A Summary Sheet of Optimization in Deep Learning

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Abstract

Newton's method provides one of the earliest insight in optimization theories. Based on gradient descent, a lot of optimization theories including momentum, adaptive learning, sign of gradient, second-order optimization, variance reduction and scheduler-free optimization have been proposed. However, there is a lack of comprehensive and clear summary of these approaches with unified notation system. This paper attempts to give a systematic, explicit and concise formulation of many of these methods with citation. I hope it can promote innovation in optimization theory in deep learning, while facilitating relevant researchers to search for references. And the related materials can be found in https://github.com/lauyikfung/A-Summary-Sheet-of-Optimization-in-Deep-Learning.

1 From Gradient Descent to Adaptive Learning

1.1 Notations

In the paper, $f(\theta_t)$ denotes the deep learning network at t-th iteration with parameter θ_t , The objective is $J(\theta_t)$ and the gradient is $\nabla_{\theta}J(\theta_t) = \nabla f(\theta_t, \boldsymbol{\xi}_t) = g_t$, where the input is $\boldsymbol{\xi}_t$ by default. Moreover, $\|\mathbf{x}\| = \|\mathbf{x}\|_2$ denotes the 2-norm, while $|\mathbf{x}|$ denotes taking the absolute value element-wisely. η is the learning rate or step size, and it may change over iterations unless specific explanation. We just omit the initialization of parameters and state variables for simplicity.

1.2 Newton's Method

For Newton's method, $f(\theta + \epsilon) = f(\theta) + \epsilon^{\top} \nabla f(\theta) + \frac{1}{2} \epsilon^{\top} \mathbf{H} \epsilon + \mathcal{O}(\|\epsilon\|^3)$, where $\mathbf{H} = \nabla^2 f(\theta)$ is the Hessian matrix (Zhang et al., 2021).

For first-order method, the second-order and higher-order terms $(\frac{1}{2}\epsilon^{\top}\mathbf{H}\epsilon + \mathcal{O}(\|\epsilon\|^3))$ are ignored since they have relatively lower influence on the convergence of training and much harder to compute, and the update rule comes to:

$$\theta_{t+1} = \theta_t - \eta \nabla f(\theta_t),$$

where $\eta = -\epsilon$ is the step size.

While in second-order methods, only the higher-order terms $(\mathcal{O}(\|\epsilon\|^3))$ are ignored. Since at the minimum of f, $\nabla_{\theta} f(\theta) = 0$, then $\epsilon = -\mathbf{H}^{-1} \nabla f(\theta)$, and it comes to:

$$\theta_{t+1} = \theta_t - \eta \mathbf{H}^{-1} \nabla f(\theta_t),$$

where η is the step size.

¹According to the limitation of time, I may miss some excellent works on optimization in deep learning. I am very pleased to communicate with others and adding more interesting works to this sheet.

1.3 Gradient Descent (GD)

Full GD:

- Using full datasets for gradient descent, 1. $\theta_{t+1} = \theta_t \eta \nabla_{\theta} J(\theta_t) = \theta_t \eta g_t$. Here and below, g_t is defined the gradient of full data/mini batch data on θ_t .
- Convergence $O(\frac{1}{T})$. Here the convergence is defined by $f(x^T) f^*$

Stochastic GD (SGD): Using one sample per step, convergence $O(\frac{1}{\sqrt{T}})$

Batch GD (BGD): Using small batch (size=b) per steps, convergence $O(\frac{1}{\sqrt{hT}} + \frac{1}{T})$

1.4 Momentum and Related

Momentum (Grum, 2023) $m_{t+1} = \gamma m_t + \eta \nabla_{\theta} J(\theta_t), \, \theta_{t+1} = \theta_t - m_{t+1}$

Nestorov's Accelerated Gradient (NAG) (Nesterov, 1983) $m_{t+1} = \gamma m_t + \eta \nabla_{\theta} J(\theta_t - \gamma m_t),$ $\theta_{t+1} = \theta_t - m_{t+1}$

BFGS (Broyden–Fletcher–Goldfarb–Shanno) (Fletcher, 1987) $d_t = -H_t g_t$, $\alpha_t = \arg\min_{\alpha} f(\theta - \alpha d_t)$, $\theta_{t+1} = \theta_t + \alpha_t d_t$, $H_{t+1} = (I - \frac{s_t y_t}{y_t^{\top} s_t})^{\top} H_t (I - \frac{y_t s_t^{\top}}{y_t^{\top} s_t}) + \frac{s_t s_t^{\top}}{y_t^{\top} s_t}$, where $s_t = \theta_{t+1} - \theta_t$, $y_t = g_{t+1} - g_t$.

L-BFGS (Liu & Nocedal, 1989) Based on BFGS, but choose α_t satisfying Wolfe conditions (try $\alpha_t = 1$ first): $f(\theta_t + \alpha_t d_t) \le f(\theta_t) + \beta' \alpha_t g_t^{\mathsf{T}} d_t$. Moreover, for $\widehat{m} = \min\{t, m-1\}$,

$$H_{t+1} = (\prod_{i=t,inv}^{t-\widehat{m}} V_i^{\top}) H_0(\prod_{i=t-\widehat{m}}^t V_i) + \sum_{j=t-\widehat{m}}^t \rho_j(\prod_{i=t,inv}^{j+1} V_i^{\top}) s_j s_j^{\top} (\prod_{i=j+1}^t V_i),$$

where $\prod_{i=t,inv}^{t'}$ denotes the product of matrices with indices from t to t' < t, and $\rho_t = 1/(y_t^\top s_t)$.

