

Model selection and KNN

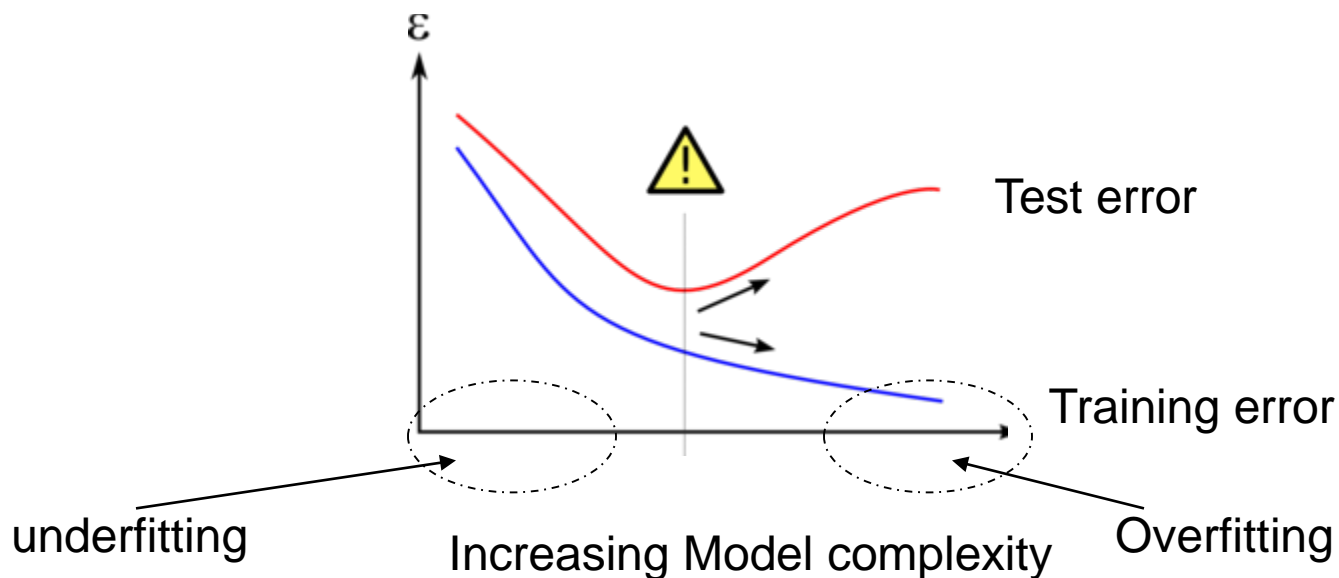
CS434

Model Selection

- **Model selection** is about choosing among different models
 - linear regression vs. quadratic regression
 - Choosing one type of regularization over another
 - Choosing the regularization parameter
 - Choosing one set of features vs. another
- Heavily studied in machine learning, crucial importance in practice

Model selection 101

If we use training error to select models, we will always choose more complex ones



(e.g., as we decrease the regularization parameter λ)

Overfitting

- Overfitting can be interpreted as:
 - Fitting to the particularities of the data
 - E.g. fitting to the noise of the data, not the general trend
 - Fitting too many parameters with too few data points
 - E.g. fitting a line to a single data point
- Over fitting can be worsened with
 - Too many parameters (or over-complex model)
 - Too few training examples

Under-fitting

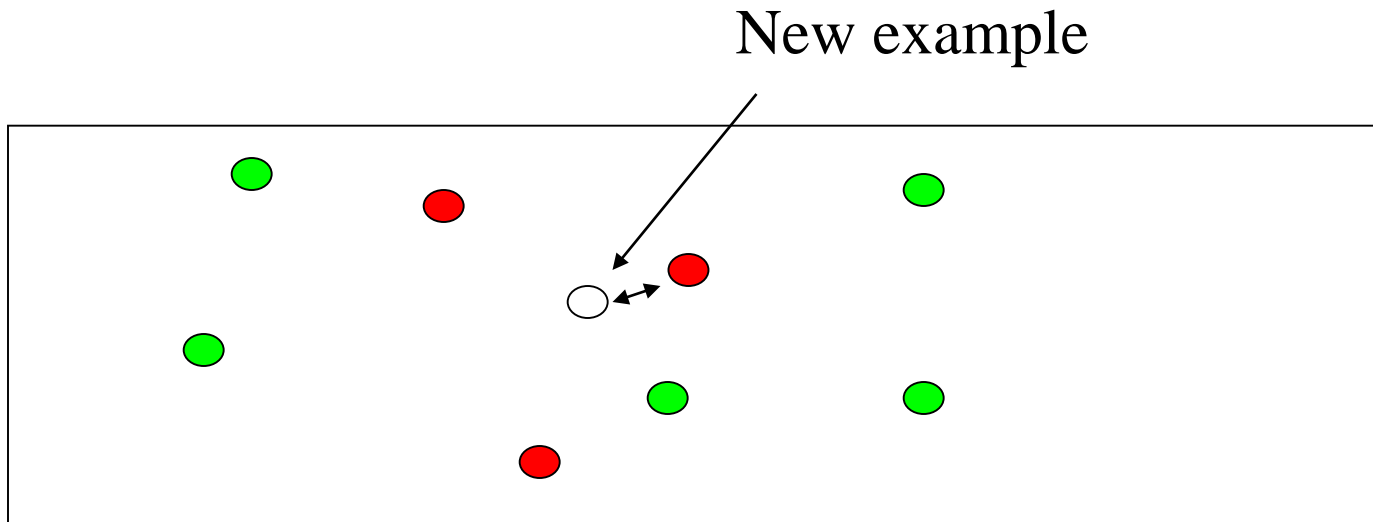
- When the model is not complex enough to capture the variability in the data
- E.g., fitting a line through a polynomial curve
- E.g., linear decision boundary for non-linearly separable data

