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Week 2. Linear Regression and Gradient Descent

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Overview

- Linear Regression – a ML algorithm for regression problems
- Gradient descent – an optimisation technique used to in ML algorithms.

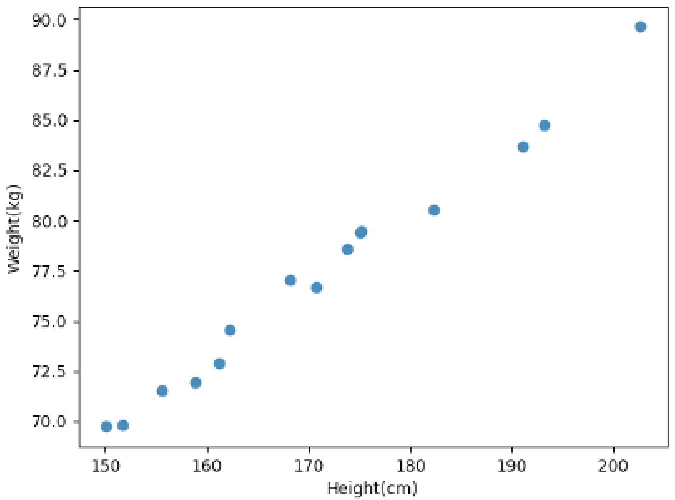
Recall: regression

- Regression means learning a function that captures the “trend” between input and output.
- The output is a continuous value.
- This function is used to predict the target values for new inputs.

Example of a regression problem

- Can we predict people's weight from their height?

Height(cm)	Weight(kg)
150.00686	69.73347
151.64326	69.83261
155.54032	71.55730
158.80535	71.92875
161.17561	72.92118
⋮	
175.15167	79.48533
182.32900	80.52182
191.11317	83.67998
193.21947	84.72086
202.68705	89.64049



- Visually, there appears to be a trend.
- A reasonable model seems to be the class of linear functions (lines).

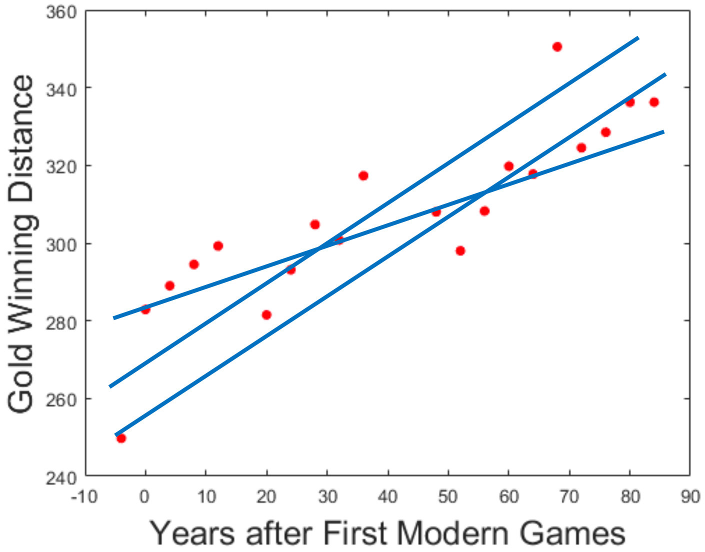
Univariate linear regression

- We have one input attribute (height) – hence the name **univariate**.

$$\underbrace{y}_{\text{dependent variable}} = f(x; \underbrace{w_0, w_1}_{\text{free parameters}}) = w_1 \underbrace{x}_{\text{independent variable}} + w_0$$

- Any line is described by this equation by specifying values for w_1 and w_0.

Our goal: find the “best” line



- Which is the “best” line? That captures the trend in the data.
- Determine the “best” values for w_0 and w_1.

Loss/cost functions

- We need a criterion that tells us how good/bad that line is.
- Such criterion is called a loss function.

