Stochastic Gradient Descent (2)

Problem Formulation

Consider the minimization of an average of functions,

$$\min_x \ \frac{1}{n}\sum_{i=1}^{n} f_i(x)$$

where f is convex and differentiable, $\mathrm{dom}(f) = \mathbb{R}^d$.

Review

Stochastic Gradient Descent (SGD)

- Initialize $x^{(0)} \in \mathbb{R}^d$
- Repeat:

$$x^{(k)} = x^{(k-1)} - t \cdot \nabla f_{i_k}\left(x^{(k-1)}\right), \quad k = 1, 2, 3, \ldots$$

where t is the step size, $i_k \in \{1, \ldots, n\}$ is an index randomly selected at iteration k.

Mini-batch Stochastic Gradient Descent (Mini-batch)

- Initialize $x^{(0)} \in \mathbb{R}^d$
- Repeat:

$$x^{(k)} = x^{(k-1)} - t \cdot \frac{1}{b}\sum_{i \in I_k} \nabla f_i\left(x^{(k-1)}\right), \quad k = 1, 2, 3, \ldots$$

where $I_k \subseteq \{1, \ldots, n\}$ is a subset of size $|I_k| = b \ll n$ randomly selected at iteration k.

Stochastic Average Gradient (SAG)[1]

- Initialize $x^{(0)}$ and $g_i^{(0)} = \nabla f_i\left(x^{(0)}\right), i = 1, \ldots, n$
- At steps $k = 1, 2, 3, \ldots$, pick random $i_k \in \{1, \ldots n\}$, then let

$$g_{i_k}^{(k)} = \nabla f_{i_k}\left(x^{(k-1)}\right)$$

Set all other $g_i^{(k)} = g_i^{(k-1)}, i \neq i_k$.

- Update

$$x^{(k)} = x^{(k-1)} - t \cdot \frac{1}{n} \sum_{i=1}^{n} g_i^{(k)}$$

SAGA[2]

- Initialize $x^{(0)}$ and $g_i^{(0)} = \nabla f_i\left(x^{(0)}\right), i = 1, \ldots, n$
- At steps $k = 1, 2, 3, \ldots$, pick random $i_k \in \{1, \ldots n\}$, then let

$$g_{i_k}^{(k)} = \nabla f_{i_k}\left(x^{(k-1)}\right)$$

Set all other $g_i^{(k)} = g_i^{(k-1)}, i \neq i_k$.

- Update

$$x^{(k)} = x^{(k-1)} - t \cdot \left(g_{i_k}^{(k)} - g_{i_k}^{(k-1)} + \frac{1}{n} \sum_{i=1}^{n} g_i^{(k-1)}\right)$$

Stochastic Variance Reduced Gradient (SVRG)[3]

- Initialize $\hat{x}^{(0)} \in \mathbb{R}^d$
- At step $k = 1, 2, 3, \ldots,$
  - Set

$$\hat{x} = \hat{x}^{(k-1)}, \ x_0 = \hat{x}$$

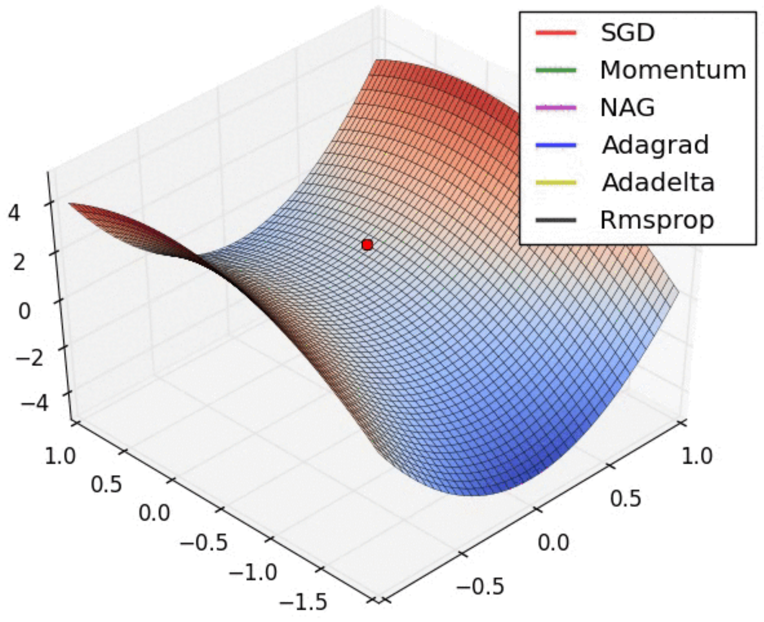
  - For $j = 1, \ldots, m$, randomly pick $i_j \in \{1, \ldots, n\}$ and update

