Gradient decent

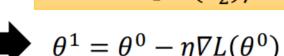
Suppose that θ has two variables $\{\theta_1, \theta_2\}$

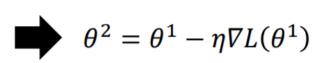
Randomly start at
$$\theta^0 = \begin{bmatrix} \theta_1^0 \\ \theta_2^0 \end{bmatrix}$$

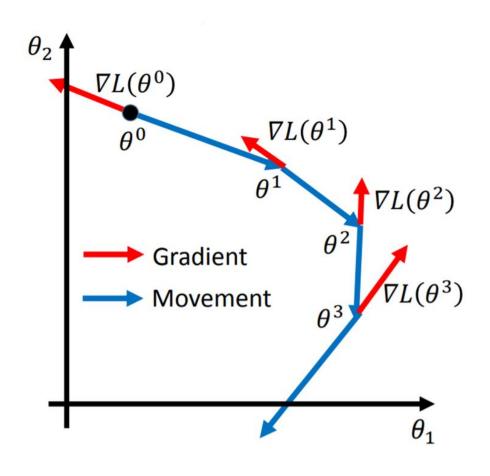
$$\nabla L(\theta) = \begin{bmatrix} \frac{\partial L(\theta_1)}{\partial \theta_2} \\ \frac{\partial L(\theta_2)}{\partial \theta_2} \end{bmatrix}$$

$$\begin{bmatrix} \theta_1^1 \\ \theta_2^1 \end{bmatrix} = \begin{bmatrix} \theta_1^0 \\ \theta_2^0 \end{bmatrix} - \eta \begin{bmatrix} \frac{\partial L(\theta_1^0)}{\partial \theta_1} \\ \frac{\partial L(\theta_2^0)}{\partial \theta_2} \end{bmatrix} \implies \theta^1 = \theta^0 - \eta \nabla L(\theta^0)$$

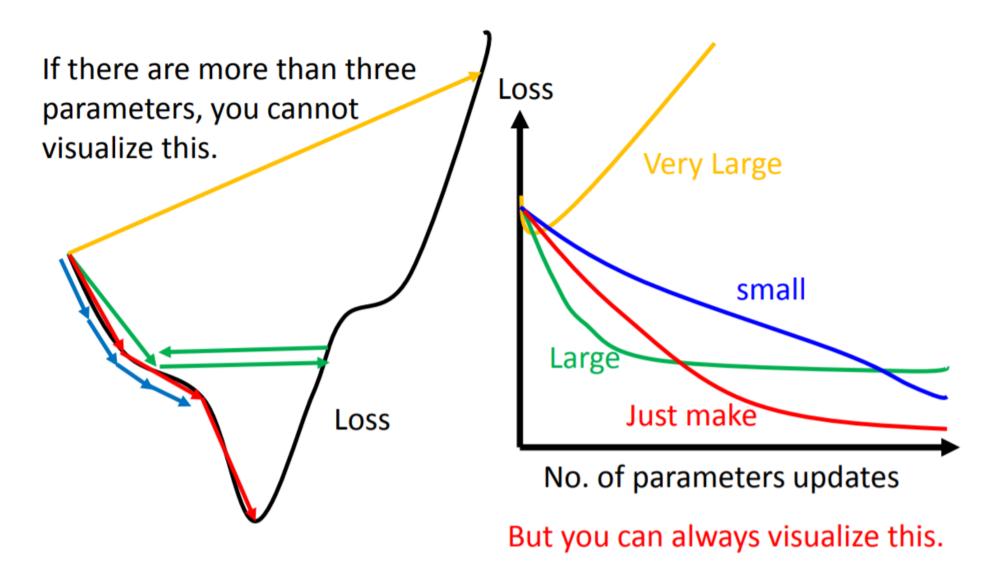
$$\begin{bmatrix} \theta_1^2 \\ \theta_2^2 \end{bmatrix} = \begin{bmatrix} \theta_1^1 \\ \theta_2^1 \end{bmatrix} - \eta \begin{bmatrix} \frac{\partial L(\theta_1^1)}{\partial \theta_1} \\ \frac{\partial L(\theta_2^1)}{\partial \theta_2} \end{bmatrix} \implies \theta^2 = \theta^1 - \eta \nabla L(\theta^1)$$





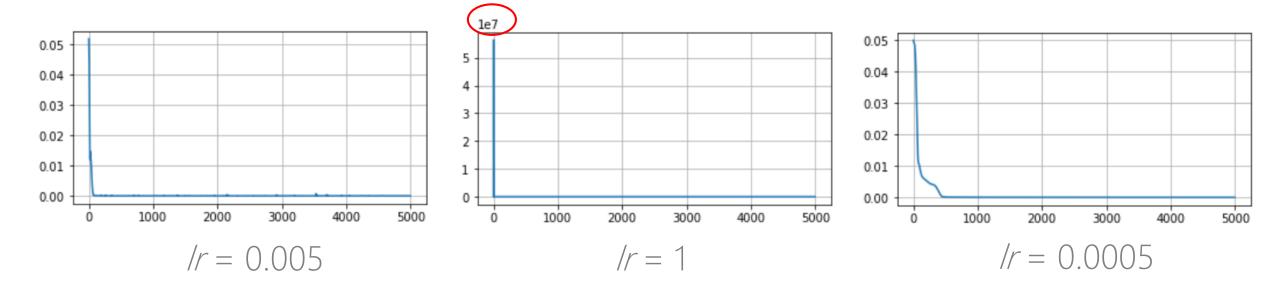


Learning rate



Practice

• Run "3.1. Learning rate" and explain why good /r is important?

