Gradient Descent

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CIVE 497 – CIVE 700: Smart Structure Technology

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UNIVERSITY OF WATERLOO
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Supervised Learning

Inputs

Learn (Input, Output)
updates internal state to
minimize an estimate loss

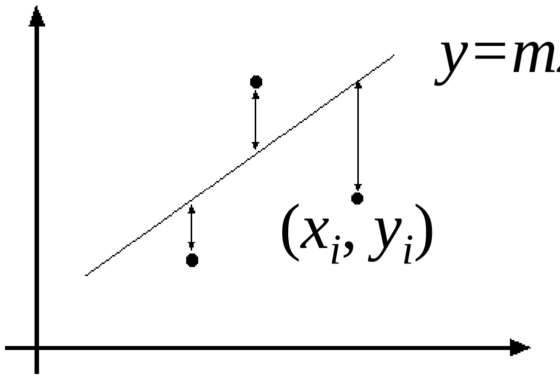
Outputs

Recall: Least Squares Line Fitting

Data (measurement): $(x_1, y_1), \ldots, (x_n, y_n)$

<u>Model: Line ($y_i = m x_i + b$)</u>

Task: Find (m, b)



Minimize $\boxed{E = J(m,b) = \sum_{i=1}^{n} (y_i - mx_i - b)^2}$

$$\frac{\partial(E)}{\partial m} = -2\sum_{i=1}^{n}[y_i - mx_i - b]x_i = 0$$

$$\frac{\partial(E)}{\partial b} = -2\sum_{i=1}^{n}[y_i - mx_i - b] = 0$$

$$\mathrm{m} = \frac{\sum_{i=1}^{n} x_i y_i - 1/n(\sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i)}{\sum_{i=1}^{n} x_i^2 - 1/n\left(\sum_{i=1}^{n} x_i\right)^2}$$

$$\mathrm{b} = \frac{1/n(\sum_{i=1}^{n} y_i)\left(\sum_{i=1}^{n} x_i^2\right) - 1/n\sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2 - 1/n\left(\sum_{i=1}^{n} x_i\right)^2}$$

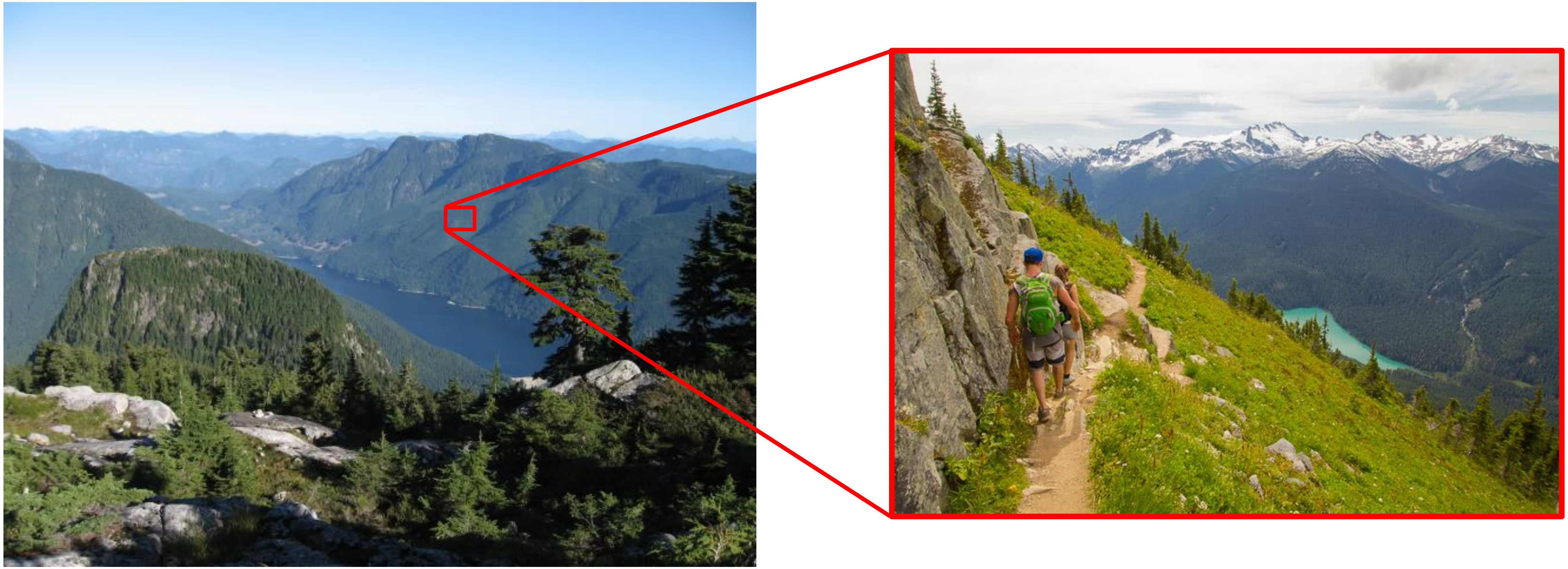
Gradient Descent

- Gradient descent is an iterative machine learning optimization algorithm to find a local minimum of a differentiable function so that we have models that makes accurate predictions.
- Cost function(J) or loss function measures **the difference between the actual output and predicted output** from the model.

Repeat until convergence

$$\theta_{j+1} \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

Gradient Descent (Continue)



$$\theta_{j+1} \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

Line Fitting using Gradient Descent

Data (measurement): $(x_1, y_1), \ldots, (x_n, y_n)$

Model: Line ($y_i = m\,x_i + b$)

Task: Find (m, b)

Minimize $\boxed{E = J(m,b) = \sum_{i=1}^{n} (y_i - m x_i - b)^2}$

Cost function:

$$J(\theta) = J(\theta^1, \theta^2) = \sum_{i=1}^{n} (y_i - \theta^1 x_i - \theta^2)^2$$

Derivatives:

$$\frac{\partial J(\theta^1, \theta^2)}{\partial \theta^1} = -2 \sum_{i=1}^{n} [y_i - \theta^1 x_i - \theta^2] x_i$$

$$\frac{\partial J(\theta^1, \theta^2)}{\partial \theta^2} = -2 \sum_{i=1}^{n} [y_i - \theta^1 x_i - \theta^2]$$

Updated rules:

$$\theta_{j+1}^1 \leftarrow \theta_j^1 - \alpha \frac{\partial}{\partial \theta_j^1} J(\theta)$$

$$\theta_{j+1}^2 \leftarrow \theta_j^2 - \alpha \frac{\partial}{\partial \theta_j^2} J(\theta)$$

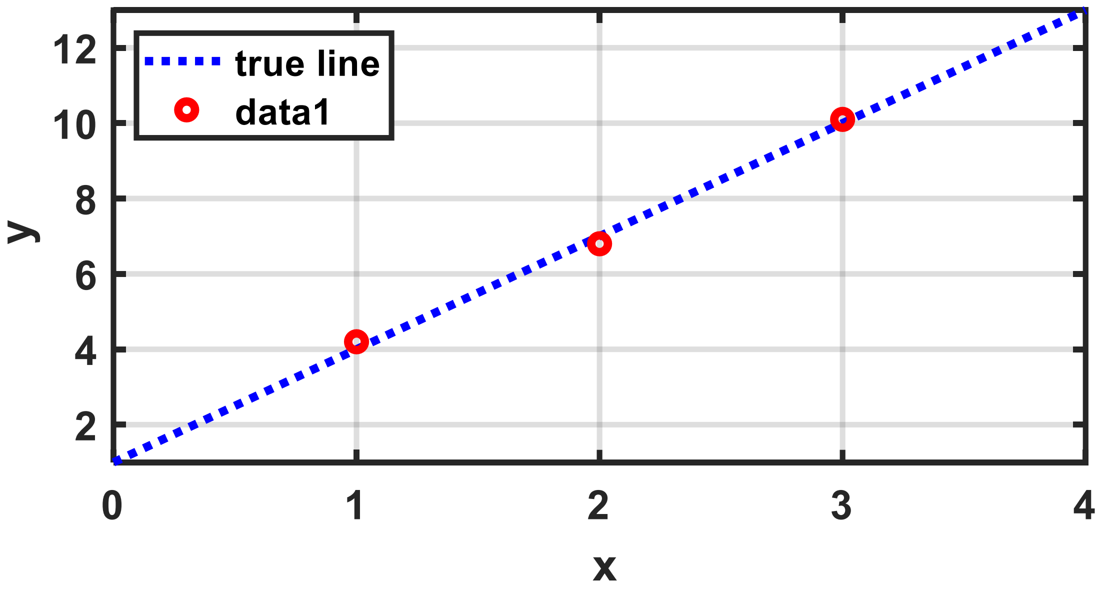
Example: Line Fitting using Gradient Descent