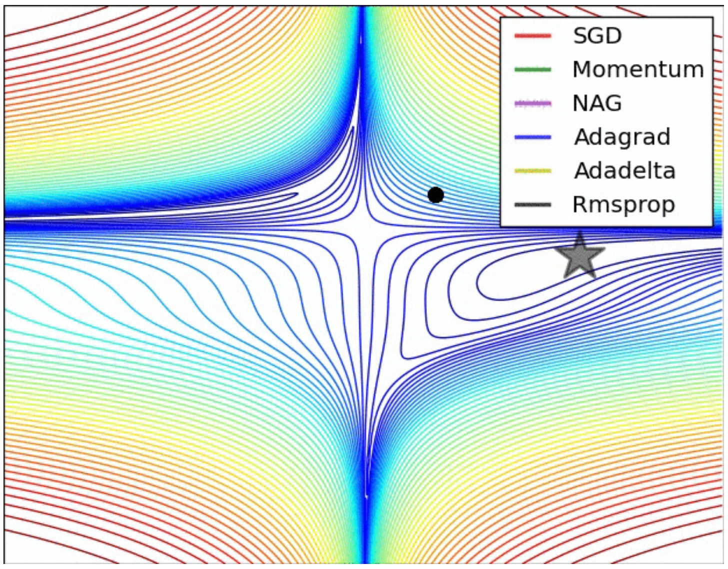
$$x_j = x_{j-1} - t\left(\nabla f_{i_j}(x_{j-1}) - \nabla f_{i_j}(\hat{x}) + \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(\hat{x})\right)$$

  - Option 1: Set $\hat{x}^{(k)} = x_m$.
    Option 2: Set $\hat{x}^{(k)} = x_j$ for randomly chosen $j \in \{1, \ldots, m\}$.

Other Improvements on Stochastic Gradient Descent

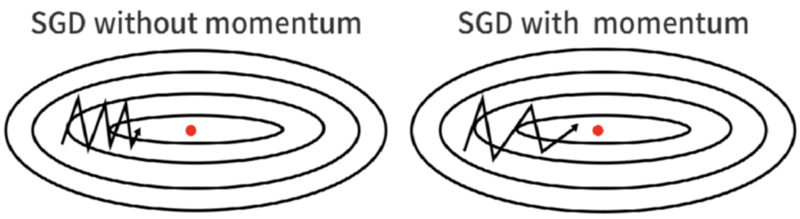
In this lecture, we are going to introduce more improvements on stochastic gradient descent. Here are some visualizations about the method we are going to introduce.





Momentum

A **momentum term**[4] is usually added to SGD to improve the speed of learning and dampens oscillations.



- Initialize $x^{(0)}, v^{(0)} \in \mathbb{R}^d$
- Repeat:

$$v^{(k)} = \gamma v^{(k-1)} + t\nabla f_{i_k}\left(x^{(k-1)}\right)$$
$$x^{(k)} = x^{(k-1)} - v^{(k)}, \quad k = 1, 2, 3, \ldots$$

where the decay factor (*momentum constant*) $0 < \gamma < 1$, t is the step size, $i_k \in \{1, \ldots, n\}$ is an index randomly selected at iteration k.

> - If $\gamma = 0$, it is SGD.
> - The update of SGD is usually unstable.
> - Momentum works by adding a fraction ($1 - \gamma$ is *the cosntant of friction*) of the update vector of the past time step to the current update vector.

