

# DATA SCIENCE

## LECTURE 4: K-NEAREST NEIGHBORS CLASSIFICATION

YUCHEN ZHAO / DAT-14

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## RECAP

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### LAST TIME:

I. DATA RETRIEVAL

II. ETL INTRO

III. VISUALIZATION

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## RECAP

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### LAST TIME:

I. DATA RETRIEVAL (API, JSON)

II. ETL INTRO (DATABASE, SQL)

III. VISUALIZATION (D3.JS)

### EXERCISES:

IV. PANDAS

V. MINING TWITTER VIA API

QUESTIONS?

**I. CLASSIFICATION PROBLEMS**

**II. BUILDING EFFECTIVE CLASSIFIERS**

**III. KNN CLASSIFICATION**

**EXERCISES:**

**IV. EXPLORING & IMPLEMENTING K-NN CLASSIFICATION**

# **I. CLASSIFICATION PROBLEMS**

	<i>continuous</i>	<i>categorical</i>
<i>supervised</i>	???	???
<i>unsupervised</i>	???	???

	<i>continuous</i>	<i>categorical</i>
<i>supervised</i>	<i>regression</i>	<i>classification</i>
<i>unsupervised</i>	<i>dimension reduction</i>	<i>clustering</i>

*Here's (part of) an example dataset:*

Fisher's *Iris* Data

Sepal length ⇅	Sepal width ⇅	Petal length ⇅	Petal width ⇅	Species ⇅
5.1	3.5	1.4	0.2	<i>I. setosa</i>
4.9	3.0	1.4	0.2	<i>I. setosa</i>
4.7	3.2	1.3	0.2	<i>I. setosa</i>
4.6	3.1	1.5	0.2	<i>I. setosa</i>
5.0	3.6	1.4	0.2	<i>I. setosa</i>
5.4	3.9	1.7	0.4	<i>I. setosa</i>
4.6	3.4	1.4	0.3	<i>I. setosa</i>
5.0	3.4	1.5	0.2	<i>I. setosa</i>

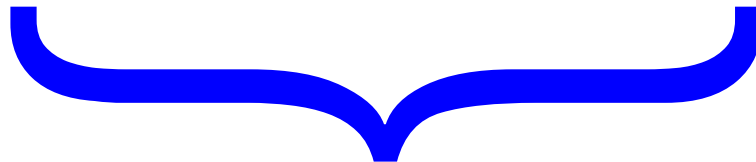


*Here's (part of) an example dataset:*

*independent  
variables*

Fisher's Iris Data

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*independent  
variables*

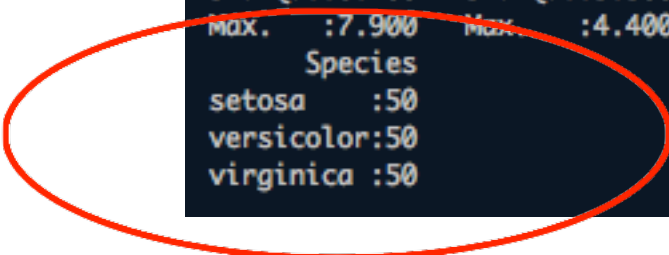
*class  
labels  
(qualitative)*

*Q: What does “supervised” mean?*

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*A: We know the labels.*

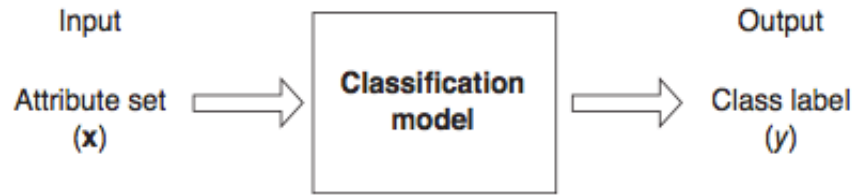
```
Welcome to R! Thu Feb 28 13:07:25 2013
> summary(iris)
  Sepal.Length  Sepal.Width  Petal.Length  Petal.Width
Min.   :4.300   Min.   :2.000   Min.   :1.000   Min.   :0.100
1st Qu.:5.100   1st Qu.:2.800   1st Qu.:1.600   1st Qu.:0.300
Median :5.800   Median :3.000   Median :4.350   Median :1.300
Mean   :5.843   Mean   :3.057   Mean   :3.758   Mean   :1.199
3rd Qu.:6.400   3rd Qu.:3.300   3rd Qu.:5.100   3rd Qu.:1.800
Max.   :7.900   Max.   :4.400   Max.   :6.900   Max.   :2.500
   Species
setosa   :50
versicolor:50
virginica :50
```



*Q: How does a classification problem work?*

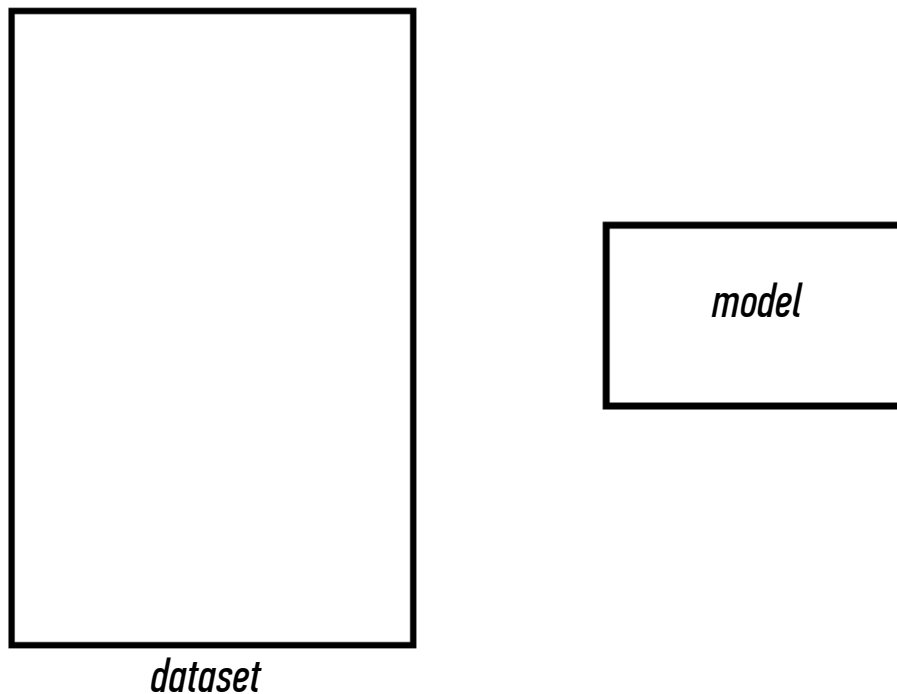
*Q: How does a classification problem work?*

