DS 100/200: Principles and Techniques of Data Science **Date: April 10, 2020**

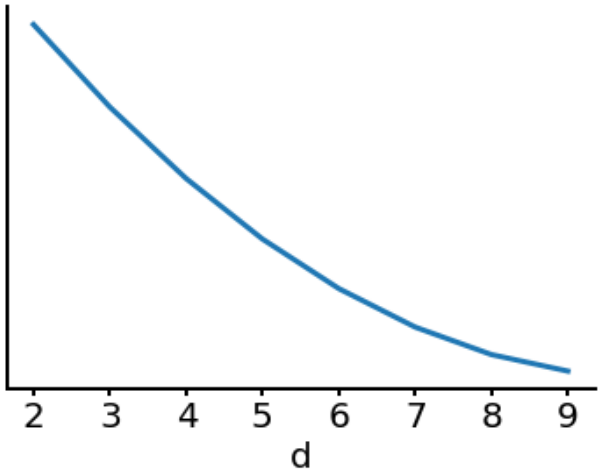
Discussion #10 Solutions

Name:

Bias-Variance Trade-Off

1. Your team would like to train a machine learning model in order to predict the next YouTube video that a user will click on based on the videos the user has watched in the past. We extract m attributes (such as length of video, view count etc) from each video and our model will be based on the previous d videos watched by that user. Hence the number of features for each data point for the model is $m \cdot d$. You're not sure how many videos to consider.

   (a) Your colleague generates the following plot, where the value d is on the x axis. However, they forgot to label the y-axis.



Which of the following could the y axis represent? Select all that apply.

☐ A. Training Error

☐ B. Validation Error

☐ C. Bias

☐ D. Variance

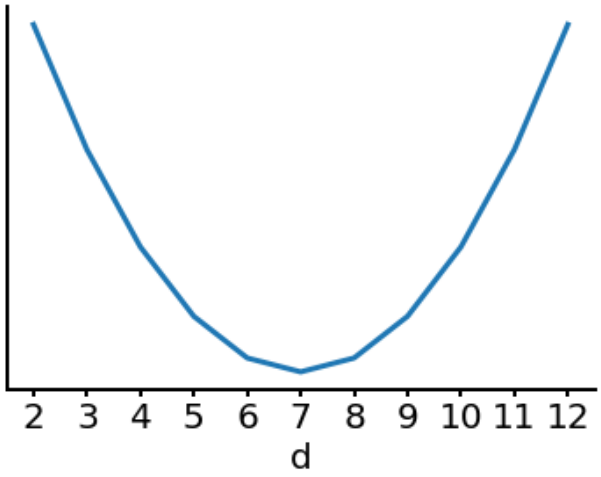
Solution:

Training Error: Training error decreases as we add more features

Validation Error: Can be true depending on the underlying complexity of the data. In part (b), we see that increasing d does not necessarily lower our validation error

Bias: Decreases with model complexity
Variance: Increases with model complexity

(b) Your colleague generates the following plot, where the value d is on the x axis. However, they forgot to label the y-axis.



Which of the following could the y axis represent? Select all that apply.

☐ A. Training Error
☐ B. Validation Error
☐ C. Bias
☐ D. Variance

Solution:
See solution in part (a)

2. We randomly sample some data $(x_i, y_i)_{i=1}^n$ and use it to fit a model $f_{\hat{\theta}}(x)$ according to some procedure (e.g. OLS, Ridge, LASSO). We then sample a new point that is independent from our existing points, but sampled from the same underlying truth as our data. Furthermore, assume that we have a function $g(x)$ and some noise generation process that produces ϵ such that $\mathbb{E}[\epsilon] = 0$ and $\text{var}(\epsilon) = \sigma^2$. Every time we query mother nature for Y at a given a x, she gives us $Y = g(x) + \epsilon$. (The true function for our data is $Y = g(x) + \epsilon$.) A new ϵ is generated each time, independent of the last. In class, we showed that

$$\underbrace{\mathbb{E}\left[(Y - f_{\hat{\theta}}(x))^2\right]}_{} = \underbrace{\sigma^2}_{} + \underbrace{(g(x) - \mathbb{E}[f_{\hat{\theta}}(x)])^2}_{} + \underbrace{\mathbb{E}\left[(f_{\hat{\theta}}(x) - \mathbb{E}[f_{\hat{\theta}}(x)])^2\right]}_{}$$