Nestorve accelerated gradient (NAG)

Inspired by the **Nesterov method**[5] for optimizing convex functions, Ilya Sutskever[6] suggested a new form of momentum that often works better.

- Initialize $x^{(0)}, v^{(0)} \in \mathbb{R}^d$
- Repeat:

$$v^{(k)} = \gamma v^{(k-1)} + t\nabla f_{i_k}\left(x^{(k-1)} - \gamma v^{(t-1)}\right)$$
$$x^{(k)} = x^{(k-1)} - v^{(k)}, \quad k = 1, 2, 3, \ldots$$

where $0 < \gamma < 1$, step size t is chosen to be fixed and small, $i_k \in \{1, \ldots, n\}$ is an index randomly selected at iteration k.

> $x^{(k)} = x^{(k-1)} - v^{(k)} = x^{(k-1)} - \gamma v^{(k-1)} - t\nabla f_{i_k}\left(x^{(k-1)} - \gamma v^{(t-1)}\right)$. So, $x^{(k-1)} - \gamma v^{(t-1)}$ is used for ∇f_{i_k} as a "look-forward" prediction.

Adaptive Gradient Algorithm (Adagrad)

Adagrad[7] uses a different learning rate for every $x_j^{(k)}$ at every time step k. Here, $x_j^{(k)}$ is the j-th component of $x^{(k)}$, $j = 1, 2, ..., d$.

- Initialize $x^{(0)} \in \mathbb{R}^d$
- Repeat:

$$x_j^{(k)} = x_j^{(k-1)} - \frac{t}{\sqrt{G_{j,j}^{(k-1)} + \epsilon}} \nabla_{x_j} f_{i_k}(x^{(k-1)}), \quad k = 1, 2, 3, \ldots$$

where $G^{(k-1)} \in \mathbb{R}^{d \times d}$ is a diagonal matrix where the j-th diagonal element is the sum of the square of the gradient with respect to x_j up to time step k

$$G_{j,j}^{(k-1)} = \sum_{l=1}^{k} \left\| \nabla_{x_j} f_{i_l}(x^{(l-1)}) \right\|^2$$

and ϵ is added to prevent division by zero. Step size t is chosen to be fixed and small, $i_k \in \{1, \ldots, n\}$ is an index randomly selected at iteration k.

> - Adagrad ***adapts the learning rate to the parameters***, performing smaller updates for parameters associated with frequently occurring features, and larger updates for parameters associated with infrequent features.
> - It is well-suited for dealing with *sparse data* and greatly improves the robustness of SGD.
> - Adagrad's main **weakness** is its accumulation of the squared gradients in the denominator. Since the accumulated sum keeps growing during training, ***the learning rate will shrink and eventually become infinitesimally small***.

Adadelta

Adadelta[8] is also proposed to solve the weakness of Adagrad.
Denote $g^{(k)} = \nabla f_{i_k}\left(x^{(k-1)}\right)$. Instead of accumulating the sum of squared gradients over all time in ADAGRAD, the running average at step k depends on the previous weighted average and the current gradient.

$$\mathbb{E}[g^2]^{(k)} = \gamma \mathbb{E}[g^2]^{(k-1)} + (1-\gamma)(g^{(k)})^2$$

> - The notation $\mathbb{E}$ in this algorithm is rather vague and heuristic, however it is exactly what has been written in the original work. $\mathbb{E}[g^2]^{(k)}$ should be treated as a variable and in fact refers to exponentially decaying average to estimate the true expectation of the stochastic g^2.
> - g^2 is the ***elementwise*** square: $g^2 = g \odot g$ is a vector with components $(g_j)^2$.

Replace the diagonal matrix in Adagrad with this decaying average yields

$$\begin{aligned}\Delta x^{(k)} &= x^{(k)} - x^{(k-1)} \\ &= -\frac{t}{\sqrt{\mathbb{E}[g^2]^{(k)} + \epsilon}} g^{(k)} \\ &= -\frac{t}{\mathrm{RMS}[g]^{(k)}} g^{(k)}\end{aligned}$$

where RMS stands for the root mean squared error. However, the authors noticed that the units in this update do not match, in which the update should have the same hypothetical units as the parameter.

