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Week 2. Linear Regression and Gradient Descent

Dr. Shuo Wang



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.



Overview

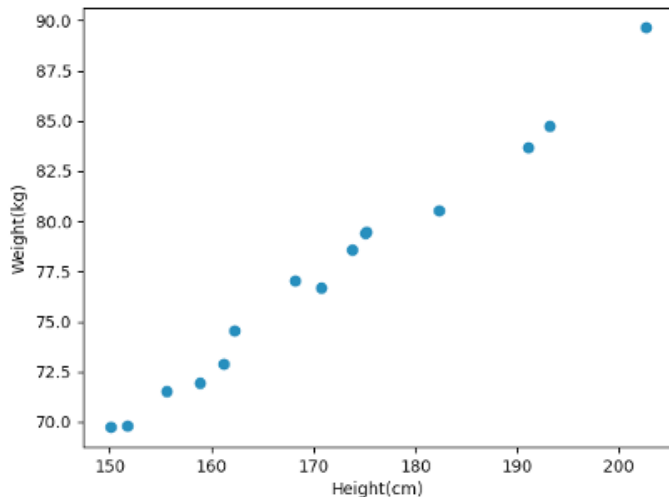
- Linear Regression – a ML algorithm for regression problems
- Gradient descent – an optimisation technique used to in ML algorithms.



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



Univariate linear regression

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

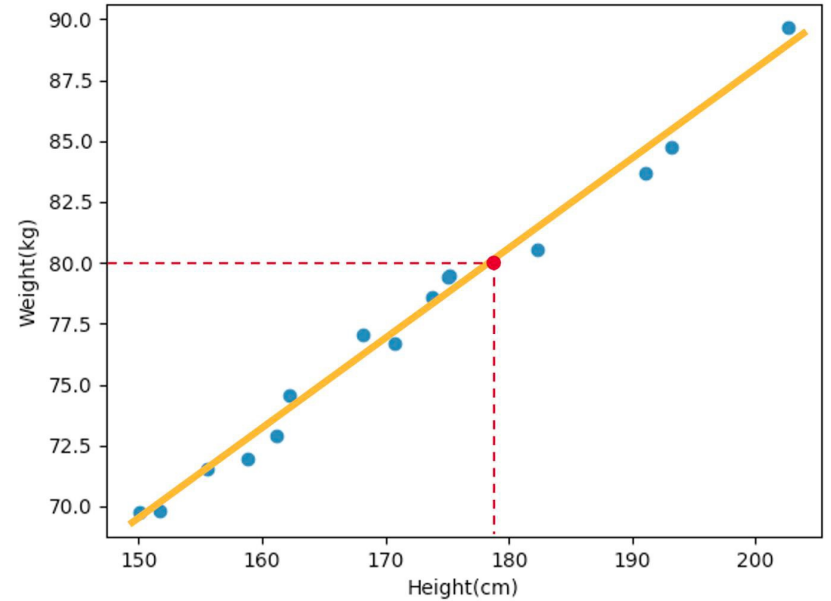
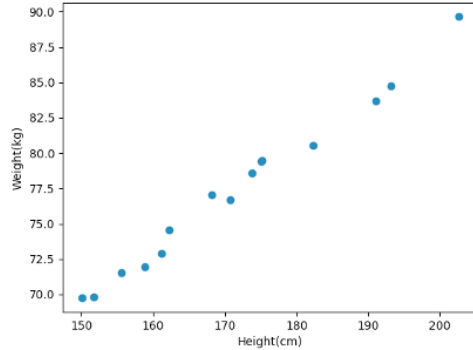
$$y = f(x; w_0, w_1) = w_1x + w_0$$

