深度學習
Deep Learning

最佳化方法

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Course GitHub

Slido # DL0924

Outline

- Recap [20 min]
- Gradient Descent (II) - Optimizers [60 min]
- Training script in PyTorch [35 min]
- Quiz [30 min]

[Recap] Gradient Descent (梯度下降)

Assume x is a trainable parameter (weight), f is a differentiable function:

Gradient descent: $$x' = x - \eta \nabla_x f(x)$$

η is the learning rate (伊塔/欸塔) used for gradient descent.

- 調整每次更新參數時的**幅度**

[Recap] Minimize a Regression Model

- 假設我們今天要用 linear regression 來訓練一層的 MLP，模型輸出是 $\hat{y} = wx + b$
- 以均方誤差 (Mean Squared Error) 為例：

$$\mathcal{L} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$ ← 模型輸出跟正確答案的平均差距

把 $(wx_\mathrm{i} + b)$ 代入 $\hat{y}_i$ →

$$\boxed{= \frac{1}{n}\sum_{i=1}^{n}\big(y_i - (wx_\mathrm{i} + b)\big)^2}$$

訓練目標是讓這個公式在n筆訓練資料的平均差距越小越好

- 其中:
  - $\mathcal{L}$ 代表 Loss function；n 代表有 n 筆訓練資料
  - y_i 爲任一筆 ground-truth、$\hat{y}_i$ 爲任一筆 prediction (model output)

[Recap] Minimize a Regression Model

$$\mathcal{L} = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (wx_{\mathrm{i}} + b)\right)^2$$

對w進行偏微分

$$\frac{\partial \mathcal{L}}{\partial w} = \frac{1}{n}\sum_{i=1}^{n} 2\left(y_{\mathrm{i}} - (wx_{\mathrm{i}} + b)\right) \cdot (-x_{\mathrm{i}})$$

對b進行偏微分

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{1}{n}\sum_{i=1}^{n} 2\left(y_i - (wx_{\mathrm{i}} + b)\right) \cdot (-1)$$

[Recap] Minimize a Regression Model

$$\frac{\partial \mathcal{L}}{\partial w} = \frac{1}{n}\sum_{i=1}^{n} 2\big(y_{\mathrm{i}} - (wx_{\mathrm{i}} + b)\big) \cdot (-x_{\mathrm{i}})$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{1}{n}\sum_{i=1}^{n} 2\big(y_i - (wx_{\mathrm{i}} + b)\big) \cdot (-1)$$

更新w：

$$w_t = w_{t-1} - \eta \frac{\partial \mathcal{L}}{\partial w_{t-1}}$$

現在這個時間點的權重值

上一次的時間點的權重值

更新b：

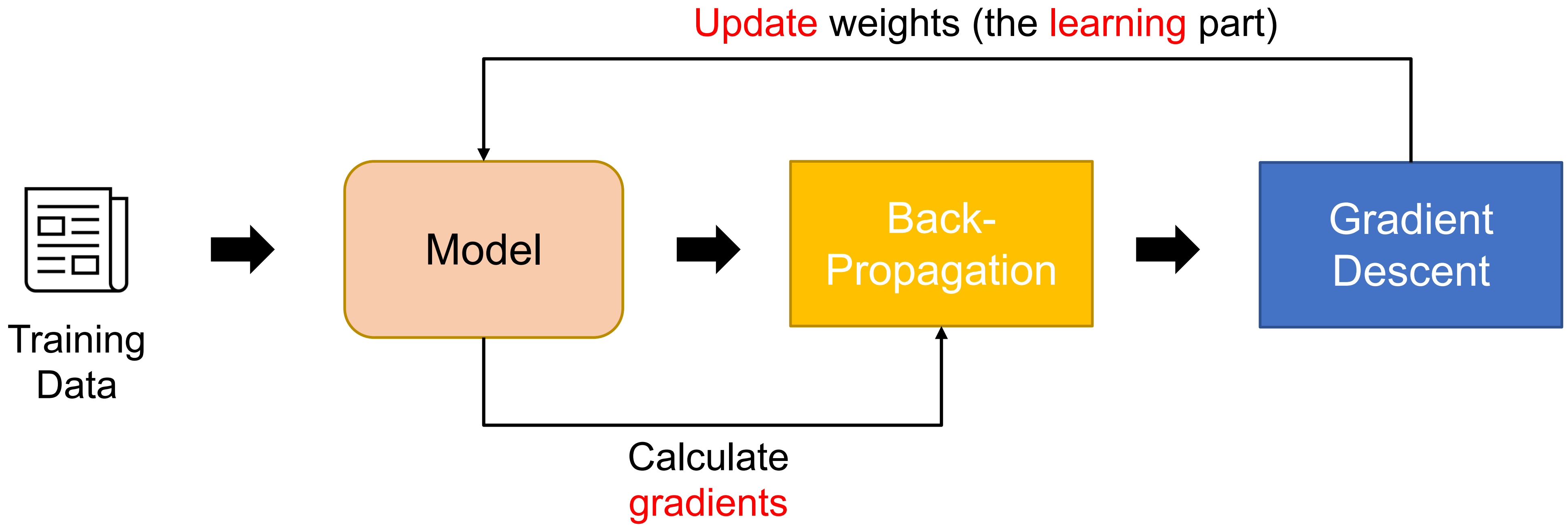
$$b_t = b_{t-1} - \eta \frac{\partial \mathcal{L}}{\partial b_{t-1}}$$

現在這個時間點的偏置項

上一次的時間點的偏置項

Training Process of a Deep Learning Model

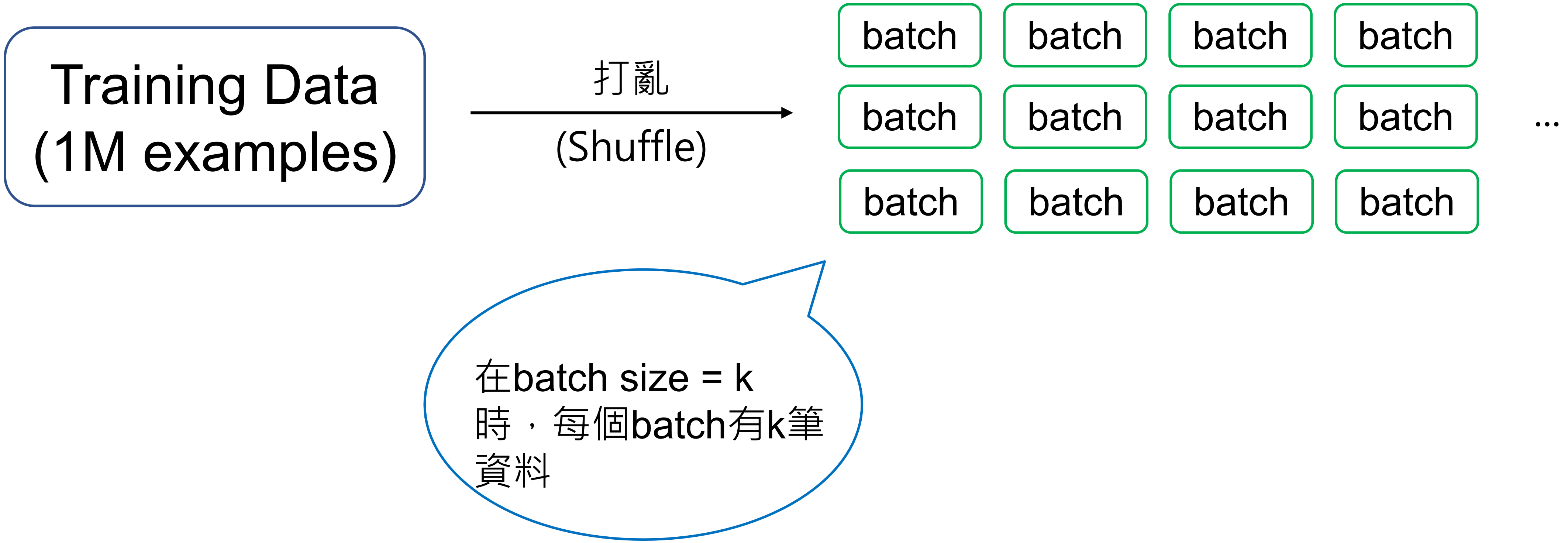
- 深度學習模型被訓練的流程



Another training approach: SGD

- 在一般的 Gradient descent (GD) 中，我們是將所有的資料算一次梯度之後，才更新一次模型
  - 資料量大的時候，單次模型更新的計算時間長 (但是平行化可以解決)
- SGD: Stochastic gradient descent
  - 把資料切成 batches，每次進行 GD 時都是隨機取其中一個 batch 來計算梯度與更新模型

