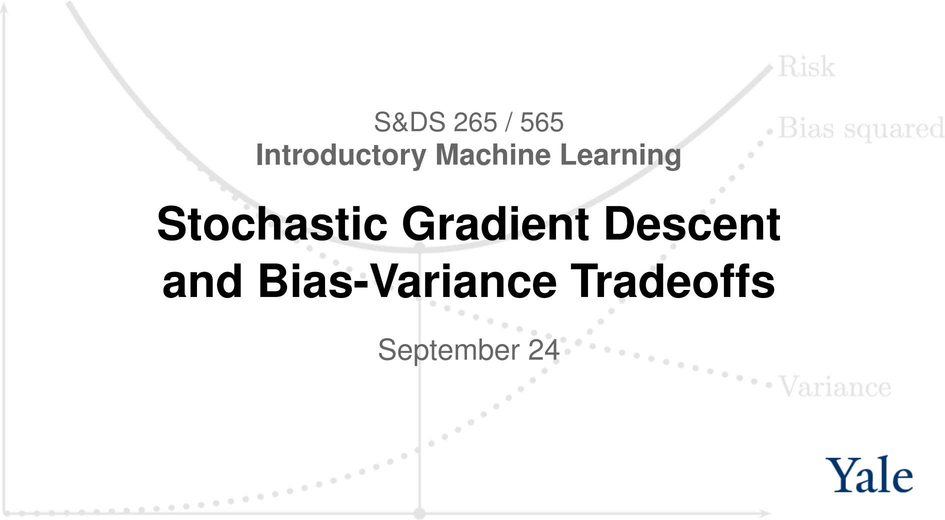
S&DS 265 / 565

Introductory Machine Learning

Stochastic Gradient Descent and Bias-Variance Tradeoffs

September 24



Yale

Goings on

- Assignment 2 is out; due next Thursday
- Quiz 2 this Thursday
- Midterm: October 15 (in class)

Outline for today

- Stochastic gradient descent (redux)
- Regularization
- Jupyter notebook example
- Bias-variance tradeoffs

SGD idea

- For each parameter β_j, see what happens to the loss if that parameter is increased a little bit.
- If the loss goes down (up), then increase (decrease) β_j proportionately
- Do this simultaneously for all of the parameters
- Rinse and repeat

Stochastic gradient descent

Initialize all parameters to zero: $\beta_j = 0$, $j = 1, \ldots, p$.

Read through the data one record at a time, and update the model.

1. Read data item x
2. Make a prediction $\widehat{y}(x)$
3. Observe the true response/label y
4. Update the parameters β so $\widehat{y}$ is closer to y

Stochastic gradient descent

Suppose we are doing *linear regression*. We initialize all parameters to zero: $\beta_j = 0$, $j = 1, \ldots, p$.

We read through the data one record at a time, and update the model.

1. Read data item x
2. Make a prediction $\widehat{y}(x) = \sum_{j=1}^{p} \beta_j x_j$
3. Observe the true response/label y
4. Update the parameters β so $\widehat{y}$ is closer to y

SGD: Computation for squared error

Change β_j by a little bit:

$$\beta_j \to \beta_j + \varepsilon$$

SGD: Computation for squared error

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$$\beta_j \to \beta_j + \varepsilon$$

What happens to the squared error?

$$\begin{aligned}\tfrac{1}{2}(y - \widehat{y})^2 &\to \tfrac{1}{2}(y - \widehat{y} - \varepsilon x_j)^2 \\ &\approx \tfrac{1}{2}(y - \widehat{y})^2 + \underbrace{(\widehat{y} - y)x_j}_{derivative\ of\ loss} \varepsilon\end{aligned}$$

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Use adjustment

$$\begin{aligned}\beta_j &\to \beta_j \overbrace{-\eta \cdot \text{derivative of loss}}^{\varepsilon} \\ &= \beta_j + \eta \cdot (y - \widehat{y})x_j\end{aligned}$$

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Squared error then decreases:

$$\tfrac{1}{2}(y - \widehat{y})^2 \approx \tfrac{1}{2}(y - \widehat{y})^2 - \eta \cdot \text{derivative of loss } \underline{\text{squared}}$$

SGD for general loss

Suppose $L(y, \beta^T x)$ is the loss for an input (x, y), e.g., $(y - \beta^T x)^2$

