CSE 242: Machine Learning

2022 Fall

Razvan Marinescu
Computer Science and Engineering

Welcome

- Instructor: Razvan Marinescu
  - ramarine@ucsc.edu
  - Class times: Tue & Thu: 9:50am – 11:25am
  - In-person class (zoom available, but only if absolutely necessary – check canvas for link)

- Two TAs: Fatemeh Elyasi & Swati Jindal
- NEW Two tutors/graders! (still in hiring process)

- Lectures & office hours:
  - Keep your conversations respectful and polite.
  - Attendancy is required, active class participation will count towards your final grade.
  - Lectures will be video-recorded and made available after the class
  - Office hours:
    - Fatimeh: Tue 1-3pm
    - Swati: Thu 12-2pm
    - Razvan: Tue 4-6pm

- Lab sessions:
  - Hosted by Fatemeh & Swati
  - Time: One of the office hours will be used, **TBD**
  - First three weeks: intro to jupyter notebook and assignment submission

- Tutors:
  - Grade your assignments
  - Host office hours to address questions related to assignments

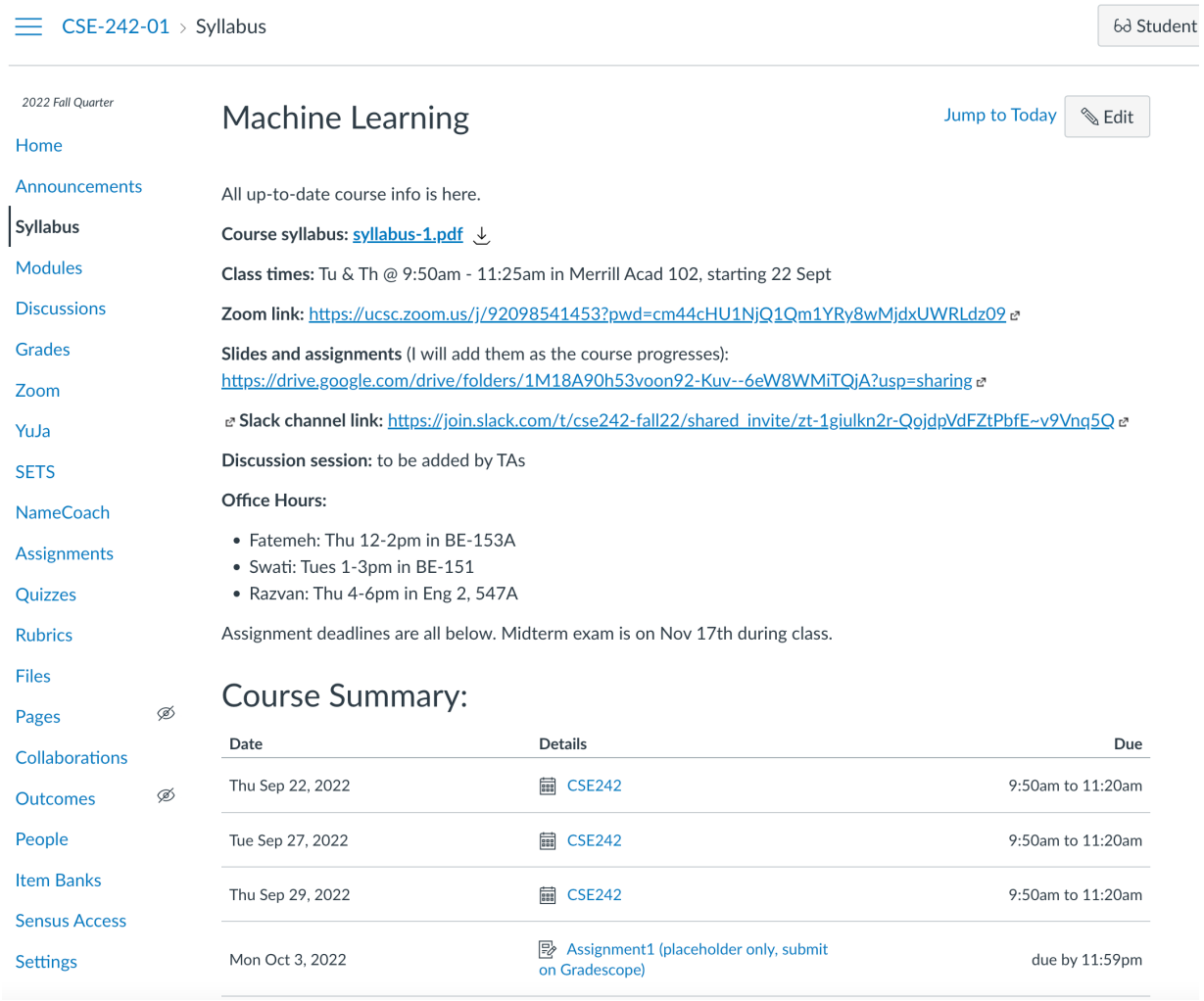
Meeting online

- Online class
  - The live lecture time will be a mixture of lectures, online discussions, meeting our teaching staffs, questions and answering

Web Info

- Emailing the instructor might ***not*** be the fastest way to get a response
- Sign up on Piazza (access code=CSe242) at
  - https://piazza.com/ucsc/fall2022/cse242
  - Use Piazza for all questions
- We will also enable Slack for asking questions
- Assignment submission on Gradescope:
- Make sure you access Canvas, Piazza and UCSC Email regularly

All up-to-date links to slides, assignments, zoom, etc … **are on Canvas**



Your course evaluation

- Midterm exam (30%): will be conducted online via Zoom
- Assignments (5 x 12% = 60%):
  - 5 assignments contribute equally to your final grade, each might consist a writing component and a programming component.
  - Will be posted on Canvas, you submit your copies on Gradescope.

```
Assignment 1: get you started
```

- Participation (10%): lectures, class exercises, discussions, attending invited talks, posting answers on piazza, etc

This course is not about

- Database
- Data mining
- Data processing
- Data visualization
- Coding a deep neural network
- Build a conversational robot

Planned Topics (tentative)

Week 1

- Basic concepts of machine learning

Week 2

- Probability reviews (MAP, MLE)
- Linear algebra (PCA)

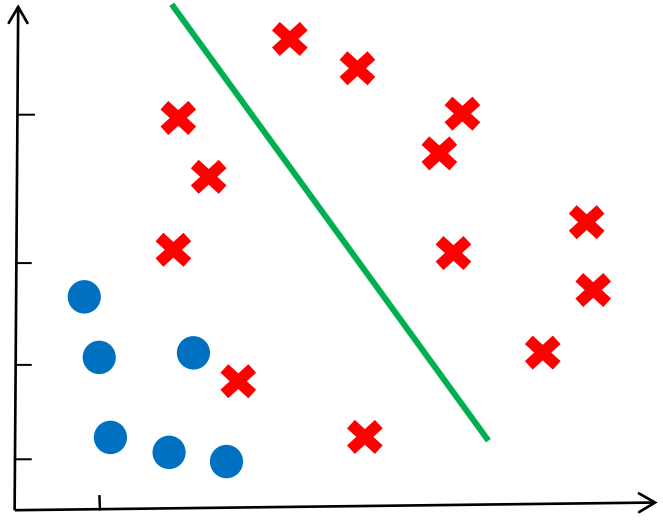
Planned Topics

Week 3 (Regression and Optimization)

- Linear regression, Logistic regression
- Risk minimization, SGD

Week 4 (Linear Models)

- Perceptron
- Support Vector Machine



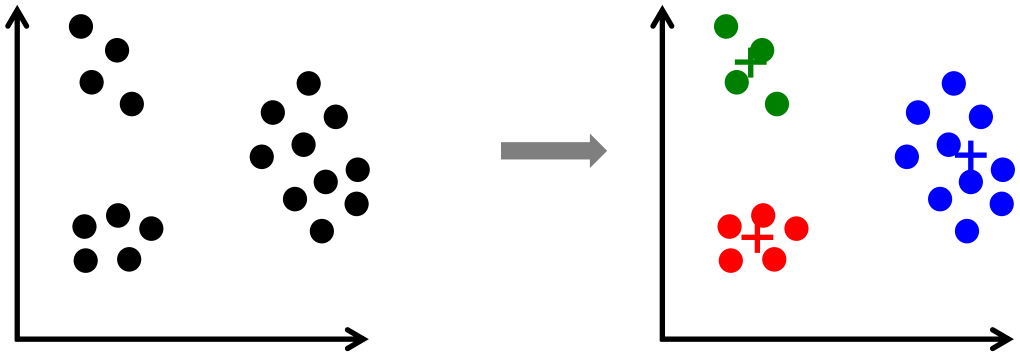
Planned Topics

Week 5 (light touch on other ML models)

- Kernel
- KNN, Naïve Bayes

Week 6

- Decision Tree
- Clustering
- EM



Planned Topics

Week 7

- Boosting
- Special topics

Week 8

- Reinforcement learning

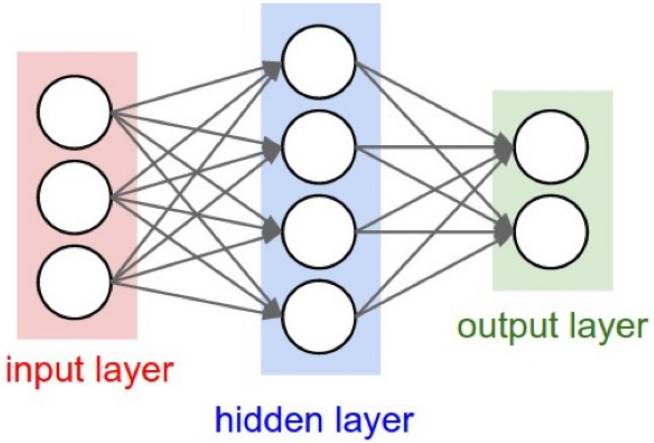
Planned Topics

Week 9

- Guest lecture
- **17th Nov: Midterm exam (during the lecture)**
- DRC students, email me in advance if you need special accommodations

Week 10

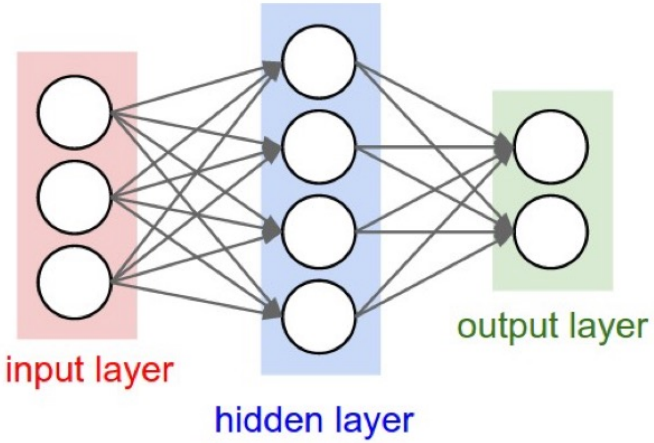
- Neural Networks
- Thanksgiving



Planned Topics

Week 11

- Generative Adversarial Networks
- Special Topics (my research on Bayesian GANs, or read a recent research paper)



A Brief Introduction

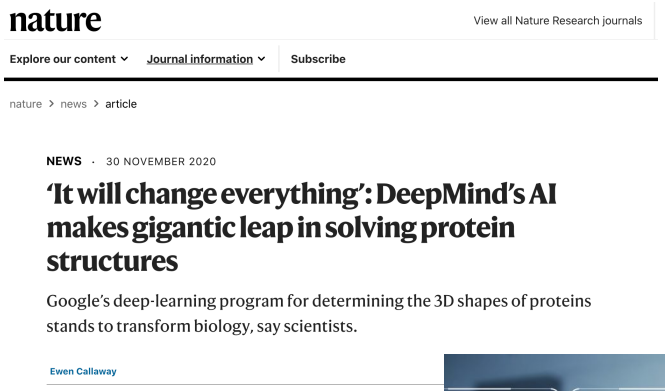
Annoucements

- We will use both Piazza and Slack for questions and discussions.
- Assignment 1 will be released later today. You will have two weeks to complete.

Classroom policy

- Quick and clarification questions are welcomed
- Vague questions ("I don't understand"; "can you repeat everything again") **=>** Office hour, online platforms, and tutoring sessions
- Frequent questions **=>** Office hour, online platforms, and tutoring sessions (think of the lecutres are serving a much broader audience than yourself)
- All other logistical questions **=>** Office hour, piazza, slack, email

Machine Learning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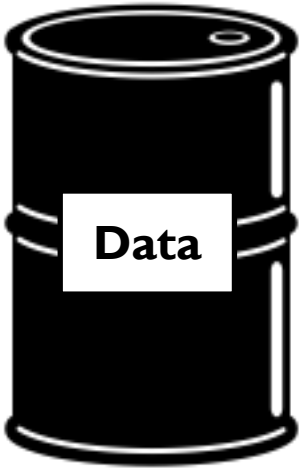
NEWS · 30 NOVEMBER 2020

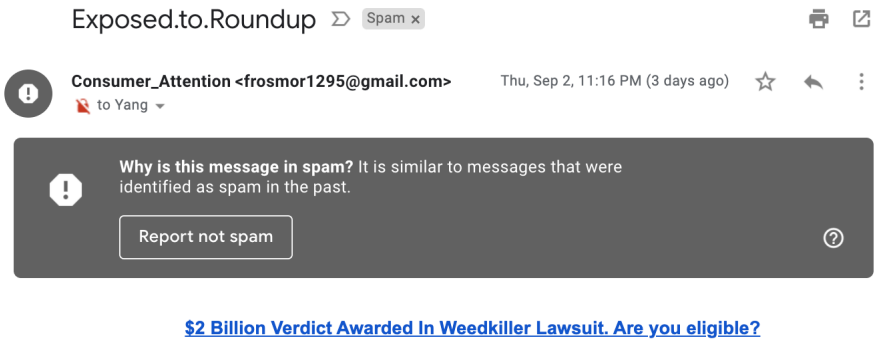
'It will change everything': DeepMind's AI makes gigantic leap in solving protein structures

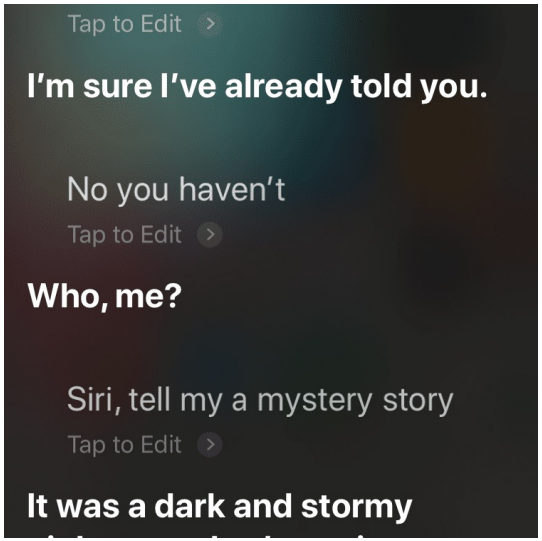
Google's deep-learning program for determining the 3D shapes of proteins stands to transform biology, say scientists.