Data (measurement): (1 4.2), (2, 6.8), (3, 10.1)

Model: Line ($y_i = m x_i + b$)

True model: y = 3x + 1

Task: Find (m, b)



Least square

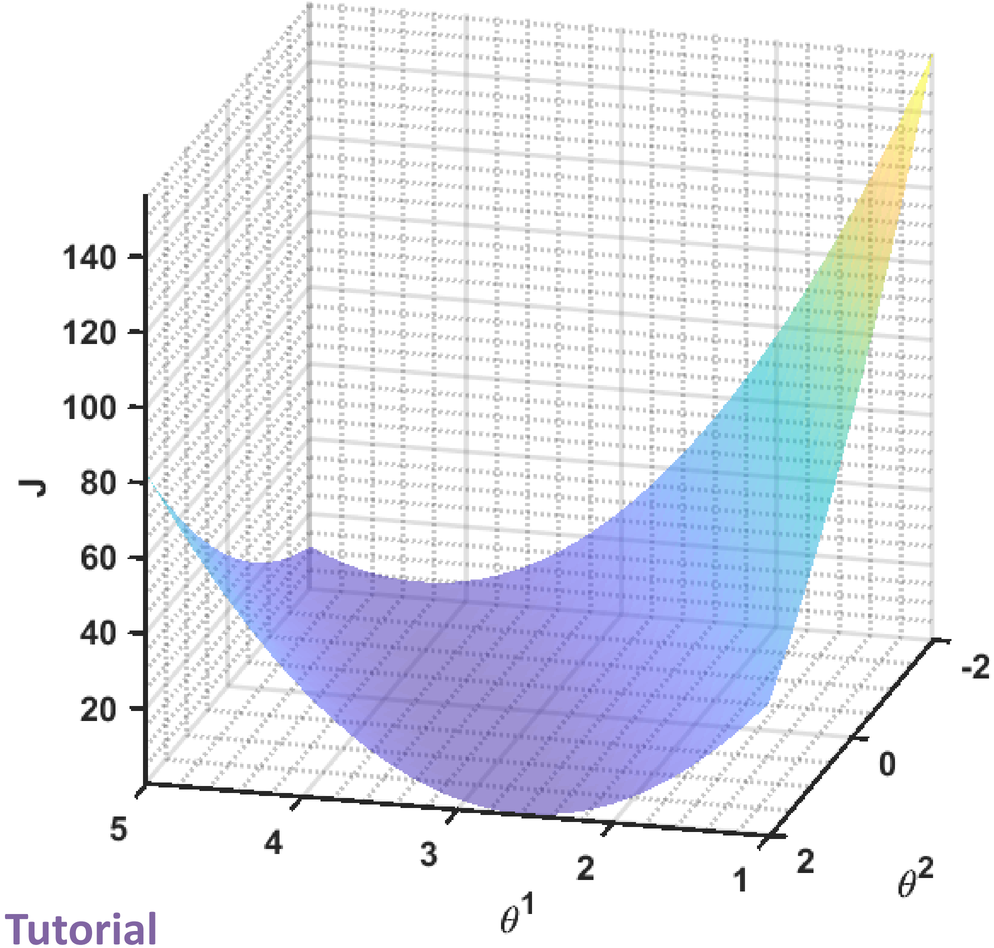
$$m = \frac{\sum_{i=1}^{n} x_i y_i - 1/n(\sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i)}{\sum_{i=1}^{n} x_i^2 - 1/n\left(\sum_{i=1}^{n} x_i\right)^2} = \frac{(4.2 + 13.6 + 30.3) - 1/3(6 * 21.1)}{14 - 1/3(6 * 6)} = \frac{5.9}{2} = 2.95$$

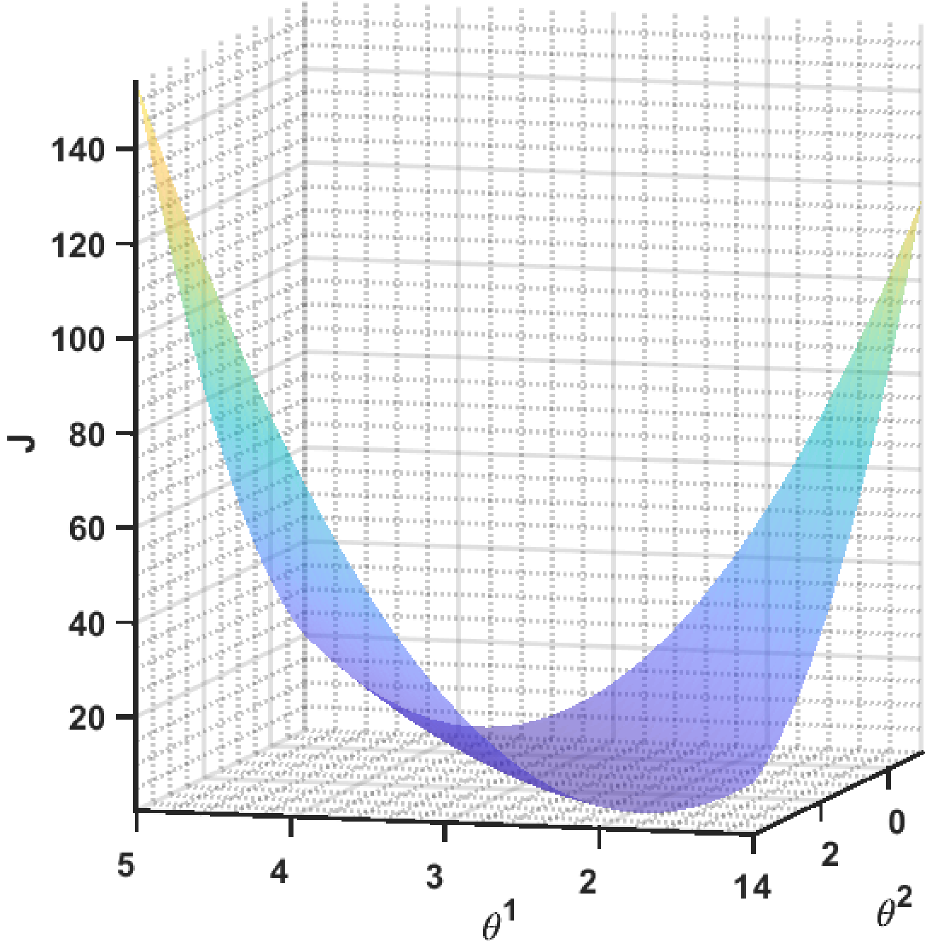
$$b = \frac{1/n(\sum_{i=1}^{n} y_i)(\sum_{i=1}^{n} x_i^2) - 1/n \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2 - 1/n\left(\sum_{i=1}^{n} x_i\right)^2} = \frac{\frac{1}{3} * 21.1 * 14 - \frac{1}{3} * 6 * (4.2 + 13.6 + 30.3)}{2} = 1.133$$

Example: Line Fitting using Gradient Descent (Continue)

Cost function: $$J(\theta) = J(\theta^1, \theta^2) = \sum_{i=1}^{n} (y_i - \theta^1 x_i - \theta^2)^2$$

