UVA CS 6316/4501 – Fall 2016 Machine Learning

Lecture 15: K-nearest-neighbor Classifier / Bias-Variance Tradeoff

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Rough Plan

- HW5 is due on Sat
- HW6 will have two coding Q – (image + audio)
- HW7 will be sample final questions
  – Final will be most contents after midterm

- Midterm grade will be released this evening
  – Mean 78 / Median 79 / Max 95
- Final will be in-class / close note / @ Dec5th

Where are we ? ➔ Five major sections of this course

- ❑ Regression (supervised)
- ❑ Classification (supervised)
- ❑ Unsupervised models
- ❑ Learning theory
- ❑ Graphical models

Where are we ? → Three major sections for classification

- We can divide the large variety of classification approaches into roughly three major types

1. Discriminative
   - directly estimate a decision rule/boundary
   - e.g., logistic regression, support vector machine, decisionTree

2. Generative:
   - build a generative statistical model
   - e.g., naïve bayes classifier, Bayesian networks

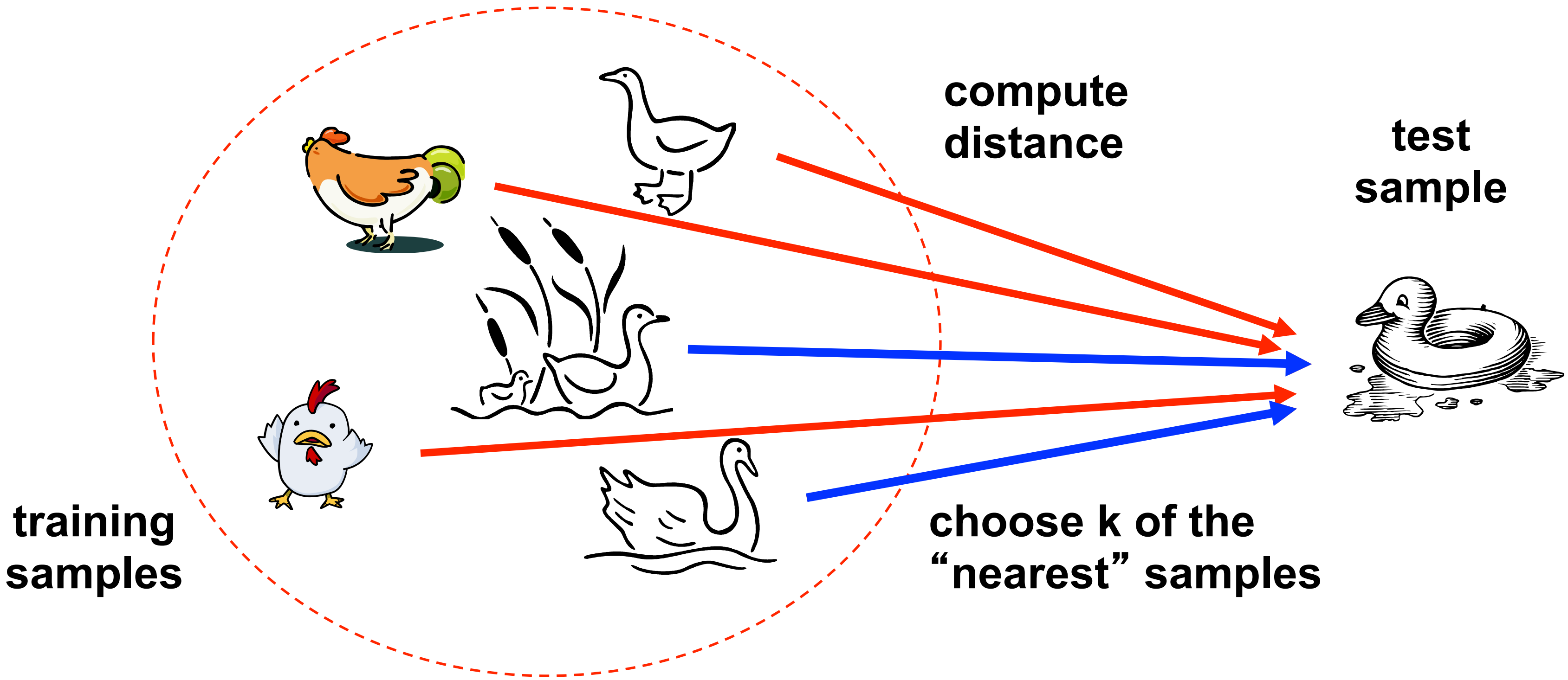
3. Instance based classifiers
   - Use observation directly (no models)
   - e.g. K nearest neighbors

Today :

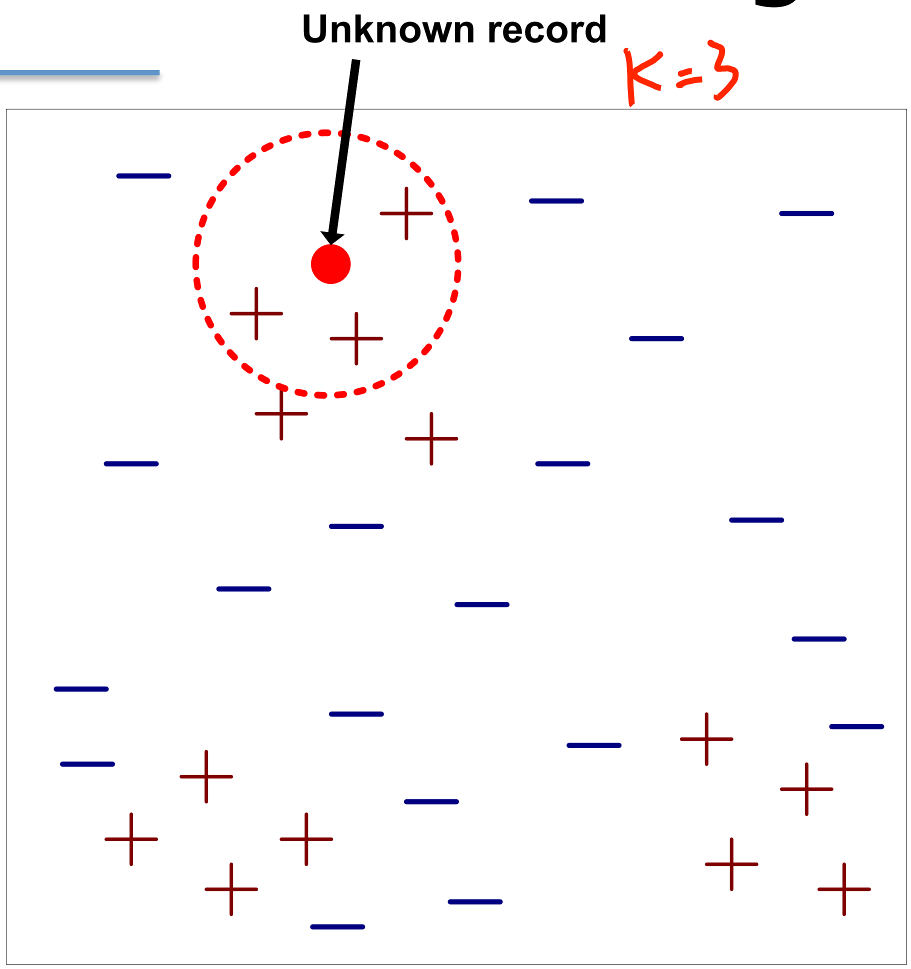
- ✓ K-nearest neighbor
- ✓ Model Selection / Bias Variance Tradeoff

Nearest neighbor classifiers

- Basic idea:
  - If it walks like a duck, quacks like a duck, then it's probably a duck