Terminology

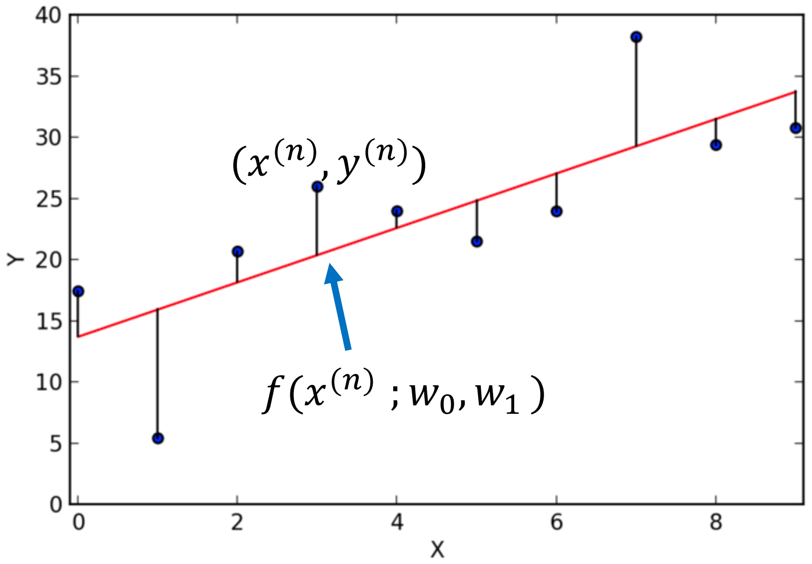
- Loss function = cost function = loss = cost = error function

We average the losses on all training examples

- For each training example (point) n = 1,…, N,

  The loss on the n-th point is the mismatch/distance between the output of the model for this point $f\left(x^{(n)}; w_0, w_1\right)$ and the observed target $y^{(n)}$.

- Average these losses.



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Loss function

- The loss expresses an error, so it must be always non-negative.
- Absolute value loss (L1 loss):

$$L1 = |f(x) - y|$$

- Mean squared error loss (L2 loss):

$$L2 = (f(x) - y)^2$$

$$\boxed{g(w_0, w_1) = \frac{1}{N}\sum_{n=1}^{N}\underbrace{\left(f\left(x^{(n)}; w_0, w_1\right) - y^{(n)}\right)^2}_{\text{Loss for the n-th training example}}}$$

Empirical loss used by LR

- 0/1 loss:

$$L_{0/1} = 0 \; if \; f(x) = y, else \; 1$$

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Univariate linear regression

- Given training data

$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots \, (x^{(N)}, y^{(N)})$$

- Fit the model

$$y = f(x; w_0, w_1) = w_1 x + w_0$$

- By minimizing the cost function

$$g(w_0, w_1) = \frac{1}{N} \sum_{n=1}^{N} \left(f\left(x^{(n)}; w_0, w_1\right) - y^{(n)}\right)^2$$

