New Optimizers for Deep Learning

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Background Knowledge

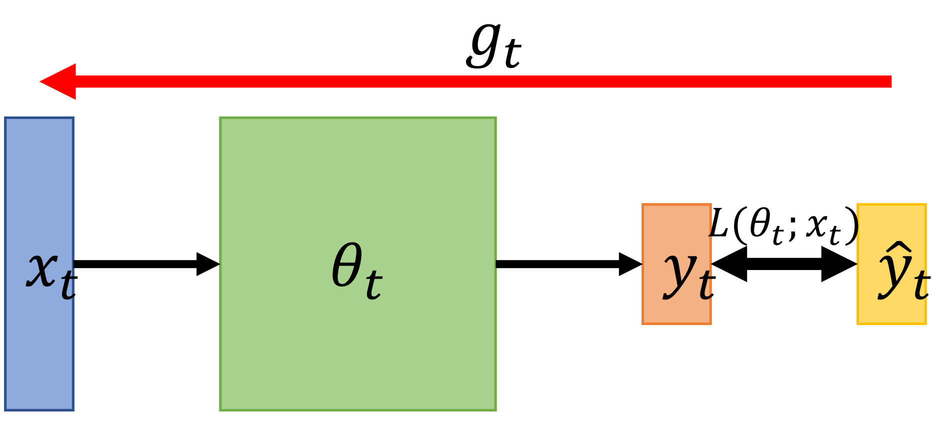
- μ-strong convexity
- Lipschitz continuity
- Bregman proximal inequality

What you have known before?

- SGD
- SGD with momentum
- Adagrad
- RMSProp
- Adam

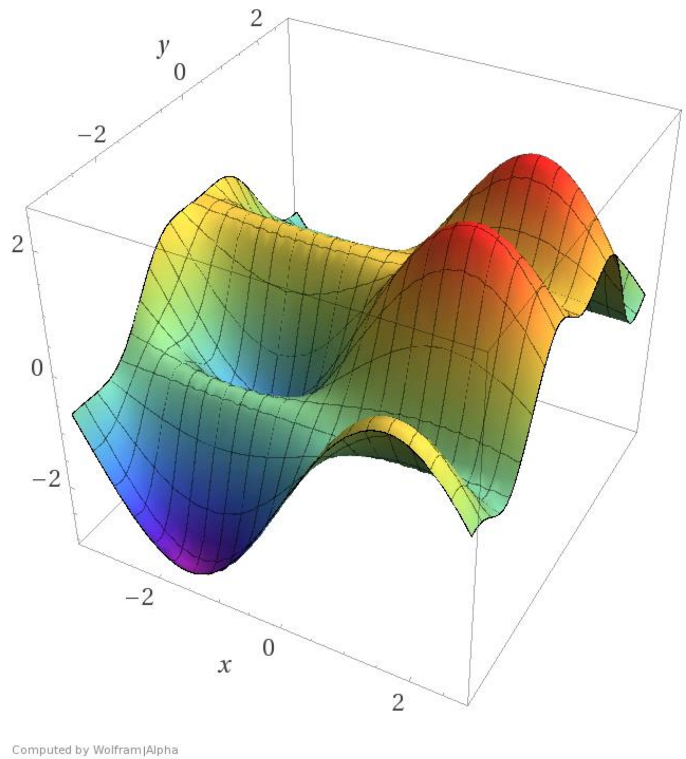
Some Notations

- θ_t : model parameters at time step t
- $\nabla L(\theta_t)$ or g_t: gradient at θ_t, used to compute θ_{t+1}
- m_{t+1}: momentum accumulated from time step 0 to time step t, which is used to compute θ_{t+1}



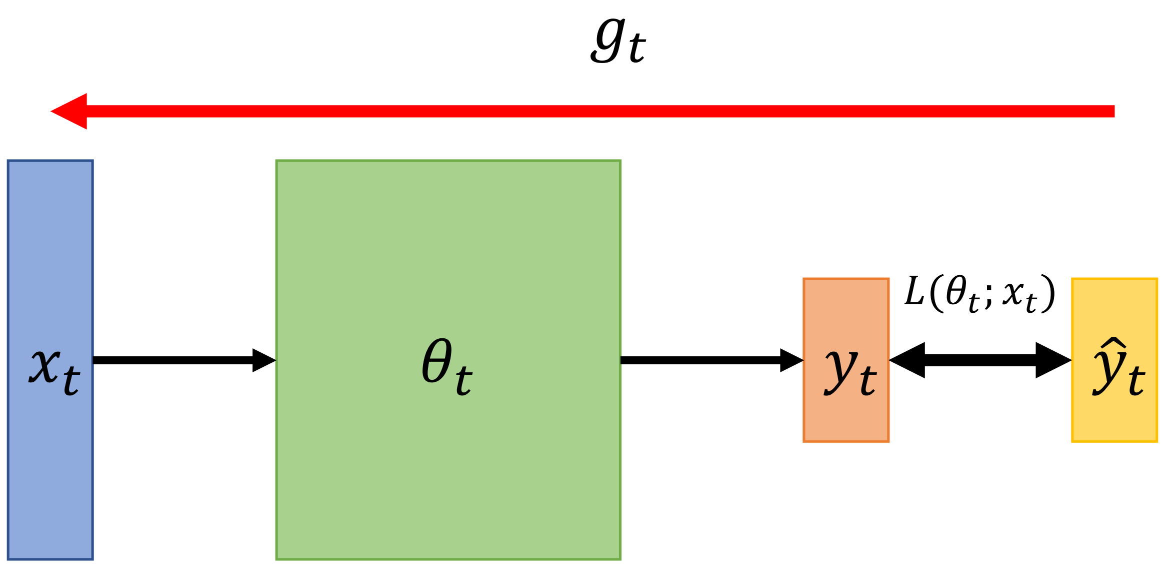
What is Optimization about?

- Find a θ to get the lowest $\sum_x L(\theta; x)$!!
- Or, Find a θ to get the lowest $L(\theta)$!!



