Stochastic Gradient Descent

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Motivation

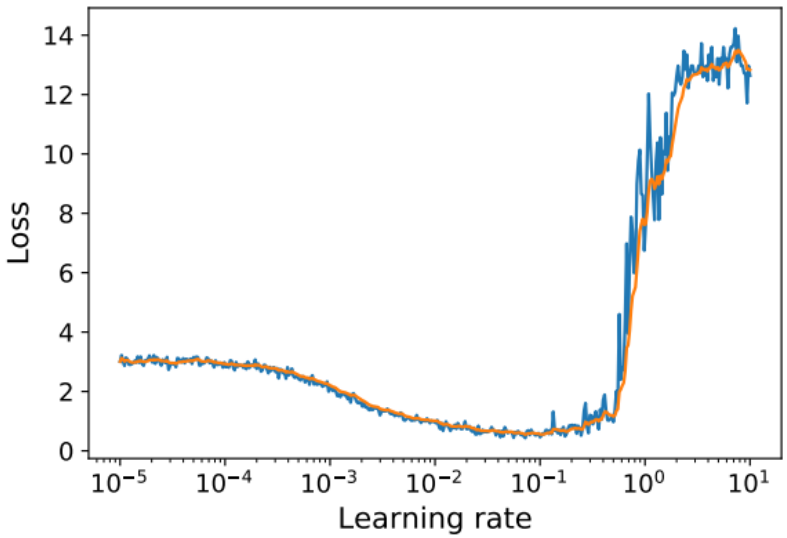


Figure 8.17: Loss vs learning rate (horizontal axis). Training loss vs learning rate for a small MLP fit to FashionMNIST using vanilla SGD. (Raw loss in blue, EWMA smoothed version in orange). Generated by lrschedule_tf.ipynb.

One heuristic

- Start with a small learning rate and gradually increase it, evaluating performance using a small number of minibatches.
- In practice, it is better to pick a rate that is slightly smaller than (i.e., to the left of) the one with the lowest loss, to ensure stability.

Learning rate schedule

- Definition:
  Learning rate schedule: Adjust the step size over time.
- Sufficient Condition for convergence:
  Robbins-Monro conditions[1]:

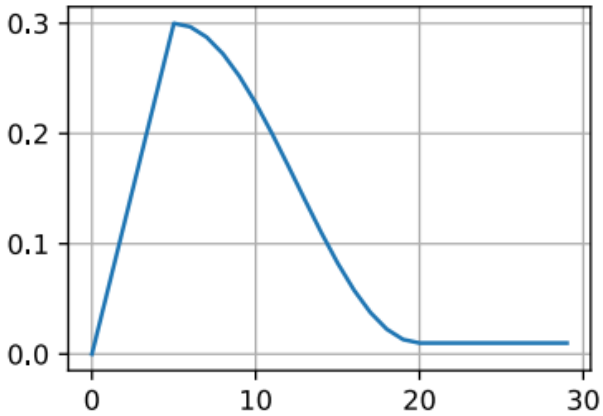
$$\eta_t \to 0, \frac{\sum_{t=1}^{\infty} \eta_t^2}{\sum_{t=1}^{\infty} \eta_t} \to 0$$

- Examples
  - piecewise constant $\eta_t = \eta_i$ if $t_i \leq t \leq t_{i+1}$
    - Step decay
    - Reduce-on-plateau
  - exponential decay $\eta_t = \eta_0 e^{-\lambda t}$
  - polynomial decay $\eta_t = \eta_0 (\beta t + 1)^{-\alpha}$
    - square-root schedule: $\alpha = 0.5, \beta = 1$

[1] Herbert Robbins and Sutton Monro. "A Stochastic Approximation Method". In: *The Annals of Mathematical Statistics* 22.3 (1951), pp. 400–407. DOI: 10.1214/aoms/1177729586. URL: https://doi.org/10.1214/aoms/1177729586.

Learning rate schedule: In deep learning community

Learning rate warmup(one-cycle learning rate schedule):

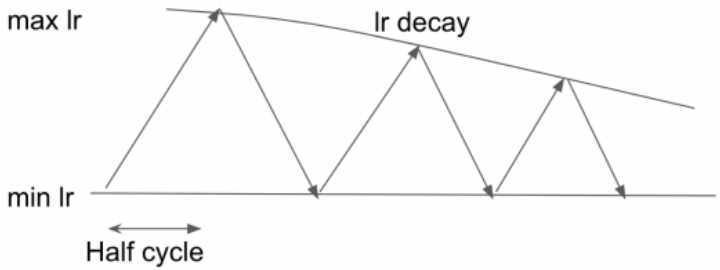


(a)

- Notice:
  To ensure convergence to a point, we must reduce the learning rate to 0.