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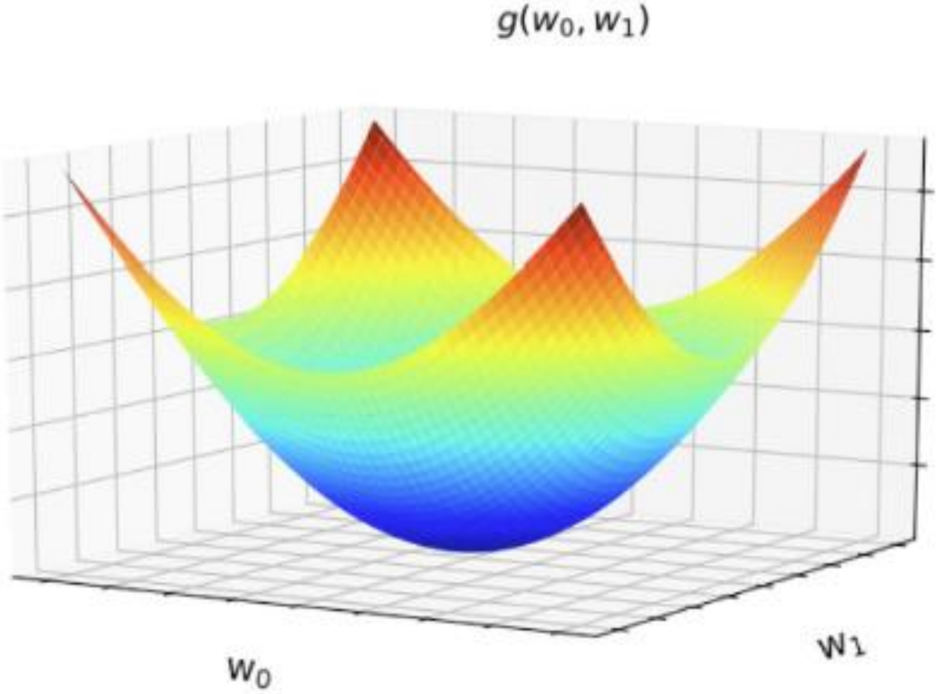
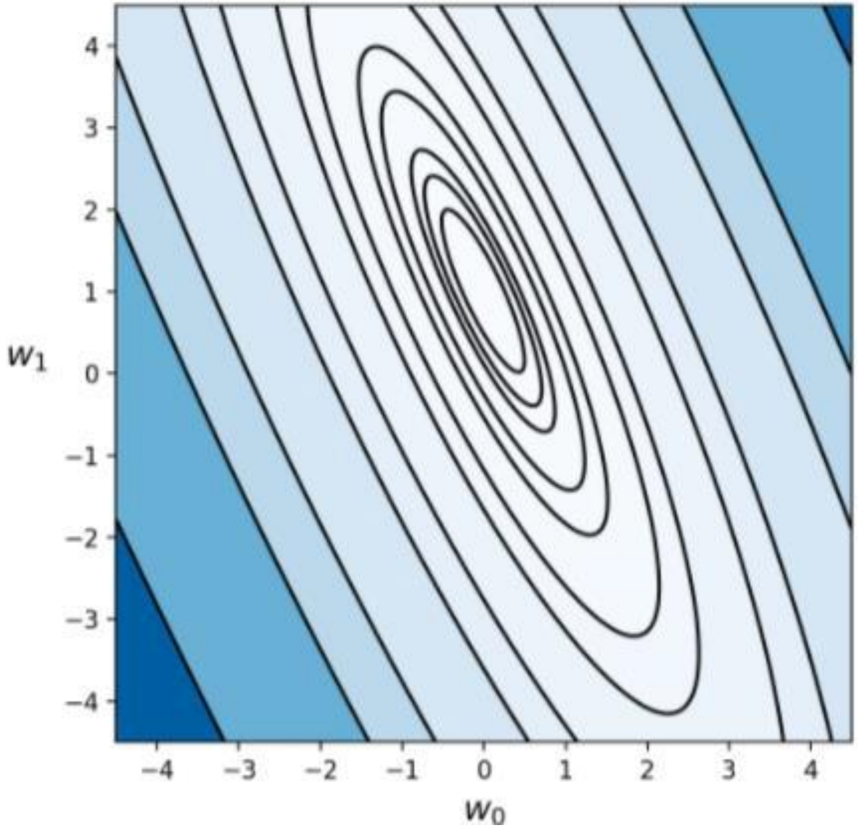
Cost function depends on the free parameter