SGD update, for a small step size $\eta > 0$:

$$\beta_j \longleftarrow \beta_j - \eta \frac{\partial L(y, \boldsymbol{\beta}^T x)}{\partial \beta_j}$$

$$\boldsymbol{\beta} \longleftarrow \boldsymbol{\beta} - \eta \nabla_\beta L(y, \boldsymbol{\beta}^T x) \quad \text{(vector notation)}$$

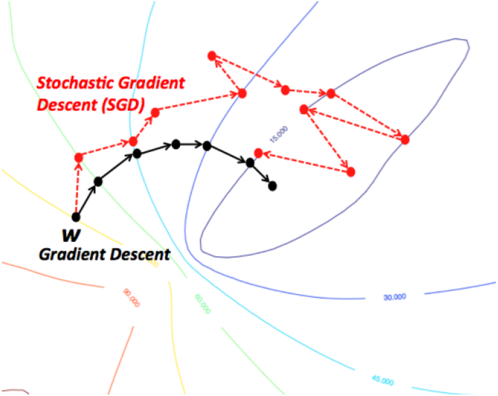
"Batch" gradient descent uses the entire training set in each step of gradient descent.

Stochastic gradient descent computes a quick approximation to this gradient, using only a single or a small "mini-batch" of data points

Batch vs. stochastic gradient descent

- The average derivative over a mini-batch can be thought of as a noisy version of the average derivative over the entire data set
- (Which can in turn be thought of as a sample estimate of a population)
- The stochastic gradient is computed more cheaply, and updating the parameters makes progress more quickly

Batch vs. stochastic gradient descent



https://wikidocs.net/3413

SGD for logistic regression

SGD Update:

$$\beta_j \longleftarrow \beta_j + \eta(y - p(x))x_j$$

$$\beta_j x_j \longleftarrow \beta_j x_j + \eta(y - p(x))x_j^2$$

$$p(x) = \frac{1}{1 + \exp(-\beta^T x)}$$

Case checking:

- Suppose $y = 1$ and probability $p(x)$ is high?

SGD for logistic regression

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Case checking:

- Suppose $y = 1$ and probability $p(x)$ is high? *small change*
- Suppose $y = 1$ and probability $p(x)$ is small?

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- Suppose $y = 1$ and probability $p(x)$ is high? *small change*
- Suppose $y = 1$ and probability $p(x)$ is small? *big change* $\uparrow$
- Suppose $y = 0$ and probability $p(x)$ is small?

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Case checking:

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- Suppose $y = 1$ and probability $p(x)$ is small? *big change* $\uparrow$
- Suppose $y = 0$ and probability $p(x)$ is small? *small change*
- Suppose $y = 0$ and probability $p(x)$ is big?

SGD for logistic regression

SGD Update:

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Case checking:

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- Suppose $y = 1$ and probability $p(x)$ is small? *big change* $\uparrow$
- Suppose $y = 0$ and probability $p(x)$ is small? *small change*
- Suppose $y = 0$ and probability $p(x)$ is big? *big change* $\downarrow$

SGD: choice of learning rate

Often the learning rate η_t is adjusted experimentally to get good convergence properties for a particular problem

We require that η_t decreases as t—the number of steps so far—increases

SGD: Regularization

A "ridge" penalty $\frac{1}{2}\lambda \sum_{j=1}^{d} \beta_j^2$ is easily handled.

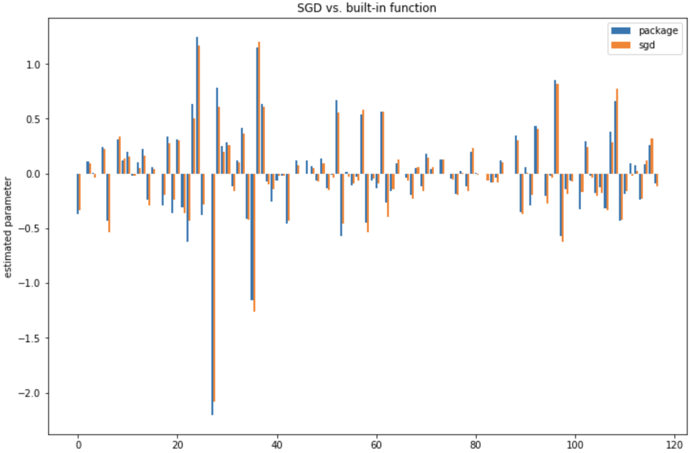
Gradient changes by an additive term $\lambda\beta_j$. Update becomes

$$\begin{aligned} \beta_j &\longleftarrow \beta_j + \eta\{(y - p(x))x_j - \lambda\beta_j\} \\ &= (1 - \eta\lambda)\beta_j + \eta(y - p(x))x_j \end{aligned}$$

Check that this "does the right thing" whether β_j wants to be large positive or negative.