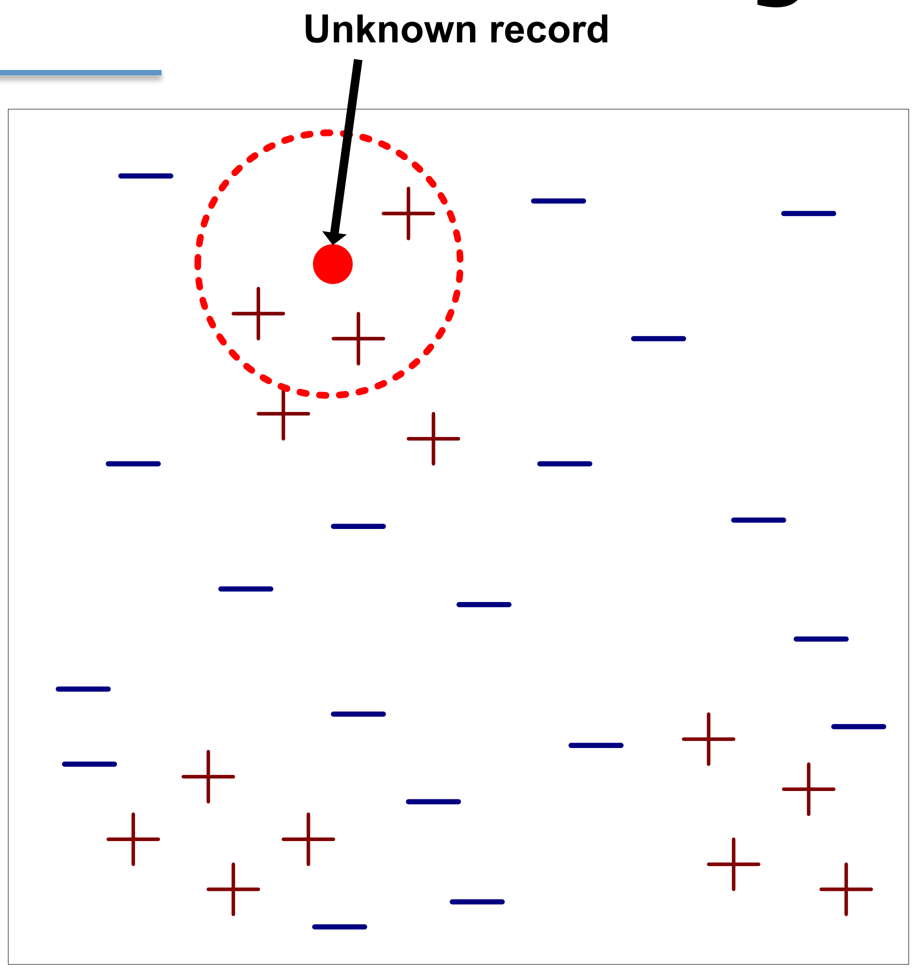
Nearest neighbor classifiers



Requires three inputs:

1. The set of stored training samples
2. Distance metric to compute distance between samples
3. The value of *k*, i.e., the number of nearest neighbors to retrieve

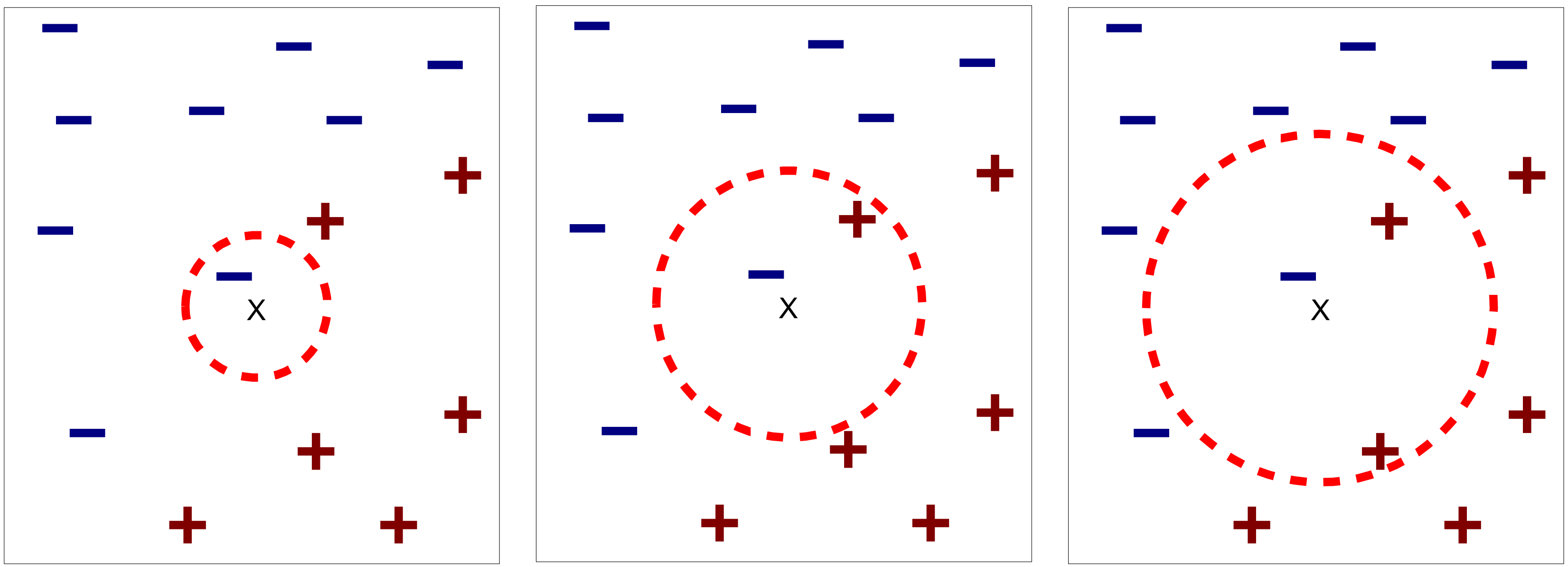
Nearest neighbor classifiers



To classify unknown sample:

1. Compute distance to other training records
2. Identify *k* nearest neighbors
3. Use class labels of nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

Definition of nearest neighbor

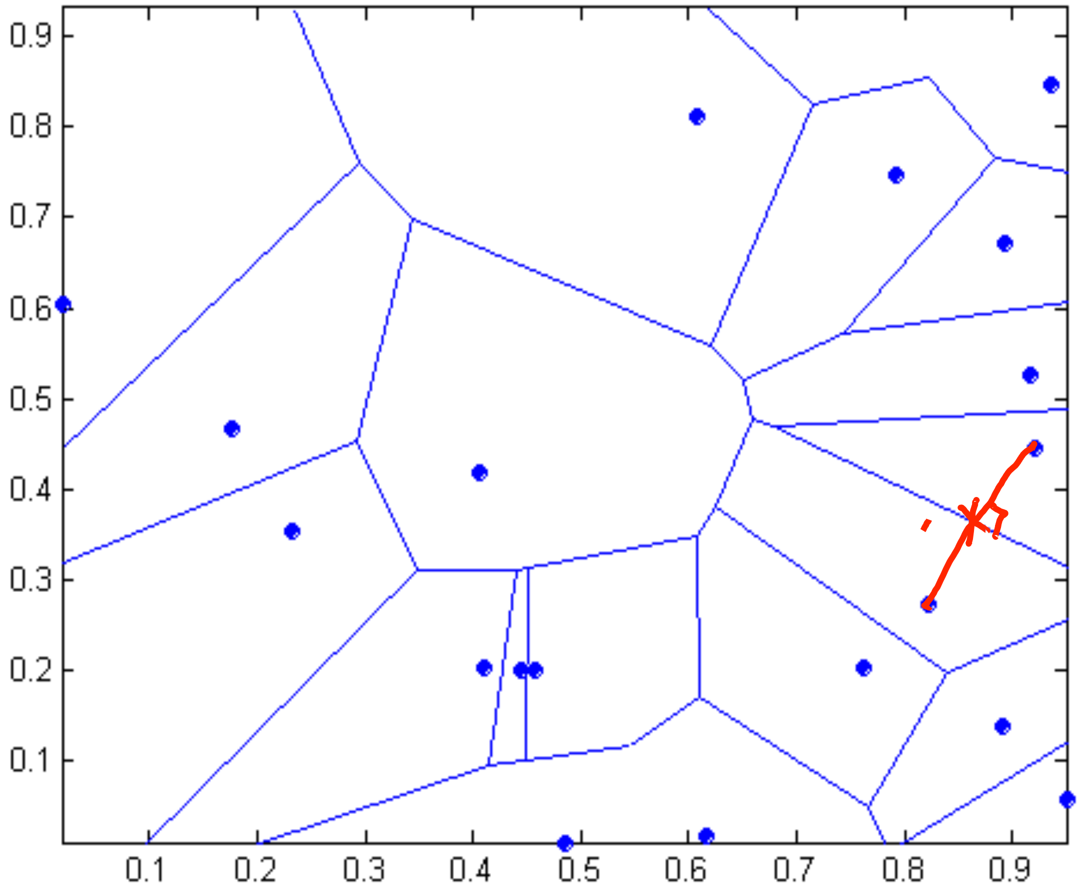


(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

k-nearest neighbors of a sample x are datapoints that have the *k* smallest distances to x

K ??

1-nearest neighbor



Voronoi diagram:

partitioning of a plane into regions based on distance to points in a specific subset of the plane.