Ewen Callaway

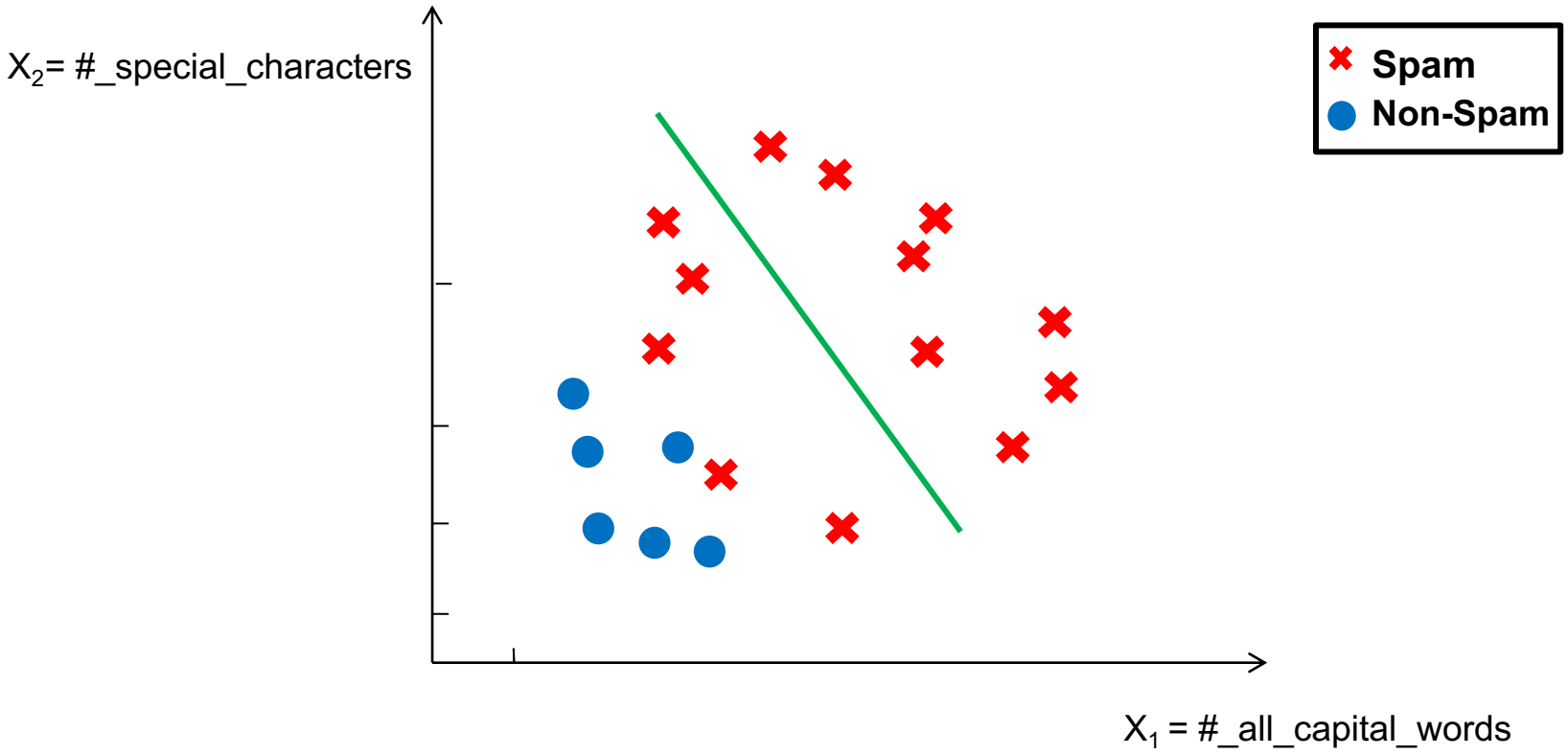
What is data?


Data


Exposed.to.Roundup
Spam
Consumer_Attention <frosmor1295@gmail.com>
Thu, Sep 2, 11:16 PM (3 days ago)
to Yang
Why is this message in spam? It is similar to messages that were identified as spam in the past.
Report not spam
$2 Billion Verdict Awarded In Weedkiller Lawsuit. Are you eligible?


Tap to Edit
I'm sure I've already told you.
No you haven't
Tap to Edit
Who, me?
Siri, tell my a mystery story
Tap to Edit
It was a dark and stormy

Representing Data



Representing Data

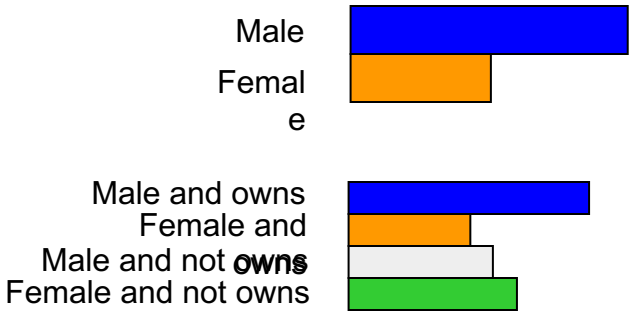
Data

Feature X **=** [
`most_recent_payment,`
`months_piad_in_full_in_last_6_months,`
`annual_salary,`
`#_loans]`

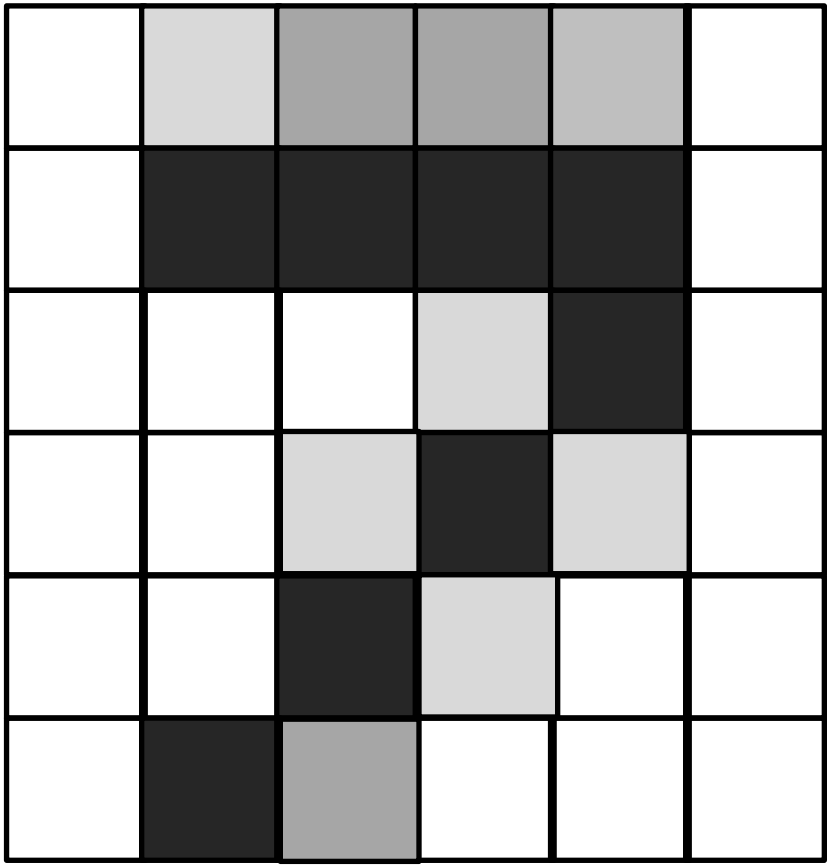
Label Y **=** [`1,0`] (Qualified)

Representing Data

id	Gender	Owns a car
1	Male	yes
2	Female	yes
3	Female	no
4	Male	yes
5	Female	yes
6	Male	no
	⋮	



Representing Data



0	100	150	150	100	0
0	255	255	255	255	0
0	0	0	100	255	0
0	0	100	255	100	0
0	0	255	100	0	0
0	255	150	0	0	0

Representing Data

0	100	150	150	100	0
0	255	255	255	255	0
0	0	0	100	255	0
0	0	100	255	100	0
0	0	255	100	0	0
0	255	150	0	0	0

```
[ 0, 100, 150, …, 0
  0, 255, 255, …, 0
  …
  0, 255, 150, 0, 0, 0 ]
```

X = `[0, 100, 150, …, 0,`
`0, 255, …, 0,…,`
`0, 255, 150, 0, 0, 0]`

Y = `[0, …, 1,…, 0]`

8th

Representing Data

0	100	150	150	100	0
0	255	255	255	255	0
0	0	0	100	255	0
0	0	100	255	100	0
0	0	255	100	0	0
0	255	150	0	0	0

$\boldsymbol{X}$ = [0, 100, 150, …, 0,
0, 255, …, 0,…,
0, 255, 150, 0, 0, 0]

Is this the best way to represent the data?

We will explore other options.

Types of data

Kind	*Order*	*Scale*	*Tendency*	*Dispersion*	*Shape*
Categorical	×	×	mode	n/a	n/a
Ordinal	√	×	median	quantiles	n/a
Quantitative	√	√	mean	range, interquartile range, variance, standard deviation	skewness, kurtosis

Statistics – calculations on the features

Supervised Batch Learning

- Assume (unknown) distribution over "things" (data)
- Things have measurable ***attributes*** or ***features***
- Get ***instances*** (feature vectors) ***X*** by drawing things from distribution and recording observations.
- Teacher ***labels*** instances making ***examples*** (***X, Y)***
- Set of labeled examples is the ***training set*** or ***sample***

Supervised Batch Learning

- Create ***hypothesis*** (rule or function) from sample
- Hypothesis predicts labels of *new* random instances, evaluated using a ***loss function*** (e.g. number of mistakes)

Supervised Learning (cont.)

- **Classification**: labels are nominal (unordered set, e.g. {ham, spam} {democrat, republican, indep.})
- **Binary Classification**
- **Regression**: labels are numeric (e.g. price of house)
- **Ranking** problems (order a set of objects)

Supervised Learning (cont.)

- **Classification**: labels are nominal (unordered set, e.g. {ham, spam} {democrat, republican, indep.}, {0,1,2,…,9})

- **Regression**: labels are numeric (e.g. price of house)

→ $10m

→ $100,000

→ $50,000

Supervised Learning (cont.)

- **Ranking** problems (order a set of objects)

Why "Learn" ?

- Machine learning is programming computers to optimize a performance criterion using example data or past experience (inference in statistics)
- To reason about data $\mathbf{X}$
- There is no need to "learn" to calculate payroll

Why "Learn" ?

- Learning is used when:
  - Human expertise does not exist (navigating on Mars),
  - Humans are unable to explain their expertise (speech recognition, object detection)
  - Solution changes in time (routing on a computer network)
  - Solution needs to be adapted or customized to particular cases (or users)

What We Talk About When We Talk About "Learning"

- Learning general models from a set of particular examples
- **To generate representation g(X) (often unsupervised)**
- **Or a prediction f(X) (often supervised)**

What We Talk About When We Talk About "Learning"

- *Data* is cheap and abundant (data warehouses, data marts); *knowledge* is expensive and scarce.
- Example in retail: Customer transactions to consumer behavior:

  People who bought "Da Vinci Code" also bought "The Five People You Meet in Heaven" (www.amazon.com)

- Build a model that is *a good and useful approximation* to the data.

What is Machine Learning?

- Training feature **X** + labels **Y (sometimes missing)**
  => programs for labeling data

- Optimize a performance criterion using example data or past experience.

- Role of Statistics: Inference from a sample

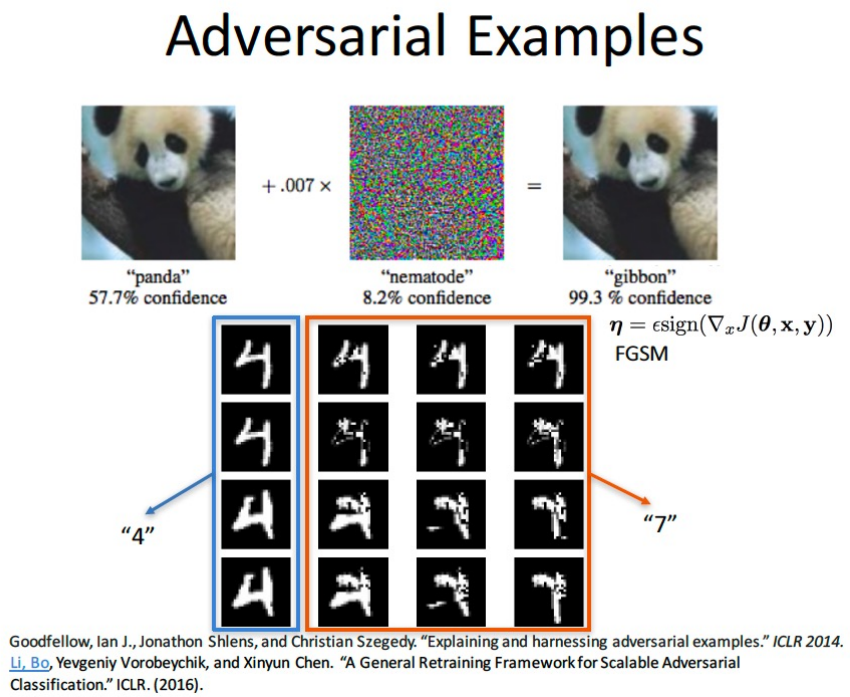
- Role of Computer science: Efficient algorithms to
  - Solve the optimization problem
  - Representing and evaluating the model for inference

Statistical Machine learning is not:

- Cognitive science (how people think/learn)
- Teaching computers to think

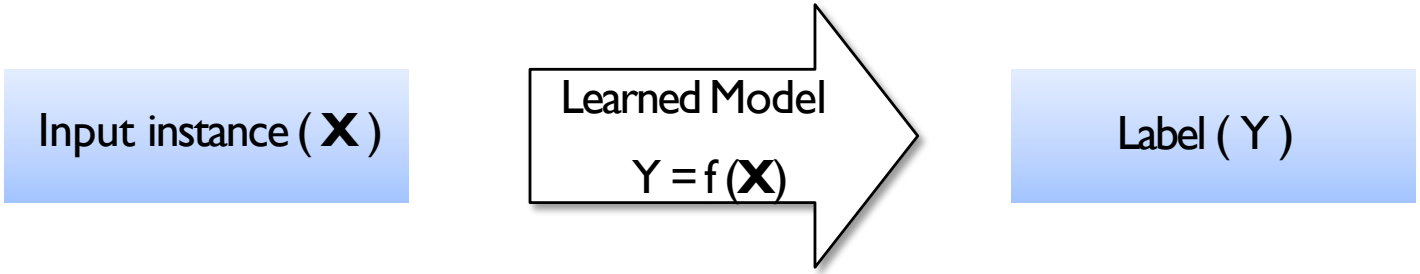
But is related to:

- Statistics
- Data Mining – Knowledge Discovery
- Control theory
- part of AI, but not "traditional" AI



Goodfellow, Ian J., Jonathon Shlens, and Christian Szegedy. "Explaining and harnessing adversarial examples." *ICLR 2014.*
Li, Bo, Yevgeniy Vorobeychik, and Xinyun Chen. "A General Retraining Framework for Scalable Adversarial Classification." ICLR. (2016).