ASGD (Polyak & Juditsky, 1992) $\theta_{t+1} = \theta_t - \eta \cdot \frac{1}{t+1} \sum_{i=1}^t g_i$

AdaGrad (Duchi et al., 2011) $r_t=r_{t-1}+g_t^2,$ $\theta_{t+1}=\theta_t-\frac{\eta}{\sqrt{r_t}+\epsilon}g_t$

AdaGrad-Norm (Ward et al., 2020) $r_t = r_{t-1} + ||g_t||^2$, $\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{r_t + \epsilon}} g_t$

AdaDelta (Zeiler, 2012) $v_t = \rho v_{t-1} + (1-\rho)g_t^2$, $\theta_t = \theta_{t-1} - \eta \frac{\sqrt{u_{t-1}}}{\sqrt{v_t + \epsilon}}g_t$, $u_t = \rho u_{t-1} + (1-\rho)\Delta\theta_t^2$, where $\Delta\theta_t = \theta_t - \theta_{t-1}$

RMSProp (Tieleman & Hinton, 2012) $v_t = \rho v_{t-1} + (1-\rho)g_t^2$ (EMA (Exponential Moving Average) of the squared gradient), $\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{v_t + \epsilon}}g_t$

2 Adam and derivatives

Adam (Kingma & Ba, 2015)

- $m_t = \beta_1 m_{t-1} + (1 \beta_1) g_t$ (EMA of gradient, use m_t below if have same expression)
- $v_t = \beta_2 v_{t-1} + (1-\beta_2)g_t^2$ (EMA of squared gradient, use v_t below if have same expression)
- $\theta_{t+1} = \theta_t \eta \frac{\widehat{m}_t}{\sqrt{\widehat{v_t}} + \epsilon}$, where $\widehat{m}_t = \frac{m_t}{1 \beta_1^t}$, $\widehat{v}_t = \frac{v_t}{1 \beta_2^t}$ (Use \widehat{m}_t or \widehat{v}_t below if have same expression)

2.1 Other forms for Adam

2.1.1 Hessian Matrices

 $\theta_{t+1} = \arg\min_{\theta} \{ \eta \langle m_t, \theta \rangle + \frac{1}{2} || \theta - \theta_t ||_{\mathbf{H}_t}^2 \}.$ In closed form: $\theta_{t+1} = \theta_t - \eta \mathbf{H}_t^{-1} m_t$.

•
$$\mathbf{H}_t = \sqrt{\operatorname{diag}(v_t)} \cdot \frac{1-\beta_1^t}{\sqrt{1-\beta_2^t}}$$
 for AdamW

•
$$\mathbf{H}_t = \sqrt{\operatorname{diag}(m_t^2)}$$
 for Lion

•
$$\mathbf{H}_t = (\sum_{\tau=1}^t \mathbf{G}_t \mathbf{G}_t^\top)^{1/4} \otimes (\sum_{\tau=1}^t \mathbf{G}_t^\top \mathbf{G}_t)^{1/4}$$
 for Shampoo

2.1.2 Matrix form of v_t

$$\theta_{t+1} = \prod_{\mathcal{F}, \sqrt{V_t}} (\theta_t - \eta_t m_t / \sqrt{\widehat{v_t}}), \text{ where } \theta \in \mathcal{F}, V_t = \text{diag}(\widehat{v_t})$$

2.2 Derivatives of Adam

In the following algorithms, if not specified, m_t , v_t , \hat{m}_t , \hat{v}_t and the updating rule are the same with Adam, or AdamW with decoupled weight decay.

2.2.1 Minute Modification

AdamW (Loshchilov & Hutter, 2019) $\theta_{t+1} = \theta_t - \eta(\frac{\widehat{m}_t}{\sqrt{\widehat{v_t}} + \epsilon} + \lambda \theta_t)$, where λ is called decoupled weight decay (hyper-parameter). And The decoupled weight decay can be applied to the algorithms below

AMSgrad (Reddi et al., 2018)
$$\widetilde{v}_t = \max(\widetilde{v}_{t-1}, v_t), \, \widehat{v}_t = \frac{\widetilde{v}_t}{1-\beta_2^t}$$

AdaMax (Loshchilov & Hutter, 2019)
$$u_t = \max(\beta_2 u_{t-1}, |g_t|), \theta_{t+1} = \theta_t - \eta \frac{\widehat{m}_t}{u_t}$$

Yogi (Zaheer et al., 2018)
$$v_t = v_{t-1} - (1 - \beta_2) \text{sign}(v_{t-1} - g_t^2) g_t^2$$

AdamX (Tran et al., 2019)
$$\widehat{m}_t=m_t, \widehat{v}_t=\max\{\frac{(1-eta_{1,t})^2}{(1-eta_{1,t-1})^2}\widehat{v}_{t-1},v_t\}$$

NAdam (Dozat, 2016) $\theta_{t+1} = \theta_t - \eta \frac{1}{\sqrt{\widehat{v_t}} + \epsilon} (\beta_1 \widehat{m}_t + \frac{1-\beta_1}{1-\beta_1^t} g_t)$, by taking $\psi = 0$ in formula below 1. In PyTorch implementation, $\theta_{t+1} = \theta_t - \eta \frac{1}{\sqrt{\widehat{v_t}} + \epsilon} (\mu_{t+1} \frac{m_t}{1-\Pi_{i=1}^{t+1} \mu_i} + \frac{(1-\mu_t)}{1-\Pi_{i=1}^t \mu_i} g_t)$, where $\mu_t = \beta_1 (1 - \frac{0.96^{t\psi}}{2})$

Padam (Chen & Gu, 2018) $\widetilde{v}_t = \max(\widetilde{v}_{t-1}, v_t)$, $\theta_{t+1} = \theta_t - \eta_t \frac{m_t}{\widetilde{v}_t^p}$. And the output is chosen from $\{\theta_t\}$ with $P(\theta_{out} = \theta_t) = \frac{\eta_{t-1}}{\sum_{t=1}^{T-1} \eta_t}$

