

Optimization for Deep Learning

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Agenda

- 1 Introduction
- 2 Gradient descent variants
- 3 Challenges
- 4 Gradient descent optimization algorithms
- 5 Parallelizing and distributing SGD
- 6 Additional strategies for optimizing SGD
- 7 Outlook

Introduction

- Gradient descent is a way to minimize an objective function $J(\theta)$
 - $\theta \in \mathbb{R}^d$: model parameters
 - η : learning rate
 - $\nabla_{\theta} J(\theta)$: gradient of the objective function with regard to the parameters
- Updates parameters **in opposite direction** of gradient.
- Update equation: $\theta = \theta - \eta \cdot \nabla_{\theta} J(\theta)$

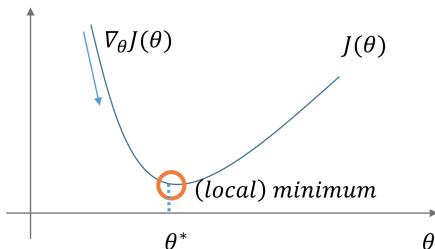


Figure: Optimization with gradient descent

Gradient descent variants

- 1 Batch gradient descent
- 2 Stochastic gradient descent
- 3 Mini-batch gradient descent

Difference: Amount of data used per update

Batch gradient descent

- Computes gradient with the **entire** dataset.
- Update equation: $\theta = \theta - \eta \cdot \nabla_{\theta} J(\theta)$

```
for i in range(nb_epochs):  
    params_grad = evaluate_gradient(  
        loss_function, data, params)  
    params = params - learning_rate * params_grad
```

Listing 1: Code for batch gradient descent update

- Pros:
 - Guaranteed to converge to **global** minimum for **convex** error surfaces and to a **local** minimum for **non-convex** surfaces.
- Cons:
 - **Very slow.**
 - Intractable for datasets that **do not fit in memory.**
 - **No online learning.**

Stochastic gradient descent

- Computes update for **each** example $x^{(i)}y^{(i)}$.
- Update equation: $\theta = \theta - \eta \cdot \nabla_{\theta} J(\theta; x^{(i)}; y^{(i)})$

```
for i in range(nb_epochs):  
    np.random.shuffle(data)  
    for example in data:  
        params_grad = evaluate_gradient(  
            loss_function, example, params)  
        params = params - learning_rate * params_grad
```

Listing 2: Code for stochastic gradient descent update

- Pros
 - **Much faster** than batch gradient descent.
 - Allows **online learning**.
- Cons
 - **High variance** updates.

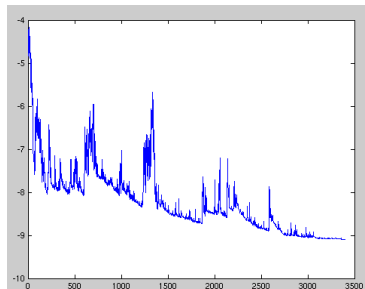


Figure: SGD fluctuation (Source: Wikipedia)

Batch gradient descent vs. SGD fluctuation

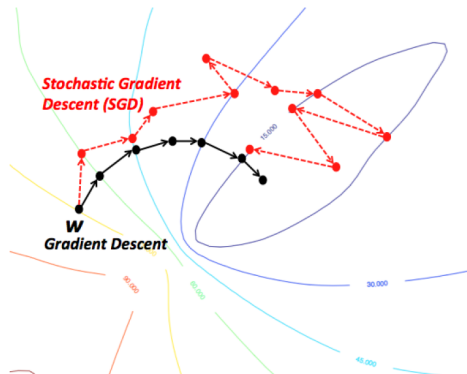


Figure: Batch gradient descent vs. SGD fluctuation (Source: wikidocs.net)

- SGD shows same convergence behaviour as batch gradient descent if learning rate is **slowly decreased (annealed)** over time.

Mini-batch gradient descent

- Performs update for every **mini-batch** of n examples.
- Update equation: $\theta = \theta - \eta \cdot \nabla_{\theta} J(\theta; x^{(i:i+n)}; y^{(i:i+n)})$

```
for i in range(nb_epochs):  
    np.random.shuffle(data)  
    for batch in get_batches(data, batch_size=50):  
        params_grad = evaluate_gradient(  
            loss_function, batch, params)  
        params = params - learning_rate * params_grad
```

Listing 3: Code for mini-batch gradient descent update

- Pros
 - **Reduces variance** of updates.
 - Can exploit **matrix multiplication** primitives.
- Cons
 - **Mini-batch size** is a hyperparameter. Common sizes are 50-256.
- Typically the algorithm of choice.
- Usually referred to as SGD even when mini-batches are used.