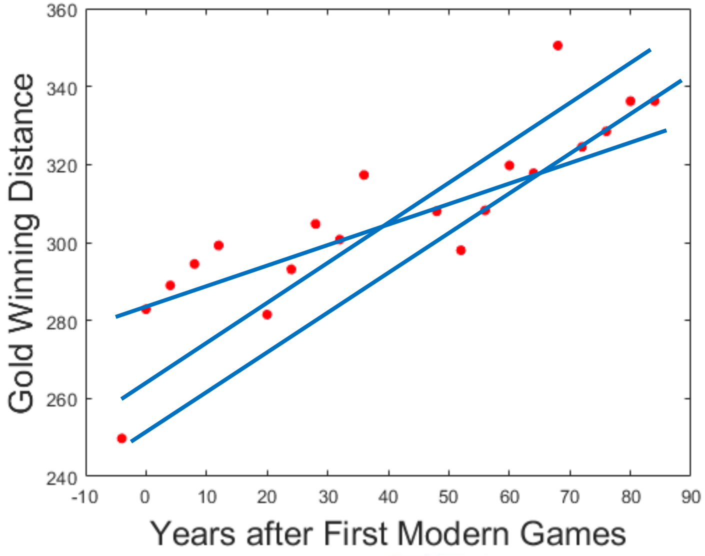


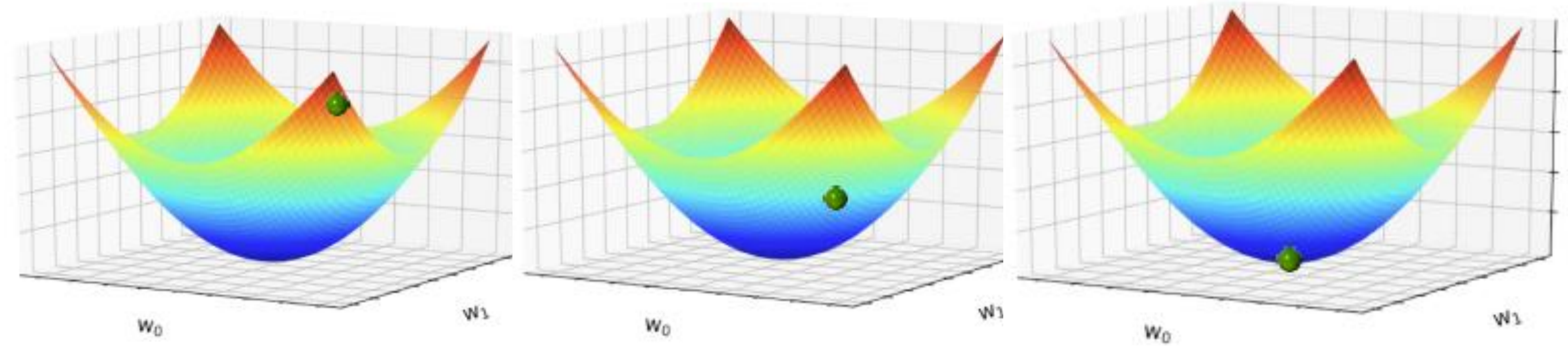


BIF

Univariate linear regression

- Every combination of (w_0, w_1) has an associated cost.
- Key training task: find the 'best' values of (w_0, w_1) such that the cost is minimum.





Gradient Descent

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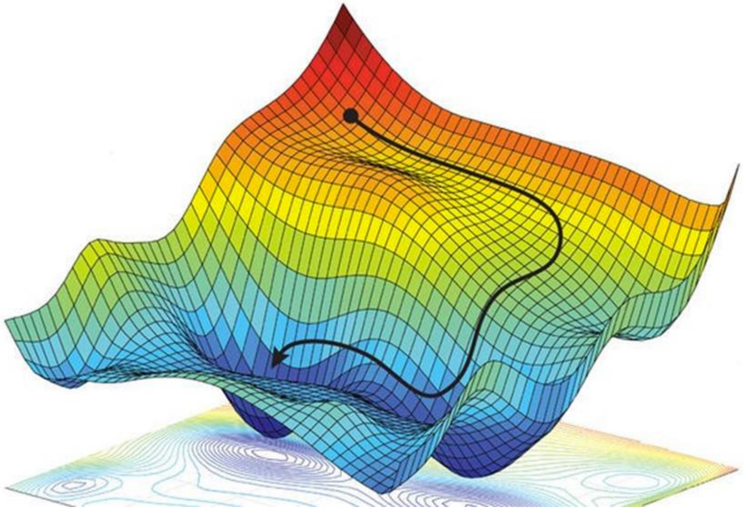
Gradient Descent

- A general strategy to minimize cost functions.