- *The penalty shrinks β_j toward zero*

Recall from demo



Each bar indicates an estimated parameter $\widehat{\beta}_j$. The estimates from SGD are very similar to those obtained using the package.

Bias and variance

Bias: How much are we off—on average?

Variance: How variable are we—on average?

Bias and variance

Bias: $\theta - \mathbb{E}\widehat{\theta}$

Variance: $\mathbb{E}(\widehat{\theta} - \mathbb{E}\widehat{\theta})^2$

Bias and variance

Examples of $\theta, \widehat{\theta}$:

Estimating height, population, election outcome, ad click rate...

Bias and variance

Bias: $\theta - \mathbb{E}\widehat{\theta}$

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Bias and variance

$$\text{Bias: } \theta - \mathbb{E}\widehat{\theta}$$

$$\text{Variance: } \mathbb{E}(\widehat{\theta} - \mathbb{E}\widehat{\theta})^2$$

- $\widehat{\theta}$ is an estimate from a sample
- $\mathbb{E}$ is the expectation (average) with respect to the sample
- So $\mathbb{E}\widehat{\theta}$ is the average estimate
- We can only directly compute $\widehat{\theta}$ for the sample we have
- *We don't know θ*

Bias and variance

In machine learning, bias and variance are two sides of a coin:
As squared bias goes up, variance goes down (and vice-versa)

Bias-variance tradeoff

$$\text{Risk} = \text{Bias}^2 + \text{Variance}$$

Bias-variance tradeoff

$$\mathbb{E}(\theta - \widehat{\theta})^2 = \mathrm{Bias}(\widehat{\theta})^2 + \mathrm{Variance}(\widehat{\theta})$$

Bias-variance tradeoff

$$\mathbb{E}(\theta - \widehat{\theta})^2 = (\theta - \mathbb{E}\widehat{\theta})^2 + \mathbb{E}(\widehat{\theta} - \mathbb{E}\widehat{\theta})^2$$

Bias-variance tradeoff

Proof:

$$\mathbb{E}(\theta - \widehat{\theta})^2 = \mathbb{E}(\theta - \mathbb{E}\widehat{\theta} + \mathbb{E}\widehat{\theta} - \widehat{\theta})^2$$

Bias-variance tradeoff

Proof:

$$
\begin{aligned}
\mathbb{E}(\theta - \widehat{\theta})^2 &= \mathbb{E}(\theta - \mathbb{E}\widehat{\theta} + \mathbb{E}\widehat{\theta} - \widehat{\theta})^2 \\
&= \mathbb{E}(\theta - \mathbb{E}\widehat{\theta})^2 - 2\mathbb{E}\left\{(\theta - \mathbb{E}\widehat{\theta})(\widehat{\theta} - \mathbb{E}\widehat{\theta})\right\} + \mathbb{E}(\widehat{\theta} - \mathbb{E}\widehat{\theta})^2
\end{aligned}
$$

Bias-variance tradeoff

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Bias-variance tradeoff

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Bias-variance tradeoff

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&= \mathbb{E}(\theta - \mathbb{E}\widehat{\theta})^2 + \mathbb{E}(\widehat{\theta} - \mathbb{E}\widehat{\theta})^2 \\
&= \mathrm{Bias}(\widehat{\theta})^2 + \mathrm{Variance}(\widehat{\theta})
\end{aligned}
$$

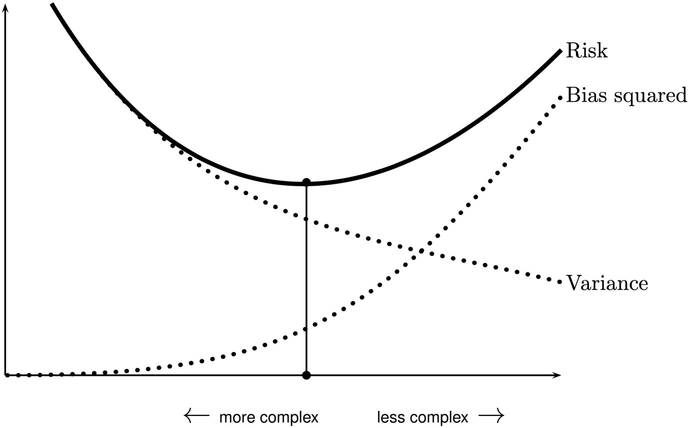
Bias-variance tradeoff

If $Y = \theta +$ noise, with $\mathbb{E}(\text{noise}) = 0$ and $Var(\text{noise}) = \sigma^2$,

$$\text{Risk} = \mathbb{E}[(Y - \widehat{\theta})^2] = \text{Bias}^2 + \text{Variance} + \sigma^2$$

Please work through the proof of this!