Mini-batch Data



Gradient Descent vs. Stochastic Gradient Descent

- 計算 $\frac{\partial \mathcal{L}}{\partial w}$ 和 $\frac{\partial \mathcal{L}}{\partial b}$

Gradient Descent:

$$\mathcal{L} = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (wx_{\mathrm{i}} + b)\right)^2$$

全部的 n，但如果 n 很大時需要計算久，且需要較大的記憶體

Stochastic Gradient Descent:

$$\mathcal{L} = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (wx_{\mathrm{i}} + b)\right)^2$$

n 改用採樣的，可能為 8 / 16 / 32 / 64 / 128

Optimization with Batches (Pseudo code)

- 假設 training data 有 5,000,000 examples，mini_batch_size = 1,000
  - Number of steps = 5000000 / 1000 = 5000
  - 代表會進行 5000 次 gradient descent (更新 5000 次參數)

```
# do shuffle
for i in range(5000):
    start_index = i * 1000
    end_index = start_index + 1000
    x = train_x[start_index: end_index]
    y = train_y[start_index: end_index]

    # Calculate gradients via BP
    # do gradient descent (update parameters)
```

Optimization with Batches

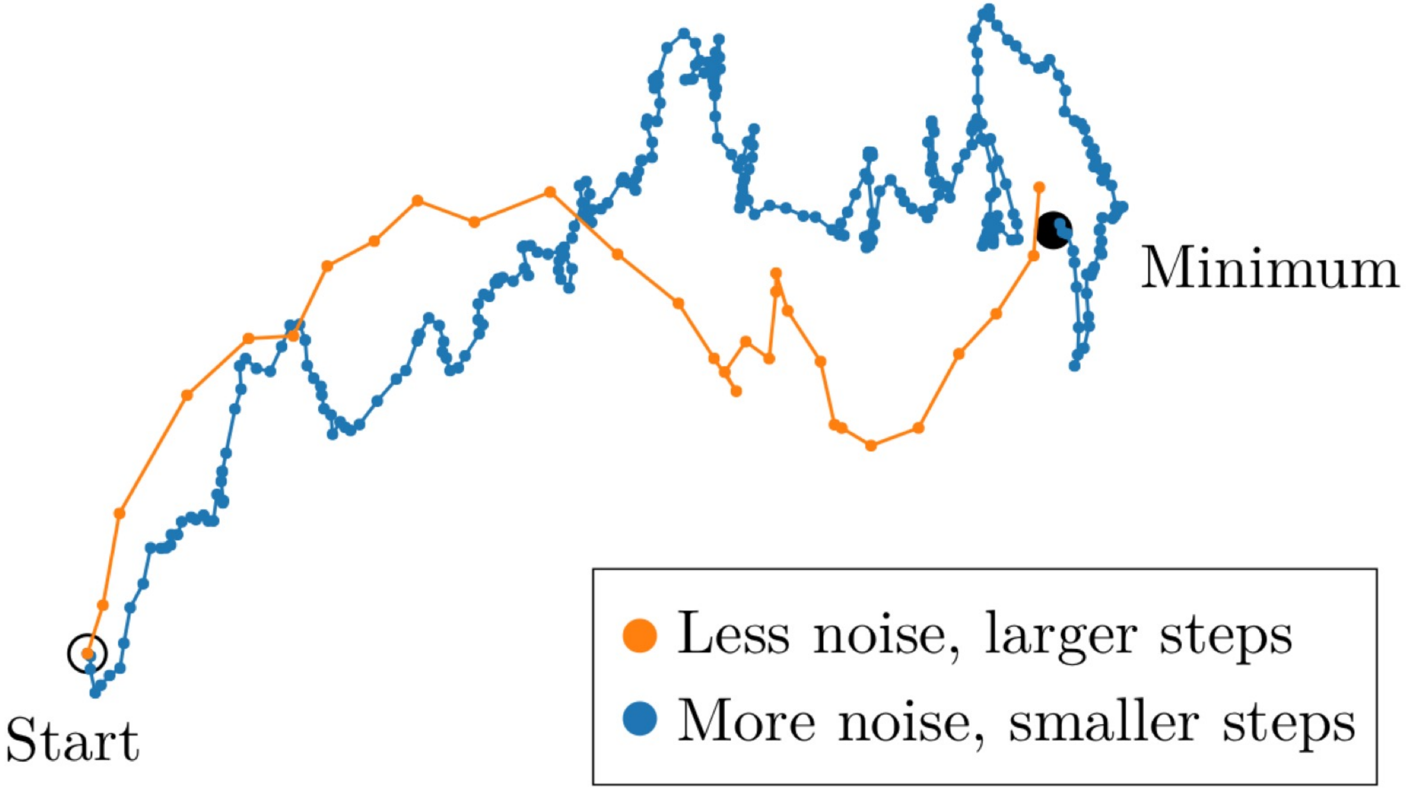
- 初始參數：θ_0

B 組 (x, y)

Batch	(x, y) 輸入到模型，forward and backward	$\theta_1 = \theta_0 - \eta\nabla_{\theta_0}\mathcal{L}(\theta_0)$
Batch	(x, y) 輸入到模型，forward and backward	$\theta_2 = \theta_1 - \eta\nabla_{\theta_1}\mathcal{L}(\theta_1)$
Batch	(x, y) 輸入到模型，forward and backward	$\theta_3 = \theta_2 - \eta\nabla_{\theta_2}\mathcal{L}(\theta_2)$

⋮

Larger batch size vs. smaller batch size



Large batch size (fewer steps)

Small batch size (more steps)

McCandlish, Sam, et al. "An empirical model of large-batch training." arXiv preprint arXiv:1812.06162 (2018).

Batching fixes the memory problem

硬體計算角度

Training Data
(1M examples)

batch

train.to("cuda:0") → ❌

mini.to("cuda:0") → ✅

- Typically, during training or test time, we use a small set of data (mini-batch) at one time for running a deep learning model on GPUs.

Figure source: https://www.league-funny.com/3c/article-343103

Question

最佳化理論角度

- 和 full batch size 的 GD 比起來，用 mini-batch 方式訓練的效果一定比較好嗎？
- Ans: full batch size 只會更新一次，容易跑到 local minimum 的位置

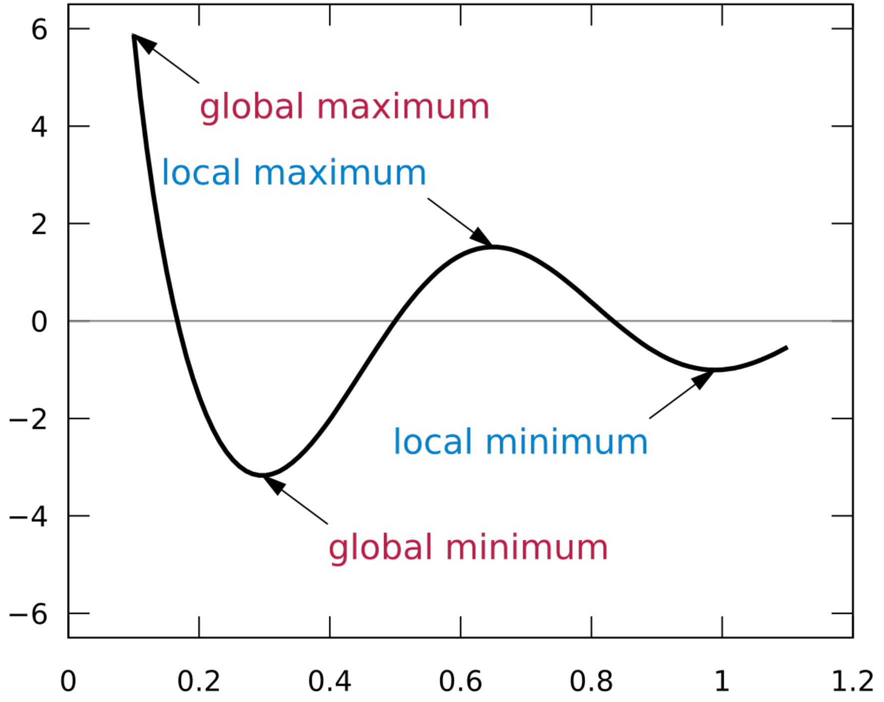


Figure source:
https://en.wikipedia.org/wiki/Maximum_and_minimum

Batch and Mini-batch Gradient Descent

比較

	Batch Gradient Descent	**Stochastic Gradient Descent**	**Mini-batch Stochastic Gradient Descent**
單次更新所使用的訓練資料筆數	Entire training set	1	mini_batch_size (Hyperparameter)
訓練穩定性	Stable	Low	Medium
訓練時期更新頻率 (number of steps)	Low 1 time per epoch	High 1 time per sample	Medium 1 time per mini-batch
缺點	Easily falling into local minimum	Training variance is too big	Hard to determine the best batch size