Gradient Descent

- A general strategy to minimize cost functions in ML algorithms.
- Goal: minimize the cost function $g(w_0, w_1)$

Start at a random point say $w_0 = 0, w_1 = 0$
Repeat until no change occurs
    Update w_0, w_1 by taking
    a small step in the direction of the steepest descent of cost
Return w_0, w_1.

Gradient Descent – More General…

- Goal: minimize the cost function $g(\boldsymbol{w}), where\ \boldsymbol{w} = (w_0, w_1, \dots)$

Input: $\alpha > 0$
Initialise $\boldsymbol{w}$. //at 0 or some random value
Repeat until convergence

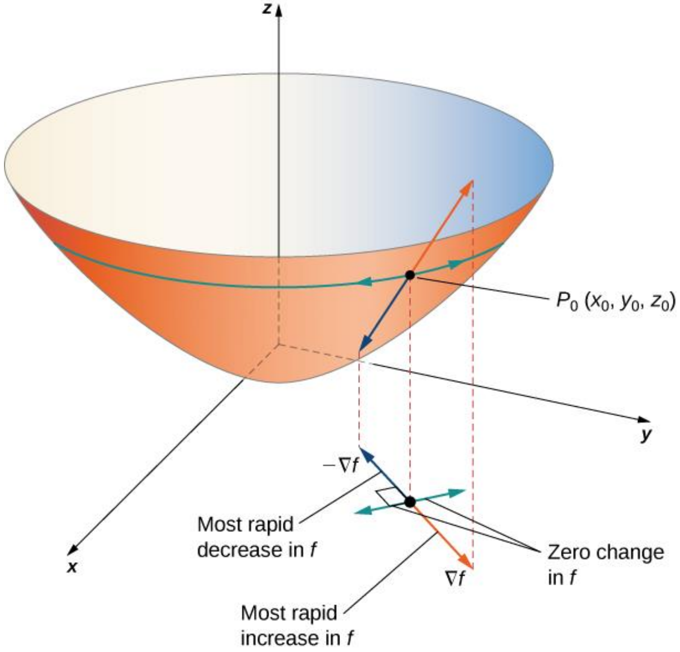
$$\boldsymbol{w} := \boldsymbol{w} - \alpha \nabla g(\boldsymbol{w})$$

Return $\boldsymbol{w}$.

Learning rate or step size, e.g. 0.01

Gradient or steepest direction

Back to Univariate Linear Regression



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Back to two dimensional function $g(w_0, w_1)$:

- The vector of partial derivatives is called the **gradient vector**.

$$\nabla g(\boldsymbol{w}) = \begin{pmatrix} \frac{\partial g}{\partial w_0} \\ \frac{\partial g}{\partial w_1} \end{pmatrix}, \text{ where } \boldsymbol{w} = \begin{pmatrix} w_0 \\ w_1 \end{pmatrix}$$

- Recall: Partial derivative with respect to one variable is the ordinary derivative of the function by treating the others as constants.
- The negative of the gradient $-\nabla g$ evaluated at a location $(\hat{w}_0, \hat{w}_1)$ gives us the direction of the steepest descent from that location.
- We take a small step in that direction – using the learning rate α.

Applying GD to solve univariate linear regression

- Recall: we aim to minimizing the cost function

$$g(w_0, w_1) = \frac{1}{N}\sum_{n=1}^{N}\left(\left(w_1 x^{(n)} + w_0\right) - y^{(n)}\right)^2$$

- Using the chain rule, we have *:

$$\frac{\partial g}{\partial w_0} = \frac{2}{N}\sum_{n=1}^{N}\left(\left(w_1 x^{(n)} + w_0\right) - y^{(n)}\right)$$

$$\frac{\partial g}{\partial w_1} = \frac{2}{N}\sum_{n=1}^{N}\left(\left(w_1 x^{(n)} + w_0\right) - y^{(n)}\right) x^{(n)}$$