RAdam (Liu et al., 2020a)
$$\rho_{\infty} = \frac{2}{1-\beta_2} - 1$$
, $\rho_t = \rho_{\infty} - \frac{2t\beta_2^t}{1-\beta_2^t}$. If $\rho_t > 4$, $l_t = \sqrt{(1-\beta_2^t)/v_t}$, $r_t = \sqrt{\frac{(\rho_t - 4)(\rho_t - 2)\rho_{\infty}}{(\rho_{\infty} - 4)(\rho_{\infty} - 2)\rho_t}}$, $\theta_{t+1} = \theta_t - \eta r_t \widehat{m}_t l_t$; otherwise $\theta_{t+1} = \theta_t - \eta \widehat{m}_t$.

Adam⁺ (Liu et al., 2020b) $\eta_t = \frac{\alpha \beta^{\gamma}}{\max(||z_t||^{1/2}, \epsilon_0)}$, $\theta_{t+1} = \theta_t - \eta z_t$, $z_{t+1} = (1 - \beta)z_t + \beta \nabla_{\theta} J((1 - \frac{1}{\beta})\theta_t + \frac{1}{\beta}\theta_{t+1})$, where I replace a in the original papar with γ for clarity

AdaX (Li et al., 2020)
$$v_t = (1 + \beta_2)v_{t-1} + \beta_2 g_t^2$$
, $\widehat{v_t} = \frac{v_t}{(1+\beta_2)^t - 1}$

AdaBelief (Zhuang et al., 2020)
$$v_t = \beta_2 v_{t-1} + (1 - \beta_2)(g_t - m_t)^2 + \epsilon$$

AdamWN (Loshchilov, 2023) $\widehat{\theta}_t = \theta_t - \eta \frac{\widehat{m}_t}{\sqrt{\widehat{v_t}} + \epsilon}$, $\theta_{t+1} = \widehat{\theta}_t - k_t (1 - \frac{r_t \|\theta_0\|}{\|\widehat{\theta}_t\|}) \widehat{\theta}_t$, $k_t \in [0, 1]$, $r_t \|\theta_0\|$ is the target weight norm for θ_t

C-Adam (Liang et al., 2024) $u_t = \frac{\widehat{m}_t}{\sqrt{\widehat{v}_t} + \epsilon}$, $\phi_t = \mathbf{1}_{u_t \circ g_t \ge 0}$, $\bar{\eta}_t = \eta \frac{d}{\|\phi_t\|_0 + 1}$, $\theta_{t+1} = \theta_t - \bar{\eta}_t (\phi_t \circ u_t + \lambda \theta_t)$

2.2.2 Clipping Involved

LARS (You et al., 2017) $m_t = \beta_1 m_{t-1} + (1-\beta_1)(g_t + \lambda \theta_t), \ \theta_{t+1} = \theta_t - \eta \frac{\text{Clip}(||\theta_t||, \gamma_t, \gamma_u)}{||\theta_t|| + \epsilon} m_t$, where $\text{Clip}(x, \gamma_l, \gamma_u) = \min(\max(x, \gamma_l), \gamma_u), \ \gamma_l$ is default to 0 if only 1 bound given

LAMB (You et al., 2020)
$$r_t = \frac{\widehat{m}_t}{\sqrt{\widehat{v_t}} + \epsilon}$$
, $\theta_{t+1} = \theta_t - \eta \frac{\text{Clip}(||\theta_t||, \gamma_t, \gamma_u)}{||r_t + \lambda \theta_t|| + \epsilon} (r_t + \lambda \theta_t)$

MARS-AdamW (Yuan et al., 2024) AdamW with variance reduction. See Section 5 for detail.

2.2.3 More EMA Involved

 $\begin{aligned} & \textbf{Prodigy} \ (\textbf{Bernstein} \ \& \ \textbf{Newhouse}, 2024) \ m_t = \beta_1 m_{t-1} + (1-\beta_1) \eta_t g_t, \ v_t = \beta_2 v_{t-1} + (1-\beta_2) \eta_t^2 g_t^2, \\ & r_t = \sqrt{\beta_2} r_{t-1} + (1-\sqrt{\beta_2}) \eta_t^2 g_t^\top (\theta_0 - \theta_t), \ s_t = \sqrt{\beta_2} s_{t-1} + (1-\sqrt{\beta_2}) \eta_t^2 g_t, \ \eta_{t+1} = \max(\eta_t, \frac{r_t}{\|s_t\|_1}), \\ & \theta_{t+1} = \theta_t - \eta_t \frac{m_t}{\sqrt{v_t}} \end{aligned}$

Adan (Xie et al., 2024)
$$v_t = (1 - \beta_2)v_{t-1} + \beta_2(g_t - g_{t-1}), n_t = (1 - \beta_3)n_{t-1} + \beta_3[g_t + (1 - \beta_2)(g_t - g_{t-1})]^2, \theta_t = \frac{1}{1 + \lambda \eta}[\theta - \frac{\eta}{\sqrt{n_t} + \epsilon} \circ (m_t + (1 - \beta_2)v_t)]$$

 $\textbf{AdEMAMix} \ (\text{Pagliardini et al., 2024}) \ r_t = \beta_3 r_{t-1} + (1-\beta_3) g_t, \ \theta_t = \theta_{t-1} - \eta (\frac{\widehat{m}_t + \alpha_t r_t}{\sqrt{\widehat{v}_t} + \epsilon} + \lambda \theta_{t-1})$