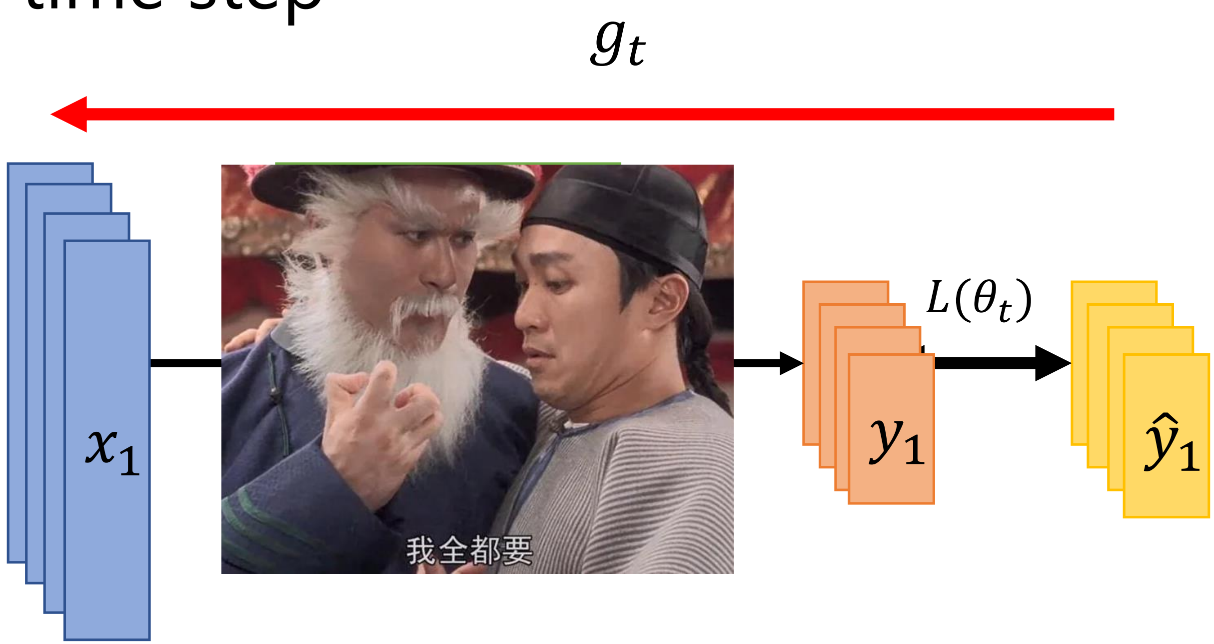
On-line vs Off-line

- On-line：one pair of $(x_t, \hat{y}_t)$ at a time step



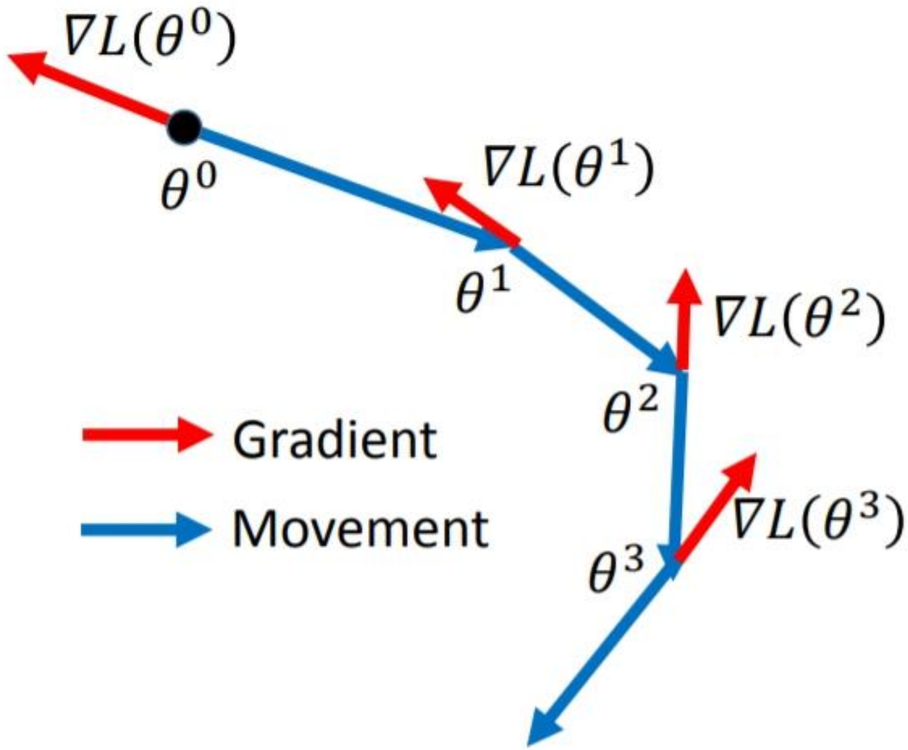
On-line vs Off-line

- Off-line：pour all $(x_t, \hat{y}_t)$ into the model at every time step



- The rest of this lecture will focus on the off-line cases

SGD



Start at position θ^0

Compute gradient at θ^0

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

Compute gradient at θ^1

Move to $\theta^2 = \theta^1 - \eta\nabla L(\theta^1)$

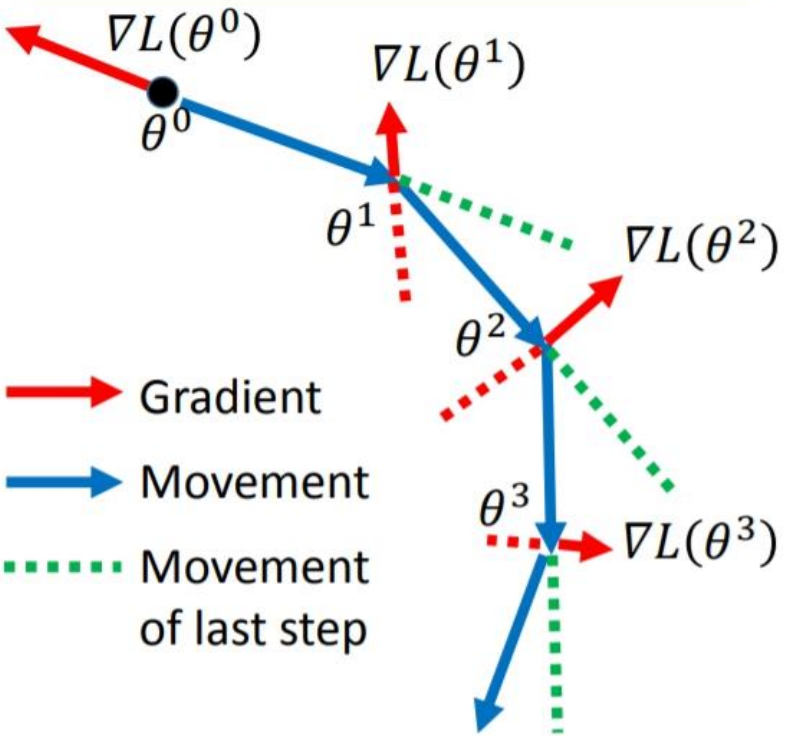
⋮

Stop until $\nabla L(\theta^t) \approx 0$

Credit to 李宏毅老師上課投影片

SGD with Momentum(SGDM)

Movement: movement of last step minus gradient at present



Start at point θ^0

Movement $v^0=0$

Compute gradient at θ^0

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

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

Compute gradient at θ^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.

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SGD with Momentum(SGDM)

v^i is actually the weighted sum of all the previous gradient: $\nabla L(\theta^0), \nabla L(\theta^1), \dots \nabla L\left(\theta^{i-1}\right)$

$$v^0 = 0$$

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

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

Start at point θ^0

Movement $v^0=0$

Compute gradient at θ^0

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

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

Compute gradient at θ^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.

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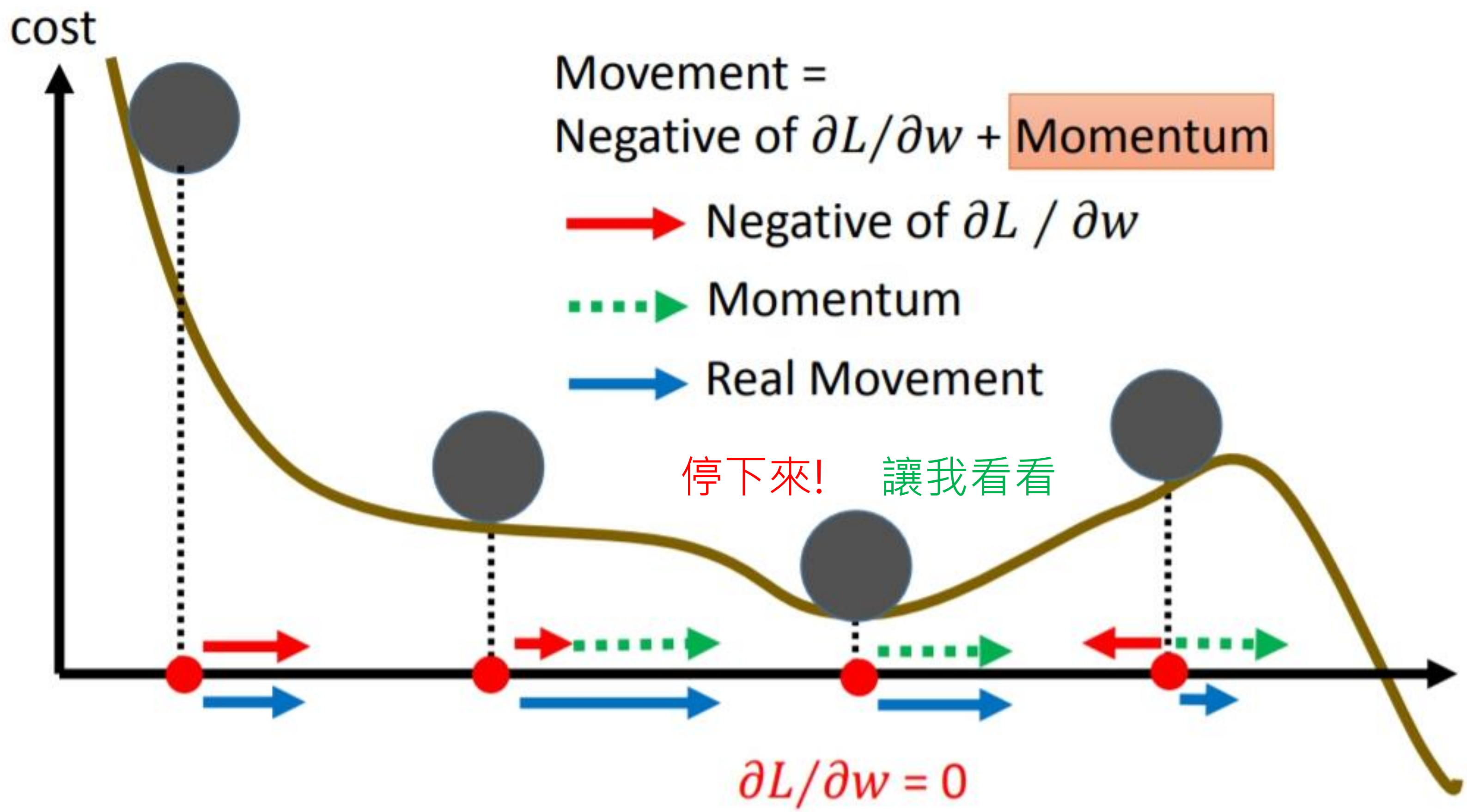
Why momentum?



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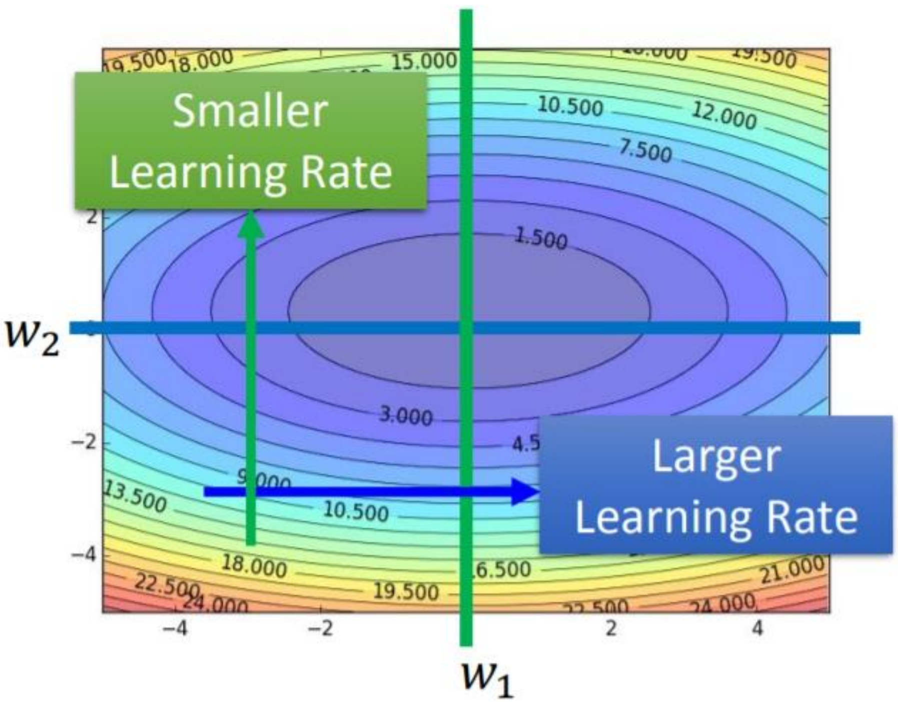
Adagrad

$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{\sum_{i=0}^{t-1}(g_i)^2}} g_{t-1}$$



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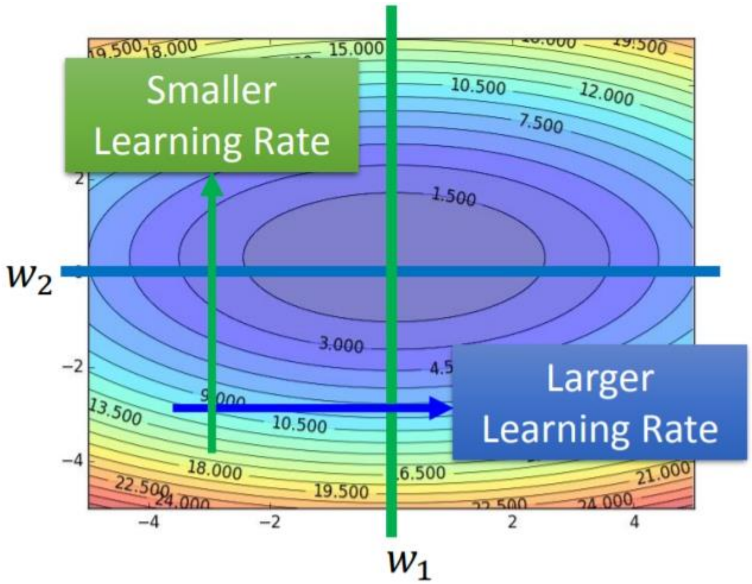
What if the gradients at the first few time steps are extremely large…

RMSProp

$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{v_t}} g_{t-1}$$

$$v_1 = {g_0}^2$$

$$v_t = \alpha v_{t-1} + (1-\alpha)(g_{t-1})^2$$



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Exponential moving average (EMA) of squared gradients is not monotonically increasing

Adam

- SGDM

$$\theta_t = \theta_{t-1} - \eta m_t$$
$$m_t = \beta_1 m_{t-1} + (1-\beta_1) g_{t-1}$$

- RMSProp

$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{v_t}} g_{t-1}$$
$$v_1 = {g_0}^2$$
$$v_t = \beta_2 v_{t-1} + (1-\beta_2)(g_{t-1})^2$$

$$\boxed{\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{\hat{v}_t} + \varepsilon} \widehat{m}_t}$$

$$\widehat{m}_t = \frac{m_t}{1-{\beta_1}^t}$$
$$\hat{v}_t = \frac{v_t}{1-{\beta_2}^t}$$

de-biasing

$$\beta_1 = 0.9$$
$$\beta_2 = 0.999$$
$$\varepsilon = 10^{-8}$$

What you have known before?