The goal of model selection is to find a middle point to avoid both over-fitting and under-fitting.

We will now introduce some of the most commonly used Model selection techniques using a very simple yet practically useful classifier --- the nearest neighbor classifier --- as an example.

Nearest Neighbor Classifier

- Store all training examples $S = \{(x_i, y_i): i = 1, \dots, n\}$
- Given a new example x to be classified, search for the training example (x_i, y_i) whose x_i is **most similar** (or **closest in distance**) to x , and predict y_i



Similarity/Distance

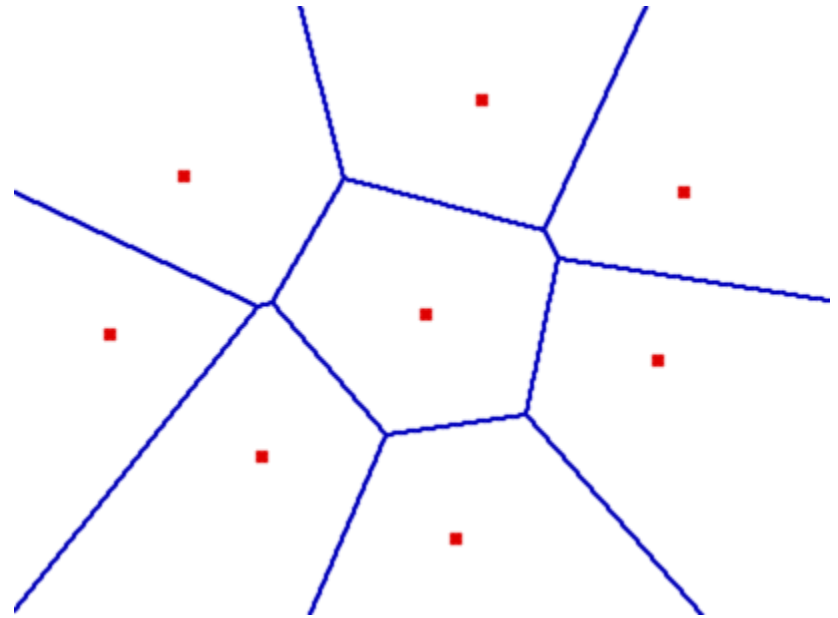
- How do we measure the similarity or distance between two examples?
- A commonly used measure is Euclidean distance (straight line distance)

$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix} \quad \mathbf{x}_i = \begin{bmatrix} x_{i1} \\ \vdots \\ x_{im} \end{bmatrix} \quad D(\mathbf{x}, \mathbf{x}_i) = \|\mathbf{x} - \mathbf{x}_i\|$$
$$= \sqrt{(\mathbf{x} - \mathbf{x}_i)^T (\mathbf{x} - \mathbf{x}_i)}$$

- Similarity can be defined as a non-increasing function of the distance
 - E.g., $S(\mathbf{x}, \mathbf{x}_i) = \exp(-\alpha D(\mathbf{x}, \mathbf{x}_i))$, where α is a parameter to control how close two things need to be for them to be considered similar