<u>廣義上</u> SGD 指的是 Mini-batch Stochastic Gradient Descent

Question

最佳化理論 / 實驗角度

- batch_size 大比較好還是 batch_size 小比較好？

SB: small batch (256)
LB: large batch (training set size*0.1)

Table 2: Performance of small-batch (SB) and large-batch (LB) variants of ADAM on the 6 networks listed in Table 1

Name	Training Accuracy SB	Training Accuracy LB	Testing Accuracy SB	Testing Accuracy LB
F_1	$99.66\% \pm 0.05\%$	$99.92\% \pm 0.01\%$	$98.03\% \pm 0.07\%$	$97.81\% \pm 0.07\%$
F_2	$99.99\% \pm 0.03\%$	$98.35\% \pm 2.08\%$	$64.02\% \pm 0.2\%$	$59.45\% \pm 1.05\%$
C_1	$99.89\% \pm 0.02\%$	$99.66\% \pm 0.2\%$	$80.04\% \pm 0.12\%$	$77.26\% \pm 0.42\%$
C_2	$99.99\% \pm 0.04\%$	$99.99\% \pm 0.01\%$	$89.24\% \pm 0.12\%$	$87.26\% \pm 0.07\%$
C_3	$99.56\% \pm 0.44\%$	$99.88\% \pm 0.30\%$	$49.58\% \pm 0.39\%$	$46.45\% \pm 0.43\%$
C_4	$99.10\% \pm 1.23\%$	$99.57\% \pm 1.84\%$	$63.08\% \pm 0.5\%$	$57.81\% \pm 0.17\%$

Keskar, Nitish Shirish, et al. "On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima." ICLR. 2017.

Small-batch vs. Large-batch Training

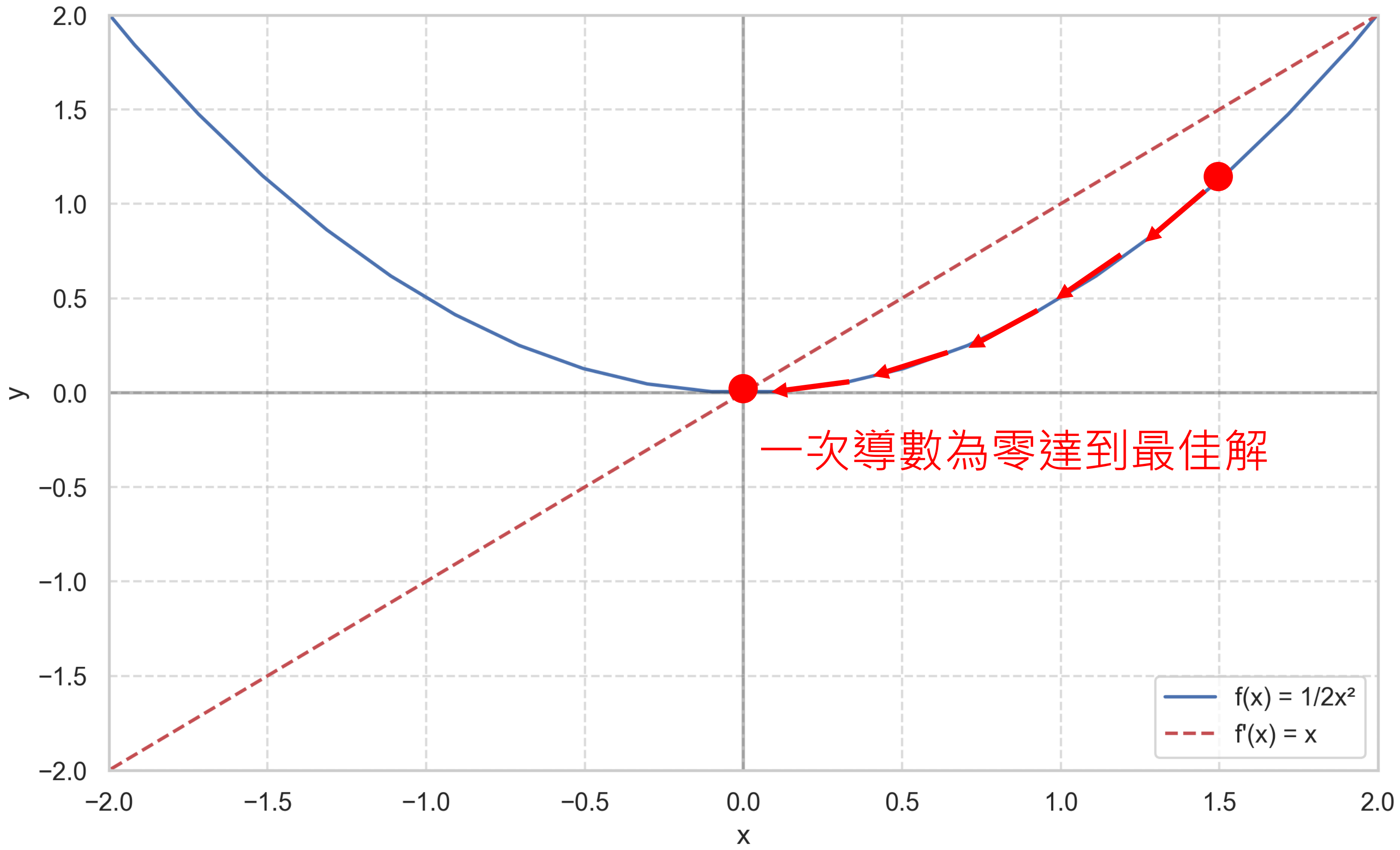
	Small batches	Large batches
單次更新所需要的時間	較短	較長 (平行化後差異縮小)
單次更新記憶體用量	較少	較多
訓練穩定性	較不穩定	較穩定
訓練時期更新頻率 (number of steps)	較多	較少
1 Epoch 訓練時間	較快	較慢 (平行化後較快)
訓練後的模型效能	可能較好	可能較差

Optimizers

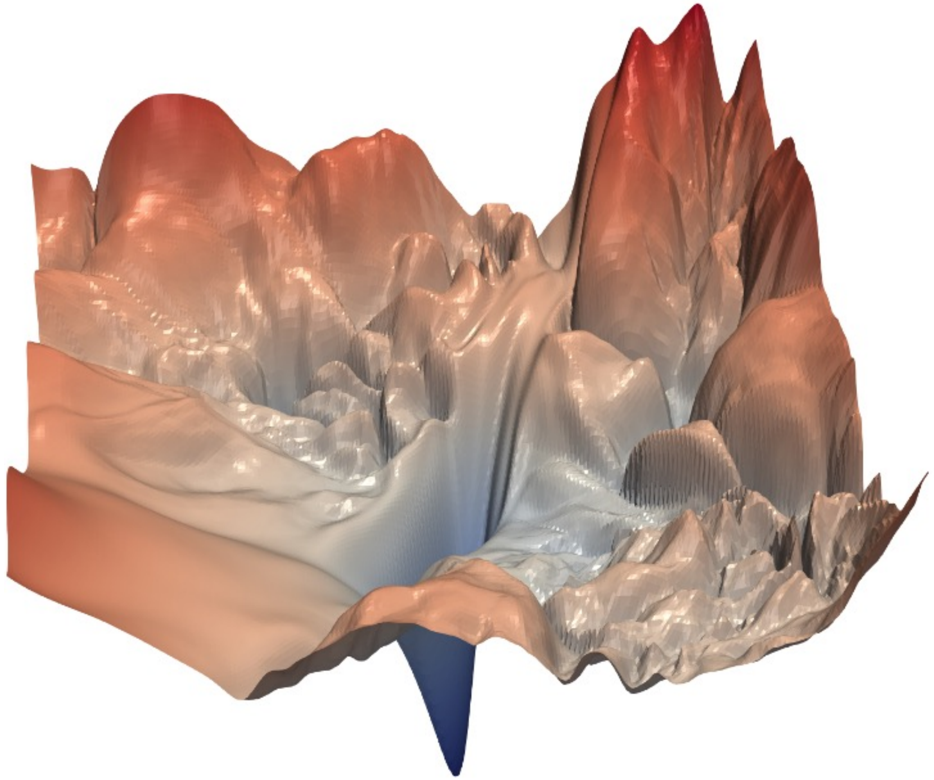
基於梯度下降的最佳化方法

Loss function 到底長怎樣？

- 使用 f(x) = $1/2x^2$ 作為簡單範例



Even more complicated ...



