情報工学実験4:データマイニング班

(week 3) 線形回帰モデルと最急降下法

1. 復習
2. scikit-learn入門
3. モデルとは？（問題設定、アルゴリズム、モデル）
4. 線形回帰モデル
5. 仮説、損失関数、目的関数
6. 最小二乗法
7. 最急降下法
8. 参考サイト

実験ページ: http://ie.u-ryukyu.ac.jp/~tnal/2017/info4/dm/

Example: *Iris* flower data set

review

http://en.wikipedia.org/wiki/Iris_flower_data_set

(1) What is experience E?
(2) What is task T?
(3) How to measure the performance P?

- Classification
  - In Classification, the samples belong to two or more classes and we want to learn from already labeled data how to predict the class of unlabeled data.
  - E.g., distinguishes the species from each other.
  - Dataset = samples vs. features and classes

- Teach data
- supervisory signal
- output data, Y
- target
- 1 class in 3 classes

- Input data, X
- 4 features or attributes

Fisher's *Iris* Data

1 sample

Sepal length	Sepal width	Petal length	Petal width	Species
5.1	3.5	1.4	0.2	*I. setosa*
4.9	3.0	1.4	0.2	*I. setosa*
4.7	3.2	1.3	0.2	*I. setosa*
4.6	3.1	1.5	0.2	*I. setosa*
5.0	3.6	1.4	0.2	*I. setosa*

Example: boston house prices dataset

http://archive.ics.uci.edu/ml/datasets/Housir

review

(1) What is experience E?
(2) What is task T?
(3) How to measure the performance P?

- Regression
  - If the desired output consists of one or more continuous variables, then the task is called *regression*.
  - E.g., concerns housing values in suburbs of Boston.
  - Dataset = samples vs. features and continuous variables

13 features

Continuous variable

1 sample

CRIM	ZN	INDUS	（中略）	LSTAT	MEDV
6.32E−03	1.80E+01	2.31E+00		4.98E+00	24.00
2.73E−02	0.00E+00	7.07E+00		9.14E+00	21.60
2.73E−02	0.00E+00	7.07E+00		4.03E+00	34.70

Example: *Iris* flower data set WITHOUT classes

http://en.wikipedia.org/wiki/Iris_flower_data_set

review

(1) What is experience E?
(2) What is task T?
(3) How to measure the performance P?

- Clustering
  - Clustering is the task of grouping a set of objects in such a way that objects in the same group (called a **cluster**) are more similar (in some sense or another) to each other than to those in other groups (clusters).
  - Training data consists of a set of input vectors x **without any corresponding target values**.
  - Dataset = samples vs. features

4 features

Don't use at learning

Fisher's *Iris* Data

Sepal length	Sepal width	Petal length	Petal width	Species
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4.6	3.1	1.5	0.2	*I. setosa*

1 sample

Terminology

review

- supervised, unsupervised learning
- classification, regression, clustering
- sample
- features, attributes
  - numerical value
  - categorical value
  - true or false
- supervisory signal, teacher, class, label, output data, target variable

- input, output
- training data / training set
- test data / test set
  - open test
  - close test
- model
- parameters
- learn, fit
- predict, estimate
- evaluation

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An introduction to machine learning with scikit-learn (1/3)

hg clone ssh://info3dm@shark//home/info3dm/HG/tnal
less sklearn_intro.py

- Loading and an example dataset
  - python --version
    - Python 3.5.2 :: Anaconda 4.1.1 (x86_64)
  - python
  - >>> from sklearn import datasets
  - >>> iris = datasets.load_iris() # datasets.load[tab]
  - >>> print(iris.DESCR)
  - >>> print(iris.data)
  - >>> print(iris.target)
  - >>> print(iris.target_names)

http://scikit-learn.org/stable/tutorial/basic/tutorial.html

An introduction to machine learning with scikit-learn (2/3)

- Learning and predicting
  - >>> from sklearn import svm
  - >>> clf = svm.SVC(gamma=0.001, C=100.)
  - >>> clf.fit(iris.data[:-1], iris.target[:-1])
  - >>> clf.predict(iris.data[-1:]]
    - sklearn 0.17以降?, サンプル1個だと書き方に注意。
  - >>> print(iris.target[-1])
  - >>> clf.score(iris.data, iris.target)

http://scikit-learn.org/stable/tutorial/basic/tutorial.html

An introduction to machine learning with scikit-learn (3/3)

- Model persistence
  - # save
  - >>> import pickle
  - >>> file = open("PredictiveModel.dump", "wb")
  - >>> pickle.dump(clf, file)
  - >>> file.close()
  - # load
  - >>> file = open("PredictiveModel.dump", "rb")
  - >>> clf2 = pickle.load(file)
  - >>> file.close()
  - >>> clf2.predict(iris.data[-1]]
  - >>> print(iris.target[-1])

http://scikit-learn.org/stable/tutorial/basic/tutorial.html

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Problems, Models, Algorithms