2.2.4 More complicated Design

Adafactor (Shazeer & Stern, 2018) $u_t = \frac{g_t}{\sqrt{\widehat{v_t}}}$, $\widehat{u}_t = \frac{u_t}{\max(1, \mathrm{RMS}(u_t)/d)}$, $\theta_{t+1} = \theta_t - \eta_t \widehat{u}_t$, where $\alpha_t = \eta \cdot \max(\epsilon_2, \mathrm{RMS}(\theta_t))$, $\beta_{2,t} = 1 - t^\tau$, and

- For weight vector $\theta_t \in \mathbb{R}^n$, $\widehat{v}_t = \beta_{2,t}\widehat{v}_{t-1} + (1 \beta_{2,t})(g_t^2 + \epsilon_1 1_n)$;
- For weight matrix $\theta_t \in \mathbb{R}^{n \times m}$, $r_t = \beta_{2,t} r_{t-1} + (1-\beta_{2,t}) (g_t^2 + \epsilon_1 \mathbf{1}_n \mathbf{1}_m^\top) \mathbf{1}_m$, $v_t = \beta_{2,t} v_{t-1} + (1-\beta_{2,t}) \mathbf{1}_n^\top (g_t^2 + \epsilon_1 \mathbf{1}_n \mathbf{1}_m^\top)$, $\hat{v}_t = r_t v_t / \mathbf{1}_n^\top r_t$.

Amos (Tian & Parikh, 2022) $c_t = (1 + \frac{1}{4}\sqrt{\eta}b_t)^{-1/2}$, $d_t = (1 + \frac{1}{4}\sqrt{\eta}\widetilde{\eta}b_t)^{-1}$, with $\widetilde{\eta}$ the expected scale for model weights θ , (Optional) $\widetilde{g}_t = \frac{\chi}{\max(\chi, \|g_t\|)}g_t$, $v_t = \beta v_{t-1} + (1-\beta)\mathrm{M}_2(\widetilde{g}_t)^2$, where $\mathrm{M}_2(a) := \sqrt{\frac{1}{k}\sum_{i=1}^k a_i^2}$ is the quadratic mean of the entries. $\widehat{v}_t = \frac{v_t}{1-\beta^t}$, $\gamma_t = c_t \frac{\eta^2}{\widehat{v}_t}\mathrm{M}_2(g_t)^2$, $\delta_t = d_t(\frac{\eta\widetilde{\eta}}{\sqrt{\widehat{v}_t}}g_t + \frac{\gamma_t}{2}\theta_t)$. $b_{t+1} = b_t + \gamma_t(1+b_t)$, (Optional) $\widetilde{\delta}_t = m_{t+1} = \mu m_t + (1-\mu)\delta_t$, $\theta_{t+1} = \theta_t - \widetilde{\delta}_t$

3 Sign of gradient

RProp (Riedmiller & Braun, 1993) for $0 < \eta^- < 1 < \eta^+$,

- If $g_t \cdot g_{t-1} > 0$, $\eta_t = \min(\eta^+ \eta_{t-1}, \eta_{max})$, $\theta_{t+1} = \theta_t \eta_t \text{Sign}(g_t)$
- If $q_t \cdot q_{t-1} < 0$, $\eta_t = \max(\eta^- \eta_{t-1}, \eta_{min})$, $\theta_{t+1} = \theta_t \Delta \theta_t$, where $\Delta \theta_t = \theta_t \theta_{t-1}$
- Otherwise $\eta_t = 1$, $\theta_{t+1} = \theta_t \eta_t \text{Sign}(q_t)$

SignSGD (Bernstein et al., 2018) $\theta_{t+1} = \theta_t - \eta \text{Sign}(g_t)$

Signum (Bernstein et al., 2018) $m_t = \beta m_{t-1} + (1-\beta)g_t$, $\theta_{t+1} = \theta_t - \eta \text{Sign}(m_t)$

Lion (Chen et al., 2023) $c_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$, $m_t = \beta_2 m_{t-1} + (1 - \beta_2) g_t$, $\theta_{t+1} = \theta_t - \eta(\operatorname{Sign}(c_t) + \lambda \theta_t)$

- Tiger (Su, 2023) (A special case of Lion when $\beta_1 = \beta_2 = \beta$) $m_t = \beta m_{t-1} + (1 \beta)g_t$, $\theta_{t+1} = \theta_t \eta(\mathrm{Sign}(m_t) + \lambda \theta_t)$. For bias and normalization parameters, $\eta_i = 0.5\eta$, $\lambda = 0$, otherwise $\eta_i = \eta \times RMS(\theta_{t,i})$, $\lambda = \mathrm{Constant} > 0$
- MARS-Lion (Yuan et al., 2024) Lion with variance reduction. See Section 5 for detail.

Grams (Cao et al., 2024) (Based on AdamW) $\theta_{t+1} = \theta_t - \eta(\operatorname{Sign}(g_t) \circ |\frac{\widehat{m}_t}{\sqrt{\widehat{v}_t} + \epsilon}| + \lambda \theta_t)$

4 Second-Order Methods

$$\theta_{t+1} = \theta_t - (\nabla^2_{\theta_t} J(\theta))^{-1} \nabla_{\theta_t} J(\theta_t) = \theta_t - \mathbf{H}_t^{-1} g_t.$$

To estimate \mathbf{H}_t , Hutchinson's method (Hutchinson, 1989) can be used: $z \sim \text{Rademacher}(0.5)$, $\frac{\partial g^\top z}{\partial \theta} = \frac{\partial g^\top}{\partial \theta} z + g^\top \frac{\partial z}{\partial \theta} = \frac{\partial g^\top}{\partial \theta} z = \mathbf{H}_t z$, $\mathbf{D} = \text{diag}(\mathbf{H}) = \mathbb{E}[z \odot (\mathbf{H}z)]$.