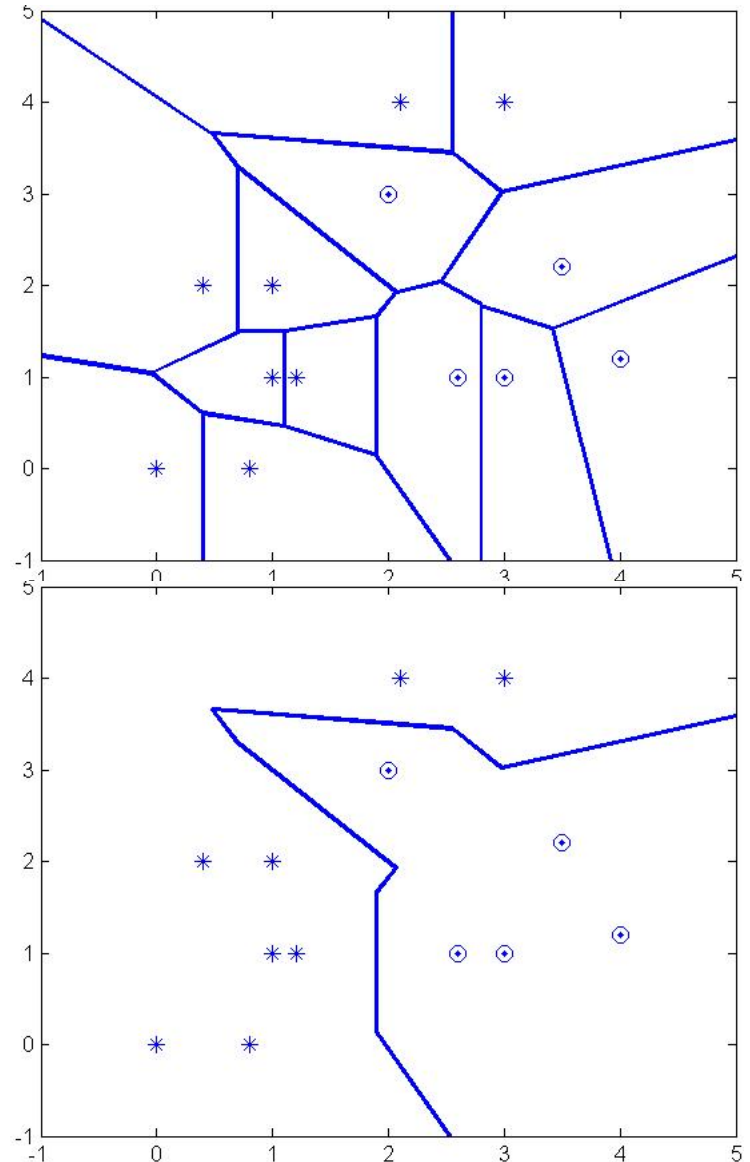
Decision Boundaries: The Voronoi Diagram

- Given a set of points, a Voronoi diagram describes the areas that are nearest to any given point.
- These areas can be viewed as zones of control
- Each zone is controlled by one of the points

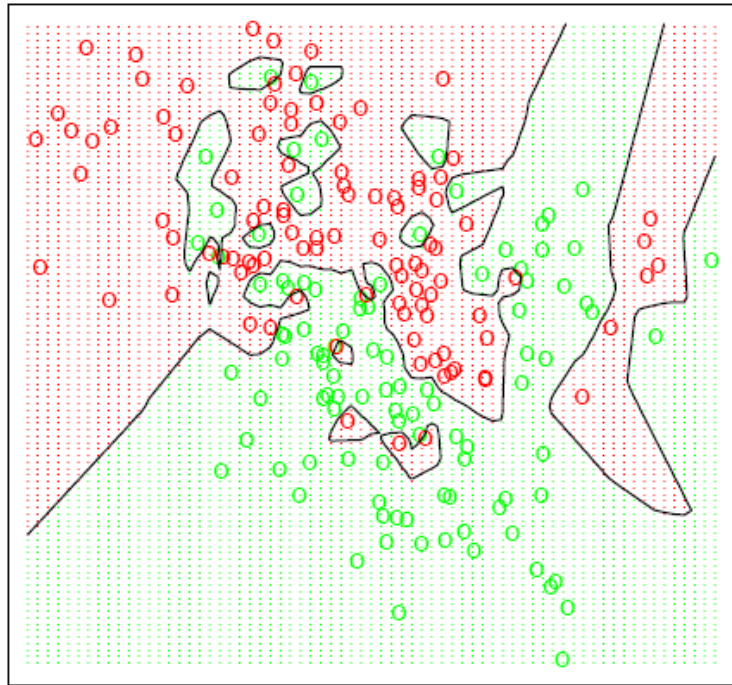


Decision Boundaries: Subset of the Voronoi Diagram

- Each example controls its own neighborhood
- Create the voronoi diagram
- Decision boundary are formed by only retaining these line segments separating different classes.
- The more training examples we have stored, the more complex the decision boundaries can become



Decision Boundaries



With large number of examples and noise in the labels, the decision boundary can become nasty!