- SGD [Cauchy, 1847]
- SGD with momentum [Rumelhart, et al., Nature'86]

Adaptive learning rate

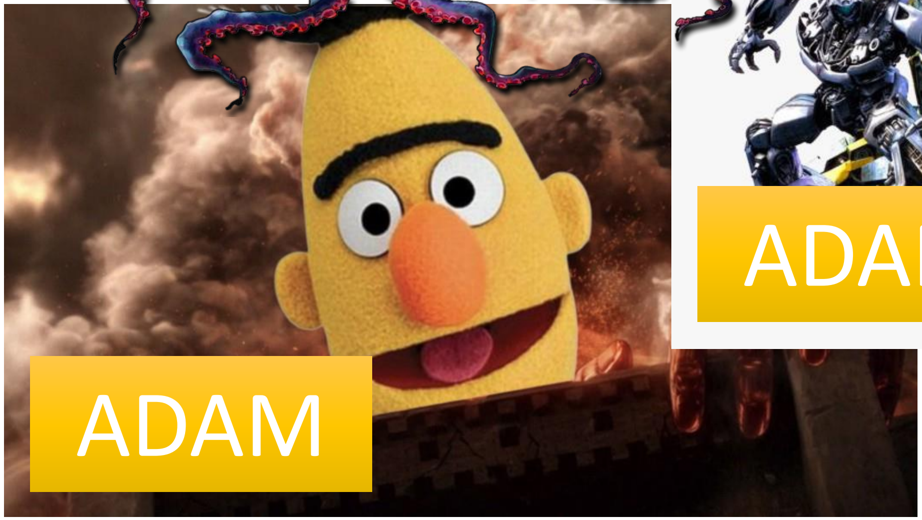
- Adagrad [Duchi, et al., JMLR'11]
- RMSProp [Hinton, et al., Lecture slides, 2013]
- Adam [Kingma, et al., ICLR'15]