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



Check your understanding

Height(cm)	Weight(kg)
150.00686	69.73347
151.64326	69.83261
155.54032	71.55730
158.80535	71.92875
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...	...
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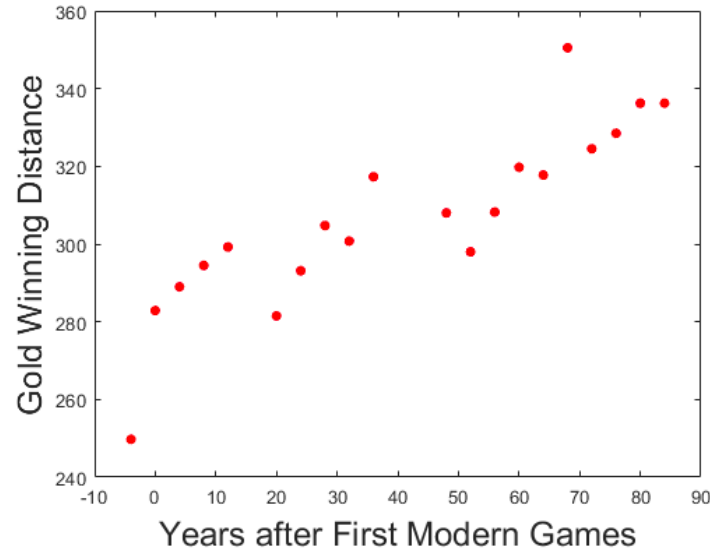
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Play around with linear functions

- Go to <https://www.desmos.com/calculator>
- Type: $y = w_1 x + w_0$
- Plug in some values for the free parameters, or set up the slider to see the effect of changing w_0 and w_1 .
- What is the role of the free parameters?
- w_0 is the intercept with the y-axis
- w_1 is the slope of the line – which is also the gradient function of the linear function $f(x; w_0, w_1) = w_1 x + w_0$ (recall last week!)
- Fixing concrete numbers for these parameters gives you specific lines.



Our goal: find the “best” line



- Which is the “best” line? That captures the trend in the data.



Loss/cost functions

- We need a criterion that tells us how good/bad that line is.
- Such criterion is called a loss function. It is a function of the free parameters.

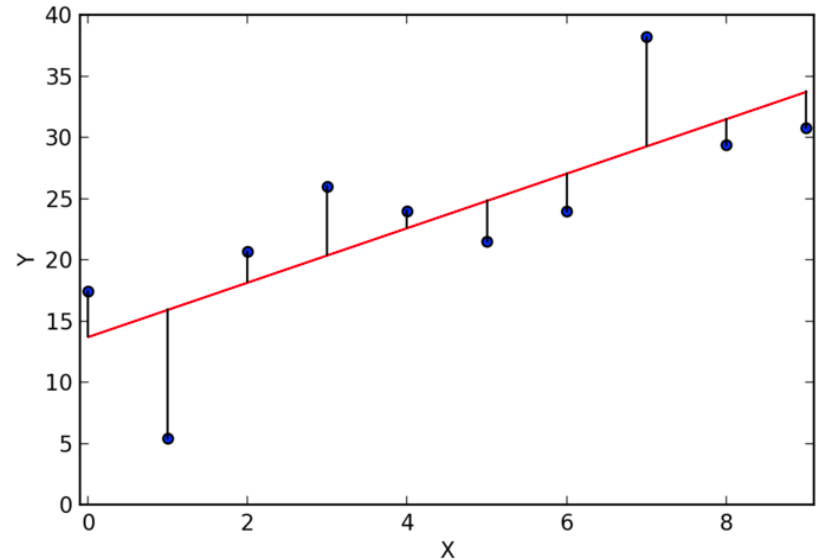
Terminology

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



We average the losses on all training examples

- For each training example (point) $n = 1, \dots, N$,
The loss on the n -th point is the mismatch/distance between the output of the model for this point $f(x^{(n)}; w_0, w_1)$ and the observed target $y^{(n)}$.
- Average these losses.



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):

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

- 0/1 loss:

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



Check your understanding

- Suppose a linear function with parameters $w_0=0.5$, $w_1=0.5$
- Computer the MSE value at the training example (1,3).