How do we learn?



- The hypothesis, f(x), is defined by parameters
  - For hypothesis = quadrangle, the parameters are its 4 corners
- How to learn the parameters?
  - Optimize a loss function

Loss function

- Learn parameters by minimizing Loss function -- L(y, y')
  - Loss function measures error of predictions y' (on train set)
  - Loss functions tells you how good f(x) or g(x) is
  - Different for different ML algorithms
  - E.g. of classification loss: L(y,y')=0 if y=y' and L(y,y')=1 o/w
  - E.g. of regression loss: $(y-y')^2$
  - Will see more examples in future

- Minimization is done using an optimization algorithm like gradient descent

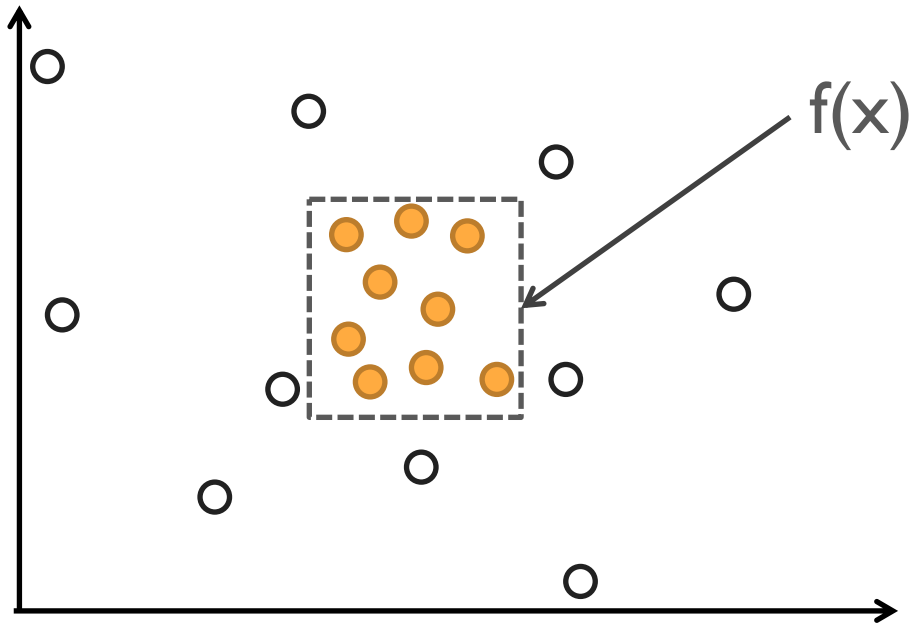
Why learning works?

- Learning is an ill-posed problem:
  If we assume nothing else, any label *Y* could be right for an unseen ***X***

Why learning works?

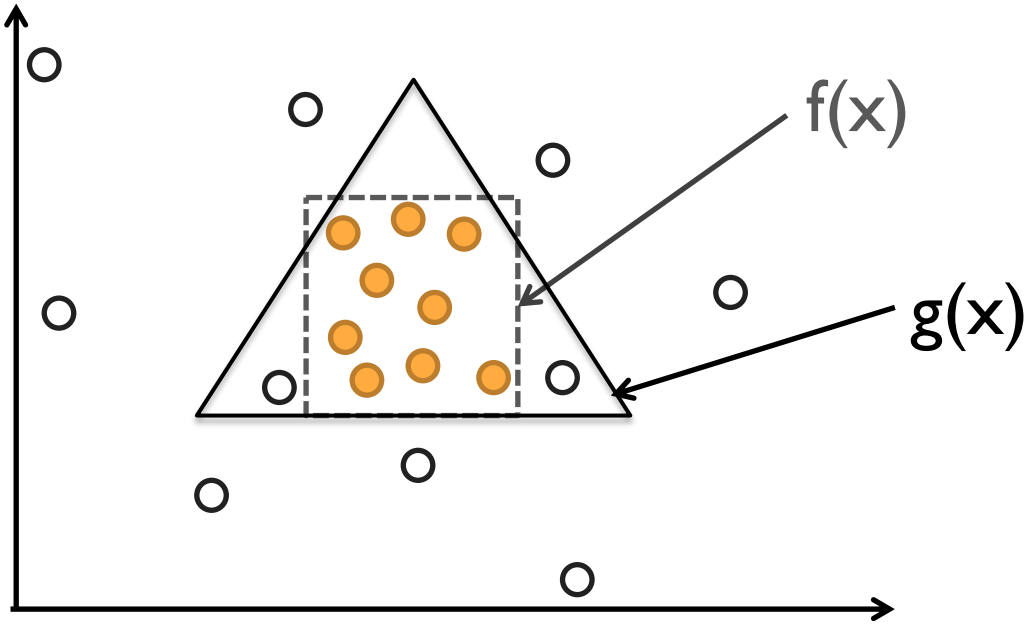
- Need an ***inductive bias*** limiting possible connections between $\boldsymbol{X}, Y$
- Often assume some kind of simplicity (e.g. linearity, neural networks) based on domain knowledge
- Bayesian approach: put *prior* on rules, and balance prior with evidence (data)

Choosing hypothesis space



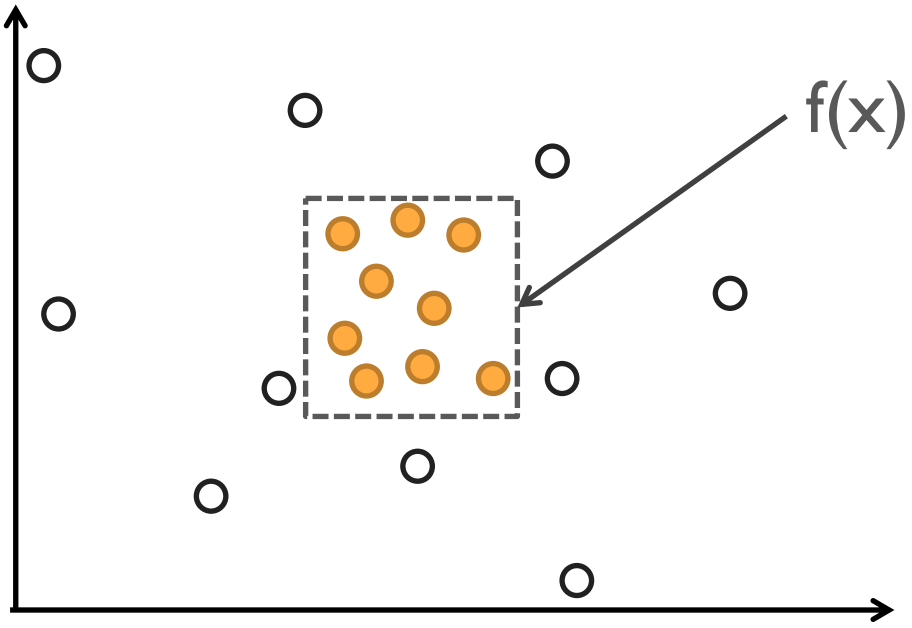
Choosing hypothesis space

- If we choose a hypothesis space that is too simple
  - Fewer parameters to learn, but less powerful
  - Model has less variance: fewer changes with changing training data
  - Model has more bias: makes more assumptions



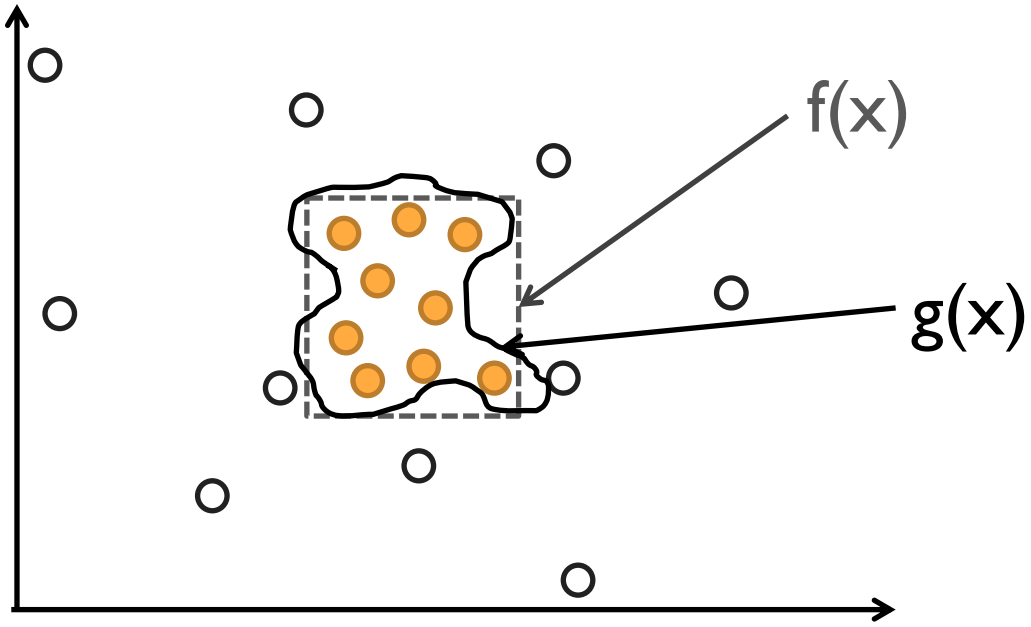
Choosing hypothesis space

- If we choose a hypothesis space that is too complex



Choosing hypothesis space

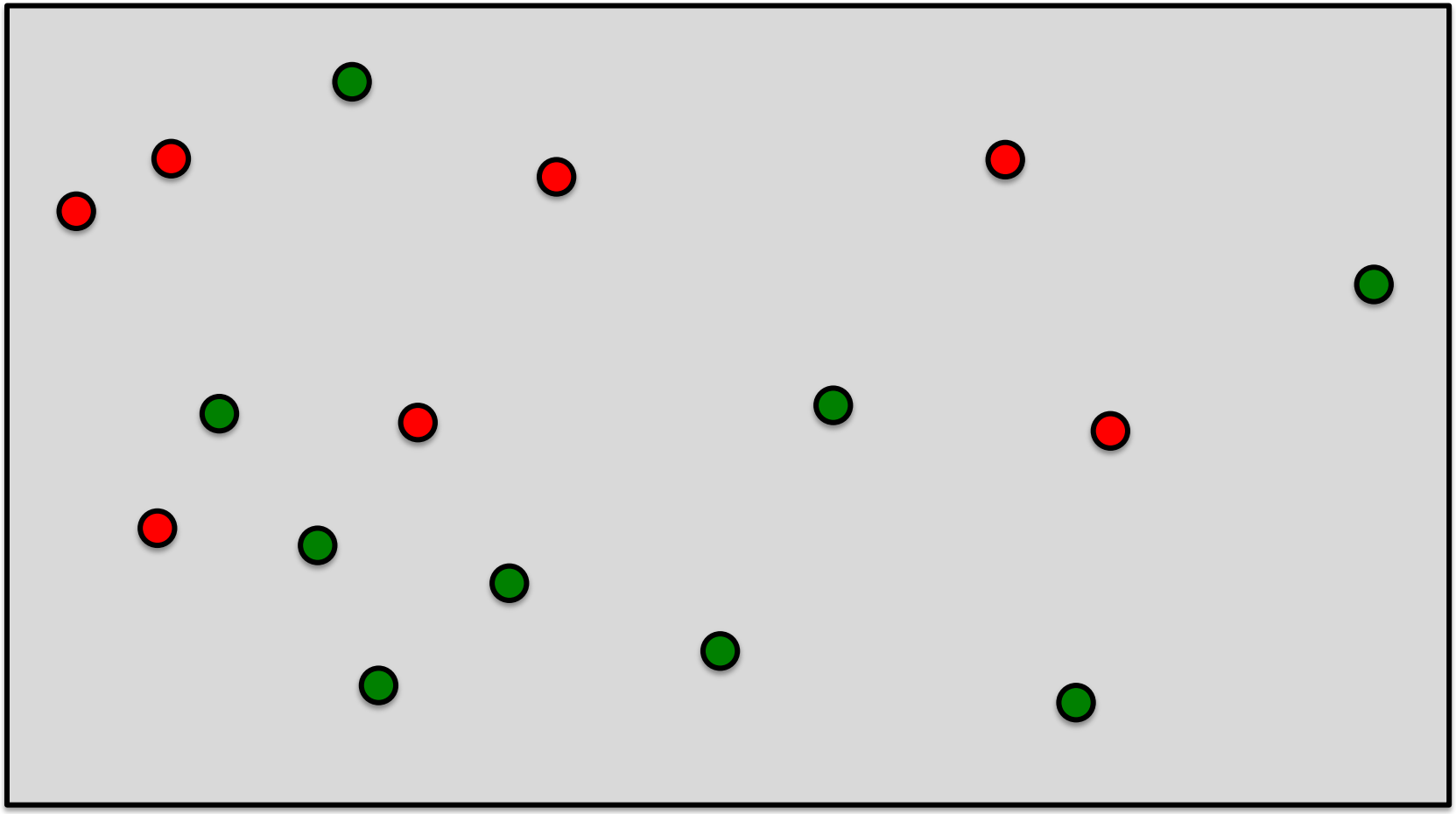
- If we choose a hypothesis space that is too complex
  - More parameters to learn but more powerful
  - Model has more variance and less bias
- This is called bias-variance tradeoff