Nearest neighbor classification

- Compute distance between two points:
  - For instance, Euclidean distance

e.g. cosine distance for text

$$d(\mathbf{x},\mathbf{y}) = \sqrt{\sum_i (x_i - y_i)^2}$$

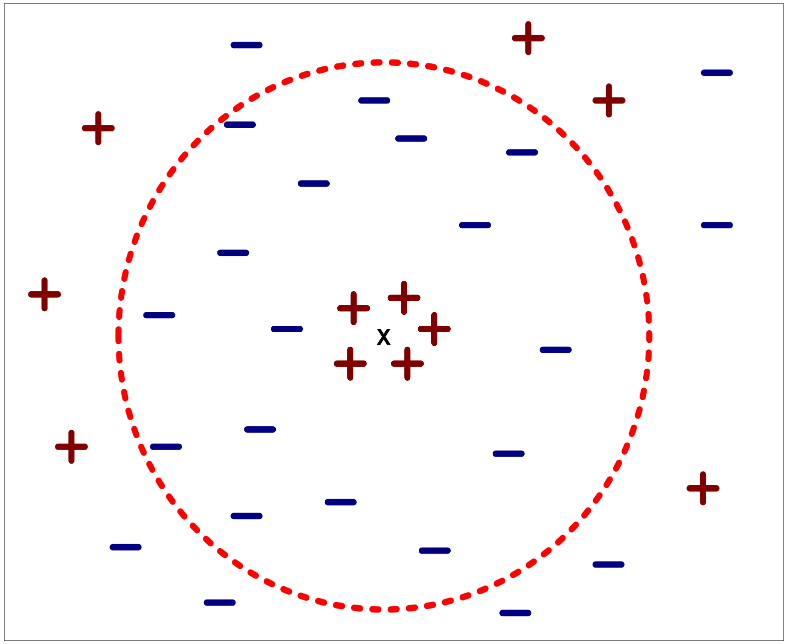
- Options for determining the class from nearest neighbor list
  - Take majority vote of class labels among the *k*-nearest neighbors
  - Weight the votes according to distance
    - example: weight factor w = 1 / d^2

Nearest neighbor classification

- Choosing the value of *k*:
  - If *k* is too small, sensitive to noise points
  - If *k* is too large, neighborhood may include points from other classes

k P
regression

P small
P large



K large

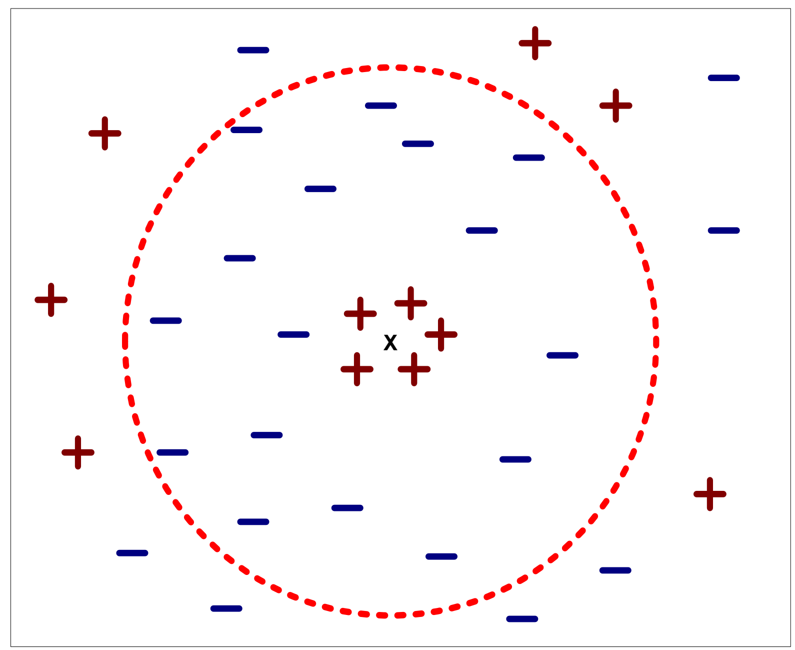
K small
flexible

Nearest neighbor classification

- Choosing the value of *k*:
  - If *k* is too small, sensitive to noise points
  - If *k* is too large, neighborhood may include points from other classes

K ↓ flexible / varies a lot

K ↑ Smooth / varies little



Nearest neighbor classification

- Scaling issues
  - Attributes may have to be scaled to prevent distance measures from being dominated by one of the attributes
  - Example:
    - height of a person may vary from 1.5 m to 1.8 m
    - weight of a person may vary from 90 lb to 300 lb
    - income of a person may vary from $10K to $1M

Nearest neighbor classification

- *k*-Nearest neighbor classifier is a lazy learner
  - Does not build model explicitly.
  - Classifying unknown samples is relatively expensive. $X_{test} \rightarrow \quad O(n) + O(\text{Sort-}n\text{-}k)$

- *k*-Nearest neighbor classifier is a local model, vs. global model of linear classifiers.

Nearest neighbor classification

- *k*-Nearest neighbor classifier is a lazy learner
  - Does not build model explicitly.
  - Classifying unknown samples is relatively expensive.

K (Xts, Xtri)

testing { KNN: num_train / all train samples
SVM: num_support vectors points

- *k*-Nearest neighbor classifier is a local model, vs. global model of linear classifiers.

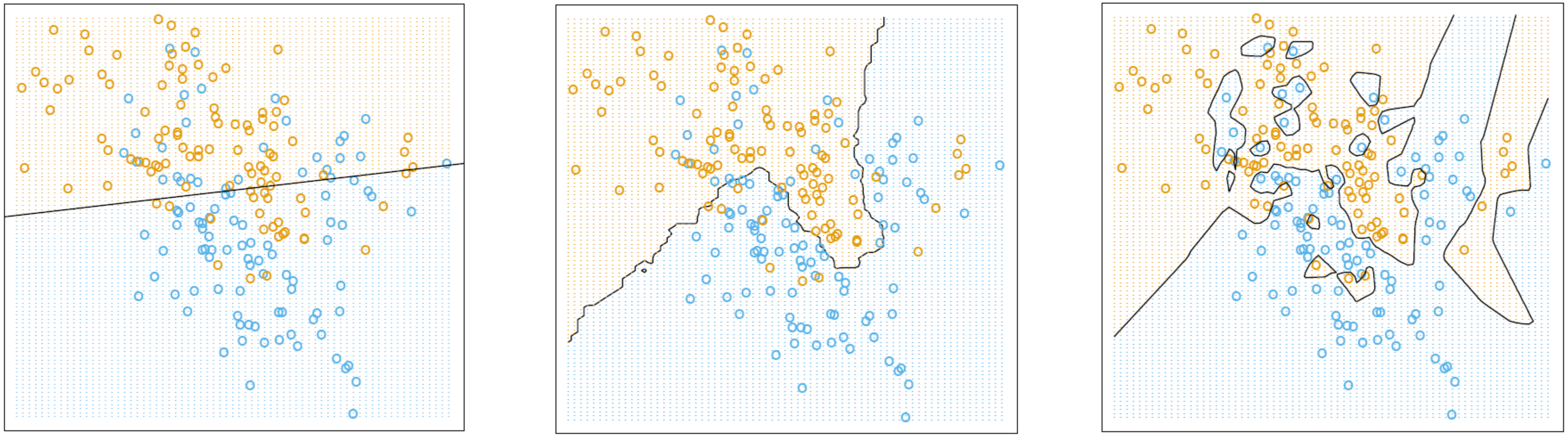
K-Nearest Neighbor

Task → Representation → Score Function → Search/Optimization → Models, Parameters

classification → Local Smoothness → NA → NA → Training Samples

Decision boundaries in global vs. local models

K=15 K=1



linear regression

- global
- stable
- can be inaccurate

15-nearest neighbor

- K acts as a smoother

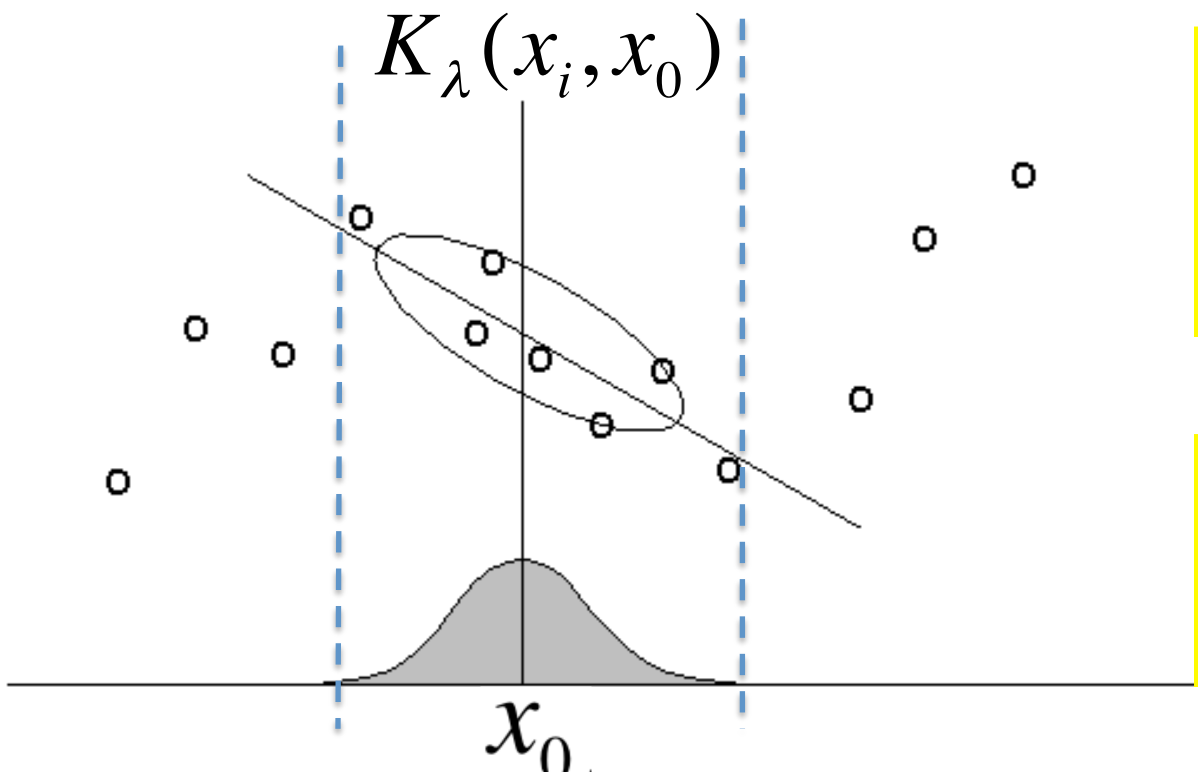
1-nearest neighbor

- local
- accurate
- unstable

What ultimately matters: ***GENERALIZATION*** vs. KNN for regression (mean of KNN)

