# Machine Learning - Introduction

CSE 4309 – Machine Learning
Vassilis Athitsos
Computer Science and Engineering Department
University of Texas at Arlington

# What is Machine Learning

- Quote by Tom M. Mitchell:

"A computer program is said to learn from experience *E* with respect to some class of tasks *T* and performance measure *P* if its performance at tasks in *T*, as measured by *P*, improves with experience *E*."

- To define a machine learning **problem**, we need to specify:
  - The experience (usually known as training data).
  - The task (classification, regression, …)
  - The performance measure (classification accuracy, squared error, …).

# Types of Machine Learning

(source: Wikipedia)

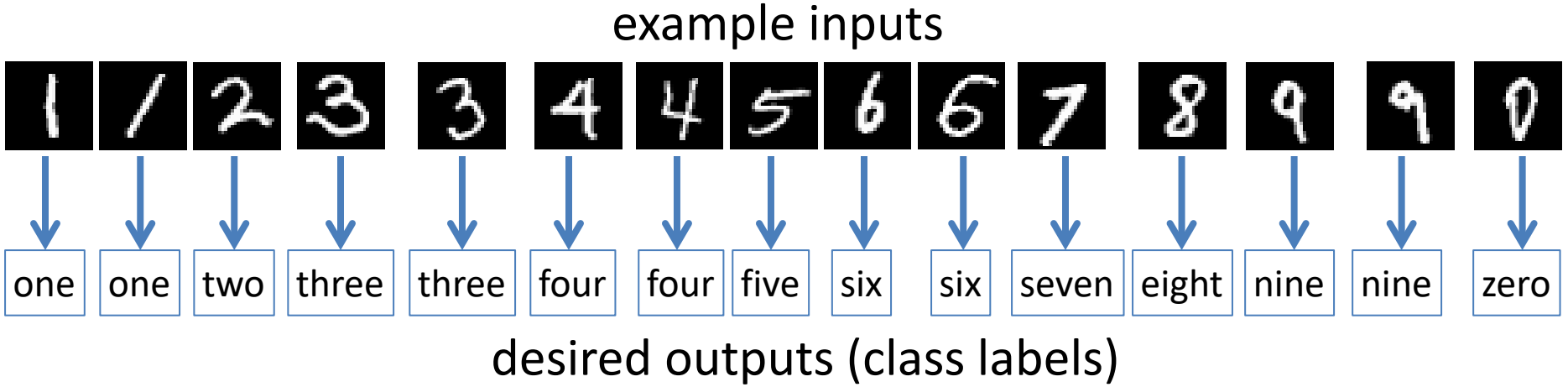
- Supervised Learning.
  - The computer is presented with example inputs and their desired outputs, given by a "teacher", and the goal is to learn a general rule that maps inputs to outputs.
- Unsupervised Learning.
  - No example outputs are given to the learning algorithm, leaving it on its own to find structure in its input.
- Reinforcement Learning.
  - A computer program interacts with a dynamic environment and must perform a certain goal (such as driving a car or playing chess). The program is provided feedback (rewards and punishments).

# Supervised Learning

- The computer is presented with example inputs and their desired outputs, given by a "teacher".
- Goal:  learn a general function that maps inputs to outputs.

# Supervised Learning

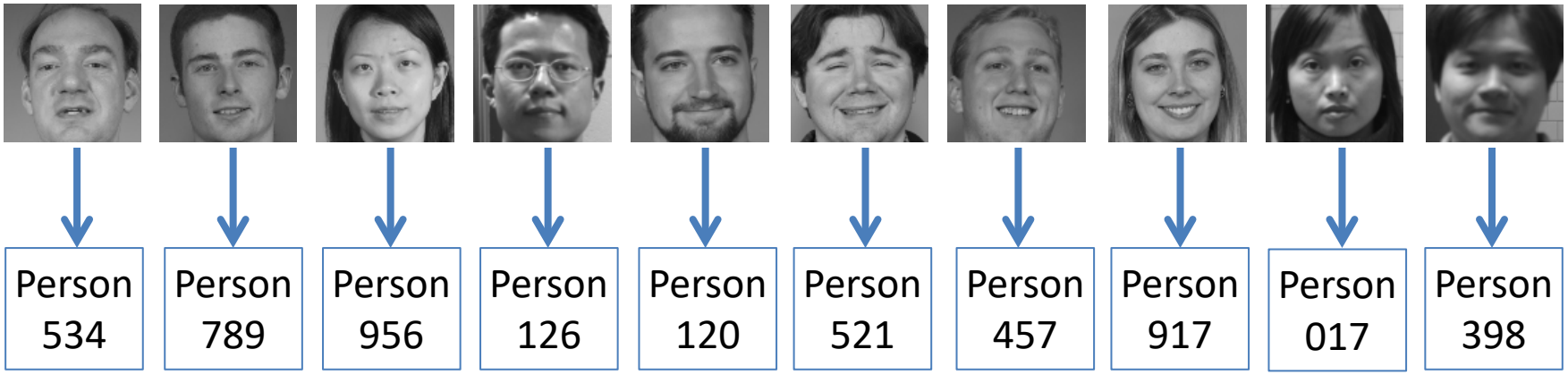
- Example: recognizing the digits of zip codes.
  - The training set consists of images of digits and the names of those digits.



# Supervised Learning

- Example: face recognition
  - The training set consists of images of faces and the IDs of those faces.

example inputs



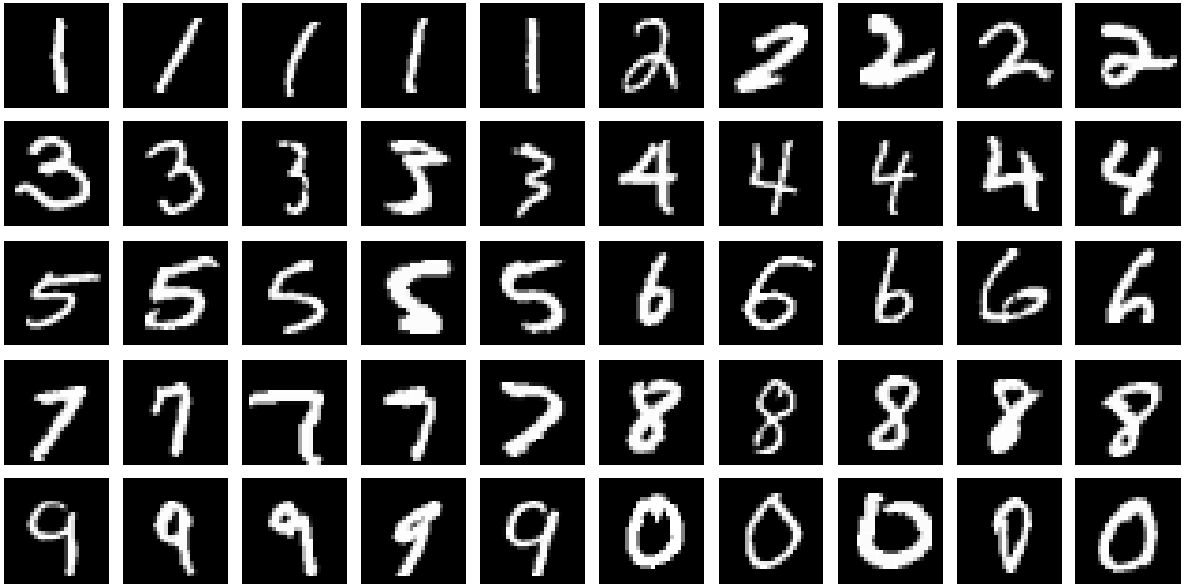

desired outputs (class labels)

# Regression, Classification, Pattern Recognition

- When the desired output belongs to one of a **finite** number of categories, then the supervised learning problem is called a **classification** problem.
- When the desired output contains one or more values from a continuous space, then the supervised learning problem is called a **regression** problem.

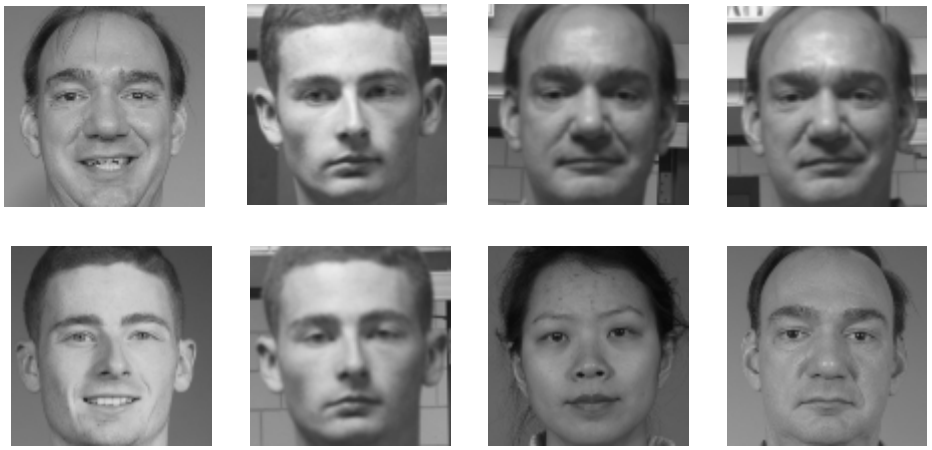
# Unsupervised Learning

- No example outputs are given to the learning algorithm, leaving it on its own to find structure in its input.
- Example: figure out how many different types of digits appear in this set:



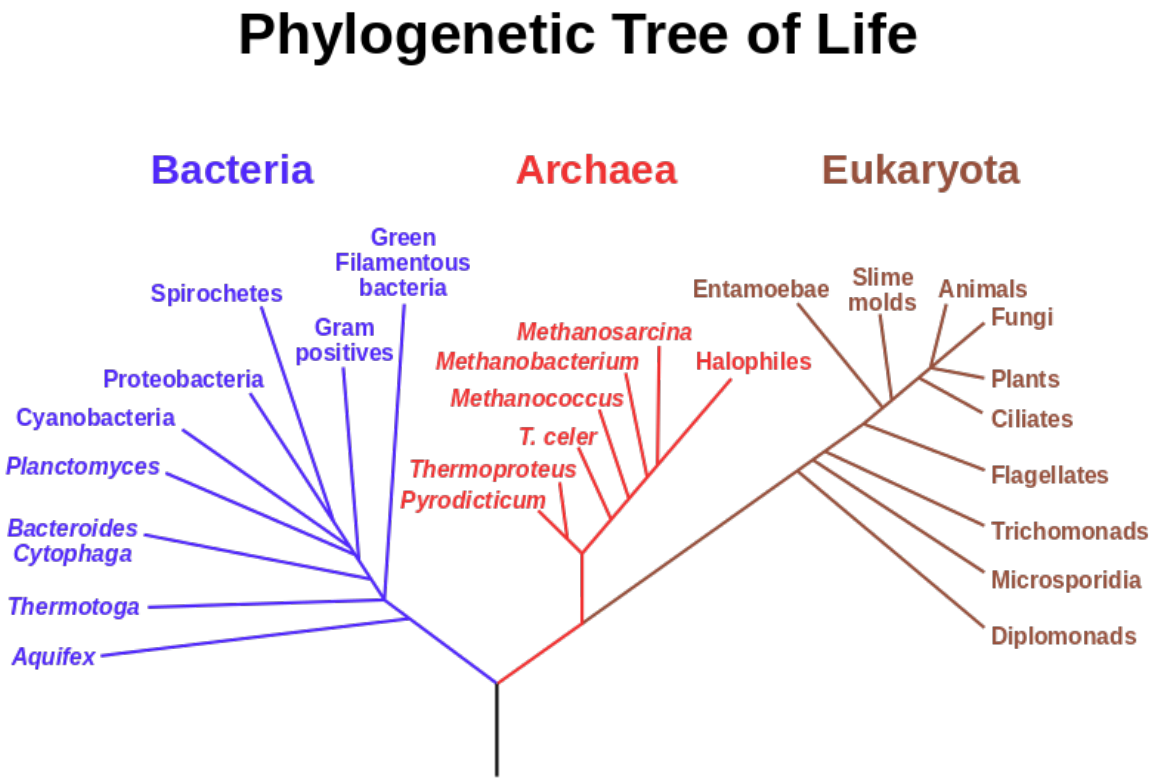
# Unsupervised Learning

- No example outputs are given to the learning algorithm, leaving it on its own to find structure in its input.
- Example: figure out how many different people appear in this set of face photos:



# Applications of Unsupervised Learning

- Clustering.
  - E.g., categorize living organisms into hierarchical groups.




