Lecture 1 - Linear Regression

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Outline

Resources

Recommended books

- Pattern Recognition and Machine Learning [Bis06]
- Machine Learning: A Probabilistic Perspective [Mur12]
- Machine Learning: The Art and Science of Algorithms That Make Sense of Data [Fla12]

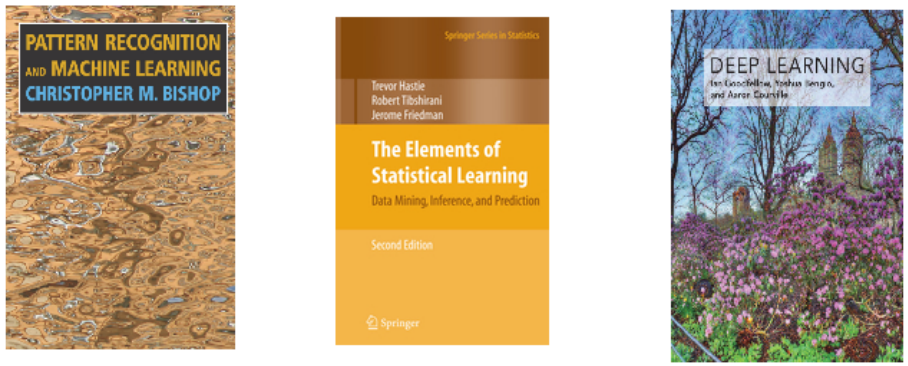

Figure 1: Recommended books

Data Sets

Figure 2: Examples datasets

Problem example

Figure 3: Netflix competition - recommendation systems

Problem visualization

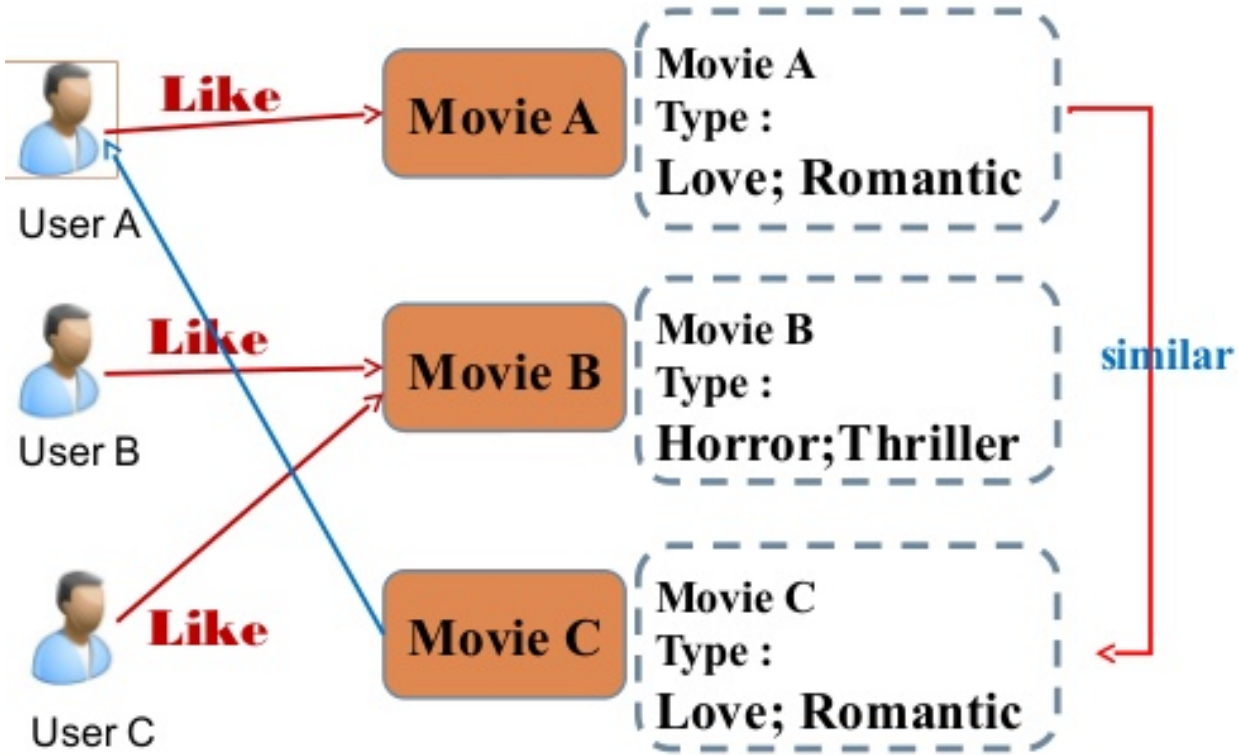

Figure 4: Visual way to describe the problem

Problem: Predicting how a viewer will rate a movie
10% improvement - 1 million dollars
The essence of machine learning:

1. A pattern exists

Problem: Predicting how a viewer will rate a movie
10% improvement - 1 million dollars
The essence of machine learning:

1. A pattern exists
2. There is no way to pin it down mathematically

The components of learning

Formalization:

1. Input x: customer behaviour

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The components of learning

Formalization:

1. Input x: customer behaviour
2. Output y: what movies does the customer like?
3. Target function: f: x $->$ y
4. Data: (x1,y1), (x2,y2), (x3,y3) ... (xn,yn)
5. Hypothesis: g: x $->$ y