Vs. Locally weighted regression

- *aka* locally weighted regression, locally linear regression, LOESS, …



linear_func(x)->y ➔ could represent only the neighbor region of x_0

Use RBF function to pick out/emphasize the neighbor region of x_0 ➔ $K_\lambda(x_i, x_0)$

Figure 2: In locally weighted regression, points are weighted by proximity to the current **x** in question using a kernel. A regression is then computed using the weighted points.

Vs. Locally weighted regression

- Separate weighted least squares **at each target point $\mathbf{x_0}$:**

x_0

$$\min_{\alpha(x_0),\beta(x_0)} \sum_{i=1}^{N} K_\lambda(x_i, x_0)[y_i - \alpha(x_0) - \beta(x_0)x_i]^2$$

$$\hat{f}(x_0) = \hat{\alpha}(x_0) + \hat{\beta}(x_0)x_0$$

$$K_\tau(\mathbf{x}_i, \mathbf{x}0) = \exp\left(-\frac{(\mathbf{x}_i - \mathbf{x}0)^2}{2\tau^2}\right)$$

Today :

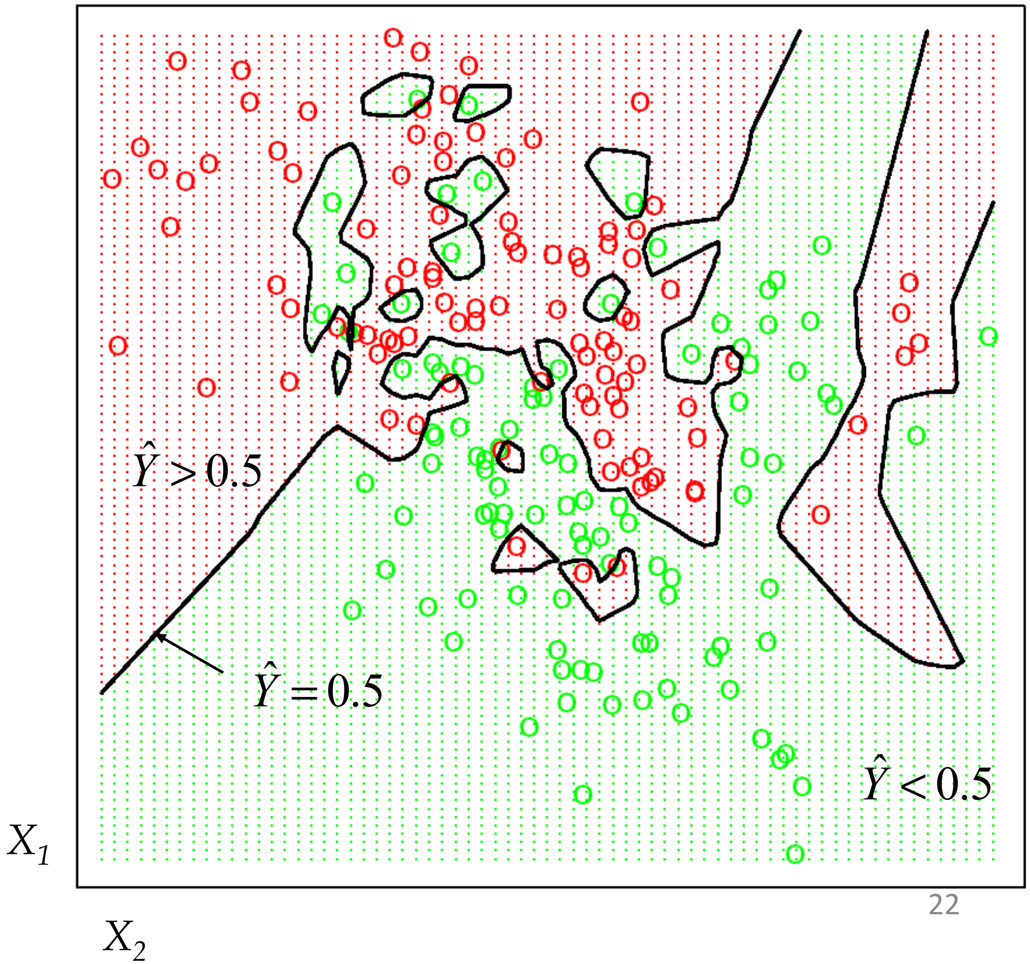
- ✓ K-nearest neighbor
- ✓ Model Selection / Bias Variance Tradeoff
  - ✓ EPE
  - ✓ Decomposition of MSE
  - ✓ Bias-Variance tradeoff
  - ✓ High bias ? High variance ? How to respond ?

e.g. Training Error from KNN, Lesson Learned

- When k = 1,
- No misclassifications (on training): Overtraining

- Minimizing training error is not always good (e.g., 1-NN)

1-nearest neighbor averaging



Statistical Decision Theory

- Random input vector: X
- Random output variable: Y
- Joint distribution: $\Pr(X, Y)$
- Loss function $L(Y, f(X))$

- Expected prediction error (EPE):
- $$\mathrm{EPE}(f) = \mathrm{E}(L(Y, f(X))) = \int L(y, f(x)) \Pr(dx, dy)$$

$$\text{e.g.} = \int (y - f(x))^2 \Pr(dx, dy)$$

Consider population distribution

e.g. Squared error loss (also called L2 loss)

Expected prediction error (EPE)

Consider joint distribution

$$\mathrm{EPE}(f) = \mathrm{E}(L(Y, f(X))) = \int L(y, f(x)) \Pr(dx, dy)$$

- **For L2 loss:** $\text{e.g.} = \int (y - f(x))^2 \Pr(dx, dy)$

under L2 loss, best estimator for EPE (Theoretically) is :

Conditional mean $\hat{f}(x) = \mathrm{E}(Y \mid X = x)$

ts

e.g. KNN

NN methods are the direct implementation (approximation)

- **For 0-1 loss:** $L(k, \ell) = 1 - d_{kl}$

$\hat{f}(X) = C_k$ if

$\Pr(C_k \mid X = x) = \max_{g \in C} \Pr(g \mid X = x)$

Bayes Classifier

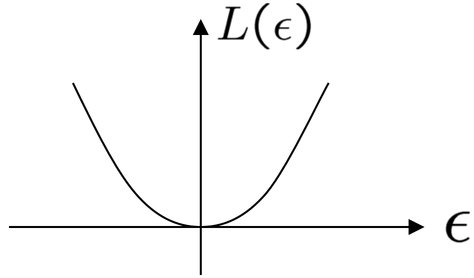
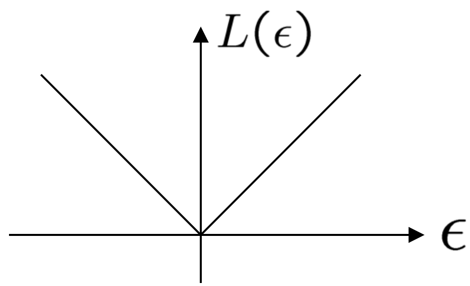
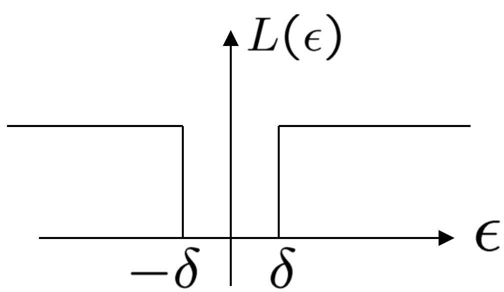
KNN FOR MINIMIZING EPE

- We know under L2 loss, best estimator for EPE (Theoretically) is :

Conditional mean $f(x) = \mathrm{E}(Y \mid X = x)$

– Nearest neighbors assumes that *f(x)* is well approximated by a locally constant function.