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*For a very detailed explanations of all steps watch: https://www.youtube.com/watch?v=sDv4f4s2SB8

Algorithm for univariate linear regression using GD

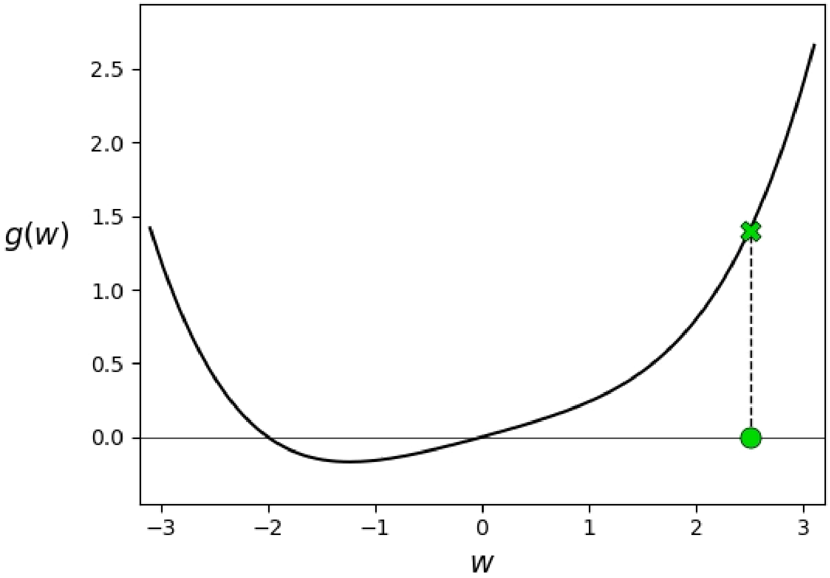
Input: $\alpha > 0$, training set $\{(x^{(n)}, y^{(n)}): n = 1,2 \ldots N\}$
Initialise $w_0 = 0, w_1 = 0$
Repeat //(first layer loop)
for n = 1, 2… N //second layer loop, more efficient to update after each data point

$$w_0 := w_0 - \alpha((w_1 x^{(n)} + w_0) - y^{(n)})$$

$$w_1 := w_1 - \alpha((w_1 x^{(n)} + w_0) - y^{(n)})x^{(n)}$$

Until change in cost remains below a very small threshold
Return w_0, w_1.

Demo Example for Gradient Descent



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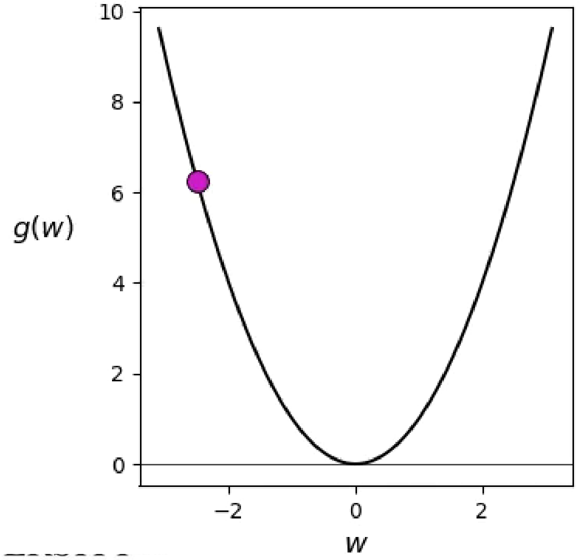
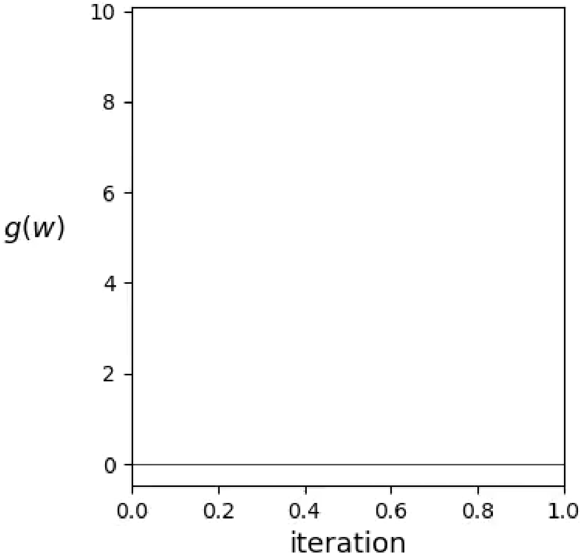
https://github.com/jermwatt/machine_learning_refined/tree/gh-pages/notes/pages/notes/3_First_order_methods/videos/animation_6.mp4

