Linear Regression

Mario Parente

A First Supervised Learning Problem

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Let's simplify the problem: devise method to easily estimate the height of a tree

A First Supervised Learning Problem

Idea?

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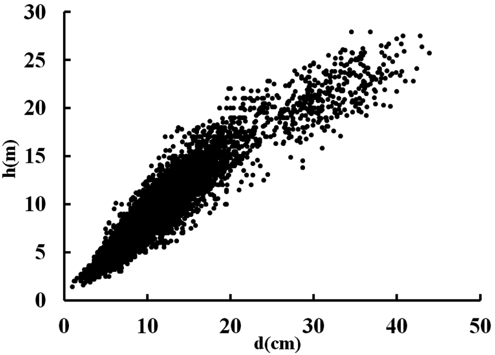
Some data

Development and Evaluation of Models for the Relationship between Tree Height and Diameter at Breast Height for Chinese-Fir Plantations in Subtropical China

Yan-qiong Li, Xiang-wen Deng, Zhi-hong Huang, Wen-hua Xiang, Wen-de Yan, Pi-feng Lei, Xiao-lu Zhou, Chang-hui Peng



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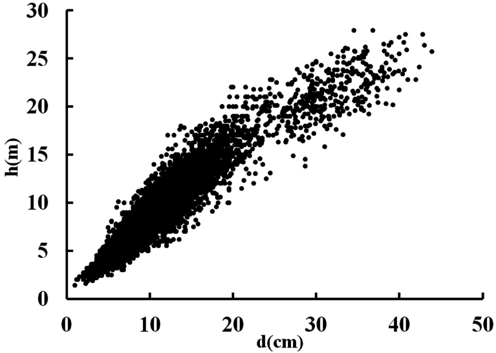

What do you predict for the height of a tree with DBH 15cm? 35cm? Why?

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What model? What algorithm? **Largely what this class is about.**

Supervised Learning

DBH (x)	Height (y)
17	63
19	65
20.5	66
...	...

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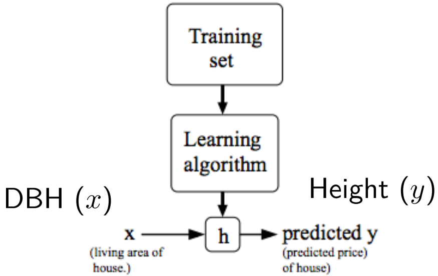
Find h such that $h(x) \approx y$



Supervised Learning: Notation and Terminology

- Observe m "training examples" of form $(x^{(i)}, y^{(i)})$
  - $x^{(i)}$: **features** / input / what we observe / DBH
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Variations: type of x, y, h

Linear Regression in One Variable

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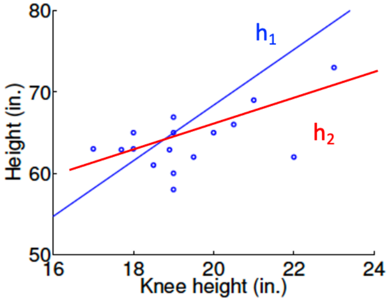
- "parameters" or "weights"

How to find "best" θ_0, θ_1?



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Exercise: which cost functions below make sense?

A. $J(\theta_1) = \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)$

B. $J(\theta_1) = \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$

C. $J(\theta_1) = \sum_{i=1}^{m} \left|h_\theta(x^{(i)}) - y^{(i)}\right|$

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5. A, B, and C

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Answer. 4

Squared Error Cost Function

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$$J(3) = (144 + 64 + 20.25)/2 = 220.25/2$$

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&= 535.125 \cdot \theta_1^2 - 3659 \cdot \theta_1 + 6275
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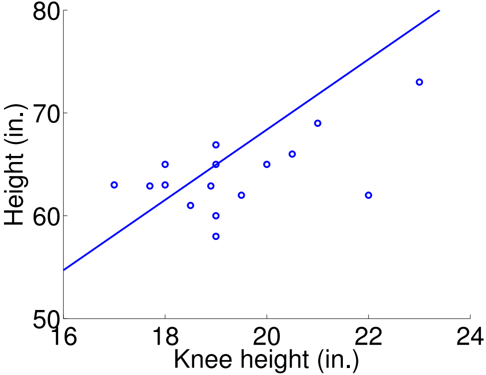
$$\theta_1 = \frac{3659}{1070.25} = 3.4188$$

(See http://www.wolframalpha.com)

Our First Algorithm In Action



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The general problem: find θ_1 to minimize

$$J(\theta_1) = \frac{1}{2} \sum_{i=1}^{m} (\theta_1 x^{(i)} - y^{(i)})^2$$

You will solve this in HW1.

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Exercise: ideas for problem one?