Review : WHEN EPE USES DIFFERENT LOSS

Loss Function	Estimator $\hat{f}(x)$
L_2 	$\hat{f}(x) = E[Y\|X = x]$
L_1 	$\hat{f}(x) = \text{median}(Y\|X = x)$
0-1 	$\hat{f}(x) = \arg\max_Y P(Y\|X = x)$ (Bayes classifier / MAP)

Today :

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  - ✓ EPE
  - ✓ Decomposition of MSE
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  - ✓ High bias ? High variance ? How to respond ?

Decomposition of EPE

- When additive error model:
- Notations $Y = f(X) + \epsilon, \ \epsilon \sim (0, \sigma^2)$
  - Output random variable: Y
  - Prediction function: f
  - Prediction estimator: $\hat{f}$

$$
\begin{aligned}
EPE(\overset{f(x_0)}{\cancel{x_0}}) &= E[(Y - \hat{f})^2 | X = x_0] \\
&= E[((Y - f) + (f - \hat{f}))^2 | X = x_0] \\
&= E[\underbrace{(Y - f)}_{\epsilon}{}^2 | X = x_0] + \underbrace{E[(f - \hat{f})^2 | X = x_0]}_{MSE} \\
&= \sigma^2 + Var(\hat{f}) + \text{Bias}^2(\hat{f})
\end{aligned}
$$

MSE component of f-hat in estimating f

Irreducible / Bayes error

Bias-Variance Trade-off for EPE:

f(x0)

EPE (~~x_0~~) = noise^2 + bias^2 + variance

Unavoidable error

Error due to incorrect assumptions

Error due to variance of training samples

Slide credit: D. Hoiem

BIAS AND VARIANCE TRADE-OFF for MSE (more general setting !!!):

more general setting of MSE

- θ: true value (normally unknown)
- $\hat{\theta}$: estimator
- $\bar{\theta} := E[\hat{\theta}]$ (mean, i.e. expectation of the estimator)

- Bias $E[(\bar{\theta} - \theta)^2]$
  - measures accuracy or quality of the estimator
  - low bias implies on average we will accurately estimate true parameter or func from training data
- Variance $E[(\hat{\theta} - \bar{\theta})^2]$
  - Measures precision or specificity of the estimator
  - Low variance implies the estimator does not change much as the training set varies

θ could be e.g. $\begin{cases} w \text{ for LR} \\ f \text{ for EPE} \end{cases}$

BIAS AND VARIANCE TRADE-OFF for MSE of parameter estimation:

e.g. In EPE case, $E[(f-\hat{f})^2 | X = X_0] \Rightarrow MSE(f(x_0))$

$\bar{\theta} = mean(\hat{\theta}) \Rightarrow$

$$
\begin{aligned}
MSE(\hat{\theta}) &= E[(\hat{\theta}-\theta)^2] \\
&= E[((\hat{\theta}-\bar{\theta})+(\bar{\theta}-\theta))^2] \\
&= E[(\hat{\theta}-\bar{\theta})^2] + E[(\bar{\theta}-\theta)^2] + 2E[(\hat{\theta}-\bar{\theta})(\bar{\theta}-\theta)] \\
&= Var(\hat{\theta}) + \text{Bias}^2(\hat{\theta}) + 0
\end{aligned}
$$

Error due to variance of training samples

Error due to incorrect assumptions

$$MSE(\hat{\theta}) = E[(\hat{\theta}-\theta)^2] = Bias^2(\hat{\theta}) + Var(\hat{\theta})$$

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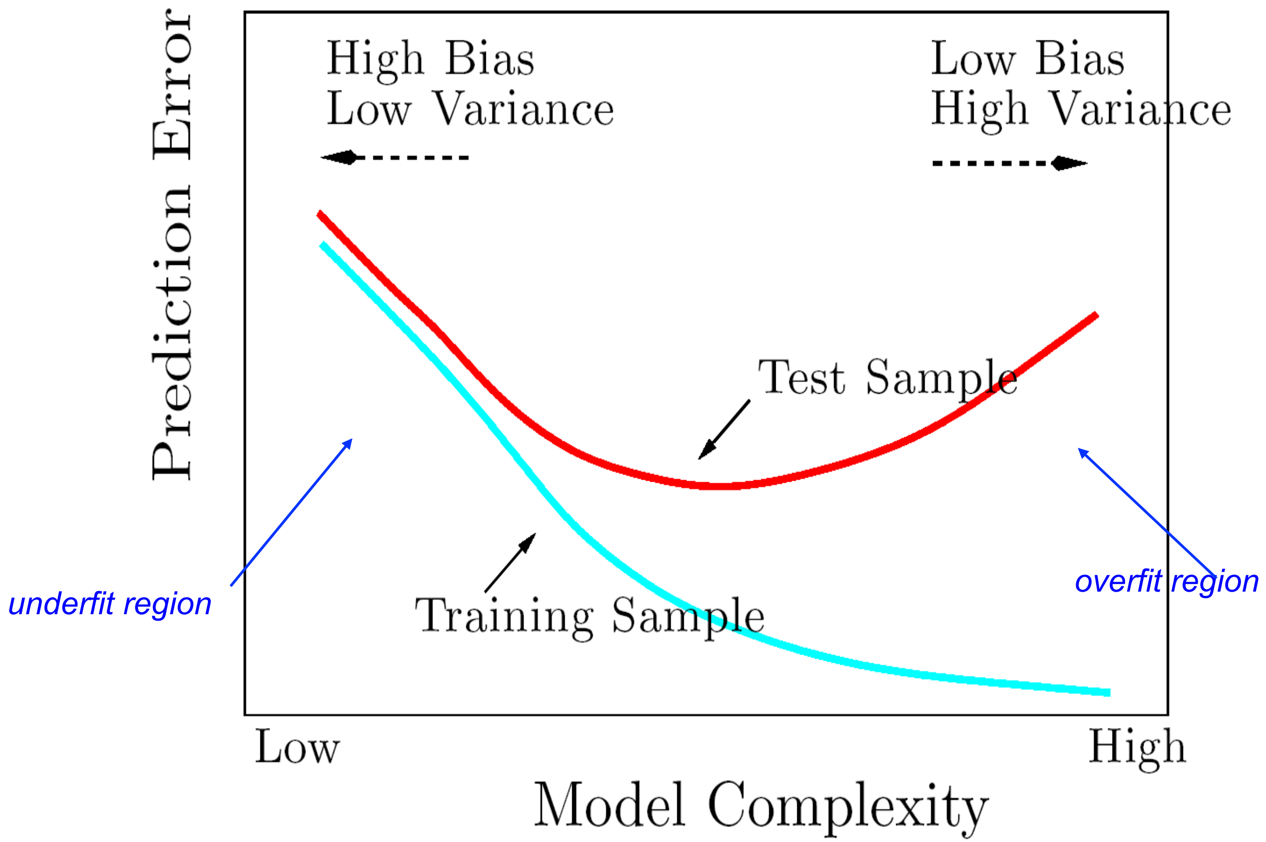
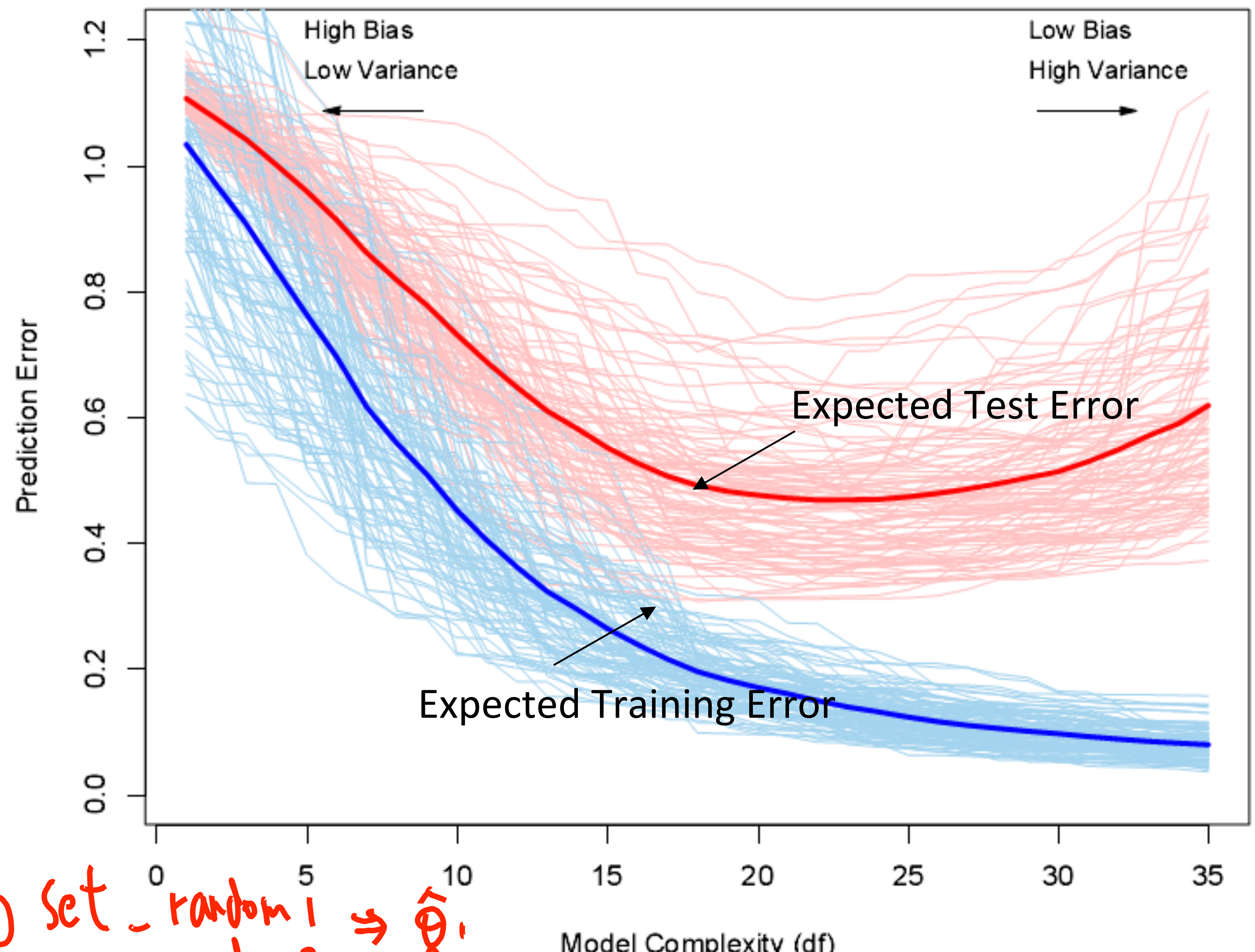
Bias-Variance Tradeoff / Model Selection