To realize this, they first define another exponentially decaying average, the squared parameter updates:

$$\mathbb{E}[\Delta x^2]^{(k)} = \gamma \mathbb{E}[\Delta x^2]^{(k-1)} + (1-\gamma)\|\Delta x^{(k)}\|^2$$

The root mean squared error of parameter updates is

$$\mathrm{RMS}[\Delta x]^{(k)} = \sqrt{\mathbb{E}[\Delta x^2]^{(k)} + \epsilon}$$

Since $\mathrm{RMS}[\Delta x]^{(k)}$ is unknown, it is approximated with $\mathrm{RMS}[\Delta x]^{(k-1)}$. Replacing the learning rate of the previous update with $\mathrm{RMS}[\Delta x]^{(k-1)}$ gives the Adadelta update rule:

- Initialize $x^{(0)} \in \mathbb{R}^d$
- Repeat:

$$\begin{aligned}\Delta x^{(k)} &= -\frac{\mathrm{RMS}[\Delta x]^{(k-1)}}{\mathrm{RMS}[g]^{(k)}} g^{(k)} \\ x^{(k+1)} &= x^{(k)} + \Delta x^{(k)}\end{aligned}$$

> - Since the step size has been eliminated from the update rule, we do not even need to set a default value. No manual setting of a learning rate.
>
> - Applying the RMS on each dimension g_j and Δx_j, we can separate dynamic learning rate per-dimension.

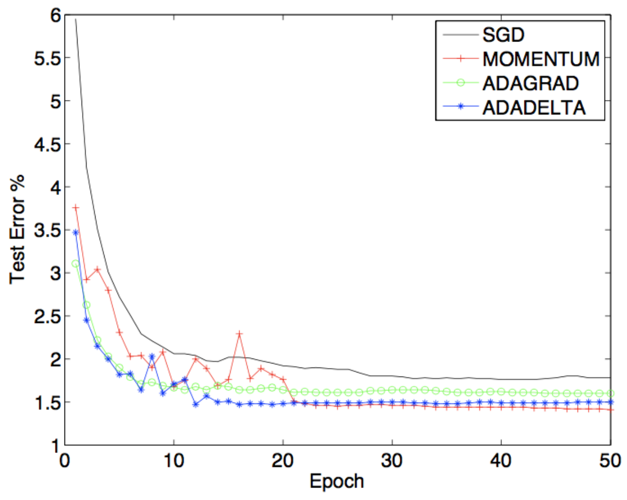


Fig. 1. Comparison of learning rate methods on MNIST digit classification for 50 epochs.

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RMSprop

RMSprop is another algorithm that deals with the weakness of Adagrad. Instead of summing up all the squared gradients, it calculates the exponentially weighted mean of the square of gradients.

- Initialize $x^{(0)}, v^{(0)} \in \mathbb{R}^d$
- Repeat:

$$v_j^{(k)} = \gamma v_j^{(k-1)} + (1-\gamma)\left(\nabla_{x_j} f_{i_k}(x^{(k-1)})\right)^2$$
$$x_j^{(k)} = x_j^{(k-1)} - \frac{t}{\sqrt{v_j^{(k)} + \epsilon}} \nabla_{x_j} f_{i_k}(x^{(k-1)})$$
$$j = 1, 2, \ldots, d, \quad k = 1, 2, 3 \ldots$$

> - RMSprop in fact is identical to *the first update rule in the deduction of Adadelta*.
> - RMSprop is not a published work, it's from Hinton's lecture note.
> - Hinton suggests γ to be set to 0.9, while a good default value for the learning rate t is 0.001.

