Learning Theory Part 3: Bias-Variance Tradeoff

CS 760@UW-Madison

Goals for the lecture

you should understand the following concepts

- estimating bias and variance
- the bias-variance decomposition

Estimation bias and variance

- How will predictive accuracy (error) change as we vary k in k-NN?
- Or as we vary the complexity of our decision trees?
- the bias/variance decomposition of error can lend some insight into these questions

note that this is a different sense of bias than in the term *inductive bias*

Background: Expected values

- the *expected value* of a random variable that takes on numerical values is defined as:

$$E[X] = \sum_x x\, P(x)$$

this is the same thing as the *mean*

- we can also talk about the expected value of a function of a random variable

$$E[g(X)] = \sum_x g(x) P(x)$$

Defining bias and variance

- consider the task of learning a regression model $f(\boldsymbol{x}; D)$ given a training set $D = \left\{ (x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)}) \right\}$

indicates the dependency of model on D

- a natural measure of the error of f is

$$E\left[\left(y - f(\mathbf{x}; D) \right)^2 \mid D \right]$$

where the expectation is taken with respect to the real-world distribution of instances

Defining bias and variance

- this can be rewritten as:

$$E\left[\left(y - f(\boldsymbol{x}; D)\right)^2 \mid \boldsymbol{x}, D\right] = E\left[\left(y - E[y \mid \boldsymbol{x}]\right)^2 \mid \boldsymbol{x}, D\right]$$

$$+ \left(f(\boldsymbol{x}; D) - E[y \mid \boldsymbol{x}]\right)^2$$

<u>error</u> of f as a predictor of y

<u>noise</u>: variance of y given $\boldsymbol{x}$; doesn't depend on D or f

Defining bias and variance

- now consider the expectation (over different data sets D) for the second term

$$E_D\left[\left(f(\boldsymbol{x};D) - E[y\,|\,\boldsymbol{x}]\right)^2\right] =$$

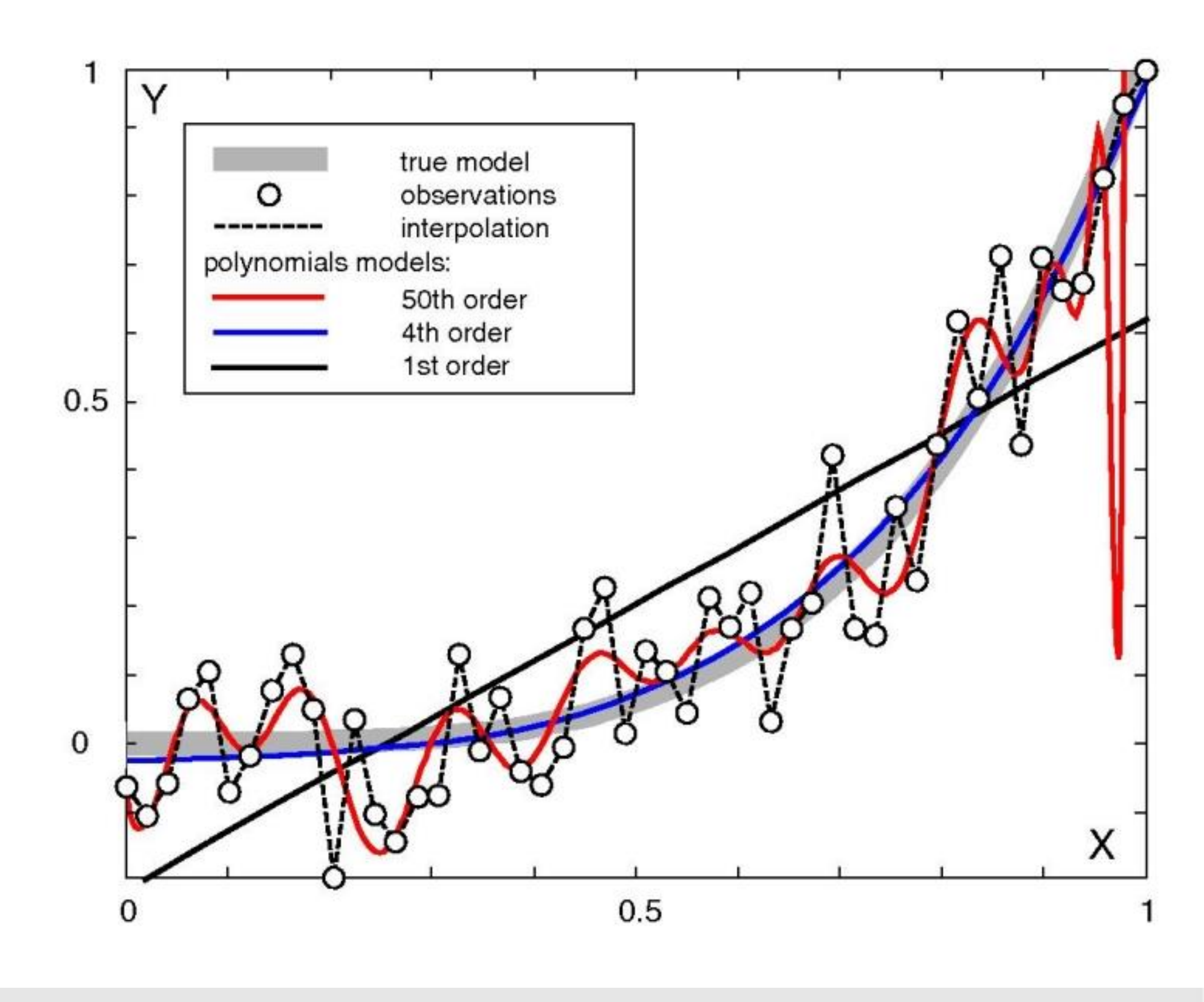
$$\left(E_D\left[f(\boldsymbol{x};D)\right] - E\left[y\,|\,\boldsymbol{x}\right]\right)^2 \qquad \text{bias}$$