(1) Training vs Test Error

- Training error can always be reduced when increasing model complexity,

- Expected Test error and CV error → good approximation of EPE



training set _ random 1 ⇒ $\hat{\theta}_1$
training set - random2 ⇒ $\hat{\theta}_2$
.... 3 ⇒ $\hat{\theta}_3$

(2) Bias-Variance Trade-off

- Models with too few parameters are inaccurate because of a large bias (not enough flexibility).

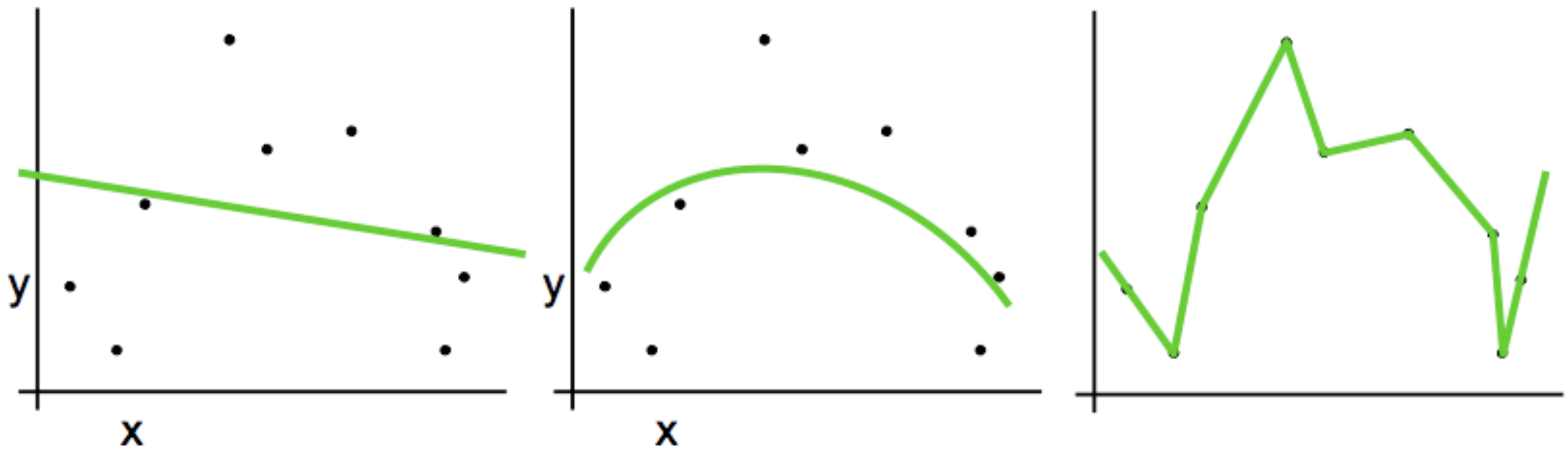
poly regression: d small
KNN: K large

- Models with too many parameters are inaccurate because of a large variance (too much sensitivity to the sample randomness).

poly regression: d large
KNN: K small

Slide credit: D. Hoiem

(2.1) Regression: Complexity versus Goodness of Fit

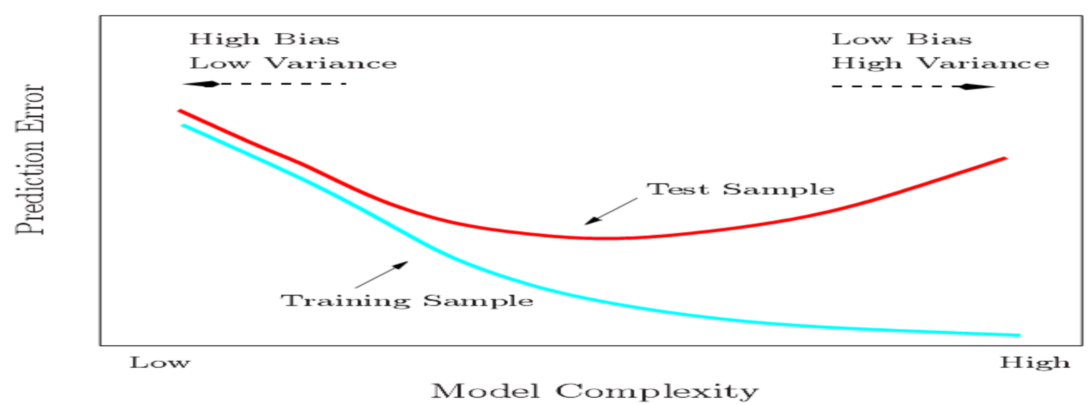


Highest Bias
Lowest variance
Model complexity = low

Medium Bias
Medium Variance
Model complexity = medium

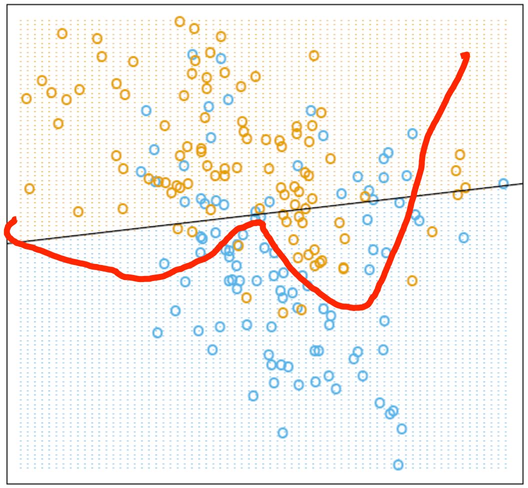
Smallest Bias
Highest variance
Model complexity = high

Low Variance / High Bias



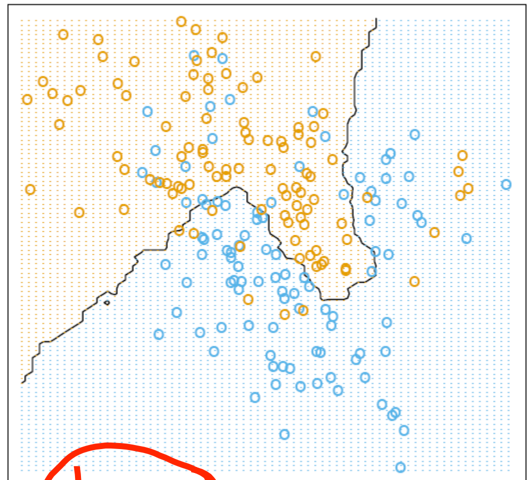
Low Bias / High Variance

(2.2) Classification, Decision boundaries in global vs. local models



Low Variance / High Bias

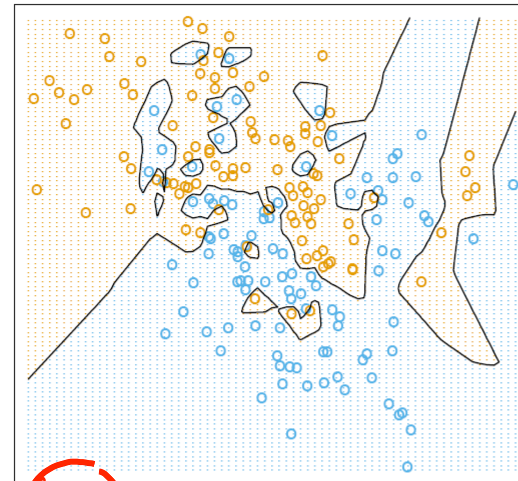
linear regression
- global
- stable
- can be inaccurate