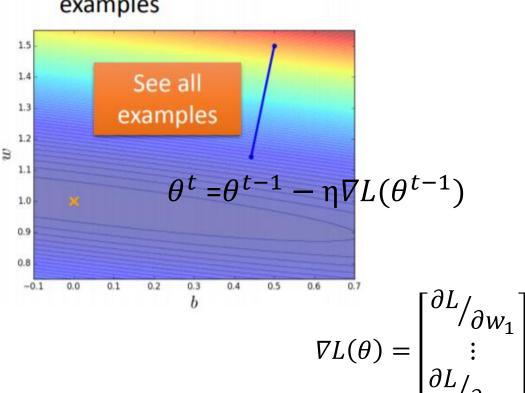




Stochastic gradient decent

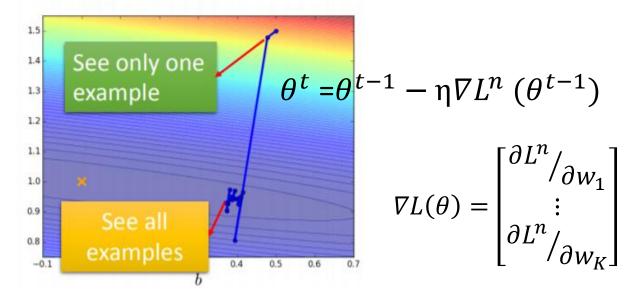
Gradient Descent

Update after seeing all examples



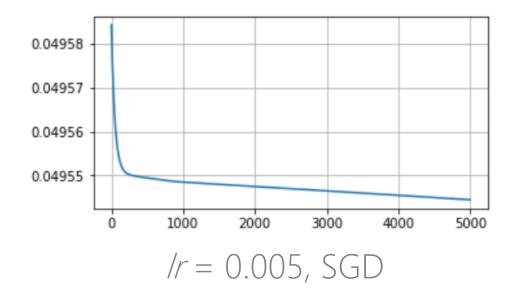
Stochastic Gradient Descent

Update for each example If there are 20 examples, 20 times faster.



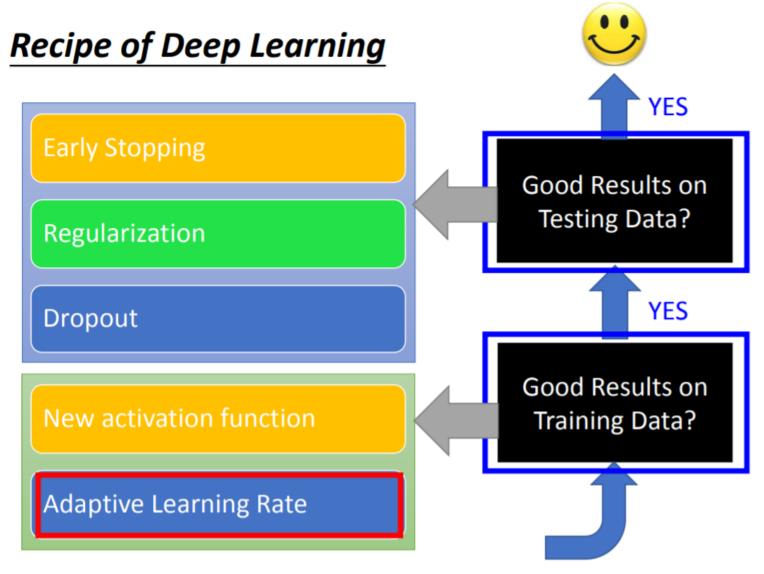
Practice

• Run "3.2. Optimizer" and discuss your loss plot.