See *demo_line_fit.m*

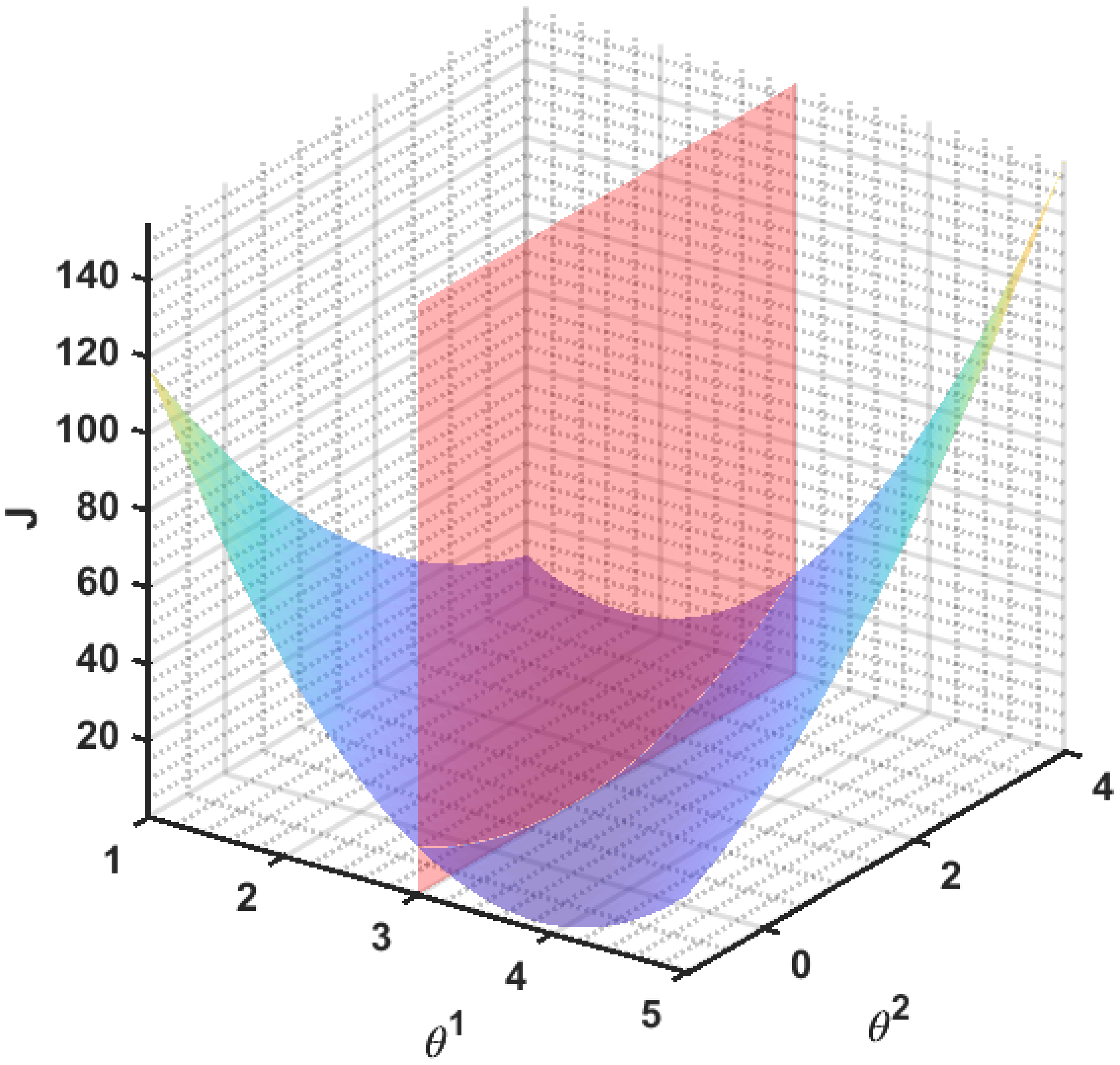


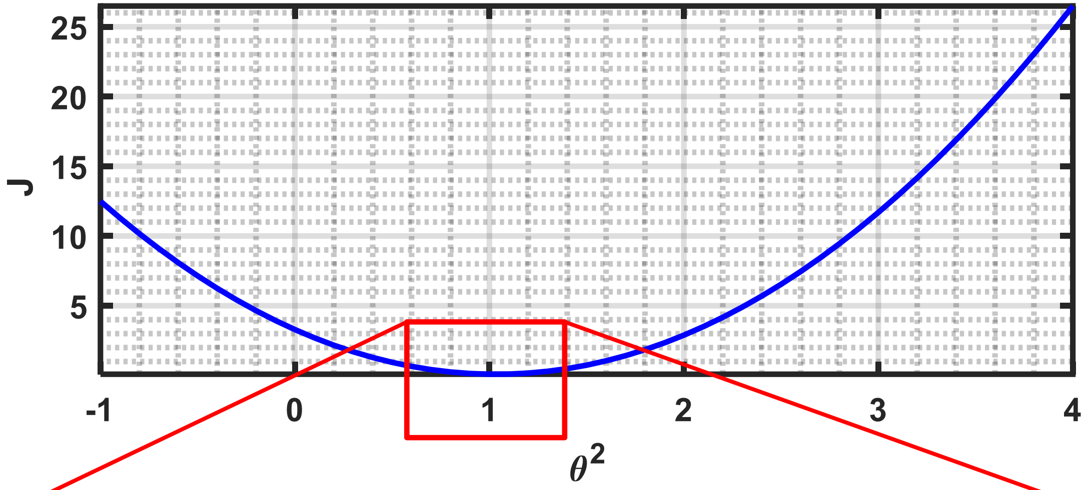


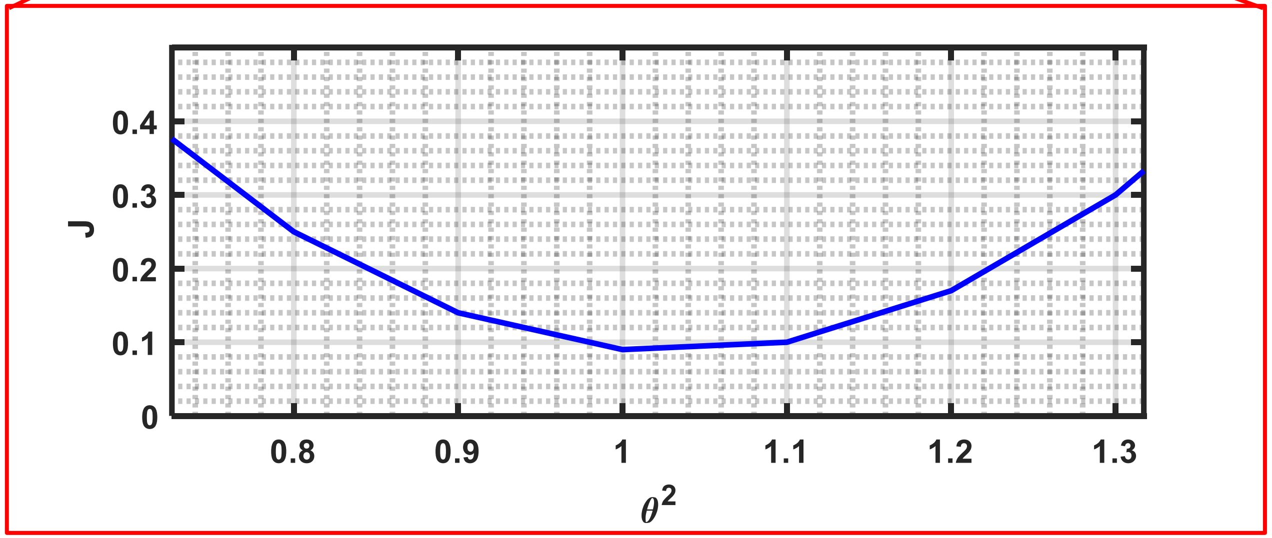
Tutorial

Example: Line Fitting using Gradient Descent (Continue)