Source: https://en.wikipedia.org/wiki/Phylogenetic_tree

# Applications of Unsupervised Learning

- Anomaly detection.
  - Figure out if someone at an airport is behaving abnormally, which may be a sign of danger.
  - Figure out if an engine is behaving abnormally, which may be a sign of malfunction/damage.
- This can also be treated as a supervised learning problem, if someone provides training examples that are labeled as "anomalies".
- If it is treated as an unsupervised learning problem, then an anomaly model must be built without such training examples.

# Reinforcement Learning

- Learn what actions to take so as to maximize reward.
- Correct pairs of input/output are not presented to the system.
- The system needs to explore different actions at different situations, to see what rewards it gets.
- However, the system also needs to exploit its knowledge so as to maximize rewards.
  - Problem: what is the optimal balance between exploration and exploitation?

# Applications of Reinforcement Learning

- A robot learning how to move a robotic arm, or how to walk on two legs.
- A car learning how to drive itself.
- A computer program learning how to play a board game, like chess, tic-tac-toe, etc.

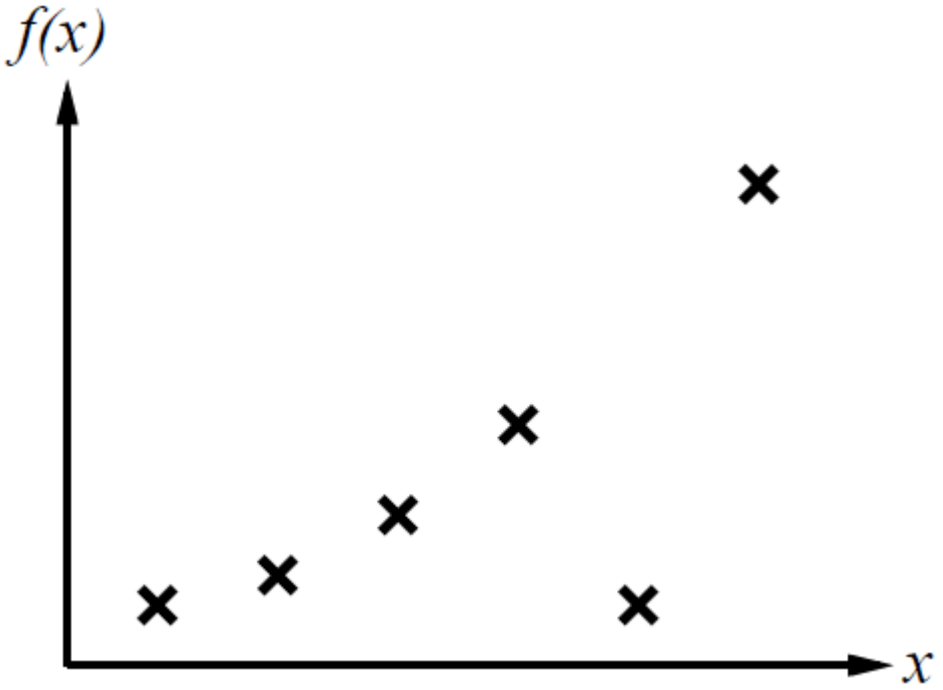
# Machine Learning and Pattern Recognition

- Machine learning and pattern recognition are **not** the same thing.
  - This is a point that confuses many people.
- You can use machine learning to learn things that are not classifiers. For example:
  - Learn how to walk on two feet.
  - Learn how to grasp a medical tool.
- You can construct classifiers without machine learning.
  - You can hardcode a bunch of rules that the classifier applies to each pattern in order to estimate its class.
- However, machine learning and pattern recognition are heavily related.
  - A big part of machine learning research focuses on pattern recognition.
  - Modern pattern recognition systems are usually exclusively based on machine learning.

# Topics for This Semester

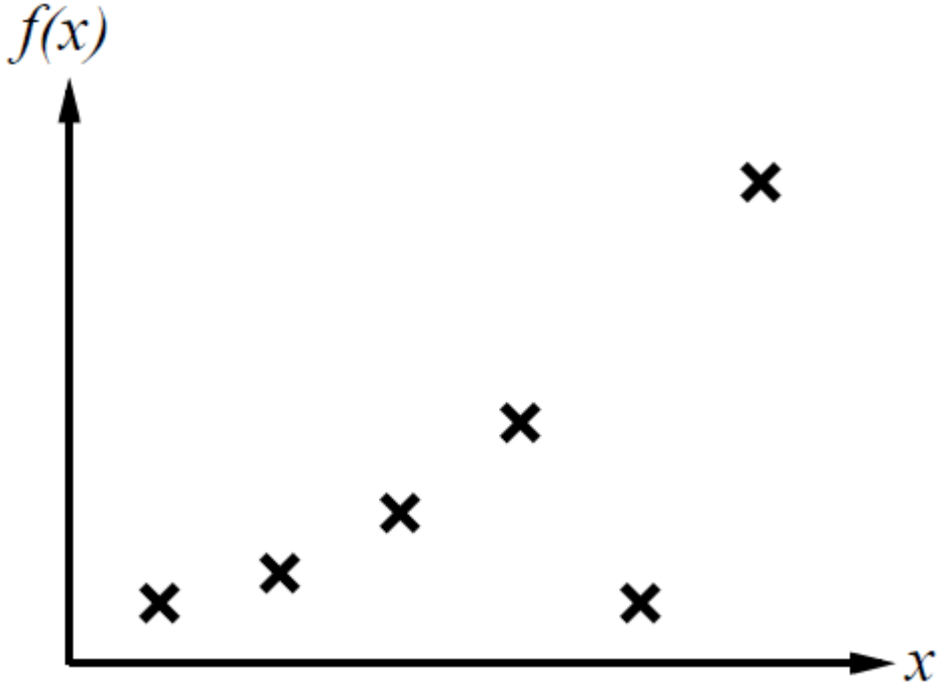
- Main emphasis: supervised learning.
- We will study several different approaches:
  - Bayesian classifiers.
  - Linear Regression.
  - Logistic Regression.
  - Neural networks.
  - Decision trees.
- Towards the end, we will briefly study unsupervised learning (clustering) and reinforcement learning.

# A Simple Learning Task



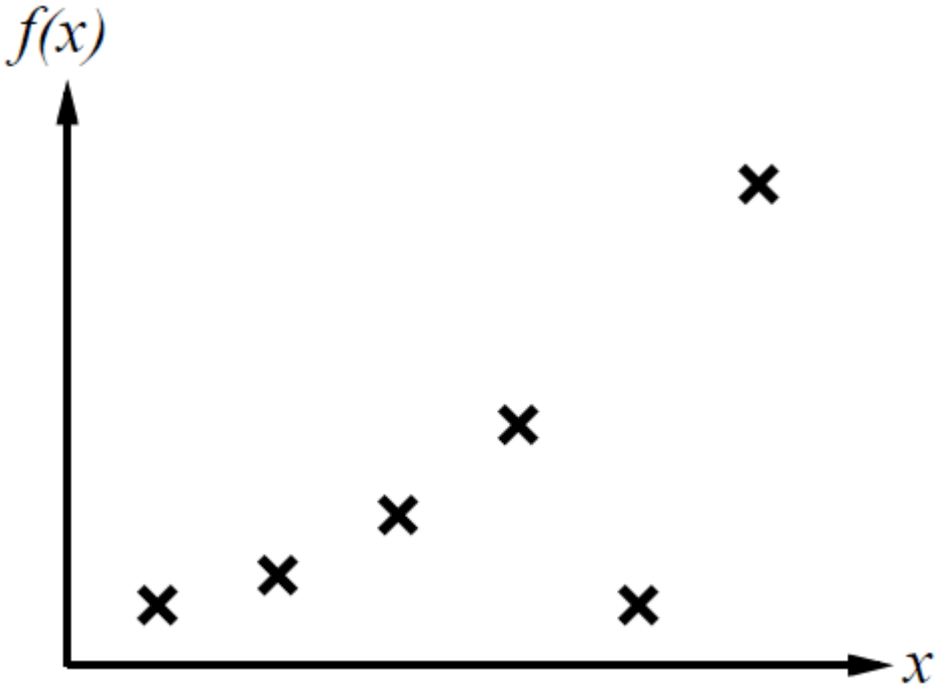

- This is a toy regression example
  - Source. S. Russell and P. Norvig, "Artificial Intelligence: A Modern Approach".
- Here, the input is a single real number.
- The output is also a real number.
- So, our target function $F_{true}$ is a function from the reals to the reals.
  - Usually patterns are much more complex.
  - In this example it is easy to visualize training examples and learned functions.

# A Simple Learning Task



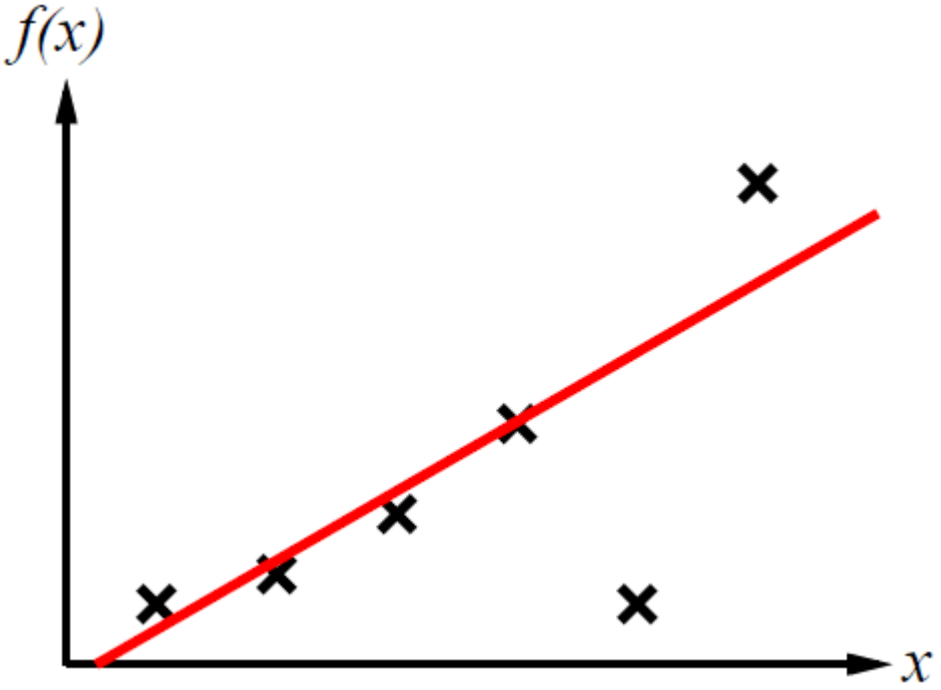

- Each training example is denoted as $(x_n, t_n)$, where:
  - $x_n$ is the example input.
  - $t_n$ is the desired output (also called target output).
- Each example $(x_n, t_n)$ is marked with $\times$ on the figure.
  - $x_n$ corresponds to the x-axis.
  - $t_n$ corresponds to the y-axis.
- Based on the figure, what do you think $F_{true}$ looks like?