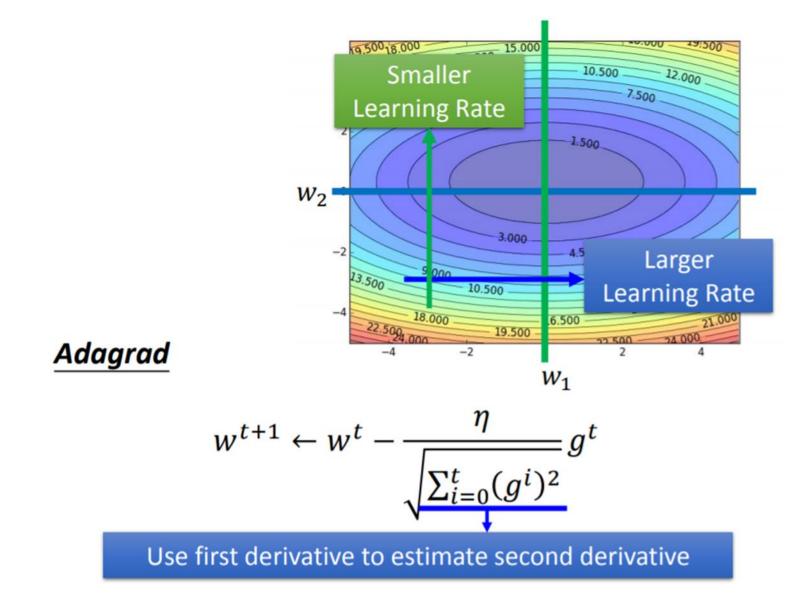




Adaptive learning rate



Adagrad



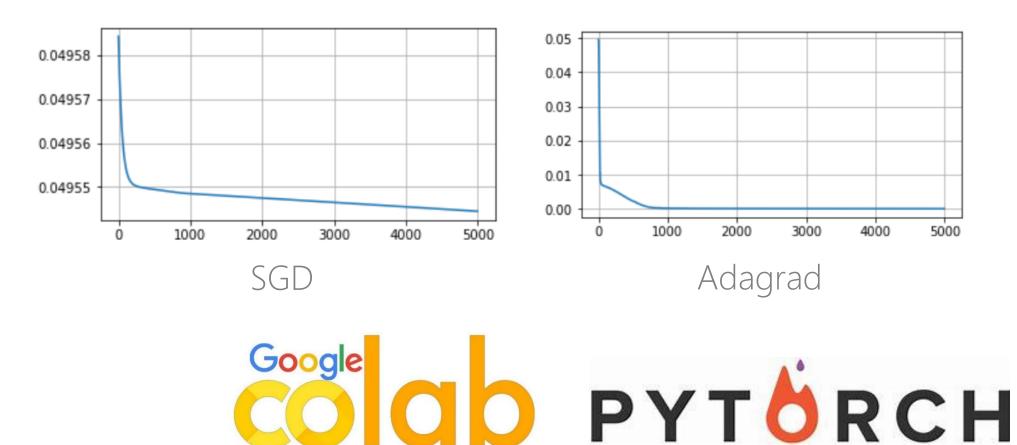
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Adagrad

$$\begin{split} w^{t+1} &\leftarrow w^t - \frac{\eta^t}{\sigma^t} g^t \qquad g^t = \frac{\partial L(\theta^t)}{\partial w} \\ w^1 &\leftarrow w^0 - \frac{\eta^0}{\sigma^0} g^0 \qquad \sigma^0 = \sqrt{(g^0)^2} \\ w^2 &\leftarrow w^1 - \frac{\eta^1}{\sigma^1} g^1 \qquad \sigma^1 = \sqrt{\frac{1}{2} [(g^0)^2 + (g^1)^2]} \\ w^3 &\leftarrow w^2 - \frac{\eta^2}{\sigma^2} g^2 \qquad \sigma^2 = \sqrt{\frac{1}{3} [(g^0)^2 + (g^1)^2 + (g^2)^2]} \\ & \vdots \\ w^{t+1} &\leftarrow w^t - \frac{\eta^t}{\sigma^t} g^t \qquad \sigma^t = \sqrt{\frac{1}{t+1} \sum_{i=0}^t (g^i)^2} \end{split}$$

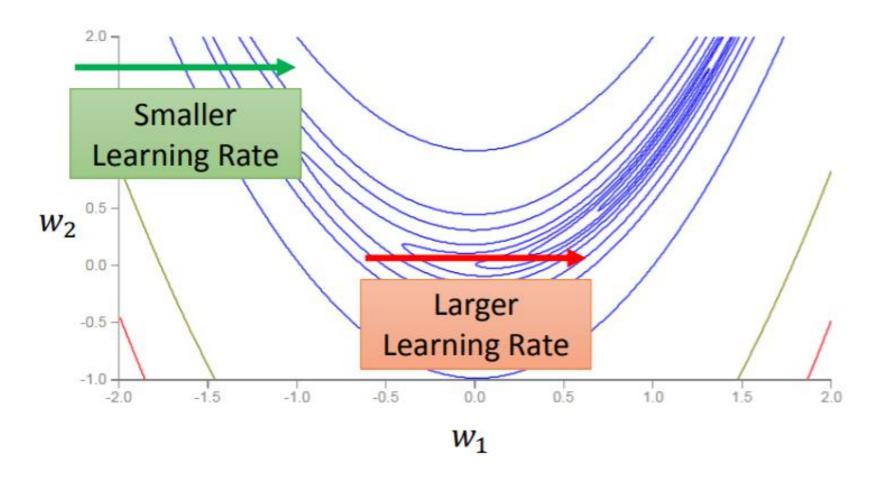
Practice

• Run "3.2. Optimizer" and discuss your loss plot.



RMS Prop

Error Surface can be very complex when training NN.