Optimizers: Real Application

Transformer

Tacotron

BERT

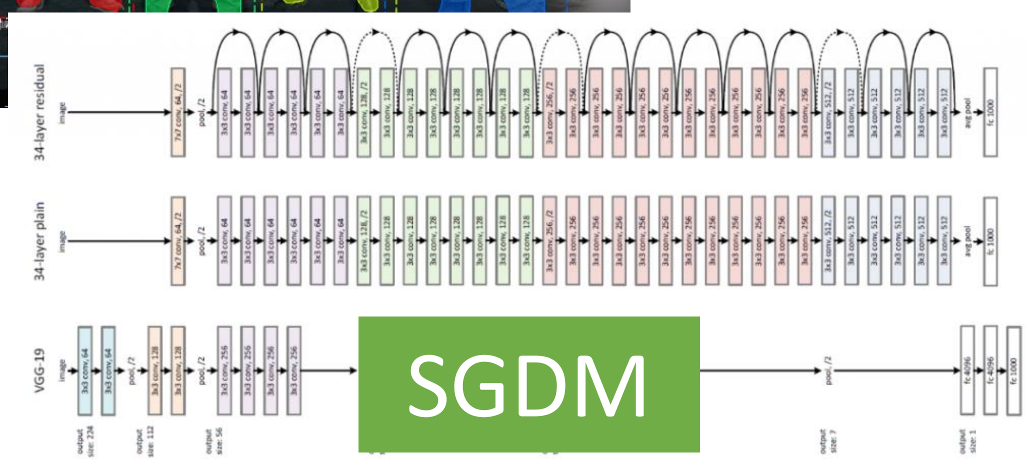


Optimizers: Real Application

Mask R-CNN

SGDM

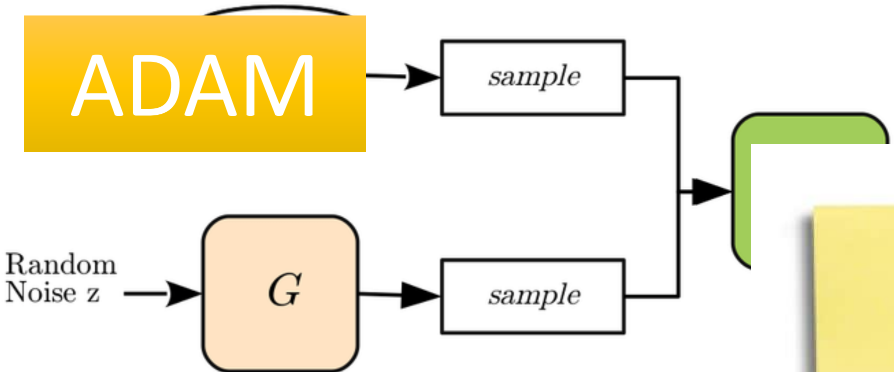
SGDM



SGDM

ResNet

Optimizers: Real Application



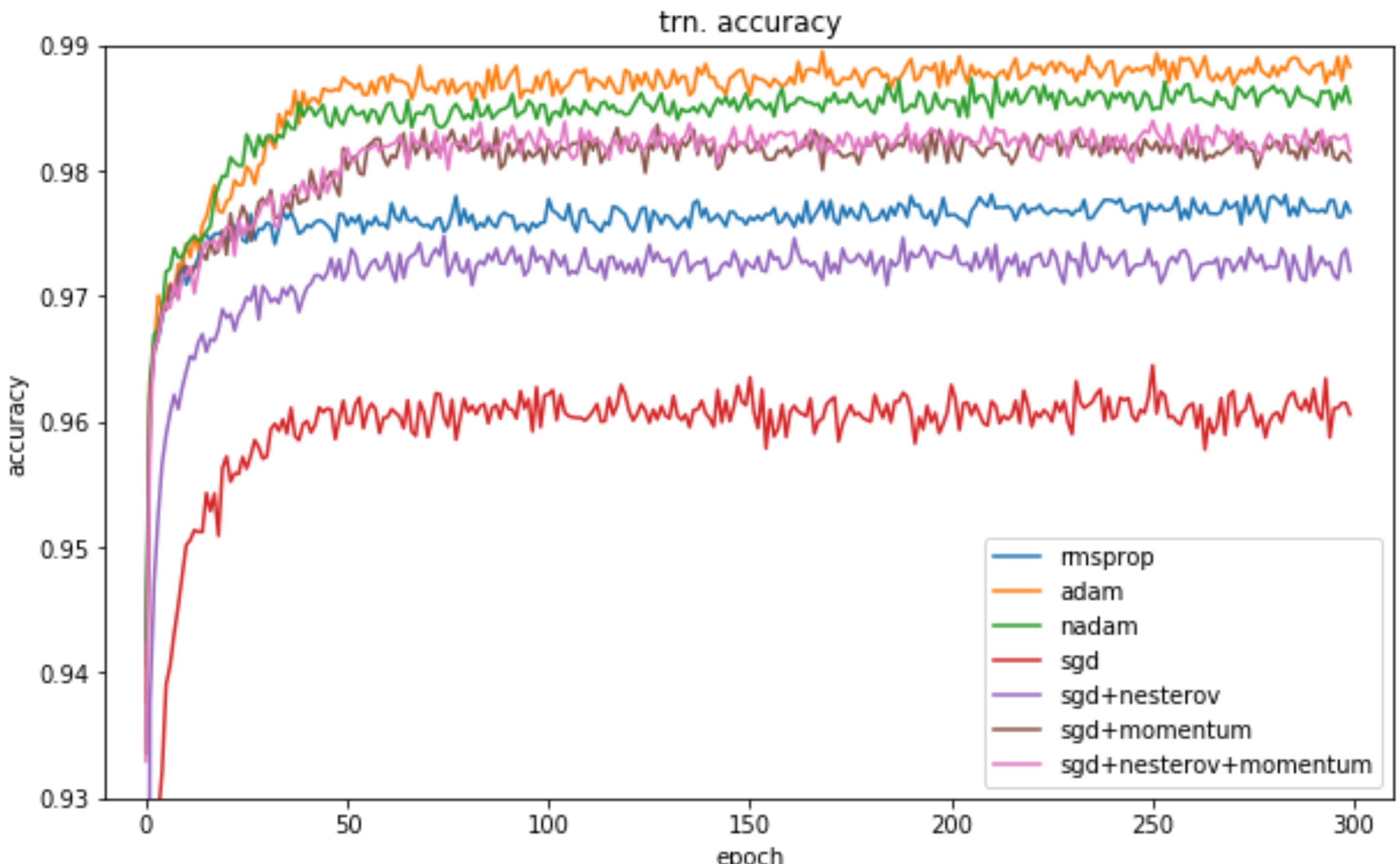
Big-GAN

MAML

Back to 2014…

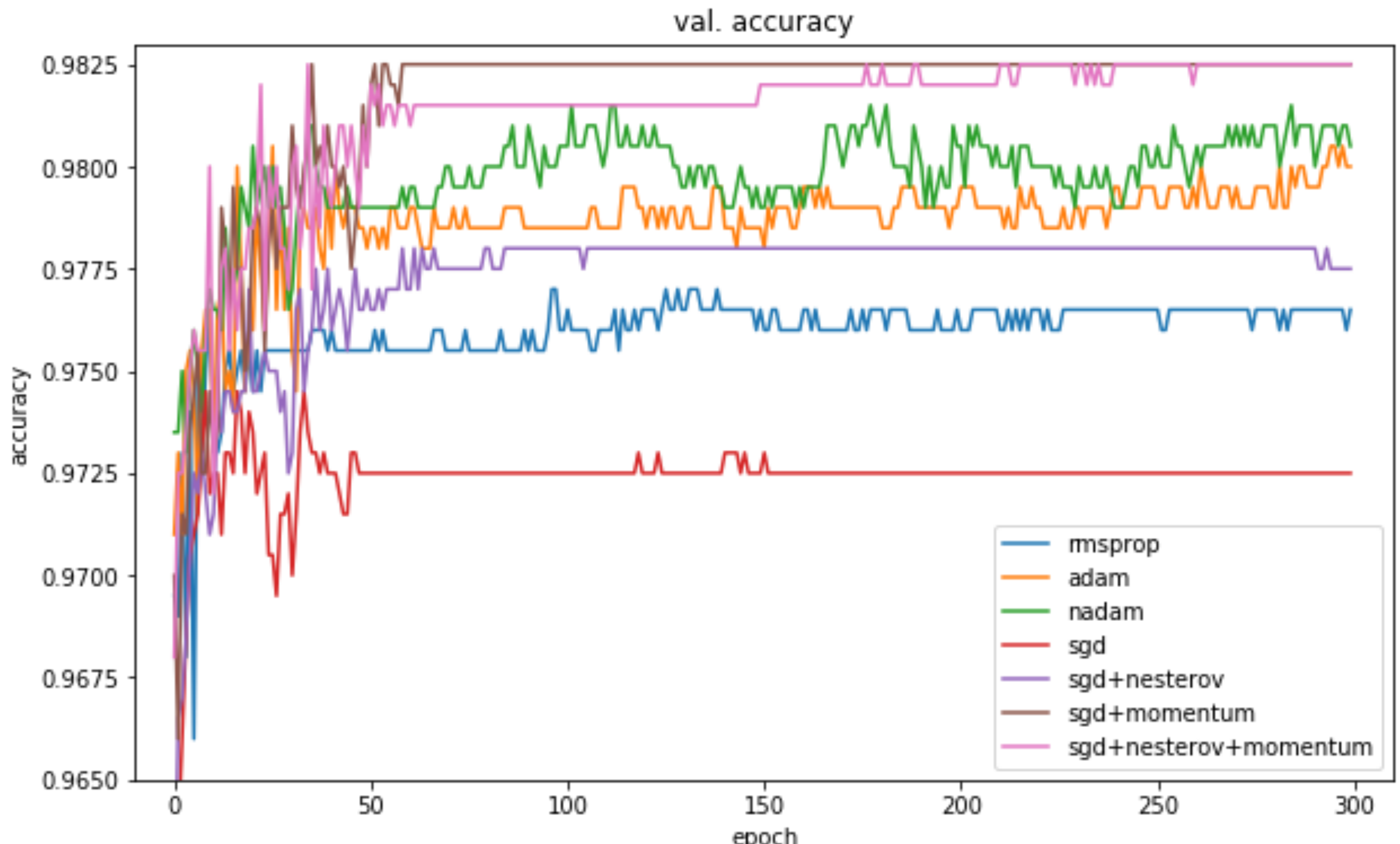
Back to 2014...

Adam vs SGDM



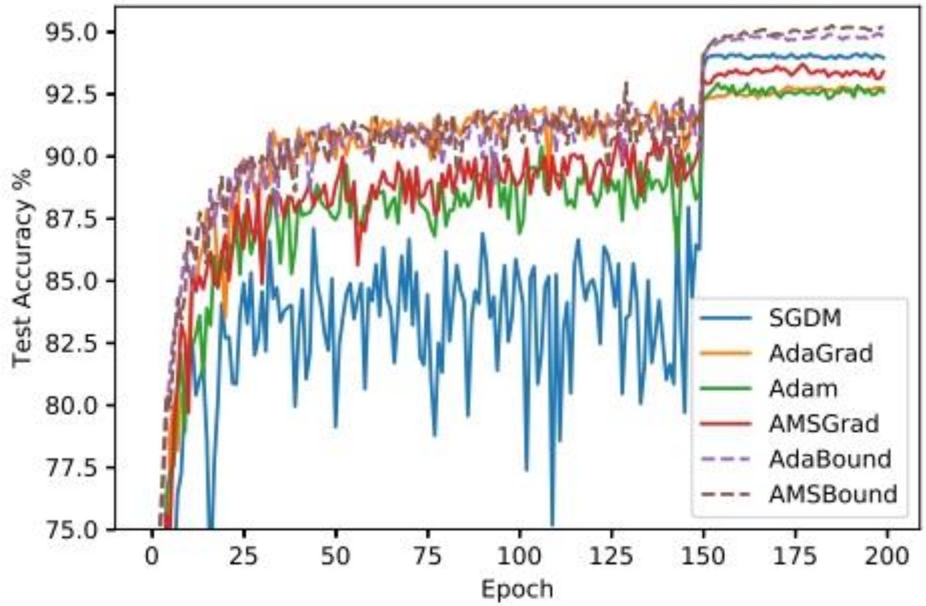
[Original article]

Adam vs SGDM



Original article

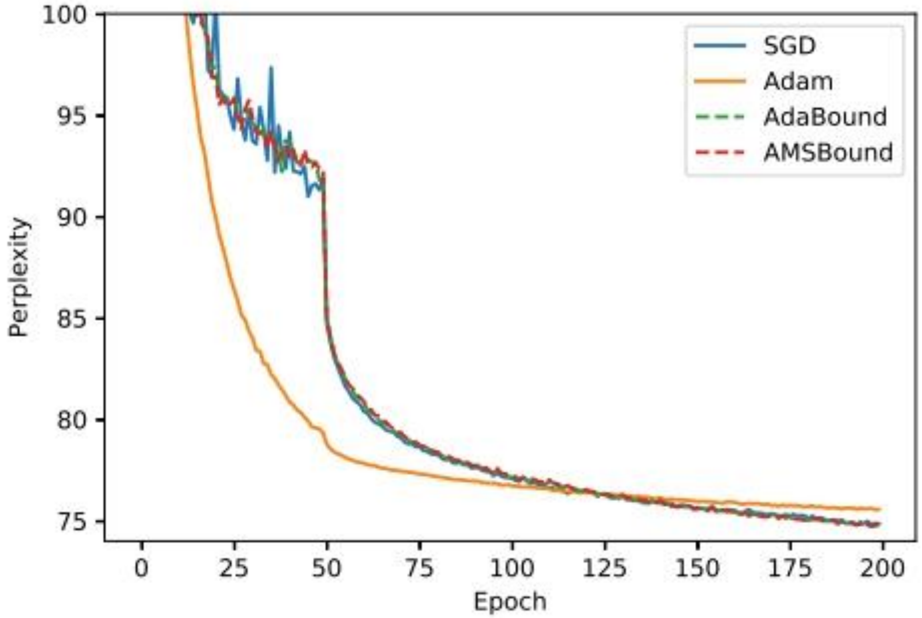
Adam vs SGDM



(d) Test Accuracy for ResNet-34

[Luo, et al., ICLR’19]

Adam vs SGDM



(a) L1: 1-Layer LSTM

[Luo, et al., ICLR'19]

Adam vs SGDM

- Adam：fast training, large generalization gap, unstable
- SGDM：stable, little generalization gap, better convergence(?)

An intuitive illustration for generalization gap

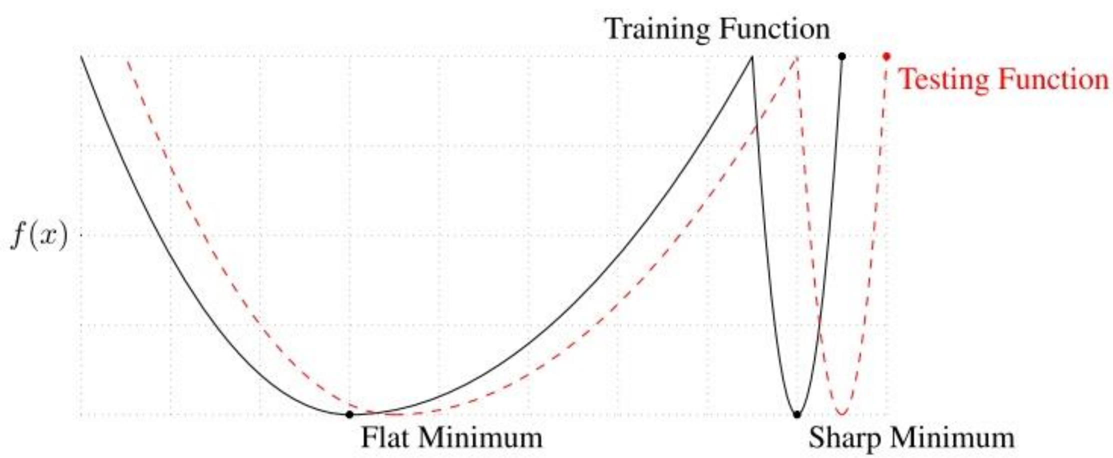
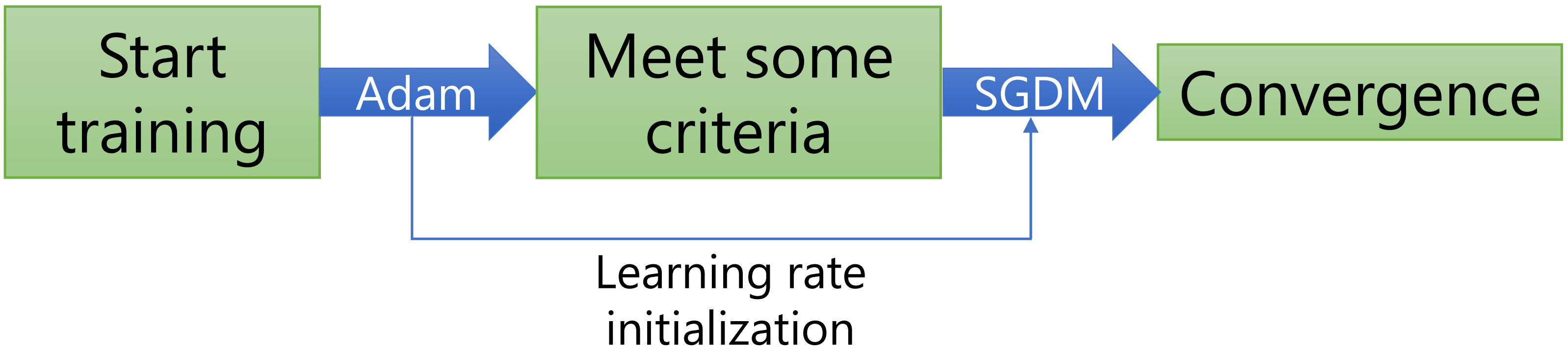


Figure 1: A Conceptual Sketch of Flat and Sharp Minima. The Y-axis indicates value of the loss function and the X-axis the variables (parameters)

Simply combine Adam with SGDM?