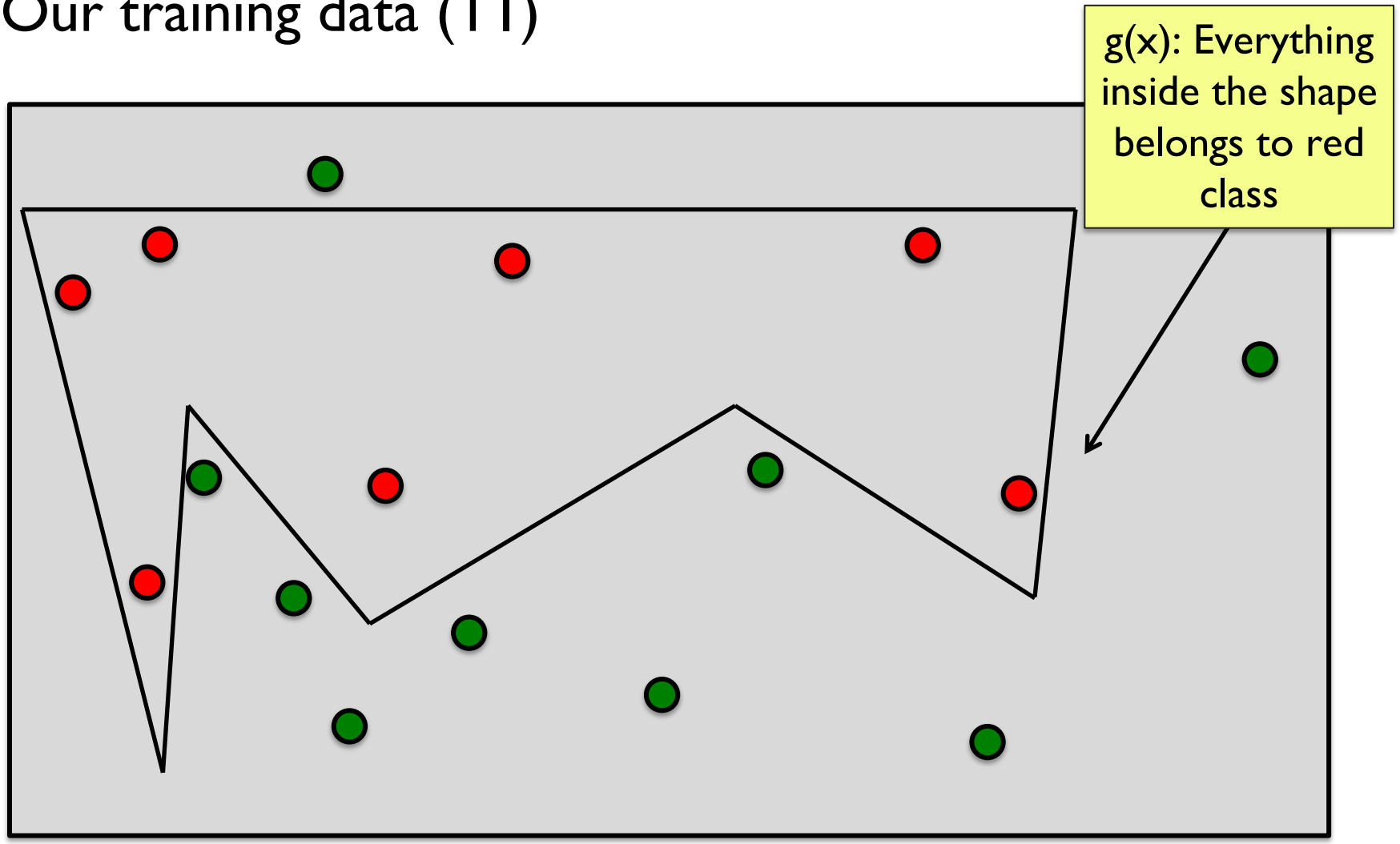
More on bias and variance

- What do we mean when we say a model from a complex model family has high variance?

Our training data (T1)



Our training data (T1)



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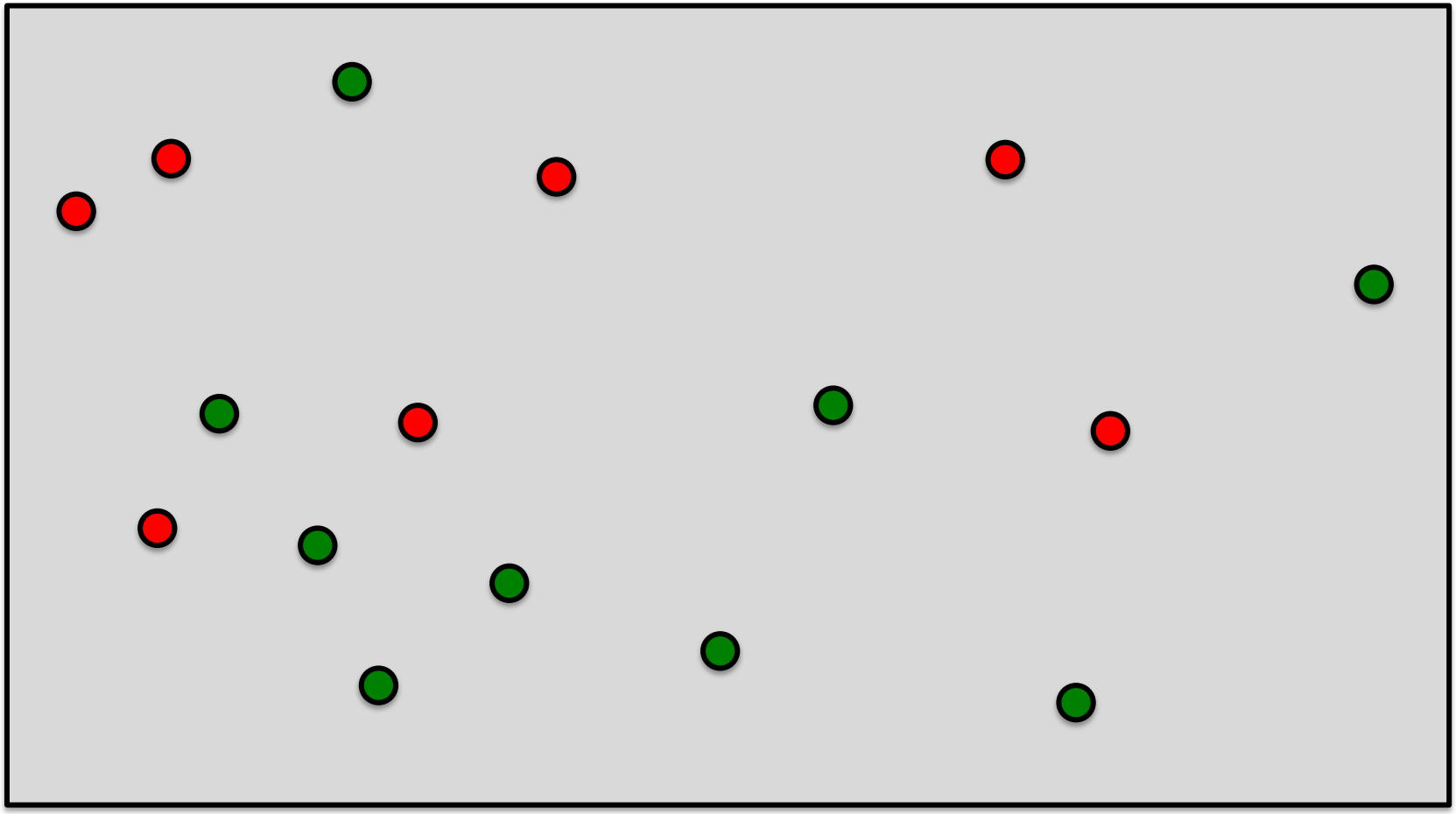
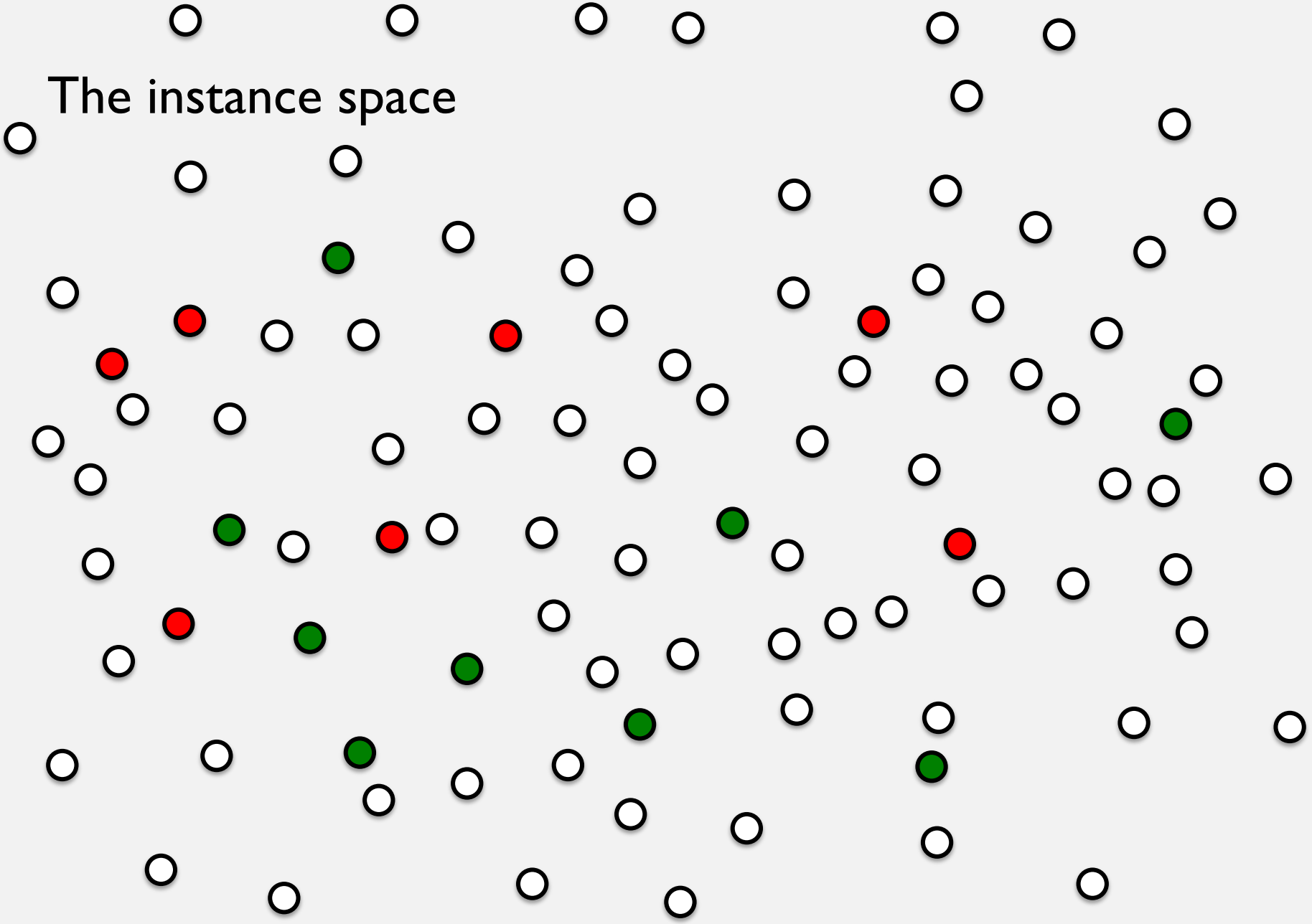
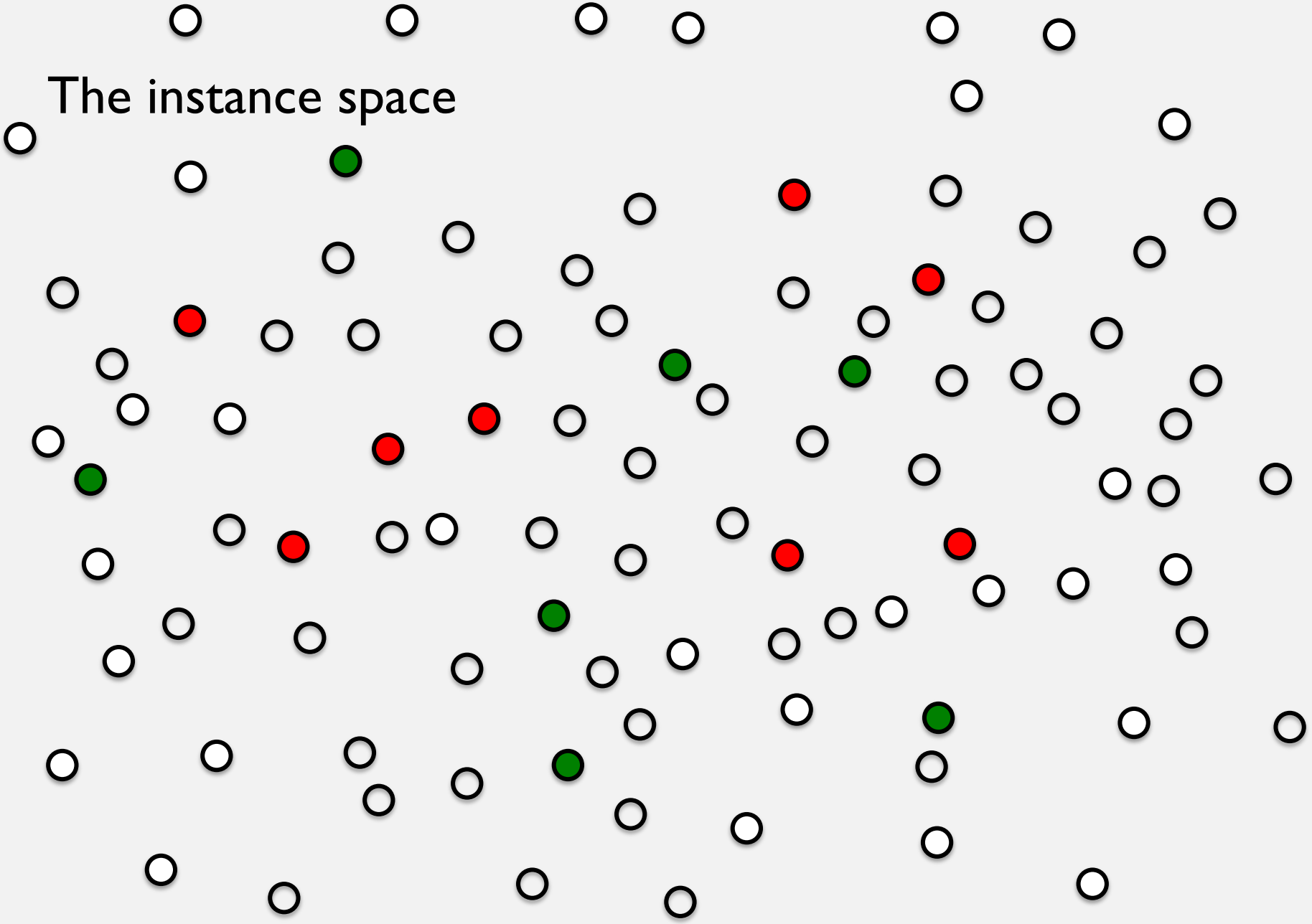


