CS 412

JAN 23RD – LINEAR MODELS

k-Nearest Neighbor

For binary classification problems

- Take the majority classification of the k-nearest neighbors (where k is odd)

For numerical output problems ← regression

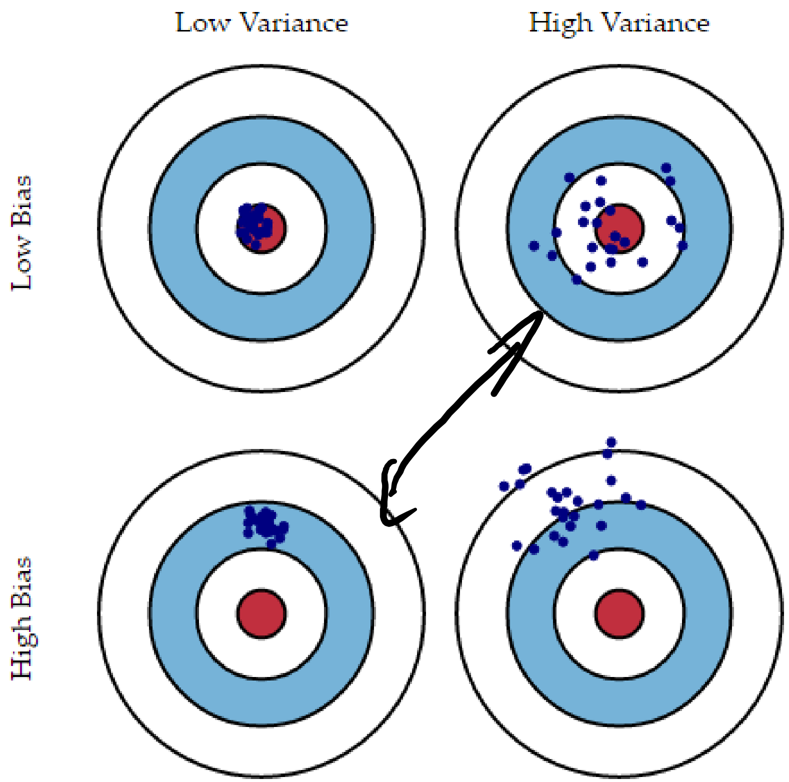
- Take the average of the k-nearest neighbors OR
- Take the weighted average of the k-nearest neighbors (Gaussian distribution)

9.0

8.7

0.6

Nearest Neighbor Regression Analysis



Bias: $\hat{E}[f_D(x)] - f(x)$

Variance: $\hat{E}[(f_D(x) - \hat{E}[f_D(x)])^2]$

problem specific

How do we evaluate a model?

EPE *(estimated prediction error)* for a given model *f*

$EPE(f) = E(Y-f(X))^2$

Where X is the vector of input attributes,
f(X) is the predicted output and
Y is the actual output

Binary classification

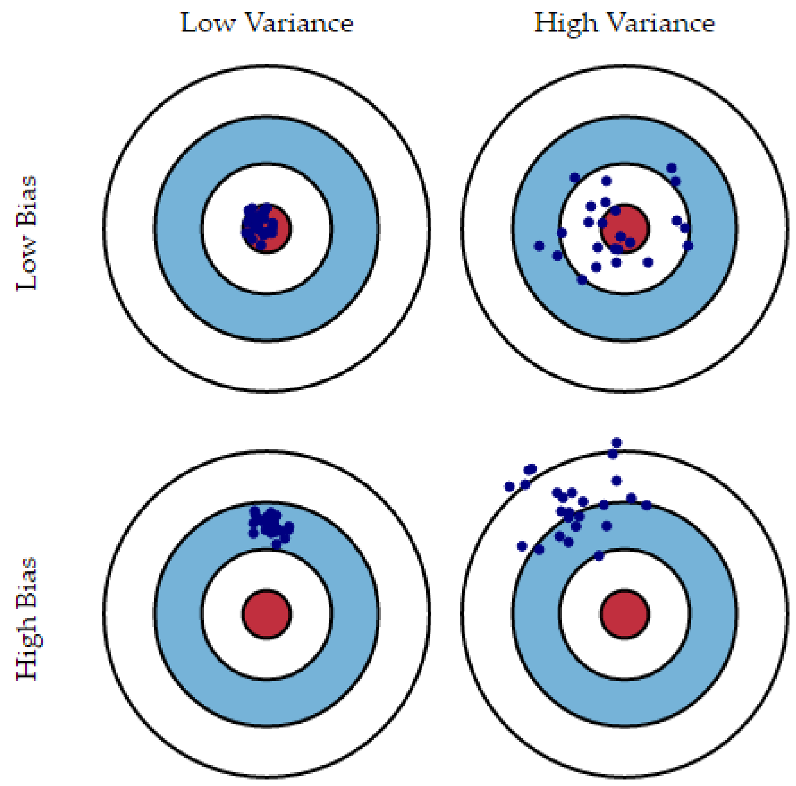
$Y \in \{0,1\}$

$f(X) \in \{0,1\}$

We will usually try to find the model which minimizes the *estimated error*, but in the classification model, this is just accuracy

This may not show the whole picture!