*A: Data in, predicted labels out.*



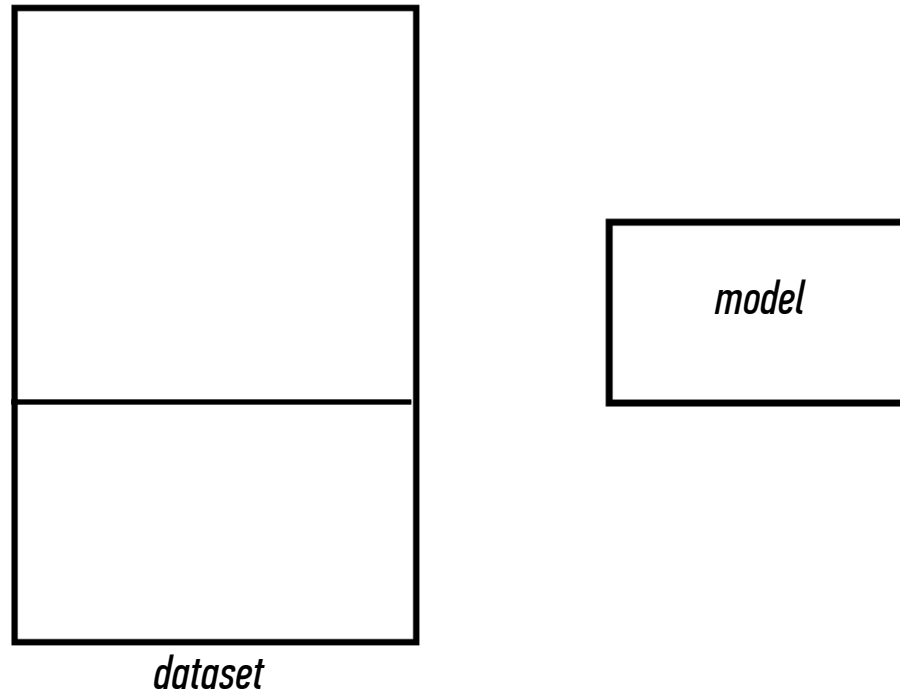
**Figure 4.2.** Classification as the task of mapping an input attribute set  $x$  into its class label  $y$ .

*Q: What steps does a classification problem require?*



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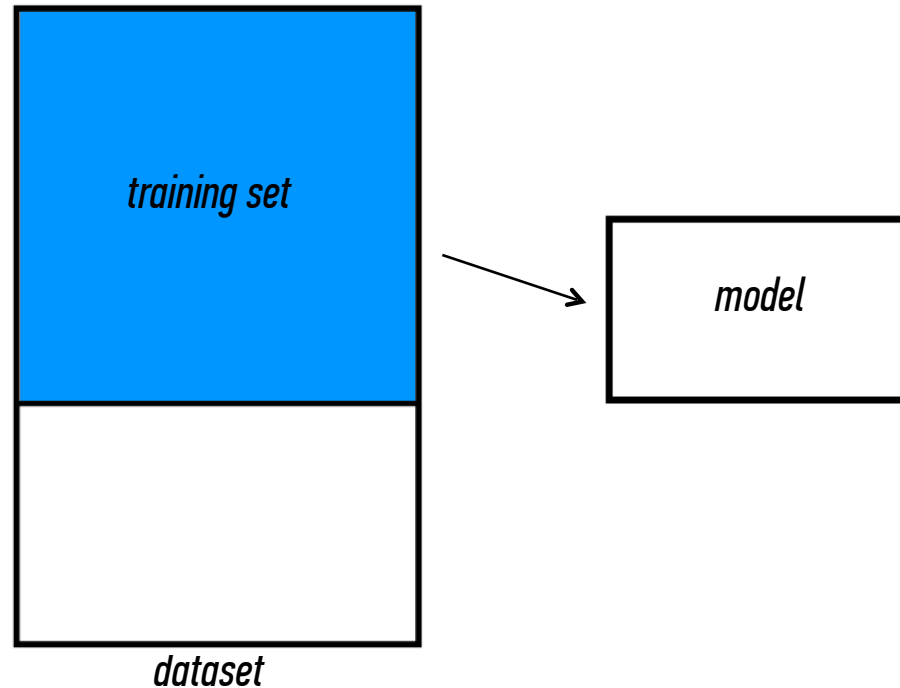
*1) split dataset*





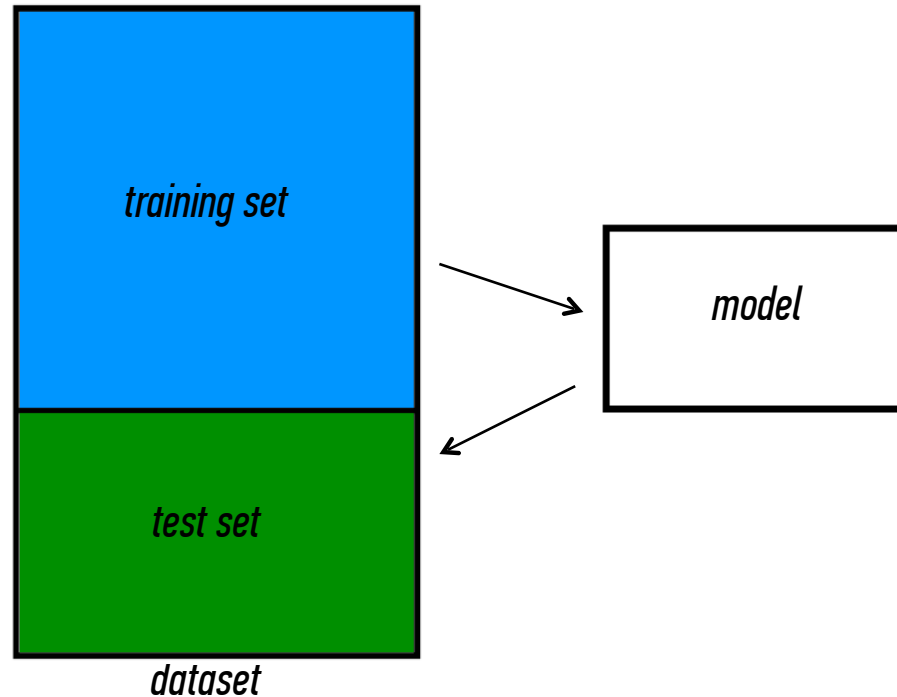
*Q: What steps does a classification problem require?*

- 1) split dataset*
- 2) train model*



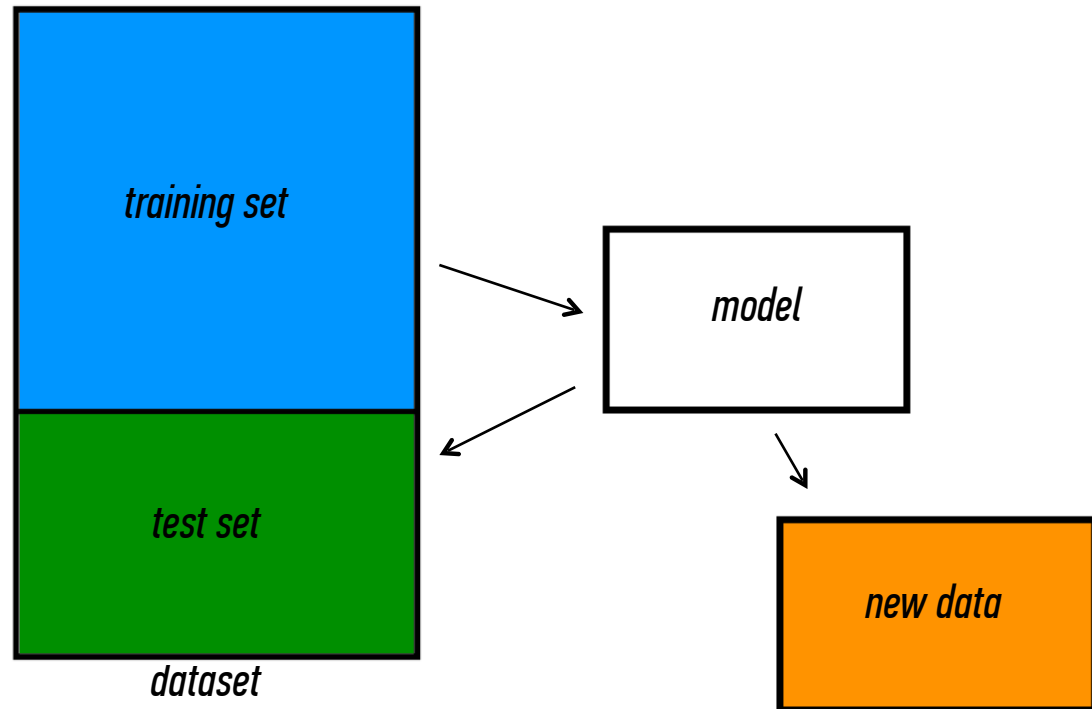
*Q: What steps does a classification problem require?*