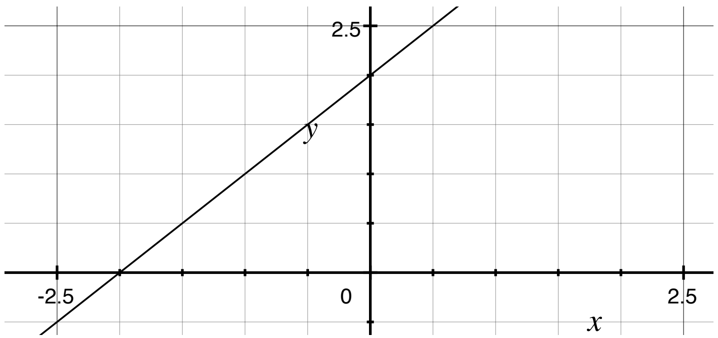
- Problems
  - Classification
  - Regression
  - Clustering
- Algorithms
  - Ordinary Least Squares
  - Gradient Descent
  - Back Propagation

- Models
  - Linear Regression Model
  - Generalized Linear Models
  - Neural Network
  - Decision Tree
  - (other kinds of models)
    - Bag-of-words document model

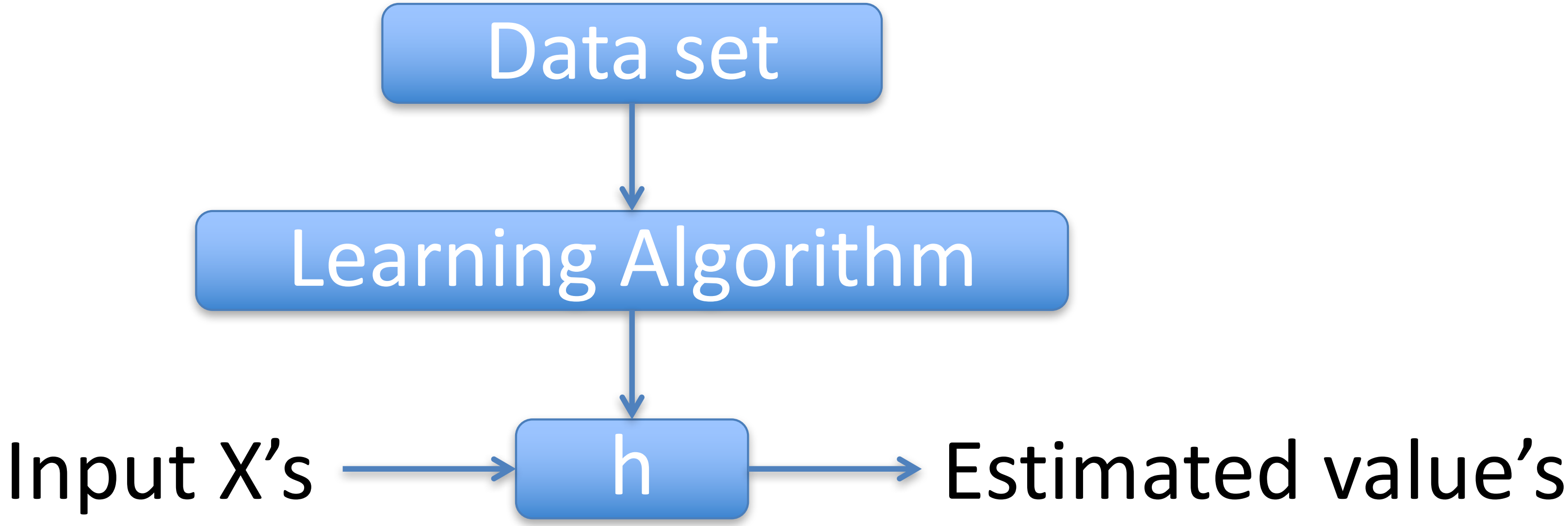
What is that?

Models

- Represent by any formulas with (sometimes one) parameters for the relationship between input X's and output Y's.
  - In machine learning, the formulas called as "hypothesis".
  - E.g., h = a*x + b
    - a, b: parameters
  - Parameterized model.
  - Predictive model. (e.g., a=1, b=2)



Problem <-> Algorithm + Model



Linear Regression Model

$$h_\theta(x) = \theta_0 x_0 + \theta_1 x_1 = \sum \theta_i x_i = \sum \theta_i \Phi_i(x)$$

$$h_\theta(x) = \theta_0 + \theta_1 x$$

- How do we prepare a model?
- How do we evaluate the goodness?
- How do we choose the appropriate parameters?