Nearest Neighbor Regression Analysis



Bias: $E[\hat{f}_D(x)] - f(x)$

want Error to be zero $\longrightarrow$ biased by base error

Variance: $E[(\hat{f}_D(x) - \hat{E}[f_D(x)])^2]$

Homework 1

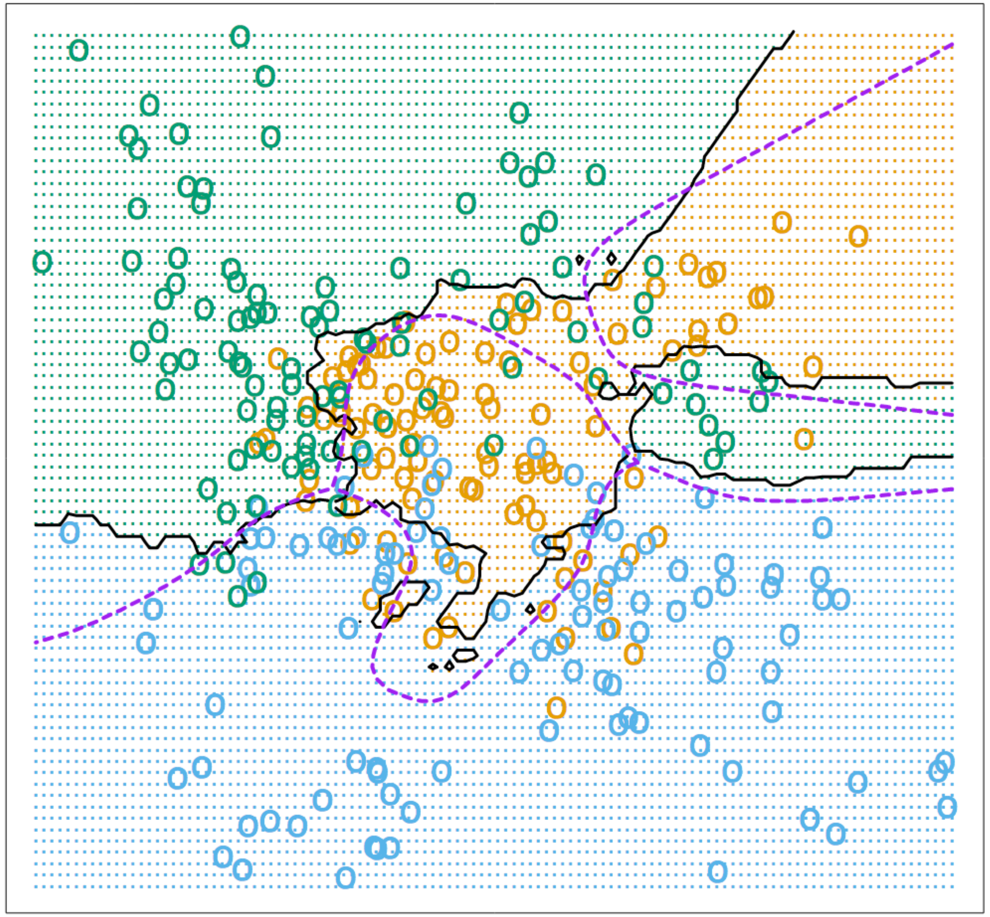
For HW 1, you'll be solving a binary classification problem with k-nearest neighbors for different levels of *k*

You will also be running your models with differing sizes of cross-validation and comparing runtimes

Make sure that you separate your test data before begin!

↳ already done

15-Nearest Neighbors



Results

What are some observations we can make about this model?

- 3 classifications
  - blue
  - orange
  - purple
- Purple line is called the Bayes decision boundary
- Does this suffer from overfitting?

Bayes boundary

numerical values

p features

Suppose that there exists some real vector $X \in \mathbb{R}^p$ and $Y \in \mathbb{R}$
with joint probability distribution $P(X,Y)$

$$P(Y|X) = \frac{P(X|Y)\,P(Y)}{P(X)}$$

Bayes boundary

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with joint probability distribution $P(X,Y)$