⬅️ The loss surfaces of ResNet-56 with/without skip connections.

https://arxiv.org/abs/1712.09913
Li, Hao, et al. "Visualizing the loss landscape of neural nets." Advances in neural information processing systems 31 (2018).

SGD Problem #1

- SGD 在訓練過程中是使用隨機的 mini-batch 進行最佳化
- 如果隨機取到的 mini-batch 突然產生很大的梯度，可能使訓練不穩定

Gradient descent: $x_{t+1} = x_t - \eta \underline{\nabla_x f(x_t)}$

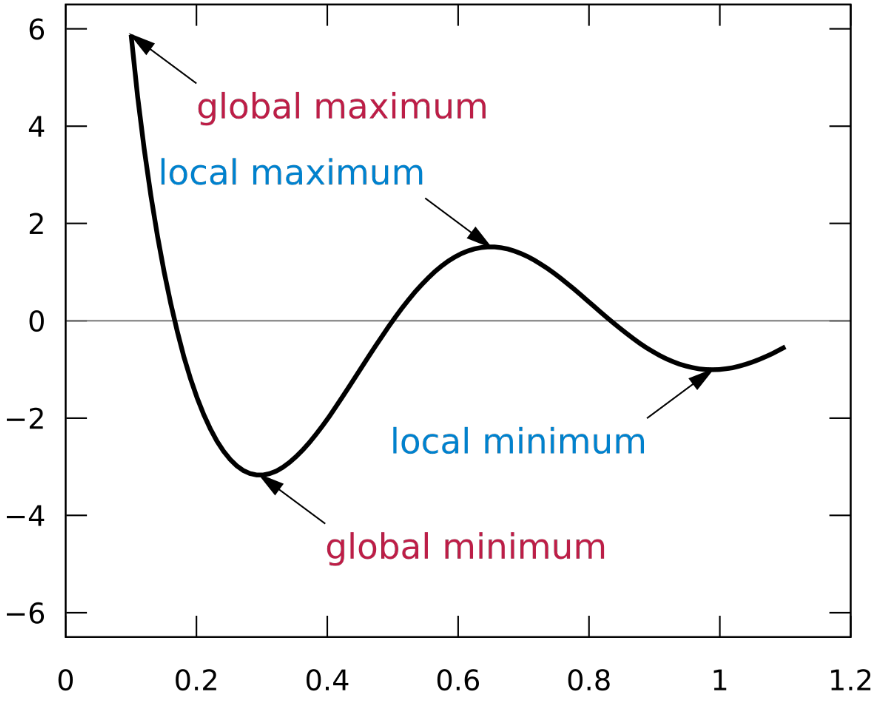
觀察梯度歷史紀錄：過去的時間點如果梯度小的話，現在這個時間點理論上梯度不該太大

調整學習率，該大的時候大一點，該小的時候小一點

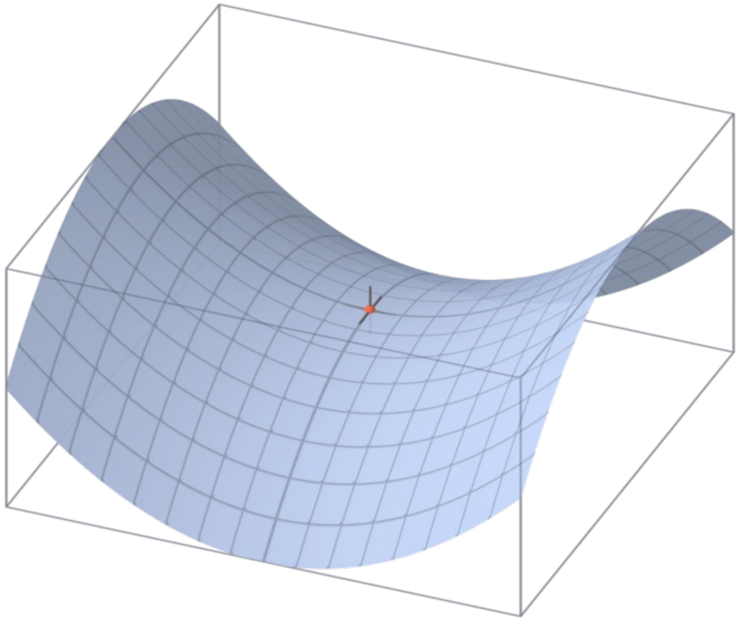
訓練不穩定代表 x_{t+1} 在不該改變很多的情況下改變太多

SGD Problem #2：容易卡住在梯度小的點

1. Local maximum / minimum



2. Saddle Point



Saddle Point
(鞍點)

Figure source:
https://en.wikipedia.org/wiki/Maximum_and_minimum
https://en.wikipedia.org/wiki/Saddle_point

如何有效訓練深度學習模型？

Optimizer:

- 對梯度動手腳
  - Momentum
  - ~~Nesterov Momentum~~ (不常用)
- 自動調整學習率
  - Adagrad
  - RMSprop
  - Adam

Momentum

https://pytorch.org/docs/main/_modules/torch/optim/sgd.html#SGD

- Momentum 將過去的梯度記錄下來
- 每次更新參數時，會考慮到上一個時間點的梯度
  - 同方向 -> 參數改變幅度大一點；不同方向 ->參數改變幅度小一點

Gradient descent: $x_{t+1} = x_t - \eta \nabla_x f(x_t)$

上一個時間點的梯度

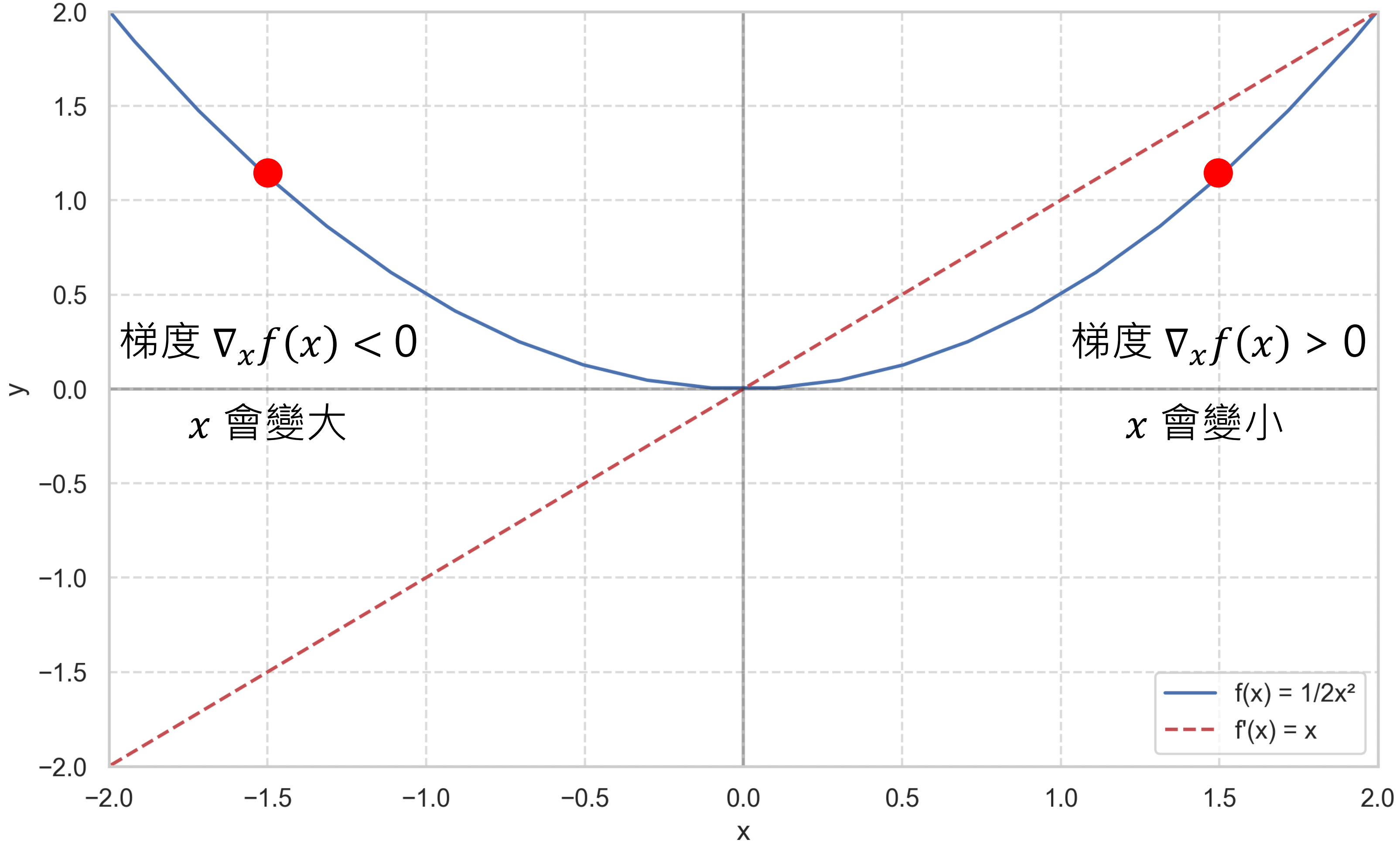
Momentum: $v_t = \gamma v_{t-1} + \eta \nabla_x f(x_t)$