Univariate linear regression

- Given training data

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

- Fit the model

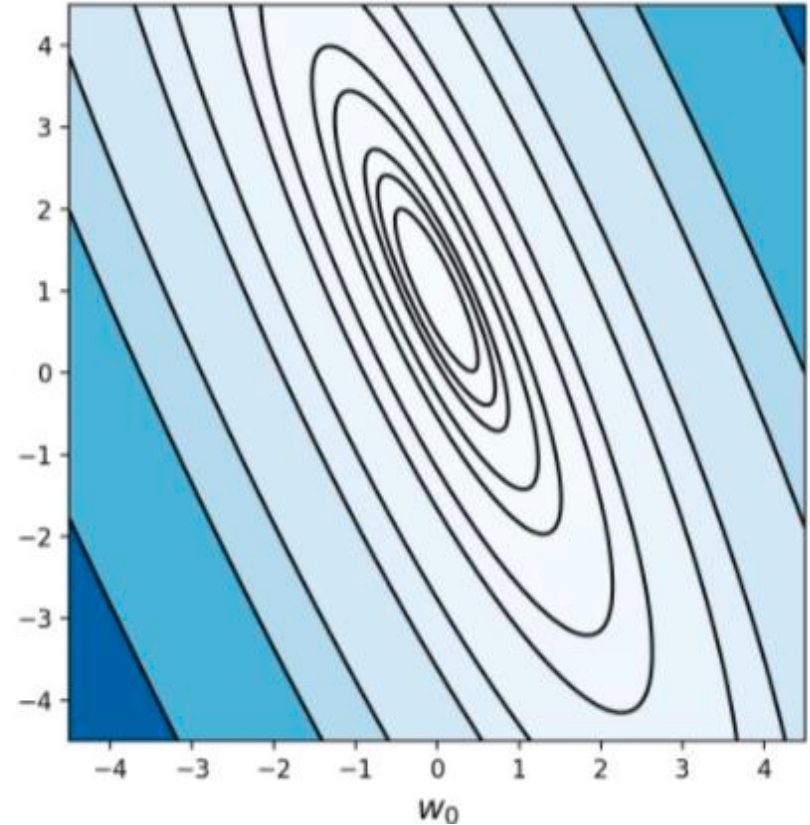
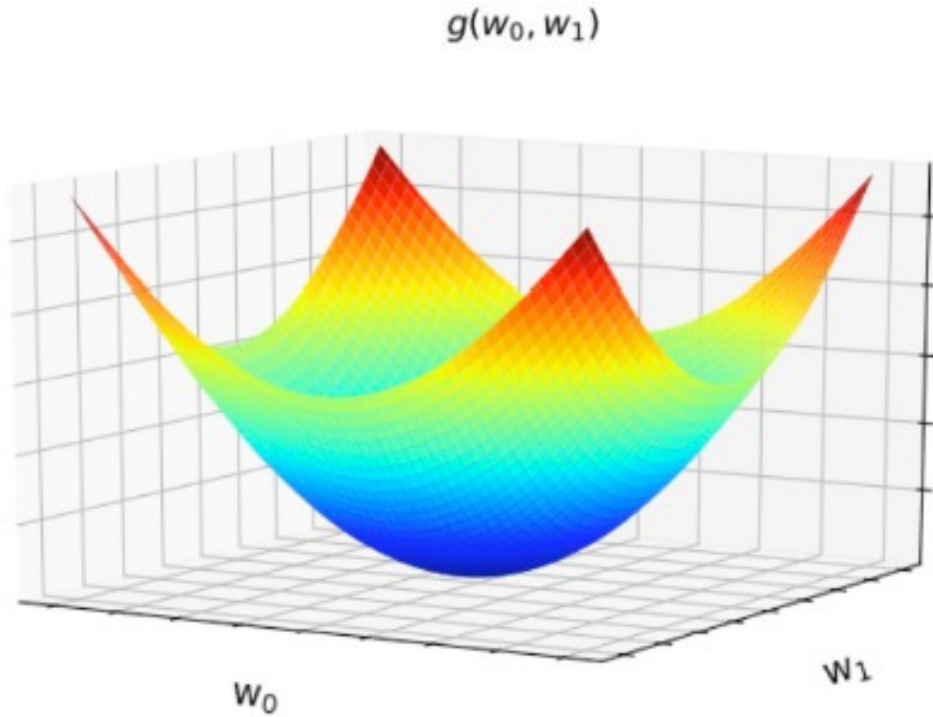
$$y = f(x; w_0, w_1) = w_1 x + w_0$$

