varepsilon) = \sigma^2 \mathrm{I}$

   There is **always** a value of λ where the ridge MSE is less than the OLS MSE:

$$\mathrm{MSE}\left(\mathbf{X}\,\hat{\boldsymbol{\beta}}^r(\lambda)\right) < \mathrm{MSE}\left(\mathbf{X}\,\hat{\boldsymbol{\beta}}^{OLS}\right)$$

Farebrother, R. W. (1976) https://www.jstor.org/stable/2984971
Theobald, C. M. (1974) https://www.jstor.org/stable/2984775

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3. Handles correlated features well -- features that are highly correlated tend to get shrunken together, i.e. they are given equal contribution to the linear model

Ridge in practice

- Don’t want to penalize the intercept
  - Before applying regularization, center columns of X and y
- Most of the time, should also scale columns of X so that we don’t penalize some coefficients more than others simply because of different scales
- These practical guidelines apply to all regularization methods

Regularization Part 2: Lasso

Next time...