Another way to estimate Hessian matrix is to compute Fisher information matrix (proposed by **H-FAC** (Martens & Grosse, 2015)):

$$F = E\left[\frac{d\log p(y|x,\theta)}{d\theta} \left(\frac{d\log p(y|x,\theta)}{d\theta}\right)^{\top}\right] = E[\mathcal{D}\theta\mathcal{D}\theta^{\top}]$$

AdaHessian (Yao et al., 2021) (Based on Adam) $v_t = \beta_2 v_{t-1} + (1-\beta_2) \mathbf{D}_t^2$, $\theta_{t+1} = \theta_t - \eta \frac{\widehat{m}_t}{(\sqrt{\widehat{v_t}})^k + \epsilon}$, where k is the Hessian power

Hessian-free (Martens et al., 2010) Define the function $B_n(d) = \mathbf{H}(\theta_t)d + \lambda d$, where $\mathbf{H}(\theta_t)d = \lim_{\epsilon \to 0} \frac{\nabla f(\theta_t + \epsilon d) - g_t}{\epsilon}$. $p_t = \text{CG-Minimize}(B_t, -g_t)$, where CG-Minimize is the linear conjugate gradient algorithm, $\theta_{t+1} = \theta_t + p_t$. λ can be adjusted by Levenberg-Marquardt style heuristic: for $\rho_t = \frac{f(\theta_t + p) - f(\theta_t)}{q_{\theta_t}(p) - q_{\theta_t}(0)}$ with $q_{\theta_t}(\cdot)$ the minimization objective of CG, if $\rho_t < \frac{1}{4}, \lambda \to \frac{3}{2}\lambda$, else if $\rho_t > \frac{3}{4}, \lambda \to \frac{2}{3}\lambda$, otherwise keep λ unchanged.

Shampoo (Gupta et al., 2018) $L_t = L_{t-1} + g_t g_t^{\top}, R_t = R_{t-1} + g_t^{\top} g_t, \theta_{t+1} = \theta_t - \eta L_t^{-1/4} g_t R_t^{-1/4}$

- Proposed by Bernstein & Newhouse (2024), $\Delta\theta = -\eta (gg^\top)^{-1/4}g(g^\top g)^{-1/4} = -\eta UV^\top$, where $g = U\Sigma V^\top$ is the SVD decomposition of the gradient. To approximate this process, they developed Newton-Schulz iteration (Higham, 2008) methods for computing UV^\top , by setting $X_0 = g/\|g\|_{l_2\to l_2}$ or $X_0 = g/\|g\|_F$, where $\|M\|_{\alpha\to\beta} := \max_x \frac{\|Mx\|_\beta}{\|x\|_\alpha}$ is the induced operator norm. Then UV^\top can be approximated by several iteration of $X_{t+1} = \frac{3}{2}X_t \frac{1}{2}X_tX_t^\top X_t$.
- MARS-Shampoo (Yuan et al., 2024): Shampoo with variance reduction. See Section 5 for detail.

SOAP (Vyas et al., 2024) (Only for 2D parameters) $g'_t = Q_L^\top g Q_R$, $m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t$, $m'_t = Q_L^\top m_t Q_R$, $v_t = \beta_2 v_{t-1} + (1-\beta_2) (g'_t)^2$, $\theta_{t+1} = \theta_t - \eta Q_L \frac{\hat{m}'_t}{\sqrt{\hat{v}_t + \epsilon}} Q_R^\top$, where $\hat{m}'_t = \frac{m'_t}{1-\beta_1^t}$, $\hat{v}_t = \frac{v_t}{1-\beta_2^t}$. $L_t = \beta_2 L_{t-1} + (1-\beta_2) g g^\top$, $R_t = \beta_2 R_{t-1} + (1-\beta_2) g^\top g$. For every k steps, obtain $Q_L = \text{QR-Eigenvectors}(LQ_L)$, $Q_R = \text{QR-Eigenvectors}(RQ_R)$, where QR-Eigenvectors returns the eigenvector matrix of the QR decomposition for the input matrix.

Muon (Jordan et al., 2024) (Only for 2D parameters) $m_t = \mu m_{t-1} + g_t$, $O_t = \text{NewtonSchulz5}(m_t)$, $\theta_{t+1} = \theta_t - \eta O_t$, where NewtonSchulz5 is the Newton-Schulz methods explained above for 5 iterations with $X_{t+1} = aX_t + bX_tX_t^{\top}X_t + c(X_tX_t^{\top})^2X_t$ for (a,b,c) = (3.4445, -4,7750, 2.0315).

Sophia (Liu et al., 2024) $m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$, if $t \mod k = 1$ for the size of the step group k, $h_t = \beta_2 h_{t-k} + (1 - \beta_2) \hat{h}_t$, where \hat{h}_t is calculated using one of the following Hessian estimators:

- Hutchinson: Draw $u \sim \mathcal{N}(0, I_d)$, $\widehat{h}_t = u \odot \nabla(\langle g_t, u \rangle)$;
- Gauss-Newton-Bartlett: Compute logits on mini-batch $\{l(\theta_t, \boldsymbol{\xi}_{t,b})\}_{b=1}^B$, sample $\widehat{y}_{t,b} \sim \operatorname{Softmax}(l(\theta_t, \boldsymbol{\xi}_{t,b})), \forall b \in [B].$ $\widehat{g} = \frac{1}{B} \nabla L(l(\theta_t, \boldsymbol{\xi}_{t,b}), \widehat{y}_{t,b})$ with loss function $l, \widehat{h} = B \cdot \widehat{g} \odot \widehat{g}$,

Otherwise, $h_t = h_{t-1}$. $\theta_{t+1} = \theta_t - \eta(\text{Clip}(\frac{m_t}{\max\{\gamma h_t, \epsilon\}}, 1) - \lambda \theta_t)$

5 Variance Reduction

SAG (Roux et al., 2012) $\theta_{t+1} = \theta_t - \frac{\eta}{n} \sum_{i=1}^n y_{i,t}$, where at each t, one ξ_{i_t} is chosen and $y_{i,t} = \nabla f(\theta_t, \xi_{i,t})$ and for other samples, keep $y_{\cdot,t}$ unchanged.