RMS Prop

$$w^{1} \leftarrow w^{0} - \frac{\eta}{\sigma^{0}} g^{0} \qquad \sigma^{0} = g^{0}$$

$$w^{2} \leftarrow w^{1} - \frac{\eta}{\sigma^{1}} g^{1} \qquad \sigma^{1} = \sqrt{\alpha(\sigma^{0})^{2} + (1 - \alpha)(g^{1})^{2}}$$

$$w^{3} \leftarrow w^{2} - \frac{\eta}{\sigma^{2}} g^{2} \qquad \sigma^{2} = \sqrt{\alpha(\sigma^{1})^{2} + (1 - \alpha)(g^{2})^{2}}$$

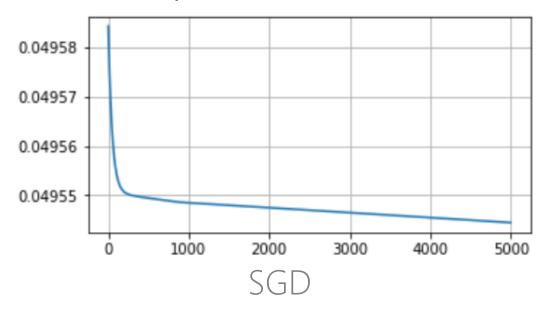
$$\vdots$$

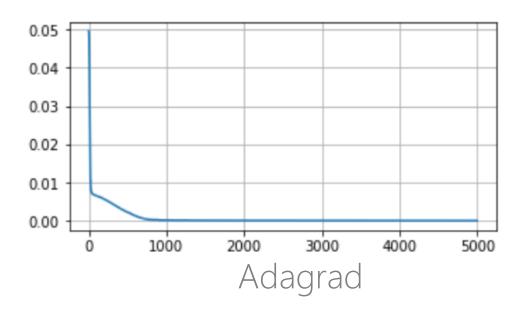
$$\vdots$$

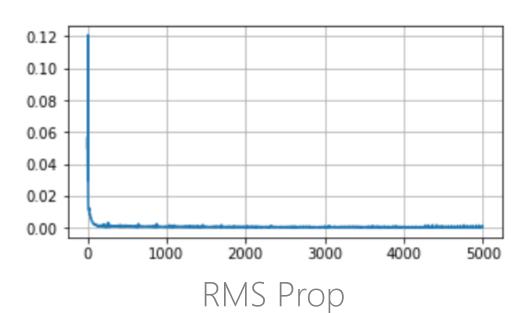
$$w^{t+1} \leftarrow w^{t} - \frac{\eta}{\sigma^{t}} g^{t} \qquad \sigma^{t} = \sqrt{\alpha(\sigma^{t-1})^{2} + (1 - \alpha)(g^{t})^{2}}$$

Root Mean Square of the gradients with previous gradients being decayed

Run "3.2. Optimizer"

