## CSC321 Lecture 2 A Simple Learning Algorithm : Linear Regression

Roger Grosse and Nitish Srivastava

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In this lecture we will

- See a simple example of a machine learning model, linear regression.
- Learn how to formulate a supervised learning problem.
- Learn how to train the model.

It's not a neural net algorithm, but it will provide a lot of useful intuition for algorithms we will cover in this course.

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## A Machine Learning Problem

Suppose we are given some data about basketball players -



What is the predicted number of points scored by a new player who is 6.5 feet tall ?

We are given labelled examples (the training set): Inputs:  $\{x^{(1)}, x^{(2)}, \dots, x^{(N)}\}$  - Height in feet. Targets:  $\{t^{(1)}, t^{(2)}, \dots, t^{(N)}\}$  - Avg points scored per game.

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• Choose a model  $\equiv$  Make an assumption about the data's behaviour. Let's say we choose -

$$y = wx + b$$

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• Learning: Extract knowledge from the data to learn the model.

$$\{x^{(1)}, x^{(2)}, \dots, x^{(N)}\} \longrightarrow w, b$$

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y = wx + b

We call w the weight and b the bias. These are the trainable parameters.

• Learning: Extract knowledge from the data to learn the model.

$$\{x^{(1)}, x^{(2)}, \dots, x^{(N)}\} = w, b$$

• Inference: Given a new x and the learned model, make a prediction y.  $x \rightarrow w, b \rightarrow y$  Design an objective function (or loss function) that is -

- Minimized when the model does what you want it to do.
- Easy to minimize (smooth, well-behaved).

Here we want y = wx + b to be close to t, for every training case.

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Design an objective function (or loss function) that is -

- Minimized when the model does what you want it to do.
- Easy to minimize (smooth, well-behaved).

Here we want y = wx + b to be close to t, for every training case. Therefore one choice could be,

$$L(w, b) = \frac{1}{2} \sum_{i=1}^{N} (wx^{(i)} + b - t^{(i)})^2$$

This is called squared loss.

Need to find w, b such that L(w, b) is minimized.

$$L(w, b) = \frac{1}{2} \sum_{i} (wx^{(i)} + b - t^{(i)})^2$$

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$$\frac{\partial L}{\partial w} = \sum_{i} (wx^{(i)} + b - t^{(i)})x^{(i)}$$
$$\frac{\partial L}{\partial b} = \sum_{i} wx^{(i)} + b - t^{(i)}$$

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$$\frac{\partial L}{\partial b} = \sum_{i} wx^{(i)} + b - t^{(i)}$$

Since L is a nonnegative quadratic function in w and b, any critical point is a minimum. Therefore, we minimize L by setting

$$\frac{\partial L}{\partial w} = 0, \frac{\partial L}{\partial b} = 0.$$

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$$w\left(\sum_{i} x^{(i)} \cdot x^{(i)}\right) + b\left(\sum_{i} x^{(i)}\right) - \left(\sum_{i} t^{(i)} x^{(i)}\right) = 0$$
$$w\left(\sum_{i} x^{(i)}\right) + bN - \left(\sum_{i} t^{(i)}\right) = 0$$

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$$w\left(\sum_{i} x^{(i)} \cdot x^{(i)}\right) + b\left(\sum_{i} x^{(i)}\right) - \left(\sum_{i} t^{(i)} x^{(i)}\right) = 0$$
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Now we have 2 linear equations and 2 unknowns w and b. Solve!

### Inference



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#### Inference



To make a prediction about a new player, just use y = wx + b.

Multi-variable : Instead of  $x \in \mathbb{R}$ , we have  $\mathbf{x} = (x_1, x_2, \dots, x_M) \in \mathbb{R}^M$ .

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Multi-variable : Instead of  $x \in \mathbb{R}$ , we have  $\mathbf{x} = (x_1, x_2, \dots, x_M) \in \mathbb{R}^M$ . For example,

Height in feet $(x_1)$	Weight in pounds $(x_2)$	Avg Points Scored Per Game $(t)$
6.8	225	9.2
6.3	180	11.7
6.4	190	15.8
6.2	180	8.6
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Choose a model -

 $y = w_1 x_1 + w_2 x_2 + \ldots + w_M x_M + b = \mathbf{w}^\top \mathbf{x} + b$ 

Parameters to be learned :  $\mathbf{w}$ , b.