$y_i = 3x_i + 1 = \theta^1 x_i + \theta^2$



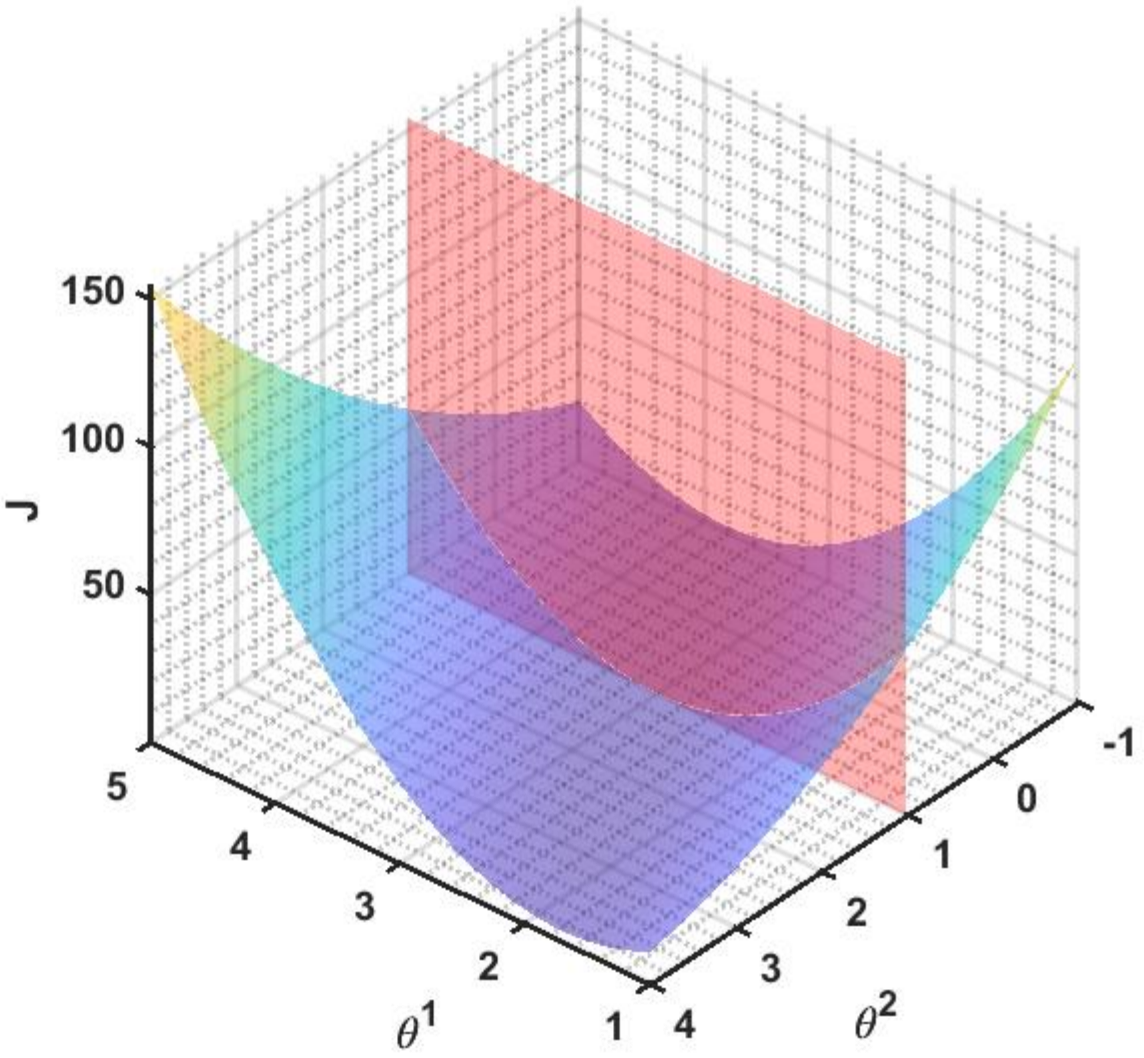


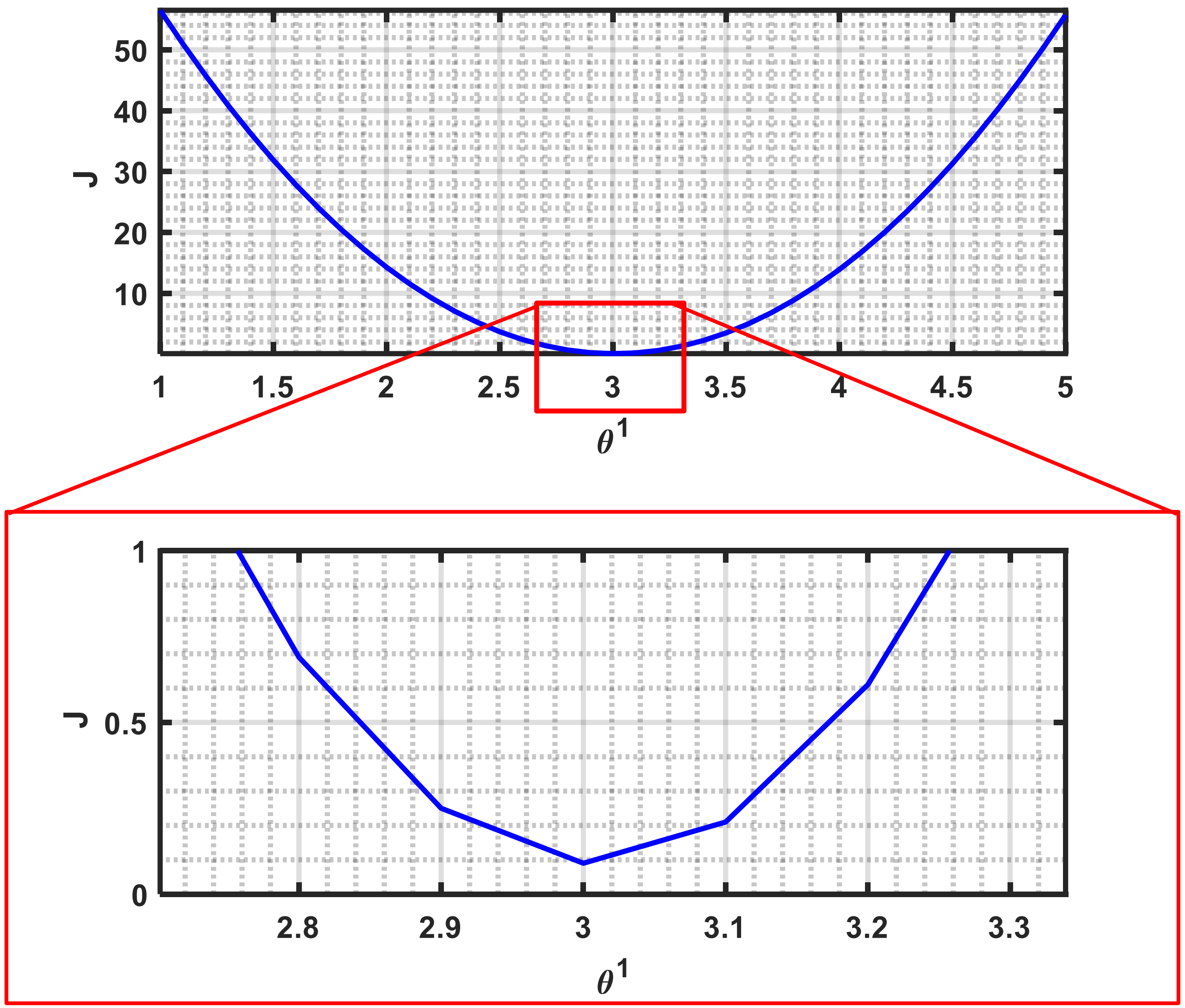


[Tutorial]

See *demo_line_fit.m*

Example: Line Fitting using Gradient Descent (Continue)