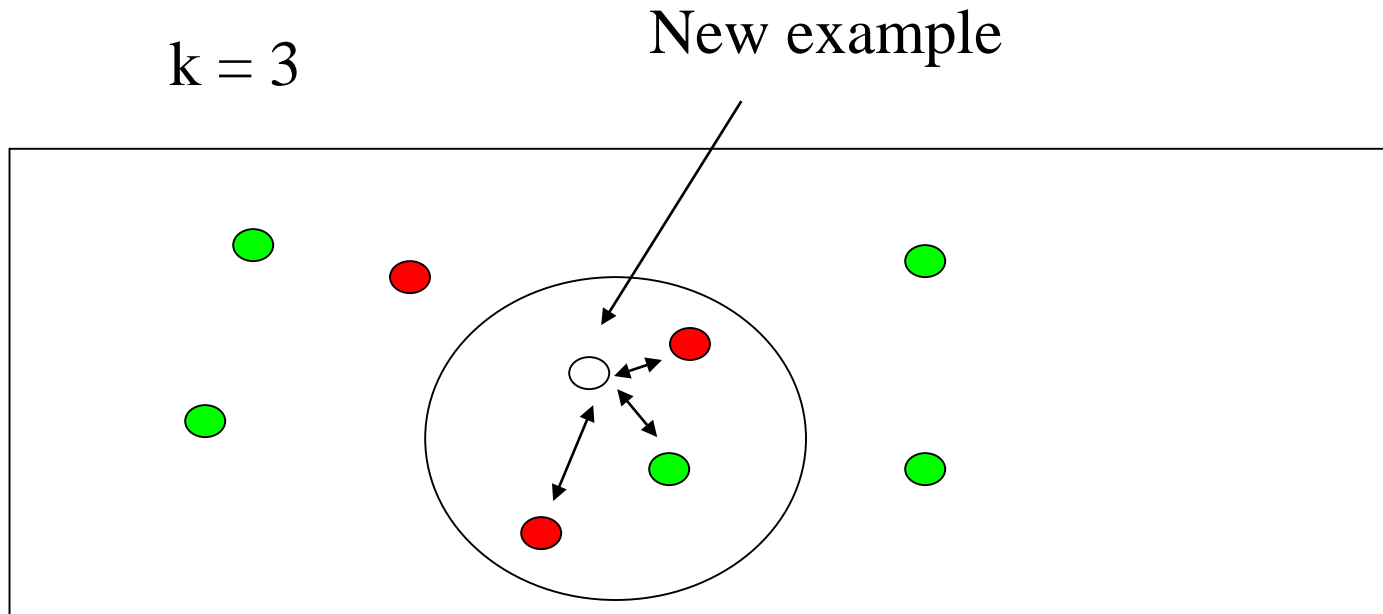
It can be bad some times – note the islands in this figure, they are formed because of noisy examples.

If the nearest neighbor happens to be a noisy point, the prediction will be incorrect!

How to deal with this issue?

k-Nearest Neighbor

Example:

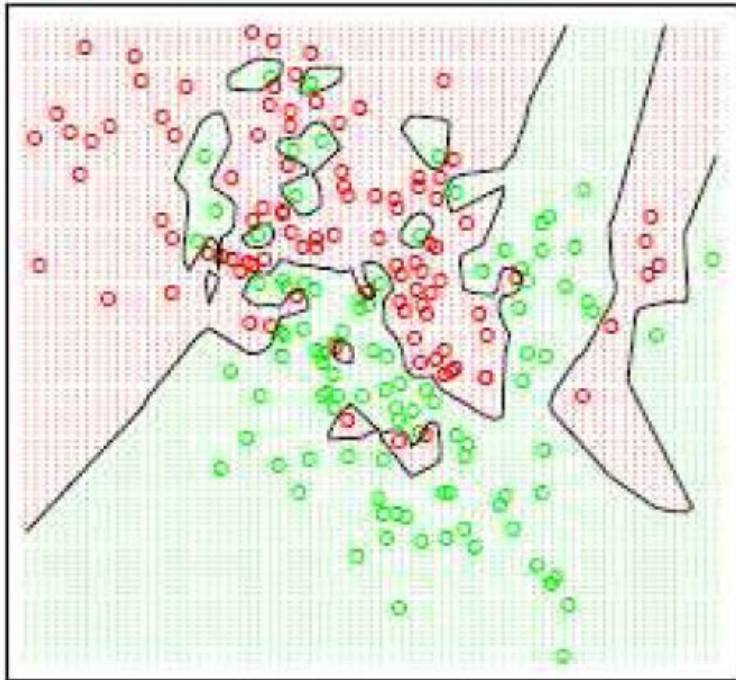


Find the ***k***-nearest neighbors and have them vote. By taking more than one neighbor, the impact of outliers can be reduced.