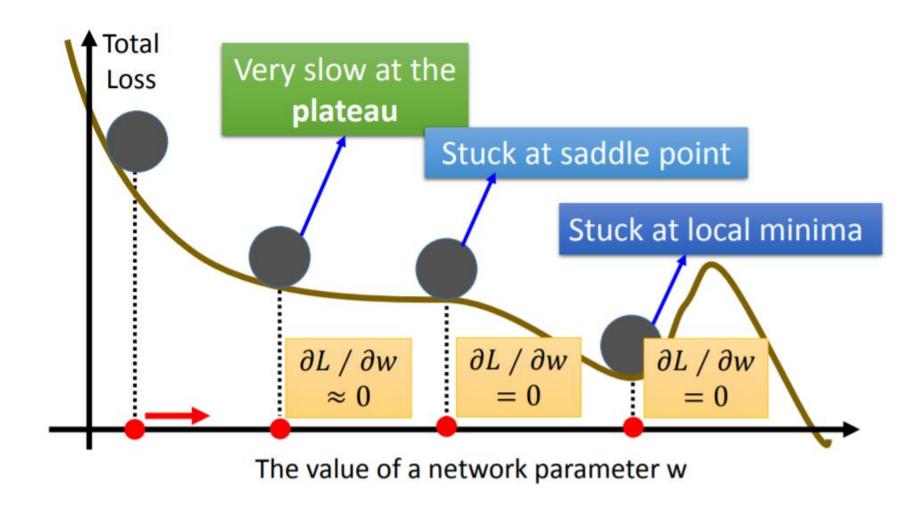






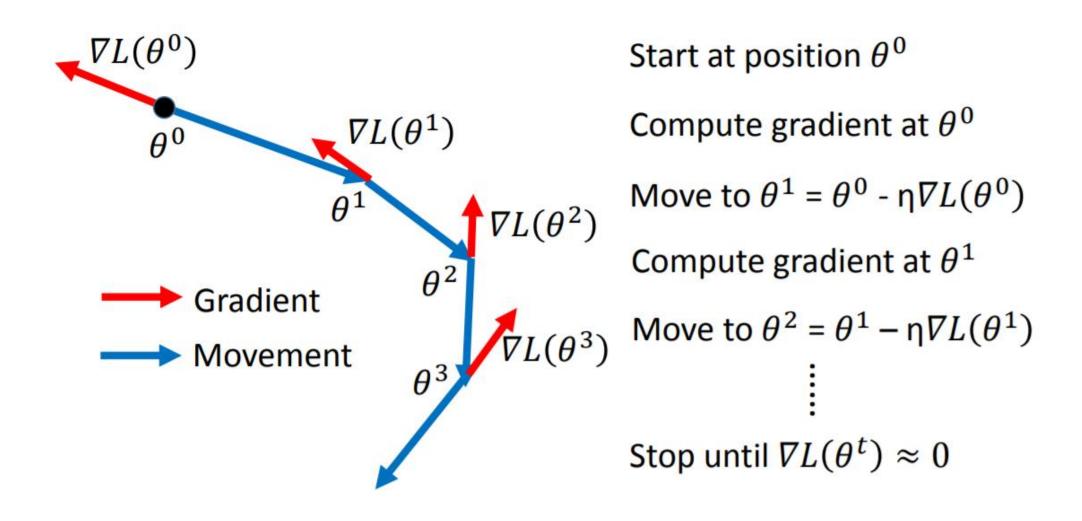


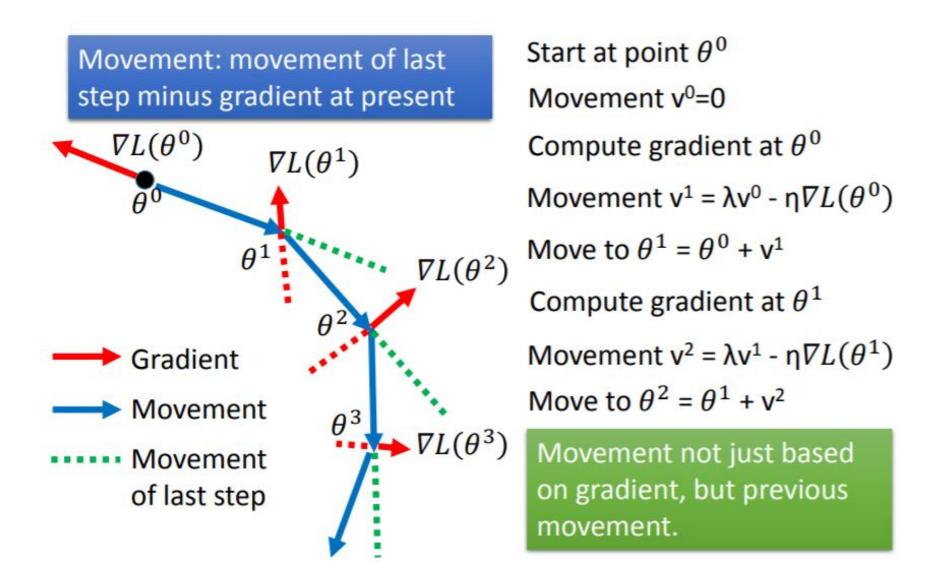
Hard to find optimal parameters



 Momentum How about put this phenomenon in gradient descent?

Vanilla gradient decent





Movement: movement of last step minus gradient at present

vⁱ is actually the weighted sum of all the previous gradient:

$$\nabla L(\theta^0), \nabla L(\theta^1), \dots \nabla L(\theta^{i-1})$$

$$v^0 = 0$$

$$v^1 = - \eta \nabla L(\theta^0)$$

$$\mathbf{v}^2 = -\lambda \, \eta \nabla L(\theta^0) - \eta \nabla L(\theta^1)$$

Start at point
$$\theta^0$$

Compute gradient at
$$\theta^0$$

Movement
$$v^1 = \lambda v^0 - \eta \nabla L(\theta^0)$$

Move to
$$\theta^1 = \theta^0 + v^1$$

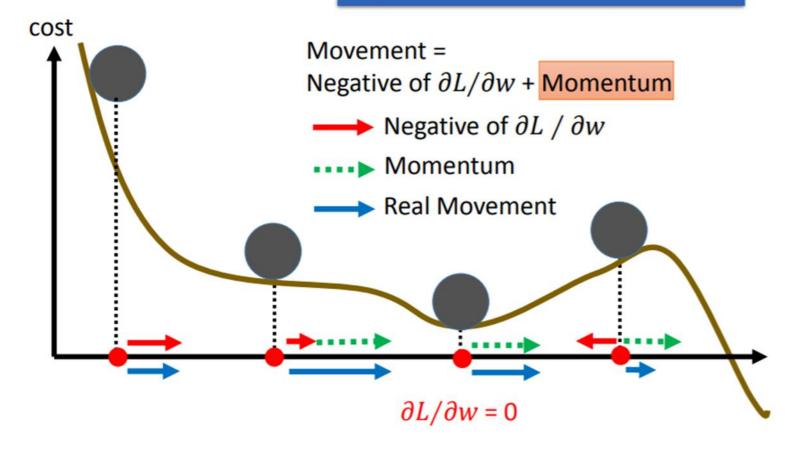
Compute gradient at
$$\theta^1$$

Movement
$$v^2 = \lambda v^1 - \eta \nabla L(\theta^1)$$

Move to
$$\theta^2 = \theta^1 + v^2$$

Movement not just based on gradient, but previous movement

Still not guarantee reaching global minima, but give some hope



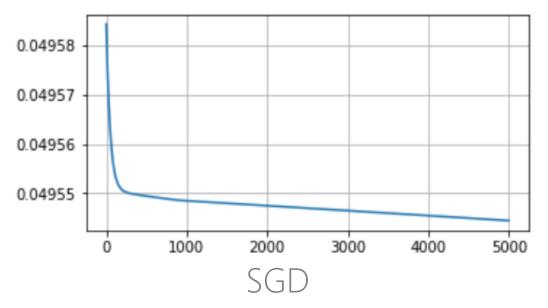
Adam

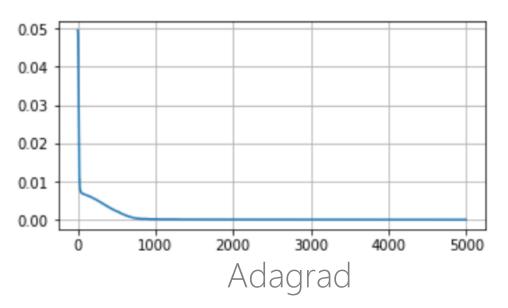
RMSProp + Momentum

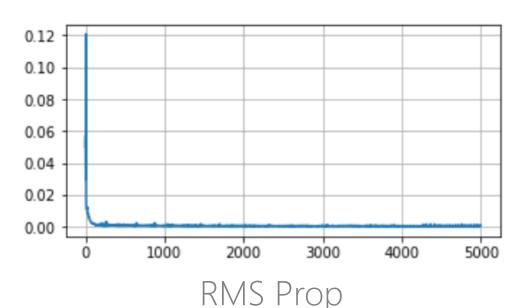
```
Algorithm 1: Adam, our proposed algorithm for stochastic optimization. See section 2 for details,
and for a slightly more efficient (but less clear) order of computation. q_t^2 indicates the elementwise
square g_t \odot g_t. Good default settings for the tested machine learning problems are \alpha = 0.001,
\beta_1 = 0.9, \, \beta_2 = 0.999 and \epsilon = 10^{-8}. All operations on vectors are element-wise. With \beta_1^t and \beta_2^t
we denote \beta_1 and \beta_2 to the power t.
Require: \alpha: Stepsize
Require: \beta_1, \beta_2 \in [0, 1): Exponential decay rates for the moment estimates
Require: f(\theta): Stochastic objective function with parameters \theta
Require: \theta_0: Initial parameter vector
  m_0 \leftarrow 0 (Initialize 1<sup>st</sup> moment vector) \rightarrow for momentum
  m_0 \leftarrow 0 (Initialize 1 moment vector) v_0 \leftarrow 0 (Initialize 2<sup>nd</sup> moment vector) for RMSprop
   while \theta_t not converged do
      t \leftarrow t + 1
      g_t \leftarrow \nabla_{\theta} f_t(\theta_{t-1}) (Get gradients w.r.t. stochastic objective at timestep t)
      m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t (Update biased first moment estimate) v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2 (Update biased second raw moment estimate)
      \widehat{m}_t \leftarrow m_t/(1-\beta_1^t) (Compute bias-corrected first moment estimate)
      \hat{v}_t \leftarrow v_t/(1-\beta_2^t) (Compute bias-corrected second raw moment estimate)
      \theta_t \leftarrow \theta_{t-1} - \alpha \cdot \widehat{m}_t / (\sqrt{\widehat{v}_t} + \epsilon) (Update parameters)
   end while
   return \theta_t (Resulting parameters)
```

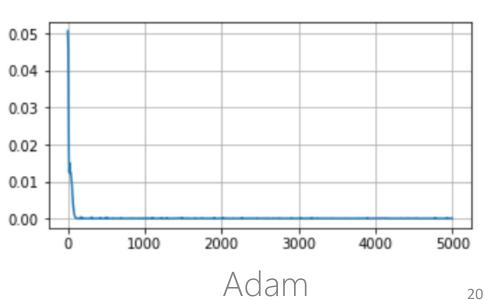
Run "3.2. Optimizer"