- SWATS [Keskar, et al., arXiv'17]

Begin with Adam(fast), end with SGDM



Towards Improving Adam…

- Trouble shooting

$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{\hat{v}_t + \varepsilon}} \hat{m}_t$$

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_{t-1}, \beta_1 = 0.$$

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2)(g_{t-1})^2, \beta_2 = 0.999$$

The "memory" of v_t keeps roughly 1000 steps!!

In the final stage of training, most gradients are small and non-informative, while some mini-batches provide large informative gradient rarely.

time step	…	100000	100001	100002	100003	…	100999	101000
gradient		1	1	1	1		100000	1
movement		η	η	η	η		$10\sqrt{10}\eta$	$10^{-3.5}\eta$

Towards Improving Adam…

- Trouble shooting

Maximum movement distance for one single update is roughly upper bounded by $\sqrt{\frac{1}{1-\beta_2}}\eta$

Non-informative gradients contribute more than informative gradients

time step	…	100000	100001	100002	100003	…	100999	101000
gradient		1	1	1	1		100000	1
movement		η	η	η	η		$10\sqrt{10}\eta$	$10^{-3.5}\eta$

1000η

Towards Improving Adam…

- AMSGrad [Reddi, et al., ICLR'18]

$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{\hat{v}_t + \varepsilon}} m_t$$

$$\hat{v}_t = \max(\hat{v}_{t-1}, v_t)$$

Reduce the influence of non-informative gradients

Remove de-biasing due to the max operation

Monotonically decreasing learning rate

Remember Adagrad vs RMSProp?

Towards Improving Adam…

- Trouble shooting

In the final stage of training, most gradients are small and non-informative, while some mini-batches provide large informative gradient rarely.

Learning rates are either extremely large(for small gradients) or extremely small(for large gradients).

Figure 1: Learning rates of sampled parameters. Each cell contains a value obtained by conducting a logarithmic operation on the learning rate. The lighter cell stands for the smaller learning rate.

Towards Improving Adam…

- AMSGrad only handles large learning rates
- AdaBound [Luo, et al., ICLR'19]

$$\theta_t = \theta_{t-1} - Clip\left(\frac{\eta}{\sqrt{\hat{v}_t + \varepsilon}}\right)\widehat{m}_t$$

$$Clip(x) = Clip\left(x, 0.1 - \frac{0.1}{(1-\beta_2)t + 1}, 0.1 + \frac{0.1}{(1-\beta_2)t}\right)$$

That's not "adaptive" at all…

Towards Improving SGDM…

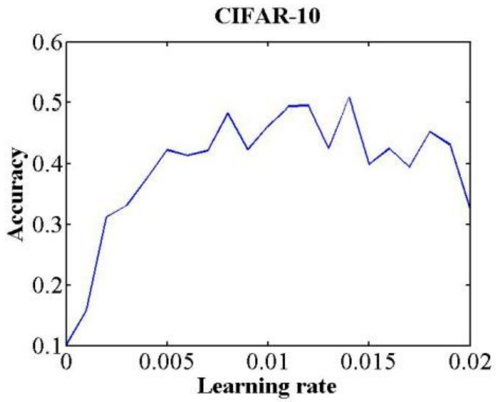
- Adaptive learning rate algorithms：dynamically adjust learning rate over time

- SGD-type algorithms：fix learning rate for all updates… too slow for small learning rates and bad result for large learning rates

There might be a “best” learning rate?

Towards Improving SGDM

- LR range test [Smith, WACV’17]



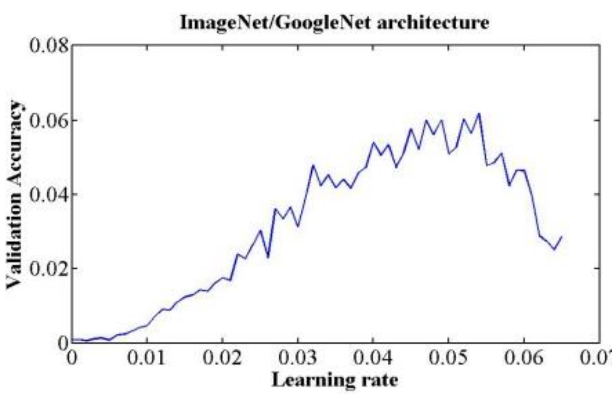


Figure 11. GoogleNet LR range test; validation classification accuracy as a function of increasing learning rate.

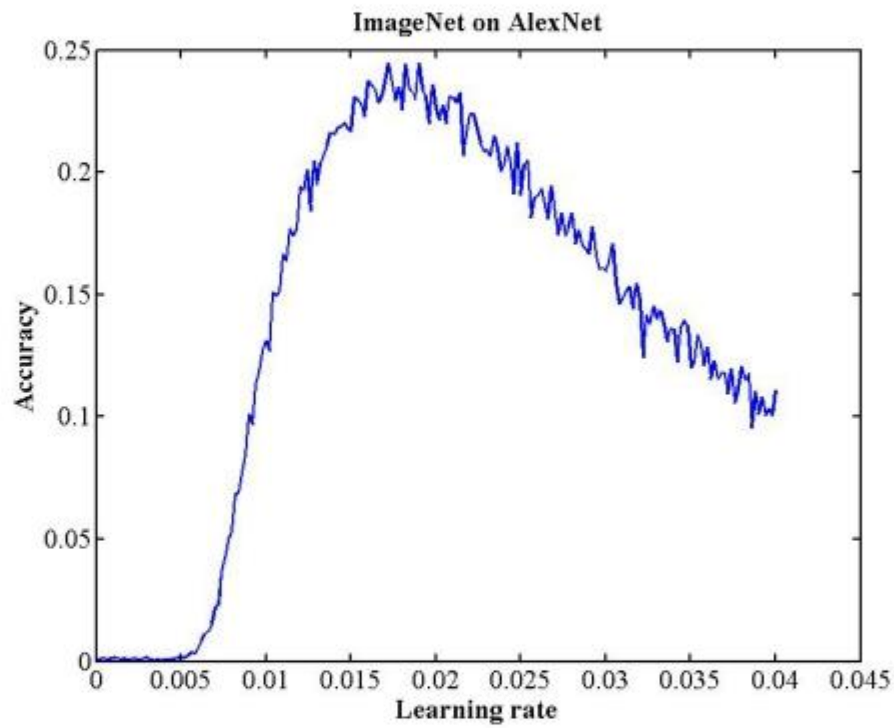
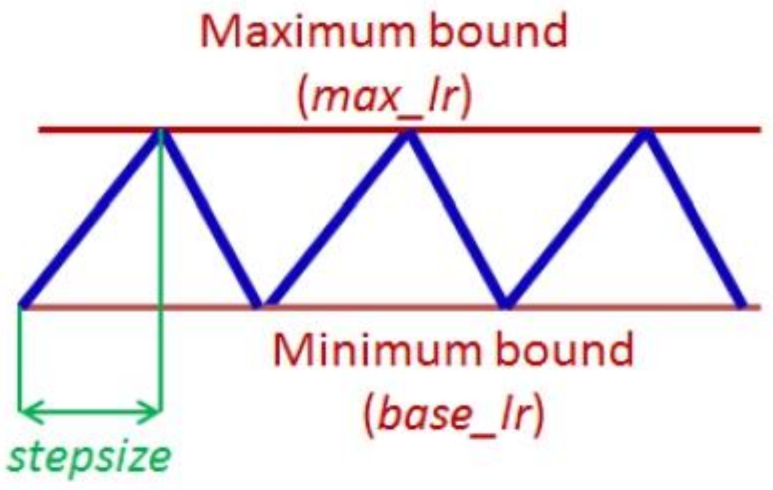


Figure 7. AlexNet LR range test; validation classification accuracy as a function of increasing learning rate.

Towards Improving SGDM

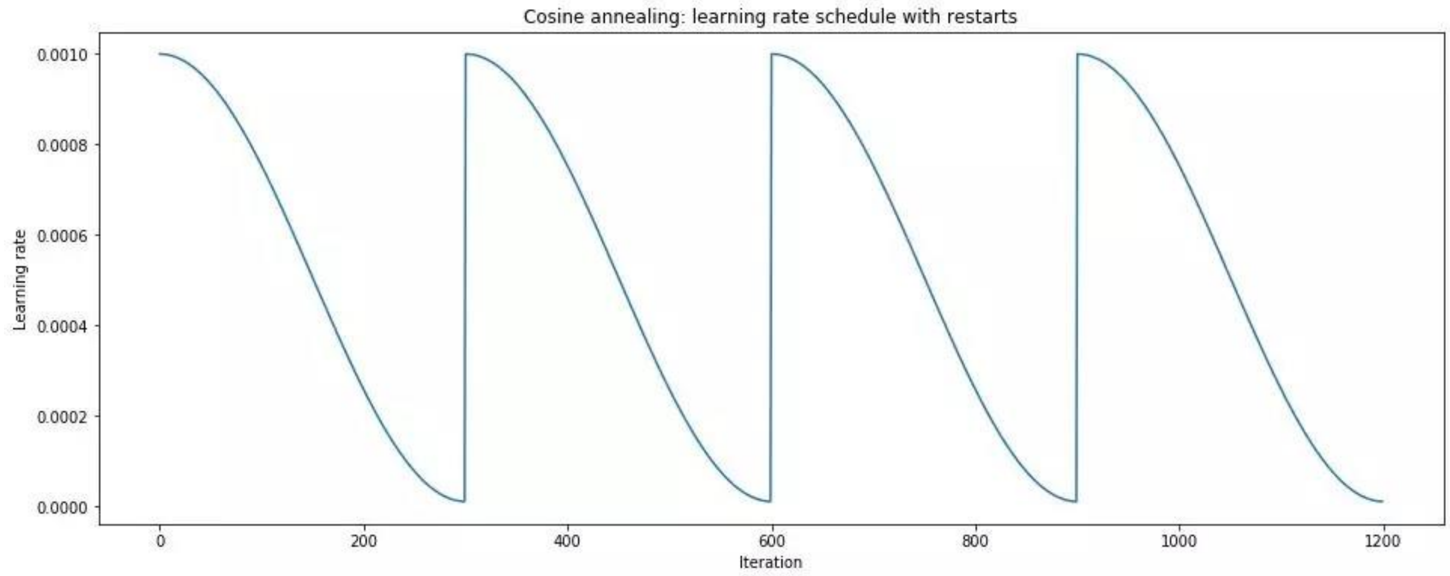
- Cyclical LR [Smith, WACV'17]
- learning rate：decide by LR range test
- stepsize：several epochs
- avoid local minimum by varying learning rate



The more exploration the better!