Adaptive Moment Estimation (Adam)

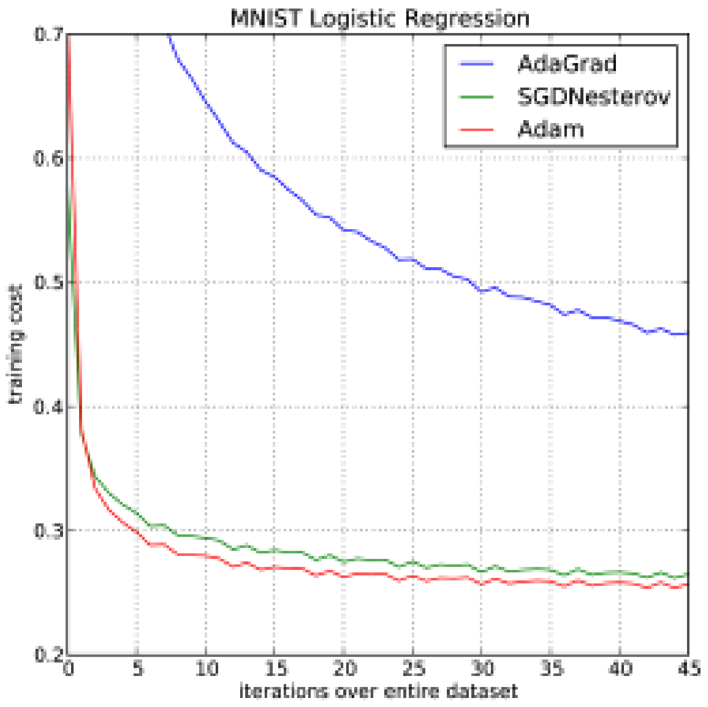
Adam[9] (Kingma & Ba, 2014) is another first-order gradient-based optimization method that computes adaptive learning rates for each parameter, based on **adaptive estimates of lower-order moments**.

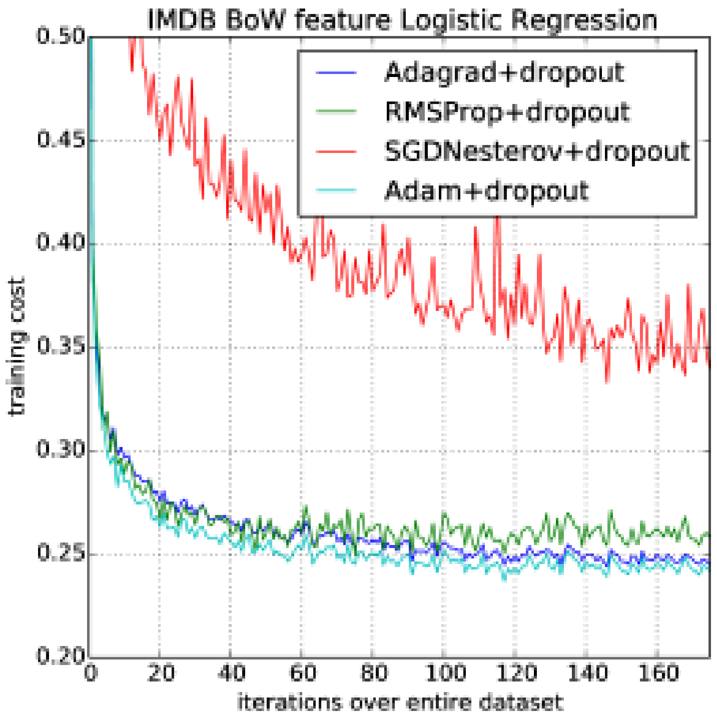
- Initialize $x^{(0)} \in \mathbb{R}^d, m^{(0)}, v^{(0)} \in \mathbb{R}$
- Repeat:

$$\begin{aligned} g^{(k)} &= \nabla f_{i_k}(x^{(k-1)}) \\ m^{(k)} &= \beta_1 m^{(k-1)} + (1-\beta_1) g^{(k)} \\ v^{(k)} &= \beta_2 v^{(k-1)} + (1-\beta_2)(g^{(k)})^2 \\ \hat{m}^{(k)} &= \frac{m^{(k)}}{1-\beta_1^k}, \quad \hat{v}^{(k)} = \frac{v^{(k)}}{1-\beta_2^k} \\ x^{(k)} &= x^{(k-1)} - t\frac{\hat{m}^{(k)}}{\sqrt{\hat{v}^{(k)}}+\epsilon} \end{aligned}$$

where $\beta_1, \beta_2 \in [0, 1)$. β_1^k and β_2^k denote β_1 and β_2 to power k. Step size t is chosen to be fixed and small, $i_k \in \{1, \ldots, n\}$ is an index randomly selected at iteration k.