Bias-variance tradeoff



Example: Regularization

Suppose that $\mathbb{E}(Y) = \theta$ and we estimate $\widehat{\theta}$ by minimizing

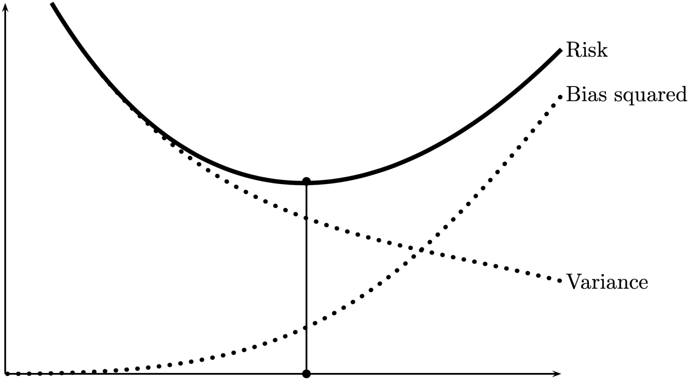
$$(Y - \theta)^2 + \lambda\theta^2$$

Then $\widehat{\theta} = \frac{Y}{1+\lambda}$. What are the squared bias and variance?

$$\text{Bias}^2 = \theta^2 \left(\frac{\lambda}{1+\lambda}\right)^2$$

$$\text{Variance} = \left(\frac{1}{1+\lambda}\right)^2 \text{Variance}(Y)$$

Bias-variance tradeoff



← less regularization   more regularization →

← less shrinkage   more shrinkage →

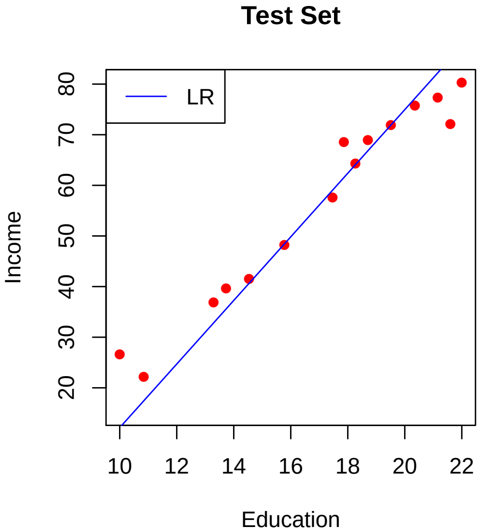
← smaller penalty   bigger penalty →

Intuition

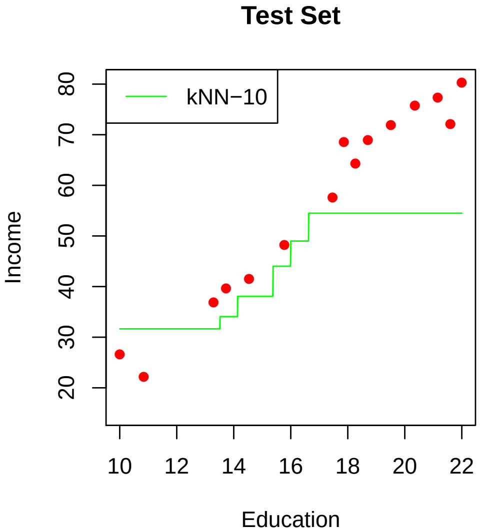
An informal description of the bias-variance tradeoff:

- As the fitted curve becomes more “wiggly” (complex) we’re seeing higher variance
- Averaging over different datasets, the “wiggles” average out to give a good fit to the data — this is low bias
- But we can’t do this averaging in practice, because we only have a single dataset