# A Simple Learning Task



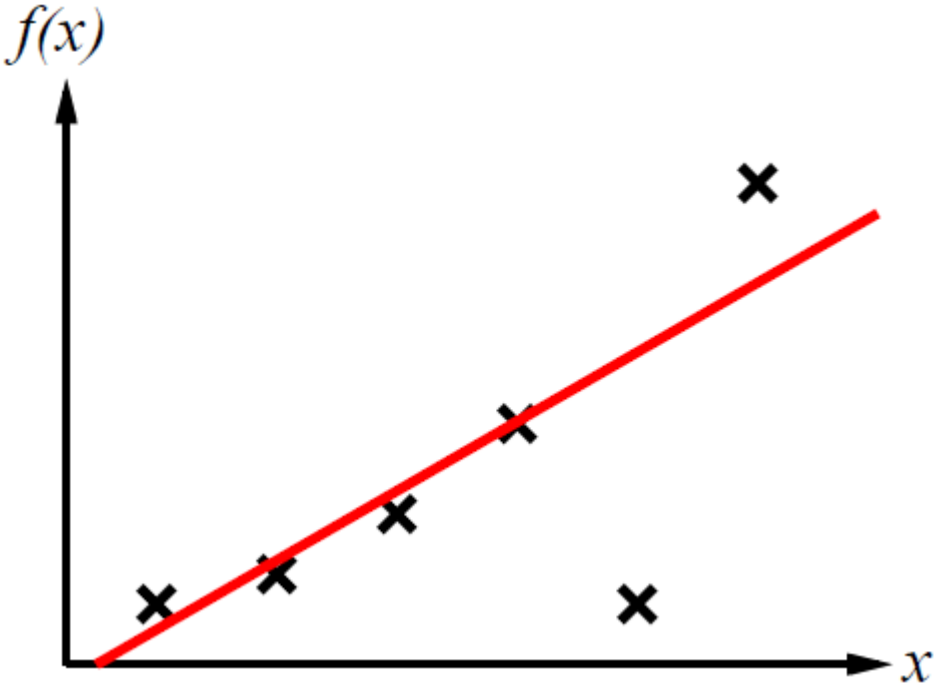

- Different people may give different answers as to what $F_{true}$ may look like.
- That shows the challenge in supervised learning: we can find some plausible functions, but:
  - How do we know which one of them is correct?
  - Given many choices for the function, how can we evaluate each choice?

# A Simple Learning Task



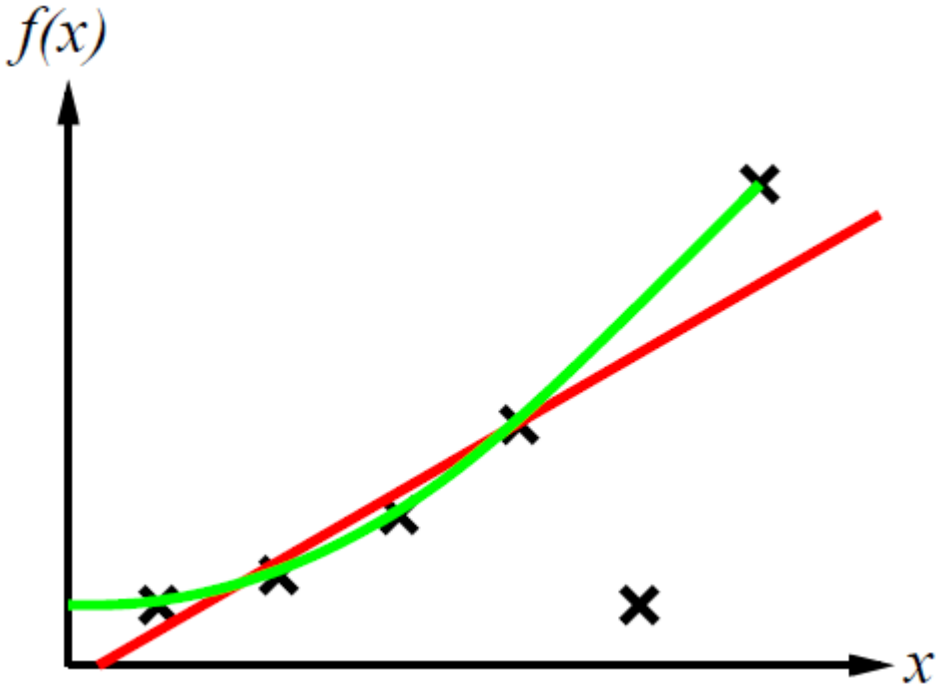

- Here is one possible function F.
- Can anyone guess how it was obtained?

# A Simple Learning Task



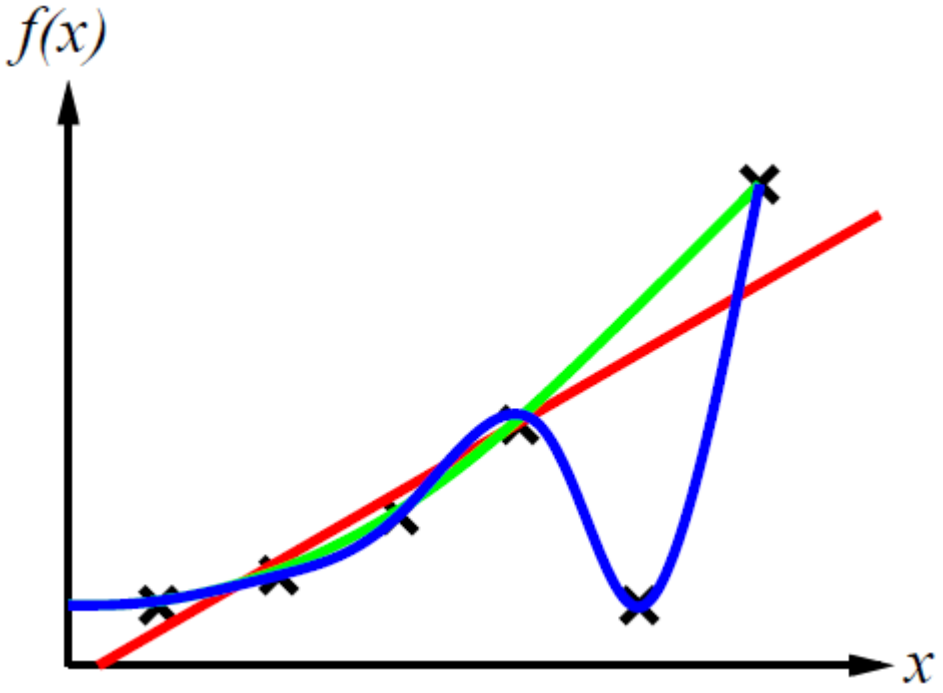

- Here is one possible function F.
- Can anyone guess how it was obtained?
- It was obtained by fitting a line to the training data.

# A Simple Learning Task



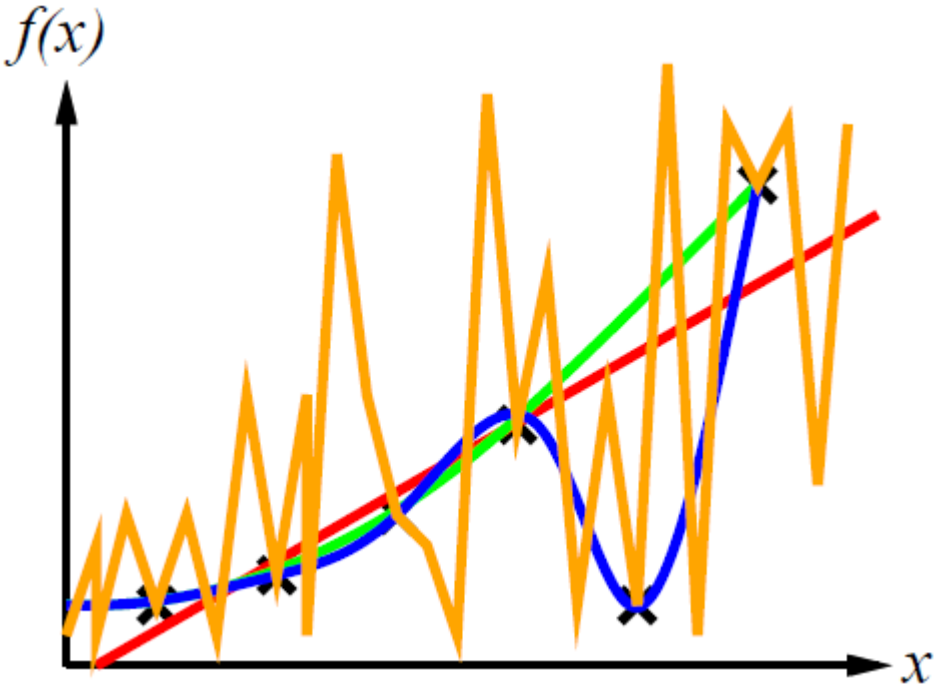

- Here we see another possible function F, shown in green.
- It looks like a quadratic function (second degree polynomial).
- It fits all the data perfectly, except for one.

# A Simple Learning Task



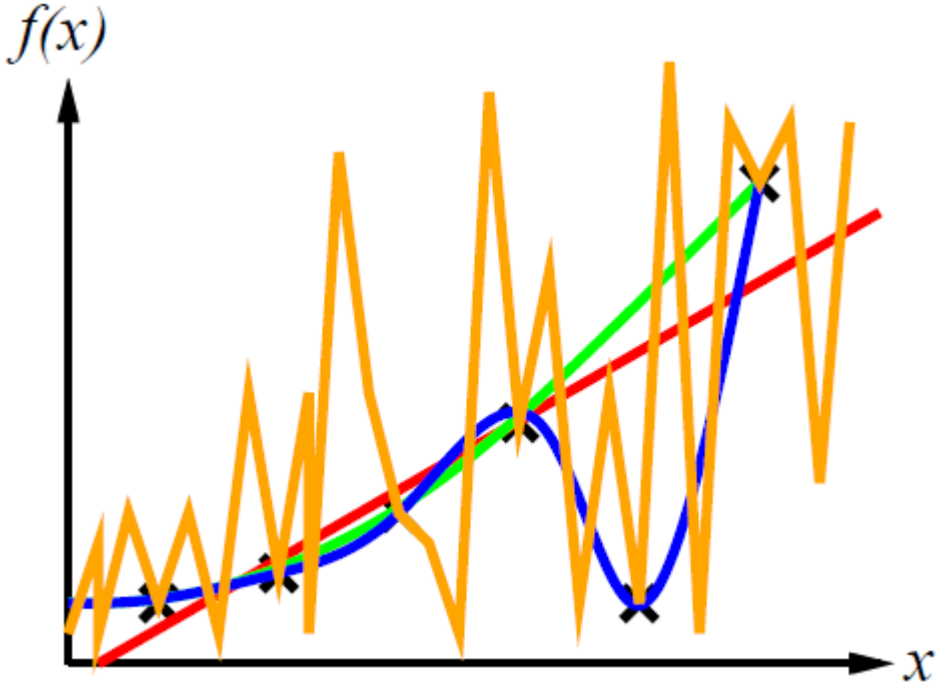

- Here we see a third possible function F, shown in blue.
- It looks like a cubic degree polynomial.
- It fits all the data perfectly.