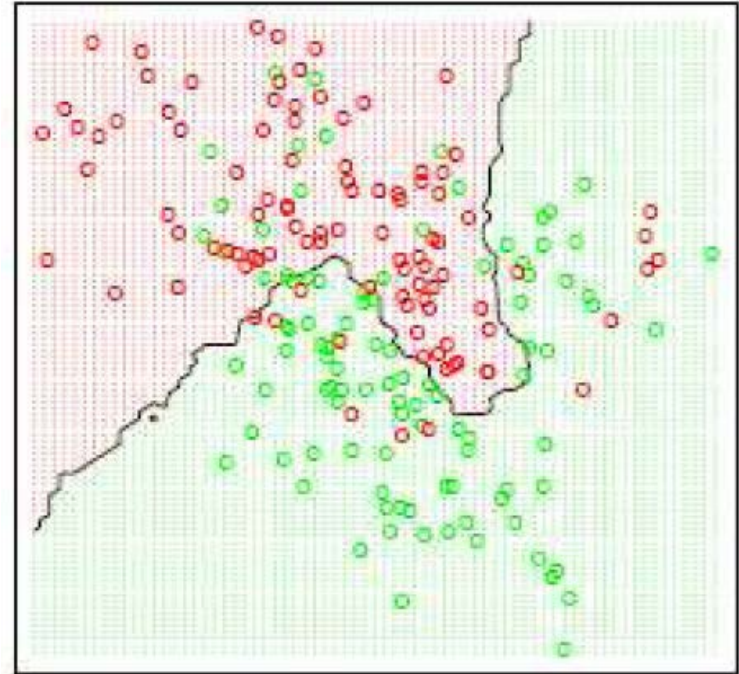
Practical note: It is typical to use an odd number for k to avoid ties

Impact of k for knn

k=1



k=15



Figures from Hastie, Tibshirani and Friedman (Elements of Statistical Learning)

Different k values give different results:

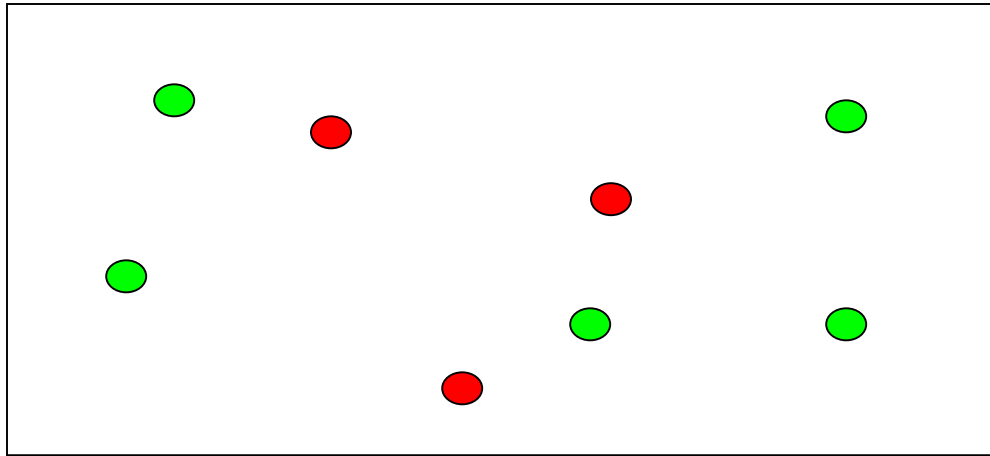
Larger k produces smoother boundaries, why?

- The impact of class label noises canceled out by one another

But when k is too large, what will happen?

k-Nearest Neighbor

What if we set $k=8$?



- We will always predict green because regardless of the location of the point, the k -nearest neighbors will contain more green points than red, simply because green is the majority
- Overly large k leads to **overly simplified** decision boundary

Question: how to choose k?