Effect of the learning rate

Whether or not we descend in the function when taking this step depends completely on how far along it we travel.





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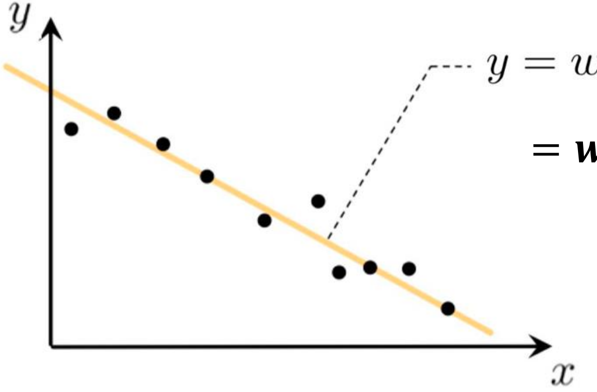
So far, univariate linear regression

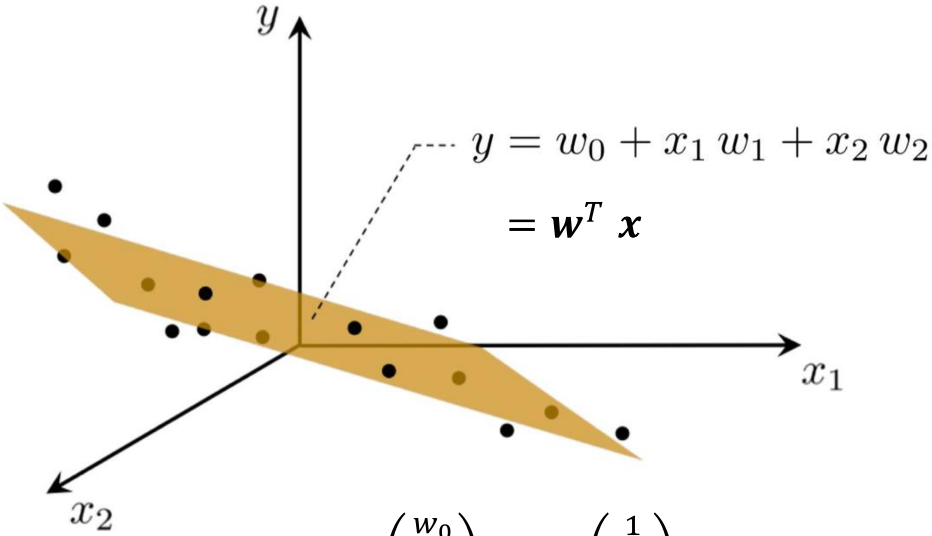
- One input variable
- Assume linear function

Multivariate linear regression



$= \boldsymbol{w}^T\ \boldsymbol{x}$

$\boldsymbol{w} = \begin{pmatrix} w_0 \\ w_1 \end{pmatrix}$, $\boldsymbol{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$



$= \boldsymbol{w}^T\ \boldsymbol{x}$

$\boldsymbol{w} = \begin{pmatrix} w_0 \\ w_1 \\ w_2 \end{pmatrix}$, $\boldsymbol{x} = \begin{pmatrix} 1 \\ x_1 \\ x_2 \end{pmatrix}$