# A Simple Learning Task



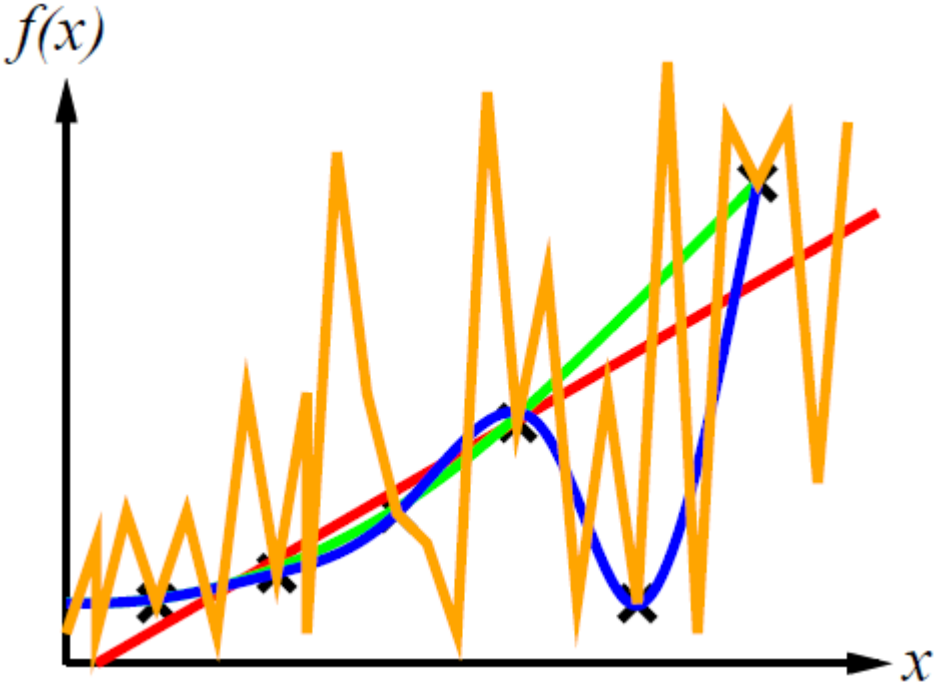

- Here we see a fourth possible function F, shown in orange.
- It zig-zags a lot.
- It fits all the data perfectly.

# The Model Selection Problem



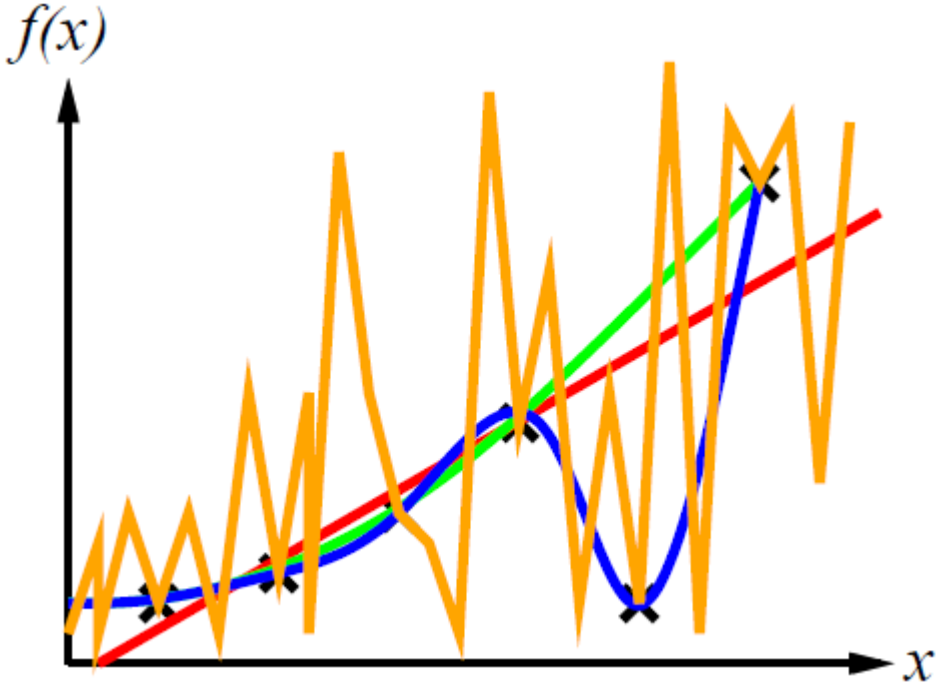

- Overall, we can come up with an infinite number of possible functions here.
- The question is, how do we choose which one is best?
- Or, an easier version, how do we choose a good one.
- This is called the **model selection problem**: out of an infinite number of possible **models** for our data, we must choose one.

# The Model Selection Problem




- An easier version of the model selection problem: given a model (i.e., a function modeling our data), how can we measure how good this model is?
- **What are your thoughts on this?**

# A Simple Learning Task

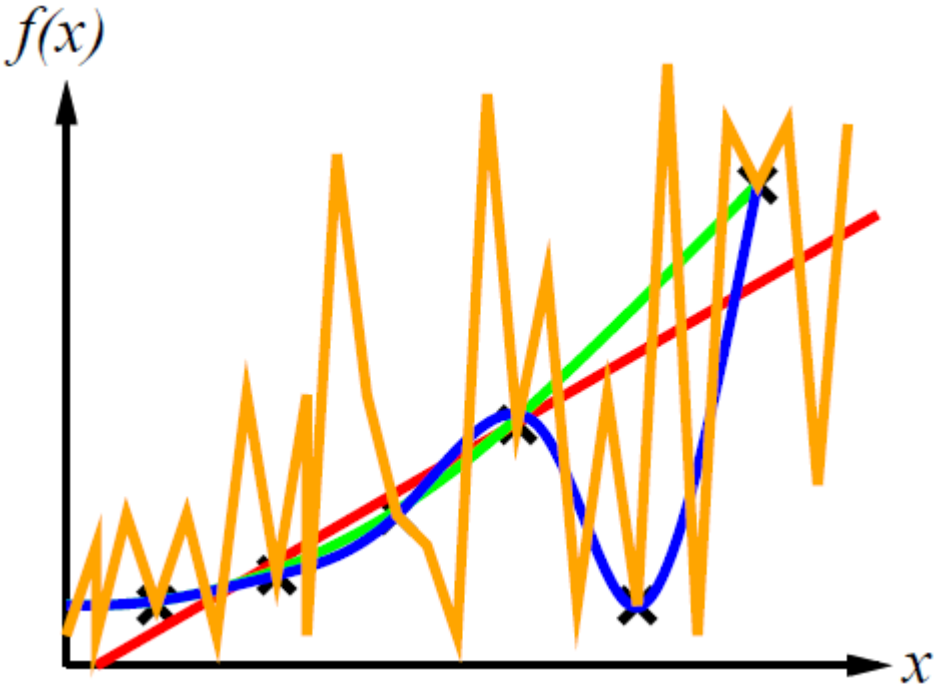



- One naïve solution is to evaluate functions based on **training error**.
- For any function F, its training error can be measured as a sum of squared errors over training patterns $x_n$:

$$\sum_n (t_n - F(x_n))^2$$

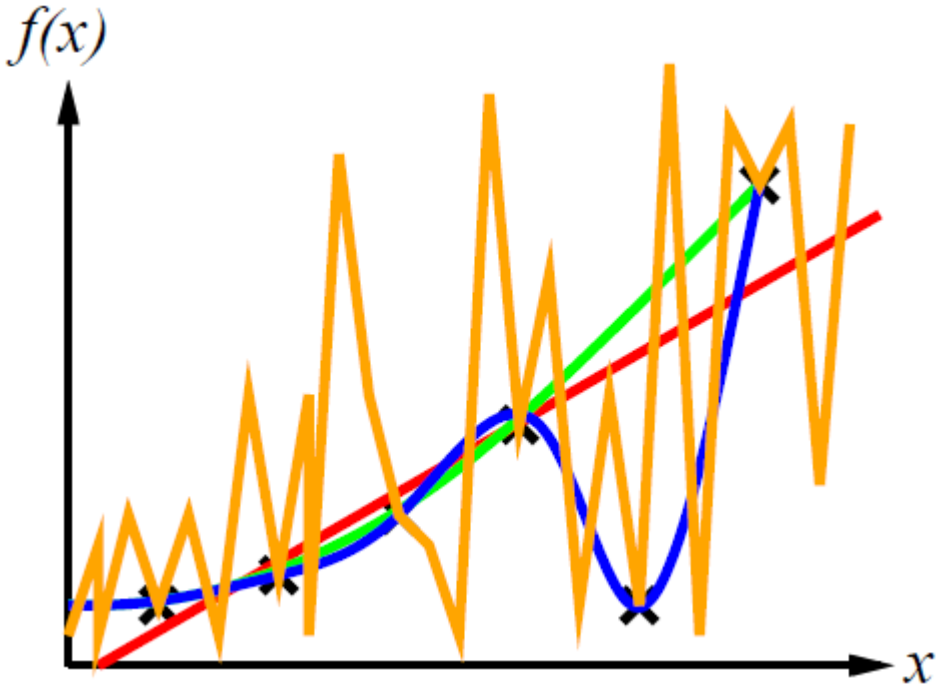
- What are the pitfalls of choosing the "best" function based on training error?

# A Simple Learning Task



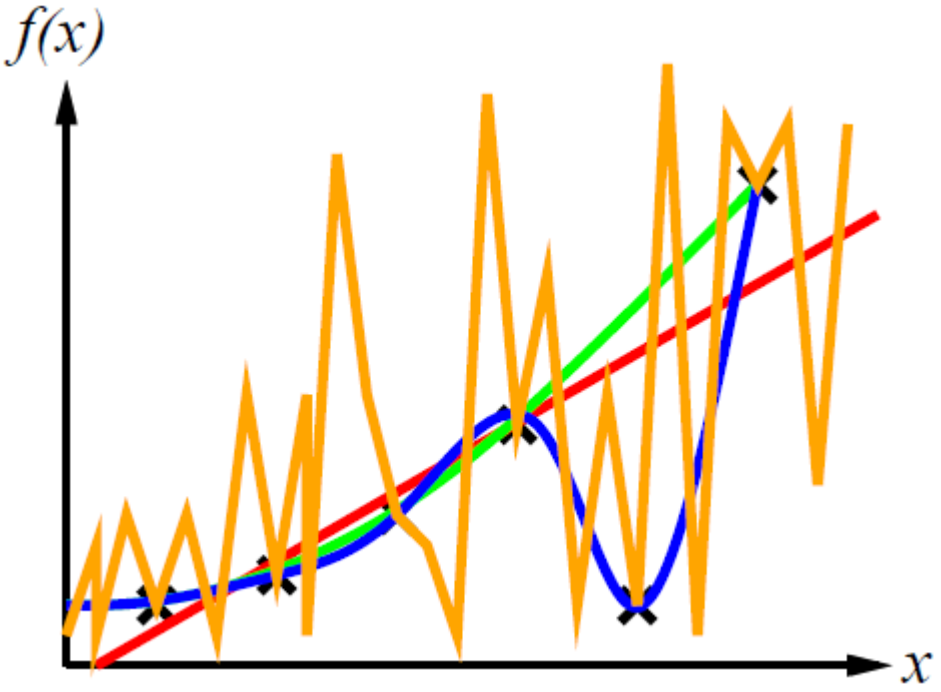

- What are the pitfalls of choosing the “best” function based on training error?
- The zig-zagging orange function comes out as “perfect”: its training error is zero.
- As a human, would you find more reasonable the orange function or the blue function (cubic polynomial)?
  - They both have zero training error.