Method	Accuracy	Update Speed	Memory Usage	Online Learning
Batch gradient descent	Good	Slow	High	No
Stochastic gradient descent	Good (with annealing)	High	Low	Yes
Mini-batch gradient descent	Good	Medium	Medium	Yes

Table: Comparison of trade-offs of gradient descent variants

Challenges

- Choosing a **learning rate**.
- Defining an **annealing schedule**.
- Updating features to **different extent**.
- **Avoiding suboptimal minima**.

Gradient descent optimization algorithms

- 1 Momentum
- 2 Nesterov accelerated gradient
- 3 Adagrad
- 4 Adadelta
- 5 RMSprop
- 6 Adam
- 7 Adam extensions

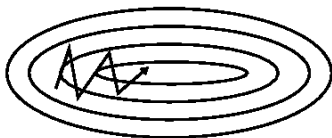
Momentum

- SGD has trouble navigating **ravines**.
- Momentum [Qian, 1999] helps SGD **accelerate**.
- Adds a fraction γ of the update vector of the past step v_{t-1} to current update vector v_t . Momentum term γ is usually set to 0.9.

$$\begin{aligned}v_t &= \gamma v_{t-1} + \eta \nabla_{\theta} J(\theta) \\ \theta &= \theta - v_t\end{aligned}\tag{1}$$



(a) SGD without momentum



(b) SGD with momentum

Figure: Source: Genevieve B. Orr

- **Reduces updates** for dimensions whose gradients **change directions**.
- **Increases updates** for dimensions whose gradients **point in the same directions**.

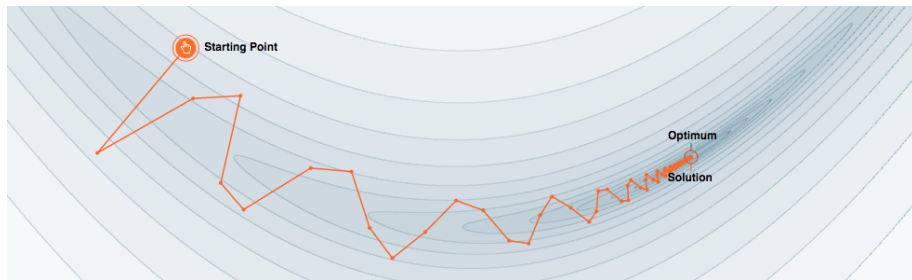


Figure: Optimization with momentum (Source: distill.pub)

Nesterov accelerated gradient

- **Momentum** **blindly accelerates** down slopes: First computes gradient, then makes a big jump.
- Nesterov accelerated gradient (NAG) [Nesterov, 1983] first makes a **big jump** in the direction of the previous accumulated gradient $\theta - \gamma v_{t-1}$. Then measures where it ends up and makes a **correction**, resulting in the **complete update vector**.

$$\begin{aligned}v_t &= \gamma v_{t-1} + \eta \nabla_{\theta} J(\theta - \gamma v_{t-1}) \\ \theta &= \theta - v_t\end{aligned}\tag{2}$$

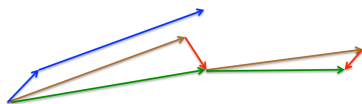


Figure: Nesterov update (Source: G. Hinton's lecture 6c)

Adagrad

- Previous methods: **Same learning rate** η for all parameters θ .
- Adagrad [Duchi et al., 2011] **adapts** the learning rate to the parameters (**large** updates for **infrequent** parameters, **small** updates for **frequent** parameters).
- SGD update: $\theta_{t+1} = \theta_t - \eta \cdot g_t$
 - $g_t = \nabla_{\theta_t} J(\theta_t)$
- Adagrad divides the learning rate by the **square root of the sum of squares of historic gradients**.
- Adagrad update:

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t \quad (3)$$

- $G_t \in \mathbb{R}^{d \times d}$: diagonal matrix where each diagonal element i , i is the sum of the squares of the gradients w.r.t. θ_i up to time step t
- ϵ : smoothing term to avoid division by zero
- \odot : element-wise multiplication

- Pros

- Well-suited for dealing with **sparse data**.
- Significantly **improves robustness** of SGD.
- Lesser need to manually tune learning rate.

- Cons

- **Accumulates squared gradients** in denominator. Causes the learning rate to **shrink** and become **infinitesimally small**.