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Linear Regression Model

- Training datasets
  - (x,y) = (4,7), (8,10), (13,11), (17,14)
- Hypothesis

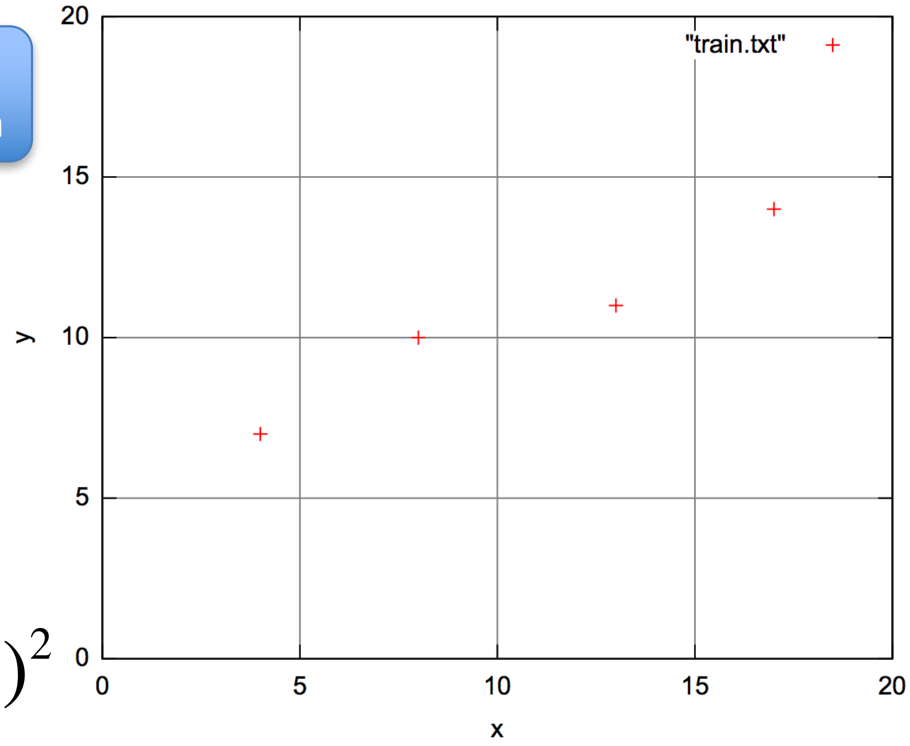
$$h_\theta(x) = \theta_0 + \theta_1 x$$

Assumption 1
Linear function

- Parameters
  - θ0, θ1
- Cost function

Assumption 2
Squared error

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



- Objective function (measurement of the goodness)

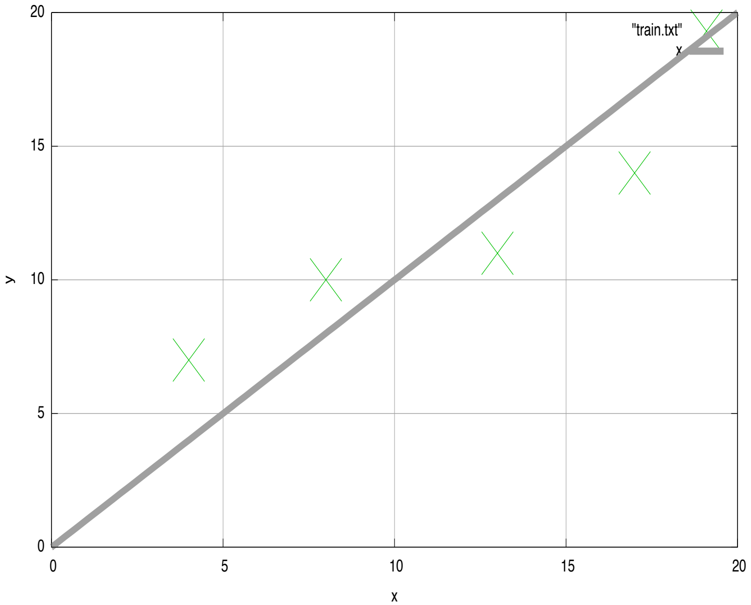
$$\min_\theta J(\theta_0, \theta_1)$$

Hypothesis vs. Cost function (θ1=1)

θ0=0, θ1=1, (x,y)=(4,7), (8,10), (13,11)

Hypothesis:

$$h(x) = x$$

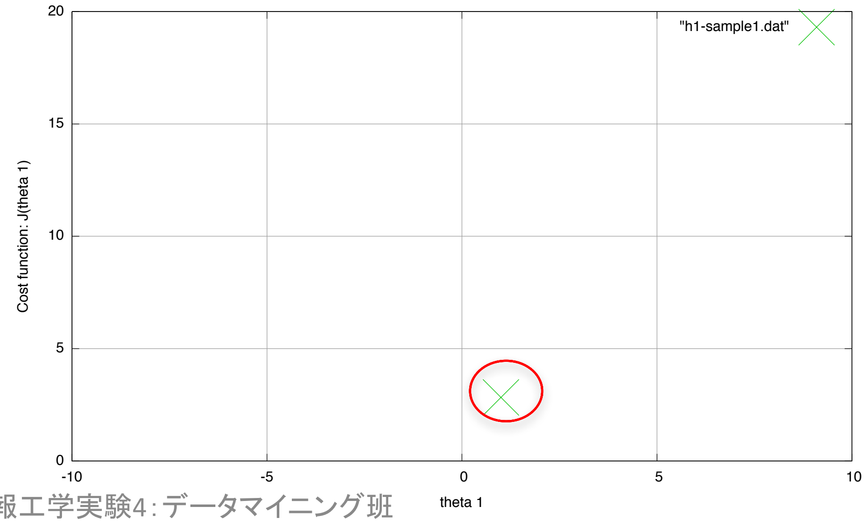


Cost function:

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

$$J(0,1) = \frac{1}{2m}((4-7)^2 + (8-10)^2 + (13-11)^2)$$

$$J(0,1) = \frac{1}{2*3}(9+4+4) = \frac{17}{6} = 2.83$$



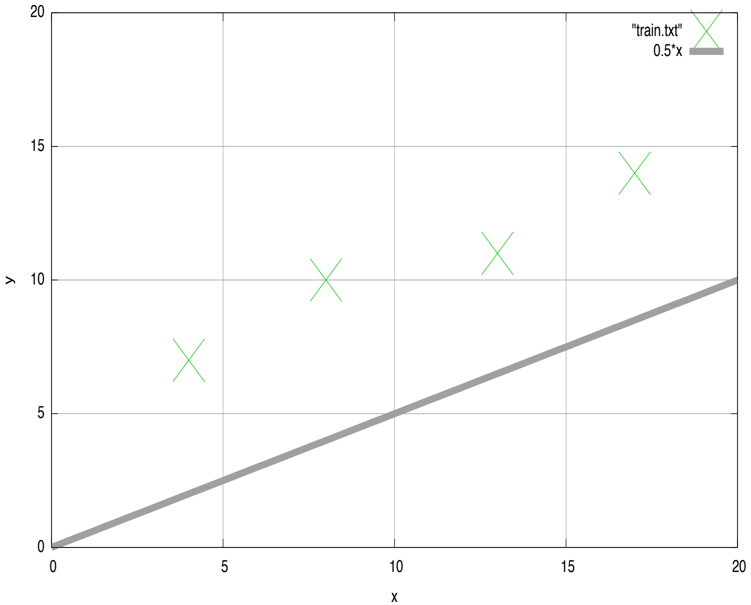
Hypothesis vs. Cost function (θ1=0.5)

θ0=0, θ1=0.5, (x,y)=(4,7), (8,10), (13,11)

Hypothesis:	Cost function:

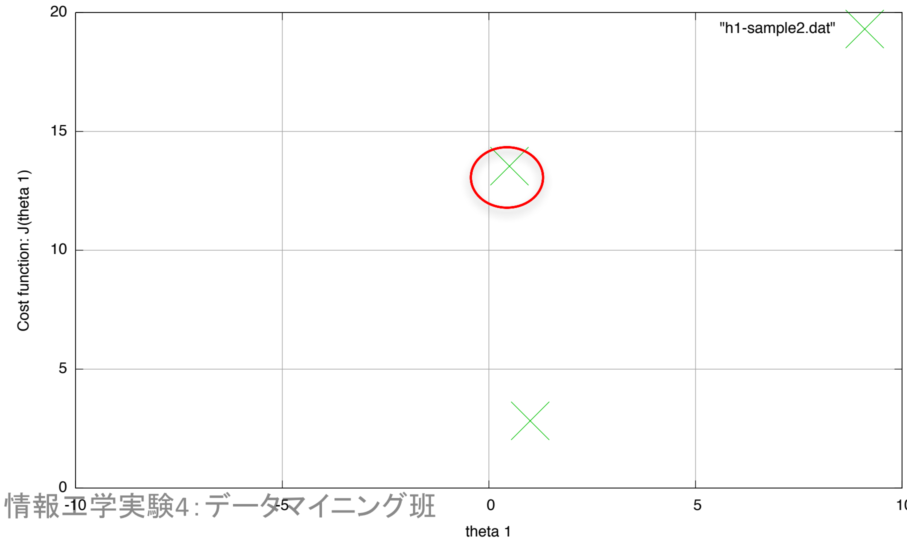
$$h(x) = 0.5 * x$$

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



$$J(0.5) = \frac{1}{2m}((2-7)^2 + (4-10)^2 + (6.5-11)^2)$$

$$J(0.5) = \frac{1}{2*3}(25 + 36 + 20.25) = \frac{81.25}{6} = 13.54$$



Hypothesis vs. Cost function (θ1=others)