> - m estimates the first order moment g, v estimate the second order moment g^2. $\hat{m}$ and $\hat{g}$ is for bias-correction.
> - g^2 indicates the elementwise square $g \odot g$: it is a vector with element $(g_i)^2$; $\sqrt{\hat{v}}$ is also elementwise sqrt. So the learning rate is different per dimension.
>
> - Adam has ***quite a lot merits***: easy to implement, computationally efficient, little memory requirements, suitable for problems with large data/parameters, suitable for problems with noisy/sparse gradients...
> - Widely used in machine learning.
> - ***Good default values*** are: $\alpha = 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 10^{-8}$.





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AdaMax

AdaMax is a variant of Adam based on the infinity norm. The $v^{(k)}$ factor in the Adam update rule scales the gradient inversely proportionally to the L^2 norm of the past and current gradient.

$$v^{(k)} = \beta_2 v^{(k-1)} + (1-\beta_2)|g^{(k)}|^2$$

This can be generalized L^p norm:

$$v^{(k)} = \beta_2^p v^{(k-1)} + (1-\beta_2^p)|g^{(k)}|^p$$

For large p, such variants become numerically unstable. However, let $p \to \infty$, the algorithm becomes surprisingly simple and stable.

- Initialize $x^{(0)} \in \mathbb{R}^d, m^{(0)}, v^{(0)} \in \mathbb{R}$
- Repeat:

$$\begin{aligned} g^{(k)} &= \nabla f_{i_k}(x^{(k-1)}) \\ m^{(k)} &= \beta_1 m^{(k-1)} + (1-\beta_1) g^{(k)} \\ u^{(k)} &= \max(\beta_2 u^{(k-1)}, \|g^{(k)}\|_\infty) \\ x^{(k)} &= x^{(k-1)} - \frac{tm^{(k)}}{(1-\beta_1^{(k)})u^{(k)}} \end{aligned}$$

where β_1^k and β_2^k denote β_1 and β_2 to power k. Step size t is chosen to be fixed and small, $i_k \in \{1, \ldots, n\}$ is an index randomly selected at iteration k.

> - AdaMax is proposed in the same work as Adam.
> - ***Good default values*** are: $\alpha = 0.002$, $\beta_1 = 0.9$ and $\beta_2 = 0.999$.

Nesterov-accelerated Adaptive Moment Estimation (Nadam)

Nadam[10] is a combination of Adam and NAG.

Recall the update rule of NAG:

$$\begin{aligned} g^{(k)} &= \nabla f_{i_k}(x^{(k)} - \gamma m^{(k-1)}) \\ m^{(k)} &= \gamma m^{(k-1)} + t g^{(k)} \\ x^{(k+1)} &= x^{(k)} - m^{(k)} \end{aligned}$$

Dozat (author of Nadam paper) rewrote this rule into:

$$
\begin{aligned}
g^{(k)} &= \nabla f_{i_k}(x^{(k)}) \\
m^{(k)} &= \gamma m^{(k-1)} + t g^{(k)} \\
x^{(k+1)} &= x^{(k)} - (\gamma m^{(k)} + t g^{(k)})
\end{aligned}
$$

Recall the Adam update rule, here $\hat{v}^{(k)}$ remains the same:

$$
\begin{aligned}
m^{(k)} &= \beta_1 m^{(k-1)} + (1-\beta_1) g^{(k)} \\
\hat{m}^{(k)} &= \frac{m^{(k)}}{1-\beta_1^k} \\
x^{(k+1)} &= x^{(k)} - \frac{t}{\sqrt{\hat{v}^{(k)} + \epsilon}} \hat{m}^{(k)}
\end{aligned}
$$

Expand the third equation with the definitions of $\hat{m}^{(k)}$ and $m^{(k)}$.