SDCA (Shalev-Shwartz & Zhang, 2013) (For machine learning task $L(\theta) = \frac{1}{n} \sum_{i=1}^{n} \phi_i(\theta^\top \boldsymbol{\xi}_i) + \frac{\lambda}{2} \|\theta\|^2$ with scalar convex function ϕ_i), for $\boldsymbol{\xi}_t = \boldsymbol{\xi}_i$, $\Delta \alpha_t = \arg \max_{\Delta \alpha} -\phi_i^* (-(\alpha_{t-1} + \Delta \alpha), \boldsymbol{\xi}_t) - \frac{\lambda n}{2} \|\theta_{t-1} + \frac{1}{\lambda n} \boldsymbol{\xi}_t \Delta \alpha\|^2$, $\alpha_t = \alpha_{t-1} + \Delta \alpha_t e_i$, $\theta_t = \theta_{t-1} + (\lambda n)^{-1} \boldsymbol{\xi}_t \Delta \alpha_t$. Output $\frac{1}{T} \sum_{i=1}^{T} \theta_{t-1}$ or randomly chosen from $\{\theta_t\}_{t=1}^T$.

SAGA (Defazio et al., 2014) Keep a $n \times d$ matrix $\phi = \{\nabla f(\theta_0, \boldsymbol{\xi}_i)\}_{i=1}^n$ storing the parameters, for $\boldsymbol{\xi}_t = \boldsymbol{\xi}_j$, $\theta_{t+1} = \arg\min_{\theta} \{h(\theta) + \frac{1}{2\gamma} \|\theta - (\theta_t - \gamma[\nabla f(\theta_t, \boldsymbol{\xi}_t) - \phi_j + \frac{1}{n}\sum_{i=1}^n \phi_i])\|^2\}$, where $h(\theta)$ is the regularization function, then update $\phi_i = \theta_t$ and keep other ϕ_i unchanged.

SVRG (Johnson & Zhang, 2013) For each epoch s, calculate the full gradient g_s for θ_s . For each iteration t, $\theta_{s,t+1} = \theta_{s,t} - \eta(\nabla f(\theta_{s,t}, \boldsymbol{\xi}_{s,t}) - \nabla f(\theta_s, \boldsymbol{\xi}_{s,t}) + g_s)$, set $\theta_s = \theta_{s,T}$ or randomly chosen from $\{\theta_{s,t}\}_{t=1}^T$

SARAH (Nguyen et al., 2017) For each epoch s, calculate the full gradient $v_{s,0} = g_s$ for θ_s , $\theta_{s,1} = \theta_{s,0} - \eta v_{s,0}$. For each iteration t, $v_{s,t} = \nabla f(\theta_{s,t}, \boldsymbol{\xi}_{s,t}) - \nabla f(\theta_s, \boldsymbol{\xi}_{s,t}) + v_{s,t-1}$, $\theta_{s,t+1} = \theta_{s,t} - \eta v_{s,t}$, set θ_s randomly chosen from $\{\theta_{s,t}\}_{t=1}^T$.

Hybrid-SGD (Tran-Dinh et al., 2019) (Hybrid SGD with SARAH) $m_t = \beta(m_{t-1} + g_t - \nabla f(\theta_{t-1}, \boldsymbol{\xi}_t)) + (1-\beta)g_t, \theta_{t+1} = \theta_t - \eta m_t$

SPIDER-SFO (Fang et al., 2018) $v_t = g_t$ for every q steps with batch size S_1 , otherwise $v_t = g_t - \nabla f(\theta_{t-1}, \boldsymbol{\xi}_t) + v_{t-1}$. Update parameters with Option I: $\theta_{t+1} = \theta_t - \eta v_t / \|v_t\|$ until $\|v_t\|$ less than some threshold, or Option II: $\theta_{t+1} = \theta_t - \eta_t v_t$ with $\eta_t = \min(\eta/\|v_t\|, \eta/(2\epsilon))$. Output θ_T or randomly choose from $\{\theta_t\}_{t=1}^T$.

SpiderBoost (Wang et al., 2019) $v_t = g_t - \nabla f(\theta_{t-1}, \xi_t) + v_{t-1}, \theta_{t+1} = \theta_t - \eta v_t / ||v_t||$

SNVRG (Zhou et al., 2020) For loop parameters $\{T_l\}$, set $T = \prod_{l=1}^K T_l$ or $T \sim \text{Geom}(1/(1+\prod_{l=1}^K T_l))$ as the total number of steps. For each step $t, r_t = \min\{j: 0 = (t \mod \prod_{l=j+1}^K T_l), 0 \le j \le K\}$. For $0 \le l \le r_t - 1$, $\theta_t^l = \theta_{t-1}^l$; otherwise $\theta_t^l = \theta_t$. For $0 \le l \le r_t - 1$, $g_t^l = g_{t-1}^l$; for $r_t + 1 \le l \le K$, $g_t^l = 0$. Then uniformly generate index set I_t with size B_{r_t} , if $r_t > 0$, $g_t^{r_t} = \frac{1}{B_{r_t}} \sum_{i \in I_t} [\nabla f(\theta_t^{r_t}, \boldsymbol{\xi}_i) - \nabla f(\theta_t^{r_{t-1}}, \boldsymbol{\xi}_i)]$, otherwise $g_t^0 = \frac{1}{B_0} \sum_{i \in I_t} \nabla f(\theta_t^0, \boldsymbol{\xi}_i)$. And $\theta_{t+1} = \theta_t - \eta \sum_{l=0}^K g_t^l$. The output parameter is randomly chosen from $\{\theta_t\}_{t=1}^T$.