- By minimizing the cost function

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

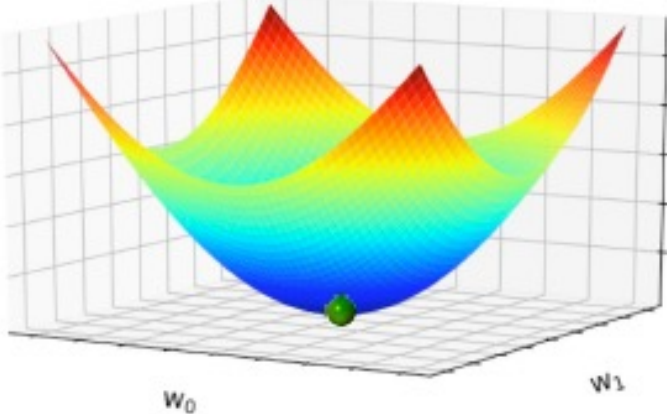
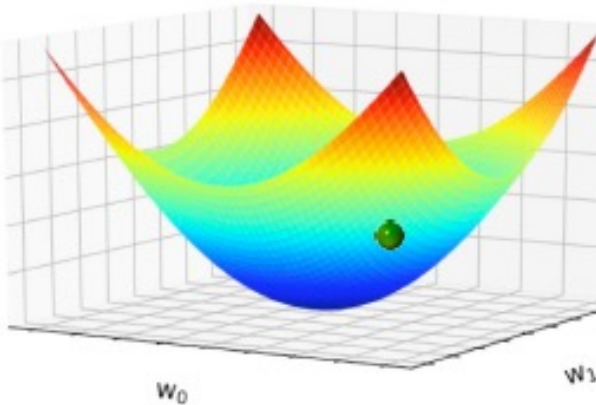
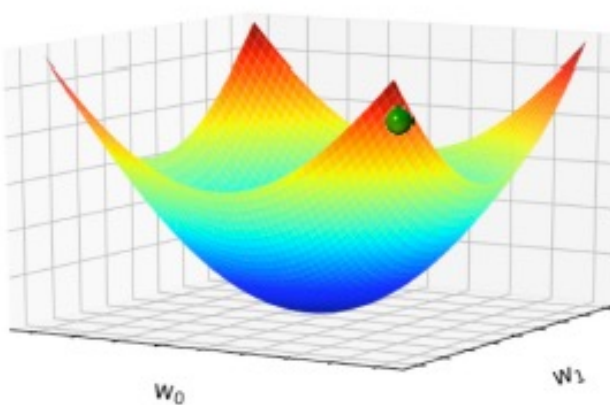
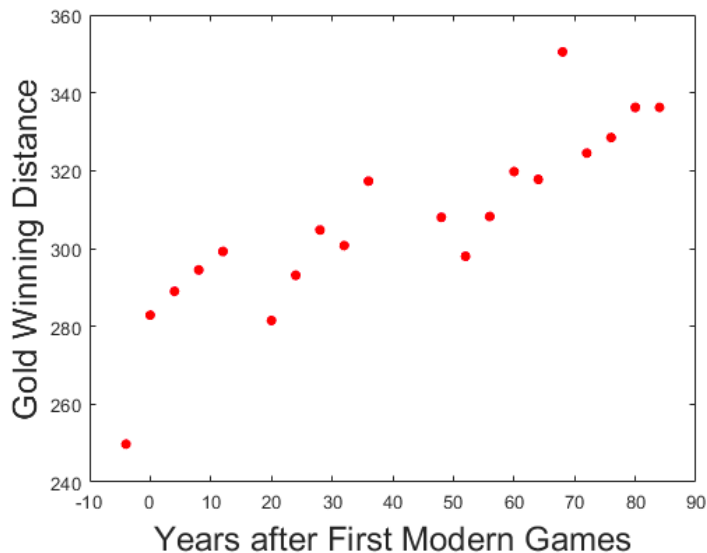


Cost function depends on the free parameter



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.