k=15

15-nearest neighbor

Low Variance / High Bias



k=1

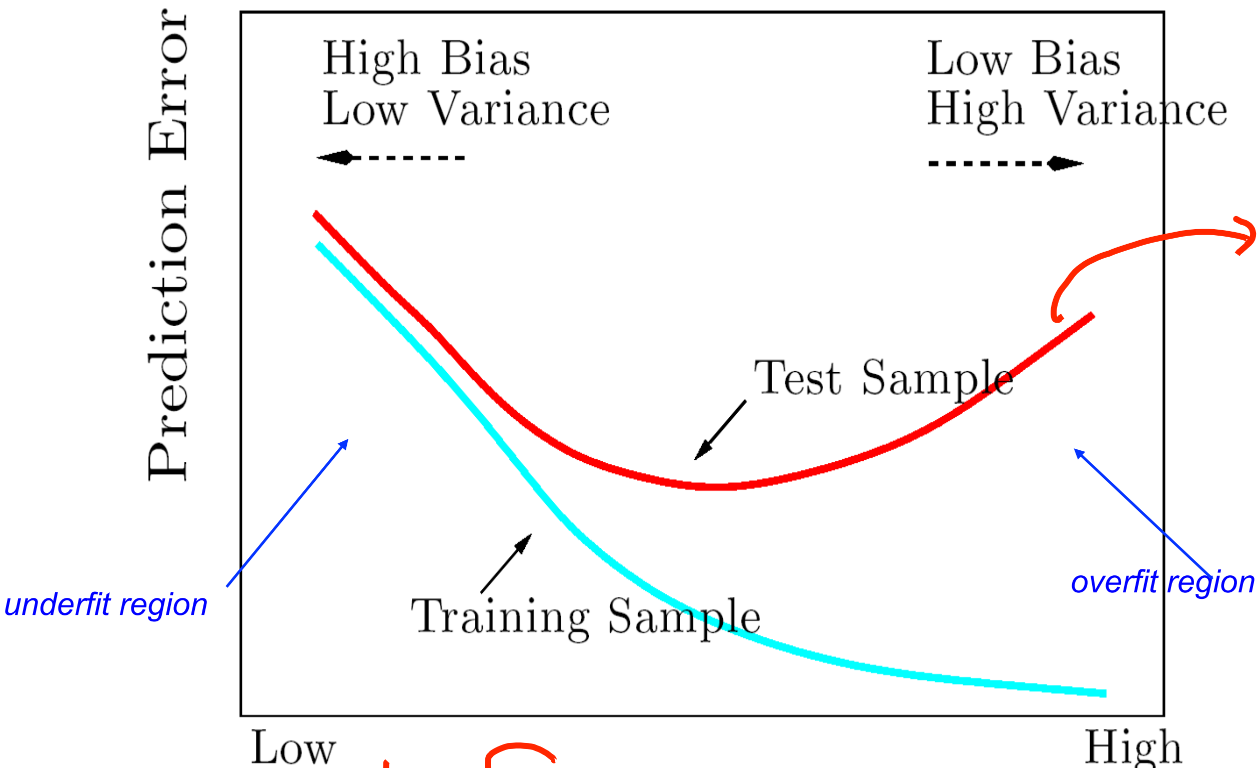
1-nearest neighbor

Low Bias / High Variance

KNN
- local
- accurate
- unstable

What ultimately matters: ***GENERALIZATION***

Bias-Variance Tradeoff / Model Selection



CV / test error
[Good approximation of EPE]

KNN: large K ← [Model Complexity] → small K

Regression: small d → large d

Model “bias” & Model “variance”

- Middle RED:
  - TRUE function

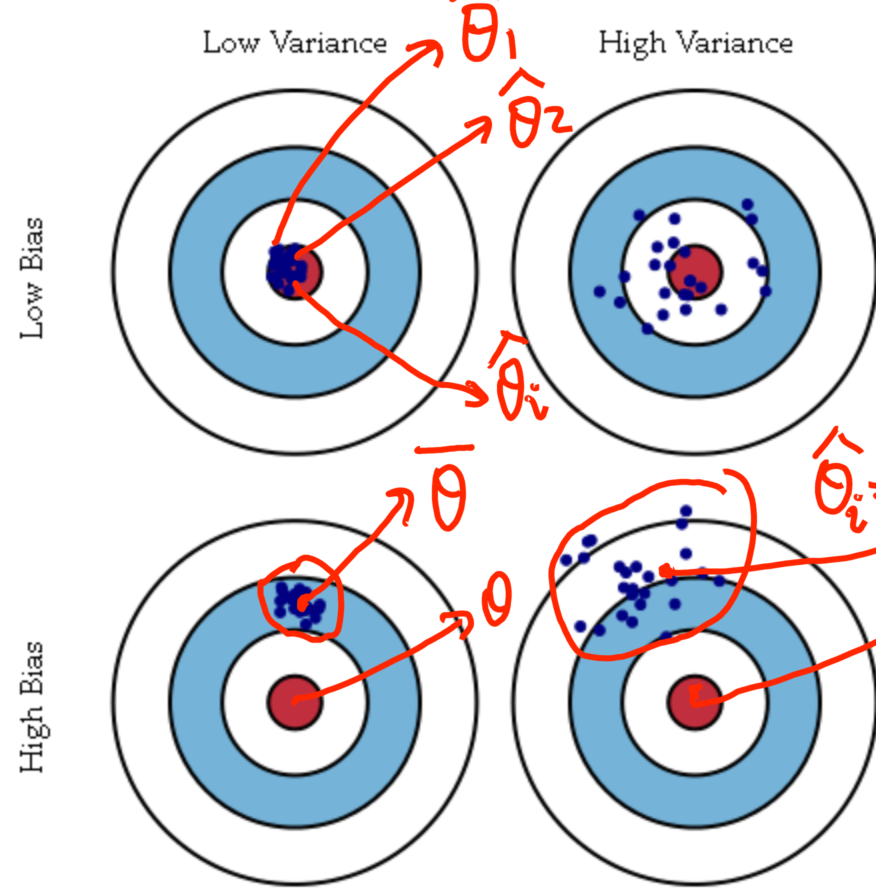
θ [middle red]

- Error due to bias:
  - How far off in general from the middle red

$$E(\theta - \bar{\theta})$$

$\underbrace{\bar{\theta}}_{\text{mean of } \hat{\theta}}$

- Error due to variance:
  - How wildly the blue points spread



$$E((\hat{\theta} - \bar{\theta})^2)$$

$\hat{\theta} \rightarrow \{\hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3, \dots\}$ Blue dots

need to make assumptions that are able to generalize

- Components of generalization error
  - **Bias:** how much the average model over all training sets differ from the true model?
    - Error due to inaccurate assumptions/simplifications made by the model
  - **Variance:** how much models estimated from different training sets differ from each other
- **Underfitting:** model is too "simple" to represent all the relevant class characteristics
  - High bias and low variance
  - High training error and high test error
- **Overfitting:** model is too "complex" and fits irrelevant characteristics (noise) in the data
  - Low bias and high variance
  - Low training error and high test error

Slide credit: L. Lazebnik

Today :

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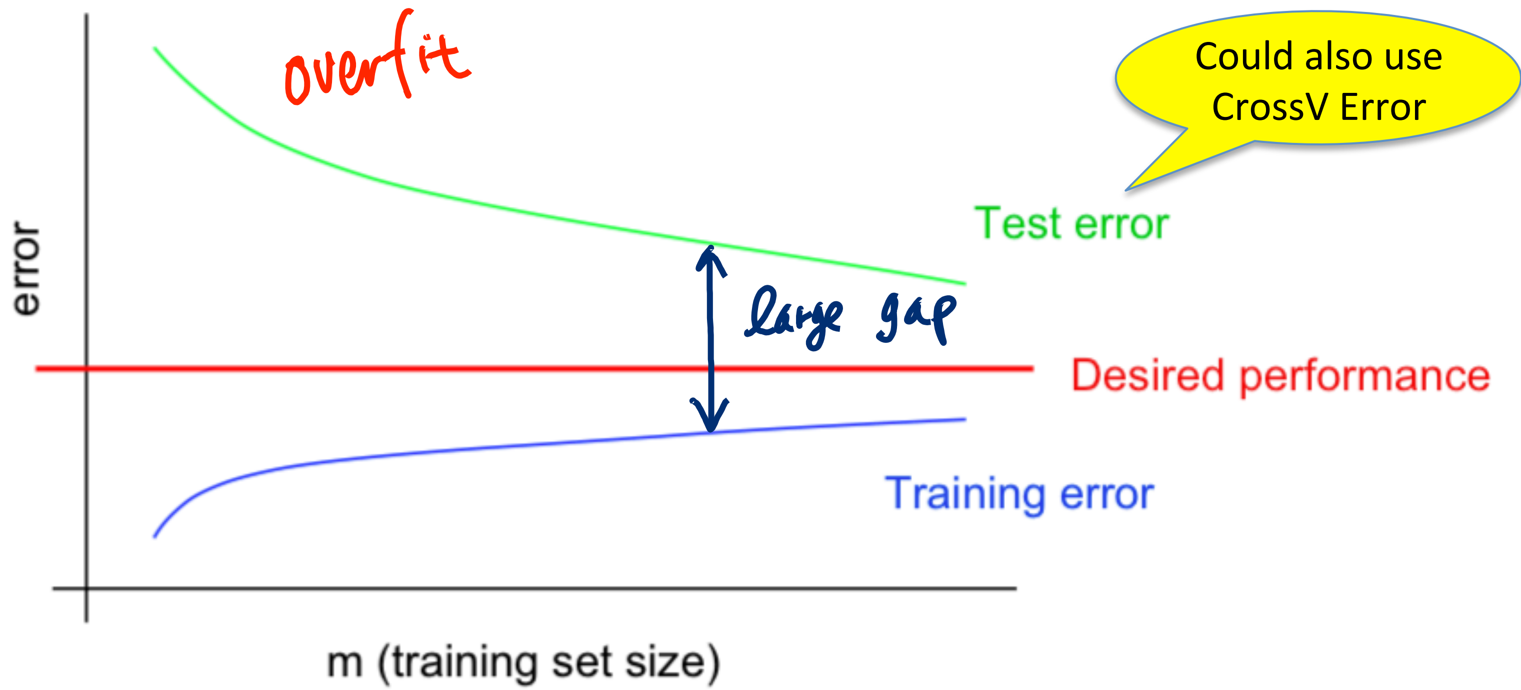
  - ✓ EPE
  - ✓ Decomposition of MSE
  - ✓ Bias-Variance tradeoff
  - ✓ High bias ? High variance ? How to respond ?