- 1) split dataset*
- 2) train model*
- 3) test model*



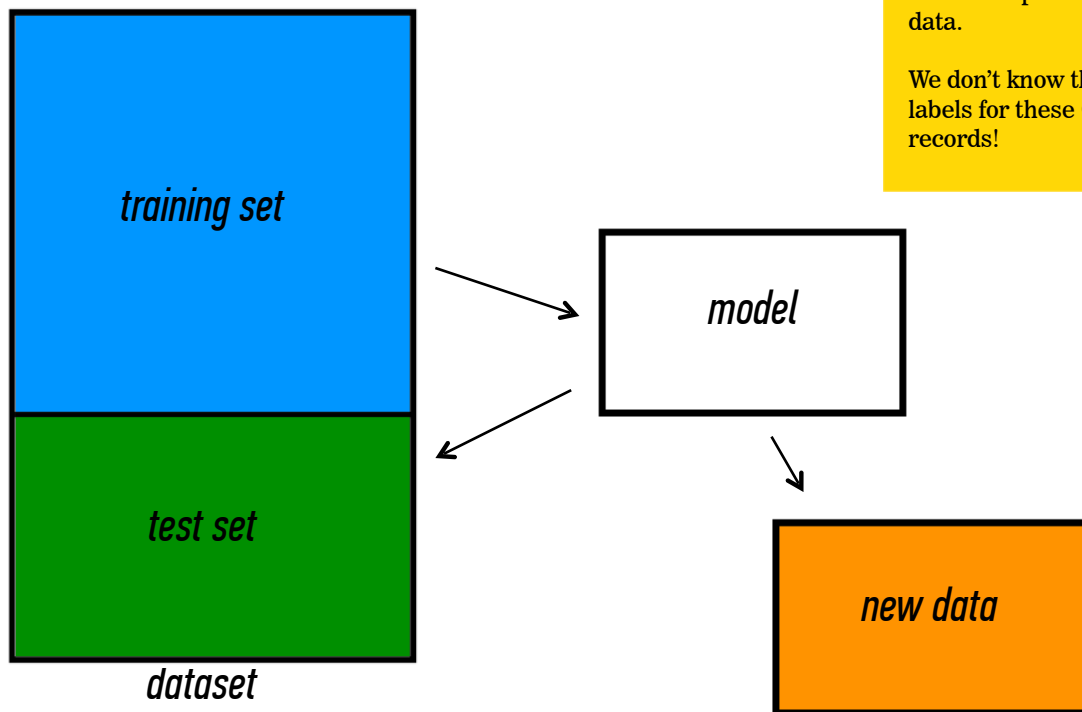
*Q: What steps does a classification problem require?*

- 1) split dataset*
- 2) train model*
- 3) test model*
- 4) make predictions*



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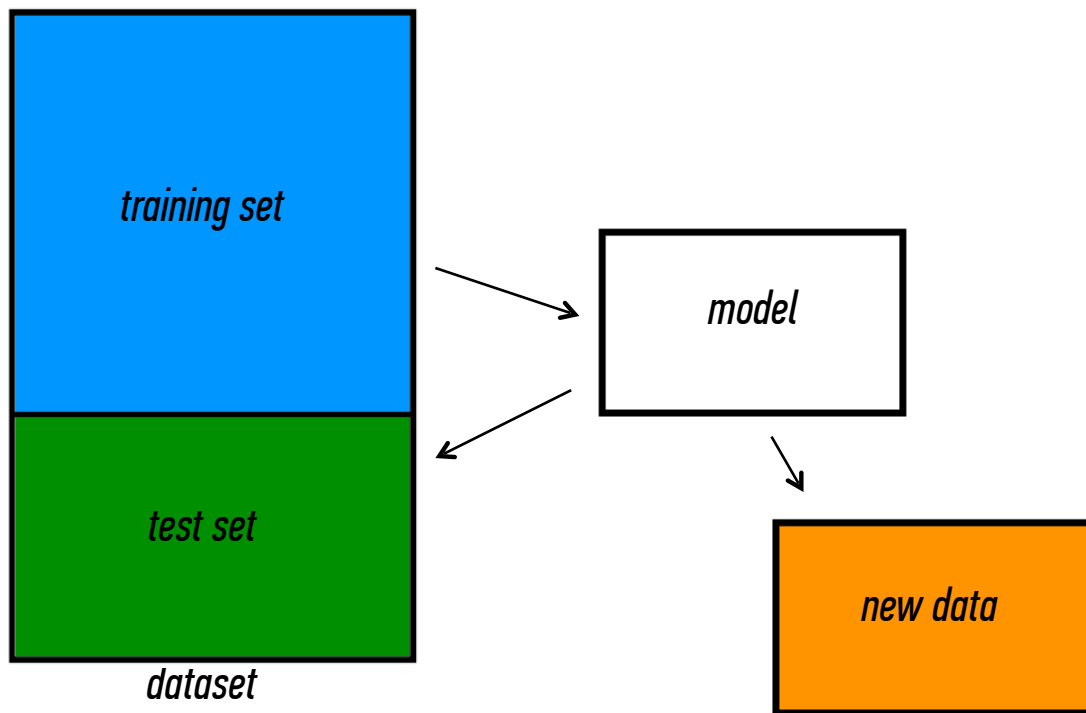
**NOTE**

This new data is called out of sample data.

We don't know the labels for these OOS records!