$$P(Y|X) = \frac{P(X|Y)\,P(Y)}{P(X)}$$

we want all possible combinations

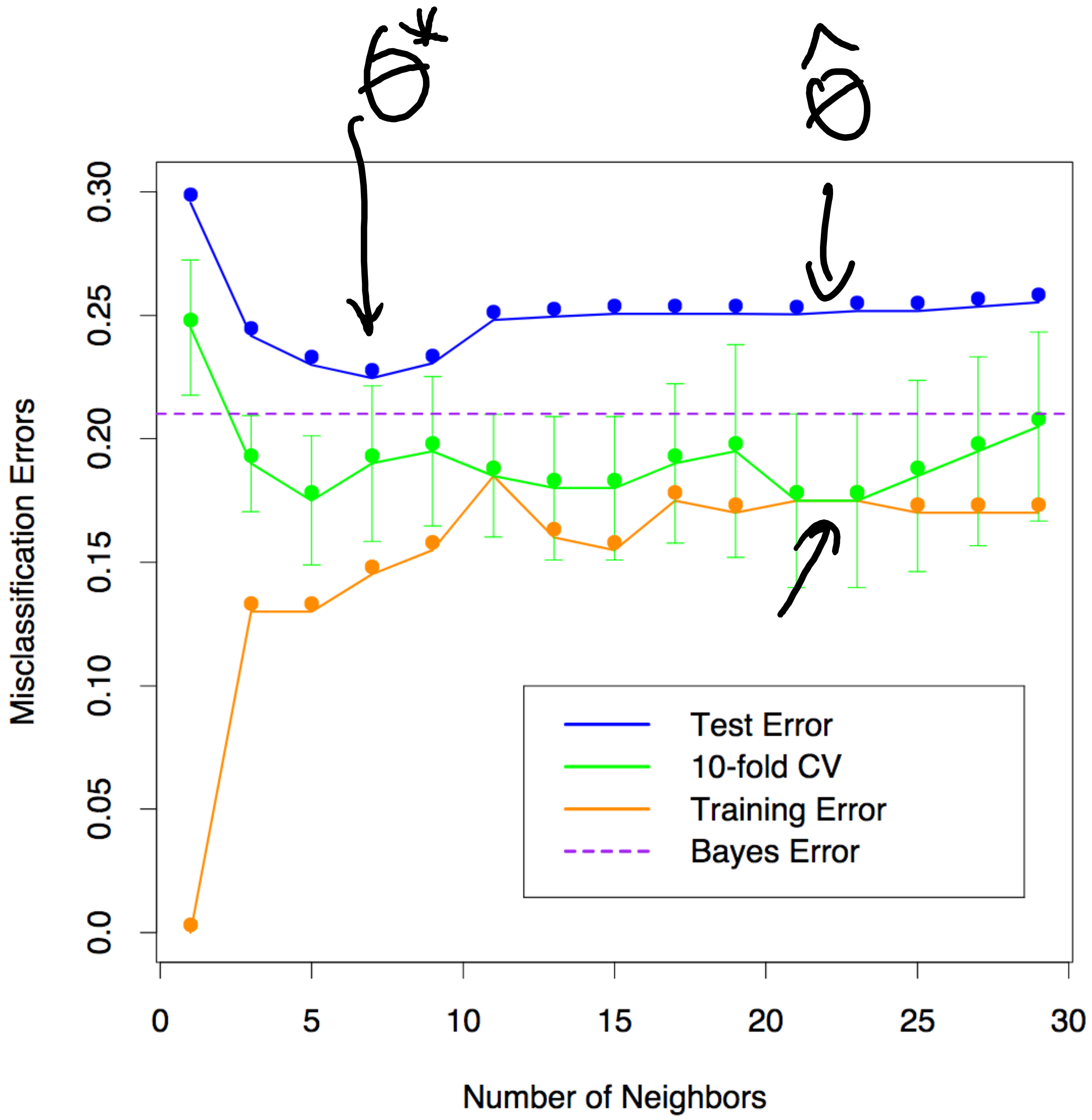
$X' \in R^k \quad k < d$

Y is the output variable, and X is the feature vector (with *p* features)

If we select the Y that has highest Bayes' probability given X,
then this is the Bayes selection