# A Simple Learning Task



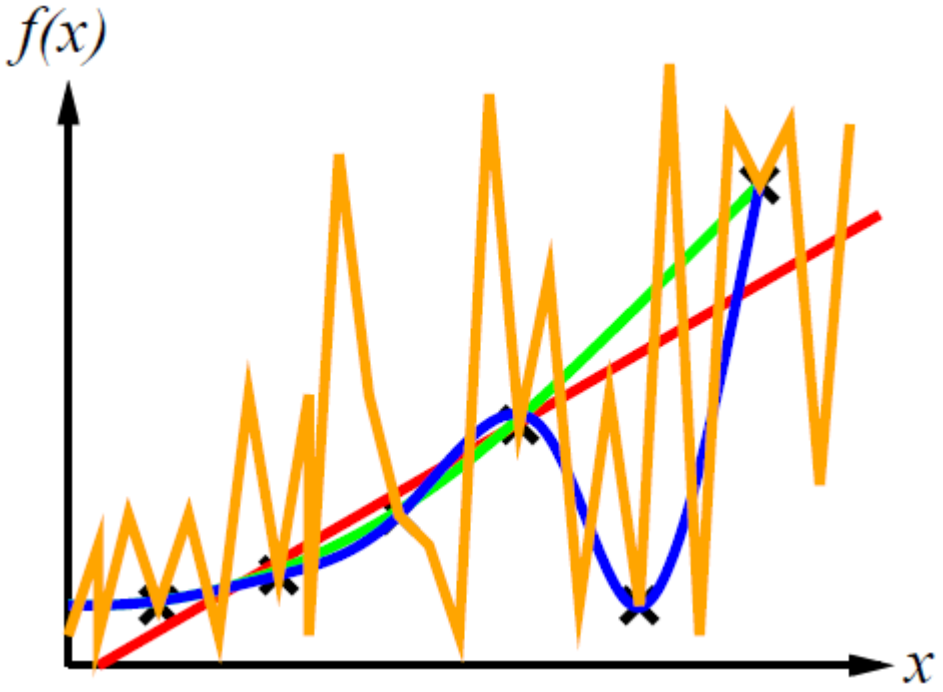

- What are the pitfalls of choosing the “best” function based on training error?
- The zig-zagging orange function comes out as “perfect”: its training error is zero.
- As a human, would you find more reasonable the orange function or the blue function (cubic polynomial)?
  - They both have zero training error.
  - However, the zig-zagging function looks pretty arbitrary.

# A Simple Learning Task



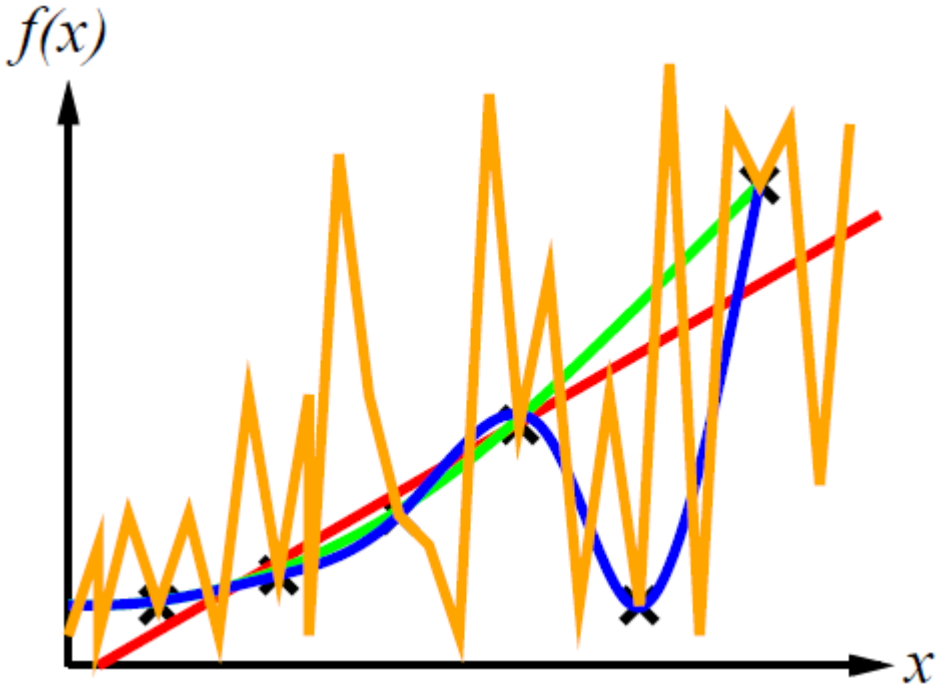

- Ockham's razor: given two equally good explanations, choose the more simple one.
  - This is an old philosophical principle (Ockham lived in the 14th century).
- Based on that, we prefer a cubic polynomial over a crazy zig-zagging function, because it is more simple, and they both have zero training error.

# A Simple Learning Task



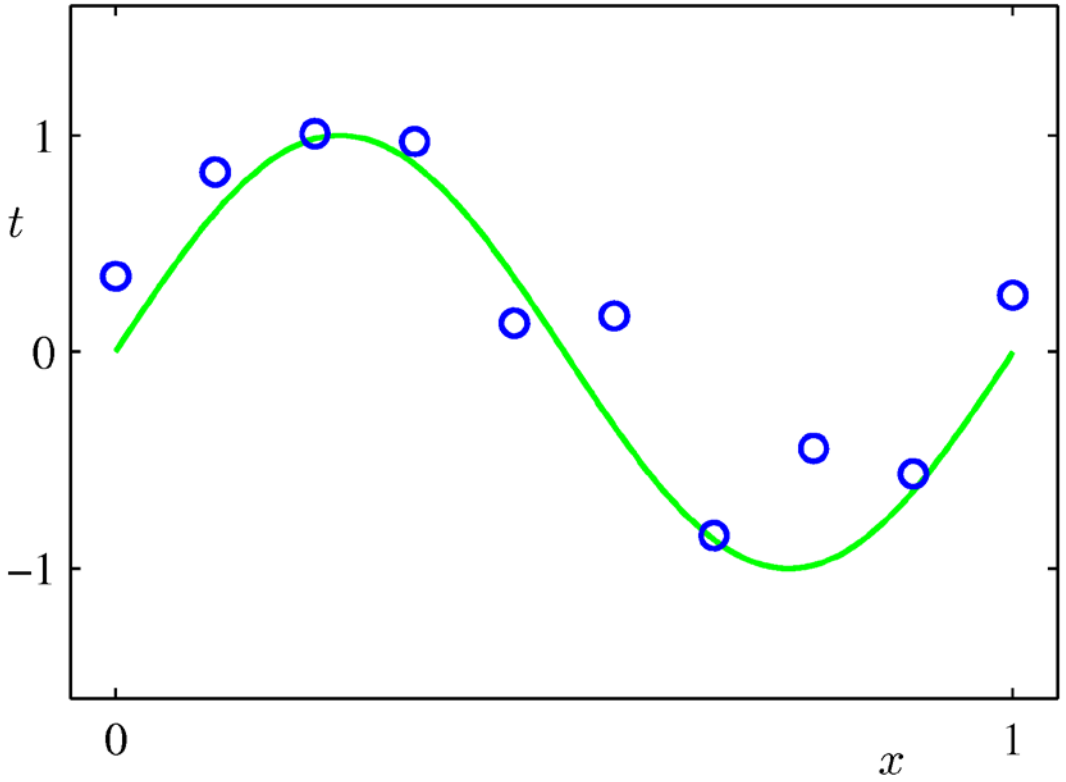

- However, real life is more complicated.
- What if none of the functions have zero training error?
- How do we weigh simplicity versus training error?

# A Simple Learning Task




- However, real life is more complicated.
- What if none of the functions have zero training error?
- How do we weigh simplicity versus training error?
- There is no standard or straightforward solution to this.
- There exist many machine learning algorithms. Each corresponds to a different approach for resolving the trade-off between simplicity and training error.

# Another Example



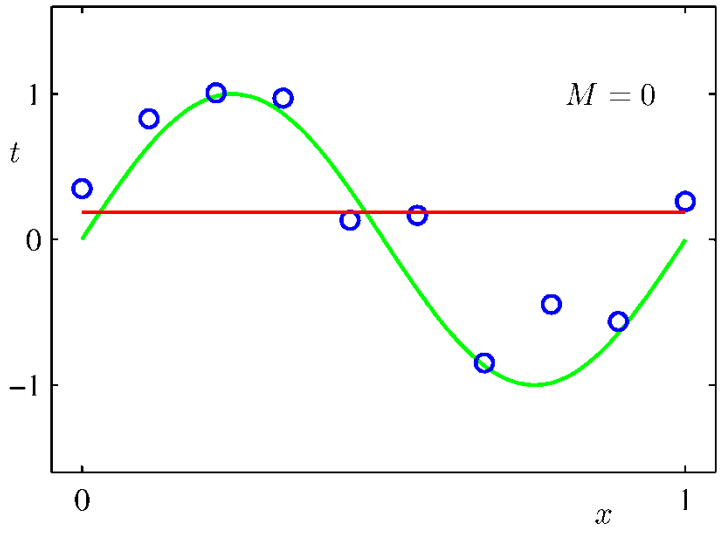

- The data here was generated as follows:
- Given $x_n$:
  - $t_n$ = $\sin(2\pi x_n)$ + noise.
  - Noise was randomly sampled from a Gaussian distribution.
- The green curve shows $\mathrm{f(x)} = \sin(2\pi x)$ without noise.
- The blue circles show the actual training examples, which are not exactly on the line because of the added noise.

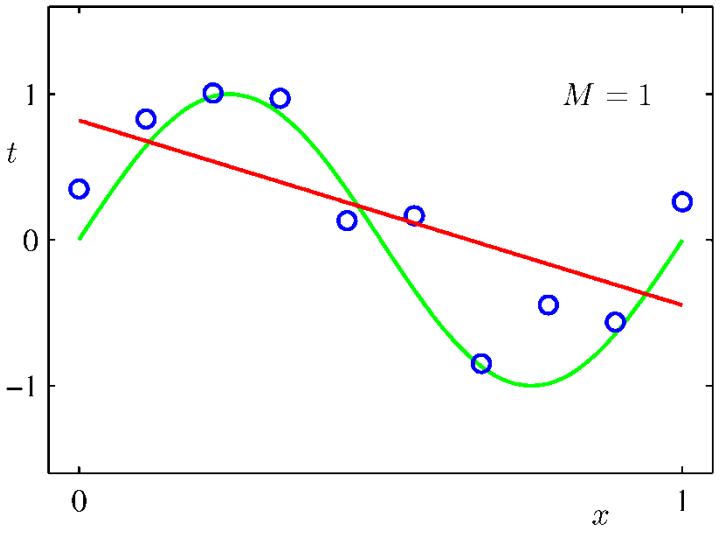
# Polynomial Fitting

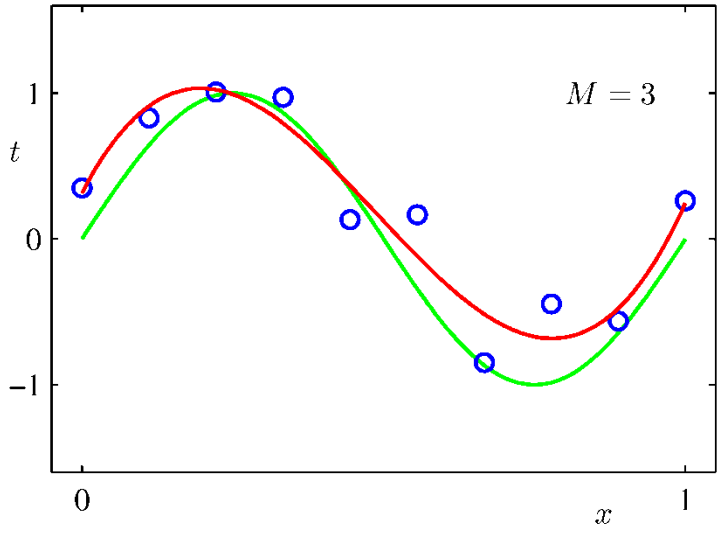
- Given the training data, if we know that the generating function is $\sin(2\pi x)$, or $\sin(cx)$ for some unknown c, the learning task is trivial.
- However, we typically do not know the underlying function.
- One common approach, that we also saw in the previous example, is to try to model the function as a polynomial.
- We estimate the parameters of the polynomial based on the training data.