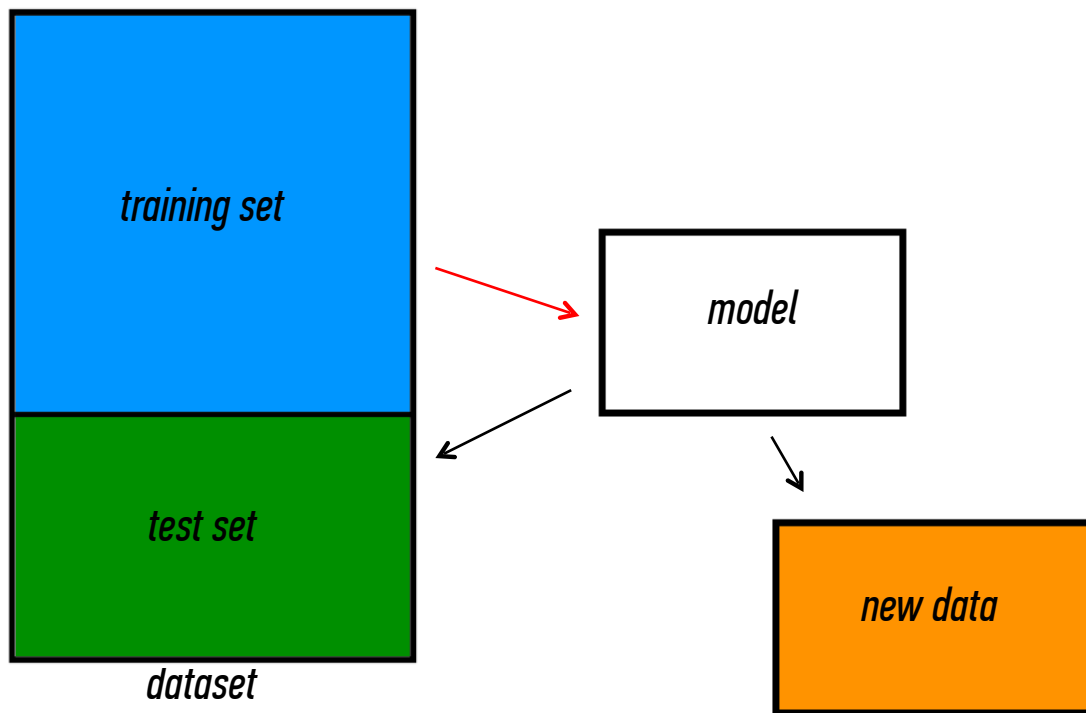
# **II. BUILDING EFFECTIVE CLASSIFIERS**

*Q: What types of prediction error will we run into?*



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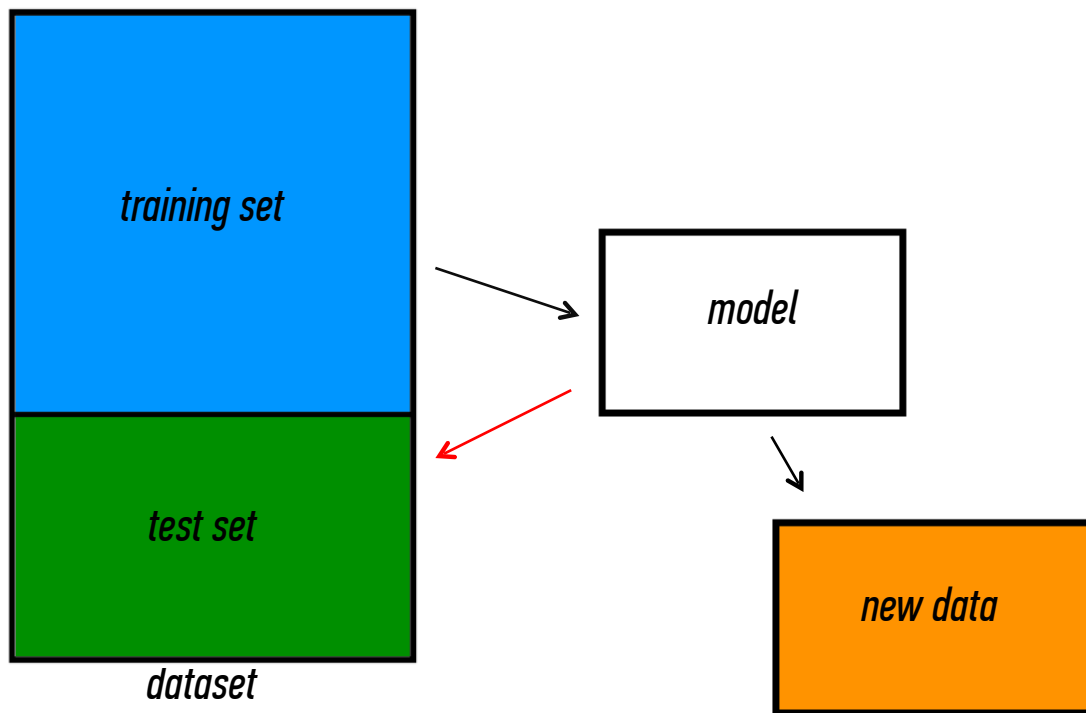
*1) training error*



*Q: What types of prediction error will we run into?*

- 1) *training error*
- 2) *generalization error*

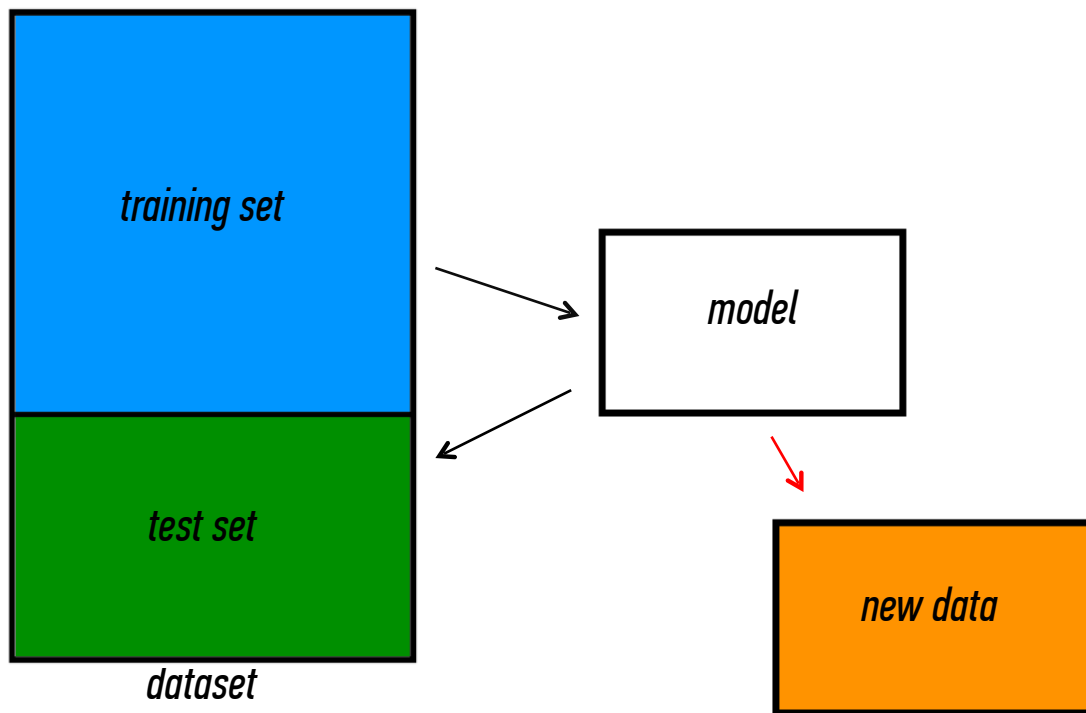
**NOTE**  
measures how  
well a learning  
machine  
generalizes to  
unseen(test) data