Adadelta

- Adadelta [Zeiler, 2012] restricts the window of accumulated past gradients to a **fixed size**. SGD update:

$$\begin{aligned}\Delta\theta_t &= -\eta \cdot g_t \\ \theta_{t+1} &= \theta_t + \Delta\theta_t\end{aligned}\tag{4}$$

- Defines **running average** of squared gradients $E[g^2]_t$ at time t :

$$E[g^2]_t = \gamma E[g^2]_{t-1} + (1 - \gamma)g_t^2\tag{5}$$

- γ : fraction similarly to momentum term, around 0.9
- Adagrad update:

$$\Delta\theta_t = -\frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t\tag{6}$$

- Preliminary Adadelta update:

$$\Delta\theta_t = -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t\tag{7}$$

$$\Delta\theta_t = -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t \quad (8)$$

- Denominator is just root mean squared (RMS) error of gradient:

$$\Delta\theta_t = -\frac{\eta}{RMS[g]_t} g_t \quad (9)$$

- Note: **Hypothetical units do not match.**
- Define **running average of squared parameter updates** and RMS:

$$\begin{aligned} E[\Delta\theta^2]_t &= \gamma E[\Delta\theta^2]_{t-1} + (1 - \gamma) \Delta\theta_t^2 \\ RMS[\Delta\theta]_t &= \sqrt{E[\Delta\theta^2]_t + \epsilon} \end{aligned} \quad (10)$$

- Approximate with $RMS[\Delta\theta]_{t-1}$, replace η for **final Adadelta update**:

$$\begin{aligned} \Delta\theta_t &= -\frac{RMS[\Delta\theta]_{t-1}}{RMS[g]_t} g_t \\ \theta_{t+1} &= \theta_t + \Delta\theta_t \end{aligned} \quad (11)$$

RMSprop

- Developed independently from Adadelta around the same time by Geoff Hinton.
- Also divides learning rate by a **running average of squared gradients**.
- RMSprop update:

$$\begin{aligned} E[g^2]_t &= \gamma E[g^2]_{t-1} + (1 - \gamma) g_t^2 \\ \theta_{t+1} &= \theta_t - \frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t \end{aligned} \tag{12}$$

- γ : decay parameter; typically set to 0.9
- η : learning rate; a good default value is 0.001

Adam

- Adaptive Moment Estimation (Adam) [Kingma and Ba, 2015] also stores **running average of past squared gradients** v_t like Adadelta and RMSprop.
- Like Momentum, stores **running average of past gradients** m_t .

$$\begin{aligned}m_t &= \beta_1 m_{t-1} + (1 - \beta_1) g_t \\v_t &= \beta_2 v_{t-1} + (1 - \beta_2) g_t^2\end{aligned}\tag{13}$$

- m_t : first moment (mean) of gradients
- v_t : second moment (uncentered variance) of gradients
- β_1, β_2 : decay rates

- m_t and v_t are initialized as 0-vectors. For this reason, they are biased towards 0.
- Compute bias-corrected first and second moment estimates:

$$\begin{aligned}\hat{m}_t &= \frac{m_t}{1 - \beta_1^t} \\ \hat{v}_t &= \frac{v_t}{1 - \beta_2^t}\end{aligned}\tag{14}$$

- Adam update rule:

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t\tag{15}$$

Adam extensions

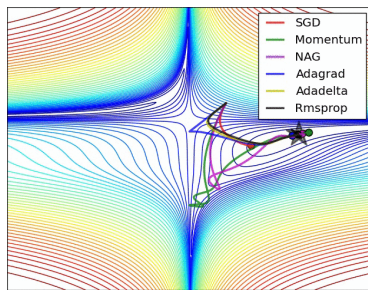
- ① AdaMax [Kingma and Ba, 2015]
 - Adam with ℓ_∞ norm
- ② Nadam [Dozat, 2016]
 - Adam with Nesterov accelerated gradient

Update equations

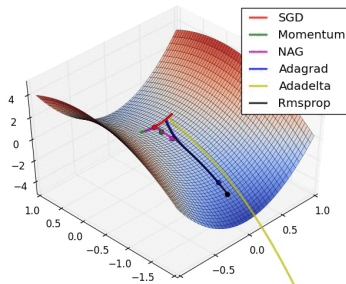
Method	Update equation
SGD	$g_t = \nabla_{\theta_t} J(\theta_t)$ $\Delta\theta_t = -\eta \cdot g_t$ $\theta_t = \theta_t + \Delta\theta_t$
Momentum	$\Delta\theta_t = -\gamma v_{t-1} - \eta g_t$
NAG	$\Delta\theta_t = -\gamma v_{t-1} - \eta \nabla_{\theta} J(\theta - \gamma v_{t-1})$
Adagrad	$\Delta\theta_t = -\frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t$
Adadelat	$\Delta\theta_t = -\frac{RMS[\Delta\theta]_{t-1}}{RMS[g]_t} g_t$
RMSprop	$\Delta\theta_t = -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t$
Adam	$\Delta\theta_t = -\frac{\eta}{\sqrt{\hat{v}_t + \epsilon}} \hat{m}_t$

Table: Update equations for the gradient descent optimization algorithms.