Learning rate schedule: In deep learning community

Cyclical learning rate:



- Motivation: To escape local minima.
- Methods: The minimum and maximum learning rates can be found based on the initial "dry run" described above, and the half-cycle can be chosen based on how many restarts you want to do with your training budget.
- Related works: **stochastic gradient descent with warm restarts(SGDR)**
  storing all the checkpoints visited after each cool down, and using all of them as members of a **model ensemble**.

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Iterate averaging

- Motivation:
  The parameter estimates produced by SGD can be very unstable over time.
- Methods:

$$\overline{\boldsymbol{\theta}}_t = \frac{1}{t}\sum_{i=1}^{t}\boldsymbol{\theta}_i = \frac{1}{t}\boldsymbol{\theta}_t + \frac{t-1}{t}\overline{\boldsymbol{\theta}}_{t-1}$$

- Advantages:
  - Achieves the best possible asymptotic convergence rate among SGD algorithms, matching that of variants using second-order information[2].
  - Statistical benefits: in the case of linear regression, this method is equivalent to ℓ_2 regularization (i.e., ridge regression)
- Related work: **Stochastic Weight Averaging (SWA)**[3]
  SWA exploits the flatness in objectives used to train deep neural networks, to find solutions which provide better generalization.

[2] Boris Polyak and Anatoli Juditsky. "Acceleration of Stochastic Approximation by Averaging". In: *SIAM Journal on Control and Optimization* 30 (July 1992), pp. 838–855. DOI: 10.1137/0330046.

[3] Pavel Izmailov et al. "Averaging Weights Leads to Wider Optima and Better Generalization". In: *arXiv e-prints*, arXiv:1803.05407 (Mar. 2018), arXiv:1803.05407. arXiv: 1803.05407 [cs.LG].

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stochastic variance reduced gradient (SVRG)

Ever so often (e.g., once per epoch), we compute the full gradient at a "snapshot" of the model parameters $\tilde{\boldsymbol{\theta}}$; the corresponding "exact" gradient is therefore $\nabla \mathcal{L}(\tilde{\boldsymbol{\theta}})$. At step t, we compute the usual stochastic gradient at the current parameters, $\nabla \mathcal{L}_t(\boldsymbol{\theta}_t)$, but also at the snapshot parameters, $\nabla \mathcal{L}_t(\tilde{\boldsymbol{\theta}})$, which we use as a baseline. We can then use the following improved gradient estimate

$$\boldsymbol{g}_t = \nabla \mathcal{L}_t(\boldsymbol{\theta}_t) - \nabla \mathcal{L}_t(\tilde{\boldsymbol{\theta}}) + \nabla \mathcal{L}(\tilde{\boldsymbol{\theta}})$$

stochastic averaged gradient accelerated (SAGA)

We first initialize by computing $\boldsymbol{g}_n^{\text{local}} = \nabla \mathcal{L}_n(\boldsymbol{\theta}_0)$ for all n, and the average, $\boldsymbol{g}^{\text{avg}} = \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{g}_n^{\text{local}}$. Then, at iteration t, we use the gradient estimate

$$\boldsymbol{g}_t = \nabla \mathcal{L}_n(\boldsymbol{\theta}_t) - \boldsymbol{g}_n^{\text{local}} + \boldsymbol{g}^{\text{avg}}$$

where $n \sim \text{Unif}\{1, \ldots, N\}$ is the example index sampled at iteration t. We then update $\boldsymbol{g}_n^{\text{local}} = \nabla \mathcal{L}_n(\boldsymbol{\theta}_t)$ and $\boldsymbol{g}^{\text{avg}}$ by replacing the old $\boldsymbol{g}_n^{\text{local}}$ by its new value.

- Unlike SVRG, it only requires one full batch gradient computation, at the start of the algorithm. While the downside is the extra memory cost.
- It is recommended for use in the sklearn logistic regression code when N is large and $\boldsymbol{x}$ is sparse.

Application to deep learning

For example, the use of batch normalization , data augmentation and dropout all break the assumptions of SVRG, since the loss will differ randomly in ways that depend not just on the parameters and the data index n.