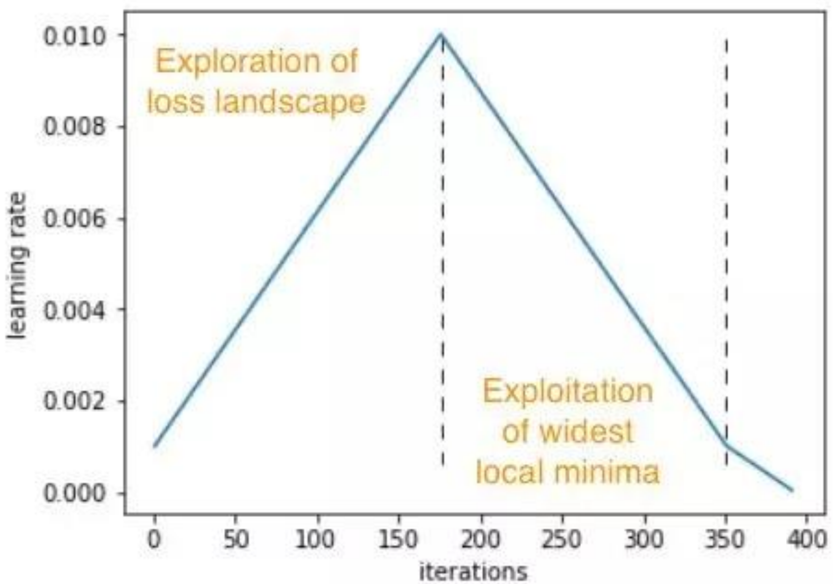
Towards Improving SGDM

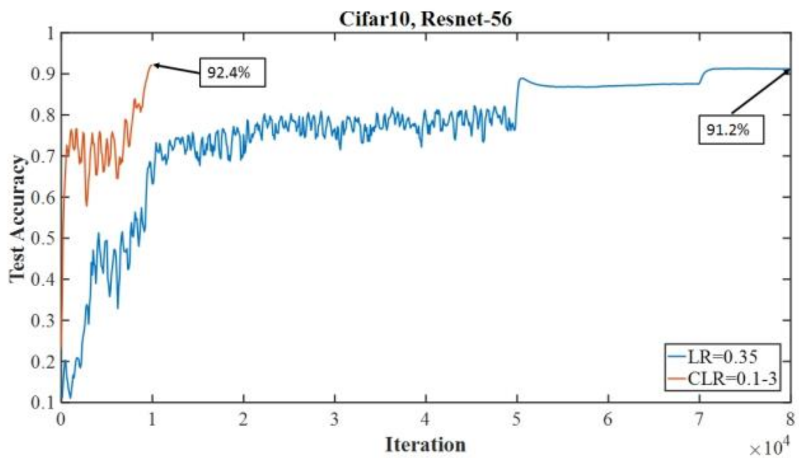
- SGDR [Loshchilov, et al., ICLR'17]



Towards Improving SGDM

- One-cycle LR [Smith, et al., arXiv'17]
  - warm-up + annealing + fine-tuning





(a) Comparison of test accuracies of super-convergence example to a typical (piecewise constant) training regime.

Does Adam need warm-up?

Of Course!

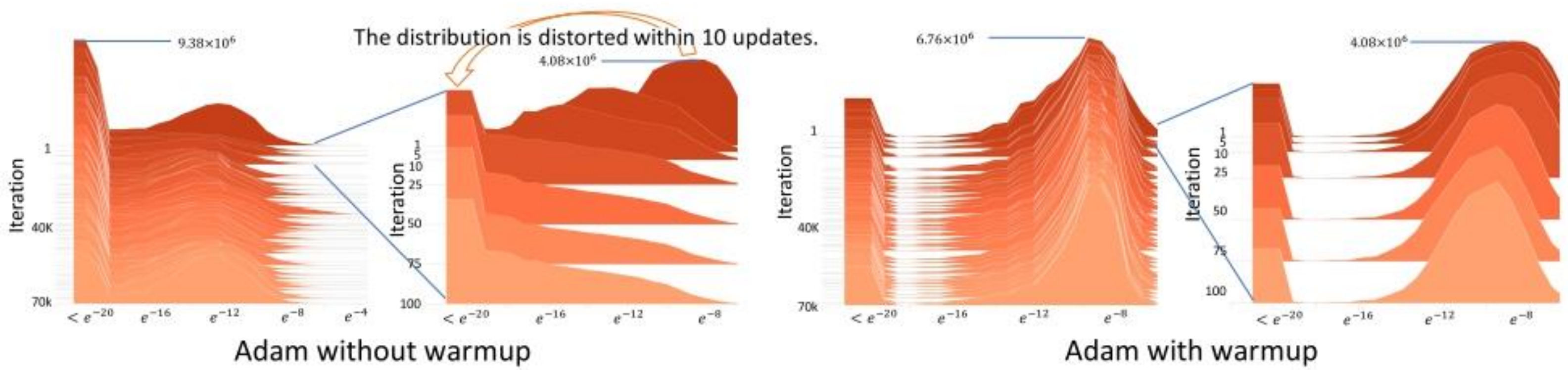


Figure 2: The absolute gradient histogram of the Transformers on the De-En IWSLT' 14 dataset during the training (stacked along the y-axis). X-axis is absolute value in the log scale and the height is the frequency. Without warmup, the gradient distribution is distorted in the first 10 steps.

Experiments show that the gradient distribution distorted in the first 10 steps

Does Adam need warm-up?

Distorted gradient

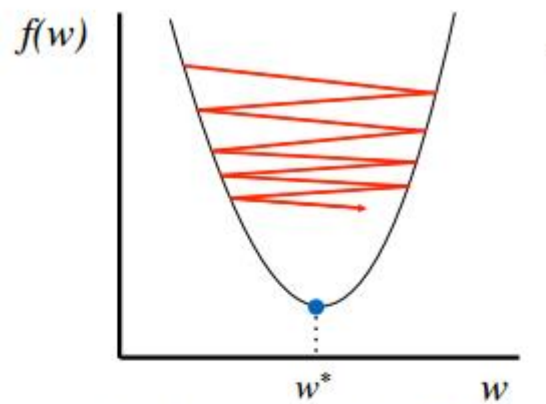
distorted EMA squared gradients

Bad learning rate

$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{\hat{v}_t + \varepsilon}} \widehat{m}_t$$

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2)(g_{t-1})^2$$

Keep your step size small at the beginning of training helps to reduce the variance of the gradients



Too big: overshoot and even diverge

Does Adam need warm-up?

- RAdam [Liu, et al., ICLR'20]

$$\rho_t = \rho_\infty - \frac{2t{\beta_2}^t}{1 - {\beta_2}^t}$$

effective memory size of EMA

$$\rho_\infty = \frac{2}{1 - \beta_2} - 1$$

max memory size ($t \rightarrow \infty$)

$$r_t = \sqrt{\frac{\rho_t - 4)(\rho_t - 2)\rho_\infty}{(\rho_\infty - 4)(\rho_\infty - 2)\rho_t}}$$

approximated $\frac{Var[\frac{1}{\hat{v}_\infty}]}{Var[\frac{1}{\hat{v}_t}]}$ (for ρ_t>4)

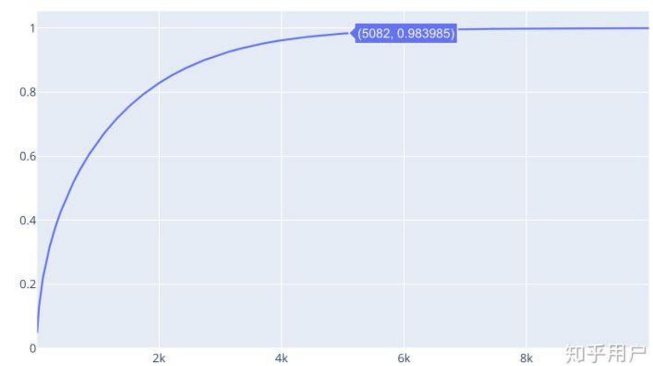
<u>When $\rho_t \leq 4$</u> (first few steps of training)

$$\theta_t = \theta_{t-1} - \eta \hat{m}_t$$

<u>When $\rho_t > 4$</u>

$$\theta_t = \theta_{t-1} - \frac{\eta r_t}{\sqrt{\hat{v}_t + \varepsilon}} \hat{m}_t$$

r_t is increasing through time!



RAdam vs SWATS

	RAdam	SWATS
Inspiration	Distortion of gradient at the beginning of training results in inaccurate adaptive learning rate	non-convergence and generalization gap of Adam, slow training of SGDM
How?	Apply warm-up learning rate to reduce the influence of inaccurate adaptive learning rate	Combine their advantages by applying Adam first, then SGDM
Switch	SGDM to RAdam	Adam to SGDM
Why switch	The approximation of the variance of $\hat{v}_t$ is invalid at the beginning of training	To pursue better convergence
Switch point	When the approximation becomes valid	Some human-defined criteria

k step forward, *1* step back

- Lookahead [Zhang, et al., arXiv'19]

universal wrapper for all optimizers

For $t = 1, 2, \ldots$ *(outer loop)*

$\theta_{t,0} = \phi_{t-1}$

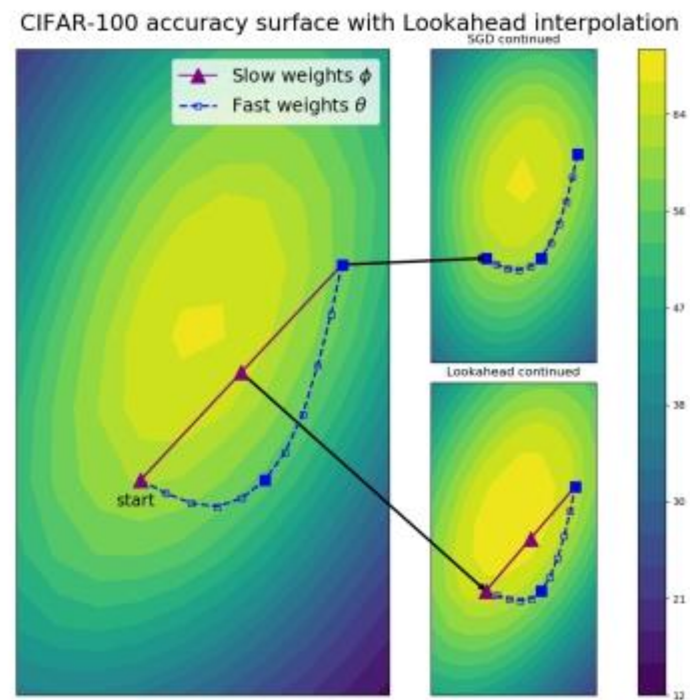
For $i = 1, 2, \ldots k$ *(inner loop)*

$\theta_{t,i} = \theta_{t,i-1} + Optim\left(Loss, data, \theta_{t,i-1}\right)$

$\phi_t = \phi_{t-1} + \alpha(\theta_{t,k} - \phi_{t-1})$

Similar to Reptile?

