Lecture 4: Model parameter estimation - gradient

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Contents of this lecture

- Basic meaning of the model regression
- Define the regression (model optimization) problem
- Estimation of the regression model (parameters)
  - Euler-Lagrange theorem (mathematically explicit solution)
  - Gradient descent algorithm (numerical approximation)
- Numerical method: the gradient descent algorithms
- Computer examples

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Model regression (1)

- **For parametric regression models, let write them in a more general form**
  - $\hat{Y} = E[Y|\boldsymbol{X}] = \beta_0 + \beta_1 f(X_1) + \beta_2 f(X_2) + \cdots$
  - $f(X_i), i = 1,2, \ldots$, represent deterministic transformation of X, such as X_n, log(X), exp(X),…
  - The regression is to find optimal values of β_0, β_1,…, to minimize cost function of optimization

Model regression (2)

- **For the nonparametric regression models (smoothing moving average)**

$$\hat{Y} = E[Y|X] = \sum_{i=1}^{k} g(x - x_i) y_i$$

  - Which kernels $g(x)$ to choose for the smoothing, e.g., $g(x)$ can be normal, box, or other functions?
  - What parameters to choose for a picked kernel $g(x)$?
  - What is the width of the smooth, i.e., k?

Model regression problem def.

The procedure for the general model regression is

Data (n obs.): $\left(y^{(1)}, x_1^{(1)}, x_2^{(1)}, x_3^{(1)}, \dots\right), \left(y^{(2)}, x_1^{(2)}, x_2^{(2)}, x_3^{(2)}, \dots\right), \dots, \left(y^{(n)}, x_1^{(n)}, x_2^{(n)}, x_3^{(n)}, \dots\right)$

Hypothesis: $\hat{f}(\boldsymbol{X}) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots$

Parameters: $\beta_0, \beta_1, \beta_2, \dots$

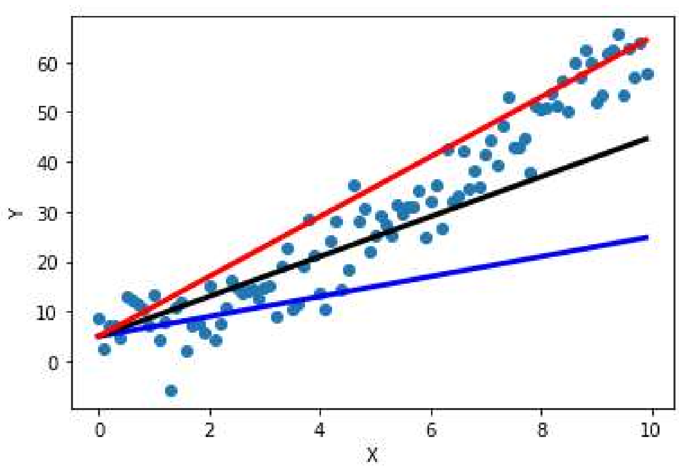
Cost Function: $J(\beta_0, \beta_1, \dots) = \frac{1}{2n}\sum_{i=1}^{n}(\hat{f}(\boldsymbol{X}^{(i)}) - y^{(i)})^2$

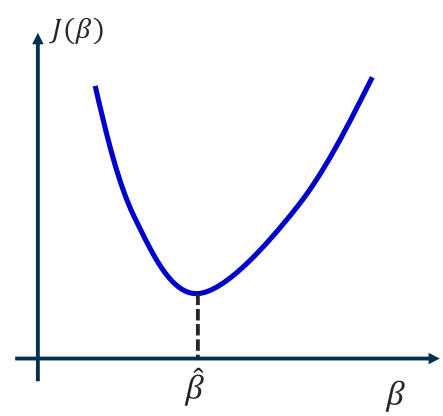
OLS, Ridge, Lasso

Goal: $\underset{\beta_0, \beta_1, \dots}{\text{minimize}}\, J(\beta_0, \beta_1, \dots)$