STORM (Cutkosky & Orabona, 2019) $\eta_t = \frac{k}{(w + \sum_{i=1}^t \|g_i\|^2)^{1/3}}, \ a_t = c\eta_{t-1}^2, \ \theta_{t+1} = \theta_t - \eta_t d_t,$ where $d_t = g_t + (1 - a_t)(d_{t-1} - \nabla f(\theta_{t-1}, \xi_t))$. Output is chosen uniformly at random from $x_1, ..., x_T$ (in practice x_T)

STORM⁺ (Levy et al., 2021) (Based on STORM) $a_{t+1} = \frac{1}{(1+\sum_{i=1}^{t} \|g_i\|^2)^{2/3}}, \quad \eta_t = \frac{1}{(\sum_{i=1}^{t} \|d_i\|^2/a_{i+1})^{1/3}}$

Super-Adam (Huang et al., 2021) (Based on Adam) $c_t = \alpha_t g_t + (1 - \alpha_t)[c_{t-1} + \tau(g_t - \nabla f(\theta_{t-1}, \boldsymbol{\xi}_t))], \tau \in \{0, 1\}, \widetilde{\theta}_t = \arg\min_{\theta} \{\eta \langle c_t, \theta \rangle + \frac{1}{2}||\theta - \theta_t||^2_{\mathbf{H}_t}\}, \theta_{t+1} = (1 - \mu_t)\theta_t + \mu_t \widetilde{\theta}_t,$ where \mathbf{H}_t is defined by one of the following cases:

- Case 1: $\mathbf{H}_t = \operatorname{diag}(\sqrt{v_t} + \lambda)$
- Case 2: $v_t = \beta v_{t-1} + (1 \beta) ||g_t||, \mathbf{H}_t = (v_t + \lambda) I_d$
- Case 3 (Barzilai-Borwein technique): $b_t = \frac{\|\langle g_t \nabla f(\theta_{t-1}, \boldsymbol{\xi}_t), \theta_t \theta_{t-1} \rangle\|}{\|\theta_t \theta_{t-1}\|}, \mathbf{H}_t = (b_t + \lambda)I_d$
- Case 4-1: $v_t = \beta_2 v_{t-1} + (1 \beta_2)(g_t m_t)^2$, $\mathbf{H}_t = \operatorname{diag}(\sqrt{v_t} + \lambda)$
- Case 4-2: $v_t = \beta_2 v_{t-1} + (1 \beta_2) \| g_t m_t \|$, $\mathbf{H}_t = (v_t + \lambda) I_d$

ROOT-SGD (Li et al., 2022) $v_t = g_t + \frac{t-1}{t}(v_{t-1} - \nabla f(\theta_{t-1}, \xi_t)), \theta_{t+1} = \theta_t - \eta v_t$

AdaSVRPS/AdaSVRLS (Jiang & Stich, 2024) $F_{\boldsymbol{\xi}_t}(\theta) = f(\theta, \boldsymbol{\xi}_t) + \mathbf{w}^\top (\nabla f(\mathbf{w}_t) - \nabla f(\mathbf{w}_t, \boldsymbol{\xi}_t)) + \frac{\mu_F}{2} \|\theta - \theta_t\|^2$, $\theta_{t+1} = \theta_t - \eta_t \nabla_\theta F_{\boldsymbol{\xi}_t}(\theta_t)$. With probability p_{t+1} , $\mathbf{w}_{t+1} = \theta_t$, otherwise $\mathbf{w}_{t+1} = \mathbf{w}_t$. Output $\frac{1}{T} \sum_{t=0}^T \theta_t$. Here

- $\bullet \ \, \eta_t = \min\{\frac{F_{\pmb{\xi}_t}(\theta_t) F^*_{\pmb{\xi}_t}}{c_p \|\nabla F_{\pmb{\xi}_t}(\theta_t)\|^2 \sqrt{\sum_{s=0}^t F_{\pmb{\xi}_s}(\theta_s) F^*_{\pmb{\xi}_s}}}, \eta_{t-1}\} \text{ for AdaSVRPS}$
- $\eta_t = \min\{\gamma_t \frac{1}{c_t\sqrt{\sum_{s=0}^t \gamma_s \|\nabla F_{\boldsymbol{\xi}_s}(\theta_s)\|^2}}, \eta_{t-1}\}$ for AdaSVRLS, where γ_t can be obtained by Armijo Backtracking line-search (Armijo, 1966; Nocedal & Wright, 2006): do $\gamma = \beta \gamma$ until $f(\theta_t \gamma \nabla f(\theta_t, \boldsymbol{\xi}_t), \boldsymbol{\xi}_t) \leq f(\theta_t, \boldsymbol{\xi}_t) \rho \gamma \|\nabla f(\theta_t, \boldsymbol{\xi}_t)\|^2$

• For AdaSPS and AdaSLS, just set $F_{\xi_t}(\theta) = f(\theta, \xi_t)$ and set $F_{\xi_t}^*$ as a predefined lower bound.