$Optim$ can be any optimizer.
E.g. Ranger= RAdam+Lookahead



k step forward, *1* step back

- Lookahead [Zhang, et al., arXiv'19]

1 step back: avoid too dangerous exploration

Look for a more flatten minimum

More stable

Better generalization

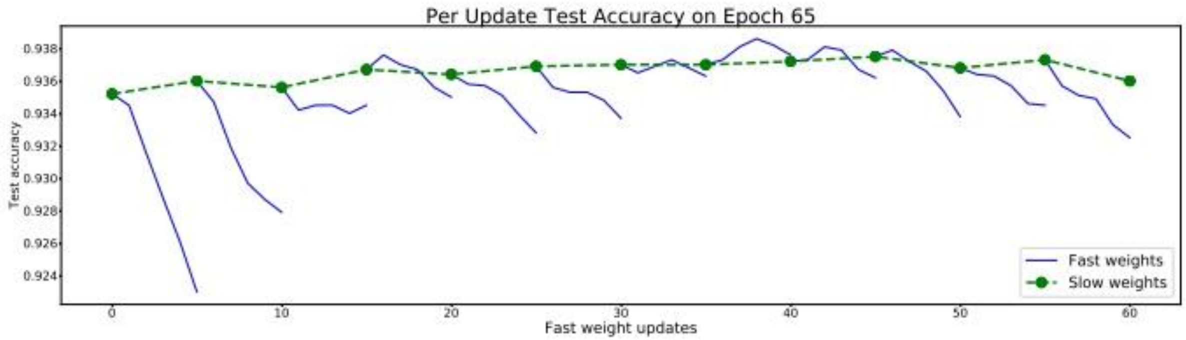
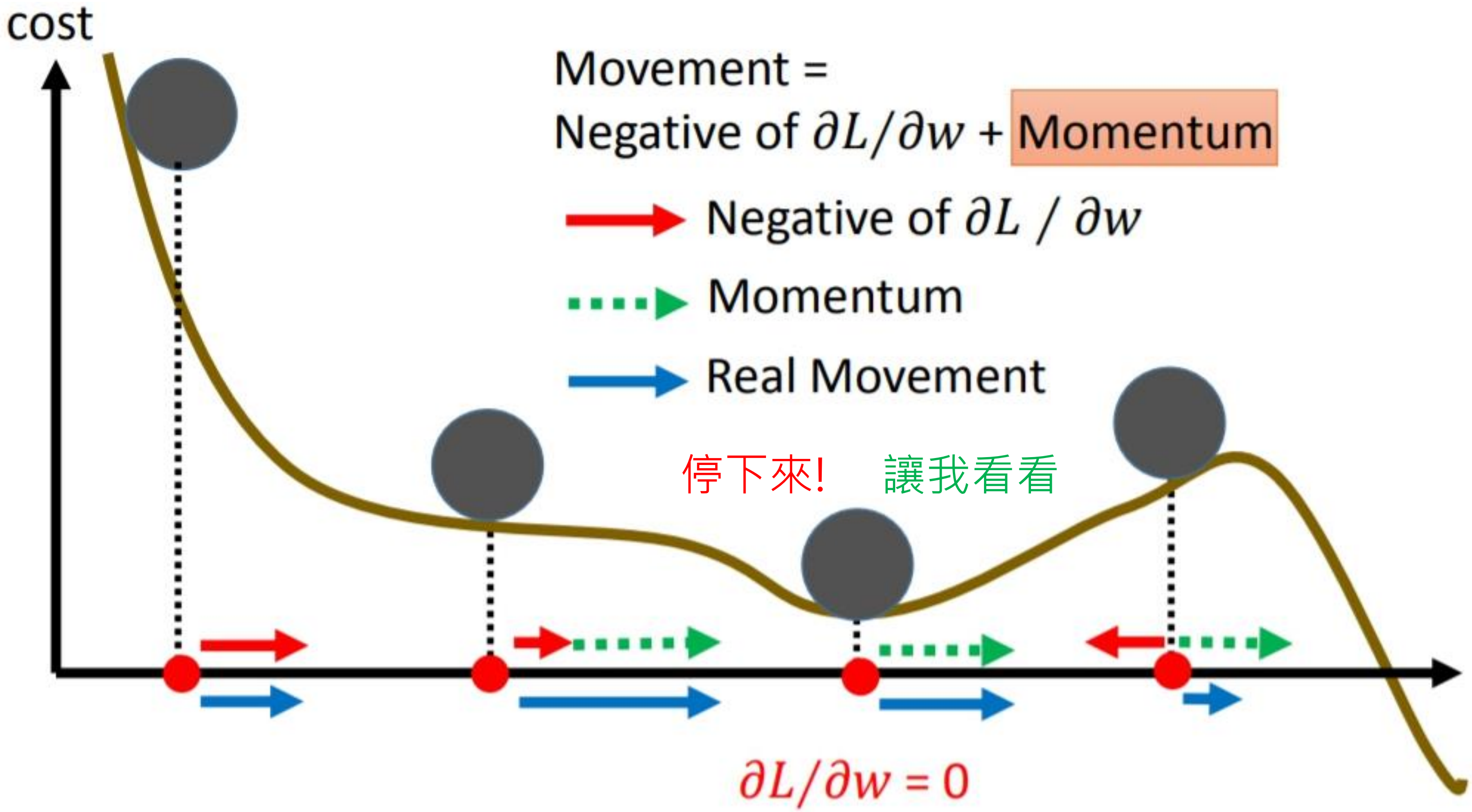


Figure 10: Visualizing Lookahead accuracy for 60 fast weight updates. We plot the test accuracy after every update (the training accuracy and loss behave similarly). The inner loop update tends to degrade both the training and test accuracy, while the interpolation recovers the original performance.

More than momentum…

- Momentum recap



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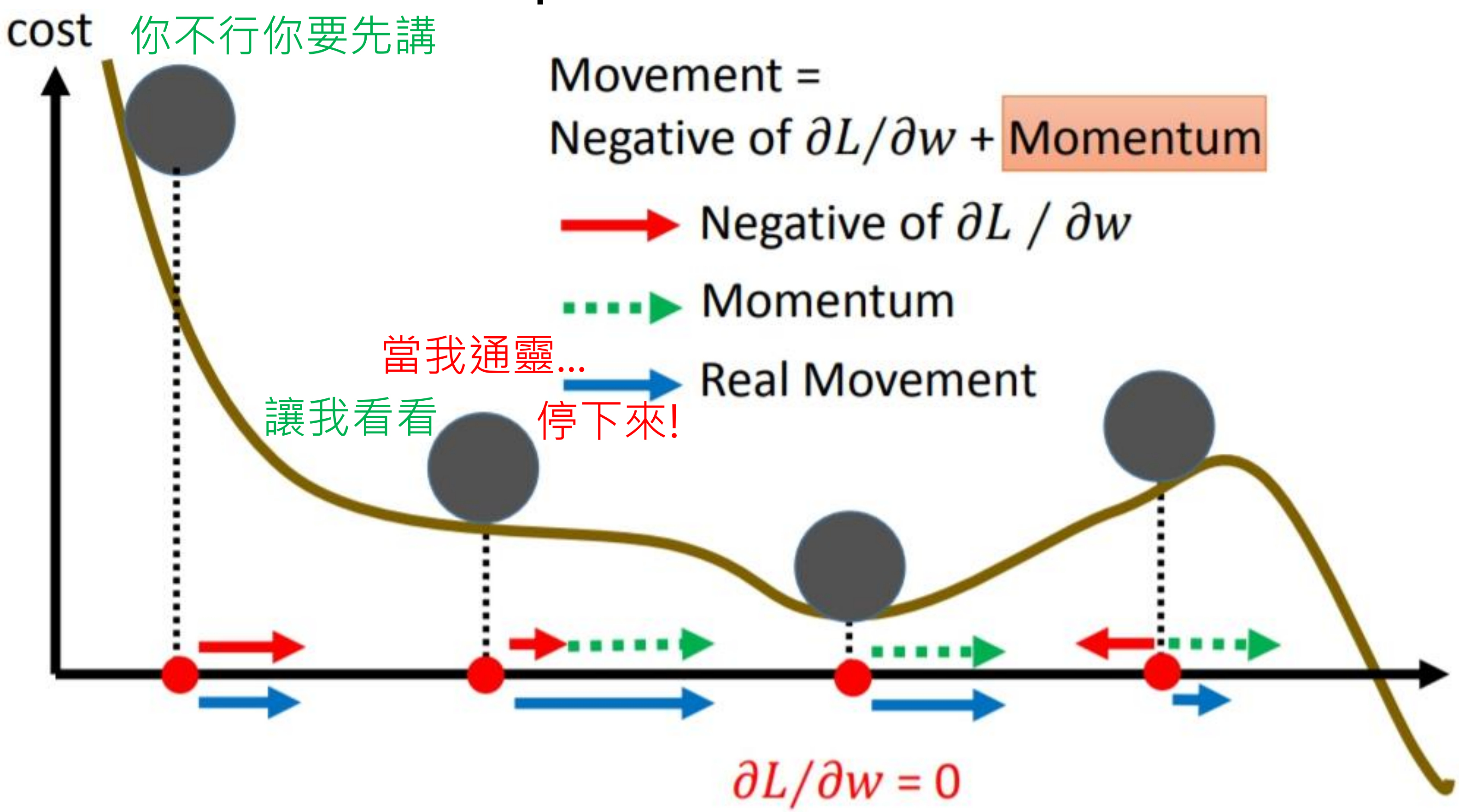
More than momentum…

- Momentum recap



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Can we look into the future?

- Nesterov accelerated gradient (NAG)

[Nesterov, jour Dokl. Akad. Nauk SSSR'83]

- SGDM

$$\theta_t = \theta_{t-1} - m_t$$
$$m_t = \lambda m_{t-1} + \eta \nabla L(\theta_{t-1})$$

Math Warning

- Look into the future...

$$\theta_t = \theta_{t-1} - m_t$$
$$m_t = \lambda m_{t-1} + \eta \nabla L(\theta_{t-1} - \lambda m_{t-1})$$

Need to maintain a duplication of model parameters?