Regression: parameter estimation

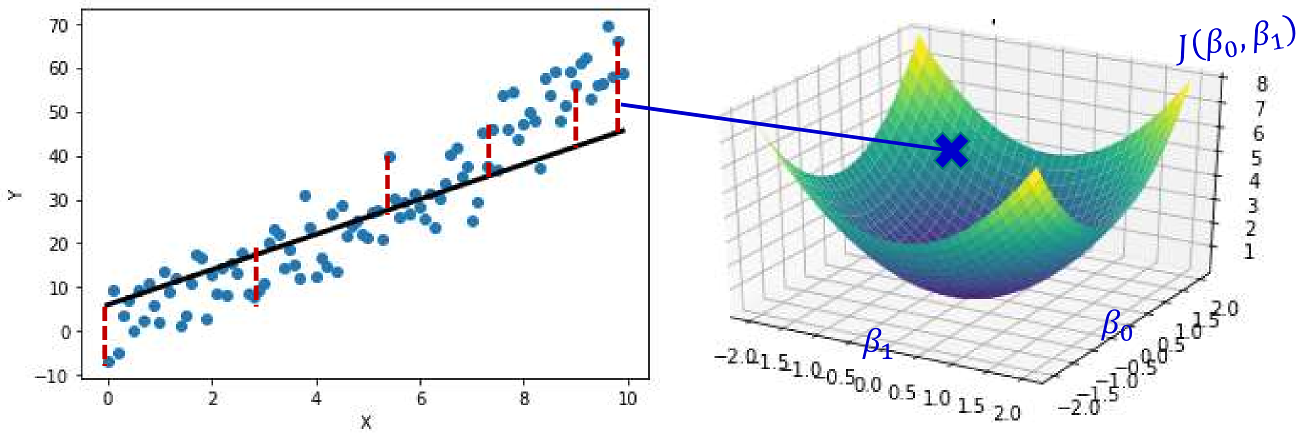
- For the cost function $J(\beta)$, the regression is to find $\hat{\beta}$ that can minimize J





Regression: parameter estimation

- For the cost function $J(\beta_0, \beta_1)$, the regression is to find $\hat{\beta}_0$ and $\hat{\beta}_1$ that can minimize J