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Choose a model -

$$y = w_1 x_1 + w_2 x_2 + \ldots + w_M x_M + b = \mathbf{w}^\top \mathbf{x} + b$$

Parameters to be learned :  $\mathbf{w}, b$ . Objective function -

$$L(\mathbf{w}, b) = \sum_{i=1}^{N} (\mathbf{w}^{\top} \mathbf{x}^{(i)} + b - t^{(i)})^2$$

We can use more general basis functions (also called "features").

$$y = w_1\phi_1(\mathbf{x}) + w_2\phi_2(\mathbf{x}) + \ldots + w_M\phi_M(\mathbf{x}) = \mathbf{w}^{\top}\Phi(\mathbf{x})$$

Parameters to be learned : w.

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Parameters to be learned :  $\mathbf{w}$ .

For example, 1-D Polynomial fitting

$$\phi_0(x) = 1$$
  

$$\phi_1(x) = x$$
  

$$\phi_2(x) = x^2$$
  

$$\phi_3(x) = x^3$$
  

$$\vdots = \vdots$$
  

$$\phi_M(x) = x^M$$
  

$$y = \overbrace{w_0\phi_0(x)}^{} + w_1\phi_1(x) + w_2\phi_2(x) + \ldots + w_M\phi_M(x) = \mathbf{w}^{\top}\Phi(x)$$

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$$\vdots = \vdots$$

$$\phi_{M}(x) = x^{M}$$

$$y = w_{0}\phi_{0}(x) + w_{1}\phi_{1}(x) + w_{2}\phi_{2}(x) + \dots + w_{M}\phi_{M}(x) = \mathbf{w}^{\top}\Phi(x)$$
Note : Linear regression means linear in parameters  $\mathbf{w}_{n}$  not linear in  $\mathbf{x}_{n}$ 

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$$\mathbf{Y} = \mathbf{W}_{0}(x) + \mathbf{W}_{1}(x) + \mathbf{W}_{2}(x) + \dots + \mathbf{W}_{M}(x) = \mathbf{W}^{\top}\Phi(x)$$

$$\mathbf{X}$$

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### Learning Multi-variable Linear Regression

Feature matrix:

$$\mathbf{\Phi} = \begin{bmatrix} \Phi(x^{(1)})^{\top} \\ \Phi(x^{(2)})^{\top} \\ \vdots \\ \Phi(x^{(N)})^{\top} \end{bmatrix} \qquad \mathbf{\Phi} \mathbf{w} = \begin{bmatrix} \mathbf{w}^{T} \Phi(x^{(1)}) \\ \mathbf{w}^{T} \Phi(x^{(2)}) \\ \vdots \\ \mathbf{w}^{T} \Phi(x^{(N)}) \end{bmatrix}$$

Vector of predictions:

Objective function

$$L(\mathbf{w}) = \frac{1}{2} \sum_{i} (\mathbf{w}^{T} \Phi(x^{(i)}) - t^{(i)})^{2}$$
$$= \frac{1}{2} ||\mathbf{\Phi}\mathbf{w} - \mathbf{t}||^{2}$$

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#### Learning Multi-variable Linear Regression

Optimum occurs where

$$\nabla_{\mathbf{w}} L(\mathbf{w}) = \mathbf{\Phi}^{\top} (\mathbf{\Phi} \mathbf{w} - \mathbf{t}) = 0$$

Therefore,

$$\mathbf{\Phi}^{\top}\mathbf{\Phi}\mathbf{w} - \mathbf{\Phi}^{\top}\mathbf{t} = 0$$
$$\mathbf{w} = \left(\mathbf{\Phi}^{\top}\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^{\top}\mathbf{t}$$

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#### Learning Multi-variable Linear Regression

Optimum occurs where

$$\nabla_{\mathbf{w}} L(\mathbf{w}) = \mathbf{\Phi}^{\top} (\mathbf{\Phi} \mathbf{w} - \mathbf{t}) = 0$$

Therefore,

$$\mathbf{\Phi}^{\top}\mathbf{\Phi}\mathbf{w} - \mathbf{\Phi}^{\top}\mathbf{t} = 0$$
$$\mathbf{w} = \left(\mathbf{\Phi}^{\top}\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^{\top}\mathbf{t}$$

Question : When will  $\mathbf{\Phi}^{\top}\mathbf{\Phi}$  be invertible ?



-Pattern Recognition and Machine Learning, Christopher Bishop.

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$$y = w_0 + w_1 x$$



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$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$

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x = 1

$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_9 x^9$$



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#### Model selection

Underfitting : The model is too simple - does not fit the data.



Overfitting : The model is too complex - fits perfectly, does not generalize.



#### Model selection

Need to select a model which is neither too simple, nor too complex.



Later in this course, we will see talk more about controlling model complexity.

#### Next class

• Another machine learning model, an early neural net : Perceptron.



- Frank Rosenblatt, with the image sensor (left) of the Mark I Perceptron40

# Reminder - Do the quizzes for video lectures A and B by 11.59pm next Monday.