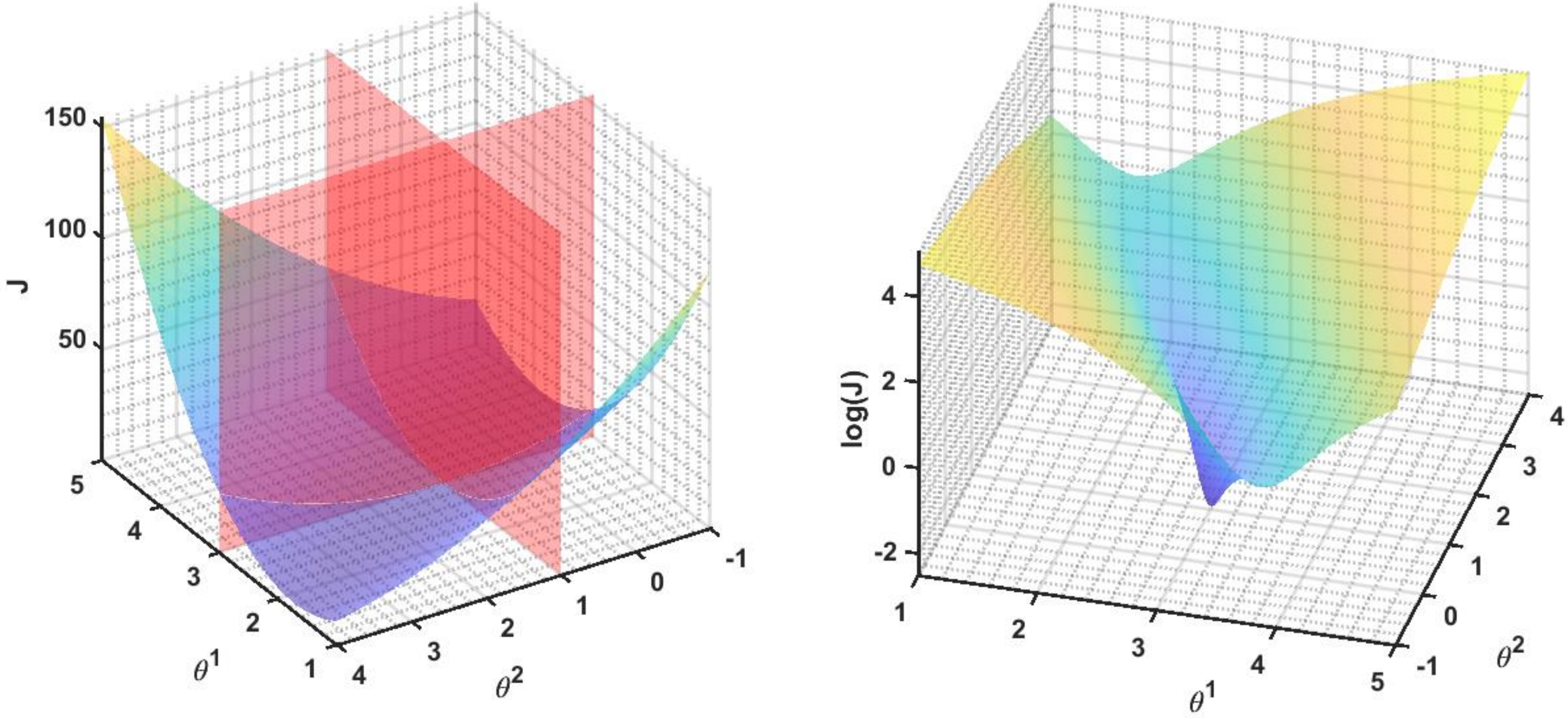




See *demo_line_fit.m*

Tutorial

Example: Line Fitting using Gradient Descent (Continue)



Tutorial

Example: Line Fitting using Gradient Descent (Continue)

$$\frac{\partial J(\theta^1,\theta^2)}{\partial\theta^1} = -2\sum_{i=1}^{n}[y_i - \theta^1 x_i - \theta^2]x_i \qquad \theta_{j+1}^1 \leftarrow \theta_j^1 - \alpha\frac{\partial}{\partial\theta_j^1}J(\theta)$$

$$\frac{\partial J(\theta^1,\theta^2)}{\partial\theta^2} = -2\sum_{i=1}^{n}[y_i - \theta^1 x_i - \theta^2] \qquad \theta_{j+1}^2 \leftarrow \theta_j^2 - \alpha\frac{\partial}{\partial\theta_j^2}J(\theta)$$

```
in_data = [1 2 3];
out_data = [4.2 6.8 10.1];

itr = 12;
l_r = 0.08;

t1 = zeros(itr,1); t1(1) = 1;
t2 = zeros(itr,1); t2(1) = 0;
```

```
J1 = @(th1, t2) -2*sum((out_data-t1*in_data-t2).*in_data);
J2 = @(th1, t2) -2*sum((out_data-t1*in_data-t2));

for ii=1:n_iter-1
    t1(ii+1) = t1(ii) - l_r*J1(t1(ii), t2(ii));
    t2(ii+1) = t2(ii) - l_r*J2(t1(ii), t2(ii));
end

```

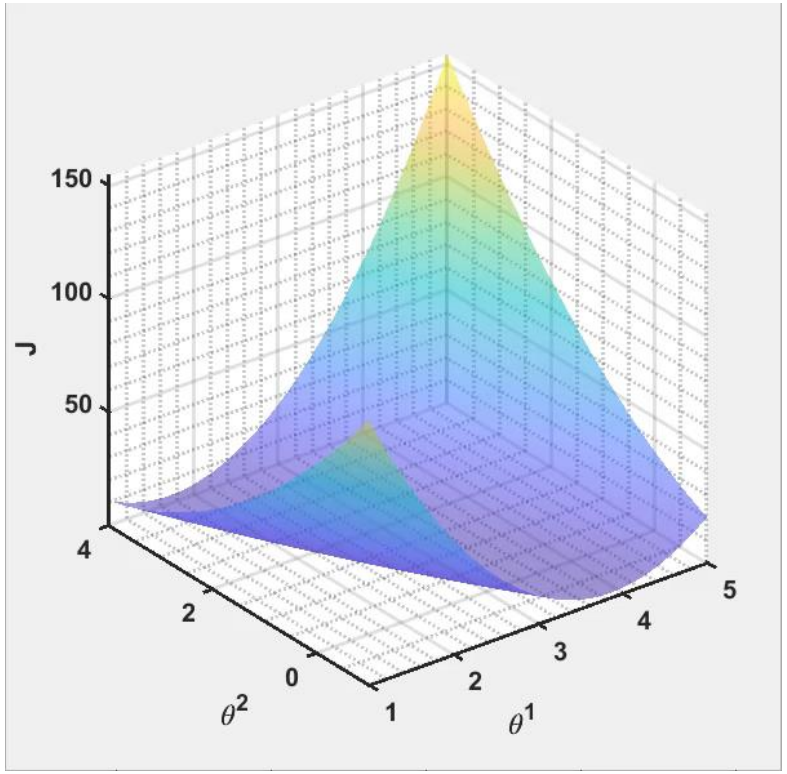
Line Fitting using Gradient Descent Depending on Learning Rates