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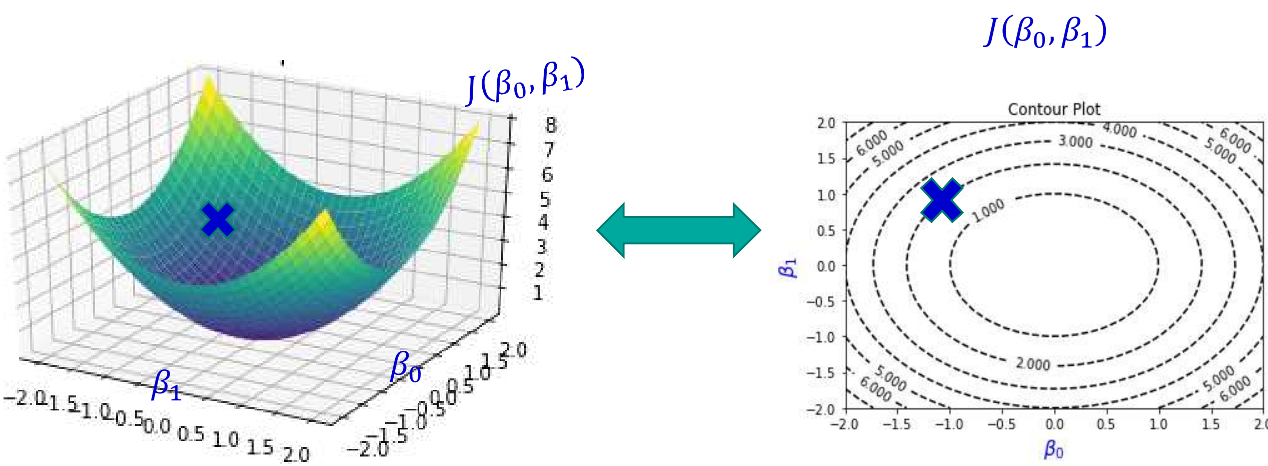
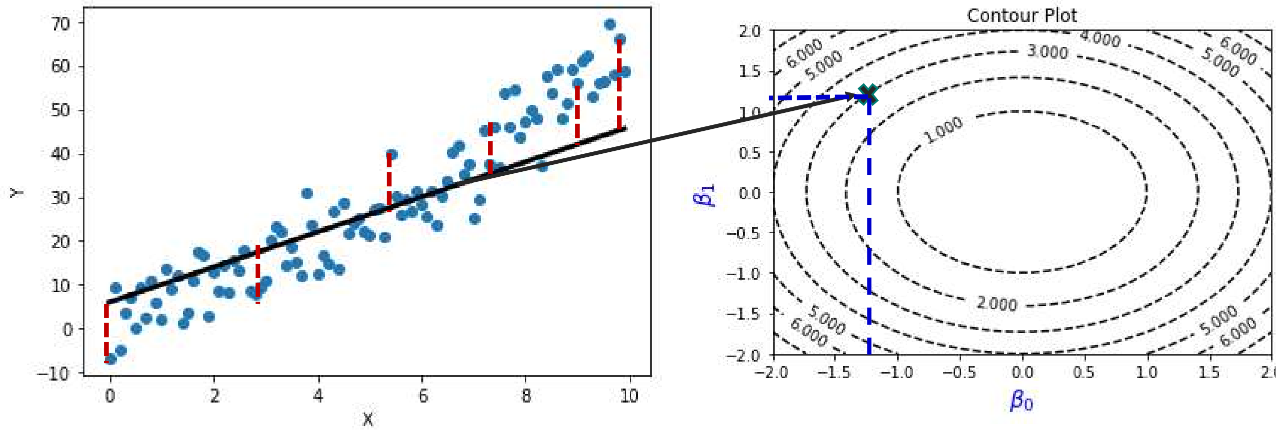


Regression: parameter estimation

For a model $Y = \beta_0 + \beta_1 X$, with data (x_i, y_i) and cost function J as follows:



Regression: parameter estimation

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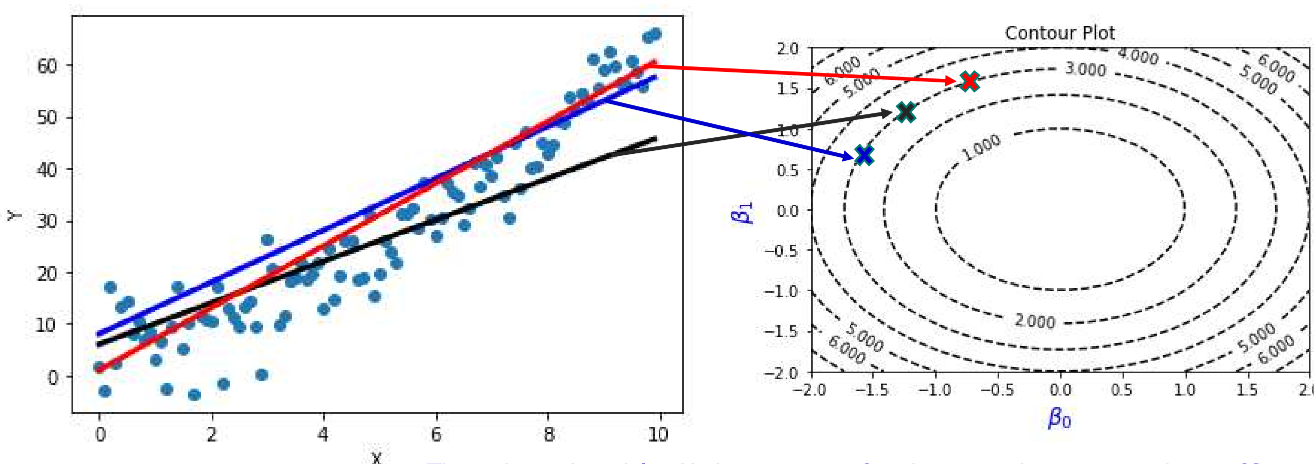
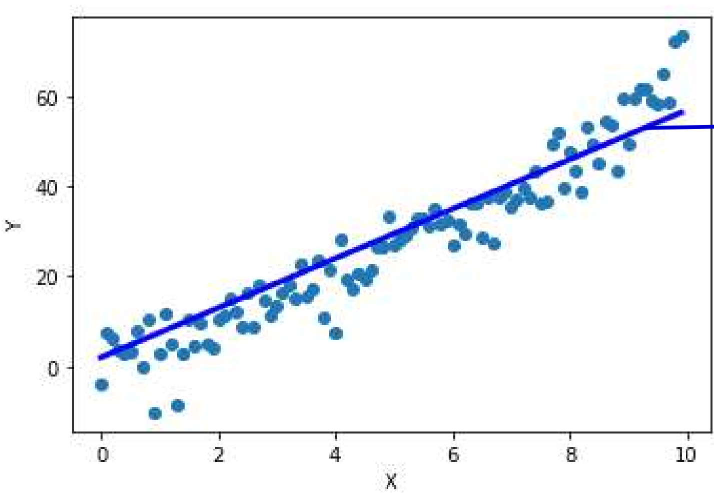
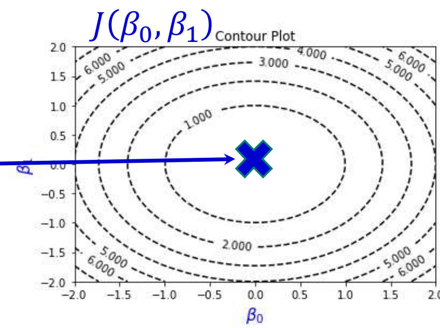