Recall: k-nearest neighbors



Recall: *k*-nearest neighbors



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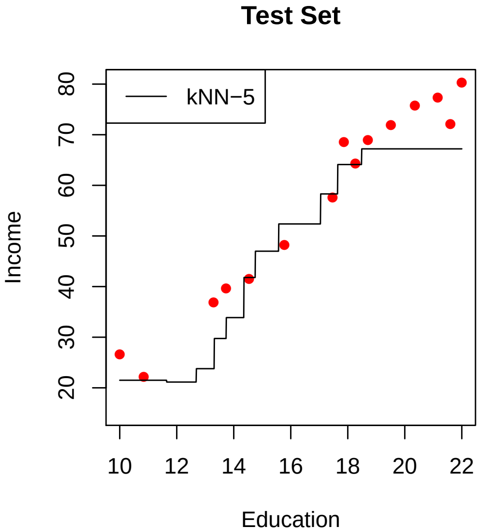

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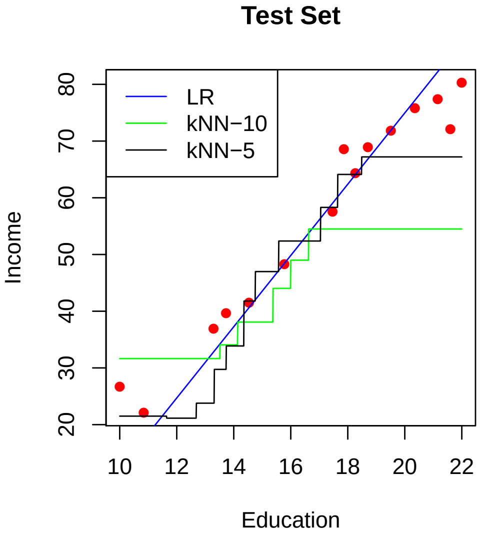

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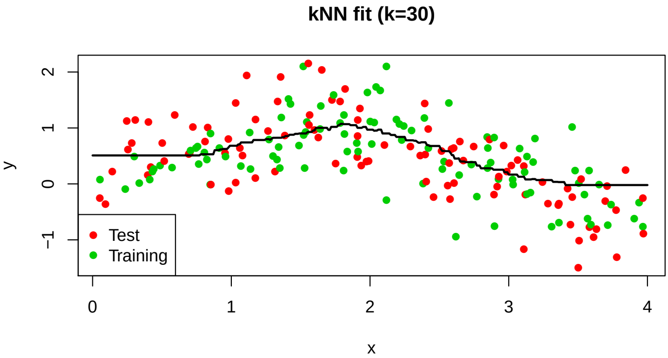

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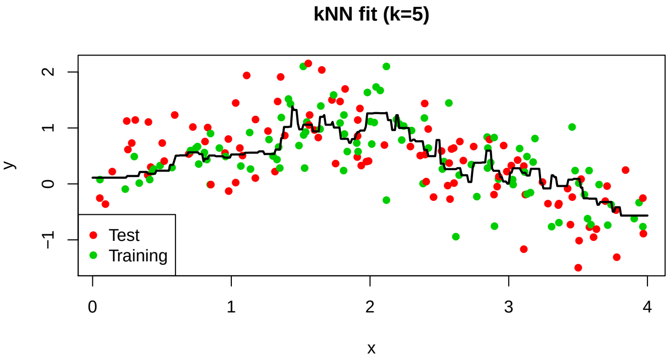
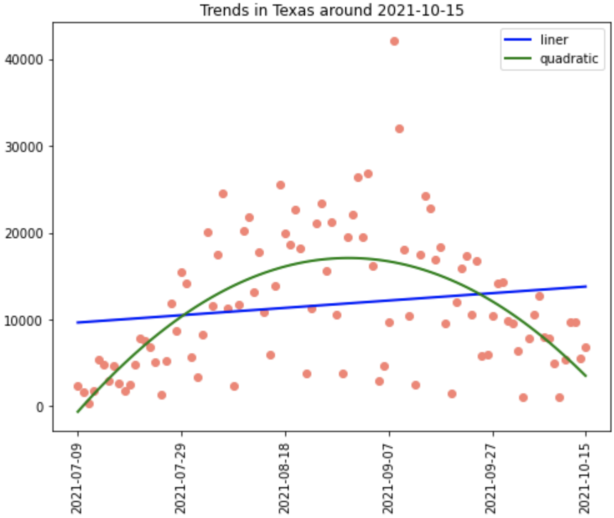


Recall: Covid example



What did we learn today?

- In SGD, a parameter is updated according to how much the loss changes when that parameter is changed by a little bit
- Mean squared error splits into squared bias plus variance
- As model complexity increases, squared bias decreases while variance increases