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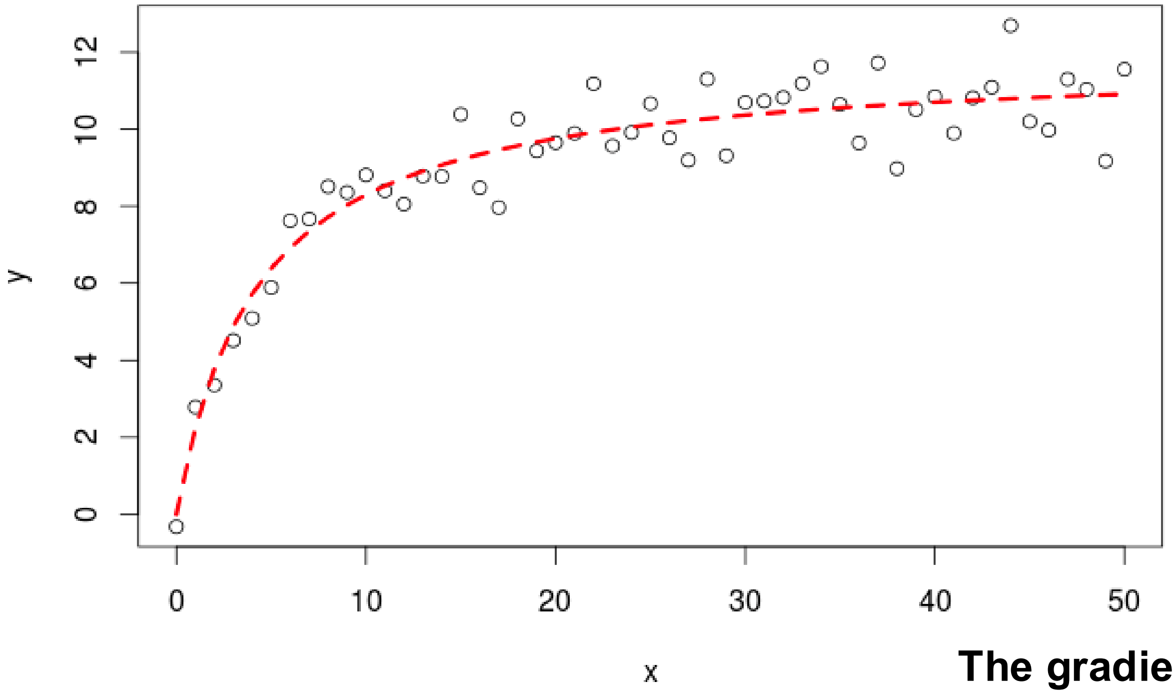
The gradient remains:

$\nabla g(\boldsymbol{w})$=$2(\boldsymbol{w}^T\boldsymbol{x}^{(n)} - y^{(n)})\boldsymbol{x}^{(n)}$

Univariate nonlinear regression

$y = w_0 + w_1 x$



$$\boldsymbol{w} = \begin{pmatrix} w_0 \\ w_1 \\ w_2 \\ \cdots \\ w_m \end{pmatrix}, \boldsymbol{x} = \begin{pmatrix} 1 \\ x \\ x^2 \\ \cdots \\ x^m \end{pmatrix}$$

This is an m-th order polynomial regression model.

The gradient remains:

$$\nabla g(\boldsymbol{w}) = 2(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)})\boldsymbol{x}^{(n)}$$

Advantages of vector notation

- Vector notation is more concise.
- With the vectors $\boldsymbol{w}$ and $\mathbf{x}$ populated appropriately (and differently in each case, as on the previous 2 slides), these models are still linear in the parameter vector.
- The cost function is the L2 as before.
- The gradient remains:

$$\nabla g(\boldsymbol{w}) = 2(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)})\boldsymbol{x}^{(n)}$$

- Ready to be plugged into the general gradient descent algorithm.

Q/A

Office Hour and Dropin Sessions
See Canvas module homepage

Figures and animations referred to:
Jeremy Watt et al. Machine Learning Refined. Cambridge University Press, 2020.
https://github.com/jermwatt/machine_learning_refined