Learning model

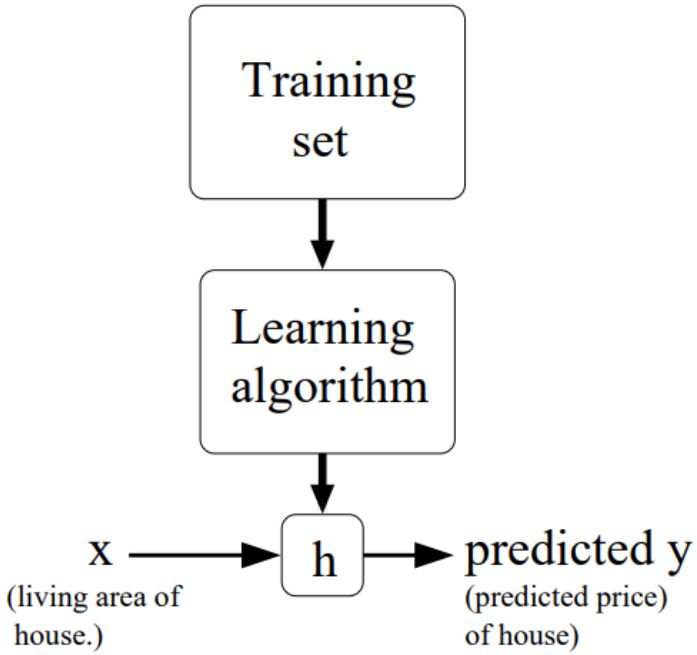


Figure 5: Learning model

Differences between a task and a learning model

...tasks are addressed by models, whereas learning problems are solved by learning algorithms that produce models.[Fla12]

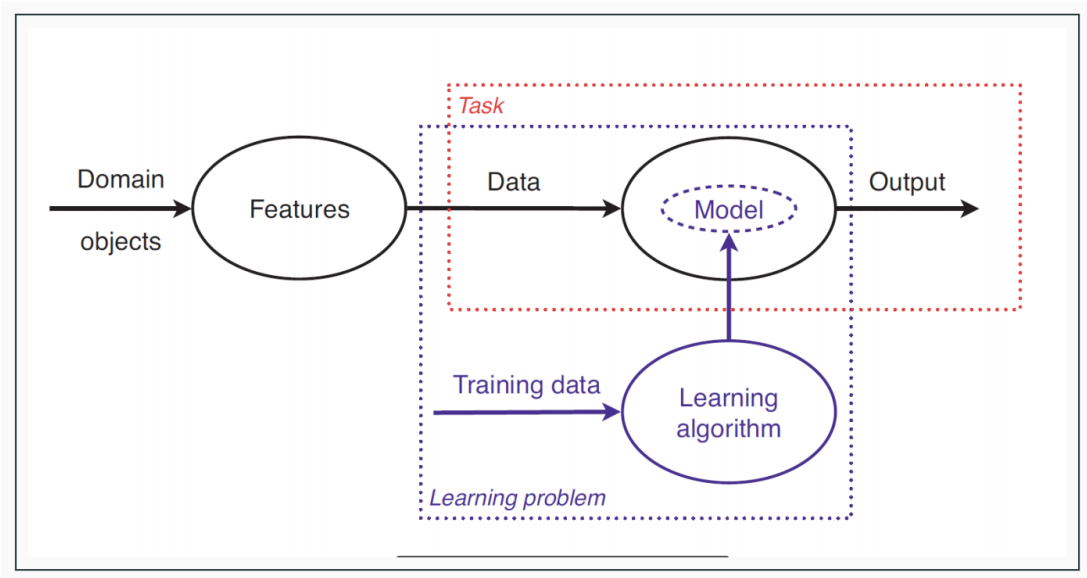
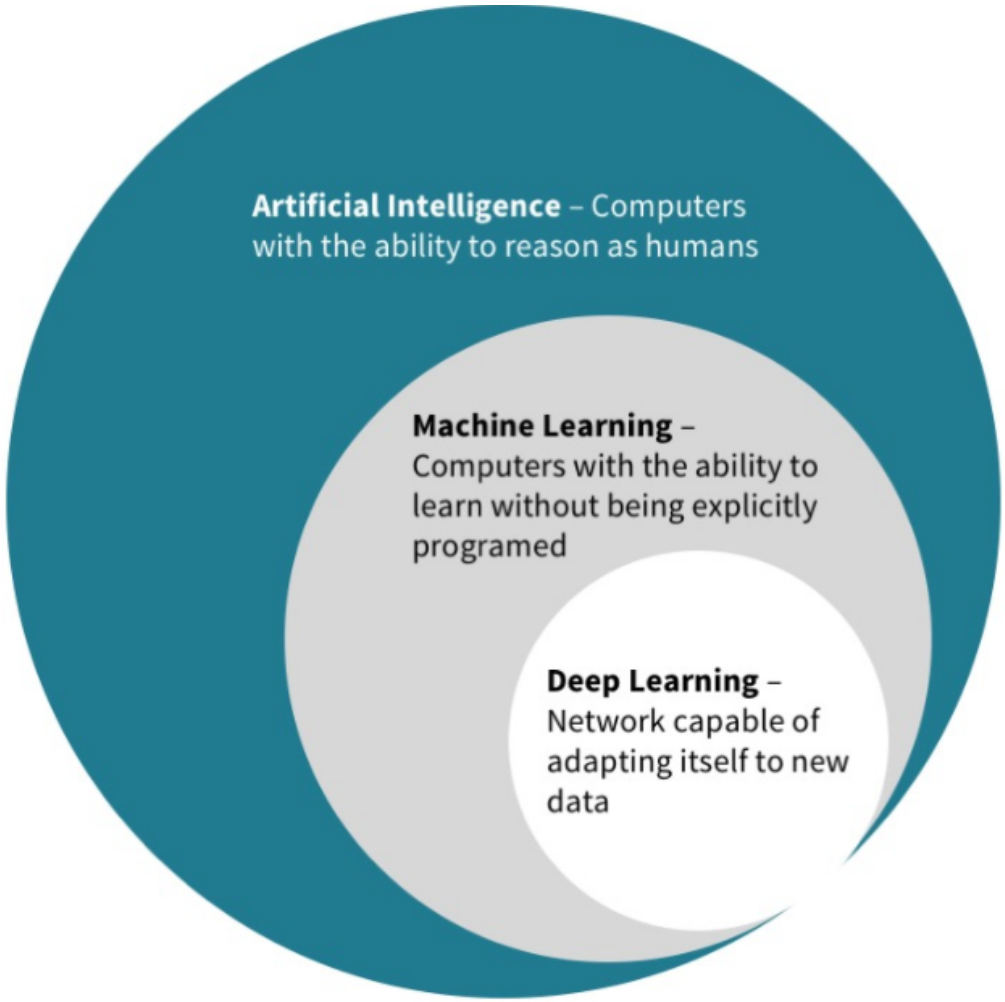