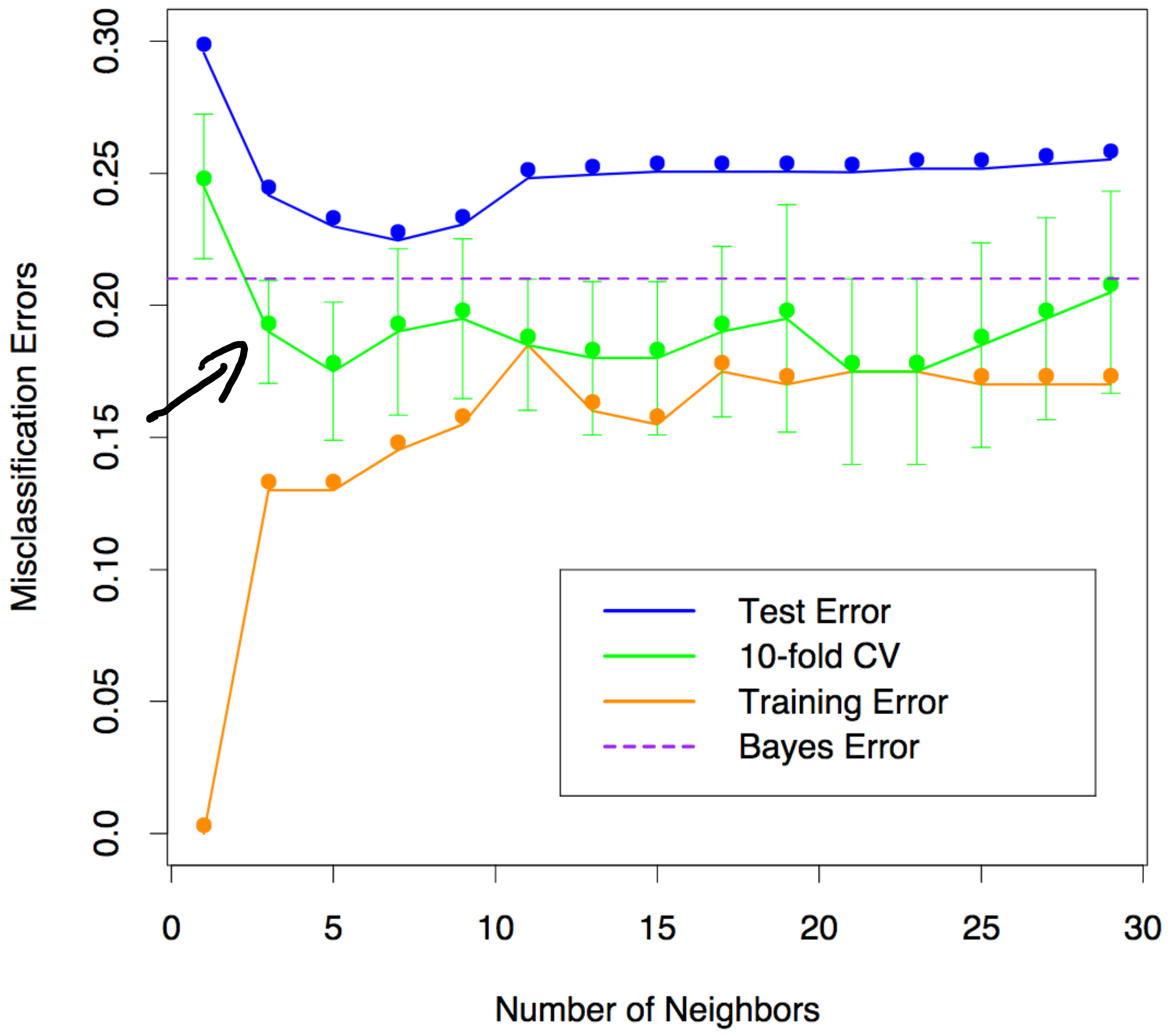
We'll talk about Bayesian classifiers later, but this is a common performance benchmark
the purple line in a lot of the figures

exponential in runtime



Results

What might be wrong with this analysis?



Results

What might be wrong with this analysis?

- *We're using the test set multiple times!*

Two common resolutions

- Set aside a validation set for this purpose
- Introduce an error
  - easy: use the Stdev of error to introduce confidence
  - more accurate: Hoeffding bound

cum. prob	$t_{.50}$	$t_{.75}$	$t_{.80}$	$t_{.85}$	$t_{.90}$	$t_{.95}$	$t_{.975}$	$t_{.99}$	$t_{.995}$	$t_{.999}$	$t_{.9995}$
one-tail	**0.50**	**0.25**	**0.20**	**0.15**	**0.10**	**0.05**	**0.025**	**0.01**	**0.005**	**0.001**	**0.0005**
two-tails	**1.00**	**0.50**	**0.40**	**0.30**	**0.20**	**0.10**	**0.05**	**0.02**	**0.01**	**0.002**	**0.001**
df											
1	0.000	1.000	1.376	1.963	3.078	6.314	12.71	31.82	63.66	318.31	636.62
2	0.000	0.816	1.061	1.386	1.886	2.920	4.303	6.965	9.925	22.327	31.599
3	0.000	0.765	0.978	1.250	1.638	2.353	3.182	4.541	5.841	10.215	12.924
4	0.000	0.741	0.941	1.190	1.533	2.132	2.776	3.747	4.604	7.173	8.610
5	0.000	0.727	0.920	1.156	1.476	2.015	2.571	3.365	4.032	5.893	6.869
6	0.000	0.718	0.906	1.134	1.440	1.943	2.447	3.143	3.707	5.208	5.959
7	0.000	0.711	0.896	1.119	1.415	1.895	2.365	2.998	3.499	4.785	5.408
8	0.000	0.706	0.889	1.108	1.397	1.860	2.306	2.896	3.355	4.501	5.041
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11	0.000	0.697	0.876	1.088	1.363	1.796	2.201	2.718	3.106	4.025	4.437
12	0.000	0.695	0.873	1.083	1.356	1.782	2.179	2.681	3.055	3.930	4.318
13	0.000	0.694	0.870	1.079	1.350	1.771	2.160	2.650	3.012	3.852	4.221
14	0.000	0.692	0.868	1.076	1.345	1.761	2.145	2.624	2.977	3.787	4.140
15	0.000	0.691	0.866	1.074	1.341	1.753	2.131	2.602	2.947	3.733	4.073
16	0.000	0.690	0.865	1.071	1.337	1.746	2.120	2.583	2.921	3.686	4.015
17	0.000	0.689	0.863	1.069	1.333	1.740	2.110	2.567	2.898	3.646	3.965
18	0.000	0.688	0.862	1.067	1.330	1.734	2.101	2.552	2.878	3.610	3.922
19	0.000	0.688	0.861	1.066	1.328	1.729	2.093	2.539	2.861	3.579	3.883
20	0.000	0.687	0.860	1.064	1.325	1.725	2.086	2.528	2.845	3.552	3.850
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28	0.000	0.683	0.855	1.056	1.313	1.701	2.048	2.467	2.763	3.408	3.674
29	0.000	0.683	0.854	1.055	1.311	1.699	2.045	2.462	2.756	3.396	3.659
30	0.000	0.683	0.854	1.055	1.310	1.697	2.042	2.457	2.750	3.385	3.646
40	0.000	0.681	0.851	1.050	1.303	1.684	2.021	2.423	2.704	3.307	3.551
60	0.000	0.679	0.848	1.045	1.296	1.671	2.000	2.390	2.660	3.232	3.460
80	0.000	0.678	0.846	1.043	1.292	1.664	1.990	2.374	2.639	3.195	3.416
100	0.000	0.677	0.845	1.042	1.290	1.660	1.984	2.364	2.626	3.174	3.390
1000	0.000	0.675	0.842	1.037	1.282	1.646	1.962	2.330	2.581	3.098	3.300
z	0.000	0.674	0.842	1.036	1.282	1.645	1.960	2.326	2.576	3.090	3.291
	0%	50%	60%	70%	80%	90%	95%	98%	99%	99.8%	99.9%
	Confidence Level										