(a) Label each of the terms above. Word bank: observation variance, model variance, observation bias^2, model bias^2, model risk, empirical mean square error.

Solution:

$$\underbrace{\mathbb{E}\left[(Y - f_{\hat{\theta}}(x))^2\right]}_{\text{model risk}} = \underbrace{\sigma^2}_{\text{observation variance}} + \underbrace{(g(x) - \mathbb{E}\left[f_{\hat{\theta}}(x)\right])^2}_{\text{model bias}^2} + \underbrace{\mathbb{E}\left[(f_{\hat{\theta}}(x) - \mathbb{E}\left[f_{\hat{\theta}}(x)\right])^2\right]}_{\text{model variance}}$$

(b) What is random in the equation above? Where does the randomness come from?

Solution: Y - this is the new observation at x. Its randomness comes from the noise generation process. $f_{\hat{\theta}}$ - this is the model fitted from the data. Its randomness comes from sampling and the noise generation process.

(c) True or false and explain. $\mathbb{E}\left[\epsilon f_{\hat{\theta}}(x)\right] = 0$

Solution: True. Since ϵ and $\hat{\theta}$ are independent,

$$\mathbb{E}\left[\epsilon f_{\hat{\theta}}(x)\right] = \mathbb{E}\left[\epsilon\right]\mathbb{E}\left[f_{\hat{\theta}}(x)\right] = 0$$

(d) Suppose you lived in a world where you could collect as many data sets you would like. Given a fixed algorithm to fit a model f_θ to your data e.g. linear regression, describe a procedure to get good estimates of $\mathbb{E}\left[f_{\hat{\theta}}(x)\right]$

Solution:

- Pick an x
- Gather a data set $\mathcal{D}_i$
- Fit a model $f_{\hat{\theta}_i}$ to that data set
- Calculate $f_{\hat{\theta}_i(x)}$
- Repeat many times
- Average over all the $f_{\hat{\theta}_i}(x)$

(e) If you could collect as many data sets as you would like, how does that affect the quality of your model $f_\theta(x)$?

Solution: By collecting many data sets, we have an unbiased estimate of the "average" model, but this does not mean our model will have unbiased prediction.

Ridge and LASSO Regression

3. Earlier, we posed the linear regression problem as follows: Find the $\vec{\theta}$ value that minimizes the average squared loss. In other words, our goal is to find $\hat{\vec{\theta}}$ that satisfies the equation below:

$$\hat{\vec{\theta}} = \underset{\vec{\theta}}{\operatorname{argmin}} L(\vec{\theta}) = \underset{\vec{\theta}}{\operatorname{argmin}} \frac{1}{n}||\vec{y} - \mathbb{X}\vec{\theta}||_2^2$$

Here, $\mathbb{X}$ is a $n \times d$ matrix, $\vec{\theta}$ is a $d \times 1$ vector and $\vec{y}$ is a $n \times 1$ vector. As we saw in lecture, the optimal $\hat{\vec{\theta}}$ is given by the closed form expression $\hat{\vec{\theta}} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^t\vec{y}$.