Figure 6: Difference between a task and learning problems

What is Machine Learning?

- Field of study that gives computers the ability to learn without being explicitly programmed. Arthur Samuel, IBM, Stanford University, 1959
- A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E. Tom Mitchell [Mit97]
- Instead of writing a program by hand, we collect lots of examples that specify the correct output for a given input. A machine learning algorithm then takes these examples and produces a program that does the job. Geoffrey Hinton [Hin14]

ML is a subset



ML solves problems with the following shape

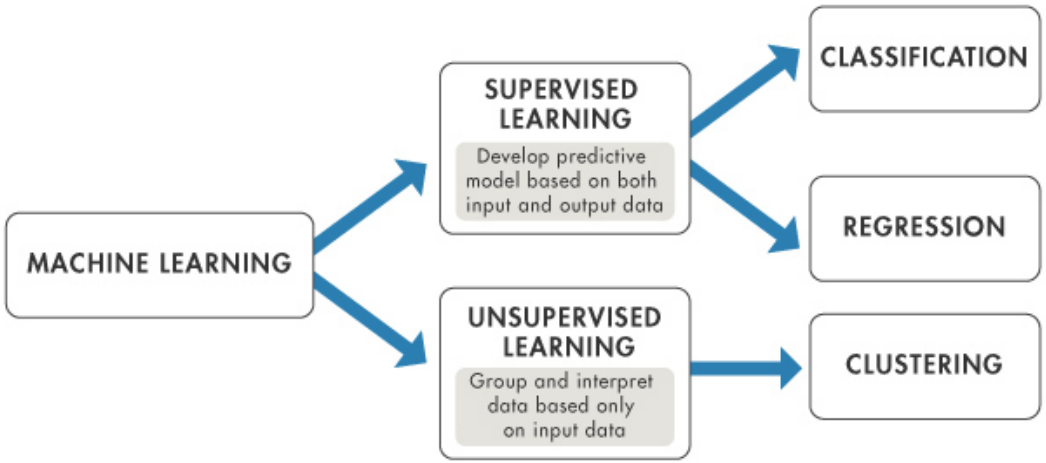
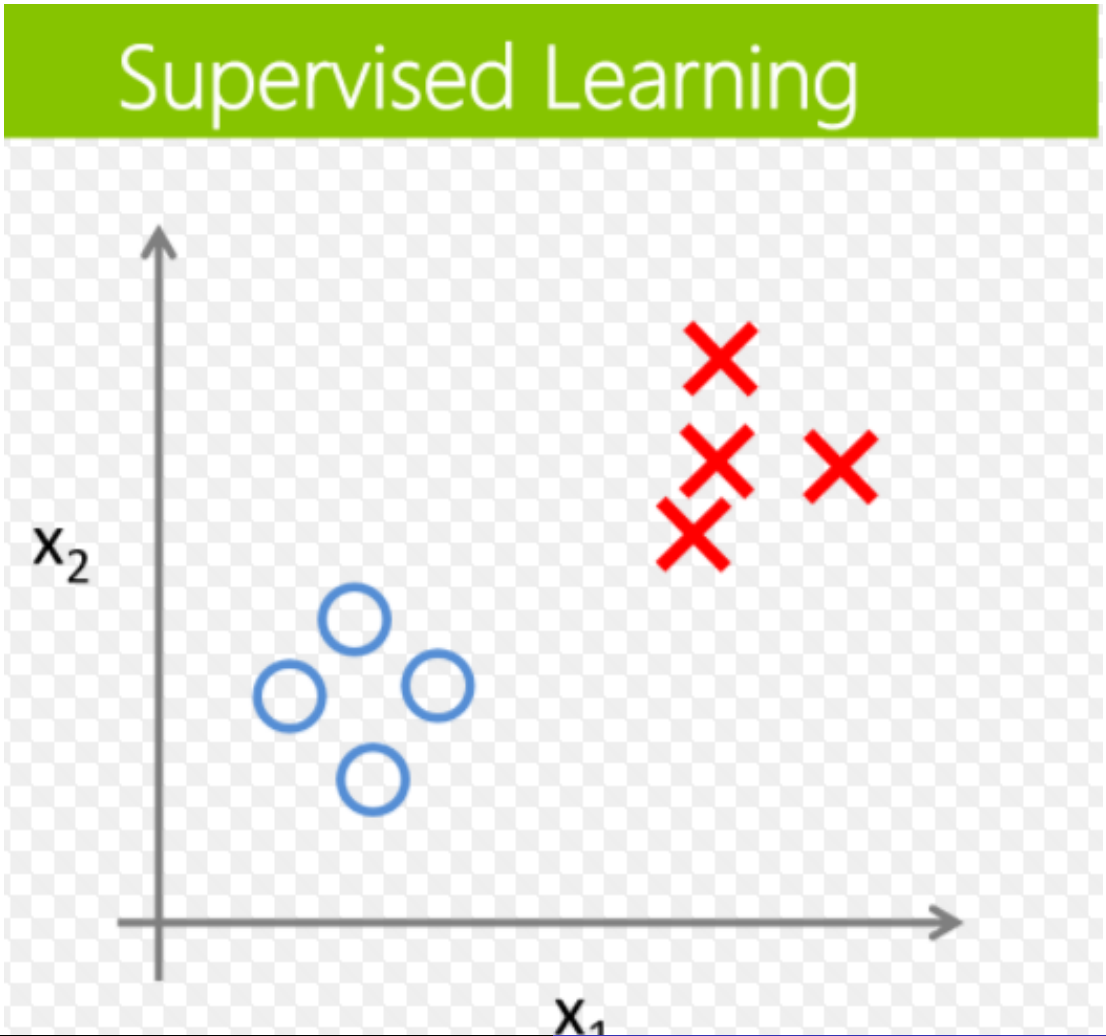
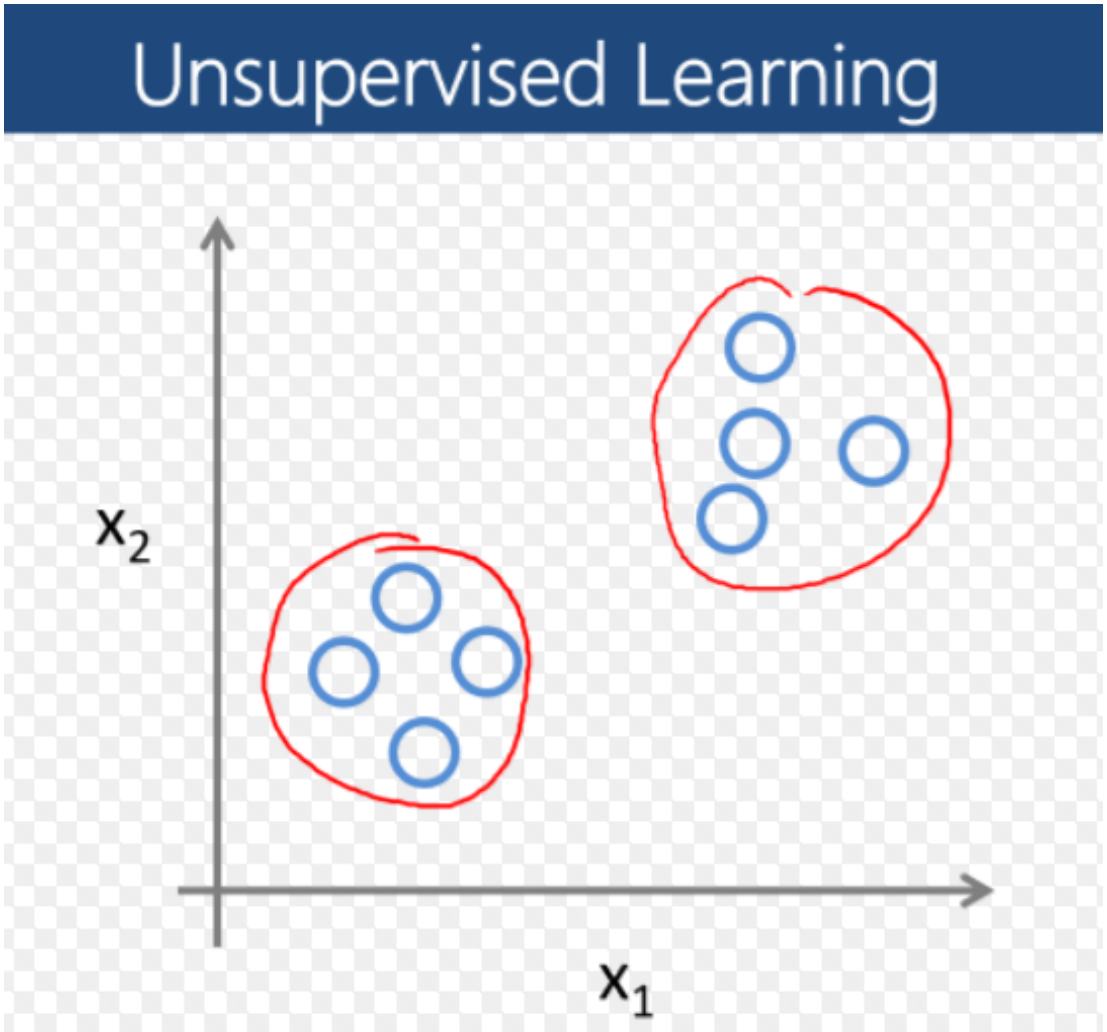