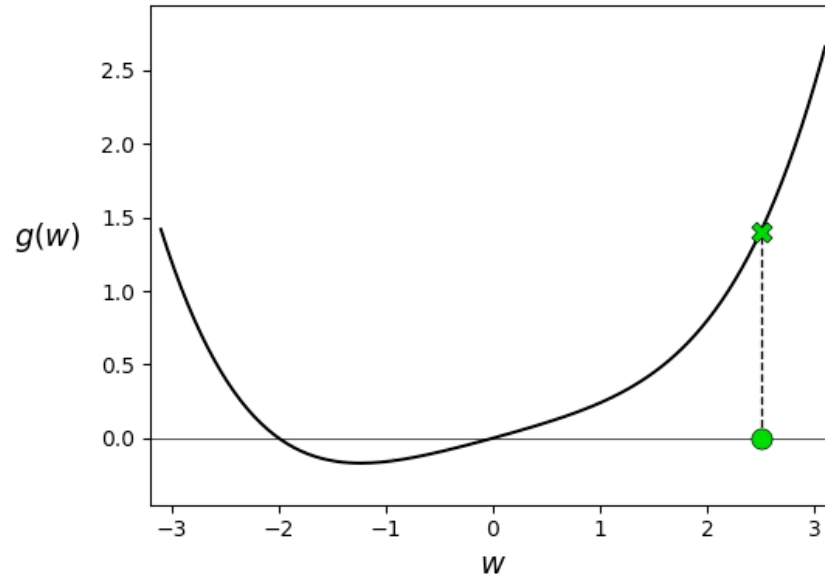


Gradient Descent



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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

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

Return w_0, w_1 .



Gradient Descent – More General...

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

Input: $\alpha > 0$

Initialise \mathbf{w} . //at 0 or some random value

Repeat until convergence

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

Return \mathbf{w} .



Algorithm for univariate linear regression using GD

Input: $\alpha > 0$, training set $\{(x^{(n)}, y^{(n)}): n = 1, 2 \dots N\}$

Initialise $w_0 = 0, w_1 = 0$

Repeat

for $n = 1, 2 \dots N$ //more efficient to update after each data point

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

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

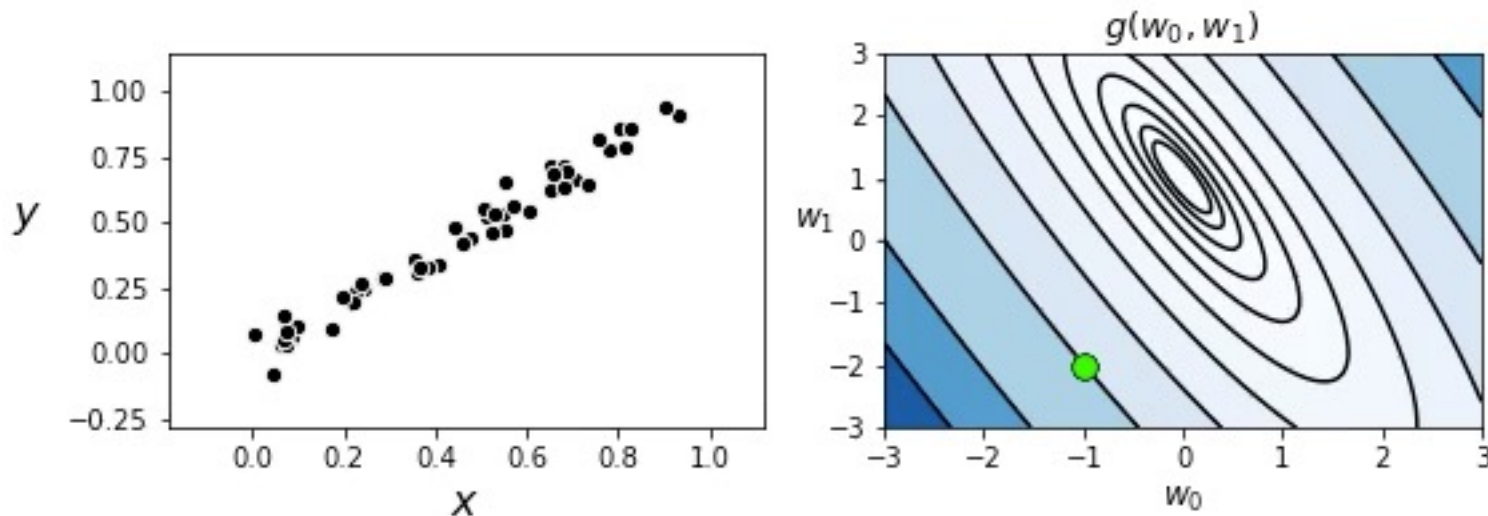
Until change in cost remains below a very small threshold

Return w_0, w_1 .