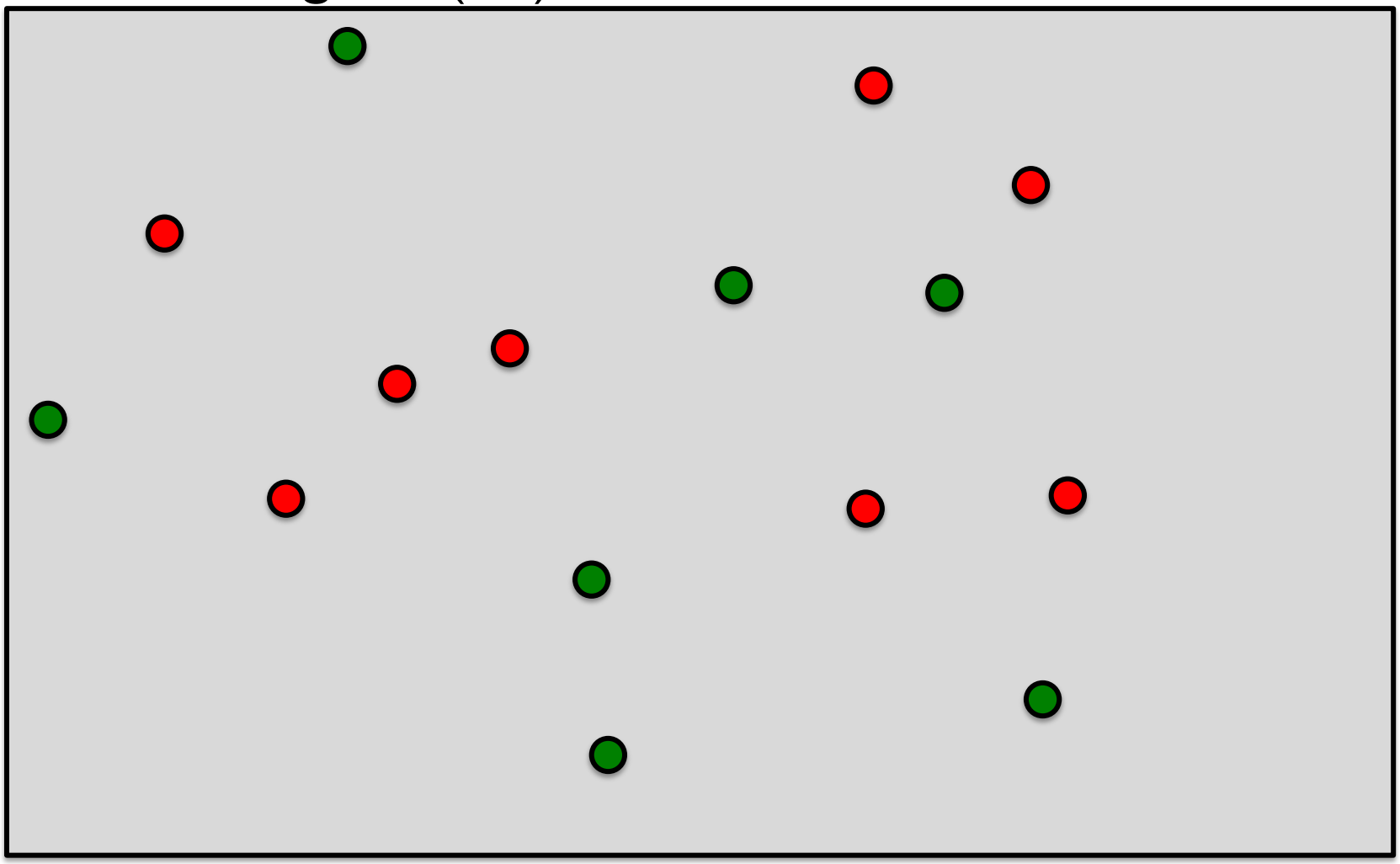
The instance space



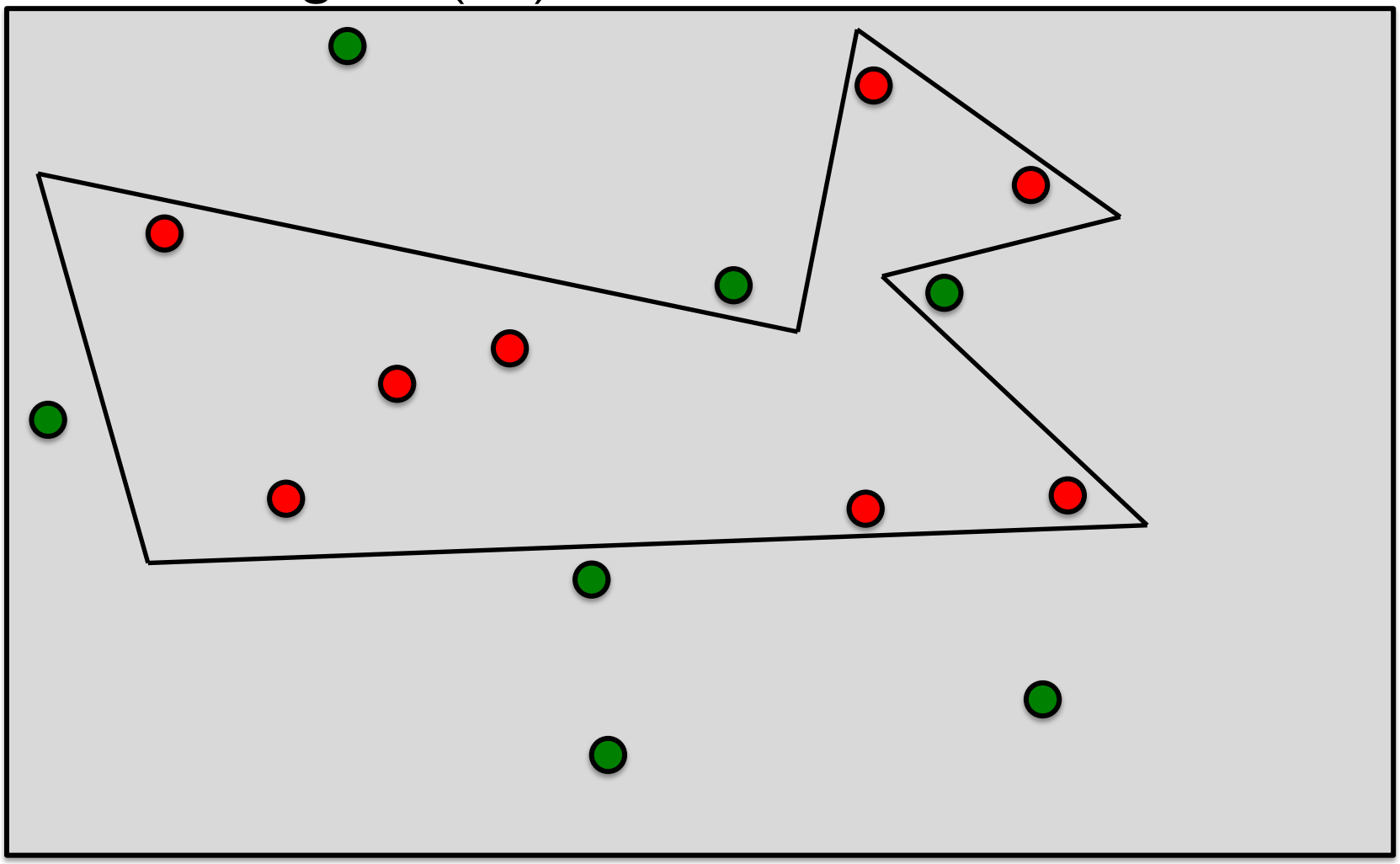
The instance space



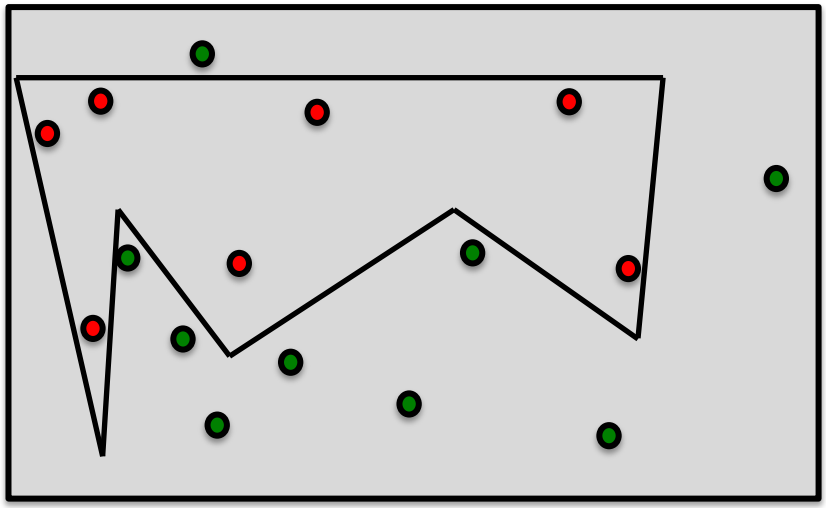
Our Training Set (T2)



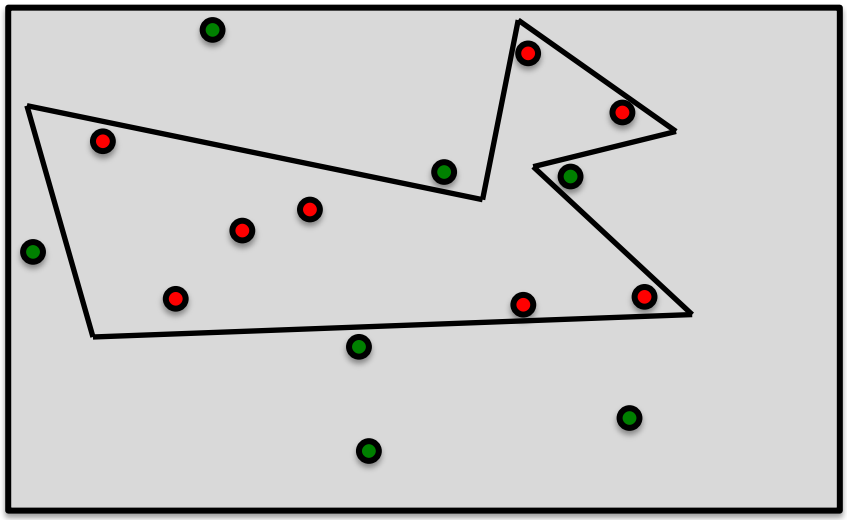
Our Training Set (T2)



High Variance



Training Set T1



Training Set T2

- T1 and T2 were different samples of the same instance space
- In principle, they represent examples for the same problem
- So, I should have learned almost identical hypothesis for both which would try to approximate the "true" decision boundary
- However, the hypotheses learned are very different, in spite of belonging to the same model family. In other words, our hypothesis changes a lot with different Ts. i.e. it has high variance

Inductive Bias

- What do we mean when we say a model has a high inductive bias?