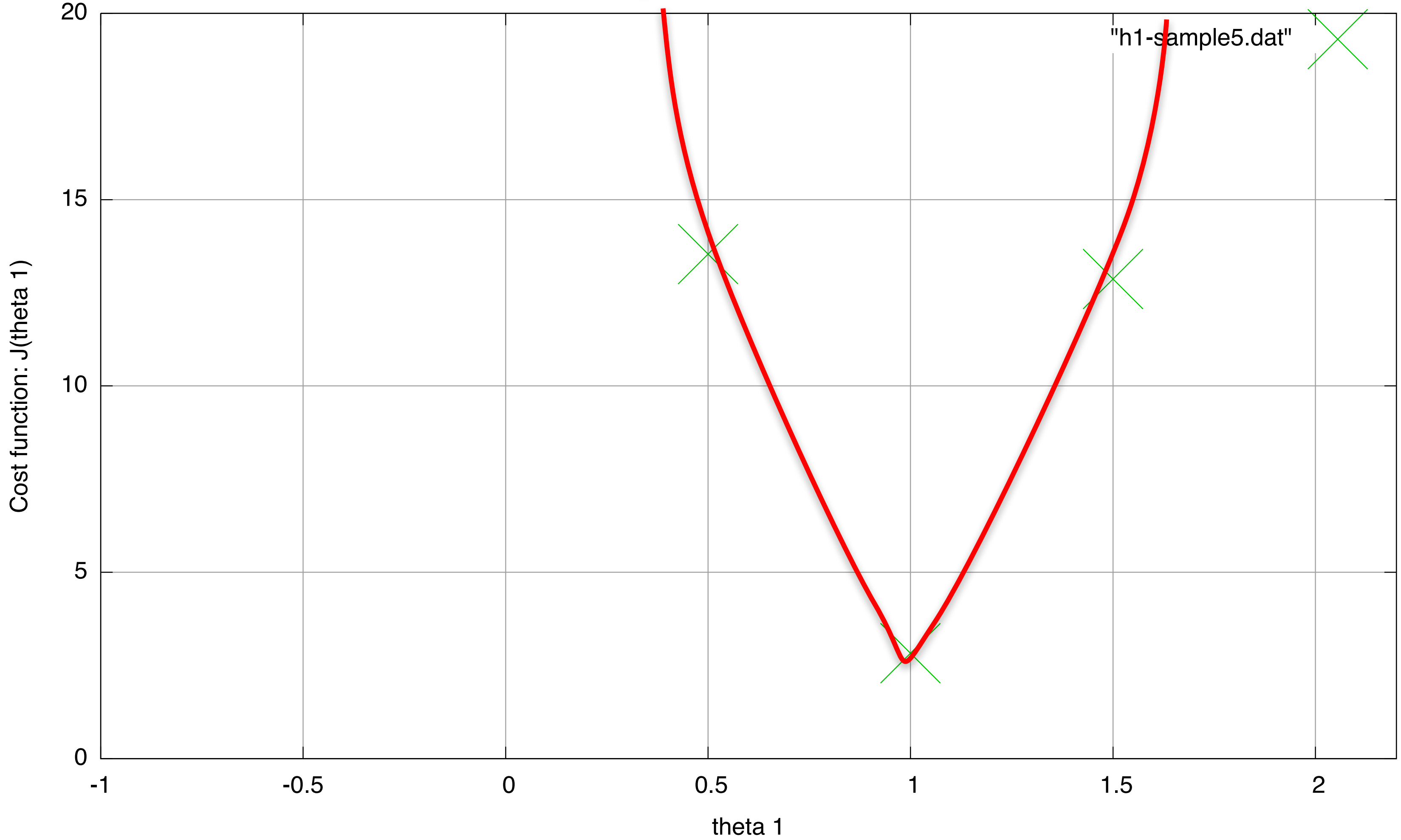
θ0=0, θ1=others, (x,y)=(4,7), (8,10), (13,11)

- θ1=0:
  - H(x)=0*x=0
  - J(0)=1/6{(0-4)^2+(0-10)^2+(0-13)^2}
    - =1/6{16+100+169}=47.5
- θ1=2:
  - H(x)=2*x
  - J(2)=1/6{(8-7)^2+(16-10)^2+(26-11)^2}
    - =1/6{1+25+225}=41.83
- θ1=1.5:
  - H(x)=1.5*x
  - J(1.5)=1/6{(6-7)^2+(12-10)^2+(19.5-11)^2}
    - =1/6{1+4+72.25}=12.87

Objective function: minimize J(θ1)

- How do we observe the shape of function?
- How do we observe the behavior of GD?

Convex function



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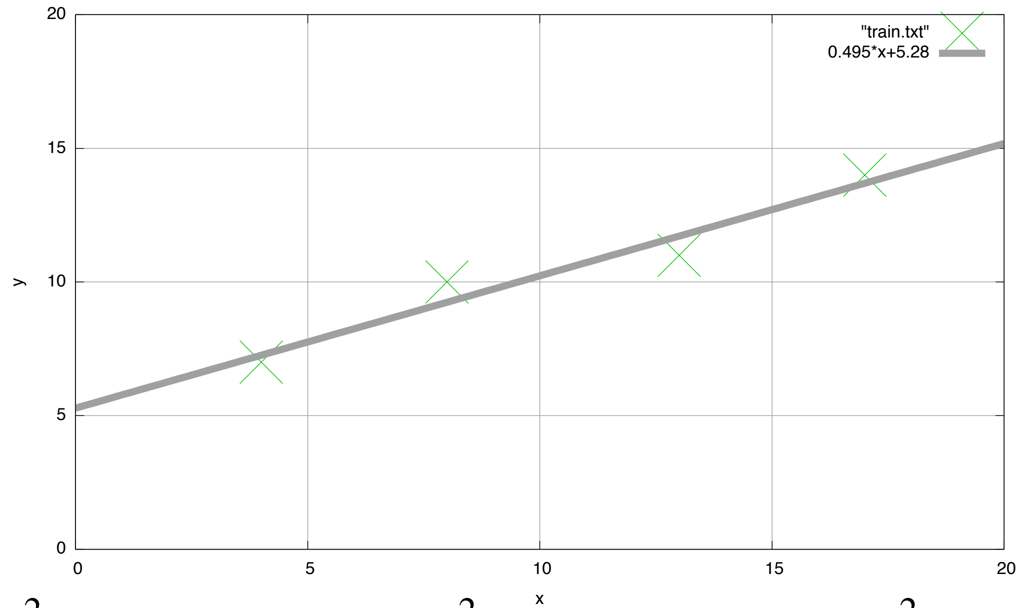
Ordinary Least Squares

problems?