Recognize this?

This is the t-table

How many standard deviations do you need to add in order to be 95% certain that the mean is within the error?

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	0%	50%	60%	70%	80%	90%	95%	98%	99%	99.8%	99.9%
	Confidence Level										

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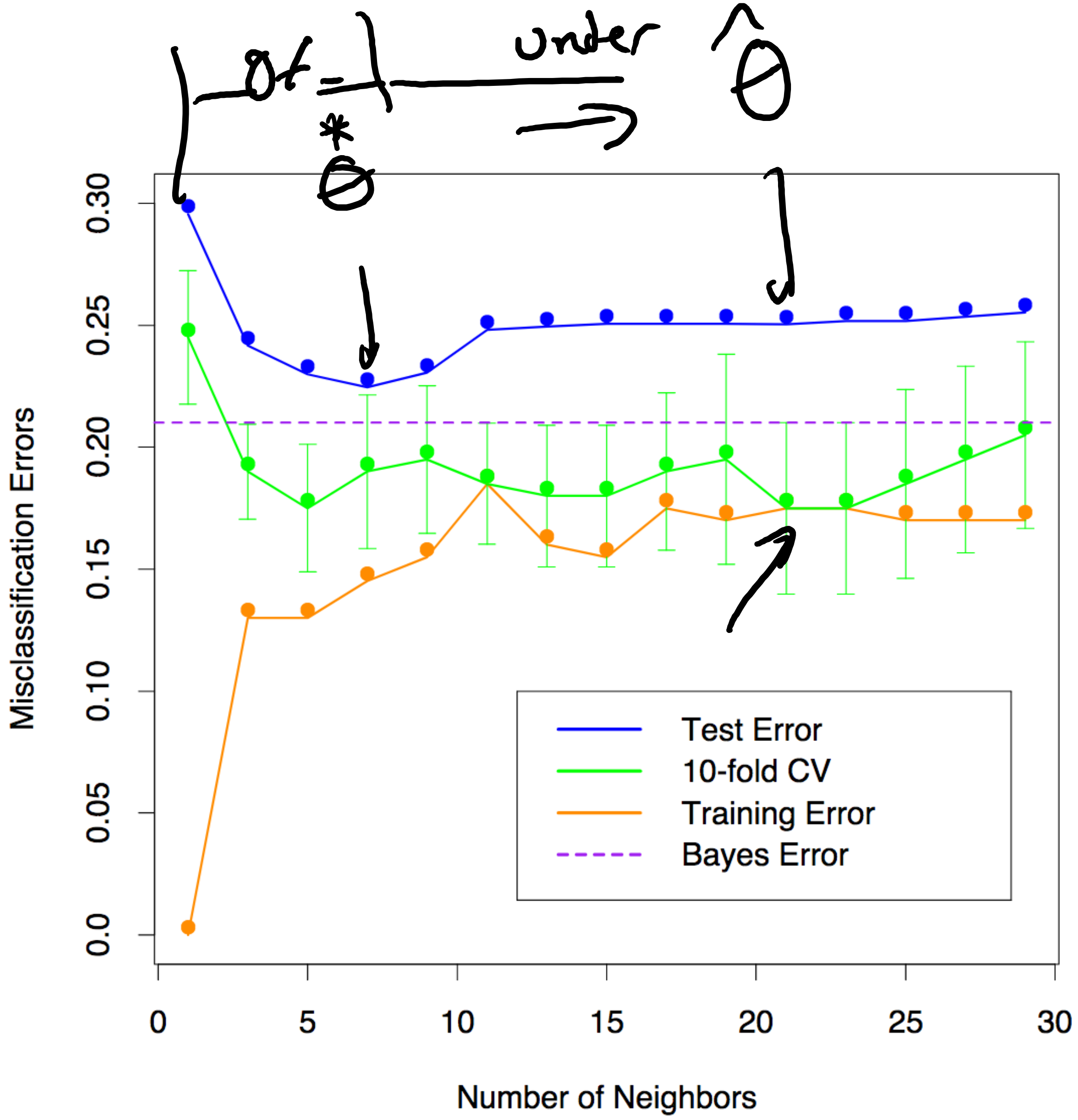
How many standard deviations do you need to add in order to be 95% certain that the mean is within the error?