Inductive Bias

- What do we mean when we say a model has a high inductive bias?
  - The model makes a lot of assumptions about the data.
  - Assumptions due to model family chosen *a-priori*

Bias-variance trade-off

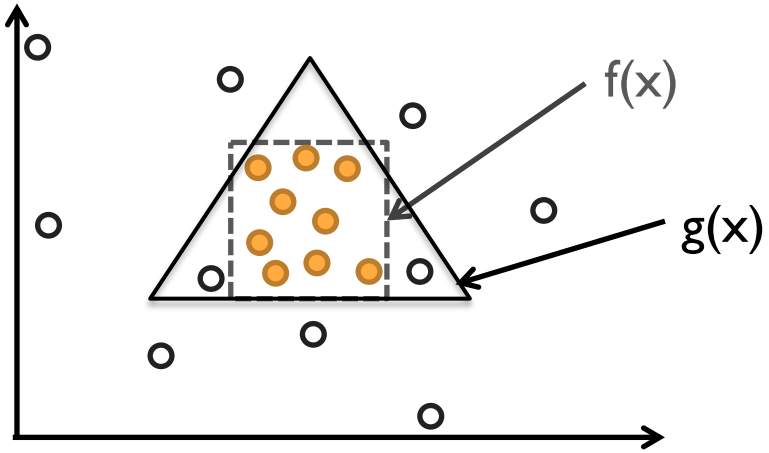
- Quality of a classifier can be decomposed into variance & bias
- Variance represents estimation error (limitations due to data)
- Bias represents approximation error (limitation of the model family)

error(g) = f(bias, variance)

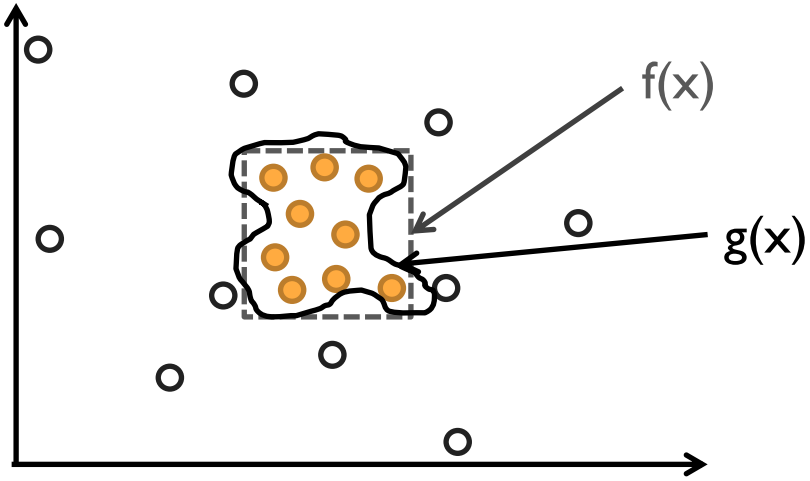
We will see this more formally
for Linear Regression

Bias-variance trade-off

- Quality of a classifier can be decomposed into variance & bias
- Variance represents **estimation error** (limitations due to data)
- Bias represents **approximation error** (limitation of the model family)



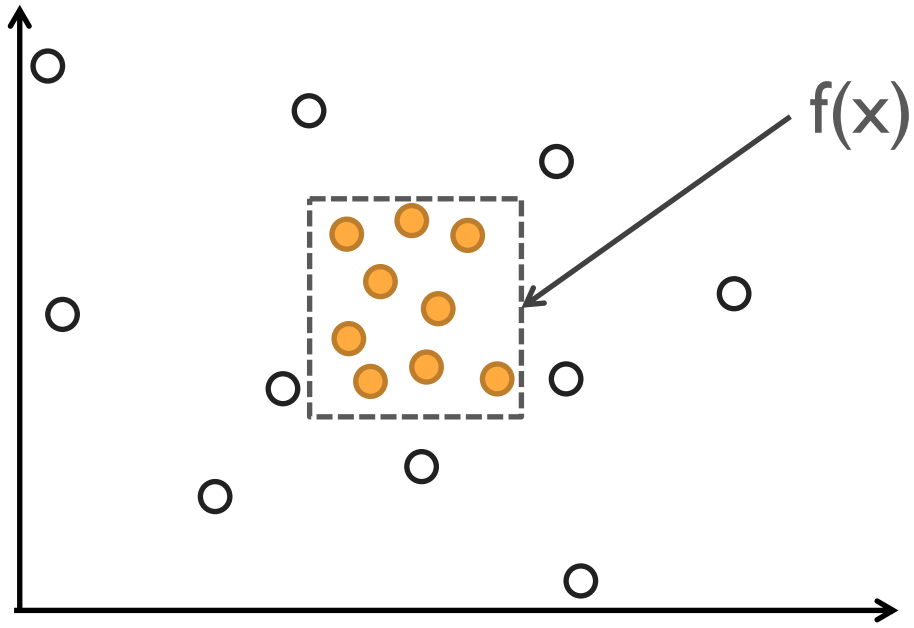
Low variance, high bias



High variance, low bias

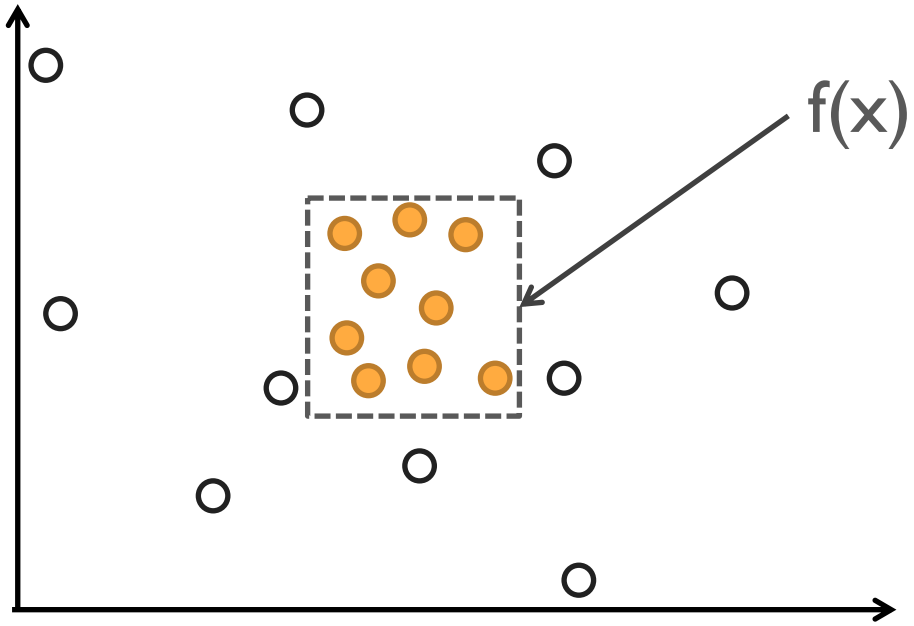
Over-fitting and Under-fitting

- Is it better to have a more complex model?



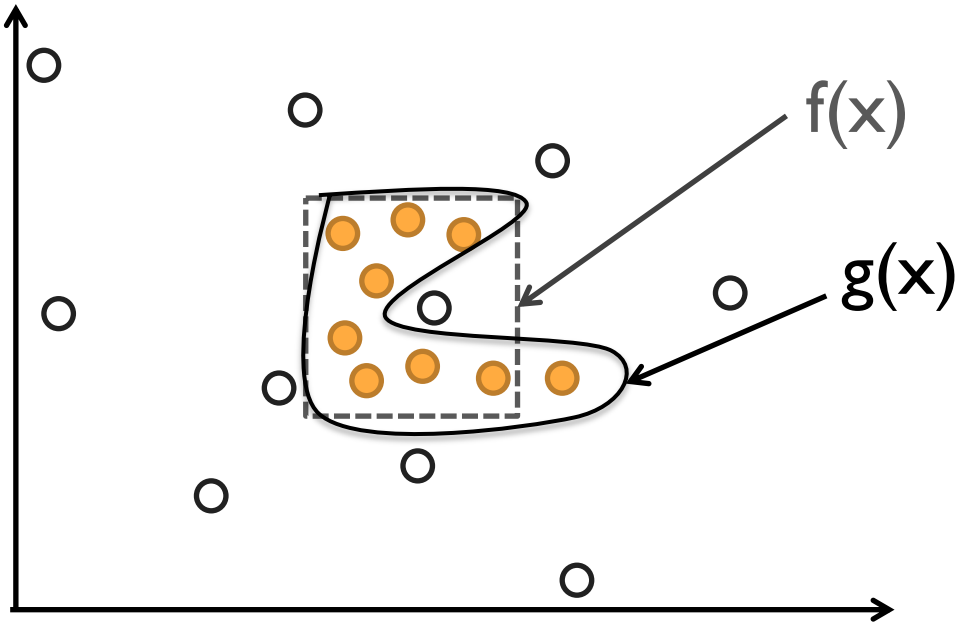
Over-fitting and Under-fitting

- Is it better to have a more complex model?
- No, follow the principle of Occam's Razor (simpler explanations are more plausible)



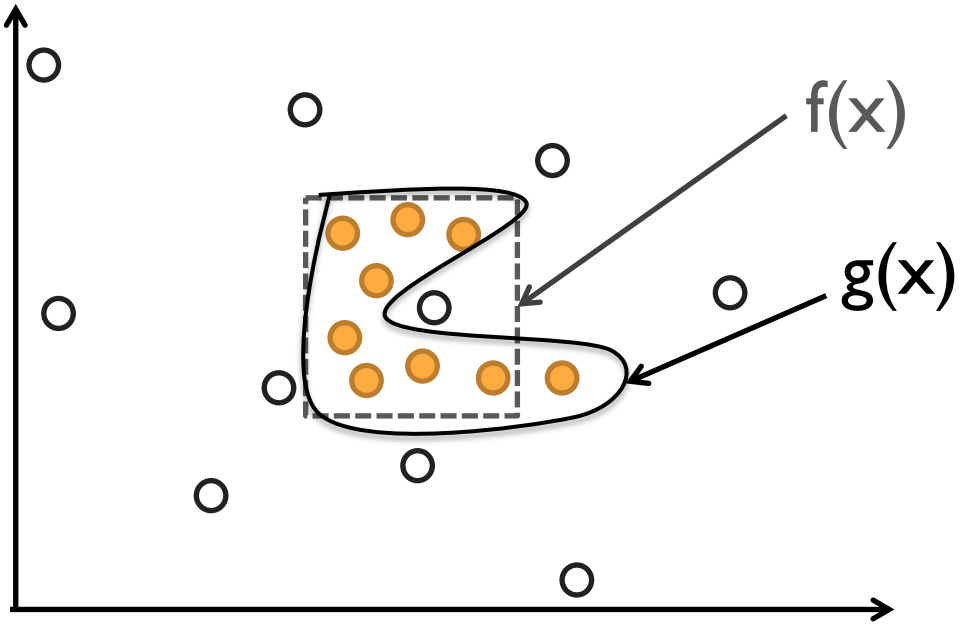
Over-fitting and Under-fitting

- Is it better to have a more complex model?
- Real world data is noisy
- You might over-fit



Over-fitting and Under-fitting

- Is it better to have a more complex model?
- real world data is noisy
- You might over-fit
- Too simple models, on the other hand, under-fit

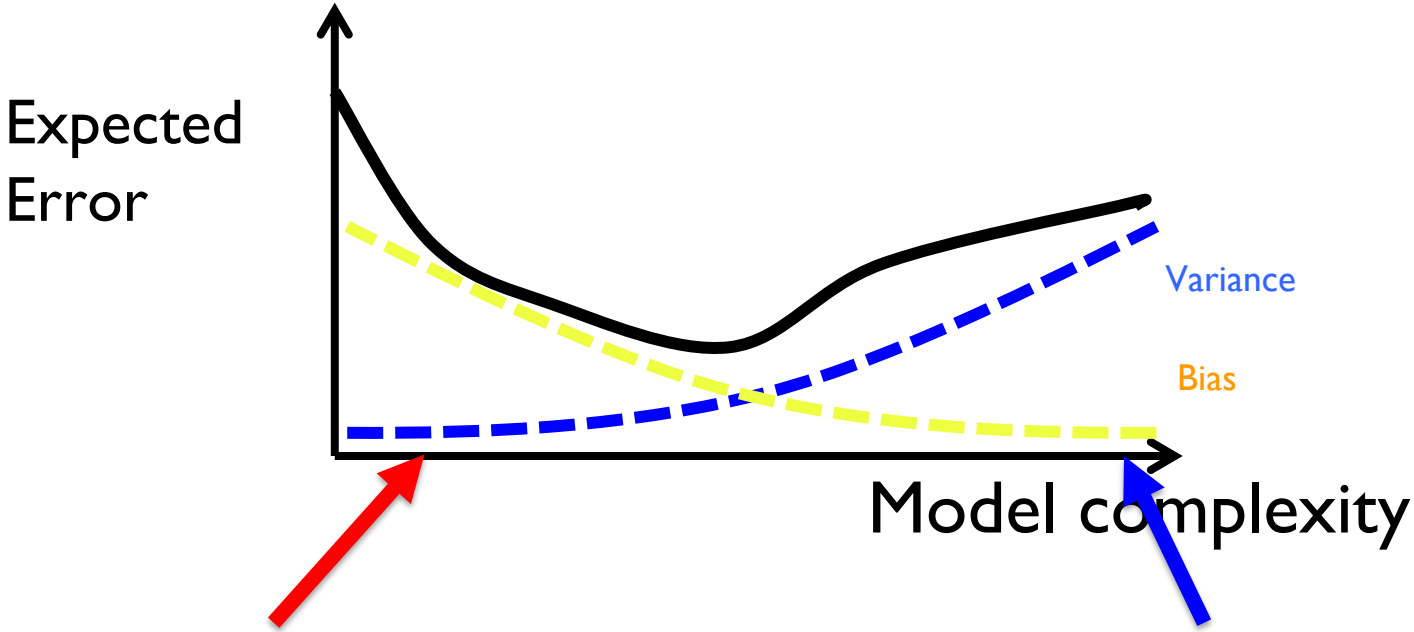


Notes on Over-fitting and Under-fitting

- Overfitting results in models that are more complex than necessary: after learning knowledge they "tend to learn noise"
- More complex models tend to have more complicated decision boundaries and tend to be more sensitive to noise, and missing examples
- Underfitting doesn't represent data well enough