Figure 8: Types of problems machine learning solves

Supervised learning - probability interpretation



Unsupervised learning - probability interpretation



Definition

- Model a single response **(dependent, continuous, outcome)** variable based on one or more input **(independent, predictor)** variables

Linear Regression example

- Suppose that we are given a training set comprising N observations of x, written **x = (x1, ..., xn)** together with corresponding observations of the values of y, denoted **y = (y1, ..., yn)**
- The input data set x in Figure 1.2 was generated by choosing values of xn, for n = 1,...,N, spaced uniformly in range [0, 1], and the target data set t was obtained by first computing the corresponding values of the function sin(2pix)

Linear Regression example

Plot of a training data set of $N = 10$ points, shown as blue circles, each comprising an observation of the input variable x along with the corresponding target variable t. The green curve shows the function $\sin(2\pi x)$ used to generate the data. Our goal is to predict the value of t for some new value of x, without knowledge of the green curve.

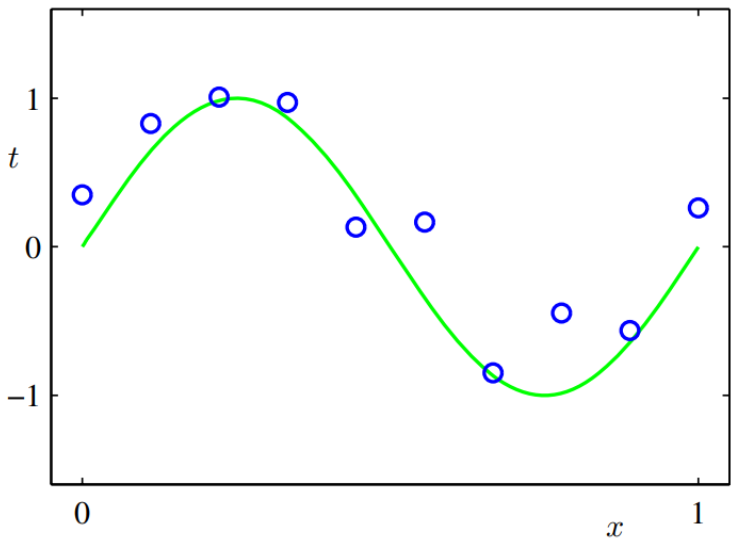


Figure 11: Target function

Curve fitting approach - Hypothesis

We shall fit the data using a polynomial function of the form:

$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Figure 12: Linear combination of learning parameters and features

Curve fitting approach - Cost function

The values of the coefficients will be determined by fitting the polynomial to the training data. This can be done by minimizing an **error function** that meaures the misfit between the function **y(x, w)**, for any given value of w, and the training set data points. The simplest error function is the **sum of squares** of the errors between the predictions **y(xn, w) for each data point xn and the corresponding target values yn, so that we minimize:**

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2$$

Figure 13: Cost function for continuous type variables

Curve fitting approach - Cost function

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2$$

The error function (1.2) corresponds to (one half of) the sum of the squares of the displacements (shown by the vertical green bars) of each data point from the function $y(x, \mathbf{w})$.

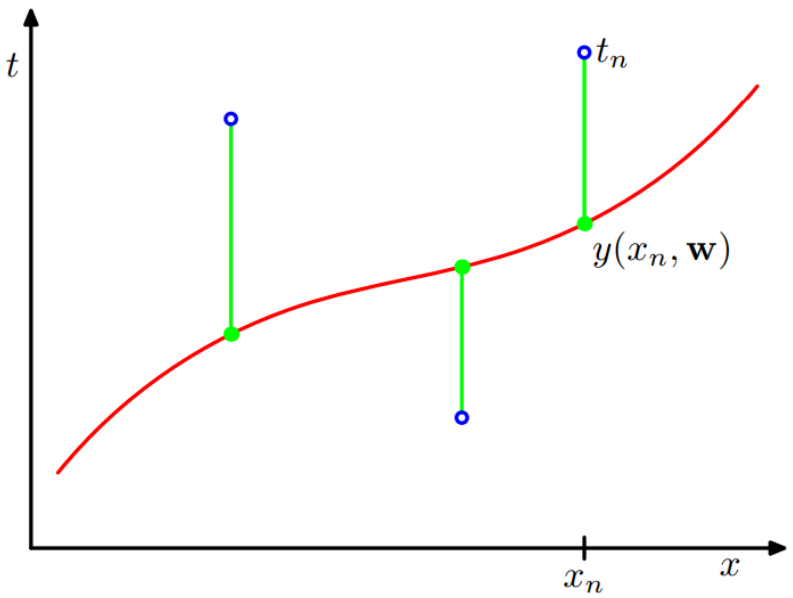
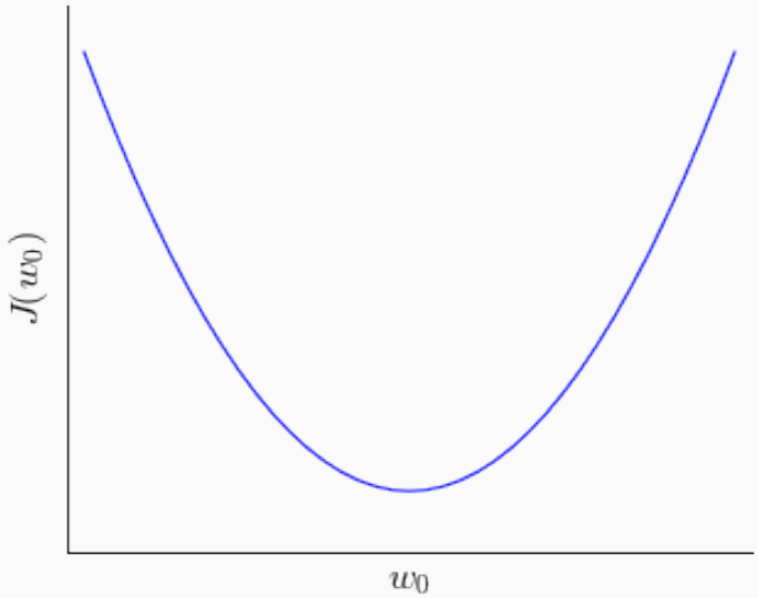