Momentum term
(超參數，常設為 0.9)

$$x_{t+1} = x_t - v_t$$

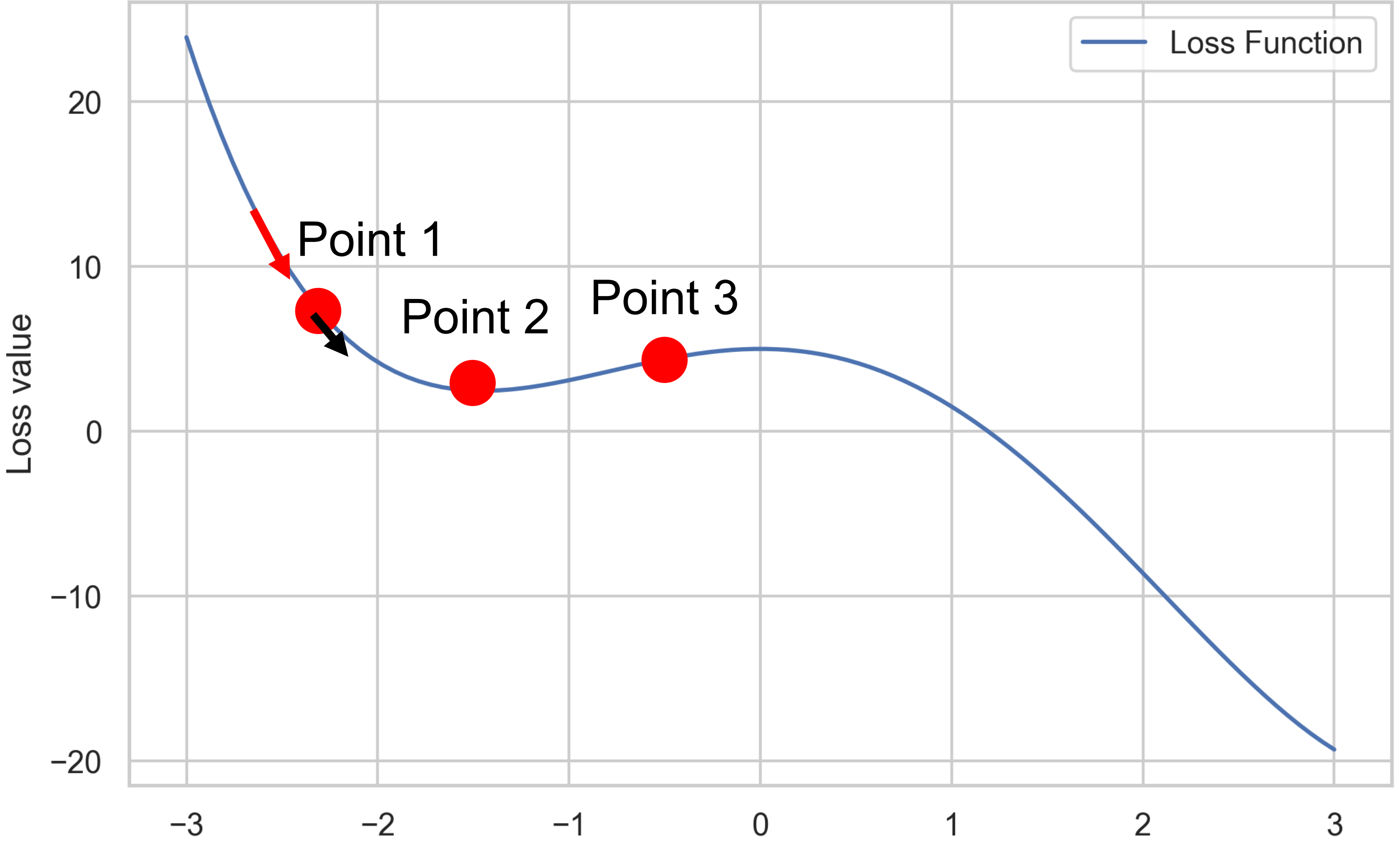
[Recap] 以兩個點來觀察 Gradient Descent 的特性

$x' = x - \eta\nabla_x f(x)$



SGD + Momentum (example)

(Point 1 ->Point 2 -> Point 3)



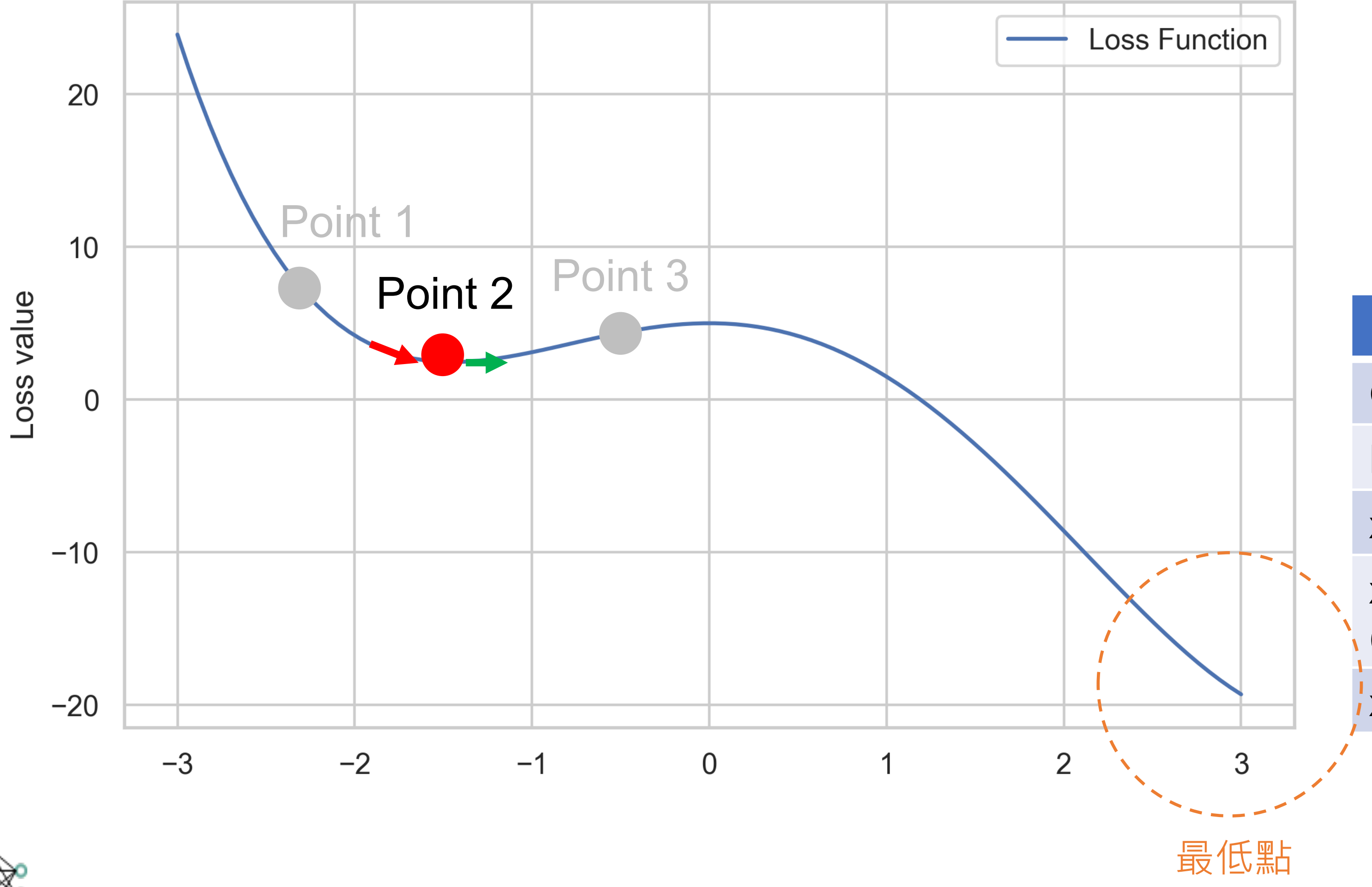
SGD + Momentum:

$$v_t = \gamma v_{t-1} + \eta \nabla_x f(x_t)$$
$$x_{t+1} = x_t - v_t$$

	P1
Gradient	-3.5
Past (v_{t-1})	-4
x 改變量 (GD)	→
x 改變量 (Momentum)	→
x 總改變量	→

SGD + Momentum (example)

(Point 1 ->Point 2 -> Point 3)



SGD + Momentum:

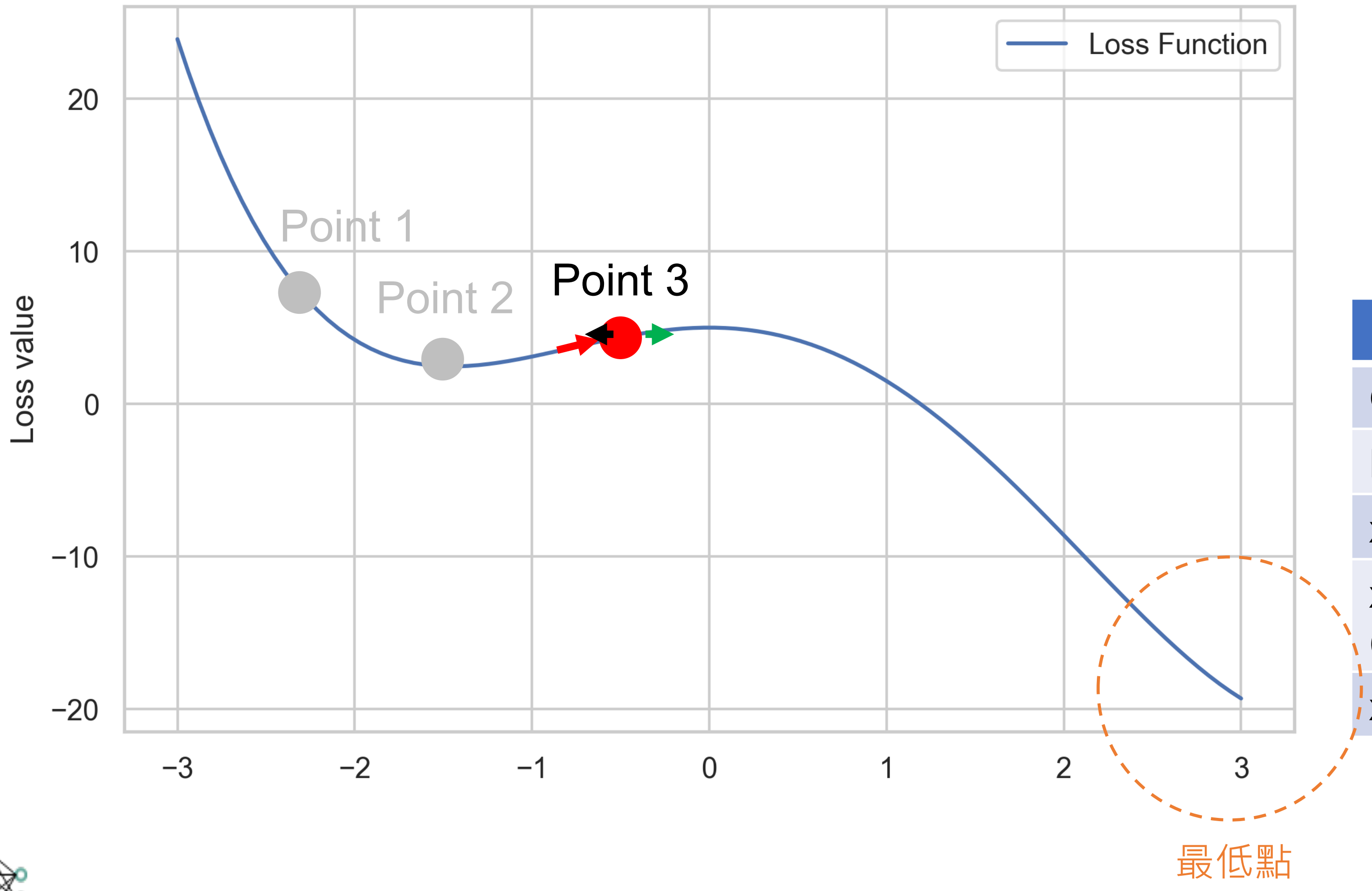
$$v_t = \gamma v_{t-1} + \eta \nabla_x f(x_t)$$

$$x_{t+1} = x_t - v_t$$

	P1	P2
Gradient	-3.5	0
Past (v_{t-1})	-4	-2
x 改變量 (GD)	→	
x 改變量 (Momentum)	→	→
x 總改變量	→	→

SGD + Momentum (example)

(Point 1 ->Point 2 -> Point 3)



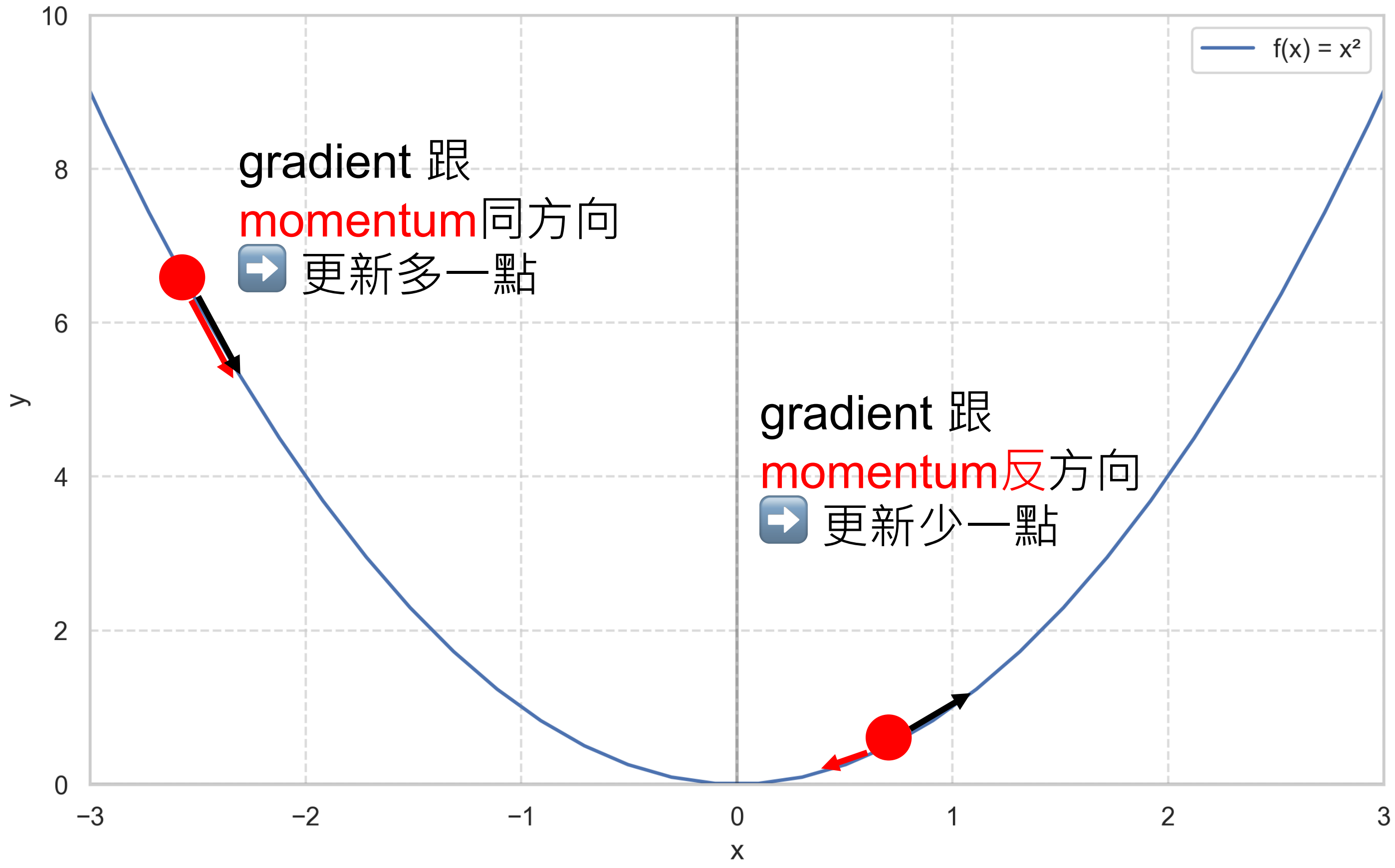
SGD + Momentum:

$$v_t = \gamma v_{t-1} + \eta \nabla_x f(x_t)$$

$$x_{t+1} = x_t - v_t$$

	P1	P2	P3
Gradient	-3.5	0	1
Past (v_{t-1})	-4	-2	-2
x 改變量 (GD)	→		←
x 改變量 (Momentum)	→	→	→
x 總改變量	→	→	→

Momentum



10
8
6
4
2
0
y
−3
−2
−1
0
1
2
3
x
f(x) = x²
gradient 跟
momentum同方向
➡️ 更新多一點
gradient 跟
momentum反方向
➡️ 更新少一點

Summary of Momentum

- SGD 可能因為隨機採樣而梯度大幅震盪，而 Momentum 可以緩衝這種震盪
- Momentum 增加歷史紀錄的功能可以：
  - 加速收斂 -> 解決 SGD Problem #1
  - 逃離鞍點 (Saddle point) -> 解決 SGD Problem #2
    - 但 Momentum 也可能超過 convergence

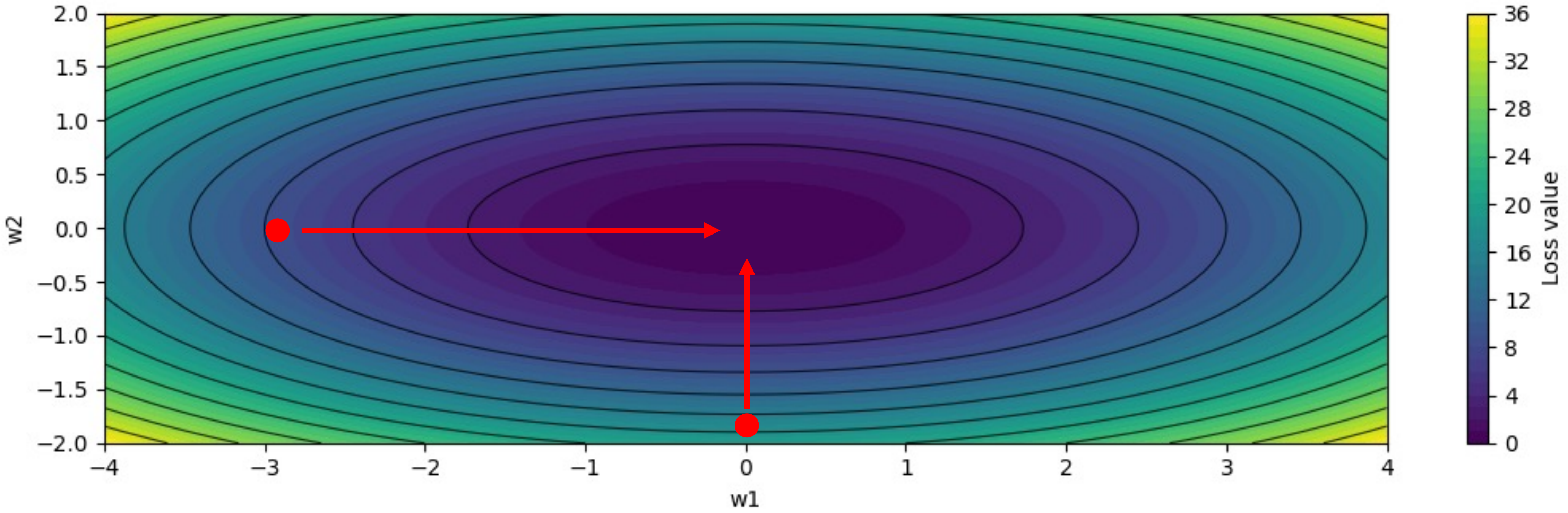
只是理論，不一定能夠做到！(Deep Learning 是很複雜的 function)

如何有效訓練深度學習模型？

Optimizer:

- 對梯度動手腳
  - Momentum
  - Nesterov Momentum
- 自動調整學習率
  - Adagrad
  - RMSprop
  - Adam

Learning rate 應該依據不同參數而不同



w1 方向的梯度通常較大（從 loss function 的橢圓形可觀察到）

w2 方向的梯度通常較小

Adagrad (Adaptative Gradient)

Journal of Machine Learning Research 12 (2011) 2121-2159 Submitted 3/10; Revised 3/11; Published 7/11

Adaptive Subgradient Methods for Online Learning and Stochastic Optimization*

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Editor: Tong Zhang

Duchi, John, Elad Hazan, and Yoram Singer. "Adaptive subgradient methods for online learning and stochastic optimization." Journal of machine learning research 12.7 (2011).

Adagrad (Adaptative Gradient)

- Adagrad 可以根據歷史梯度總和自動調整 learning rate
  - 需要一個 r 來記錄歷史梯度 (平方和)

Gradient descent:

$$x_{t+1} = x_t - \boxed{\eta} \nabla_x f(x_t)$$

Adagrad:

$$x_{t+1} = x_t - \boxed{\frac{\eta}{\delta + \sqrt{r_t}}} \nabla_x f(x_t)$$

$$r_t = r_{t-1} + g \odot g$$

其中 $g = \nabla_x f(x_t)$

- δ 是一個很小的數字，讓分母不要為0

Element-wise Scaling

- 在多維度情況 (有多個變數 x, Multivariate)下，梯度是所有偏導數的向量：

$$\nabla_{x} f = \left[\frac{\partial f}{\partial x_1}, \quad \dots, \quad \frac{\partial f}{\partial x_n}\right]$$

每個項的 g 都不同，進而能得出不同 r ，
最終每個項的 learning rate 都不同

$$x_{n,t+1} = x_{n,t} - \boxed{\frac{\eta}{\delta + \sqrt{r_{n,t}}}} \nabla_x f(x_{n,t})$$

Element-wise Multiplication

$$r_t = r_{t-1} + \boxed{g \odot g} \qquad \text{其中 } g = \nabla_x f(x_t)$$

- 在多維度情況 (有多個變數 x, Multivariate)下，梯度是所有偏導數的向量：

$$\nabla_{\mathrm{x}} f = \left[\frac{\partial f}{\partial x_1}, \quad \dots, \quad \frac{\partial f}{\partial x_n}\right]$$

$$g \odot g = \left[\left(\frac{\partial f}{\partial x_1}\right)^2, \quad \dots, \quad \left(\frac{\partial f}{\partial x_n}\right)^2\right]$$

對 Adagrad 的觀察與思考

Adagrad: $r_t = r_{t-1} + g \odot g$ 其中 $g = \nabla_x f(x_t)$

$$x_{t+1} = x_t - \frac{\eta}{\delta + \underline{\sqrt{r_t}}} \nabla_x f(x_t)$$

- 特性：梯度大的學習率自動調小一點；梯度小的學習率自動調大一點
- 缺點：Learning rate 或許會下降太快 (因為 r_t 持續累積平方和)
  - 不適用於許多深度學習模型 (實驗角度)

RMSProp

- RMSProp (Root Mean Square Propagation) 是 Adagrad 的改版，為了避免 r 很快就變很大，使得學習率很快就變得很低 (此時神經網路會很難更新)
- Hinton, Geoffrey, Nitish Srivastava, and Kevin Swersky. "Neural networks for machine learning lecture 6a overview of mini-batch gradient descent." Cited on 14.8 (2012): 2.