$$h(x) = \theta_0 + \theta_1 x$$

(x,y)=(4,7), (8,10), (13,11), (17,14)



$$7 = \theta_0 + 4\theta_1$$

$$0 = \theta_0 + 4\theta_1 - 7$$

$$e_1 := \theta_0 + 4\theta_1 - 7$$

$$e_1^2 = (\theta_0 + 4\theta_1 - 7)^2$$

$$E = \sum e_i^2 \geq 0$$

$$= (\theta_0 + 4\theta_1 - 7)^2 + (\theta_0 + 8\theta_1 - 10)^2 + (\theta_0 + 13\theta_1 - 11)^2 + (\theta_0 + 17\theta_1 - 14)^2$$

$$= 538\theta_1^2 + 84\theta_0\theta_1 + 4\theta_0^2 - 978\theta_1 - 84\theta_0 + 466$$

$$= (2\theta_1 + 21\theta_0 - 21)^2 + 97(\theta_0 - 48/97)^2 + 121/97$$

θ0=1029/194≒5.28, θ1=48/97≒0.495

h(x) = 5.28 + 0.495x

Ref., http://gihyo.jp/dev/serial/01/machine-learning/0008

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Gradient descent algorithm

Repeat until convergence {

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

}

(1) Start with any parameters.
(2) Update the parameters simultaneously, until convergence.