For large n, 1.96

What's wrong with this approach?

This assumes a random sample,
not that we selected the best value,
which will have higher error



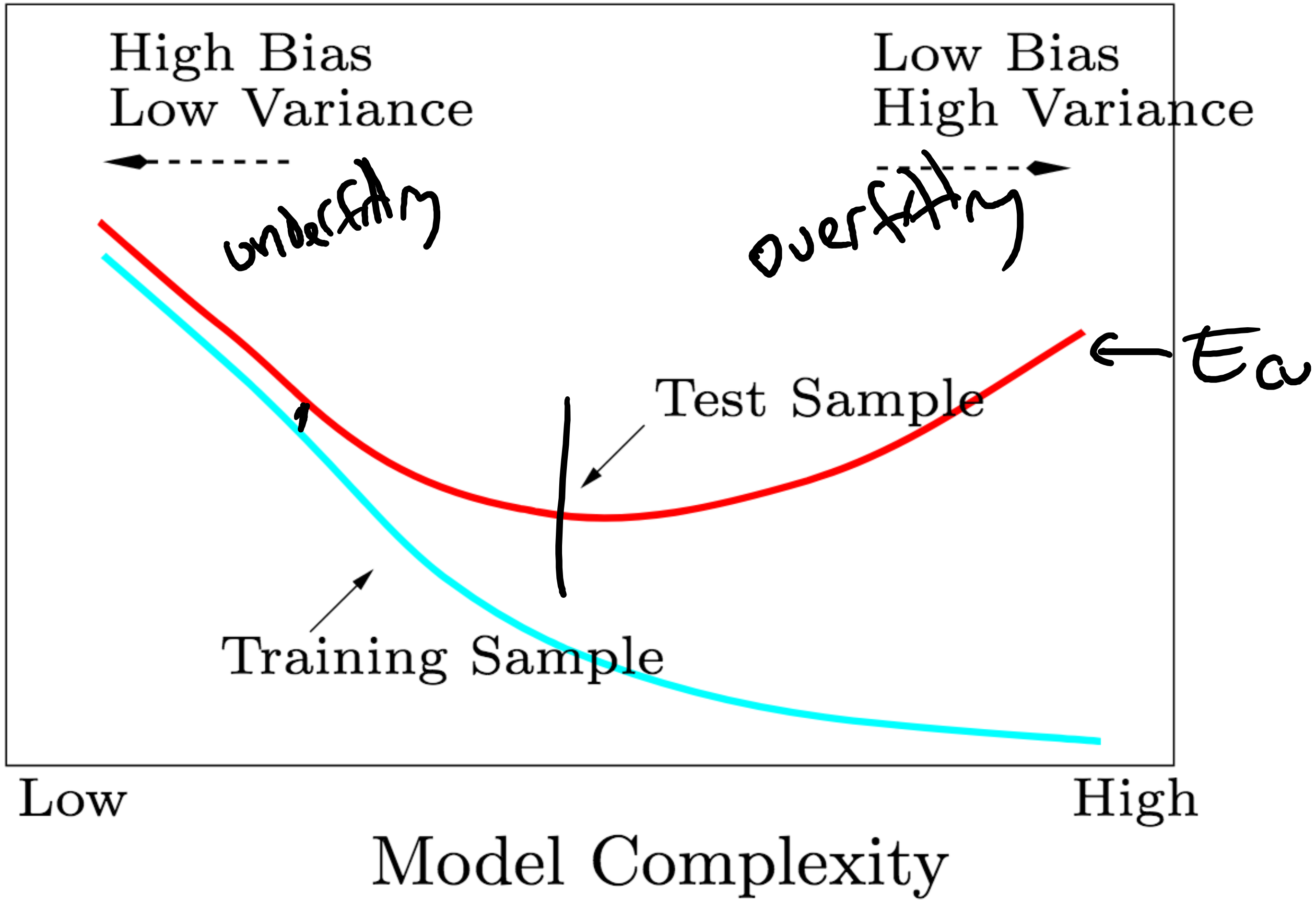
Results

This illustrates a common trade-off

Bias vs. Variance

The more we test (and the more complicated our model), the lower our bias is.