$$+\,E_D\left[\left(f(\boldsymbol{x};D) - E_D\left[f(\boldsymbol{x};D)\right]\right)^2\right] \qquad \text{variance}$$

- bias: if on average $f(\boldsymbol{x};D)$ differs from $E[y\,|\,\boldsymbol{x}]$ then $f(\boldsymbol{x};D)$ is a biased estimator of $E[y\,|\,\boldsymbol{x}]$
- variance: $f(\boldsymbol{x};D)$ may be sensitive to D and vary a lot from its expected value

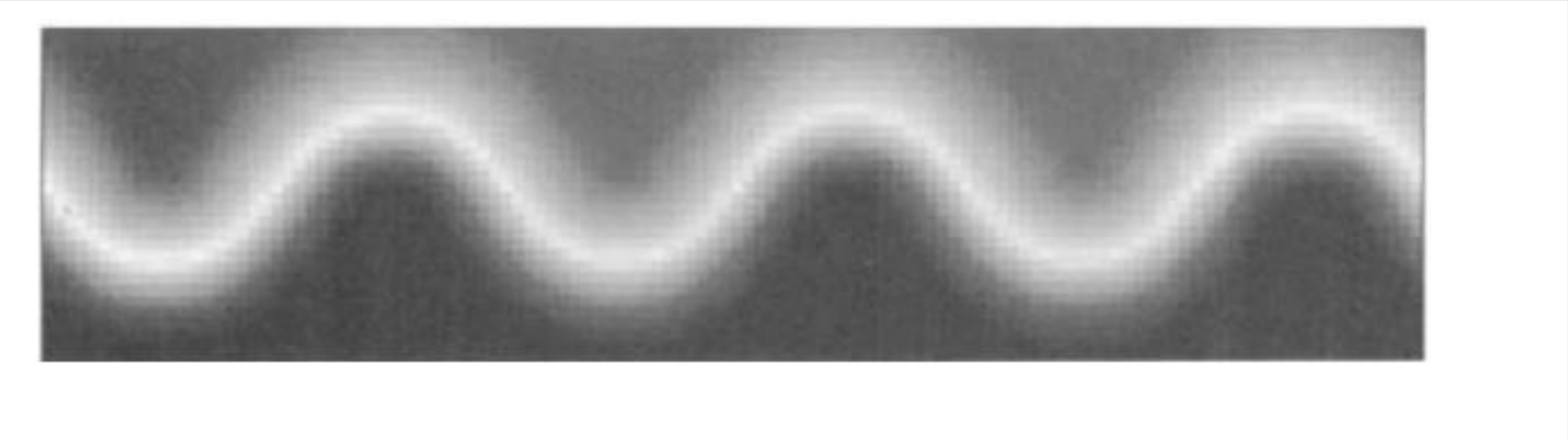
Bias/variance for polynomial interpolation

- the 1st order polynomial has high bias, low variance
- 50th order polynomial has low bias, high variance
- 4th order polynomial represents a good trade-off



Bias/variance trade-off for k-NN regression

- consider using k-NN regression to learn a model of this surface in a 2-dimensional feature space