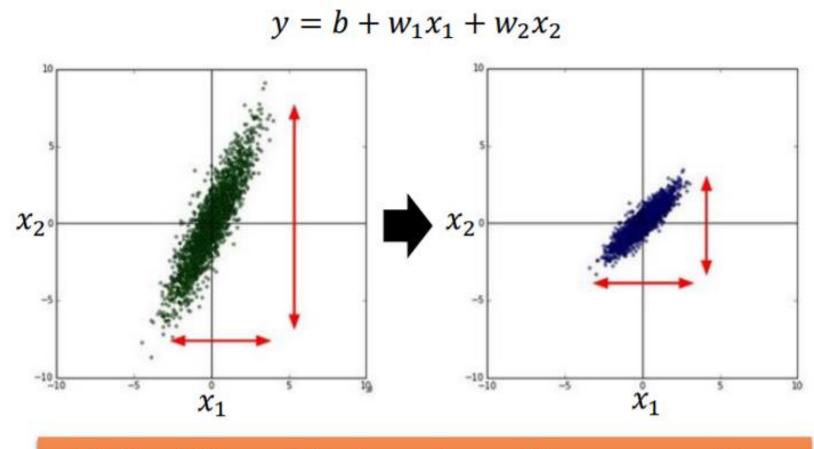








Feature scaling



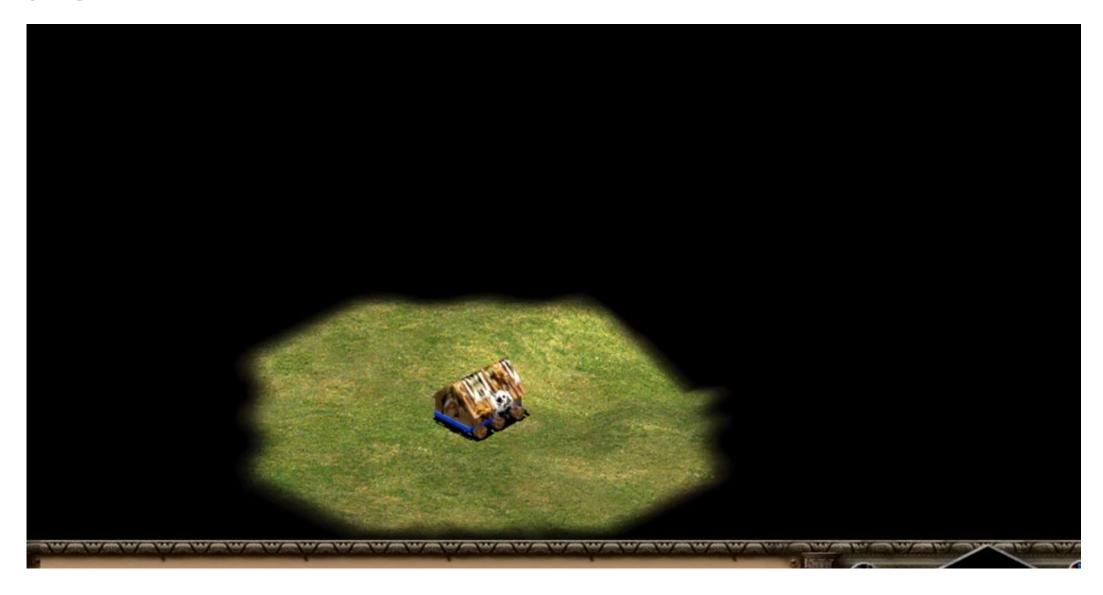
Make different features have the same scaling

Practice – Why feature scaling is important?

- Run "1. 2.1 MLP regression practice (1).ipynb".
- Run "1. 2.1 MLP regression practice (2).ipynb".



Why gradient decent can find local minimum?



Why gradient decent can find local minimum?

Based on Taylor Series:

If the red circle is **small enough**, in the red circle

$$L(\theta) \approx L(a,b) + \frac{\partial L(a,b)}{\partial \theta_{1}}(\theta_{1}-a) + \frac{\partial L(a,b)}{\partial \theta_{2}}(\theta_{2}-b)$$

$$s = L(a,b)$$

$$u = \frac{\partial L(a,b)}{\partial \theta_{1}}, v = \frac{\partial L(a,b)}{\partial \theta_{2}}$$

$$L(\theta)$$

$$\approx s + u(\theta_{1}-a) + v(\theta_{2}-b)$$

$$\frac{\partial L(a,b)}{\partial \theta_{2}}(\theta_{1}-a) + \frac{\partial L(a,b)}{\partial \theta_{2}}(\theta_{2}-b)$$

Why gradient decent can find local minimum?

Red Circle: (If the radius is small)

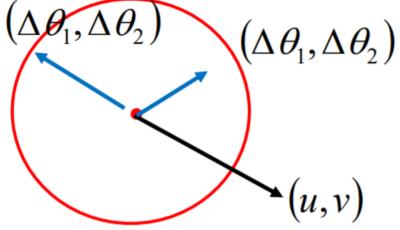
$$L(\theta) \approx s + u(\underline{\theta_1} - a) + v(\underline{\theta_2} - b)$$

$$\Delta \theta_1 \qquad \Delta \theta_2 \qquad (\Delta \theta_1, \Delta \theta_2)$$
Find θ_1 and θ_2 in the red circle

minimizing $L(\theta)$

$$\frac{\left(\underline{\theta_1} - a\right)^2 + \left(\underline{\theta_2} - b\right)^2 \le d^2}{\Delta \theta_1}$$