To prevent overfitting, we saw that we can instead minimize the sum of the average squared loss plus a regularization function $\alpha\mathcal{S}(\vec{\theta})$. If use the function $\mathcal{S}(\vec{\theta}) = ||\vec{\theta}||_2^2$, we have "ridge regression". If we use the function $\mathcal{S}(\vec{\theta}) = ||\vec{\theta}||_1$, we have "LASSO regression". For example, if we choose S($\vec{\boldsymbol{\theta}}$) = $||\vec{\theta}||_2^2$, our goal is to find $\hat{\vec{\theta}}$ that satisfies the equation below:

$$\hat{\theta} = \underset{\vec{\theta}}{\operatorname{argmin}} L(\vec{\theta}) = \underset{\vec{\theta}}{\operatorname{argmin}} \frac{1}{n}||\vec{y} - \mathbb{X}\vec{\theta}||_2^2 + \alpha||\vec{\theta}||_2^2 = \underset{\vec{\theta}}{\operatorname{argmin}} \frac{1}{n}\sum_{i=1}^{n}(y_i - \mathbb{X}_{i,\cdot}^T\vec{\theta})^2 + \alpha\sum_{j=1}^{d}\theta_j^2$$

Recall that α is a hyperparameter that determines the impact of the regularization term. Though we did not discuss this in lecture, we can also find a closed form solution to ridge regression: $\hat{\vec{\theta}} = (\mathbb{X}^T\mathbb{X} + n\alpha\mathbf{I})^{-1}\mathbb{X}^T\vec{y}$. It turns out that $\mathbb{X}^T\mathbb{X} + n\alpha\mathbf{I}$ is guaranteed to be invertible (unlike $\mathbb{X}^T\mathbb{X}$ which might not be invertible).

(a) As model complexity increases, what happens to the bias and variance of the model?

> **Solution:** Model complexity is inversely related to the regularization parameter α. As α increases, Bias tends to increase and variance tends to decrease.

(b) In terms of bias and variance, how does a regularized model compare to ordinary least squares regression?

> **Solution:** Regularized regression has higher bias and lower variance relative to ordinary least squares regression.

(c) In ridge regression, what happens if we set $\alpha = 0$? What happens as α approaches ∞?

> **Solution:** If we set $\alpha = 0$ we end up with OLS. As α approaches ∞ then $\boldsymbol{\theta}$ goes to $\mathbf{0}$.

(d) How does model complexity compare between ridge regression and ordinary least squares regression? How does this change for large and small values of α?

Solution: Ridge regression in general will result in simpler models, as we penalize for large components in of $\boldsymbol{\theta}$. α is inversely related to model complexity, e.g. larger values of α represent larger penalties, meaning even lower model complexity.

(e) If we have a large number of features (10,000+) and we suspect that only a handful of features are useful, which type of regression (Lasso vs Ridge) would be more helpful in interpreting useful features?

Solution: LASSO would be better as it sets many values to 0, so it would be effectively selecting useful features and "ignoring" bad ones.

(f) What are the benefits of using ridge regression?

Solution: If $\mathbf{X}^T\mathbf{X}$ is not full rank (not invertible), then we end up with infinitely many solutions for least squares. But if we use ridge regression, $\hat{\boldsymbol{\theta}} = (\mathbf{X}^T\mathbf{X} + n\alpha\mathbf{I})^{-1}\mathbf{X}^T\mathbf{Y}$. This guarantees invertbility and a unique solution, for $\alpha > 0$.

Random Variables

4. The average response time for a question on Piazza this semester was 11 minutes. As always, the number of questions answered by each TA is highly variable, with a few TAs going above and beyond the call of duty. Below are the number of contributions for the top four TAs (out of $20,000$ total Piazza contributions):

TA	# contributions
Daniel	2000
Suraj	1800
Manana	700
Allen	500

Suppose we take a sample with replacement of size $n = 500$ contributions from the original $20,000$ contributions. We will also define some random variables:

- $D_i = 1$ when the i^{th} contribution in our sample is made by Daniel; else $D_i = 0$.
- $S_i = 1$ when the i^{th} contribution in our sample is made by Suraj; else $S_i = 0$.
- $M_i = 1$ when the i^{th} contribution in our sample is made by Manana; else $M_i = 0$.
- $A_i = 1$ when the i^{th} contribution in our sample is made by Allen; else $A_i = 0$.