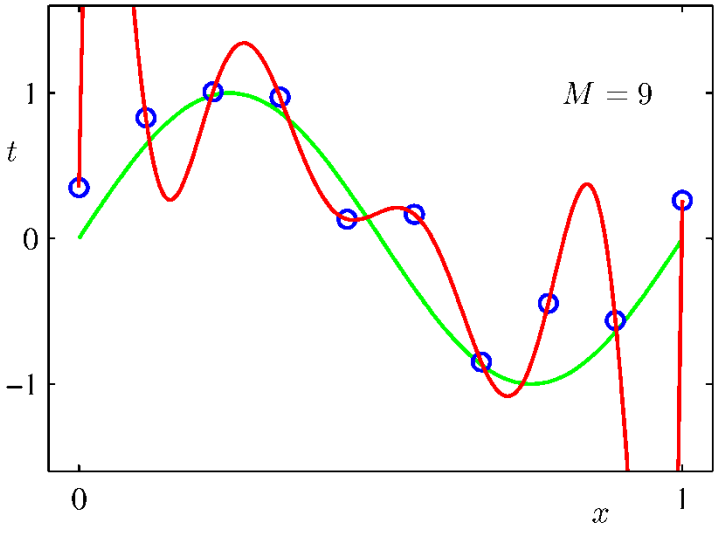
# Polynomial Fitting

Here are estimated polynomials of degrees 0, 1, 3, 9.



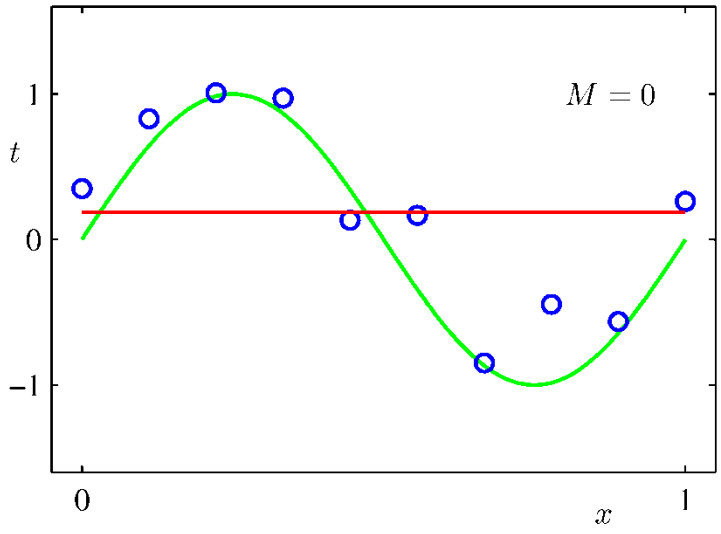



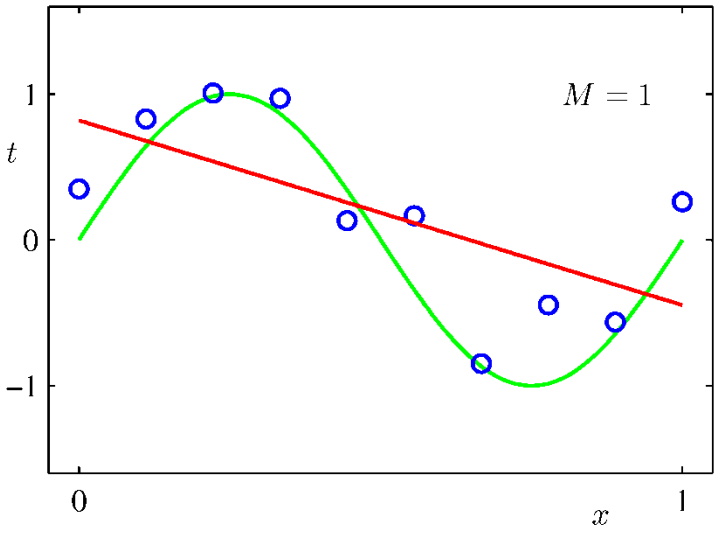



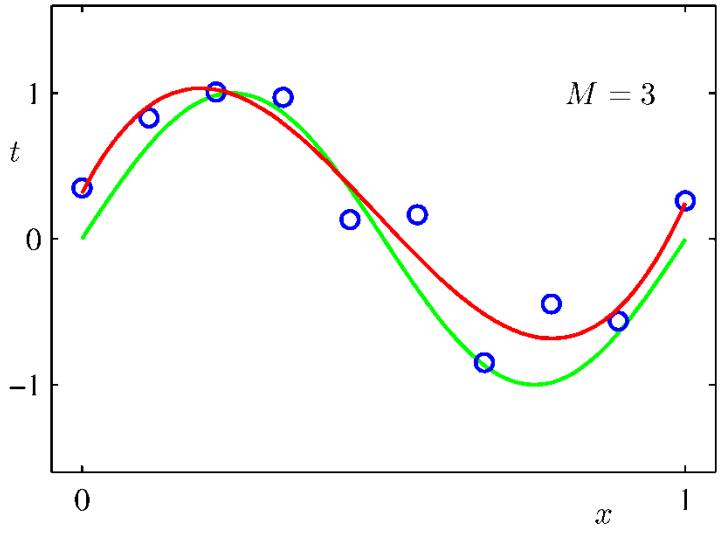



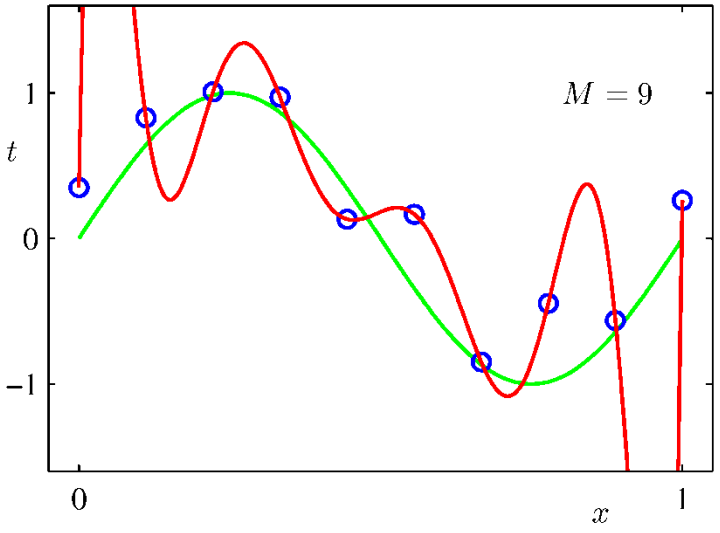
# Polynomial Fitting

Notice the overfitting problem with the 9th degree polynomial.