Figure 14: Cost function for continuous type variables

Curve fitting approach - Intuition about solving the problem

We can solve the curve fitting problem by choosing the value of w for which E(w) is as small as possible. Because the error function is a quadratic function of the coefficients w, its derivatives with respect to the coefficients will be linear in the elements of w, and so the minimization of the error function has a unique solution, denoted by w$*$, which can be found in closed form. The resulting polynomial is given by the function y(x, w$*$).

Curve fitting approach - Gradient Descent



Update rule

$$\frac{d}{dw_0}J(w_0)$$

$$w_0 := w_0 - \alpha\frac{d}{dw_0}J(w_0)$$

- A positive $\alpha\frac{d}{dw_0}J(w_0)$ moves w_0 to the left
- A negative $\alpha\frac{d}{dw_0}J(w_0)$ moves w_0 to the right

Figure 15: Gradient descent

BGD, SGD

Batch gradient descent

BGD, SGD

Stochastic gradient descent

Gradient Descent - Multiple Regression problem

$$\boldsymbol{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}^T$$

$$\boldsymbol{y} = \{y_1, y_2, \ldots, y_N\}^T$$

$$\boldsymbol{w} = \{w_0, w_1, \ldots, w_D\}^T$$

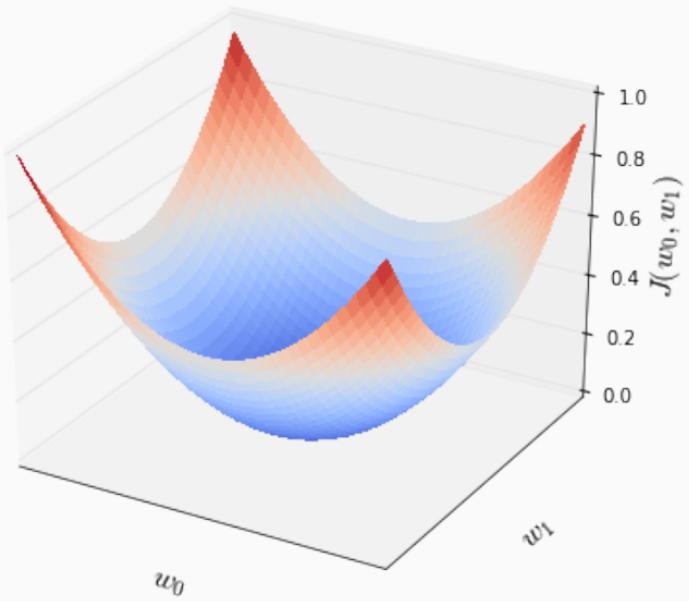
$$w_j := w_j - \alpha \frac{\partial}{\partial w_j} J(\boldsymbol{w})$$

$$\frac{\partial}{\partial w_j} J(\boldsymbol{w}) = \frac{\partial}{\partial w_j} \frac{1}{2N} \sum_{i=1}^{N} (\hat{y}_i - y_i)^2 = \frac{1}{2N} \sum_{i=1}^{N} \frac{\partial}{\partial w_j} (\hat{y}_i - y_i)^2 =$$

$$\frac{1}{2N} \sum_{i=1}^{N} 2(\hat{y}_i - y_i)^2 \frac{\partial}{\partial w_j} (\hat{y}_i - y_i) = \frac{1}{N} \sum_{i=1}^{N} (\hat{y}_i - y_i) x_i$$

Figure 16: Multiple parameters increase the dimensionality of the parameters' vector

Curve fitting approach - How many features?



Solution

$$\frac{\partial}{\partial w_j} J(w_0, w_1)$$

repeat until convergence {

Simultaneously update for every j:

$$w_j := w_j - \alpha \frac{\partial}{\partial w_j} J(\boldsymbol{w})$$

}

Figure 17: Multi-dimensional cost function

Curve fitting approach - How many features?