Univariate linear regression

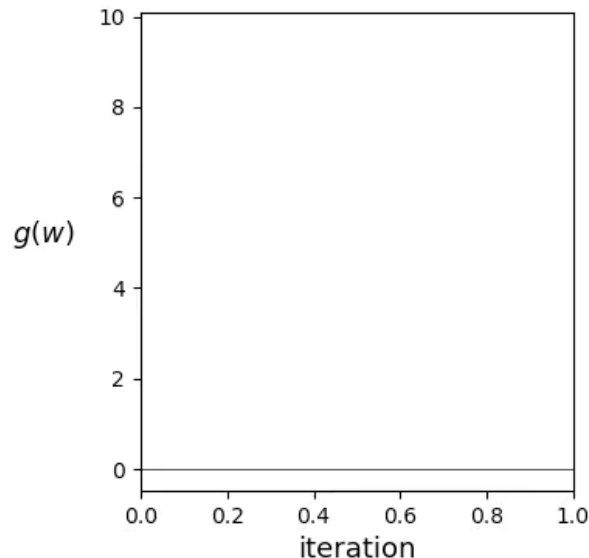
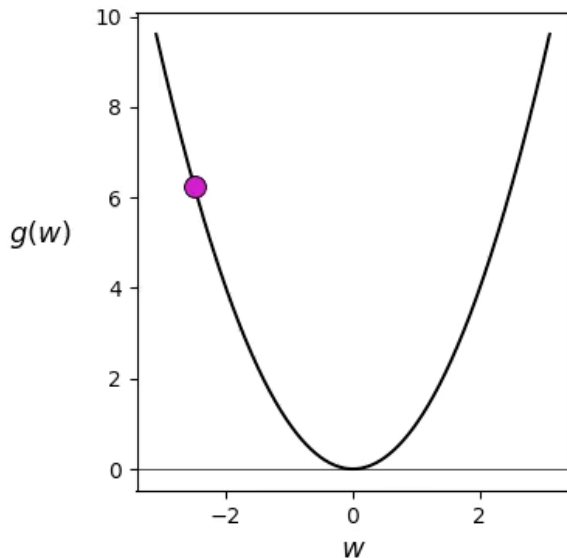
- Every combination of (w_0, w_1) has an associated cost.
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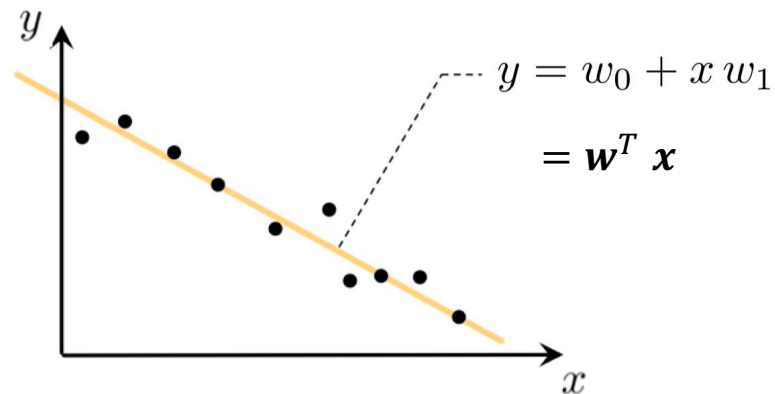
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Effect of the learning rate