$$
\begin{aligned}
x^{(k+1)} &= x^{(k)} - \frac{t}{\sqrt{\hat{v}^{(k)} + \epsilon}} \left(\frac{\beta_1 m^{(k-1)}}{1-\beta_1^k} + \frac{(1-\beta_1) g^{(k)}}{1-\beta_1^k} \right) \\
x^{(k+1)} &= x^{(k)} - \frac{t}{\sqrt{\hat{v}^{(k)} + \epsilon}} \left(\beta_1 \hat{m}^{(k-1)} + \frac{(1-\beta_1) g^{(k)}}{1-\beta_1^k} \right)
\end{aligned}
$$

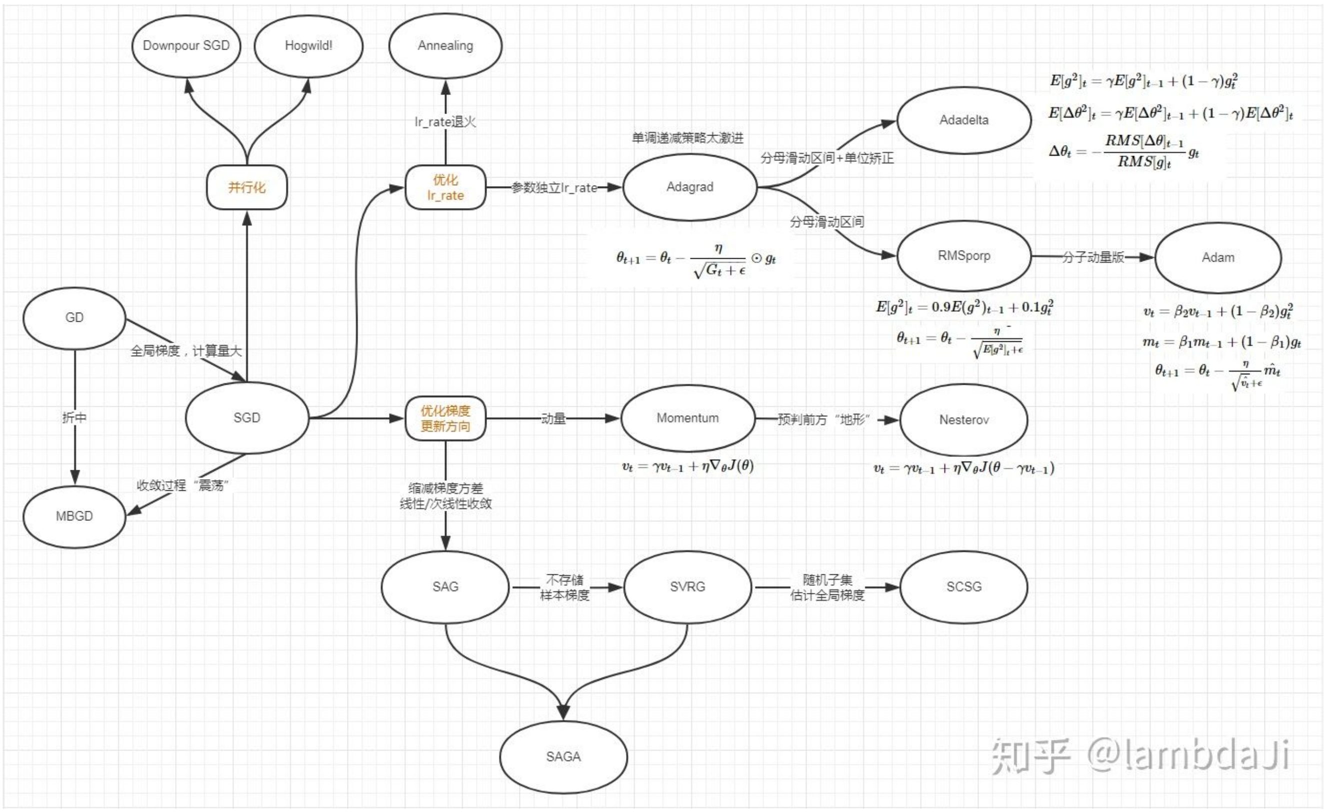
Note that for simplicity, we ignore that the denominator is $1-\beta_1^k$ and not $1-\beta_1^{k-1}$. The Nadam update rule is:

- Initialize $x^{(0)} \in \mathbb{R}^d, m^{(0)}, v^{(0)} \in \mathbb{R}$
- Repeat:

$$
\begin{aligned}
g^{(k)} &= \nabla f_{i_k}(x^{(k-1)}) \\
m^{(k)} &= \beta_1 m^{(k-1)} + (1-\beta_1) g^{(k)} \\
v^{(k)} &= \beta_2 v^{(k-1)} + (1-\beta_2) \| g^{(k)} \|^2 \\
\hat{m}^{(k)} &= \frac{m^{(k)}}{1-\beta_1^k}, \quad \hat{v}^{(k)} = \frac{v^{(k)}}{1-\beta_2^k} \\
x^{(k+1)} &= x^{(k)} - \frac{t}{\sqrt{\hat{v}^{(k)} + \epsilon}} \left(\beta_1 \hat{m}^{(k-1)} + \frac{(1-\beta_1) g^{(k)}}{1-\beta_1^k} \right)
\end{aligned}
$$

where β_1^k and β_2^k denote β_1 and β_2 to power k. Step size t is chosen to be fixed and small, $i_k \in \{1, \ldots, n\}$ is an index randomly selected at iteration k.

In summary, the following diagram might be useful.


Downpour SGD
Hogwild!
Annealing
lr_rate退火
并行化
优化 lr_rate
参数独立lr_rate
单调递减策略太激进
Adagrad
$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t$
分母滑动区间+单位矫正
Adadelta
$E[g^2]_t = \gamma E[g^2]_{t-1} + (1-\gamma) g_t^2$
$E[\Delta\theta^2]_t = \gamma E[\Delta\theta^2]_{t-1} + (1-\gamma) E[\Delta\theta^2]_t$
$\Delta\theta_t = -\frac{RMS[\Delta\theta]_{t-1}}{RMS[g]_t} g_t$
分母滑动区间
RMSporp
$E[g^2]_t = 0.9E(g^2)_{t-1} + 0.1g_t^2$
$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{E[g^2]_t + \epsilon}}$
分子动量版
Adam
$v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2$
$m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t$
$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v}_t + \epsilon}} \hat{m}_t$
GD
全局梯度，计算量大
折中
SGD
收敛过程“震荡”
MBGD
优化梯度 更新方向
动量
Momentum
$v_t = \gamma v_{t-1} + \eta \nabla_\theta J(\theta)$
预判前方“地形”
Nesterov
$v_t = \gamma v_{t-1} + \eta \nabla_\theta J(\theta - \gamma v_{t-1})$
缩减梯度方差 线性/次线性收敛
SAG
不存储 样本梯度
SVRG
随机子集 估计全局梯度
SCSG
SAGA
知乎 @lambdaJi

There are more and more methods with more complications. e.g., AdaBelief Optimizer

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1. https://arxiv.org/pdf/1309.2388.pdf ↩

2. https://papers.nips.cc/paper/5258-saga-a-fast-incremental-gradient-method-with-support-for-non-strongly-convex-composite-objectives.pdf ↩

3. https://papers.nips.cc/paper/4937-accelerating-stochastic-gradient-descent-using-predictive-variance-reduction.pdf ↩

4. https://www.sciencedirect.com/science/article/pii/S0893608098001166?via%3Dihub ↩

5. http://mpawankumar.info/teaching/cdt-big-data/nesterov83.pdf ↩

6. https://www.cs.utoronto.ca/~ilya/pubs/ilya_sutskever_phd_thesis.pdf ↩

7. https://jmlr.org/papers/volume12/duchi11a/duchi11a.pdf ↩

8. https://arxiv.org/pdf/1212.5701.pdf ↩

9. https://arxiv.org/pdf/1412.6980.pdf ↩

10. https://openreview.net/pdf/OM0jvwB8jIp57ZJjtNEZ.pdf ↩