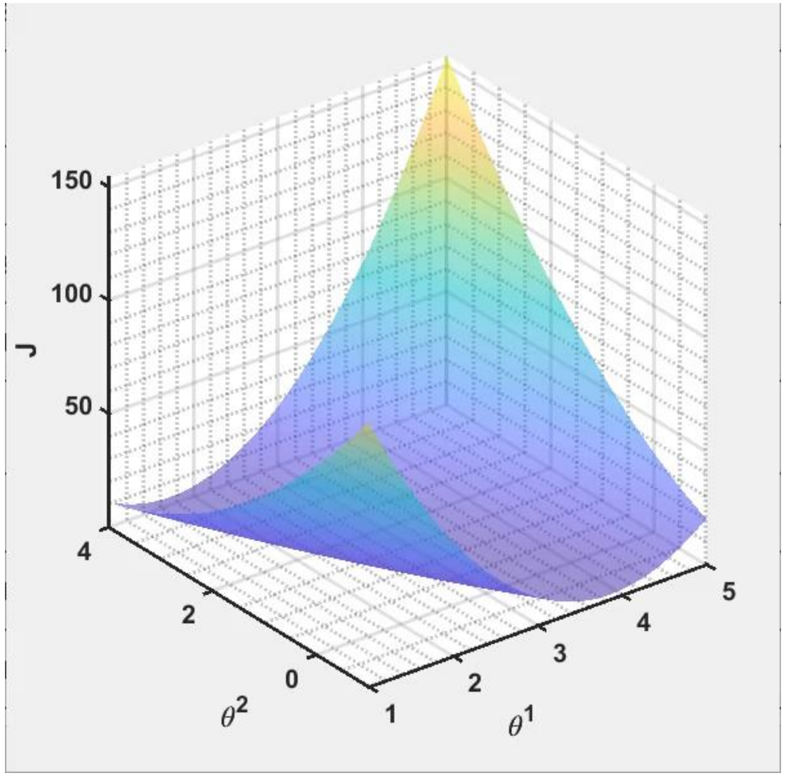
$\alpha = 0.01$

Iter.	1	2	3	4	5	6	7	8	9	10	11	12
θ^1	**1**	**1.682**	**2.1368**	**2.440011**	**2.642082**	**2.776673**	**2.866242**	**2.925774**	**2.965265**	**2.991388**	**3.008593**	**3.019848**
θ^2	**0**	**0.302**	**0.50404**	**0.639382**	**0.730217**	**0.791354**	**0.832672**	**0.860763**	**0.880024**	**0.893391**	**0.902821**	**0.909621**

$\alpha = 0.001$

Iter.	1	2	3	4	5	6	7	8	9	10	11	12
θ^1	**1**	**1.0682**	**1.134128**	**1.19786**	**1.259468**	**1.319024**	**1.376595**	**1.432248**	**1.486047**	**1.538053**	**1.588325**	**1.636923**
θ^2	**0**	**0.0302**	**0.0594**	**0.087634**	**0.114934**	**0.141331**	**0.166855**	**0.191535**	**0.215398**	**0.238473**	**0.260786**	**0.282361**





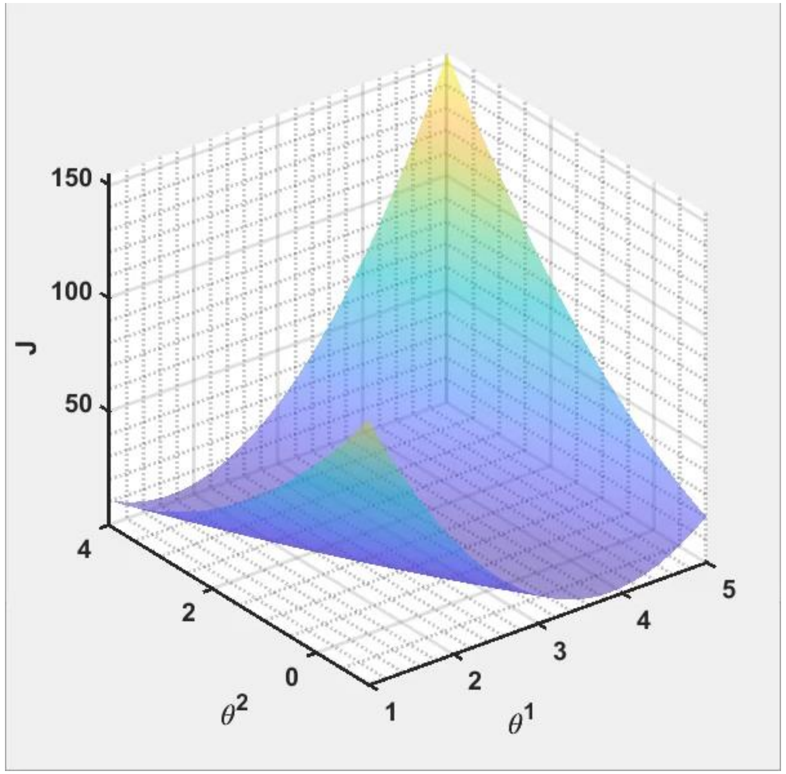
Line Fitting using Gradient Descent Depending on Learning Rates (Continue)

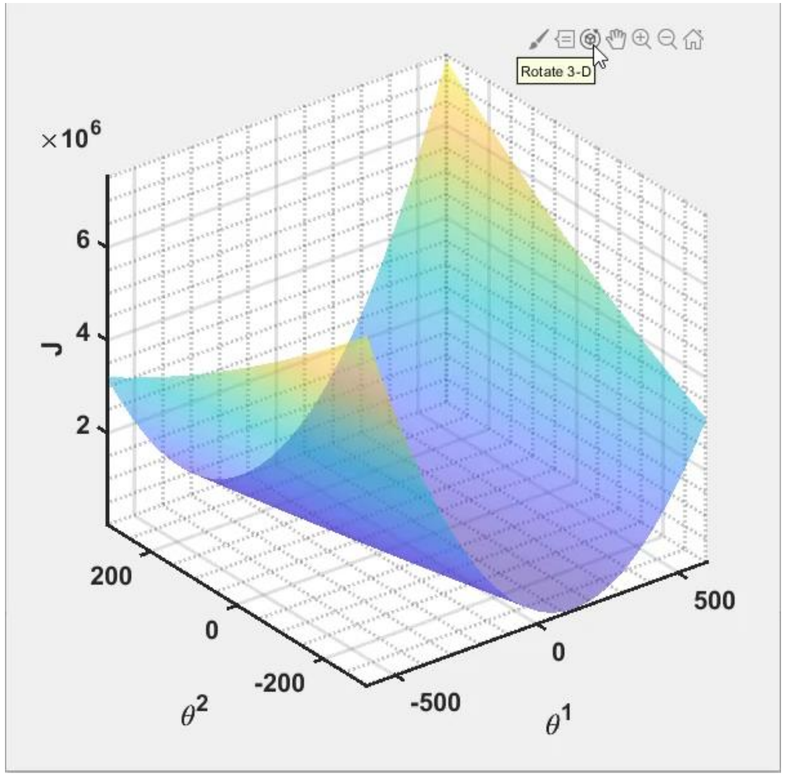
$\alpha = 0.05$

Iter.	1	2	3	4	5	6	7	8	9	10	11	12
θ^1	**1**	**4.41**	**2.14**	**3.6414**	**2.63902**	**3.299202**	**2.855733**	**3.145209**	**2.948232**	**3.074404**	**2.98619**	**3.040475**
θ^2	**0**	**1.51**	**0.521**	**1.1907**	**0.75865**	**1.057643**	**0.870829**	**1.00614**	**0.927173**	**0.990081**	**0.958415**	**0.989177**