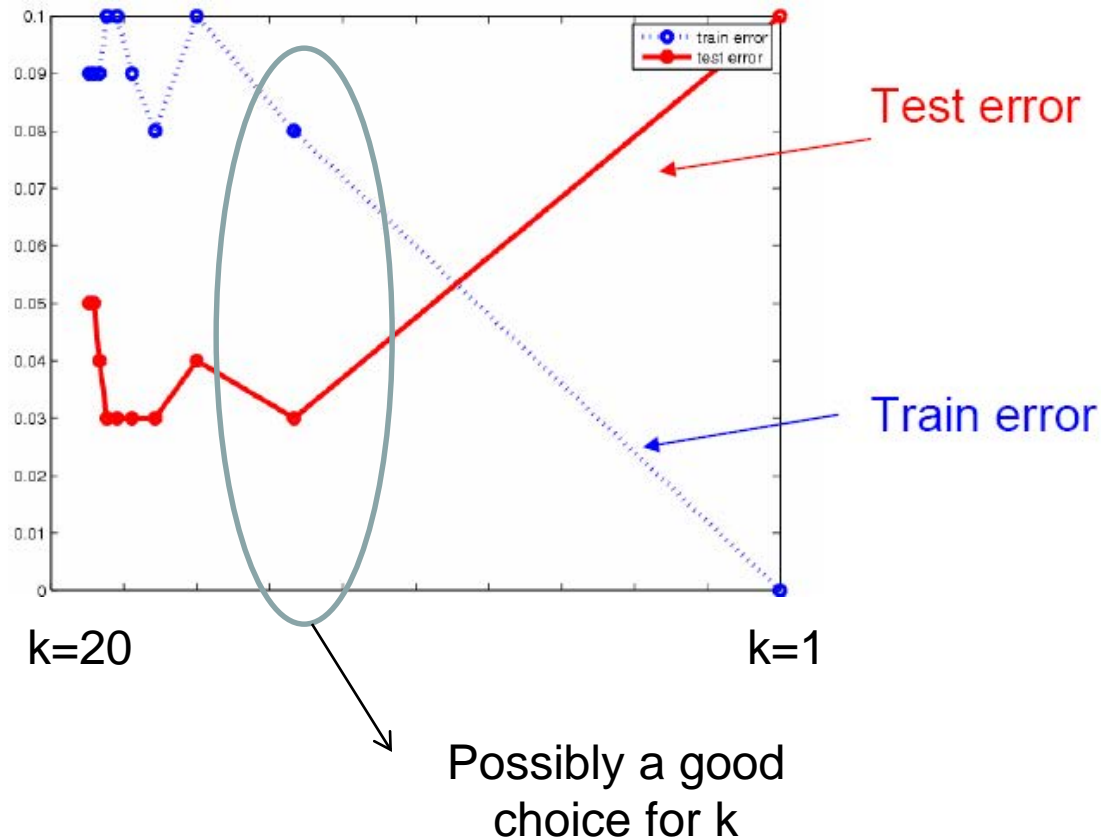
- Can we choose k to minimize the mistakes that we make on training examples (*training error*)?
- Let's first define training error
 - Given a training set \mathbf{S} , learn a classifier h
 - for every example (\mathbf{x}_i, y_i) in \mathbf{S}
 - If $h(\mathbf{x}_i) \neq y_i$ $\varepsilon_{tr} = \varepsilon_{tr} + 1$
- What is training error of 1-nearest neighbor?
 - $\varepsilon_{tr} = 0$
 - Because for any training example, its nearest neighbor in \mathbf{S} is always itself

We cannot use training error to select k because it will always select $k=1$

Continue: how to choose k?

- Can we choose k to minimize the mistakes that we make on a set of separate test examples (**test error**)?
- Let's first define test error
 - Given a training set **S** and a separate set **T**, learn a classifier h on **S** (without looking at **T**)
 - for every example (x_i, y_i) in **T**
 - If $h(x_i) \neq y_i$ $\epsilon_{te} = \epsilon_{te} + 1$
- How do ϵ_{tr} and ϵ_{te} change as we change the value of k?

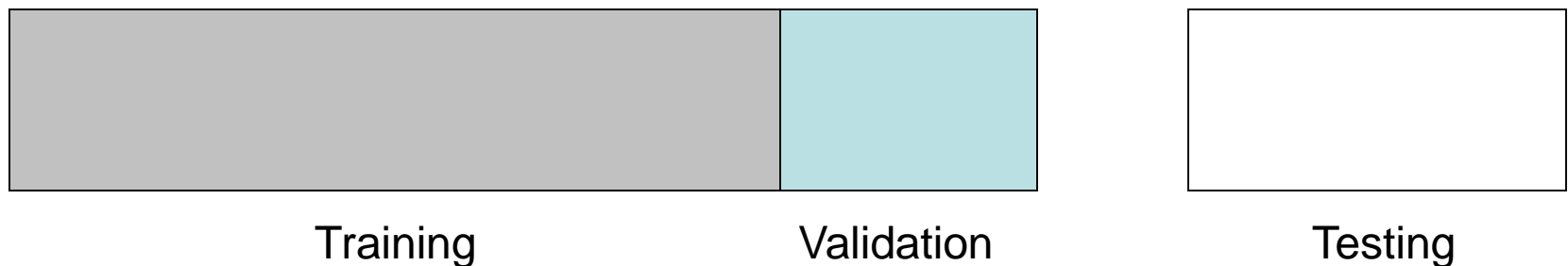
For the Previous Example



But choosing the model based on test data is not practical --- in practice we will have make the choice before seeing the test cases!