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Preconditioned SGD

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta_t \mathbf{M}_t^{-1} \boldsymbol{g}_t$$

- The noise in the gradient estimates make it difficult to reliably estimate the Hessian.
- Most practitioners use a diagonal preconditioner

AdaGrad

$$\theta_{t+1,d} = \theta_{t,d} - \eta_t \frac{1}{\sqrt{s_{t,d} + \epsilon}} g_{t,d}$$

where $d = 1 : D$ indexes the dimensions of the parameter vector, and

$$s_{t,d} = \sum_{i=1}^{t} g_{i,d}^2$$

is the sum of the squared gradients and $\epsilon > 0$ is a small term to avoid dividing by zero.

RMSprop and AdaDelta

Motivation: the denominator get larger over time. However, it might hurt performance as the denominator gets large too fast.

RMSprop

$$s_{t+1,d} = \beta s_{t,d} + (1-\beta) g_{t,d}^2$$

- We apply the EWMA of the past squared gradients rather than their sum.
- In practice we usually use $\beta \sim 0.9$, which puts more weight on recent examples.

RMSprop and AdaDelta

AdaDelta

$$\Delta\boldsymbol{\theta}_t = -\eta_t \frac{\sqrt{\boldsymbol{\delta}_{t-1} + \epsilon}}{\sqrt{\boldsymbol{s}_t + \epsilon}} \boldsymbol{g}_t$$

where

$$\boldsymbol{\delta}_t = \beta \boldsymbol{\delta}_{t-1} + (1-\beta)\left(\Delta\boldsymbol{\theta}_t\right)^2$$

- Eliminate the need to tune learning rate η_t, since the "units" of the numerator and denominator cancel, so we are just elementwise-multiplying the gradient by a scalar.[4]

However, since these adaptive learning rates need not decrease with time (unless we choose η_t to explicitly do so), these methods are not guaranteed to converge to a solution.

[4] Matthew Zeiler. "ADADELTA: An adaptive learning rate method". In: 1212 (Dec 2012).

Adam

Adam=RMSProp + momentum

$$\boldsymbol{m}_t = \beta_1 \boldsymbol{m}_{t-1} + (1-\beta_1)\,\boldsymbol{g}_t$$
$$\boldsymbol{s}_t = \beta_2 \boldsymbol{s}_{t-1} + (1-\beta_2)\,\boldsymbol{g}_t^2$$