<u>Simple example</u>

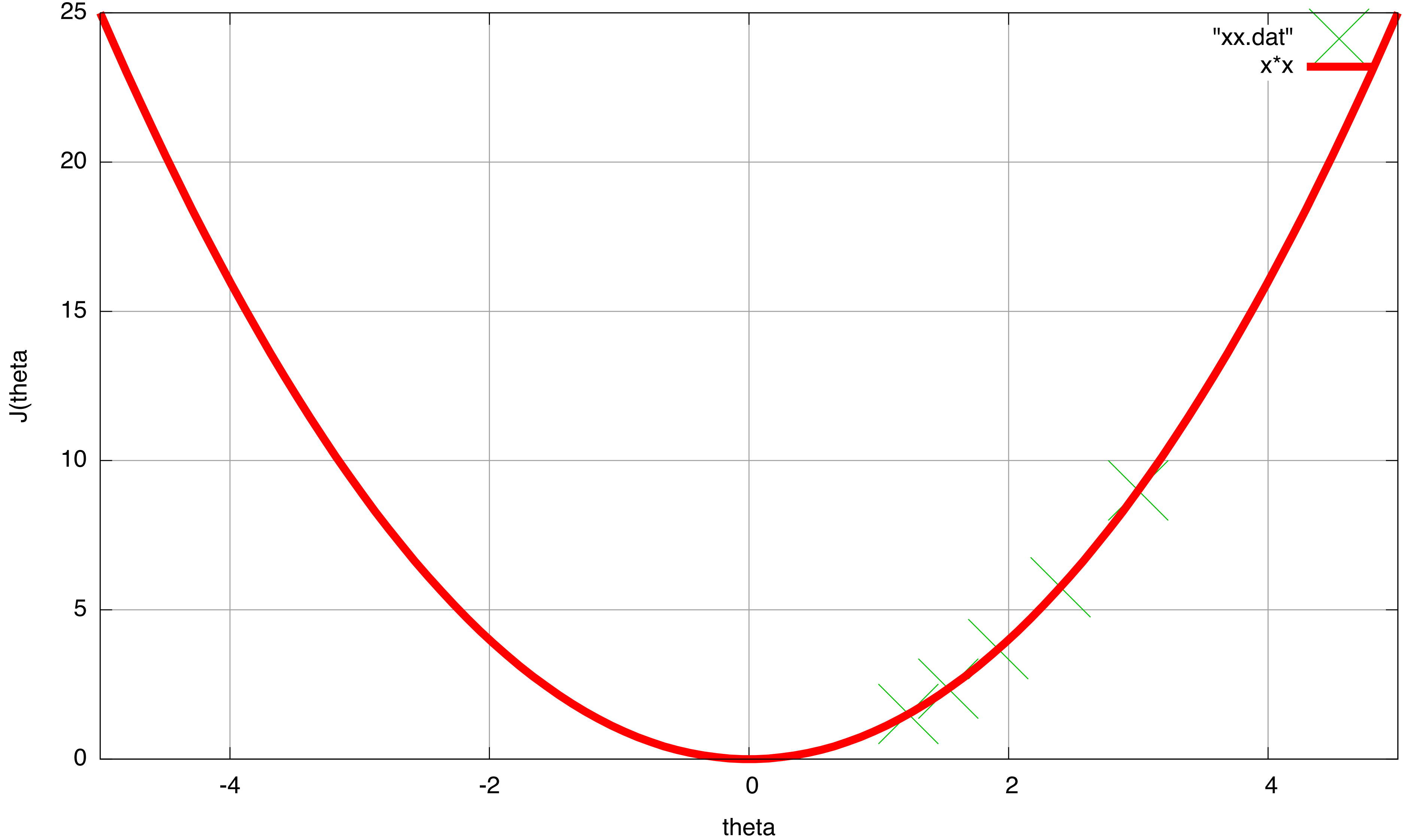
$$J(\theta) = \theta^2, \alpha = 0.1$$

$$new\_\theta = \theta - \alpha \frac{d}{d\theta} J(\theta)$$

$$= \theta - 0.1 * 2\theta = \theta - 0.2\theta = 0.8\theta$$

- e.g., α=0. 1, θ=3, J(θ)=9
- 1st update
  - New_θ = 0.8*3 = 2.4
  - J(θ) = 2.4**2 = 5.76
- 2nd update
  - New_θ = 0.8*2.4 = 1.92
  - J(θ) = 1.92**2 = 3.6864
- 3rd update
  - New_θ = 1.536
  - J(θ) = 2.359296
- 4th update
  - New_θ = 1.2288000000000001
  - J(θ) = 1.5099494400000002

Cont.) the behavior of GD



Gradient descent for Linear Regression

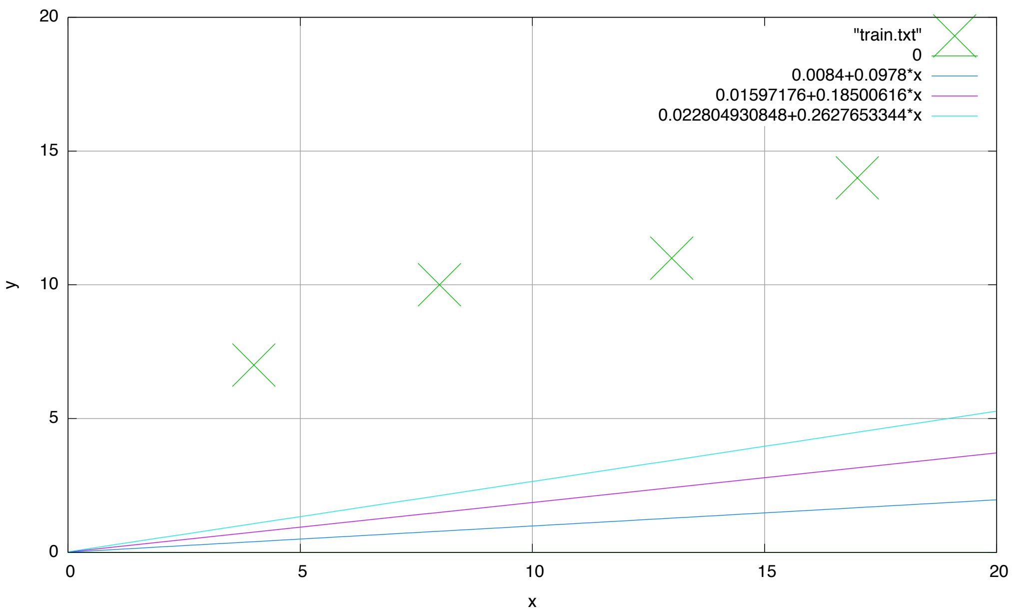
$$\theta_i := \theta_i - \alpha \frac{\partial}{\partial \theta_i} J(\theta_0, \theta_1)$$

$$h_\theta(x) = \theta_0 + \theta_1 x$$ (x,y) = (4,7), (8,10), (13,11), (17,14)

$$J(\theta_0, \theta_1) = 538\theta_1^2 + 84\theta_0\theta_1 + 4\theta_0^2 - 978\theta_1 - 84\theta_0 + 466$$

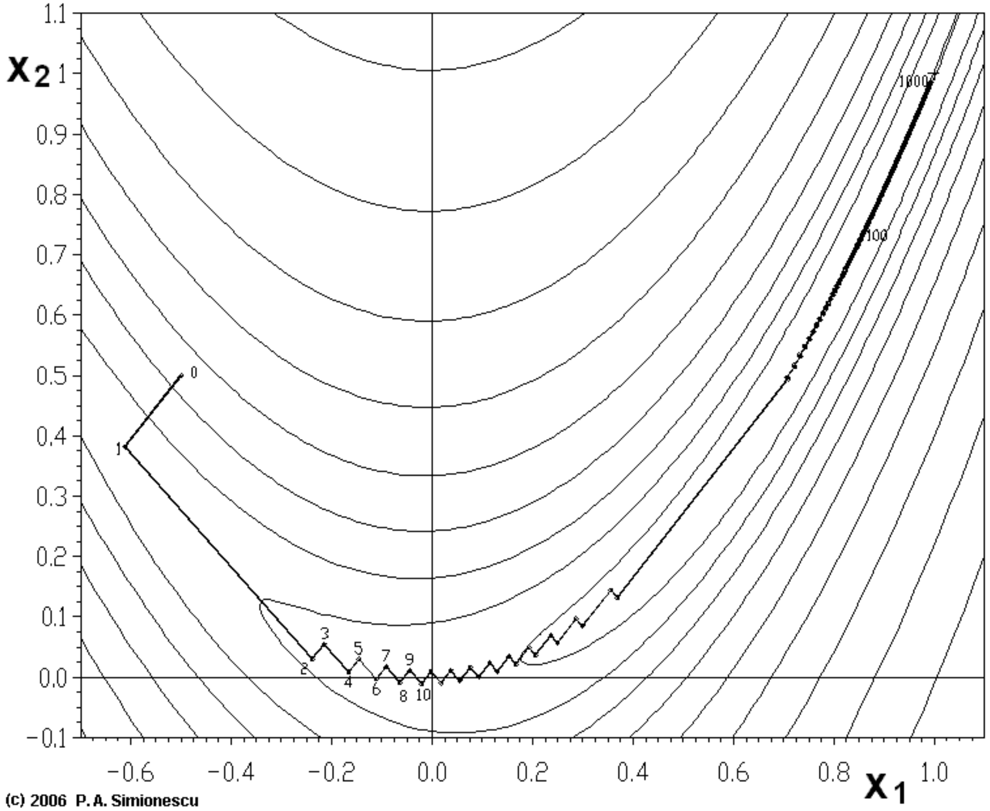
$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = 84\theta_1 + 8\theta_0 - 84$$