However, we introduce more variance, which is represented in the test data.



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Another model

k-NN is not a model, so much as it is a way of extracting values from the data itself

- No model is ever constructed
- All of the data must be present to estimate (unless we choose representatives)
- Difficult to apply a statistical bound on performance of the 'model'
- LOOCV is easier to test, however. *Why?*

↳ n-Fold CV

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Let's now consider an actual model that we can build from the data

The Linear Model

The linear model assumes that E(Y|X) is a linear combination of inputs $X_1, X_2, \ldots, X_p$

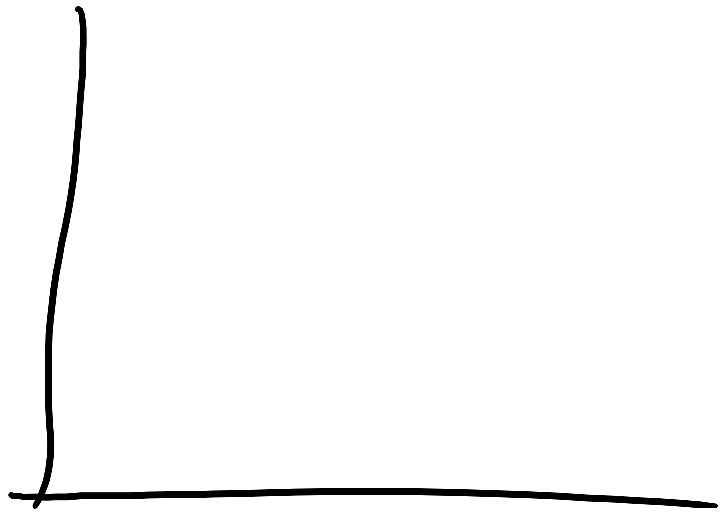
Under this assumption, how do we produce our 'linear model'

Choose the value that minimizes our EPE!

For a linear model, what is the EPE?

- Recall: $EPE(f) = E(Y - f(X))^2$

This minimization problem is the least squares!



kNN Summary

Very simple non-linear classification technique

Works well with large amounts of data

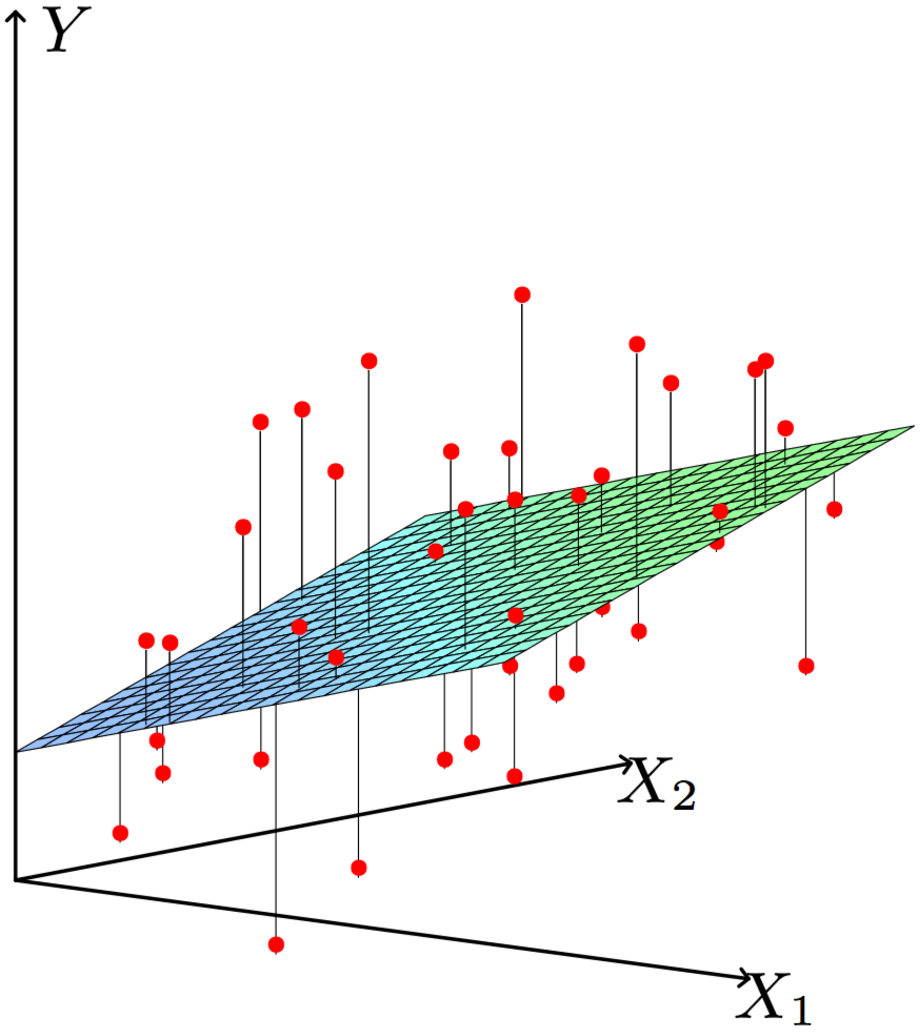
Related to very sophisticated machine learning technique: kernel methods!