The estimated models with the same cost function mean the same goodness of fit.
Their values are shown as marks on the same contour line.

Regression: parameter estimation

- For the cost function $J(\beta_0, \beta_1)$, the regression is to find $\hat{\beta}_0$ and $\hat{\beta}_1$ that can minimize J





According to the Lagrange multiplier theorem, the solution of parameters to minimize the cost function J is set:

$$\frac{\partial J(\beta_0, \beta_1)}{\partial \beta_0} = 0 \qquad \frac{\partial J(\beta_0, \beta_1)}{\partial \beta_1} = 0$$

Regression: parameter estimation (1)

- When the cost function is very complex, it means that the mathematical solution to the differential equations with respect to parameters is not that straightforward.
- Some numerical methods, e.g., implementation of the gradient descent, could be used to get the parameters of a model to minimize the cost function for the regression
- Let the cost function represented by $J(\beta_0, \beta_1)$, the procedure to get β_0, β_1 minimizing J is:

Regression: parameter estimation (2)

- **Workflow for gradient descent for numerical approximation:**
  - Start with some initial values ($\beta_0 = \beta_{0,0}, \beta_1 = \beta_{1,0}$)
  - Updating the values of (β_0, β_1) iteratively according to the gradient of cost functions until the cost function reaches to a minimum point (not always successful for global minimum)