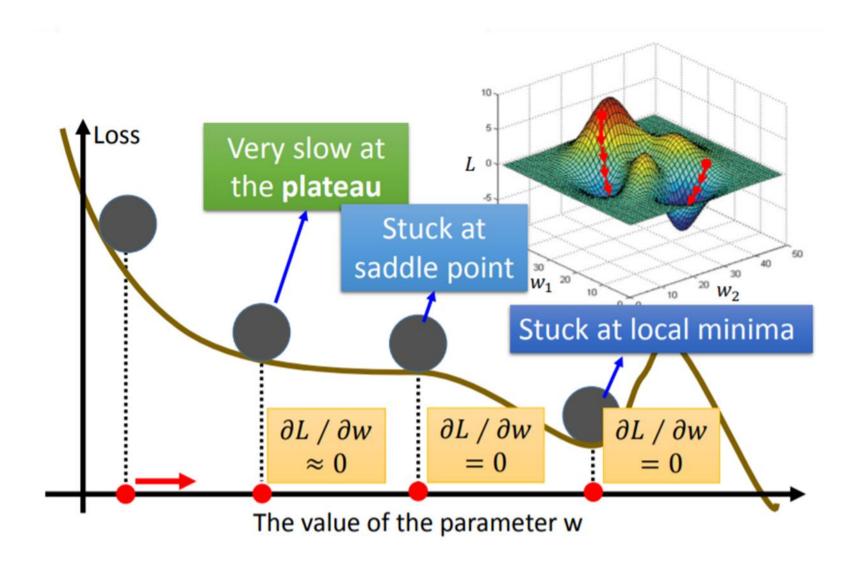
$$\Delta \theta_2$$



To minimize $L(\theta)$

$$\begin{bmatrix} \Delta \theta_1 \\ \Delta \theta_2 \end{bmatrix} = -\eta \begin{bmatrix} u \\ v \end{bmatrix} \qquad \qquad \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix} - \eta \begin{bmatrix} u \\ v \end{bmatrix}$$

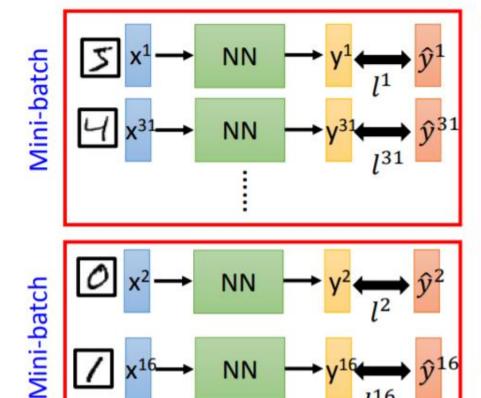
Limitation of gradient decent



Mini-batches

We do not really minimize total loss!

Mini-batch



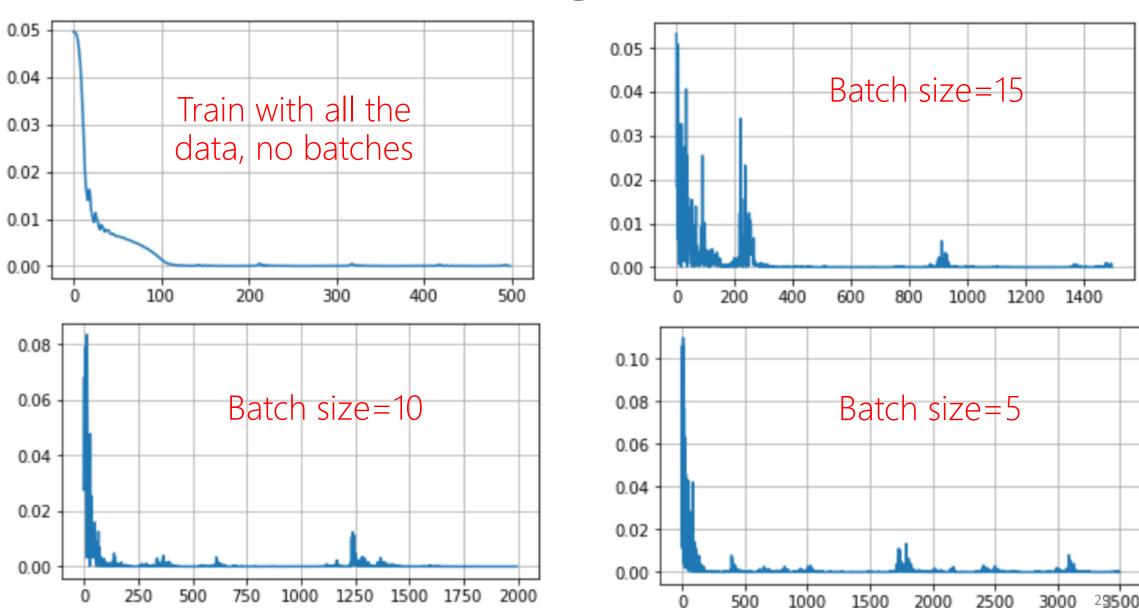
- Randomly initialize network parameters
- Pick the 1st batch $L' = l^1 + l^{31} + \cdots$ Update parameters once
- Pick the 2^{nd} batch $L'' = l^2 + l^{16} + \cdots$ Update parameters once :
- Until all mini-batches have been picked

one epoch

Repeat the above process

Run "3.3. Mini_Batch_Training" Color PYTÖRCH





Batch size influences both speed and performance. You have to tune it.

Speed

Very large batch size can yield worse performance

- Smaller batch size means more updates in one epoch
 - E.g. 50000 examples
 - batch size = 1, 50000 updates in one epoch 166s 1 epoch
 - batch size = 10. 5000 updates in one epoch 17s 10 epoch