Model selection: *Validation* Set

- We can keep part of the labeled data aside as the validation data
- Evaluate different k values based on the prediction accuracy on the validation data
- Choose k that minimize validation error



Testing is typically reserved for final evaluation purpose, whereas ***Validation*** is used for model selection purpose.

The impact of validation set size

- If we only reserve one point in our validation set, should we trust the validation error as a reliable estimate of our classifier's performance?
- No. The larger the validation set, the more reliable our model selection choices are
- When the total labeled set is small, we might not be able to get a big enough validation set – leading to unreliable model selection decisions

Model selection: K -fold Cross Validation

- Note the use of capital K – not the k in knn
- Randomly split the training set into K equal-sized subsets
 - The subsets should have similar class distribution
- Perform learning/testing K times
 - Each time reserve one subset for validation, train on the rest

Example: A 5-fold cross validation

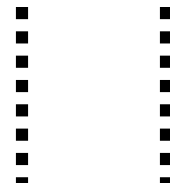
S1	S2	S3	S4	S5
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Train on S2, S3, S4, S5, test on S1 $\rightarrow \epsilon_1$

S1	S2	S3	S4	S5
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Train on S1, S3, S4, S5, test on S2 $\rightarrow \epsilon_2$

S1	S2	S3	S4	S5
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S1	S2	S3	S4	S5
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S1	S2	S3	S4	S5
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Train on S1, S2, S3, S4, test on S5 $\rightarrow \epsilon_5$

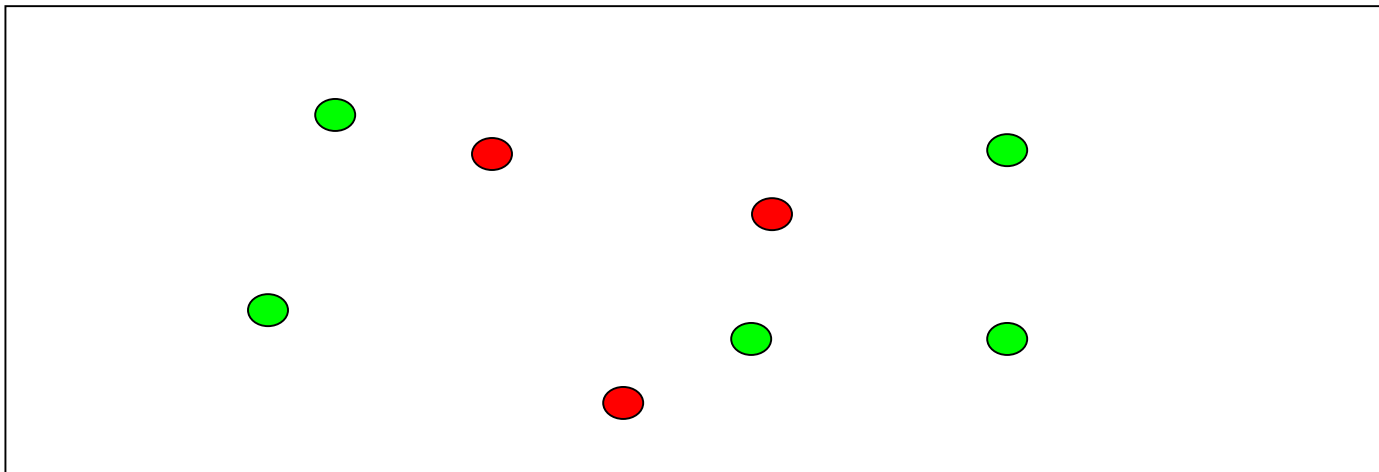
$$\epsilon = \frac{1}{5} \sum_{i=1}^5 \epsilon_i$$

Model Selection: K -fold Cross Validation

- For each candidate model, e.g. for k -nn we consider each possible value of k (1,3,5...)
 - Perform K -fold cross-validation on the training set (e.g., $K = 10$)
 - Measure its cross-validation error
- Select the model with lowest Cross-Validation error

Leave-one-out Cross Validation

- If we set K , the number of folds to $|\mathbf{S}|$, we end up with what we call leave-one-out cross validation
- Each time we leave one example out for validation



What is the leave-one-out error of 1-nearest neighbor on this data set?