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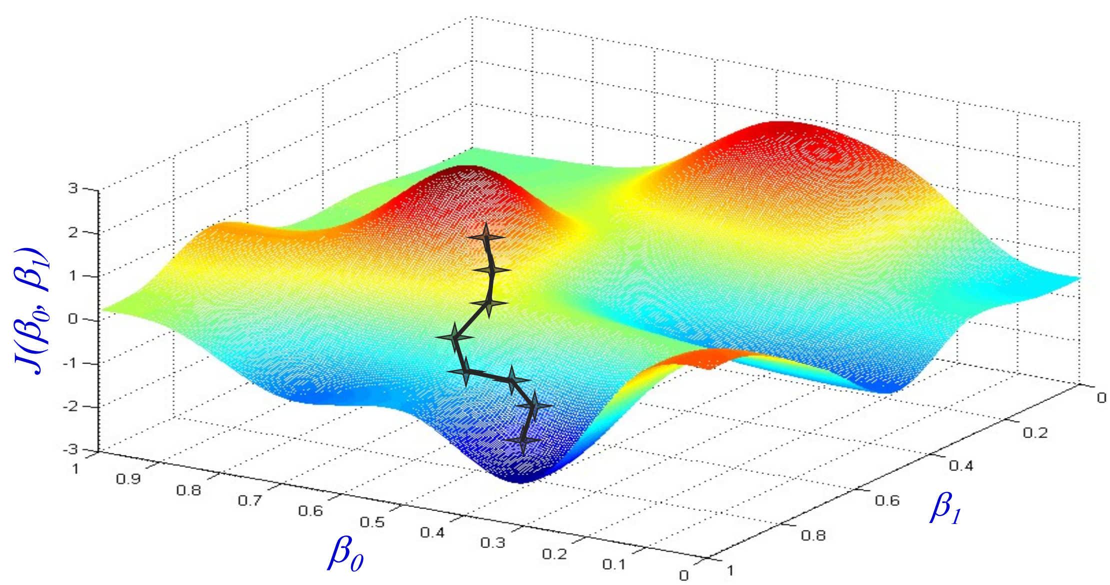
Gradient descent for approximation



From Andrew Ng's lecture notes

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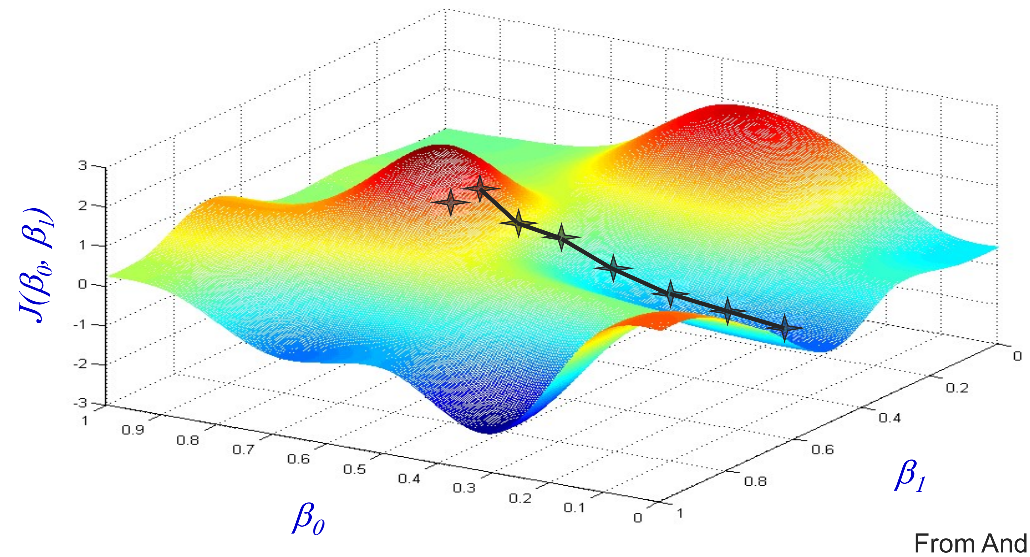
Initial values matter for approximation



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(Batch) Gradient descent algorithm

Procedures to implement the gradient descent algorithm

1. Select initial values of (β_0, β_1) according to your experiences, i.e., $(\beta_{0,0}, \beta_{1,0})$
2. Choose a learning rate coefficient α
3. Estimate the gradient of the cost function J at the values of $(\beta_{0,0}, \beta_{1,0})$, i.e.,
   $\frac{\partial}{\partial \beta_0} J(\beta_{0,0}, \beta_{1,0})$, and $\frac{\partial}{\partial \beta_1} J(\beta_{0,0}, \beta_{1,0})$
4. Update all the model parameters simultaneously according to the learning rate
   $\beta_{0,1} = \beta_{0,0} - \alpha \frac{\partial}{\partial \beta_0} J(\beta_{0,0}, \beta_{1,0})$,
   $\beta_{1,1} = \beta_{1,0} - \alpha \frac{\partial}{\partial \beta_1} J(\beta_{0,0}, \beta_{1,0})$
5. Repeat steps (3-4) until the cost function J convergence to a minimum point

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Stochastic Gradient descent Algor.