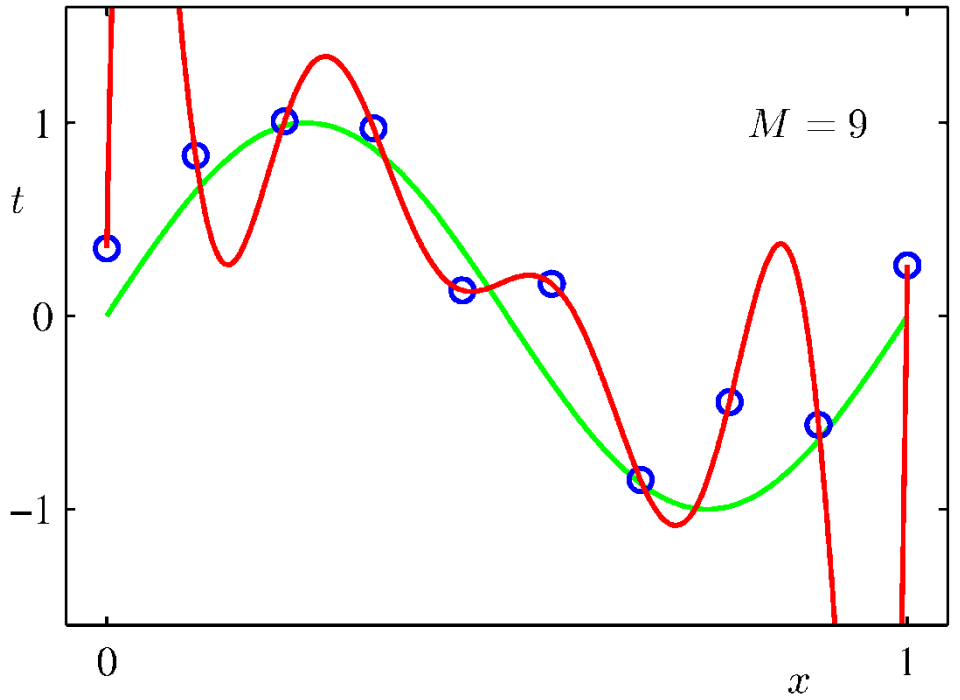


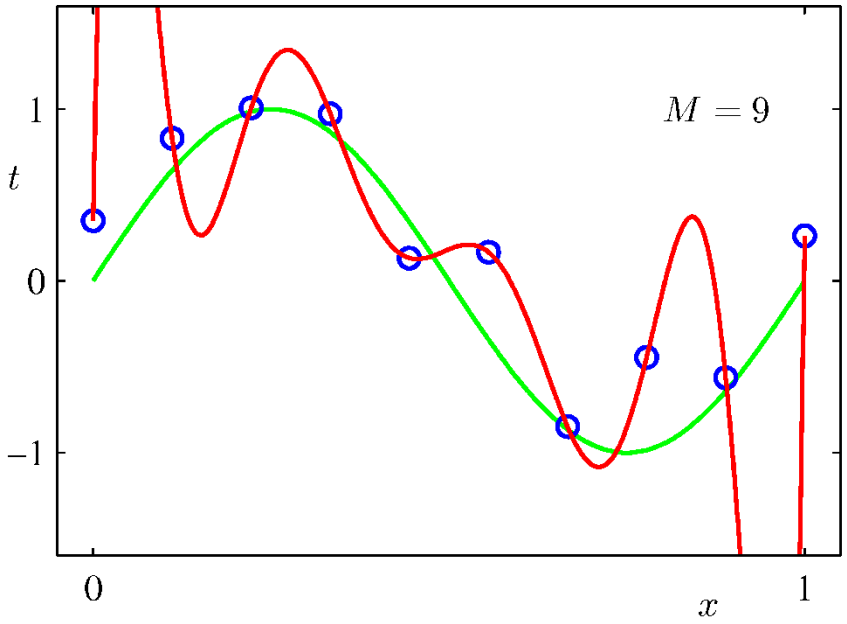
# Overfitting

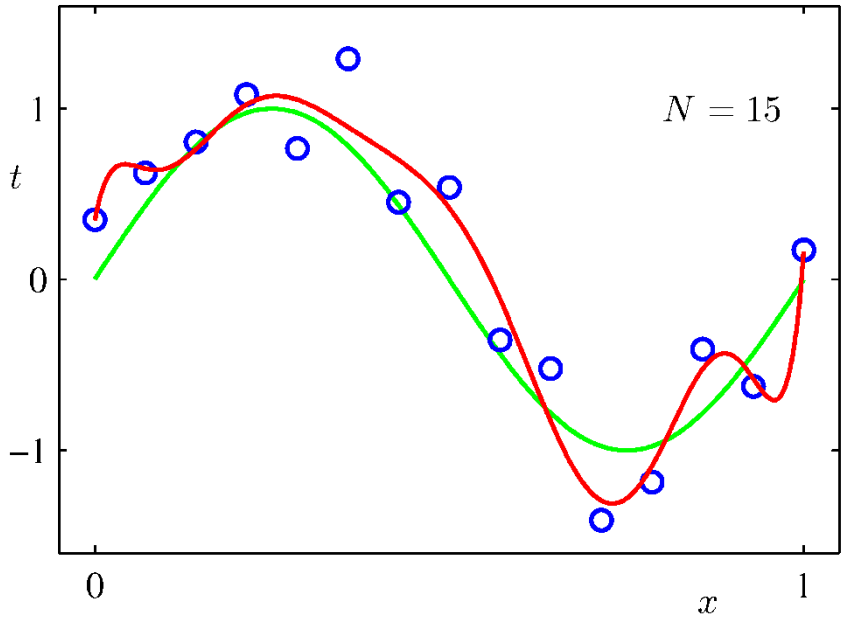


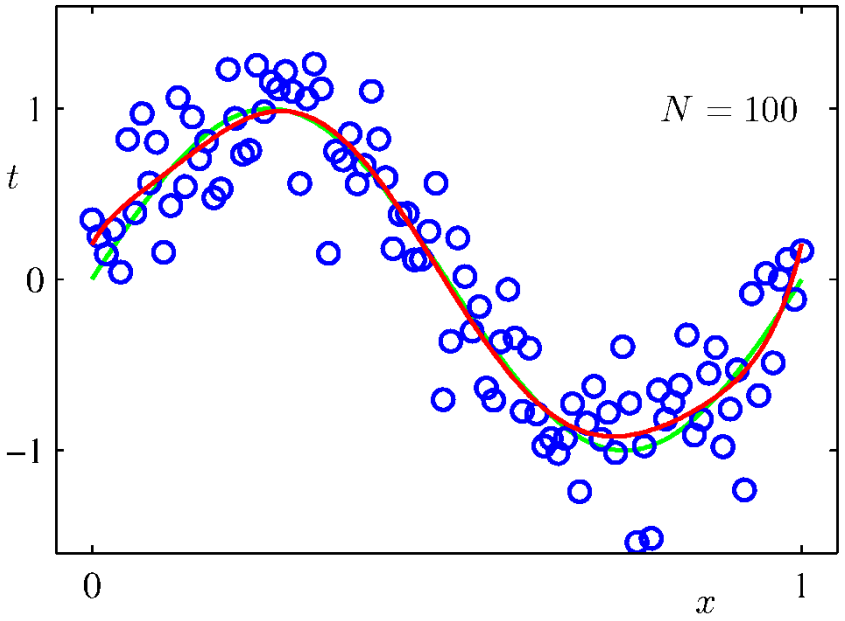

- Overfitting is a **huge** problem in machine learning.
- Overfitting means that the learned function fits very well (or perfectly) the training data, but works very poorly on test data.
- Some times, when our models have too many parameters (like a $9^{th}$ degree polynomial), those parameters get tuned to match the noise in the data.

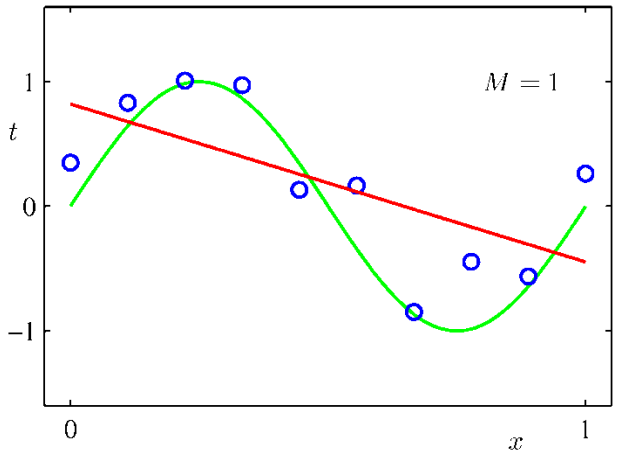
# More Training, Less Overfitting

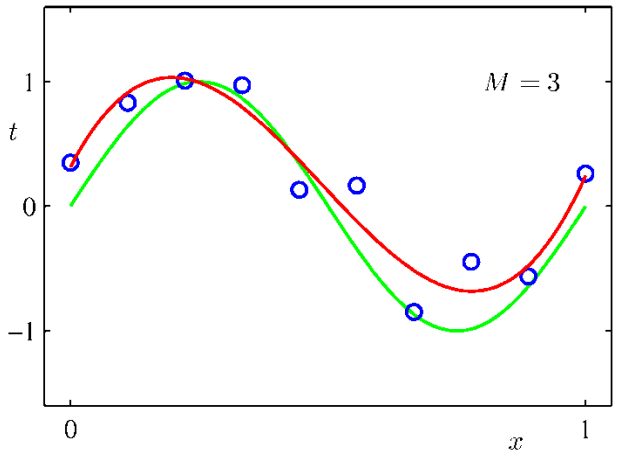
- Increasing the amount of training data (from 10 to 15, and then to 100) reduces overfitting.

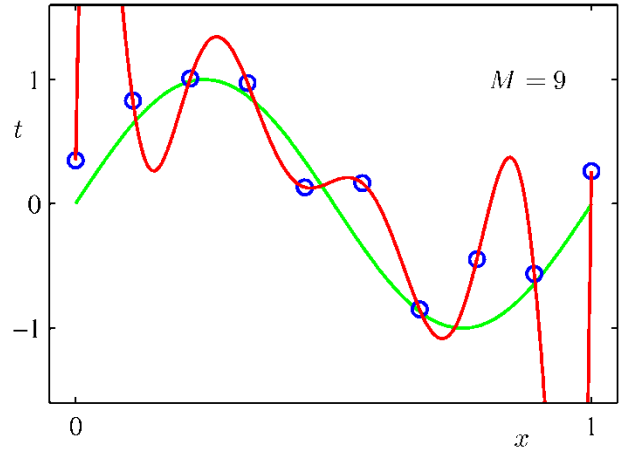




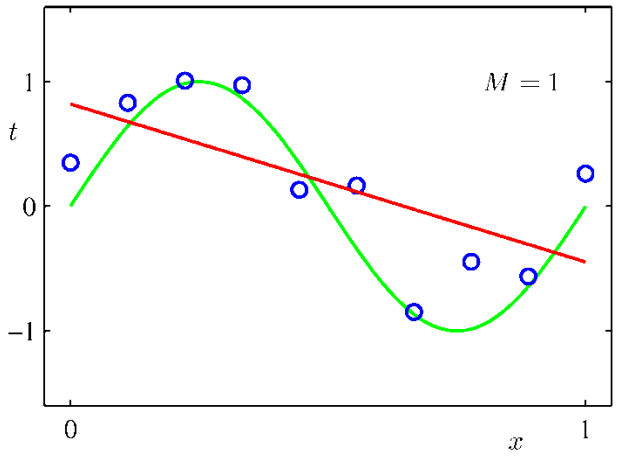



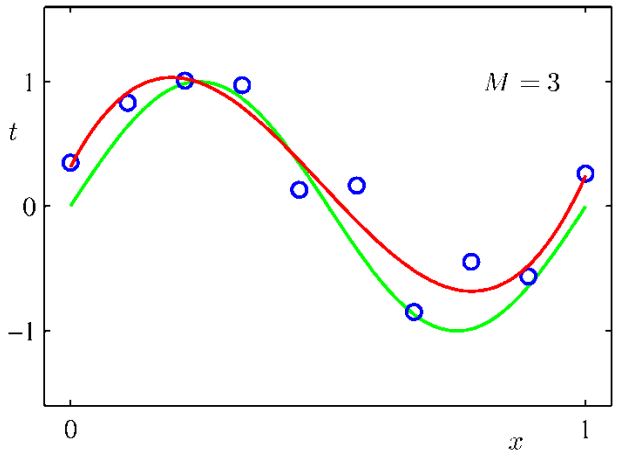



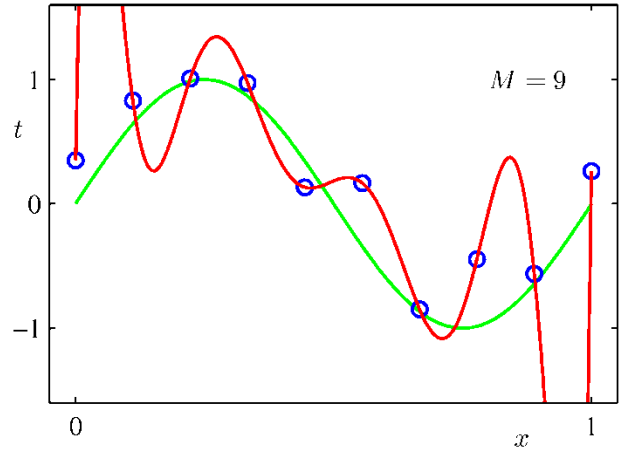

# Regularization

- These are the parameters for some estimated polynomials.

| | Degree 1 | Degree 3 | Degree 9 |
|---|---|---|---|
| $w_0$ | 0.82 | 0.31 | 0.35 |
| $w_1$ | -1.27 | 7.99 | 232.37 |
| $w_2$ | | -25.43 | -5321.83 |
| $w_3$ | | 17.37 | 48568.31 |
| $w_4$ | | | -231639.30 |
| $w_5$ | | | 640042.26 |
| $w_6$ | | | -1061800.52 |
| $w_7$ | | | 1042400.18 |
| $w_8$ | | | -557682.99 |
| $w_9$ | | | 125201.43 |




# Regularization

- Overfitting leads to very large magnitudes of parameters.

| | Degree 1 | Degree 3 | Degree 9 |
|---|---|---|---|
| $w_0$ | 0.82 | 0.31 | 0.35 |
| $w_1$ | -1.27 | 7.99 | 232.37 |
| $w_2$ | | -25.43 | -5321.83 |
| $w_3$ | | 17.37 | 48568.31 |
| $w_4$ | | | -231639.30 |
| $w_5$ | | | 640042.26 |
| $w_6$ | | | -1061800.52 |
| $w_7$ | | | 1042400.18 |
| $w_8$ | | | -557682.99 |
| $w_9$ | | | 125201.43 |