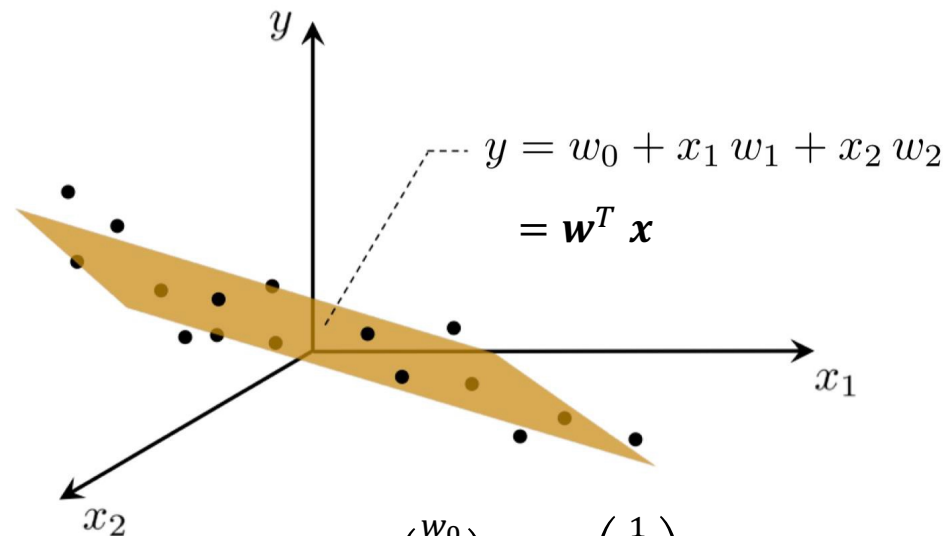
Whether or not we descend in the function when taking this step depends completely on how far along it we travel.



Multivariate linear regression



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

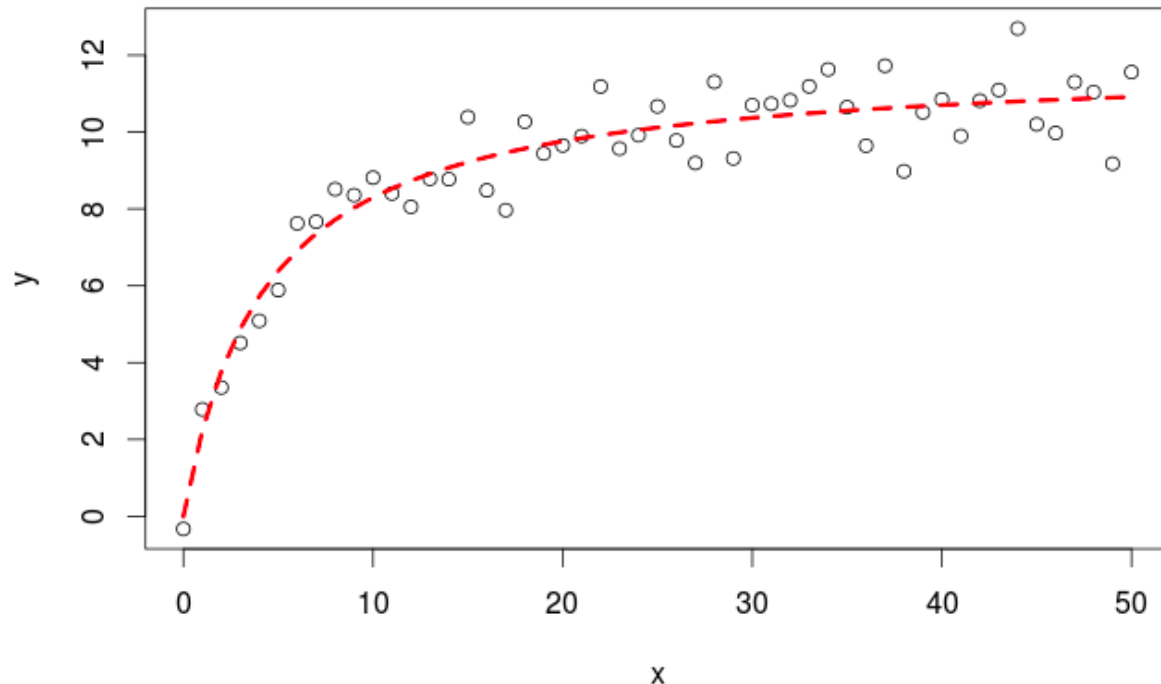


$$\mathbf{w} = \begin{pmatrix} w_0 \\ w_1 \\ w_2 \end{pmatrix}, \mathbf{x} = \begin{pmatrix} 1 \\ x_1 \\ x_2 \end{pmatrix}$$