Solve the problem using different dimensionalities for x

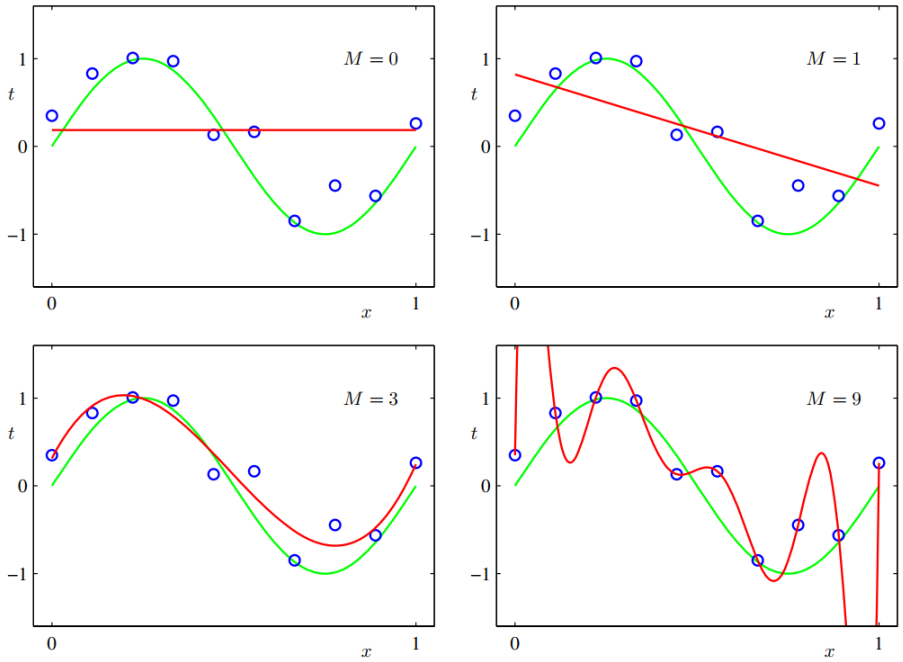


Figure 18: Multi-dimensional cost function

Curve fitting approach - Addressing overfitting (variance) and underfitting (bias)

Which is the correct number of features to be used?

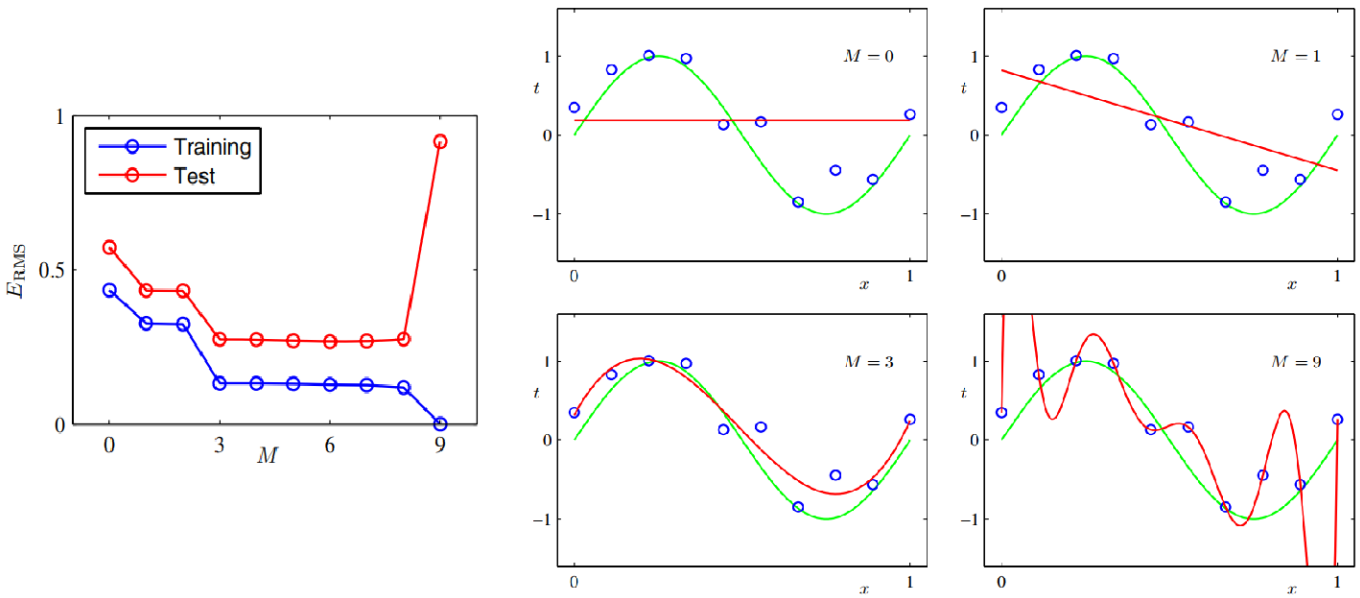


Figure 19: Diagnosing Overfitting and underfitting

Curve fitting approach - Addressing overfitting (variance) and underfitting (bias)

Table of the coefficients $\mathbf{w}^\star$ for polynomials of various order. Observe how the typical magnitude of the coefficients increases dramatically as the order of the polynomial increases.

	$M=0$	$M=1$	$M=6$	$M=9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

Figure 20: Why overfitting and underfitting?

Curve fitting approach - Causes of Overfitting

- Extensive search in hypothesis
- Too many features (curse of dimensionality)
- Insufficient examples

Curve fitting approach - Causes of Underfitting

- Not enough data points
- Not enough features
- Not enough polynomial terms to capture non-linearity

Curve fitting approach - Solve overfitting underfitting with regularization

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

$$\text{where } \|\mathbf{w}\|^2 \equiv \mathbf{w}^{\mathrm{T}}\mathbf{w} = w_0^2 + w_1^2 + \ldots + w_M^2.$$

Curve fitting approach - Solve overfitting underfitting with regularization

Table of the coefficients $\mathbf{w}^\star$ for $M = 9$ polynomials with various values for the regularization parameter λ. Note that $\ln \lambda = -\infty$ corresponds to a model with no regularization, i.e., to the graph at the bottom right in Figure 1.4. We see that, as the value of λ increases, the typical magnitude of the coefficients gets smaller.