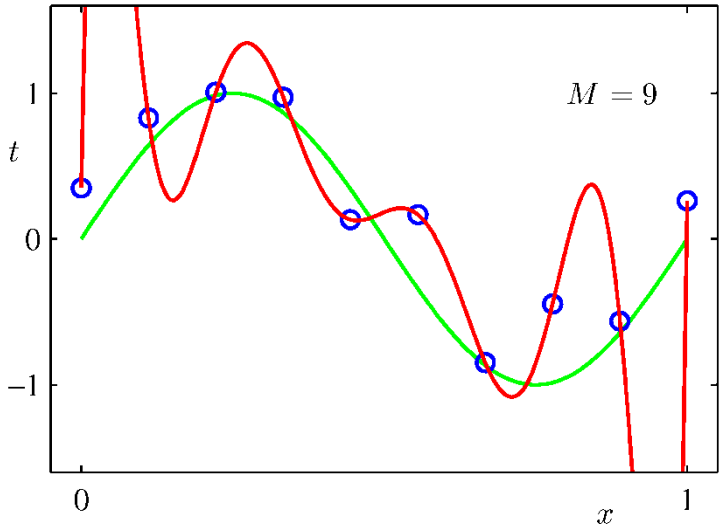
# Regularization

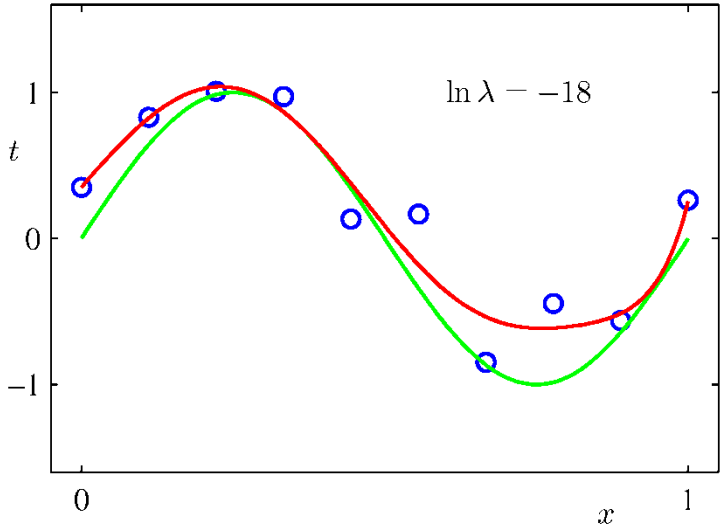
- If we are confident that large magnitudes of polynomial parameters are due to overfitting, we can penalize them in the error function:

$$\left(\sum_n (t_n - F(x_n))^2\right) + \lambda \|w\|^2$$

- The blue part is the sum-of-squares error that we saw before.
- The red part is what is called a **regularization term**.
- $\|w\|^2$ is the sum of squares of the parameters $w_i$.
- $\lambda$ is a parameter that you have to specify.
  - It controls how much you penalize large $\|w\|^2$ values.

# Regularization



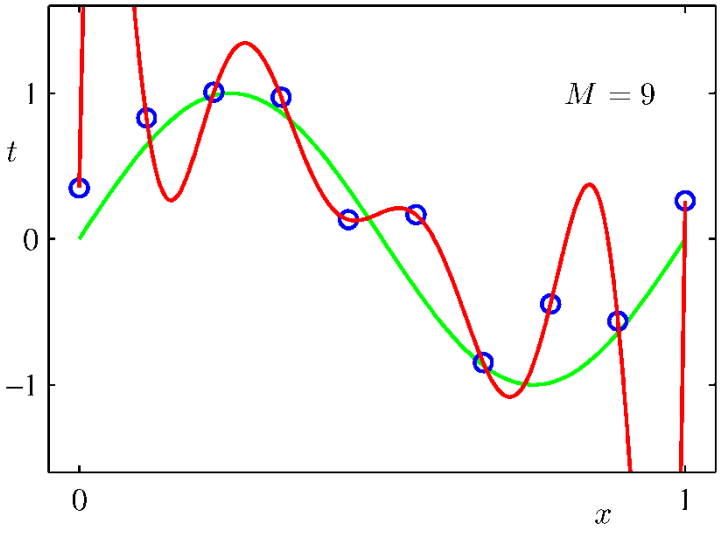

| | $\lambda = 0$ | $\lambda = e^{-18}$ |
|---|---|---|
| $w_0$ | 0.35 | 0.35 |
| $w_1$ | 232.37 | 4.74 |
| $w_2$ | -5321.83 | -0.77 |
| $w_3$ | 48568.31 | -31.97 |
| $w_4$ | -231639.30 | -3.89 |
| $w_5$ | 640042.26 | 55.28 |
| $w_6$ | -1061800.52 | 41.32 |
| $w_7$ | 1042400.18 | -45.95 |
| $w_8$ | -557682.99 | -91.53 |
| $w_9$ | 125201.43 | 72.68 |

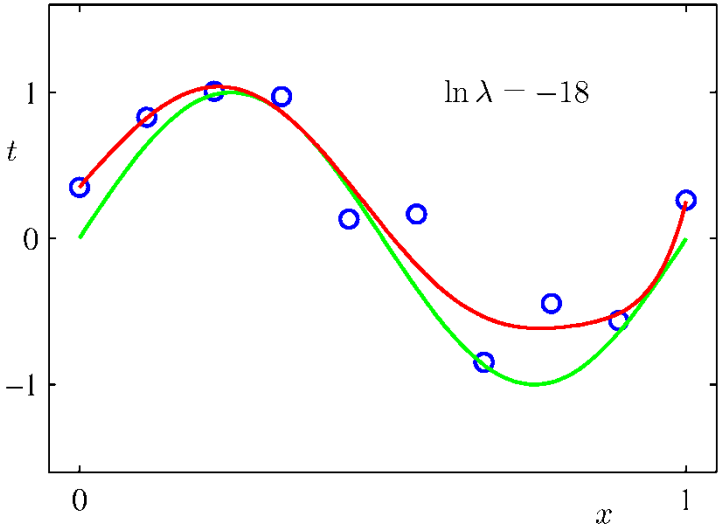
A small λ solves the overfitting problem in this case.

# Hyperparameters

- Parameter $\lambda$ in the previous example is an example of what we call a **hyperparameter**.
- A hyperparameter is a parameter that we (the humans) need to choose, as opposed to parameters that our machine learning algorithm is supposed to learn.
- To find good hyperparameter values:
  - We typically try many different values, and we see which one works best.
  - We typically try how well these values work on a **validation set** (see next slide).

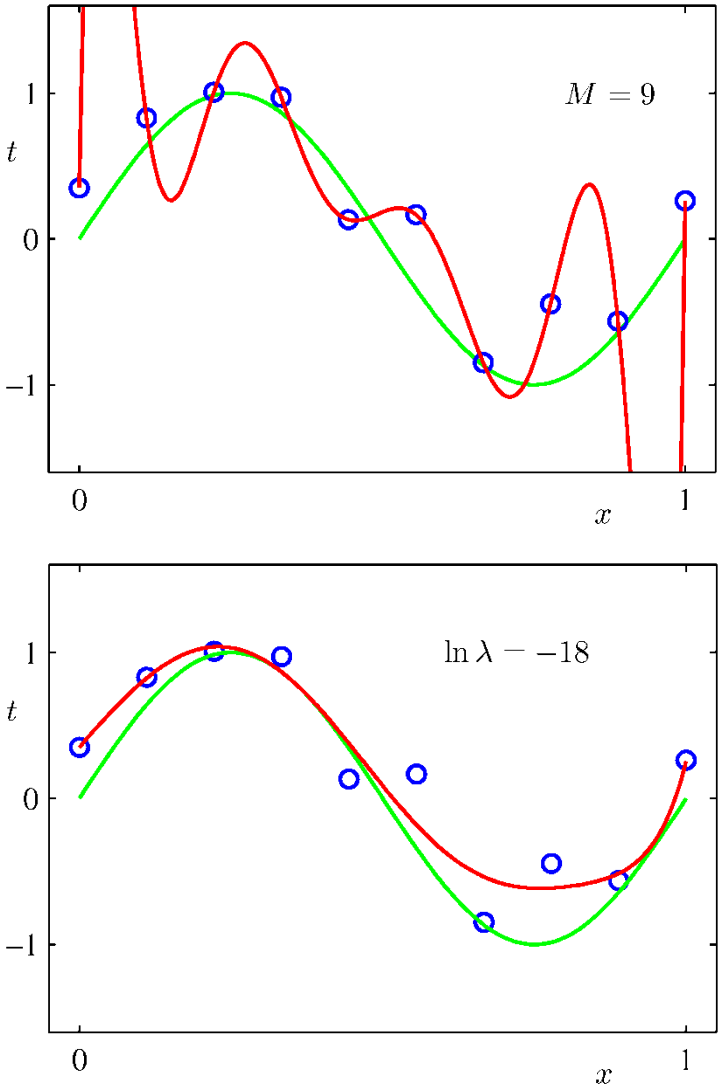
# Using a Validation Set



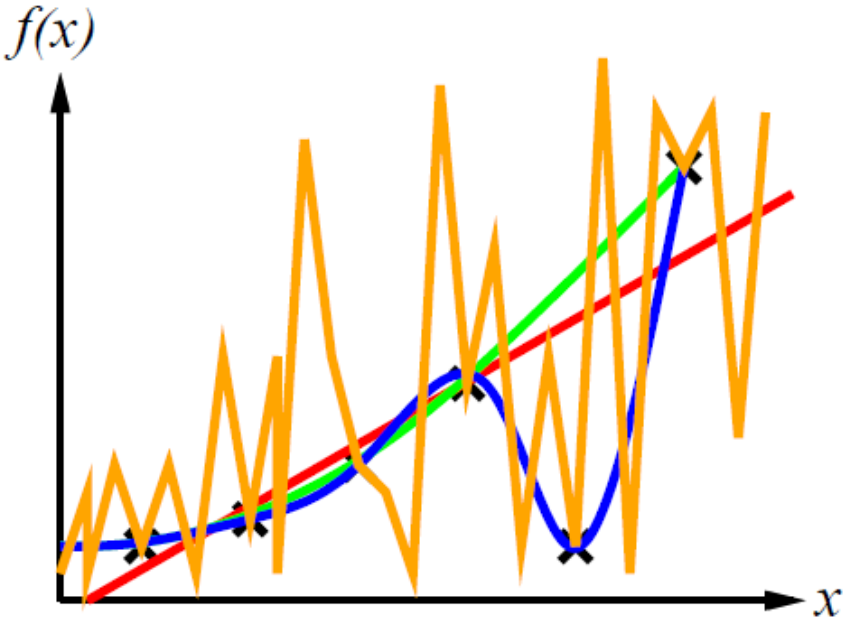

- How can we choose a good value for λ?
- A standard approach is to use a **validation set**.
  - Like the training set, the validation set is a set of example inputs and associated outputs.
  - However, the objects in the validation set should **not** appear in the training set.
- We use the training set to fit polynomials using many different values for λ.
- We choose the λ that gives best results on the validation set.

# Using a Validation Set




- Strictly speaking, choosing a good value for λ is part of the training task.
- Oftentimes, we have a general method for solving a problem, which requires that we choose some hyperparameters.
- Typically, the training set is used to solve our problem multiple times, with different choices of those hyperparameters.
- The validation set is used to decide which choice of hyperparameters works best.

# Using a Test Set




- If we want to evaluate one or more methods, to see how well they work, we use a **test set**.
- Test examples should **not** appear either in the training set or in the validation set.
- Error rates on the test set are a reliable estimate of how well a function generalizes to data outside training.
  - Error rates on the training set are **not** reliable for that task.
  - Error rates on the validation set are still not quite reliable, as the validation set was used to choose some parameters.

# Recap: Training, Validation, Test Sets

- Training set: use to learn the function that we want to learn, that maps inputs to outputs.
- Validation set: use to evaluate different values of hyperparameters (like λ for regularization) that need to be hardcoded during training.
  - Train with different values, and then see how well each resulting function works on the validation set.
- Test set: use to evaluate the final product (after the choice of hyperparameters has been finalized).