Practical issues with KNN

- Suppose we want to build a model to predict a person's shoe size
- Use the person's height and weight to make the prediction
- P1: (6', 175), P2: (5.7', 168), PQ:(6.1', 170)

$$D(\mathbf{PQ}, \mathbf{P1}) = \sqrt{0.1^2 + 5^2} \approx 5 \quad D(\mathbf{PQ}, \mathbf{P2}) = \sqrt{0.4^2 + 2^2} \approx 2.04$$

- There is a problem with this

Because weight has a much larger range of values, the differences is dominated numerically by weight

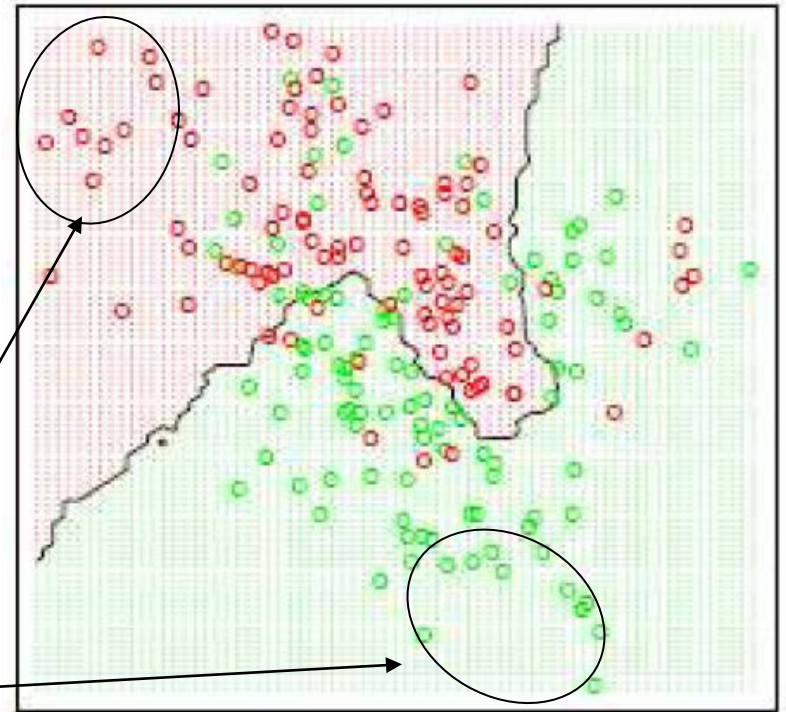
Features should be normalized to have the same range of values (e.g., [0,1]), otherwise features with larger ranges will have higher impact on the distance.

Practical issues with KNN

- Our data may also contain the GPAs
- Should we include this attribute into the calculation?
- When collecting data, people tend to collect as much information as possible regardless whether they are useful or not for the question in hand
- It is critical to recognize and remove such attributes when building your classification models
- Curse of dimensionality:
 - In high dimensional space (e.g., over 20), data becomes so sparse that the nearest neighbor is still very far, not informative any more
 - Often need to be used with dimension reduction

Other issues

- It can be computationally expensive to find the nearest neighbors for large data
 - $O(Nd)$ for every test point (as opposed to $O(d)$ for linear classifier)
 - Speed up the computation by using smart data structures (kd-tree) to quickly search for approximate solutions
- For massive data sets, it also requires a lot of memory
 - Remove unimportant examples



Final words on KNN

- KNN is what we call *lazy learning* (vs. *eager learning*)
 - Lazy: learning only occur when you see the test example
 - Eager: learn a model before you see the test example, training examples can be thrown away after learning
- Advantage:
 - Conceptually simple, easy to understand and explain
 - Very flexible decision boundaries
- Disadvantage
 - It can be hard to find a good distance measure
 - Irrelevant features and noise can be very detrimental
 - Typically can not handle more than a few dozen attributes unless a good distance measure can be learned
 - Computational cost: requires significant computation and memory

Final words on model selection

- Model selection is typically done by holding out some portion of the labeled data to be used for selecting the best model
- If there is large amounts of labeled data, using a single hold-out set for validation might be sufficient
 - E.g., NLP community often use fixed train/validation/testing split for replicability of the results.
- Cross-validation allows every training example to be considered while making the model selection choices
 - The larger the K , the more computationally intensive but more robust model selection decision