Visualization of algorithms



(a) SGD optimization on loss surface contours



(b) SGD optimization on saddle point

Figure: Source and full animations: Alec Radford

Which optimizer to choose?

- Adaptive learning rate methods (Adagrad, Adadelata, RMSprop, Adam) are **particularly useful for sparse features**.
- Adagrad, Adadelata, RMSprop, and Adam work well in similar circumstances.
- [Kingma and Ba, 2015] show that bias-correction helps Adam **slightly outperform RMSprop**.

Parallelizing and distributing SGD

- ① Hogwild! [Niu et al., 2011]
 - Parallel SGD updates on CPU
 - Shared memory access **without parameter lock**
 - Only works for **sparse input data**
- ② Downpour SGD [Dean et al., 2012]
 - **Multiple replicas** of model on subsets of training data run in parallel
 - Updates sent to parameter server; **updates fraction of model parameters**
- ③ Delay-tolerant Algorithms for SGD [McMahan and Streeter, 2014]
 - Methods also adapt to **update delays**
- ④ TensorFlow [Abadi et al., 2015]
 - Computation graph is split into a **subgraph for every device**
 - Communication takes place using Send/Receive node pairs
- ⑤ Elastic Averaging SGD [Zhang et al., 2015]
 - **Links parameters elastically** to a center variable stored by parameter server

Additional strategies for optimizing SGD

- ① Shuffling and Curriculum Learning [Bengio et al., 2009]
 - Shuffle training data after every epoch to **break biases**
 - Order training examples to **solve progressively harder problems**; infrequently used in practice
- ② Batch normalization [Ioffe and Szegedy, 2015]
 - **Re-normalizes every mini-batch** to zero mean, unit variance
 - Must-use for computer vision
- ③ Early stopping
 - *"Early stopping (is) beautiful free lunch"* (Geoff Hinton)
- ④ Gradient noise [Neelakantan et al., 2015]
 - Add Gaussian noise to gradient
 - Makes model **more robust to poor initializations**

Outlook

- ① Tuned SGD vs. Adam
- ② SGD with restarts
- ③ Learning to optimize
- ④ Understanding generalization in Deep Learning
- ⑤ Case studies

Tuned SGD vs. Adam

- Many recent papers use **SGD with learning rate annealing**.
- SGD with tuned learning rate and momentum is **competitive with Adam** [Zhang et al., 2017b].
- Adam **converges faster**, but **underperforms SGD** on some tasks, e.g. Machine Translation [Wu et al., 2016].
- Adam with **2 restarts and SGD-style annealing** converges faster and outperforms SGD [Denkowski and Neubig, 2017].
- **Increasing the batch size** may have the same effect as decaying the learning rate [Smith et al., 2017].

SGD with restarts

- At each restart, the learning rate is initialized to some value and decreases with cosine annealing [Loshchilov and Hutter, 2017].
- Converges $2\times$ to $4\times$ faster with comparable performance.

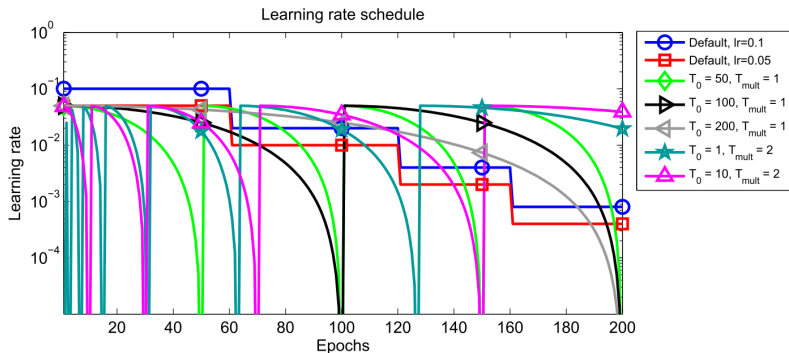


Figure: Learning rate schedules with warm restarts [Loshchilov and Hutter, 2017]

Snapshot ensembles

- 1 Train model until convergence with cosine annealing schedule.
- 2 Save model parameters.
- 3 Perform warm restart and repeat steps 1-3 M times.
- 4 Ensemble saved models.