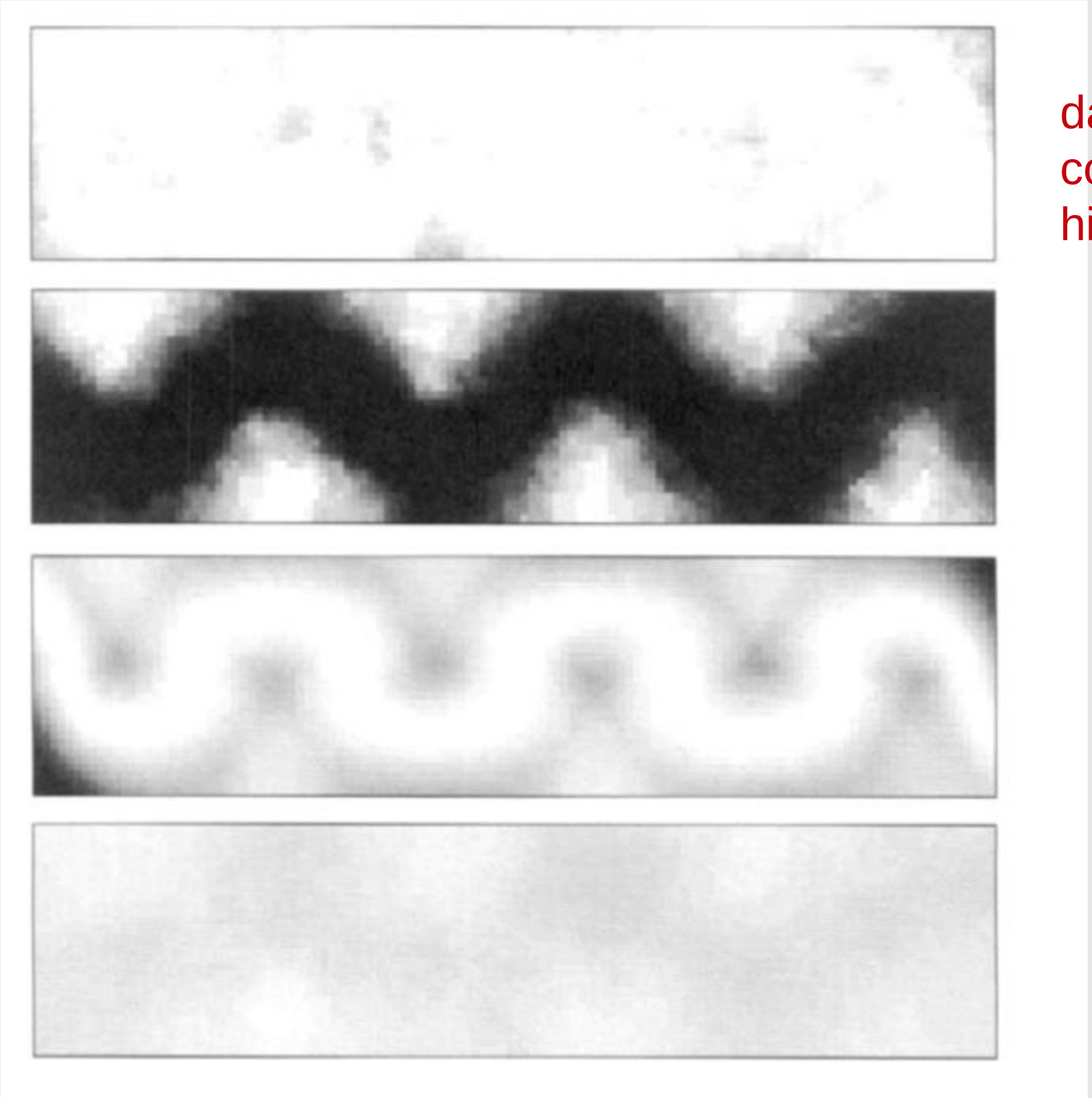
Bias/variance trade-off for k-NN regression