Can we look into the future?

- Nesterov accelerated gradient (NAG)

$$\theta_t = \theta_{t-1} - m_t$$
$$m_t = \lambda m_{t-1} + \eta \nabla L(\theta_{t-1} - \lambda m_{t-1})$$

$$\begin{aligned} Let\ \theta_t{}' &= \theta_t - \lambda m_t \\ &= \theta_{t-1} - m_t - \lambda m_t \\ &= \theta_{t-1} - \lambda m_t - \lambda m_{t-1} - \eta \nabla L(\theta_{t-1} - \lambda m_{t-1}) \\ &= \theta_{t-1}{}' - \lambda m_t - \eta \nabla L(\theta_{t-1}{}') \end{aligned}$$
$$m_t = \lambda m_{t-1} + \eta \nabla L(\theta_{t-1}{}')$$

No need to maintain a duplication of model parameters

你也懂超前部署？

- SGDM

$$\theta_t = \theta_{t-1} - m_t$$
$$m_t = \lambda m_{t-1} + \eta \nabla L(\theta_{t-1})$$

or

$$\theta_t = \theta_{t-1} - \lambda m_{t-1} - \eta \nabla L(\theta_{t-1})$$
$$m_t = \lambda m_{t-1} + \eta \nabla L(\theta_{t-1})$$

Adam in the future

- Nadam [Dozat, ICLR workshop'16]

$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{\hat{v}_t + \varepsilon}} \hat{m}_t$$

$$\hat{m}_t = \frac{\beta_1 m_t}{1 - {\beta_1}^{t+1}} + \frac{(1 - \beta_1) g_{t-1}}{1 - {\beta_1}^{t}}$$

- SGDM

$$\hat{m}_t = \frac{1}{1 - {\beta_1}^{t}} (\beta_1 m_{t-1} + (1 - \beta_1) g_{t-1})$$

$$= \frac{\beta_1 m_{t-1}}{1 - {\beta_1}^{t}} + \frac{(1 - \beta_1) g_{t-1}}{1 - {\beta_1}^{t}}$$

Do you really know your optimizer?

- A story of L2 regularization…

$$L_{l_2}(\theta) = L(\theta) + \gamma||\theta||^2$$

SGD

$$\begin{aligned}\theta_t &= \theta_{t-1} - \nabla L_{l_2}(\theta_{t-1})\\ &= \theta_{t-1} - \nabla L(\theta_{t-1}) - \gamma\theta_{t-1}\end{aligned}$$

SGDM

$$\theta_t = \theta_{t-1} - \lambda m_{t-1} - \eta(\nabla L(\theta_{t-1}) + \gamma\theta_{t-1})$$
$$m_t = \lambda m_{t-1} + \eta(\nabla L(\theta_{t-1}) + \gamma\theta_{t-1}) \ ?$$
$$m_t = \lambda m_{t-1} + \eta(\nabla L(\theta_{t-1})) \ ?$$

Adam

$$m_t = \lambda m_{t-1} + \eta(\nabla L(\theta_{t-1}) + \gamma\theta_{t-1}) \ ?$$
$$v_t = \beta_2 v_{t-1} + (1 - \beta_2)(\nabla L(\theta_{t-1}) + \gamma\theta_{t-1})^2 \ ?$$

Do you really know your optimizer?

- AdamW & SGDW with momentum [Loshchilov, arXiv'17]

SGDWM

$$\theta_t = \theta_{t-1} - m_t - \gamma\theta_{t-1}$$
$$m_t = \lambda m_{t-1} + \eta(\nabla L(\theta_{t-1}))$$

AdamW

$$m_t = \beta_1 m_{t-1} + (1-\beta_1)\nabla L(\theta_{t-1})$$
$$v_t = \beta_2 v_{t-1} + (1-\beta_2)(\nabla L(\theta_{t-1}))^2$$
$$\theta_t = \theta_{t-1} - \eta(\frac{1}{\sqrt{\hat{v}_t}+\varepsilon}\hat{m}_t + \gamma\theta_{t-1})$$

L2 regularization or weight decay?

Something helps optimization…

- Shuffling
- Dropout
- Gradient noise [Neelakantan, et al., arXiv'15]

$$g_{t,i} = g_{t,i} + N(0, {\sigma_t}^2)$$

$$\sigma_t = \frac{c}{(1+t)^{\gamma}}$$

The more exploration, the better!

Something helps optimization…

- Warm-up
- Curriculum learning [Bengio, et al., ICML'09]

  Train your model with easy data(e.g. clean voice) first, then difficult data.

  Perhaps helps to improve generalization
- Fine-tuning

Teach your model patiently!

Something helps optimization…

- Normalization

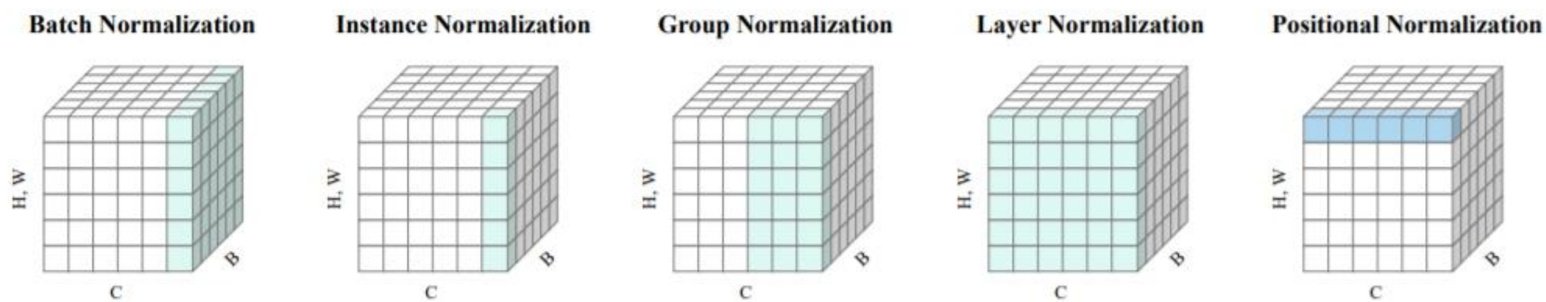

Figure 2: Positional Normalization together with previous normalization methods. In the figure, each subplot shows a feature map tensor, with B as the batch axis, C as the channel axis, and (H, W) as the spatial axis. The entries colored in green or blue (ours) are normalized by the same mean and standard deviation. Unlike previous methods, our method processes each position independently, and compute both statistics across the channels.

- Regularization

What we learned today?

Team SGD	Team Adam
• SGD • SGDM • Learning rate scheduling • NAG • SGDWM	• Adagrad • RMSProp • Adam • AMSGrad • AdaBound • Learning rate scheduling • RAdam • Nadam • AdamW

Extreme values of learning rate

SWATS

Lookahead

What we learned today?

SGDM	Adam
• Slow	• Fast
• Better convergence	• Possibly non-convergence
• Stable	• Unstable
• Smaller generalization gap	• Larger generalization gap

Advices

SGDM	Adam
• Computer vision image classification segmentation object detection	• NLP QA machine translation summary • Speech synthesis • GAN • Reinforcement learning

Universal Optimizer?

No Way!!!

What I think I am going to learn in this class

What I actually learned in this class

Reference

- [Ruder, arXiv'17] Sebastian Ruder, "An Overview of Gradient Descent Optimization Algorithms", arXiv, 2017
- [Rumelhart, et al., Nature'86] David E. Rumelhart, Geoffrey E. Hinton and Ronald J. Williams, "Learning Representations by Back-Propagating Errors", Nature, 1986
- [Duchi, et al., JMLR'11] John Duchi, Elad Hazan and Yoram Singer, "Adaptive Subgradient Methods for Online Learning and Stochastic Optimization", JMLR, 2011
- [Hinton, et al., Lecture slides, 2013] Geoffrey Hinton, Nitish Srivastava and Kevin Swersky, "RMSProp", Lecture slides, 2013
- [Kingma, et al., ICLR'15] Diederik P. Kingma and Jimmy Ba, "A Method for Stochastic Optimization", ICLR, 2015

Reference

- [Keskar, et al., arXiv'17] Nitish Shirish Keskar and Richard Socher, "Improving Generalization Performance by Switching from Adam to SGD", arXiv, 2017
- [Reddi, et al., ICLR'18] Sashank J. Reddi, Satyen Kale and Sanjiv Kumar, "On the Convergence of Adam and Beyond", ICLR, 2018
- [Luo, et al., ICLR'19] Liangchen Luo, Yuanhao Xiong, Yan Liu and Xu Sun, "Adaptive Gradient Methods with Dynamic Bound of Learning Rate", ICLR, 2019
- [Smith, WACV'17] Leslie N. Smith, "Cyclical Learning Rates for Training Neural Networks", WACV, 2017
- [Loshchilov, et al., ICLR'17] Ilya Loshchilov and Frank Hutter, "SGDR: Stochastic Gradient Descent with Warm Restarts", ICLR, 2017

Reference

- [Smith, et al., arXiv'17] Leslie N. Smith and Nicholay Topin, "Super-Convergence: Very Fast Training of Neural Networks Using Large Learning Rates", arXiv, 2017
- [Liu, et al., ICLR'20] Liyuan Liu, Haoming Jiang, Pengcheng He, Weizhu Chen, Xiaodong Liu, Jianfeng Gao and Jiawei Han, "On the Variance of the Adaptive Learning Rate and Beyond", ICLR, 2020
- [Zhang, et al., arXiv'19] Michael R. Zhang, James Lucas, Geoffrey Hinton and Jimmy Ba, "Lookahead Optimizer: k Step Forward, 1 Step Back", arXiv, 2019
- [Nesterov, jour Dokl. Akad. Nauk SSSR'83] Yu. E. Nesterov, "A Method of Solving a Convex Programming Problem with Convergence Rate O(1/k^2)""

Reference

- [Dozat, ICLR workshop’16] Timothy Dozat, “Incorporating Nesterov Momentum into Adam”, ICLR workshop, 2016
- [Loshchilov, arXiv’17] Ilya Loshchilov and Frank Hutter, “Fixing Weight Decay Regularization in Adam”, arXiv, 2017
- [Neelakantan, et al., arXiv’15] Arvind Neelakantan, Luke Vilnis, Quoc V. Le, Ilya Sutskever, Lukasz Kaiser, Karol Kurach and James Martens, “Adding Gradient Noise Improves Learning for Very Deep Networks”, arXiv, 2015
- [Bengio, et al., ICML’09] Yoshua Bengio, Jèrôme Louradour, Ronan Collobert and Jason Weston, “Curriculum Learning”, ICML, 2015