$\alpha = 0.08$

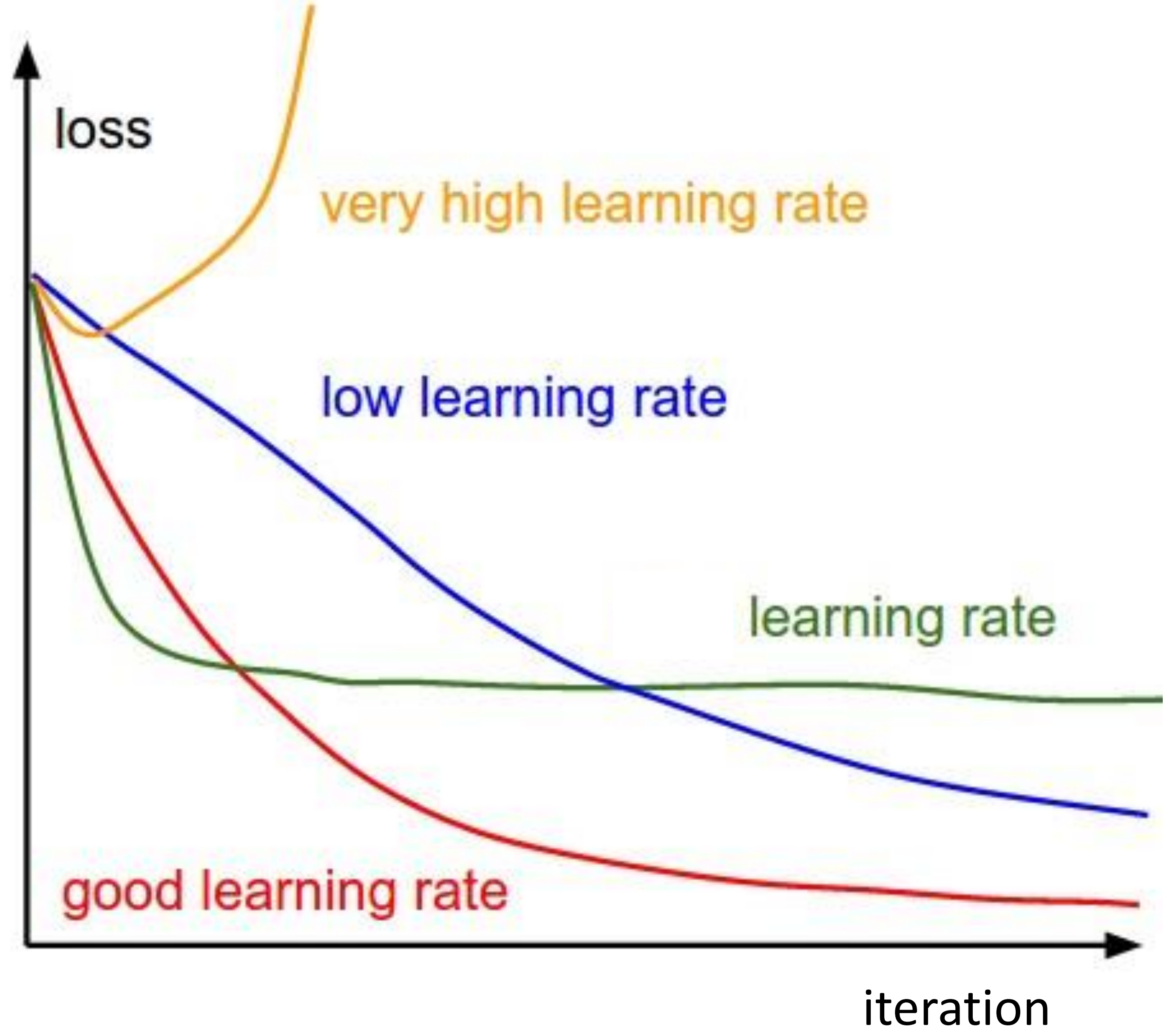
Iter.	1	2	3	4	5	6	7	8	9	10	11	12
θ^1	**1**	**6.456**	**-2.6288**	**12.45853**	**-12.6348**	**29.06521**	**-40.2649**	**74.97162**	**-116.597**	**201.8388**	**-327.509**	**552.42**
θ^2	**0**	**2.416**	**-1.56544**	**5.085619**	**-5.93967**	**12.41676**	**-18.0699**	**32.63401**	**-51.6271**	**88.46348**	**-144.388**	**242.7028**





Tutorial

Effect of Learning Rates



Higher or lower

Stochastic Gradient Decent

Batch (Vanilla) Gradient Descent

$$\theta_{j+1} \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

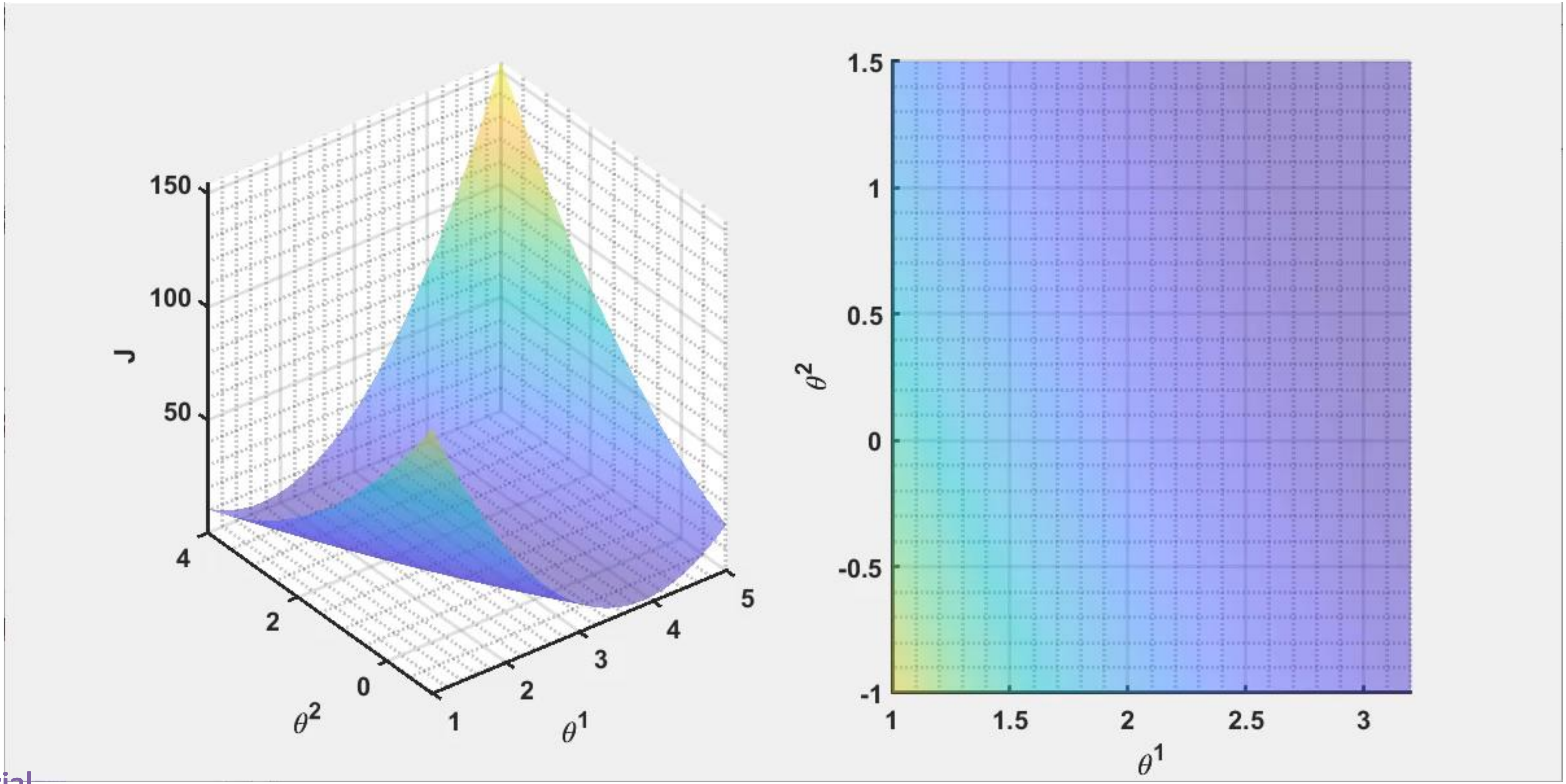
Stochastic Gradient Descent

$$\theta_{j+1} \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(x^i, y^j; \theta)$$