bias for 1-NN

variance for 1-NN

bias for 10-NN

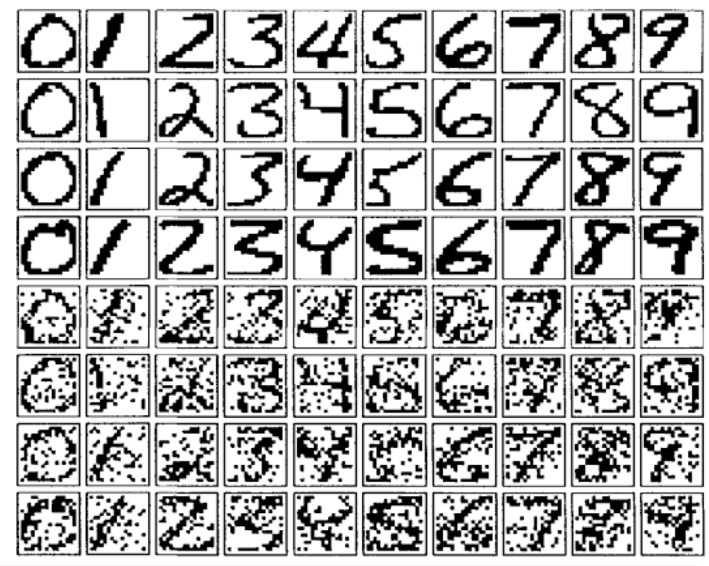
variance for 10-NN

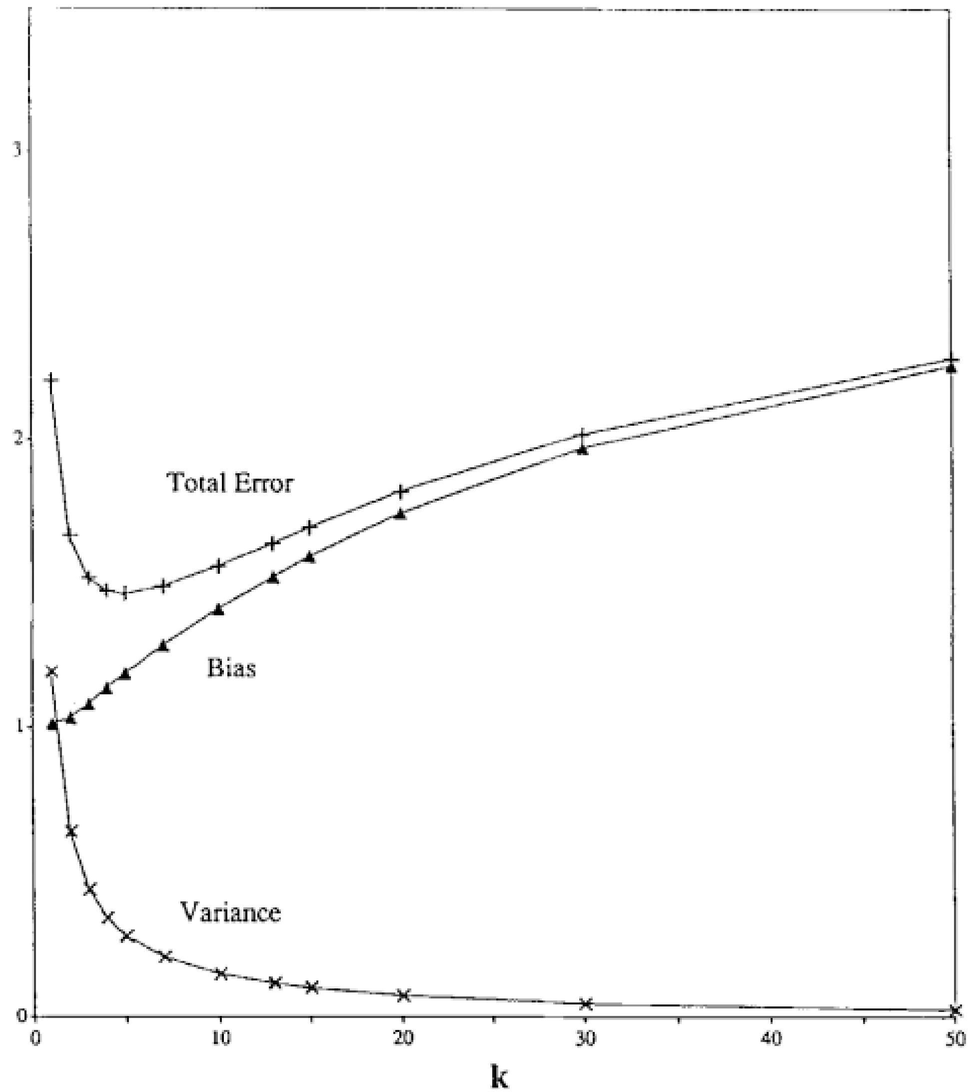


darker pixels correspond to higher values

Bias/variance trade-off

- consider k-NN applied to digit recognition





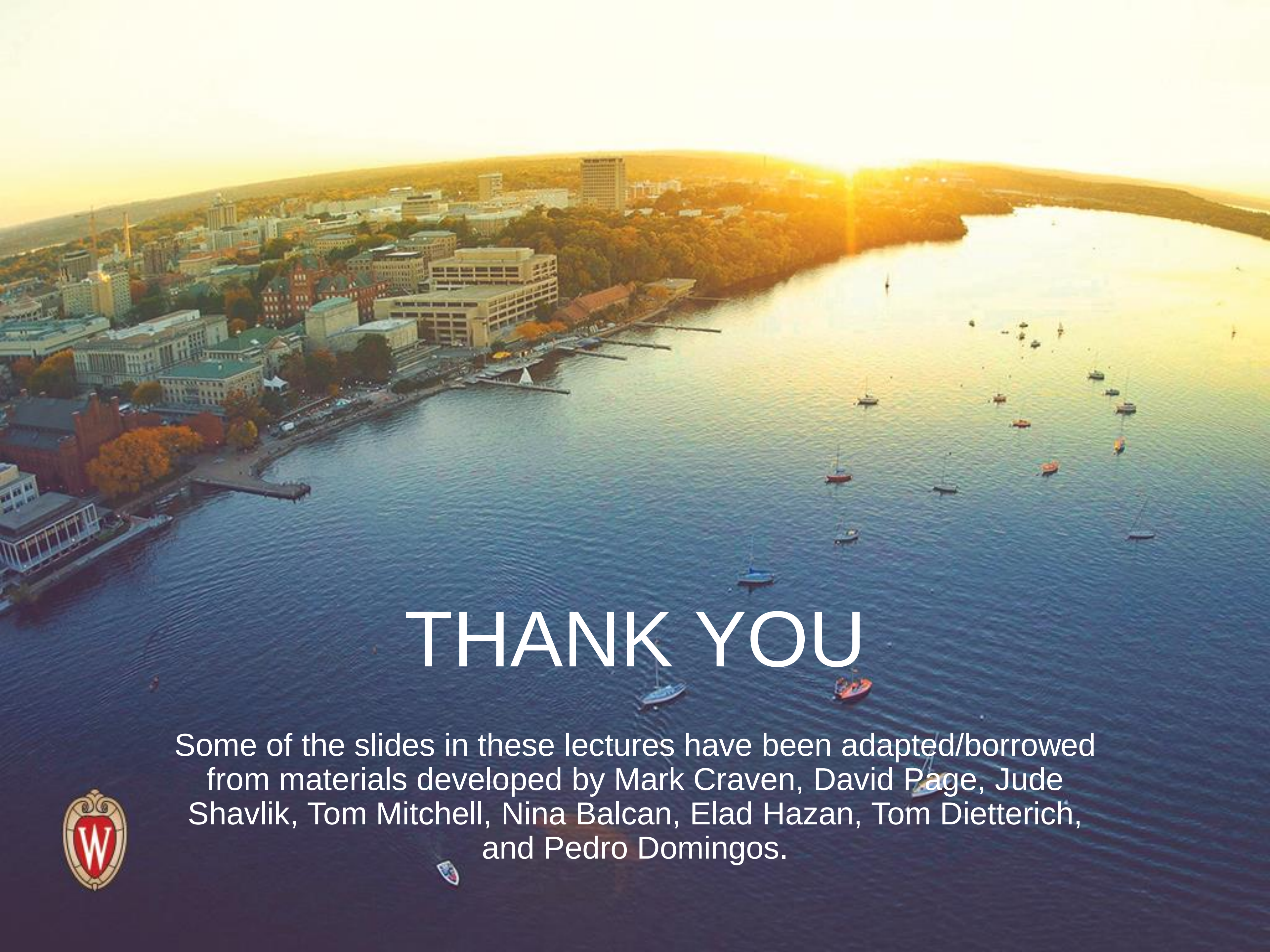
Bias/variance discussion

- predictive error has two controllable components
  - expressive/flexible learners reduce *bias*, but increase *variance*
- for many learners we can trade-off these two components (e.g. via our selection of k in k-NN)
- the optimal point in this trade-off depends on the particular problem domain and training set size
- this is not necessarily a strict trade-off; e.g. with ensembles we can often reduce bias and/or variance without increasing the other term

Bias/variance discussion

the bias/variance analysis

- helps explain why simple learners can outperform more complex ones
- helps understand and avoid overfitting


THANK YOU
Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Elad Hazan, Tom Dietterich, and Pedro Domingos.