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$	1042400.18	-45.95	-0.00
$w_8^\star$	-557682.99	-91.53	0.00
$w_9^\star$	125201.43	72.68	0.01

Curve fitting approach - Solve overfitting underfitting with regularization

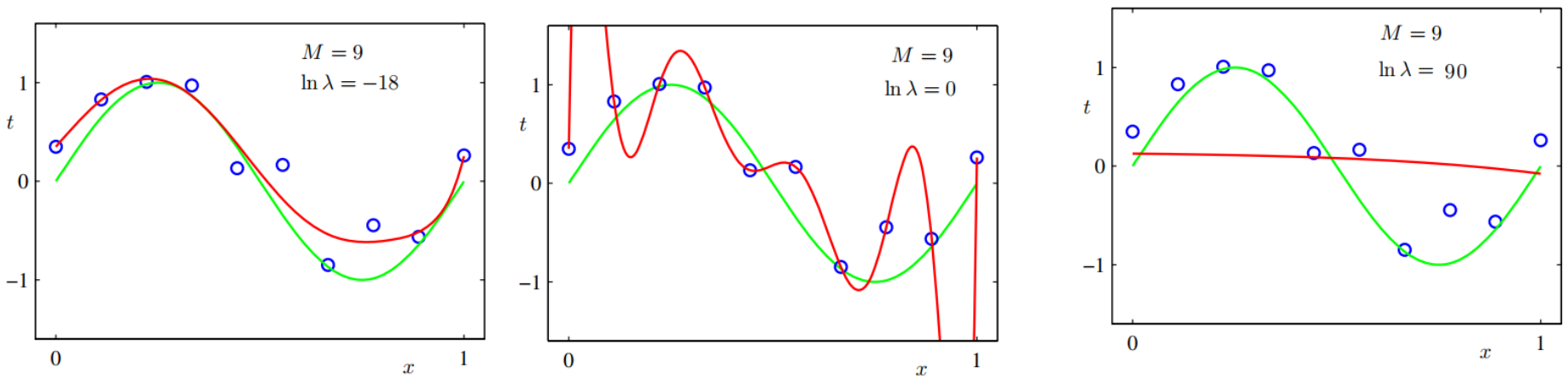


Figure 23: Apllying regularization

Curve fitting approach - Solve overfitting underfitting adding more data (always works)

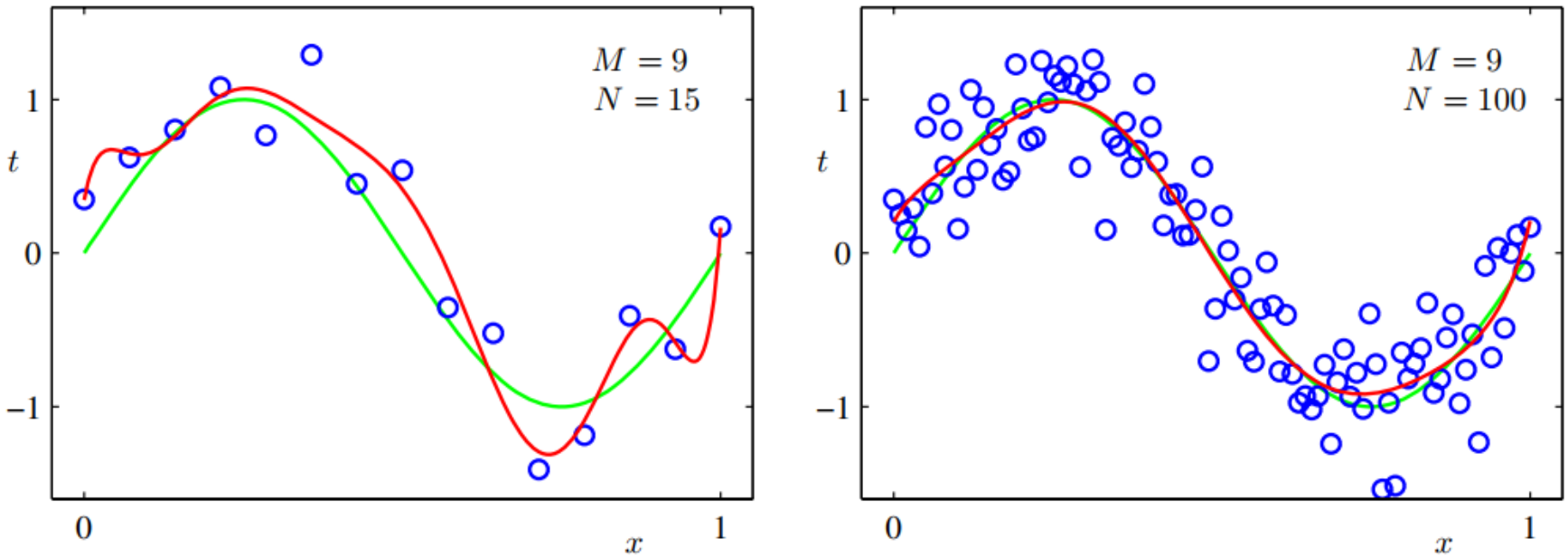


Figure 24: The more data, the better

Summary

- Hypothesis
- Cost function
- Learning algorithm

Summary - Hyperparameters

Hyperparameters:

References I

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