Procedures to implement the gradient descent algorithm

1. Select initial values of (β_0, β_1) according to your experiences, i.e., $(\beta_{0,0}, \beta_{1,0})$
2. Choose a learning rate coefficient α
3. Estimate the error of the first instance (data point), i.e., $\varepsilon = y_i - \beta_{0,0} - \beta_{1,0}X_i$
4. Update all the model parameters simultaneously according to the learning rate

   $\beta_{0,1} = \beta_{0,0} - \alpha \times \varepsilon,$

   $\beta_{1,1} = \beta_{1,0} - \alpha \times \varepsilon \times X_i,$
5. Repeat steps (3-4) until the parameters converge to stable parameters

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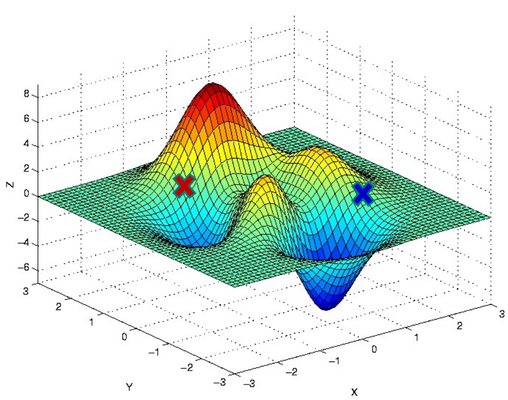
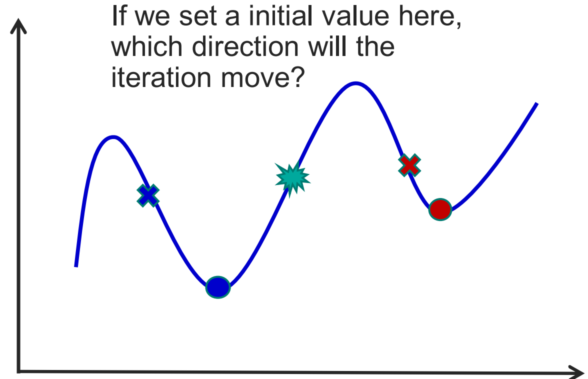
Key elements in Gradient algorithm

- **Initial values of the model parameters are important for the convergence study**
- **Not necessarily always convergence to a global minimum cost value**





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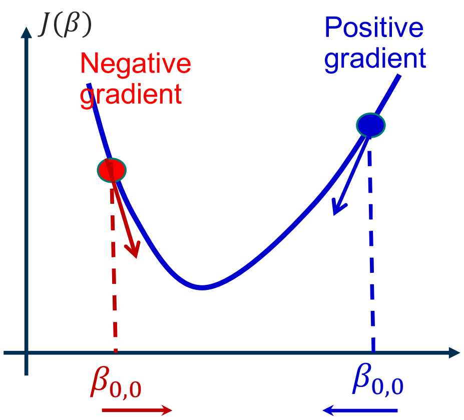
Key elements in Gradient algorithm

- Movement of parameter update in continuous iterations



$$\beta_{0,1} = \beta_{0,0} - \alpha \frac{\partial}{\partial \beta_0} J(\beta_{0,0}, \beta_{1,0}),$$

Let the learning rate α as a positive value

- On the negative side, since the derivative is negative, the parameter increments will be positive, i.e., move right
- On the negative side, the parameter increments will move Left
- So, on both side, the parameters will move toward the minimum location of the cost function