We want to neither overfit nor underfit

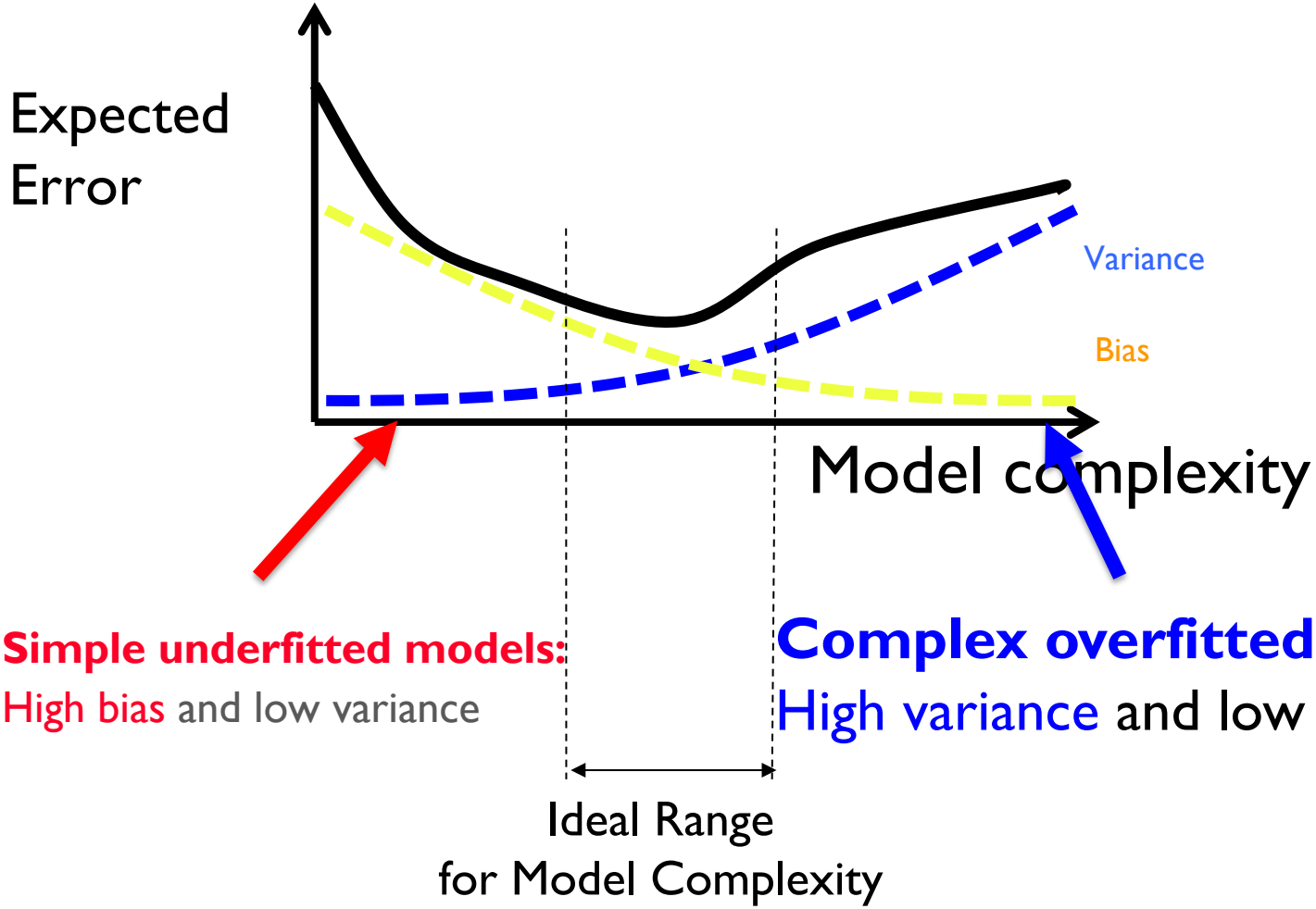
Model complexity



- **Simple underfitted models:**
  High bias and low variance

Complex overfitted models:
High variance and low bias

Model complexity



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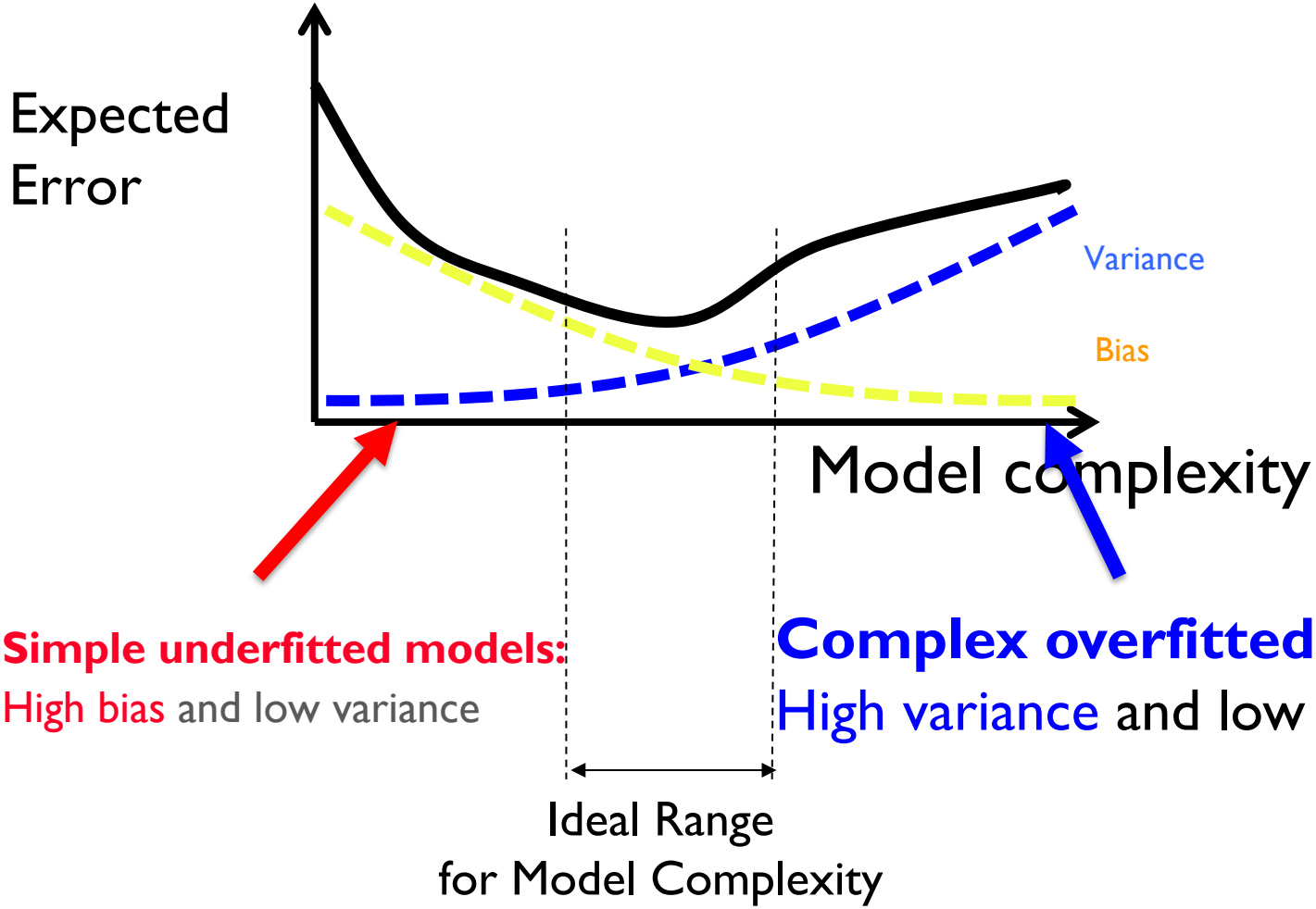
Complex overfitted models:
High variance and low bias

Model complexity



- **Simple underfitted models:**
  High bias and low variance

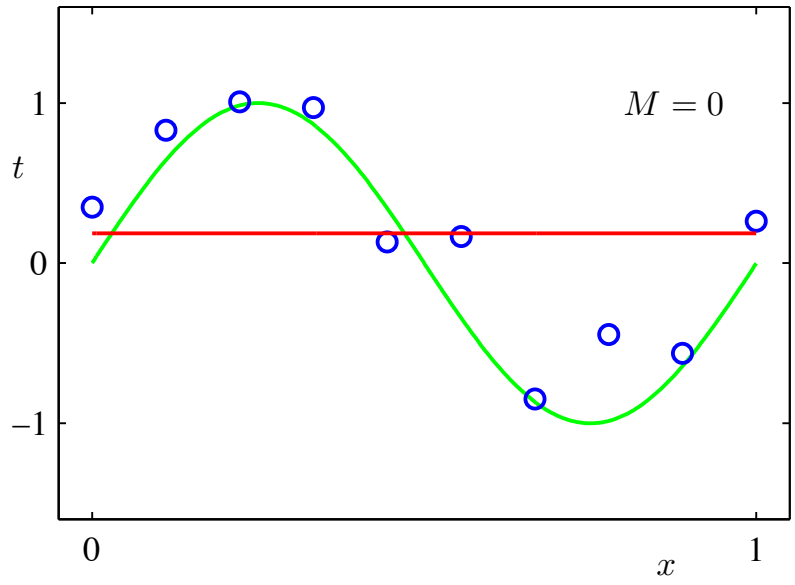
Complex overfitted models:
High variance and low bias

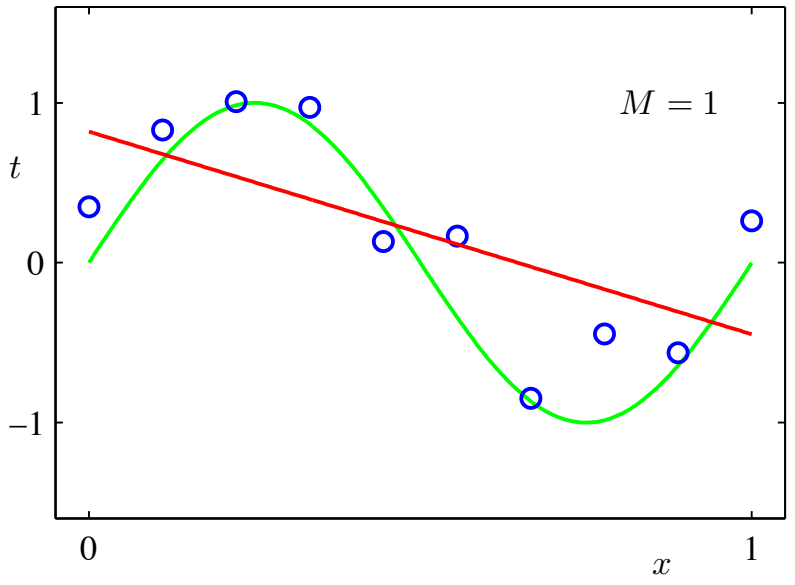
We need to find the "ideal range"

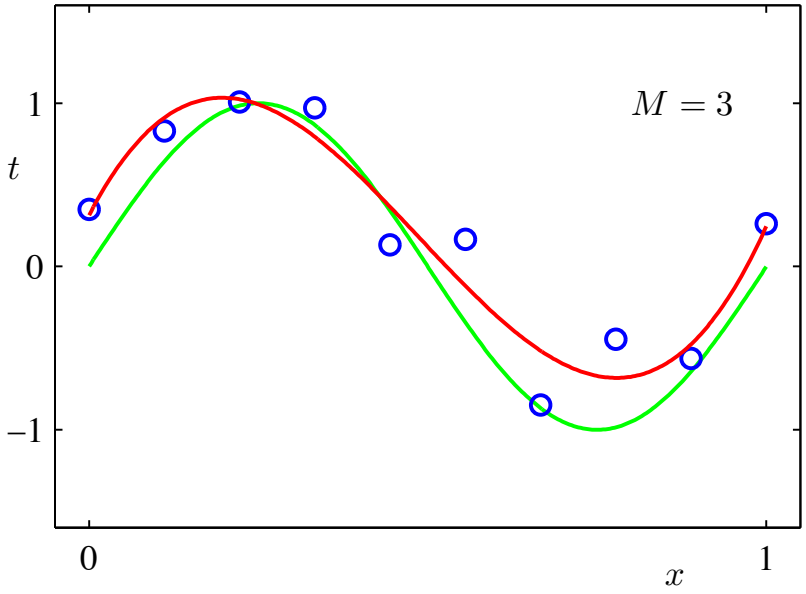
Overfitting and Underfitting

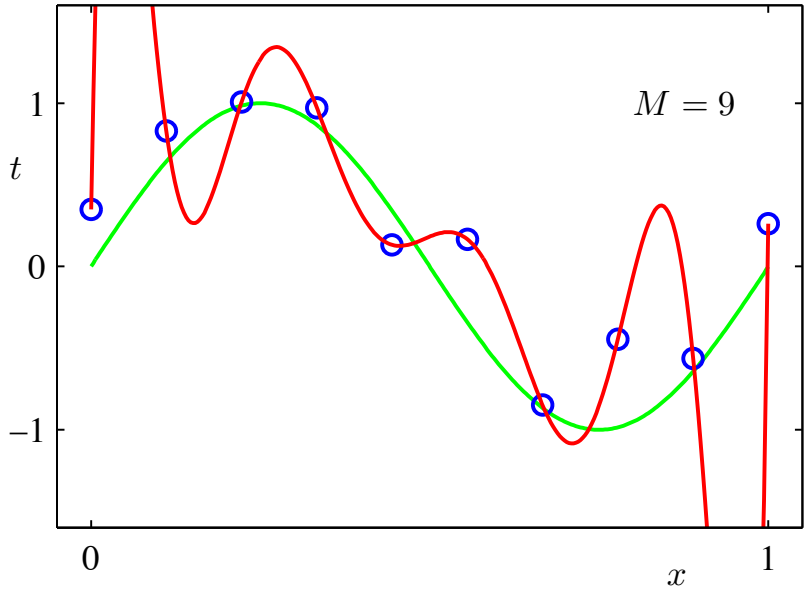
- **Overfitting** happens when the hypothesis is too complex for the "truth"
- **Underfitting** happens when the hypothesis is too simple.

Bishop fig 1.4









How to find the "ideal" range?