Mini-batch Gradient Descent

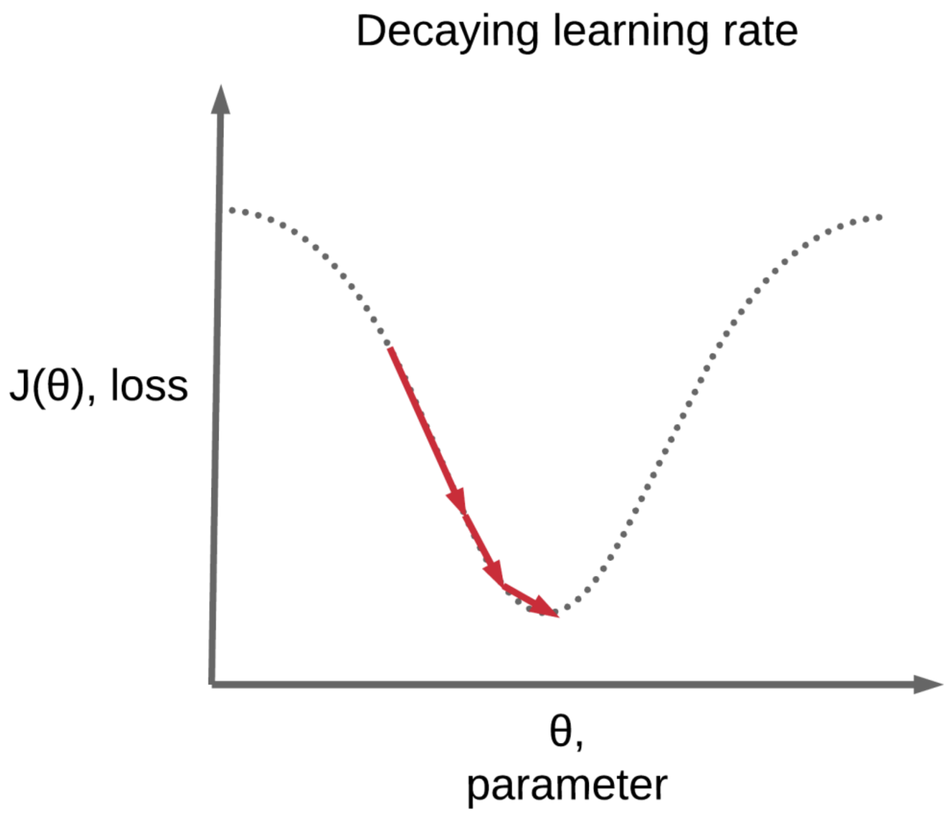
$$\theta_{j+1} \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(x^{\{i:i+b\}}, y^{\{i:i+b\}}; \theta)$$

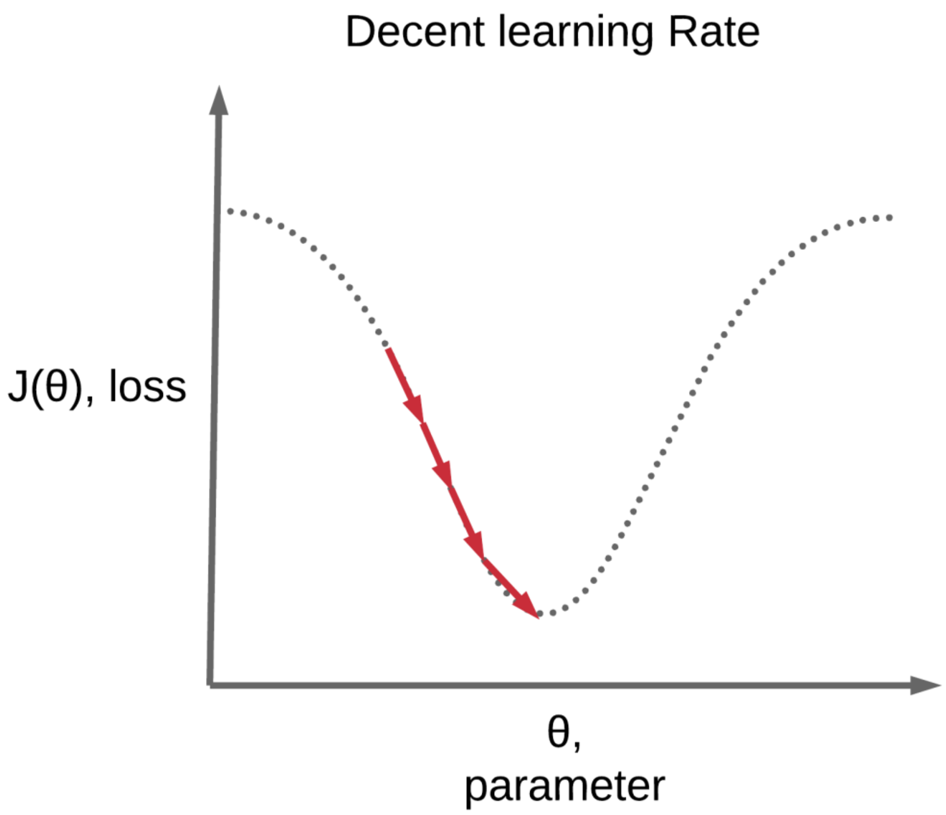
Stochastic Gradient Decent (Simulation)



Tutorial

Variations (Adaptive Learning Rate or Learning Rate Scheduling)





$$\theta_{j+1} \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

$$\alpha_{\mathrm{j}} = \alpha_{\mathrm{j}} \gamma \quad \text{where } \gamma = 0.1$$

Variations (Momentum)

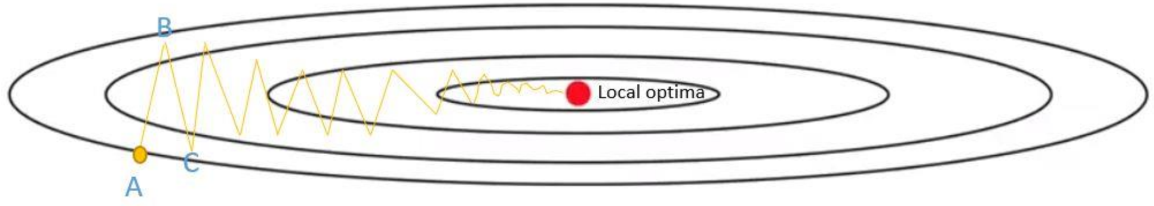
Without momentum:

$$w_{t+1} = w_t - \eta \nabla w_t$$

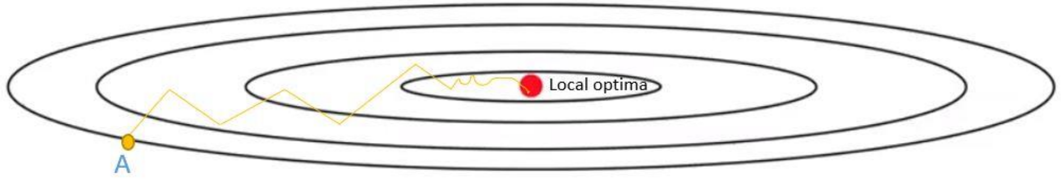
With momentum:

$$update_t^w = \gamma \cdot update_{t-1}^w + \eta \nabla w_t$$
$$w_{t+1} = w_t - update_t^w$$

$$
\begin{aligned}
update_0 &= 0 \\
update_1 &= \gamma \cdot update_0 + \eta \nabla w_1 = \eta \nabla w_1 \\
update_2 &= \gamma \cdot update_1 + \eta \nabla w_2 = \gamma \cdot \eta \nabla w_1 + \eta \nabla w_2 \\
update_3 &= \gamma \cdot update_2 + \eta \nabla w_3 = \gamma(\gamma \cdot \eta \nabla w_1 + \eta \nabla w_2) + \eta \nabla w_3 \\
&= \gamma \cdot update_2 + \eta \nabla w_3 = \gamma^2 \cdot \eta \nabla w_1 + \gamma \cdot \eta \nabla w_2 + \eta \nabla w_3 \\
update_4 &= \gamma \cdot update_3 + \eta \nabla w_4 = \gamma^3 \cdot \eta \nabla w_1 + \gamma^2 \cdot \eta \nabla w_2 + \gamma \cdot \eta \nabla w_3 + \eta \nabla w_4 \\
&\vdots \\
update_t &= \gamma \cdot update_{t-1} + \eta \nabla w_t = \gamma^{t-1} \cdot \eta \nabla w_1 + \gamma^{t-2} \cdot \eta \nabla w_1 + \ldots + \eta \nabla w_t
\end{aligned}
$$



Without momentum



With momentum

https://towardsdatascience.com/learning-parameters-part-2-a190bef2d12

$$\theta_{j+1} \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$