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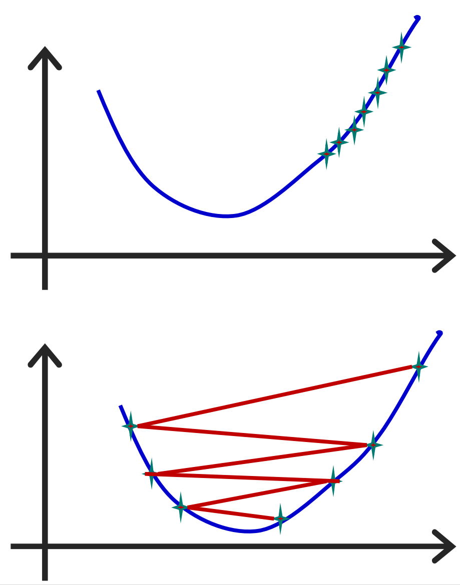
Key elements in Gradient algorithm

The results will be sensitive to values of the learning rate:

- If α is too small, the convergence of gradient descent will be slow
- If α is too large, the convergence can overshoot the minimum, or even diverge

$$\beta_{0,1} = \beta_{0,0} - \alpha \frac{\partial}{\partial \beta_0} J(\beta_{0,0}, \beta_{1,0}),$$



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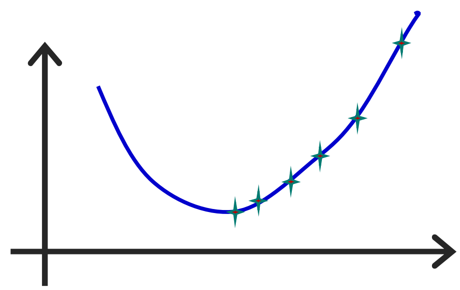
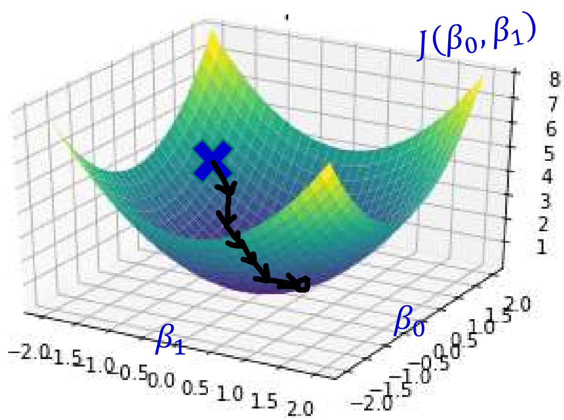
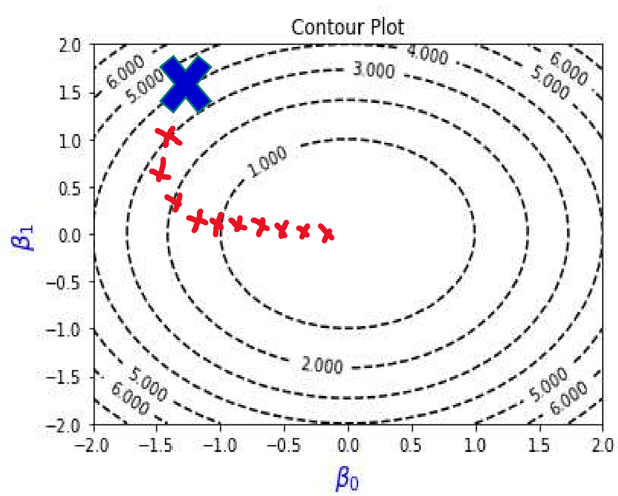
Key elements in Gradient algorithm

- Should the value of α be adjusted (reduced) in each iteration when the cost function approaches to its minimum location?
- *Probably not, because gradient descent can automatically help the iteration take smaller steps, because the derivative also decreases.*



Gradient descent for multivariate regression





Final remarks on gradient descent

- For each iteration of the gradient descent method, all the data should be used to estimate the cost for the pre-assumed model parameters.
- The gradient descents ideas have been also widely used in other machine learning algorithms.
- For example, to be combined with the boosting method, the so-called XG boost method is one of the most powerful ML algorithm for the model estimation.

Introduction of assignment project 2

- Prediction of ship power consumption in terms of other parameters

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