- $O_i = 1$ when the i^{th} contribution is made by anyone other than Daniel, Suraj, Manana, or Allen; else, $O_i = 0$

(a) i. What is $P(A_1 = 1)$?

$P(A_1 = 1)$ =

Solution: $\frac{500}{20000} = \frac{1}{40}$

ii. What is $\mathbb{E}[S_1]$?

$\mathbb{E}[S_1]$ =

Solution: $\frac{1800}{20000} = \frac{9}{100}$

iii. What is $\mathbb{E}[M_{100}]$?

$\mathbb{E}[M_{100}]$ =

Solution: $\frac{700}{20000} = \frac{7}{200}$

iv. What is Var$[D_{50}]$?

Var$[D_{50}]$ =

Solution: $D_{50} \sim$ Bernoulli$(\frac{2000}{20000} = \frac{1}{10})$. $Var(D_{50}) = \frac{1}{10} \cdot (1 - \frac{1}{10}) = \frac{9}{100}$

v. What is $D_{400} + S_{400} + A_{400} + M_{400} + O_{400}$?

$D_{400} + S_{400} + A_{400} + M_{400} + O_{400}$ =

Solution: 1. The 400th contribution must be made by Daniel, Suraj, Manana, or other so one of the 5 random variables must 1 and the rest are 0s.

(b) For parts b.i and b.ii, let:

- $N_D = \sum_{i=1}^{500} D_i$

- $N_S = \sum_{i=1}^{500} S_i$
- $N_M = \sum_{i=1}^{500} M_i$
- $N_A = \sum_{i=1}^{500} A_i$
- $N_O = \sum_{i=1}^{500} O_i$

i. What is $\mathbb{E}[N_A]$?

$\mathbb{E}[N_A]$ =

Solution:

$$\begin{aligned}\mathbb{E}[N_A] &= \mathbb{E}[\sum_{i=1}^{500} A_i] \\ &= \sum_{i=1}^{500} \mathbb{E}[A_i] \\ &= \sum_{i=1}^{500} \frac{500}{20000} \\ &= 500 \cdot \frac{500}{20000} \\ &= \frac{25}{2}\end{aligned}$$

ii. What is Var$(N_D + N_S + N_A + N_M + N_O)$?

Var$(N_D + N_S + N_A + N_M + N_O)$ =

Solution: 0. $N_D + N_S + N_A + N_M + N_O = 500$. $Var(500) = 0$. The variance of a constant is 0.

(c) Now, suppose we take a sample with replacement of 20 contributions, what is the probability that 7 were by Daniel?

Probability =

Solution: This is a binomial distribution where $P(\text{Daniel}) = \frac{2000}{20000}$, $P(\text{Contributor other than Daniel}) = \frac{18000}{20000}$ and the number of trials $n = 20$.

Then,

$$P(7 \text{ Daniel}, 13 \text{ Contributor other than Daniel} = \binom{20}{7} \cdot \left(\frac{2000}{20000}\right)^7 \cdot \left(\frac{18000}{20000}\right)^3$$

(d) Finally, suppose we take a sample with replacement of 10 contributions. What is the probability that 3 were by Daniel, 3 were by Suraj, and 4 were by Manana? (Note: Refer to Lecture 2 to refresh your knowledge on how to calculate this type of probability)

Probability =

Solution: This is a multinomial distribution where $P(\text{Daniel}) = \frac{2000}{20000}$, $P(\text{Suraj}) = \frac{1800}{20000}$ and $P(\text{Manana}) = \frac{700}{20000}$ and the number of trials $n = 10$.

Then,

$$P(3 \text{ Daniel}, 3 \text{ Suraj}, 4 \text{ Manana}) = \frac{10!}{3!3!4!} \cdot \left(\frac{2000}{20000}\right)^3 * \left(\frac{1800}{20000}\right)^3 \cdot \left(\frac{700}{20000}\right)^4$$