RMSProp

Hinton, Geoffrey, Nitish Srivastava, and Kevin Swersky. "Neural networks for machine learning lecture 6a overview of mini-batch gradient descent." Cited on 14.8 (2012): 2.

Adagrad:

$$r_t = r_{t-1} + g \odot g$$

其中 $g = \nabla_x f(x_t)$

$$x_{t+1} = x_t - \frac{\eta}{\delta + \sqrt{r_t}} \nabla_x f(x_t)$$

Running average (moving average)，依照比例抑制 $g \odot g$ 所造成 r 的增長

RMSProp:

$$r_t = p r_{t-1} + (1 - p) g \odot g$$

p 為 decay rate (常設為 0.9)

$$x_{t+1} = x_t - \frac{\eta}{\sqrt{\delta + r_t}} \nabla_x f(x_t)$$

δ 是一個很小的數字，讓分母不要為0

Adam

- Adam: adaptive moment estimation
- 結合了 Momentum 和 RMSProp 的概念

Kingma, Diederik P., and Jimmy Ba. "Adam: A method for stochastic optimization." ICLR 2015. https://arxiv.org/abs/1412.6980

Adam

Kingma, Diederik P., and Jimmy Ba. "Adam: A method for stochastic optimization." ICLR 2015. https://arxiv.org/abs/1412.6980

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. g_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 β_1^t and β_2^t we denote β_1 and β_2 to the power t.

Require: α: Stepsize Learning rate
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector
  $m_0 \leftarrow 0$ (Initialize 1st moment vector) momentum
  $v_0 \leftarrow 0$ (Initialize 2nd moment vector) Adagrad, RMSProp
  $t \leftarrow 0$ (Initialize timestep)
  while θ_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)
    $\widehat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (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) Adagrad
  end while
  return θ_t (Resulting parameters)

移動平均取自 RMSProp

[Adam]
m 記錄梯度
v 記錄梯度平方

訓練初期的問題

[Adam]
m 記錄梯度
v 記錄梯度平方

假設 $\beta_1 = 0.9$

Momentum歷史記錄 $m_t = \beta_1 m_{t-1} + (1-\beta_1)\nabla_x f(x_t)$

0 0.1 0.5

$\boxed{\widehat{m}_t \leftarrow m_t/(1-\beta_1^t) \text{ (Compute bias-corrected first moment estimate)}}$
$\widehat{v}_t \leftarrow v_t/(1-\beta_2^t)$ (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)

(以 β_1^t 為例) $\beta_1^t = \beta_1^1 \times \beta_1^2 \times \cdots \times \beta_1^t$

$\beta_1^t = 0.9$	無校正 (即 m_t)	校正後
$\widehat{m}_t$	0.1 * 0.5 = 0.05	0.1 * 0.5 / 0.1 = 0.5

代表訓練初期參數更新幅度小 ☹

訓練初期的問題 (t 次項)

[Adam]
m 記錄梯度
v 記錄梯度平方

$\widehat{m}_t \leftarrow m_t / \boxed{(1-\beta_1^t)}$ (Compute bias-corrected first moment estimate)

$\beta_1^t = \beta_1^1 \times \beta_1^2 \times \cdots \times \beta_1^t$

t	β_1^t	校正項 $1-\beta_1^t$
1	0.9	0.1
2	$0.9^2 = 0.81$	0.19
3	$0.9^3 = 0.729$	0.271
10	$0.9^{10} = 0.3487$	0.6513
100	$0.9^{100} = 0.000026$	0.999974

$1-\beta_1^t$ 越來越接近1

代表隨著訓練時間增加，
越來越不需要校正

比較參數更新

[Adam]
m 記錄梯度
v 記錄梯度平方

Adam: $\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \boxed{\widehat{m}_t}/(\boxed{\sqrt{\widehat{v}_t} + \epsilon})$ (Update parameters)

其中 α 是學習率

Momentum:

$$v_t = \gamma v_{t-1} + \eta \nabla_x f(x_t)$$

$$x_{t+1} = x_t \boxed{- v_t}$$

其中 η 是學習率

Adagrad:

$$r_t = r_{t-1} + g \odot g$$

$$x_{t+1} = x_t - \frac{\eta}{\boxed{\delta + \sqrt{r_t}}} \nabla_x f(x_t)$$

其中 $g = \nabla_x f(x_t)$

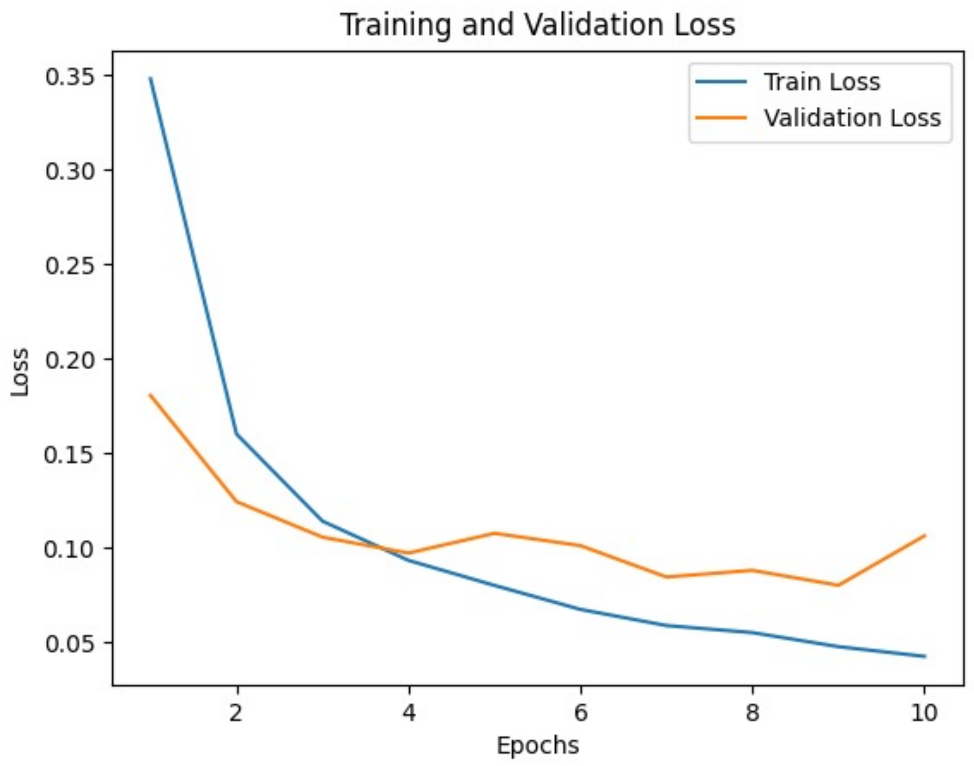
再加上移動平均紀錄的概念，Adam 是 Momentum, RMSProp, Adagrad 的集大成

https://x.com/DBahdanau/status/1916666861808456176

訓練完成之後

Convergence

- Convergence (收斂) 是指在模型訓練過程中，loss 的變化逐漸趨於穩定，可能已經到達最佳解，表示模型的學習進度減緩
- 收斂表示模型可能已達到某個局部或全局最小值，但不一定代表它找到了最佳解 (因為有可能只是局部最小值)，也不保證模型此時具備良好的泛化能力 (val_loss 也同樣很低)



Convergence and gradients

- 在經過很多個 steps (t 很大) 的更新之後，gradients 等於零的情況：

$$\nabla_{\theta_t}\mathcal{L}(\theta_t) = 0$$

- $\mathcal{L}$: loss function
- θ_t: 在 t 個時間點 (step) 的的參數組合 (包含各層的w跟b)
- $\nabla_{\theta_t}\mathcal{L}(\theta_t)$: 梯度

此時代表模型可能已經達到目標函數的最佳解

Additional Links

- Optimizers
  - https://www.ruder.io/optimizing-gradient-descent/#fn5
- Saddle point
  - https://www.youtube.com/watch?v=8aAU4r_pUUU
- Deep Learning Book Chapter 8
  - https://www.deeplearningbook.org/contents/optimization.html

Thank you!

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