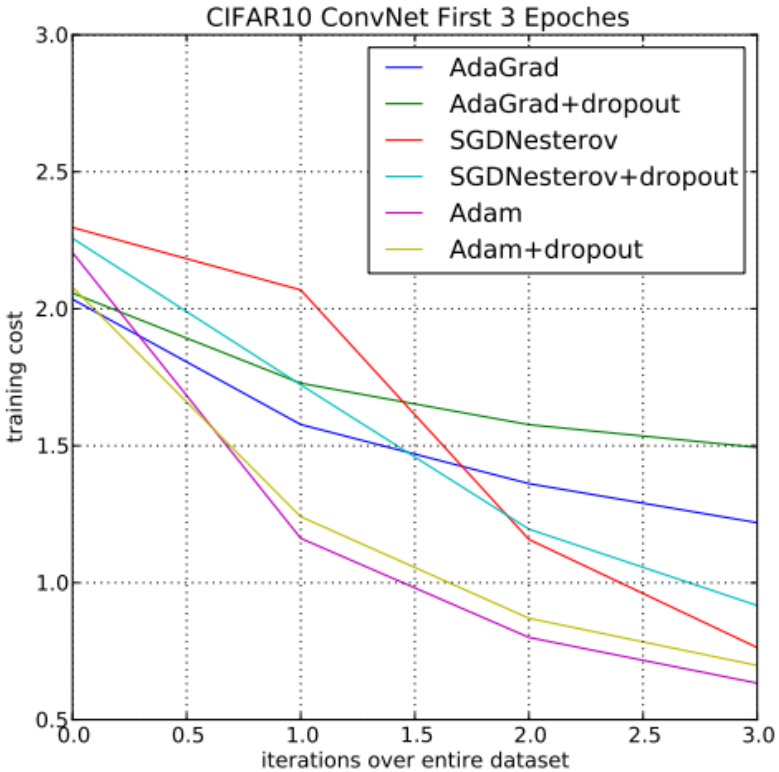
We then perform the update

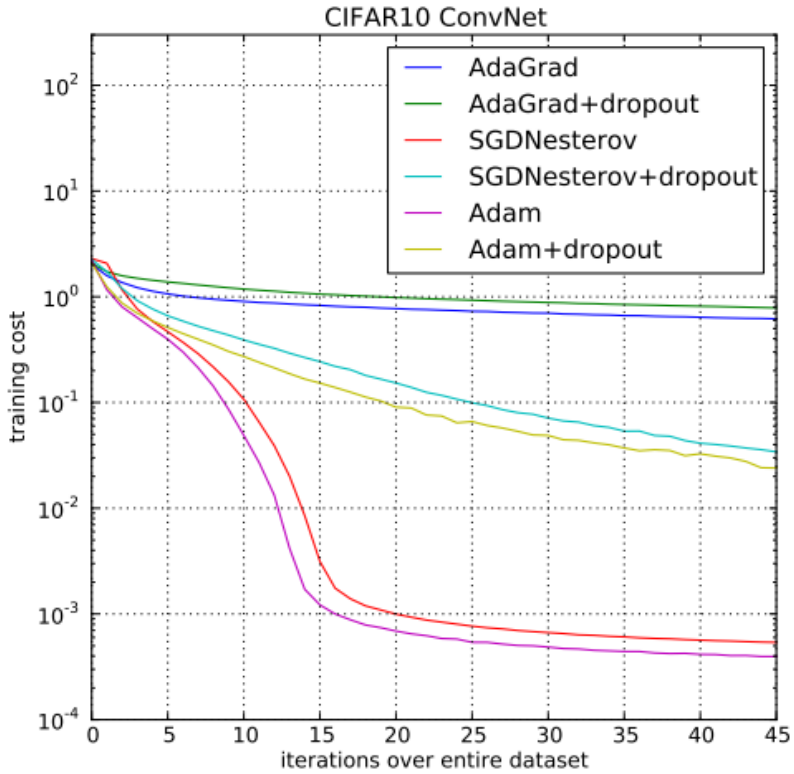
$$\Delta\boldsymbol{\theta}_t = -\eta_t \frac{1}{\sqrt{\boldsymbol{s}_t} + \epsilon}\boldsymbol{m}_t$$

If we initialize with $\boldsymbol{m}_0 = \boldsymbol{s}_0 = \mathbf{0}$, then initial estimates will be biased towards small values. The authors therefore recommend using the bias-corrected moments, which increase the values early in the optimization process. These estimates are given by

$$\hat{\boldsymbol{m}}_t = \boldsymbol{m}_t / \left(1-\beta_1^t\right)$$
$$\hat{\boldsymbol{s}}_t = \boldsymbol{s}_t / \left(1-\beta_2^t\right)$$

Adam


CIFAR10 ConvNet First 3 Epoches
AdaGrad
AdaGrad+dropout
SGDNesterov
SGDNesterov+dropout
Adam
Adam+dropout
training cost
iterations over entire dataset
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0


CIFAR10 ConvNet
AdaGrad
AdaGrad+dropout
SGDNesterov
SGDNesterov+dropout
Adam
Adam+dropout
training cost
iterations over entire dataset
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
0
5
10
15
20
25
30
35
40
45

Issues with adaptive learning rates

- Although it is called adaptive learning rate methods, it still needs to set the base learning rate η_0
- Since the EWMA methods are typically used in the stochastic setting where the gradient estimates are noisy, their learning rate adaptation can result in non-convergence even on convex problems.

Non-diagonal preconditioning matrices

Motivation: Although the methods we have discussed above can adapt the learning rate of each parameter, they do not solve the more fundamental problem of ill-conditioning due to correlation of the parameters, and hence do not always provide as much of a speed boost over vanilla SGD as one may hope.[5]

[5] Rohan Anil et al. "Scalable Second Order Optimization for Deep Learning". In: (Mar. 2021).

References

[1] Herbert Robbins and Sutton Monro. "A Stochastic Approximation Method". In: *The Annals of Mathematical Statistics* 22.3 (1951), pp. 400–407. DOI: 10.1214/aoms/1177729586. URL: https://doi.org/10.1214/aoms/1177729586.

[2] Boris Polyak and Anatoli Juditsky. "Acceleration of Stochastic Approximation by Averaging". In: *SIAM Journal on Control and Optimization* 30 (July 1992), pp. 838–855. DOI: 10.1137/0330046.

[3] Pavel Izmailov et al. "Averaging Weights Leads to Wider Optima and Better Generalization". In: *arXiv e-prints*, arXiv:1803.05407 (Mar. 2018), arXiv:1803.05407. arXiv: 1803.05407 [cs.LG].

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