Bias-Variance decomposition

- Must find a good balance!

Leave-on-out cross validation

- Very efficient for nearest neighbors



Linear Regression

Regression problems are trying to predict some output value ($Y \in \mathbb{R}$) which is a function of the input variables ($X \in \mathbb{R}^2$)

This is a different problem than *classification*

- kNN can be used for both
- So can linear models

Start with linear regression and move to logistic regression

A note about preqreqs

A note about the linear algebra

- Not a prerequisite for the course
- Whatever linear algebra we'll need, I'll give in class
- Mostly helpful for notation

numpy

Linear Regression

Assume that the output variable is some linear combination of input variables

Linear Regression

Assume that the output variable is some linear combination of input variables

This is probably uncommon. → underfitting

Why learn linear regression models then?

- Basis for kernel methods
- Can be a good baseline performance
- More expressive than you'd initially expect

Linear Regression

Assume that the output variable is some linear combination of input variables

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Why learn linear regression models then?

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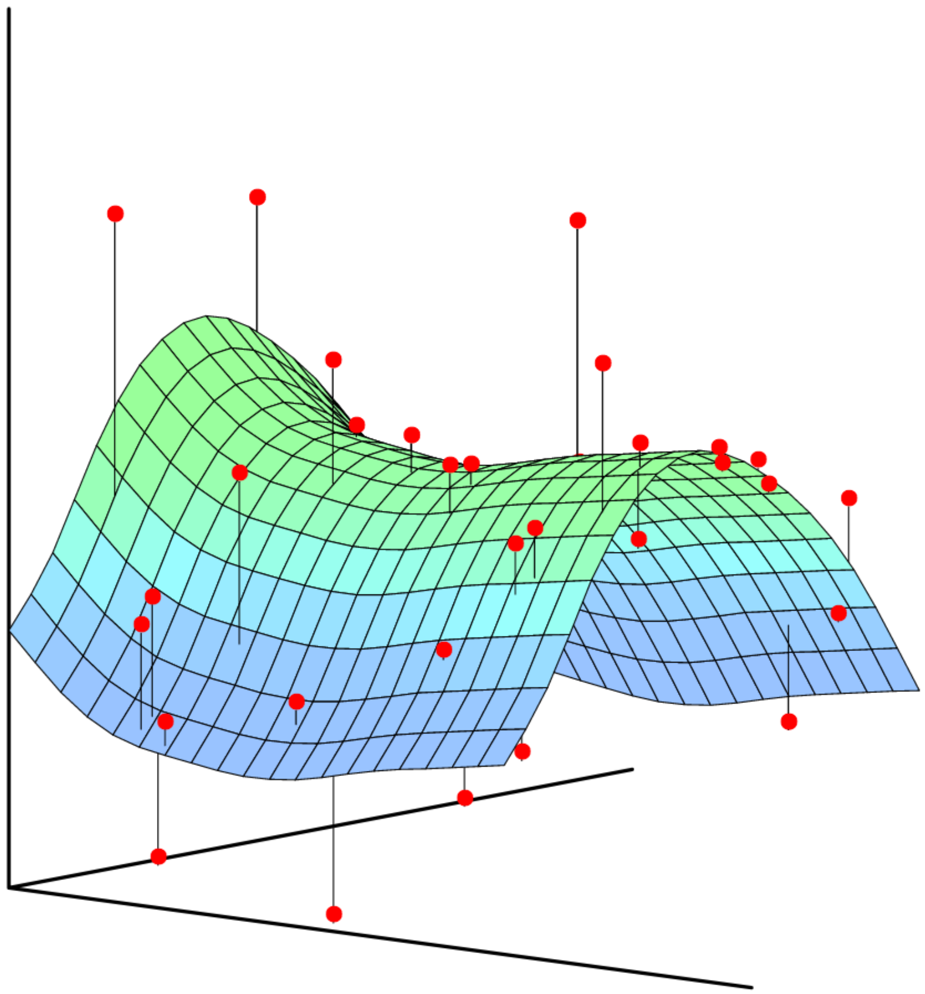
- Can be a good baseline performance
- More expressive than you'd initially expect

Variables are not restricted to being just the inputs (X), they can also be:

- Transformations or interactions ($\log(X_1)$, X_1X_2)
- Dummy encodings
- Polynomial expansions

Feature expansion

Kernel



Linear Regression

The more variables we include:

- higher our risk for overfitting
- higher our expected error
- more complex data can be modeled

Since this is a statistical approach, we can directly bound the error of the model

This is an easy approach for a more robust statistical (and interpretable) result