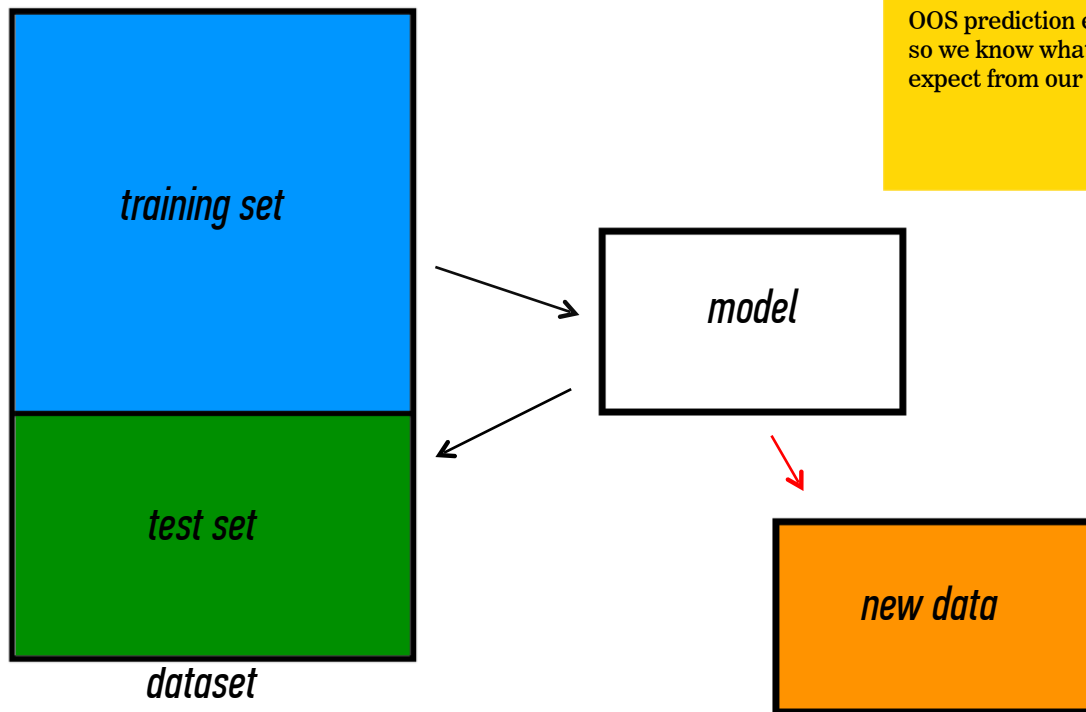
*Q: What types of prediction error will we run into?*

- 1) training error*
- 2) generalization error*
- 3) OOS error*



*Q: What types of prediction error will we run into?*

- 1) *training error*
- 2) *generalization error*
- 3) *OOS error*



### NOTE

We want to estimate OOS prediction error so we know what to expect from our model.

*Q: Why should we use training & test sets?*

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*Thought experiment:*

*Suppose instead, we train our model using the entire dataset.*

*Q: Why should we use training & test sets?*

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*Q: How low can we push the training error?*

- We can make the model arbitrarily complex (effectively “memorizing” the entire training set).*

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*A: Down to zero!*

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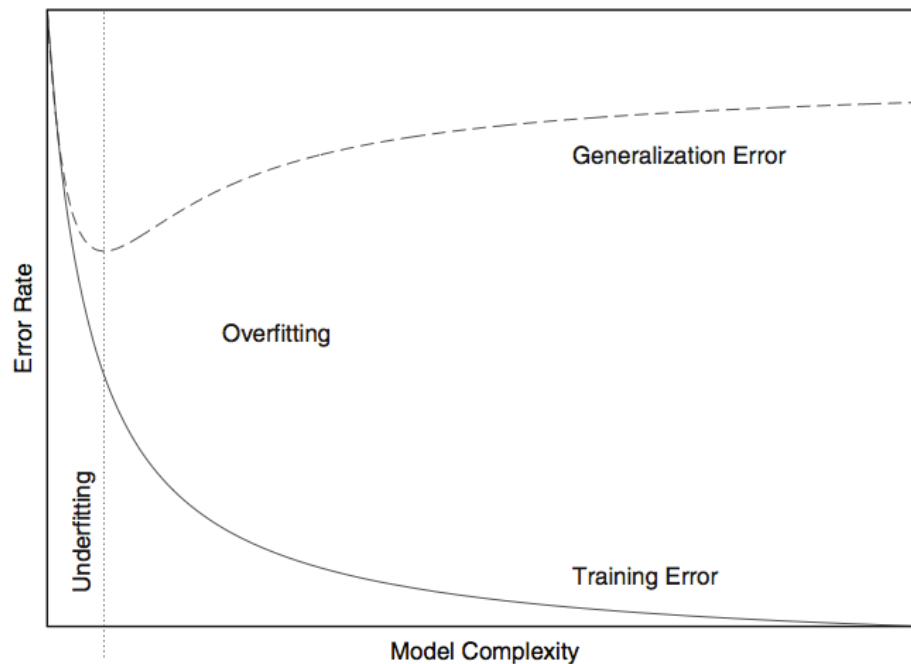
- We can make the model arbitrarily complex (effectively “memorizing” the entire training set).*

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### NOTE

This phenomenon is called overfitting.

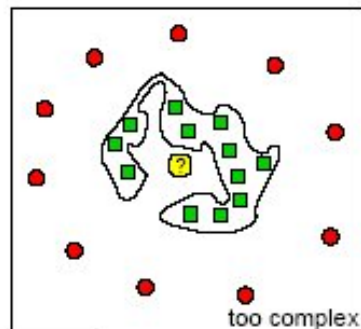
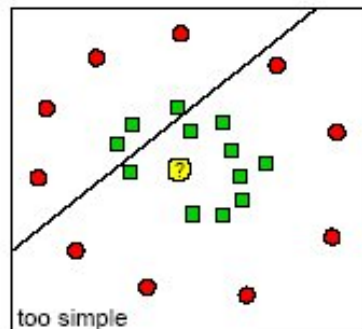




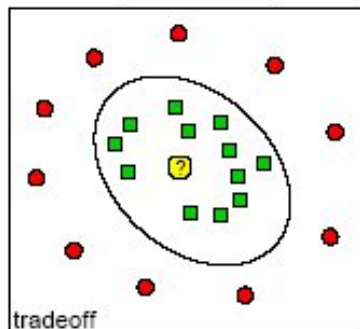
*FIGURE 18-1. Overfitting: as a model becomes more complex, it becomes increasingly able to represent the training data. However, such a model is overfitted and will not generalize well to data that was not used during training.*

## OVERFITTING - EXAMPLE

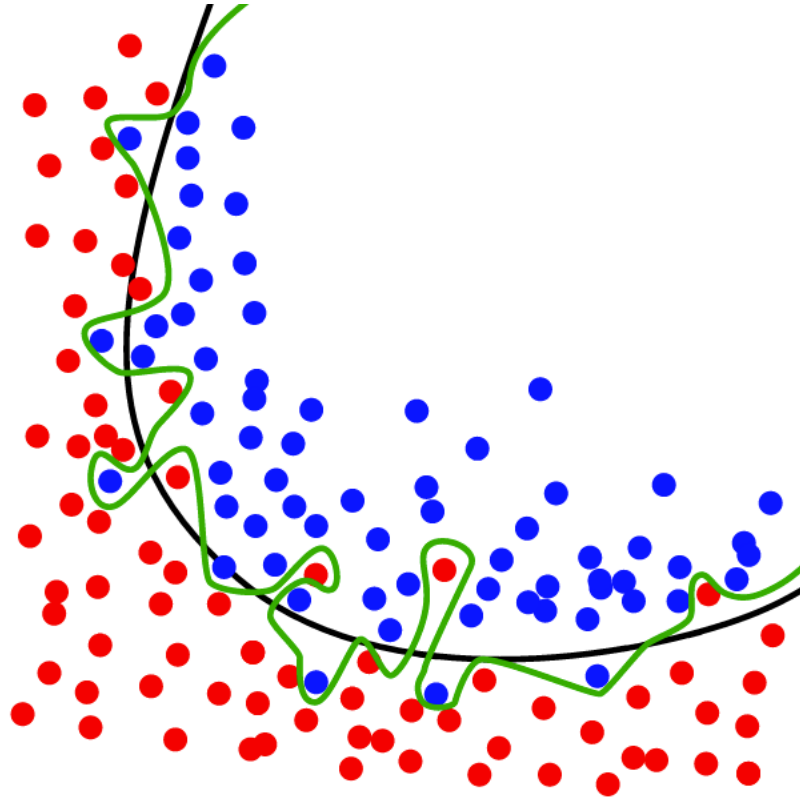
### Underfitting and Overfitting



- negative example
- positive example
- new patient



## OVERFITTING - EXAMPLE



*Q: Why should we use training & test sets?*

*Thought experiment:*

*Suppose instead, we train our model using the entire dataset.*

*Q: How low can we push the training error?*

- We can make the model arbitrarily complex (effectively “memorizing” the entire training set).*