Solution to Problem One

Design a cost function that takes two parameters:

$$
\begin{aligned}
J(\theta_0, \theta_1) &= \frac{1}{2} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2 \\
&= \frac{1}{2} \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)}\right)^2
\end{aligned}
$$

Find θ_0, θ_1 to minimize $J(\theta_0, \theta_1)$

Functions of multiple variables!

Here is an example cost function:

$$
\begin{aligned}
J(\theta_0, \theta_1) = {} & \tfrac{1}{2}(\theta_0 + 17 \cdot \theta_1 - 63)^2 + \tfrac{1}{2}(\theta_0 + 19 \cdot \theta_1 - 65)^2 \\
& + \tfrac{1}{2}(\theta_0 + 20.5 \cdot \theta_1 - 66)^2 + \tfrac{1}{2}(\theta_0 + 18.9 \cdot \theta_1 - 62.9)^2 + \ldots
\end{aligned}
$$

Gain intuition on http://www.wolframalpha.com

- Surface plot
- Contour plot

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- **Gradient descent** is a general purpose optimization algorithm. A "workhorse" of ML.
- Idea: repeatedly take steps in steepest downhill direction, with step length proportional to "slope"
- Illustration: contour plot and pictorial definition of gradient descent

Gradient Descent

To minimize a function $J(\theta_0, \theta_1)$ of two variables

- Intialize θ_0, θ_1 arbitrarily
- Repeat until convergence

$$\theta_0 := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$

  - $\alpha =$ step-size or **learning rate** (not too big)

Partial derivatives

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$$\frac{\partial}{\partial v} 5u^2v^3 = ??$$

Partial derivative intuition

Interpretation of partial derivative: $\frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$ is the rate of change along the θ_j axis

Example: illustrate function with elliptical contours

- Sign of $\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$?
- Sign of $\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$?
- Which has larger absolute value?

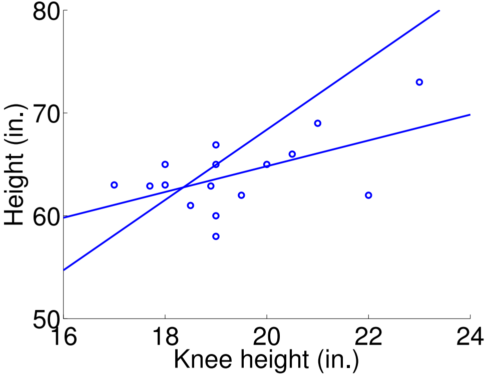
Gradient Descent

- Repeat until convergence

$$\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$
$$\theta_1 = \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$

- Issues (explore in HW1)
  - Pitfalls
  - How to set step-size α?
  - How to diagnose convergence?

The Result in Our Problem



$$h_\theta(x) = 39.75 + 1.25x$$

Gradient descent intuition

$$\theta_0 := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$

- Why does this move in the direction of steepest descent?
- What would we do if we wanted to maximize $J(\theta_0, \theta_1)$ instead?

Gradient descent for linear regression

Algorithm

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \quad \text{for } j = 0, 1$$

Cost function

$$J(\theta_0, \theta_1) = \sum_{i=1}^{m} \frac{1}{2} \big(h_\theta(x^{(i)}) - y^{(i)}\big)^2$$

We need to calculate partial derivatives.

Linear regression partial derivatives

Let's first do this with a single training example (x, y):

$$\frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) = \frac{\partial}{\partial \theta_j} \frac{1}{2} \big(h_\theta(x) - y\big)^2$$

Linear regression partial derivatives

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$$\begin{aligned}\frac{\partial}{\partial\theta_j}J(\theta_0,\theta_1) &= \frac{\partial}{\partial\theta_j}\frac{1}{2}\big(h_\theta(x)-y\big)^2 \\ &= 2\cdot\frac{1}{2}(h_\theta(x)-y)\cdot\frac{\partial}{\partial\theta_j}(h_\theta(x)-y)\end{aligned}$$

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&= \big(h_\theta(x) - y\big) \cdot \frac{\partial}{\partial \theta_j} \Big(\theta_0 + \theta_1 x - y\Big)
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\end{aligned}$$

So we get

$$\begin{aligned}
\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) &= \big(h_\theta(x) - y\big) \\
\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) &= \big(h_\theta(x) - y\big) x
\end{aligned}$$

Linear regression partial derivatives

More generally, with many training examples (work this out):

$$\frac{\partial}{\partial\theta_0} J(\theta_0, \theta_1) = \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)$$

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So the algorithm is:

$$\theta_0 := \theta_0 - \alpha \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)$$

$$\theta_1 := \theta_1 - \alpha \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right) x^{(i)}$$

Demo: parameter space vs. hypotheses

Show gradient descent demo

Summary

- What to know
  - Supervised learning setup
  - Cost function
    - Convert a learning problem to an optimization problem
    - Squared error
  - Gradient descent
- Next time
  - More on gradient descent
  - Linear algebra review