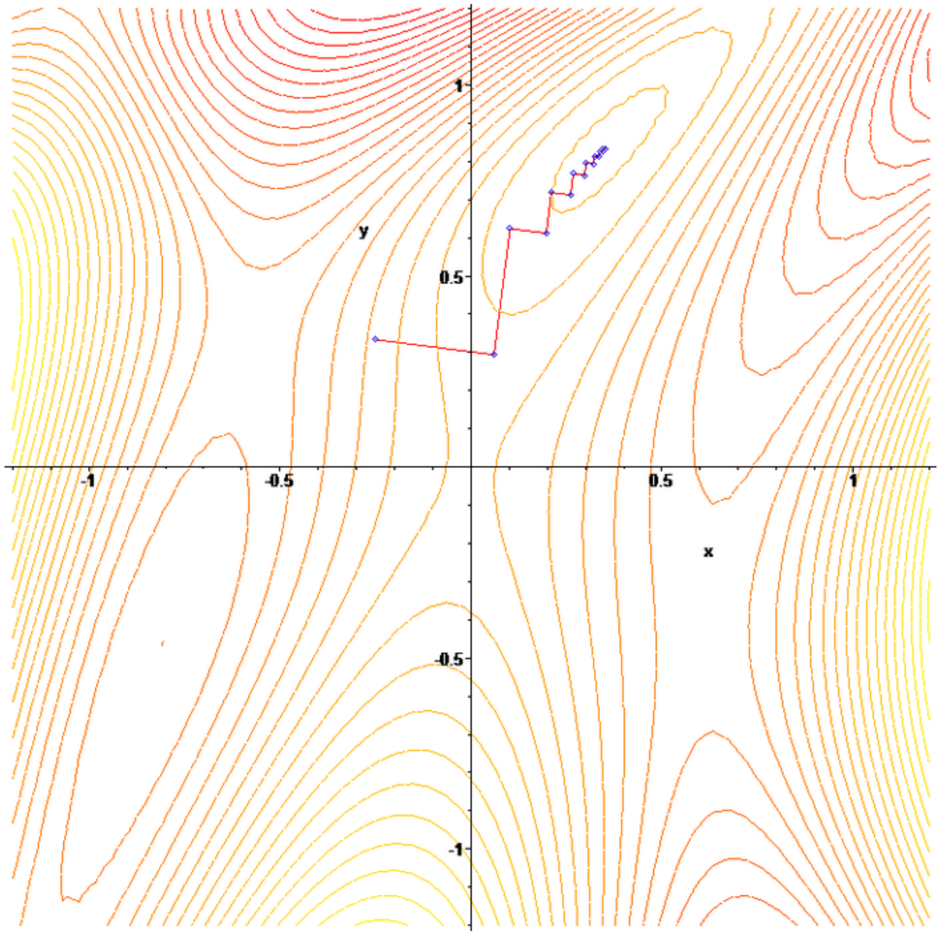
$$\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = 1076\theta_1 + 84\theta_0 - 978$$



- e.g., α=0.001, θ0=0, θ1=0, J(θ)=466
- 1st update
  - New_θ0 = 0 – 0.001*(-84) = 0.0084
  - New_θ1 = 0 – 0.001*(-978) = 0.0978
  - J(θ) = 374.86117384
- 2nd update
  - New_θ0 = 0.01597176
  - New_θ1 = 0.18500616
  - J(θ) = 302.3858537133122
- 3rd update
  - New_θ0 = 0.022804930848
  - New_θ1 = 0.2627653344
  - J(θ) = 244.7518701063334
- 4th update
  - New_θ0 = 0.028979458094 3616
  - New_θ1 = 0.332100222999 4368
  - J(θ) = 198.9198100267 7187

(optional) zig-zagging behavior





Ref., http://en.wikipedia.org/wiki/Gradient_descent

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