Univariate nonlinear regression

$$y = w_0 + w_1x + w_2x^2 + w_3x^3 + \cdots + w_mx^m = \mathbf{w}^T \mathbf{x}$$



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

This is an m -th order polynomial regression model.

Advantages of vector notation

- Vector notation is more concise.
- With the vectors \mathbf{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:

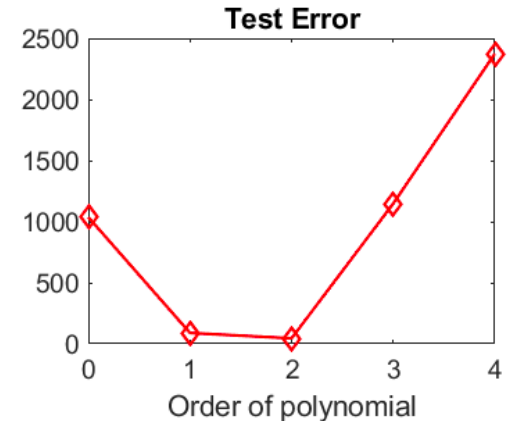
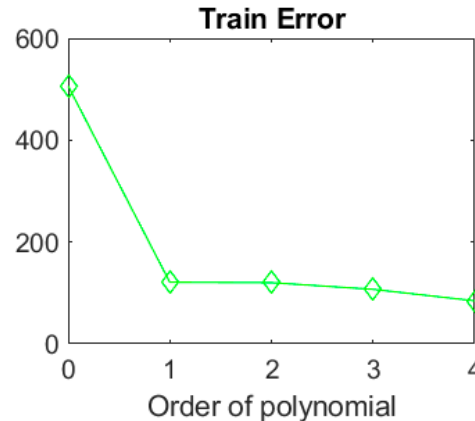
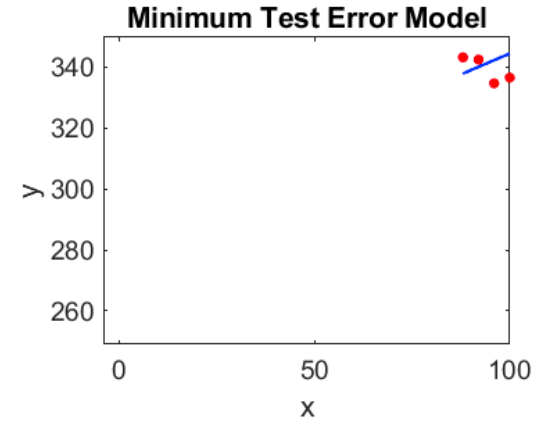
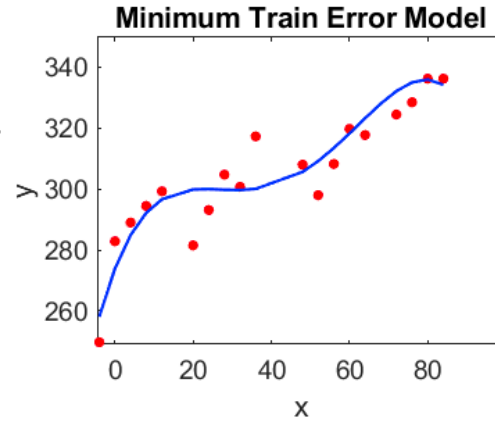
$$\nabla g(\mathbf{w}) = 2(\mathbf{w}^T \mathbf{x}^{(n)} - y^{(n)}) \mathbf{x}^{(n)}$$

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



Overfitting

- Linear regression also has overfitting problems. The model can be over-complex.
- What order of polynomial would you choose?





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Q/A

Teams Channel for Week2
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/jeremwatt/machine_learning_refined