*A: Down to zero!*

*A: Training error is not a good estimate of OOS accuracy.*

**NOTE**

This phenomenon is called overfitting.

---

**GENERALIZATION ERROR**

---

*Suppose we do the train/test split.*

## GENERALIZATION ERROR

---

*Suppose we do the train/test split.*

*Q: How well does generalization error predict OOS accuracy?*

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*Q: Would the generalization error remain the same?*



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*Q: Would the generalization error remain the same?*

*A: Of course not!*

*Suppose we do the train/test split.*

*Q: How well does generalization error predict OOS accuracy?*

*Thought experiment:*

*Suppose we had done a different train/test split.*

*Q: Would the generalization error remain the same?*

*A: Of course not!*

*A: On its own, not very well.*

*Suppose we do the train/test split.*

*Q: How well does generalization error predict OOS accuracy?*

*Thought experiment:*

*Suppose we had done a different train/test split.*

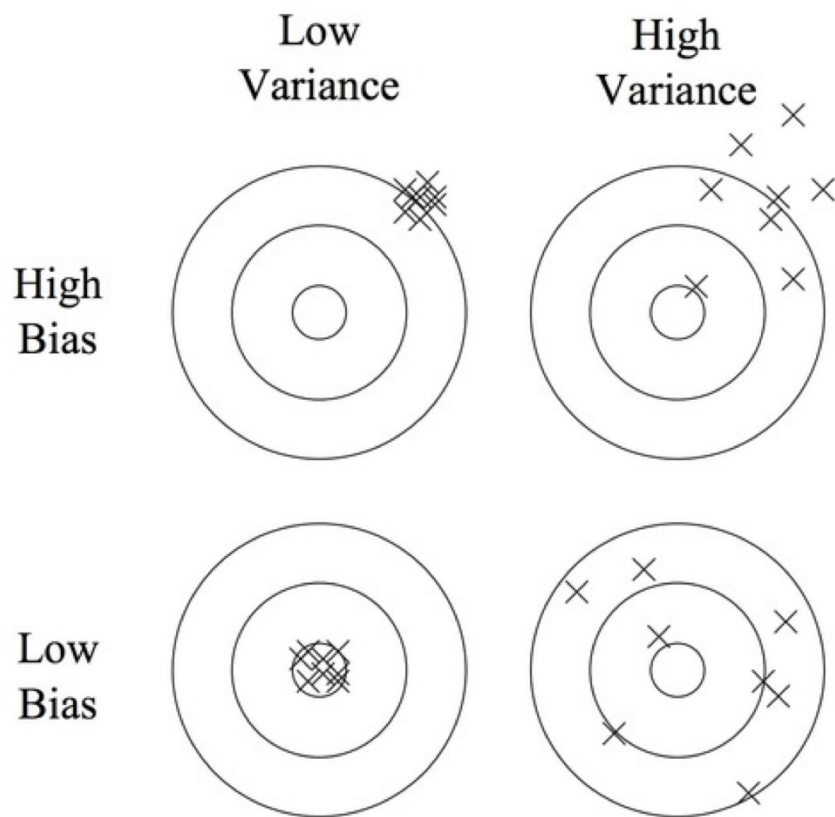
*Q: Would the generalization error remain the same?*

*A: Of course not!*

*A: On its own, not very well.*

**NOTE**

The generalization error gives a high-variance estimate of OOS accuracy.



---

**GENERALIZATION ERROR**

---

*Something is still missing!*

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*Q: How can we do better?*

## GENERALIZATION ERROR

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*Something is still missing!*

*Q: How can we do better?*

*Thought experiment:*

*Different train/test splits will give us different generalization errors.*

*Something is still missing!*

*Q: How can we do better?*

*Thought experiment:*

*Different train/test splits will give us different generalization errors.*

*Q: What if we did a bunch of these and took the average?*



*Something is still missing!*

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*Different train/test splits will give us different generalization errors.*

*Q: What if we did a bunch of these and took the average?*

*A: Now you're talking!*

*Something is still missing!*

*Q: How can we do better?*

*Thought experiment:*

*Different train/test splits will give us different generalization errors.*

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*A: Now you're talking!*

*A: Cross-validation.*

# **CROSS-VALIDATION**

*Steps for  $n$ -fold cross-validation:*

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- 1) Randomly split the dataset into  $n$  equal partitions.*

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- 3) Find generalization error.*

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- 4) Repeat steps 2-3 using a different partition as the test set at each iteration.*



### *Steps for $n$ -fold cross-validation:*

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- 2) Use partition 1 as test set & union of other partitions as training set.*
- 3) Find generalization error.*
- 4) Repeat steps 2-3 using a different partition as the test set at each iteration.*
- 5) Take the average generalization error as the estimate of OOS accuracy.*

## CROSS-VALIDATION: 5-FOLD EXAMPLE

Dataset	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	<u>Accuracy</u>
1	Test	Train	Train	Train	Train	$k_1 \%$
2	Train	Test	Train	Train	Train	$k_2 \%$
3	Train	Train	Test	Train	Train	$k_3 \%$
4	Train	Train	Train	Test	Train	$k_4 \%$
5	Train	Train	Train	Train	Test	$k_5 \%$

*overall accuracy:*  $(k_1 + k_2 + k_3 + k_4 + k_5) / 5$

*Features of  $n$ -fold cross-validation:*

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- 1) More accurate estimate of OOS prediction error.*

### *Features of $n$ -fold cross-validation:*

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  - Each record in our dataset is used for both training and testing.*

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  - Each record in our dataset is used for both training and testing.*
- 3) Presents tradeoff between efficiency and computational expense.*
  - 10-fold CV is 10x more expensive than a single train/test split*