- Cannot find it using Training error
- Training performance is often a poor indicator of generalization
  - Keep improving train accuracy => overfit
  - Stop too early => underfit
  - Both are bad!
- Generalization is what we really care about in ML
- Test performance is a good indicator of generalization
- Testing performance is not accessible during training
- Keep a small fraction (10-20%) of the data as held-out development set

Imperfect measurements

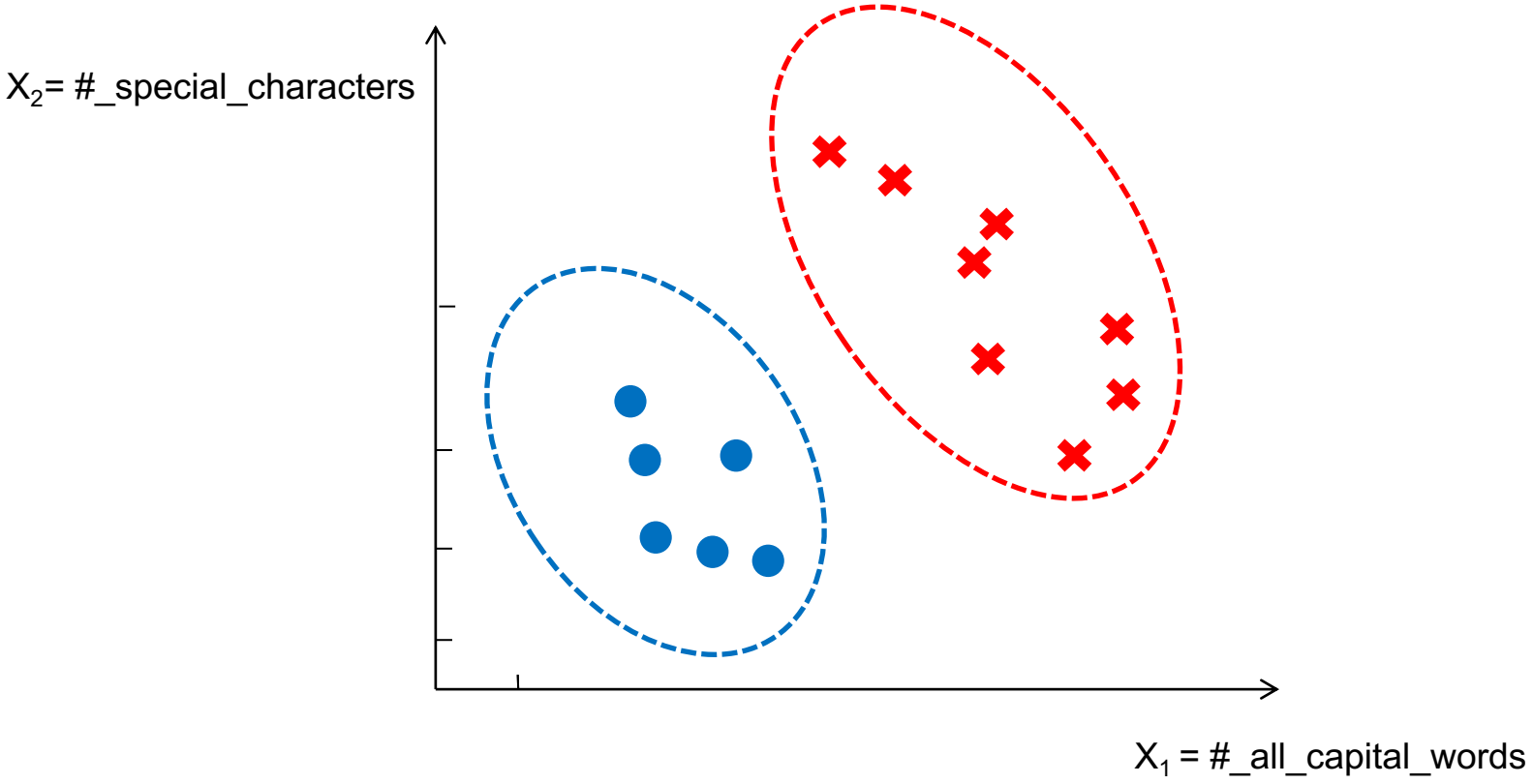
- Unmeasured Features
- Attribute noise (random or systemic)
- Label noise (random or systemic)
- Inductive bias errors may look like noise

Other kinds of supervised learning

- **Reinforcement learning -** learning a policy for influencing or reacting to environment
  - Game playing/robot in a maze, etc.
  - No supervised output, but delayed rewards
- **On-line learning**: predict on each instance in turn
- **Semi-supervised learning** uses both labeled and unlabeled data
- **Active learning** – request labels for particular instances

Unsupervised Learning

- Learning "what normally happens" in ***X***, no labels *Y*
- Clustering: Grouping similar instances



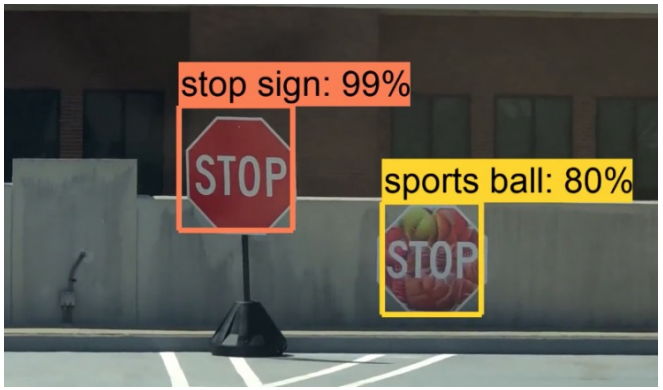
Unsupervised Learning

- Example applications
  - Segmentation in customer relationship mgmt
  - Image compression: Color quantization
  - Identifying unusual Airplane landings
  - Autoencoding – learn the "features"

```
Assignment 4: applying unsupervised
learning to solve supervised learning
problem
```

Other topics

- Security
- Privacy
- Bias



`Assignment 5: explore data bias`

Evaluation: Measuring Predictive Performance

Measuring Predictive Performance

- Various evaluation measures exist in literature that can evaluate predictive performance
- Most popular for classification:
  - Accuracy and Error Rate
  - Precision Recall and F - measure

Accuracy and Error Rate

$$\text{accuracy} = \frac{\#\text{ correct predictions}}{\#\text{ test instances}}$$

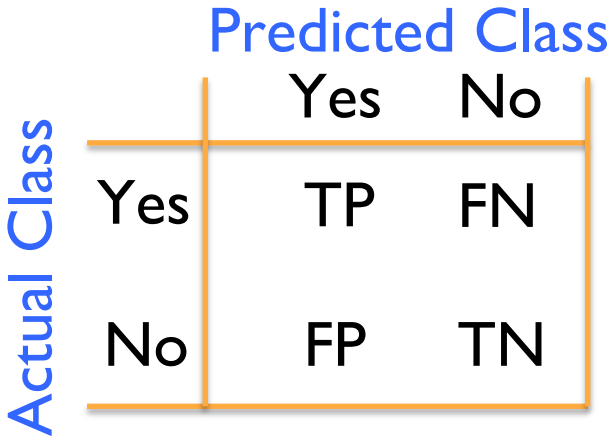
$$\text{error} = 1 - \text{accuracy} = \frac{\#\text{ incorrect predictions}}{\#\text{ test instances}}$$

Useful in "X vs Y" type of problems: both classes are equally important

Examples?

Confusion Matrix

- Given a dataset of positive instances and negative instances:



TP = True Positives
TN = True Negatives
FP = False Positives
FN = False Negatives

Example

	Predicted: Yes	Predicted: No
Actual: Yes	TP = 100	FN=5
Actual: No	FP = 10	TN = 50

Total number of instances in the corpus, N = ??

Total number of predicted yes's = ??
Total number of predicted no's = ??

Total number of actual yes's = ??
Total number of actual no's = ??

Example

N = 165	Predicted: Yes	Predicted: No	Total
Actual: Yes	TP = 100	FN=5	105
Actual: No	FP = 10	TN = 50	60
Total	110	55	

Total number of instances in the corpus, N = 165

Total number of predicted yes's = 110
Total number of predicted no's = 55

Total number of actual yes's = 105
Total number of actual no's = 60

Example

N = 165	Predicted: Yes	Predicted: No	Total
Actual: Yes	TP = 100	FN=5	105
Actual: No	FP = 10	TN = 50	60
Total	110	55	

Accuracy = ??

Example

N = 165	Predicted: Yes	Predicted: No	Total
Actual: Yes	TP = 100	FN=5	105
Actual: No	FP = 10	TN = 50	60
Total	110	55	

Accuracy = (TP+TN)/N = (100+50)/165 = 0.91

Precision, Recall and F-measure

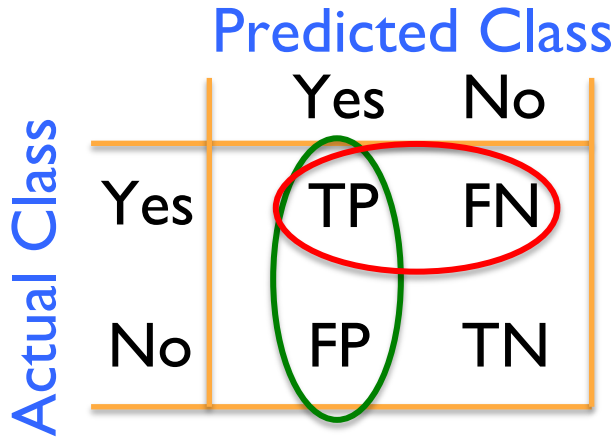
- Accuracy is useful in "X versus Y" type of problems

$$\text{accuracy} = \frac{\#\ \text{correct predictions}}{\#\ \text{test instances}}$$

- What about "X versus non-X"type of problems: one of the classes is more interesting
  - E.g. spam versus not-spam
  - E.g. information retrieval: Retrieve all relevant documents from a given list of documents

Precision, Recall and Accuracy

- Given a dataset of P positive instances and N negative instances:



$$\text{accuracy} = \frac{TP + TN}{P + N}$$

$$\text{precision} = \frac{TP}{TP + FP}$$

$$\text{recall} = \frac{TP}{TP + FN}$$

Precision measures what fraction of the retrieved documents were relevant

Recall measures what fraction of the relevant records were retrieved

F measure

$$\text{F1 measure} = \frac{2 * P * R}{P + R}$$

Inverse relationship between Precision and Recall

Example

N = 165	Predicted: Yes	Predicted: No	Total
Actual: Yes	TP = 100	FN=5	105
Actual: No	FP = 10	TN = 50	60
Total	110	55	

Accuracy = (TP+TN)/N = (100+50)/165 = 0.91

Precision = ??
Recall = ??
F1 score = ??

Example

N = 165	Predicted: Yes	Predicted: No	Total
Actual: Yes	TP = 100	FN=5	105
Actual: No	FP = 10	TN = 50	60
Total	110	55	

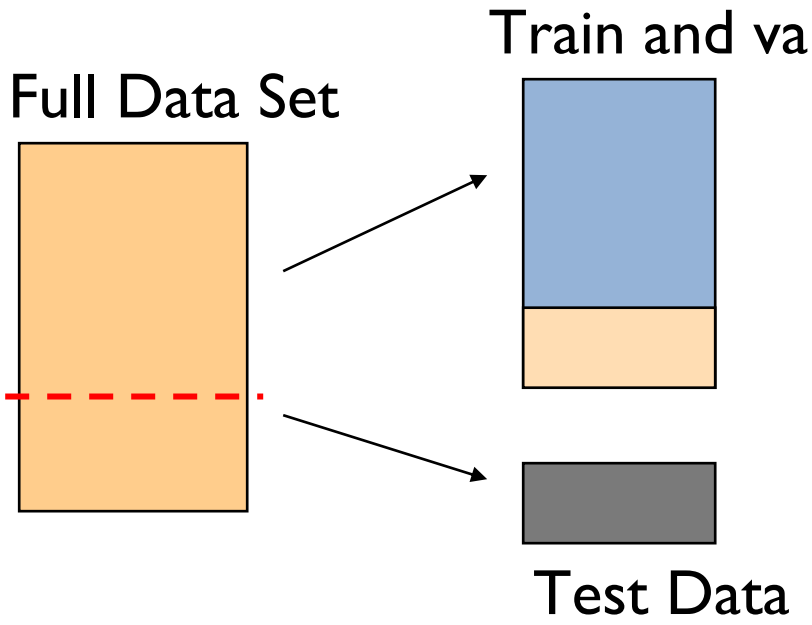
Accuracy = (TP+TN)/N = (100+50)/165 = 0.91

Precision = TP/(TP + FP) = 100/110 = 0.91
Recall = TP /(TP + FN) = 100/105 = 0.95
F1 score = 2*0.91*0.95/(0.91+0.95) = 0.93

How to report performance?

- Train data: data used to build the model

  Use held-out validation/dev set if needed
- Test data: new data, not used in the training process



Usually 80-20 split

Idea:
Train a model on the "training data"...

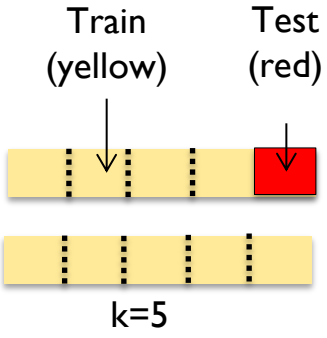
...AND THEN test model's performance on the test data

** In perfect world, you wouldn't have to hold out a test set, but instead have access to a human evaluator

k-fold cross validation

- Why just choose one particular "split" of the data as test set?
  - In principle, we should do this multiple times since performance may be different for each split
    - Run k iterations
    - In each iteration, hold out a different portion of the data as test set
  - This would improve robustness of the reported result

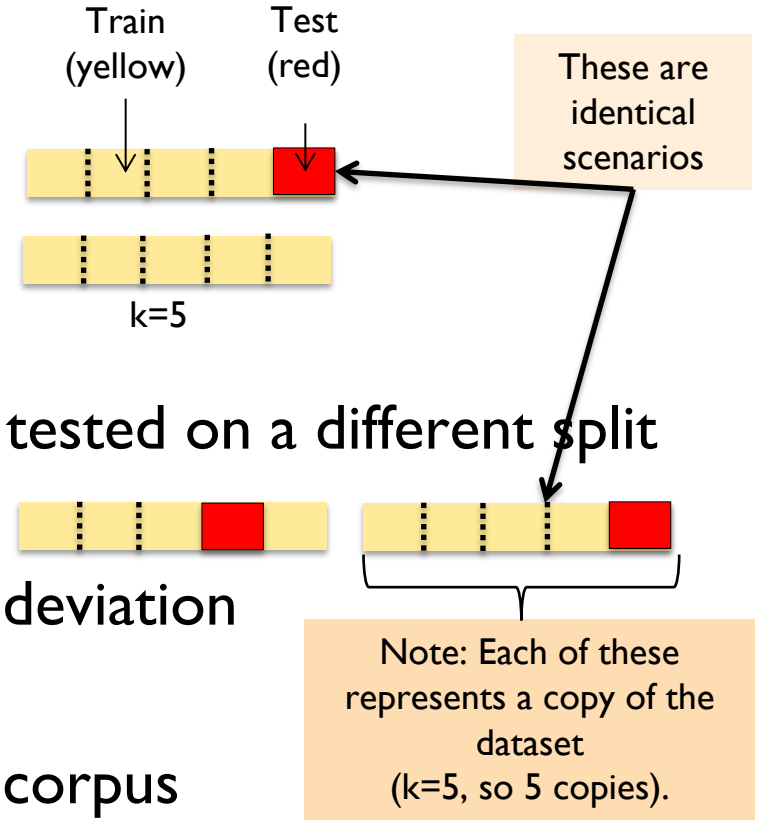
k-fold cross validation



- Instead of testing on only one split:
- Split data into k equal-sized parts:
- Train and test k **different** classifiers
- Each of the k classifier is trained and tested on a different split

- Report average accuracy & standard deviation of the accuracies across all k splits
- Leave-one-out(LOO) CV: k= size of corpus

k-fold cross validation



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