(1) High variance

Typical learning curve for high variance:



- Test error still decreasing as m increases. Suggests larger training set will help.
- Large gap between training and test error.
- Low training error and high test error

Slide credit: A. Ng

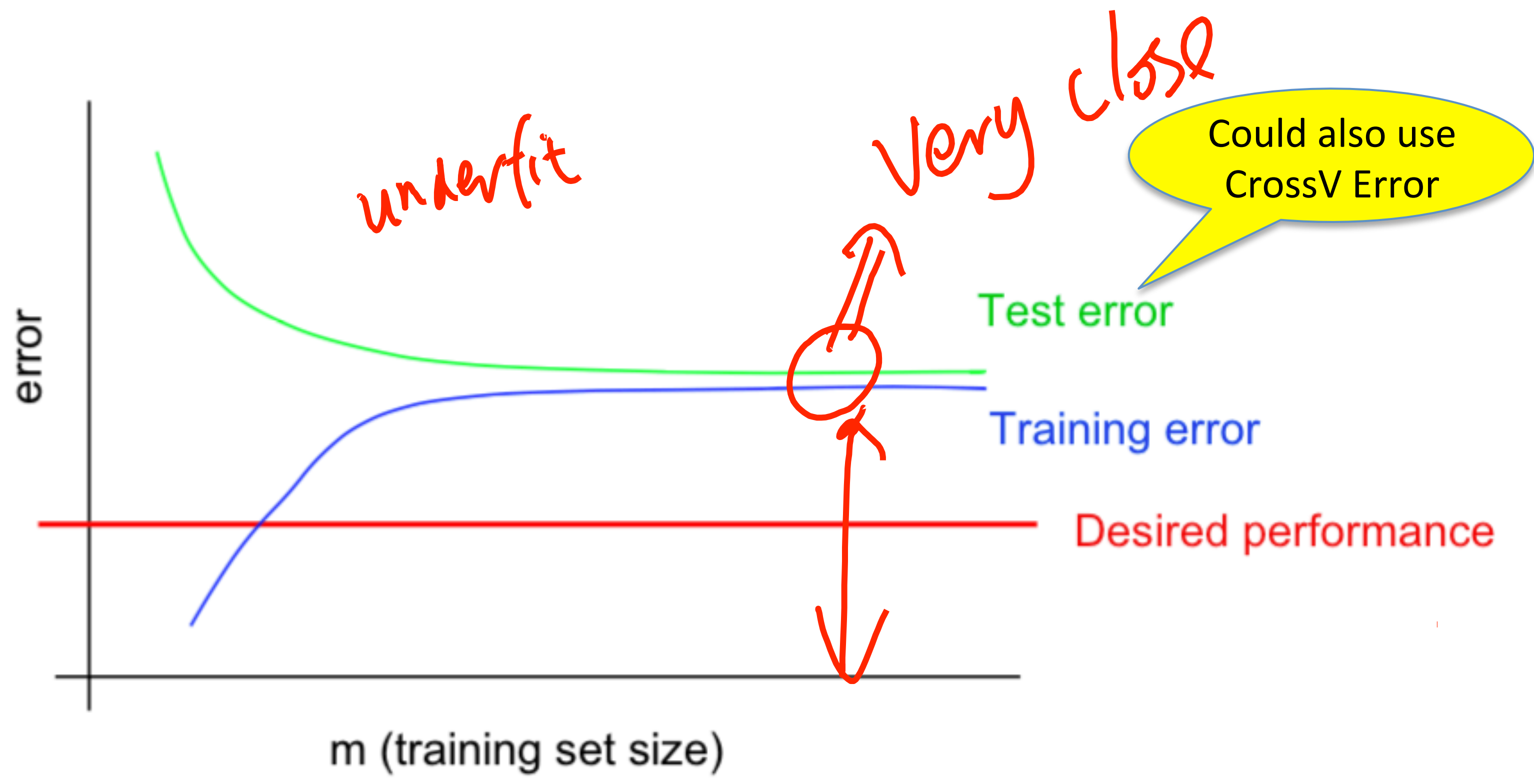
How to reduce variance?

- Choose a simpler classifier
- Regularize the parameters
- Get more training data
- Try smaller set of features

Slide credit: D. Hoiem

(2) High bias

Typical learning curve for high bias:



- Even training error is unacceptably high.
- Small gap between training and test error.

High training error and high test error

How to reduce Bias ?

- E.g.

- Get additional features
- Try adding basis expansions, e.g. polynomial
- Try more complex learner

(3) For instance, if trying to solve "spam detection" using (Extra)

L2 - logistic regression, implemented with gradient descent.

Fixes to try: If performance is not as desired

- Try getting more training examples. Fixes high variance.
- Try a smaller set of features. Fixes high variance.
- Try a larger set of features. Fixes high bias.
- Try email header features. Fixes high bias.
- Run gradient descent for more iterations. Fixes optimization algorithm.
- Try Newton's method. Fixes optimization algorithm.
- Use a different value for λ. Fixes optimization objective.
- Try using an SVM. why ??? Fixes optimization objective.

Slide credit: A. Ng

(4) Model Selection and Assessment

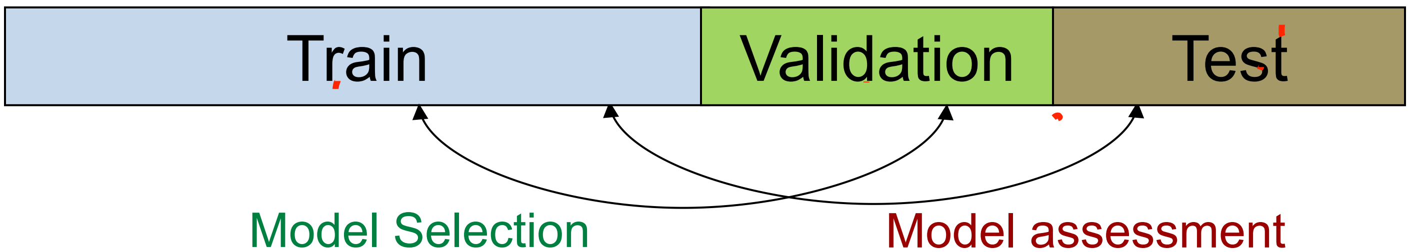
- Model Selection
  - Estimating performances of different models to choose the best one

- Model Assessment
  - Having chosen a model, estimating the <u>prediction error</u> on new data

Model Selection and Assessment

(Extra)

- Data Rich Scenario: Split the dataset



- Insufficient data to split into 3 parts
  - Approximate validation step analytically
    - AIC, BIC, MDL, SRM
  - Efficient reuse of samples
    - Cross validation, bootstrap

Today Recap:

- ✓ K-nearest neighbor
- ✓ Model Selection / Bias Variance Tradeoff
  - ✓ EPE
  - ✓ Decomposition of MSE
  - ✓ Bias-Variance tradeoff
  - ✓ High bias ? High variance ? How to respond ?

References

- Prof. Tan, Steinbach, Kumar's "Introduction to Data Mining" slide
- Prof. Andrew Moore's slides
- Prof. Eric Xing's slides
- Hastie, Trevor, et al. *The elements of statistical learning*. Vol. 2. No. 1. New York: Springer, 2009.