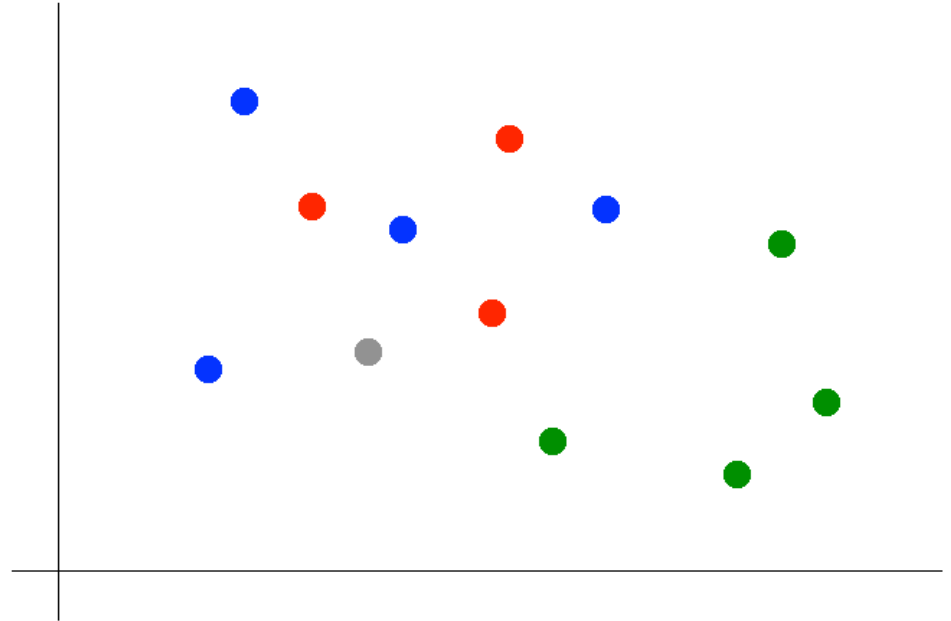
### *Features of n-fold cross-validation:*

- 1) *More accurate estimate of OOS prediction error.*
- 2) *More efficient use of data than single train/test split.*
  - *Each record in our dataset is used for both training and testing.*
- 3) *Presents tradeoff between efficiency and computational expense.*
  - *10-fold CV is 10x more expensive than a single train/test split*
- 4) *Can be used for model selection.*

# **III. KNN CLASSIFICATION**

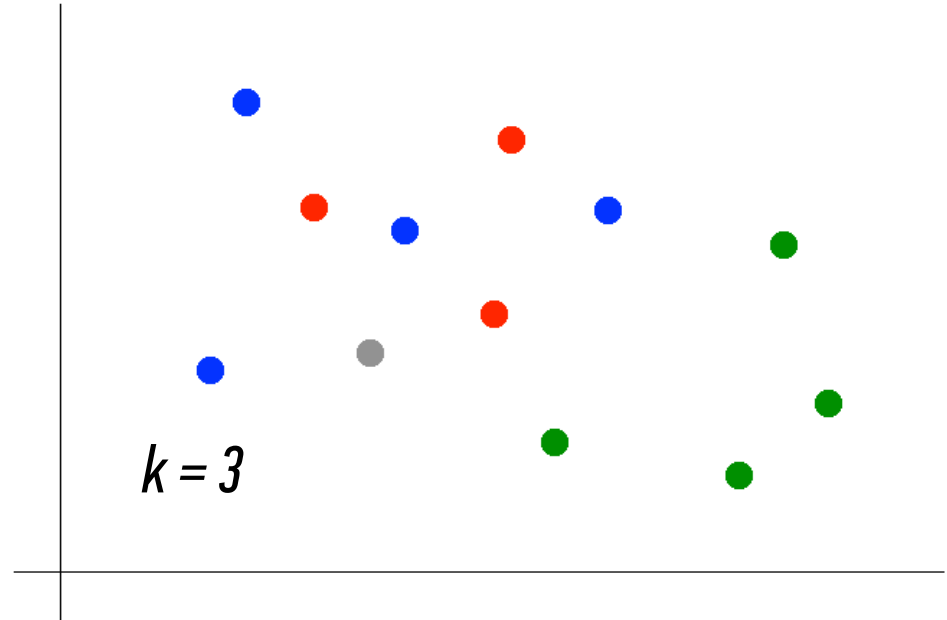


*Suppose we want to predict the color of the grey dot.*



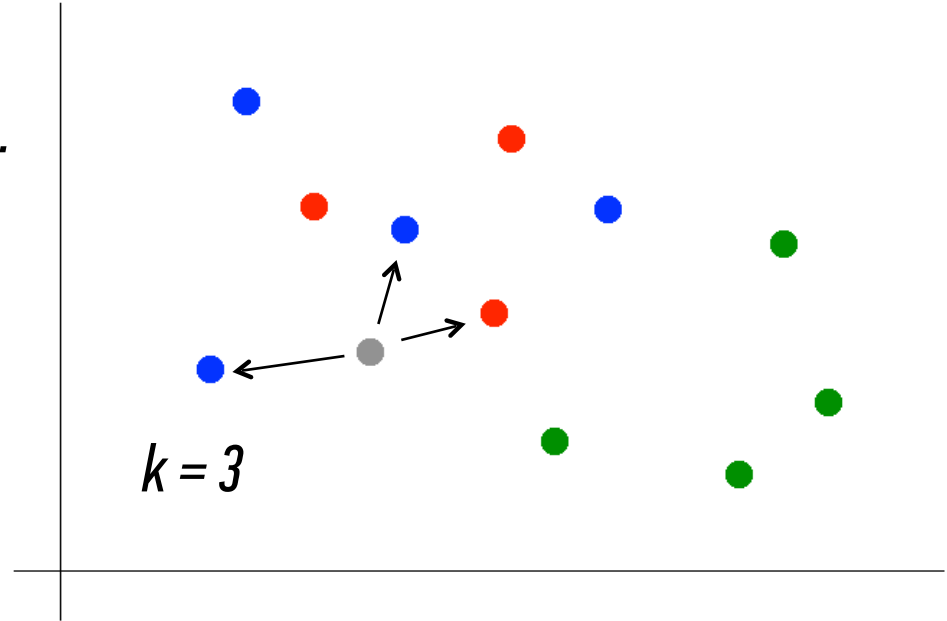
*Suppose we want to predict the color of the grey dot.*

*1) Pick a value for  $k$ .*



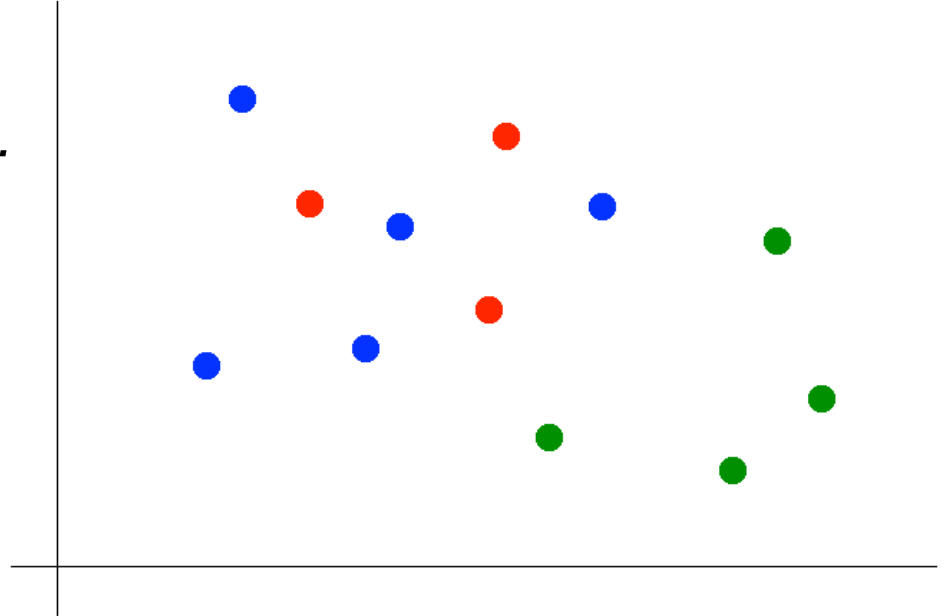
*Suppose we want to predict the color of the grey dot.*