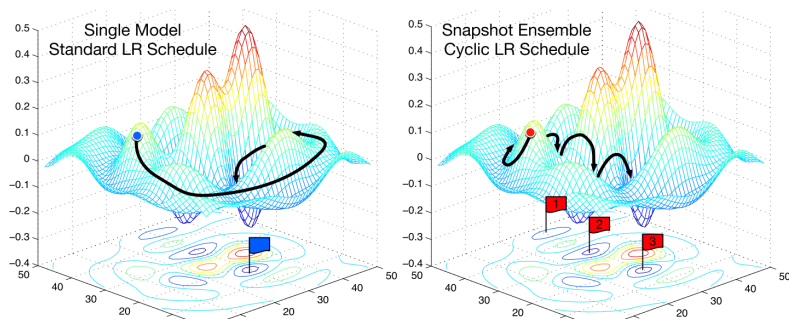


Figure: SGD vs. snapshot ensemble [Huang et al., 2017]

Learning to optimize

- Rather than manually defining an update rule, **learn it**.
- Update rules outperform existing optimizers and transfer across tasks.

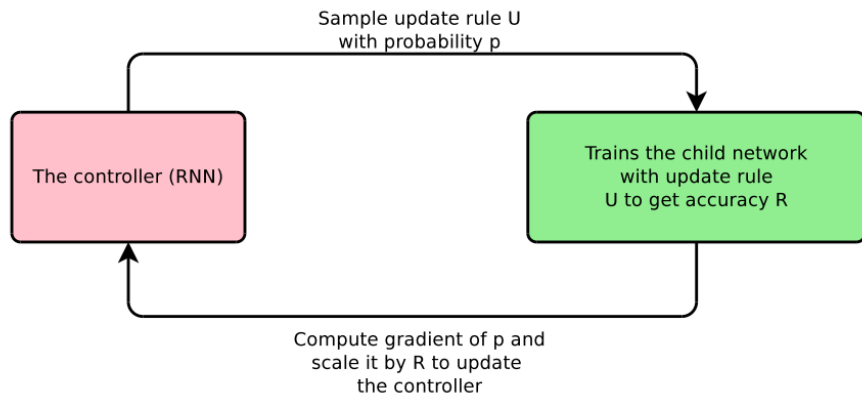


Figure: Neural Optimizer Search [Bello et al., 2017]

Discovered update rules

- **PowerSign:**

$$\alpha^{f(t) * \text{sign}(g) * \text{sign}(m)} * g \quad (16)$$

- α : often e or 2
- f : either 1 or a decay function of the training step t
- m : moving average of gradients
- Scales update by $\alpha^{f(t)}$ or $1/\alpha^{f(t)}$ depending on whether the direction of the gradient and its running average agree.

- **AddSign:**

$$(\alpha + f(t) * \text{sign}(g) * \text{sign}(m)) * g \quad (17)$$

- α : often 1 or 2
- Scales update by $\alpha + f(t)$ or $\alpha - f(t)$.

Understanding generalization in Deep Learning

- **Optimization** is closely tied to **generalization**.
- The number of possible local minima **grows exponentially with the number of parameters** [Kawaguchi, 2016].
- Different local minima **generalize to different extents**.
- Recent insights in understanding generalization:
 - Neural networks can **completely memorize random inputs** [Zhang et al., 2017a].
 - Sharp minima found by batch gradient descent have **high generalization error** [Keskar et al., 2017].
 - Local minima that generalize well can be **made arbitrarily sharp** [Dinh et al., 2017].
- Several submissions at ICLR 2018 on understanding generalization.

Case studies

- Deep Biaffine Attention for Neural Dependency Parsing [Dozat and Manning, 2017]
 - Adam with $\beta_1 = 0.9$, $\beta_2 = 0.9$
 - Report large positive impact on final performance of lowering β_2
- Attention is All You Need [Vaswani et al., 2017]
 - Adam with $\beta_1 = 0.9$, $\beta_2 = 0.98$, $\epsilon = 10^{-9}$, learning rate η
 - $\eta = d_{\text{model}}^{-0.5} \cdot \min(\text{step_num}^{-0.5}, \text{step_num} \cdot \text{warmup_steps}^{-1.5})$
 - $\text{warmup_steps} = 4000$

Thank you for attention!

For more details and derivations of the gradient descent optimization algorithms, refer to [Ruder, 2016].

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