- 1) Pick a value for  $k$ .*
- 2) Find colors of  $k$  nearest neighbors.*



*Suppose we want to predict the color of the grey dot.*

- 1) Pick a value for  $k$ .*
- 2) Find colors of  $k$  nearest neighbors.*
- 3) Assign the most common color to the grey dot.*

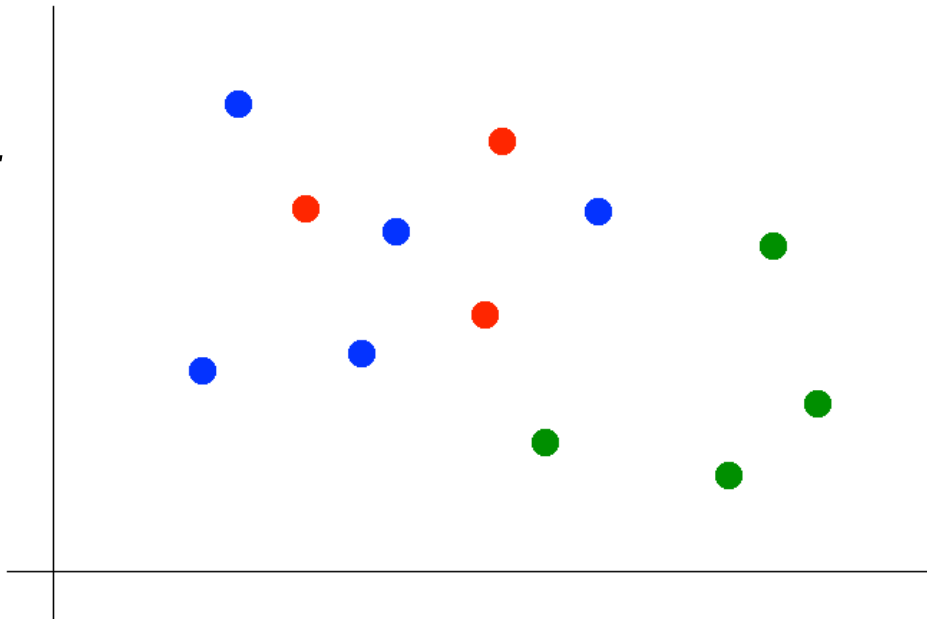


*Suppose we want to predict the color of the grey dot.*

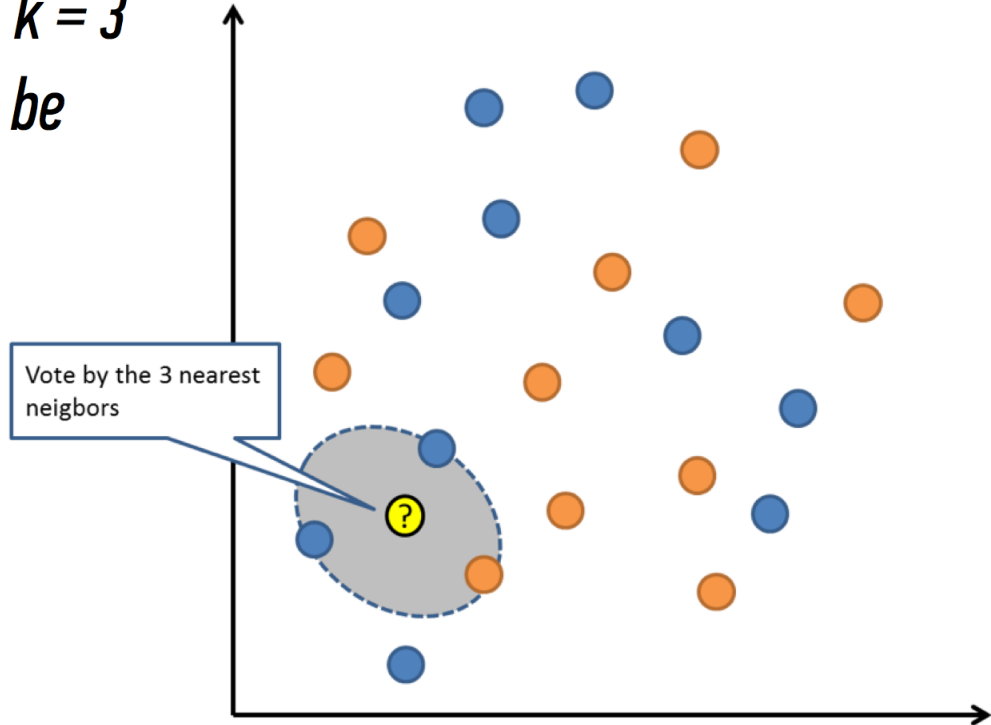
- 1) Pick a value for  $k$ .*
- 2) Find colors of  $k$  nearest neighbors.*
- 3) Assign the most common color to the grey dot.*

**OPTIONAL NOTE**

Our definition of “nearest” implicitly uses the Euclidean distance function.



*Another example with  $k = 3$   
Will our new example be  
blue or orange?*



## KNN CLASSIFICATION - HOW TO CHOOSE K?

---

*In theory, if **infinite** number of samples available, the larger is  $k$ , the better is classification*

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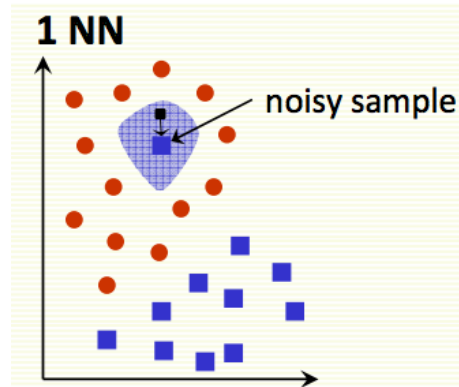
*The caveat is that all  $k$  neighbors have to be close*

- Possible when infinite # samples available*
- Impossible in practice since # samples is finite*



*Rule of thumb is  $k < \sqrt{n}$ ,  $n$  is number of examples*

- interesting theoretical properties*
- In practice,  $k = 1$  is often used for efficiency, but can be sensitive to “noise”*



## KNN CLASSIFICATION - HOW TO CHOOSE K?

---

*larger  $k$  may improve performance, but too large  $k$  destroys locality,  
i.e. end up looking at samples that are not neighbors*

*cross-validation may be used to choose  $k$*



### *Advantages*

- *Can be applied to the data from any distribution*



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---

## KNN CLASSIFICATION SUMMARY

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### *Advantages*

- *Can be applied to the data from any distribution*
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- *Good classification if the number of samples is large enough*



### *Disadvantages*

- *Choosing  $k$  may be tricky*



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- *Can be applied to the data from any distribution*
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- *Choosing  $k$  may be tricky*
- *Test stage is computationally expensive (no training stage)*



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- *Choosing  $k$  may be tricky*
- *Test stage is computationally expensive (no training stage)*
- *Need large number of samples for accuracy*



# **K-NN: WHAT ARE THE PROS AND CONS?**



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### *Disadvantages*

- *Choosing  $k$  may be tricky*
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## INTRO TO DATA SCIENCE

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# LAB