MARS (Yuan et al., 2024) (Based on AdamW/Lion/Shampoo) $c_t = g_t + \gamma_t \frac{\beta_1}{1-\beta_1} (g_t - \nabla f(\theta_{t-1}, \boldsymbol{\xi}_t)),$ $\widetilde{c}_t = \operatorname{Clip}(c_t, 1), \ m_t = \beta_1 m_{t-1} + (1-\beta_1) \widetilde{c}_t, \ \theta_{t+1} = \arg \min_{\theta} \{ \eta \langle m_t, \theta \rangle + \frac{1}{2} \| \theta - \theta_t \|_{\mathbf{H}_t}^2 \}, \text{ or } \theta_{t+1} = \arg \min_{\theta} \{ \eta \langle m_t, \theta \rangle + \frac{1}{2} \| \theta - (1-\eta\lambda)\theta_t \|_{\mathbf{H}_t}^2 \}$ with weight decay.

- MARS-AdamW: $v_t = \beta_2 v_{t-1} + (1 \beta_2) \tilde{c}_t^2$, $\mathbf{H}_t := \sqrt{\operatorname{diag}(v_t)} \cdot \frac{1 \beta_1^t}{\sqrt{1 \beta_2^t}}$, (equivalently, $\theta_{t+1} = \theta_t \eta(\frac{\hat{m}_t}{\sqrt{\hat{m}_t} + \epsilon} + \lambda \theta_t)$)
- MARS-Lion: $\mathbf{H}_t = \sqrt{\operatorname{diag}(m_t^2)}$, (equivalently, $\theta_{t+1} = \theta_t \eta(\operatorname{Sign}(m_t) + \lambda \theta_t)$)
- MARS-Shampoo: $\mathbf{H}_t = (\sum_{\tau=1}^t g_\tau g_\tau^\top)^{1/4} \otimes (\sum_{\tau=1}^t g_\tau^\top g_\tau)^{1/4}$, (equivalently, $U_t, \Sigma_t, V_t = \mathrm{SVD}(m_t) \; \theta_{t+1} = \theta_t \eta(U_t V_t^\top + \lambda \theta_t)$), and use Newton-Schulz iteration methods to approximate SVD decomposition (See Section 4 for detail).

6 Scheduler-Free Methods

Schedule-Free AdamW (Defazio et al., 2024)

- (Form 1) $y_t = (1 \beta_1)z_t + \beta_1\theta_t$, $g_t = \nabla_{\theta}J(y_t)$, $\eta_t = \eta\sqrt{1 \beta_2^t}\min(1, t/T_{\text{warmup}})$, $z_{t+1} = z_t \eta_t(\frac{g_t}{\sqrt{v_t} + \epsilon} + \lambda y_t)$, $\theta_{t+1} = (1 c_{t+1})\theta_t + c_{t+1}z_{t+1}$, where $c_{t+1} = \frac{\eta_t^2}{\sum_{i=1}^t \eta_i^2}$
- (Form 2) $\eta_t = \eta \sqrt{1 \beta_2^t} \min(1, t/T_{\text{warmup}}), \ g_t = \nabla_{\theta} J(y_t), \ \Delta_t = \eta_t (\frac{g_t}{\sqrt{v_t + \epsilon}} + \lambda y_t), \ y_{t+1} = y_t + \frac{\beta_1 c_{t+1}}{1 \beta_1} (y_t \theta_t) [\beta_1 c_{t+1} + (1 \beta_1)] \Delta_t, \ \theta_{t+1} = \theta_t + \frac{c_{t+1}}{1 \beta_1} (y_t \theta_t) c_{t+1} \Delta_t, \ \text{where } c_{t+1} = \frac{\eta_t^2}{\sum_{i=1}^t \eta_i^2}$

D-Adaptation (Defazio & Mishchenko, 2023)

- Dual Averaging: $m_t = m_{t-1} + d_{t-1}g_t$, $\eta_t = \frac{1}{\sqrt{\sum_{i=0}^k \|g_i\|^2}}$. For \widehat{d}_t , option I: $\widehat{d}_t = \frac{\eta_t \|m_t\|^2 \sum_{i=0}^{t-1} \eta_i d_i^2 \|g_{i+1}\|^2}{2\|m_t\|}$ or option II: $\widehat{d}_t = \frac{\sum_{i=0}^{t-1} d_i \eta_i \langle g_{i+1}, m_i \rangle}{\|m_t\|}$, $d_t = \max(d_{t-1}, \widehat{d}_t)$, $\theta_{t+1} = \theta_t \eta_t m_t$. Output $\frac{1}{\sum_{t=0}^{T-1} d_t} \sum_{t=1}^T d_{t-1}\theta_t$
- Gradient Descent: $\eta_t = \frac{d_{t-1}}{\sqrt{G^2 + \sum_{i=0}^t \|g_i\|^2}}, m_t = m_{t-1} + \eta_t g_t, \widehat{d}_t = \frac{\|m_t\|^2 \sum_{i=0}^t \eta_i^2 \|g_{i+1}\|^2}{2\|m_t\|}, d_t = \max(d_{t-1}, \widehat{d}_t), \theta_{t+1} = \theta_t \eta_t m_t. \text{ Output } \frac{1}{\sum_{t=0}^T \eta_t} \sum_{t=0}^T \eta_t \theta_t$
- AdaGrad: $m_t = m_{t-1} + d_{t-1}g_t$, $a_t^2 = a_{t-1}^2 + g_t^2$, $A_t = \operatorname{diag}(a_t)$, $\widehat{d}_t = \frac{\|m_t\|_{A_t^{-1}}^2 \sum_{i=0}^{t-1} d_i^2 \|g_{i+1}\|_{A_i^{-1}}^2}{2\|m_t\|_1}$, $d_t = \max(d_{t-1}, \widehat{d}_t)$, $\theta_{t+1} = \theta_t A_t^{-1}m_t$. Output $\frac{1}{\sum_{t=0}^{T-1} d_t} \sum_{t=1}^{T} d_{t-1}\theta_t$
- SGD: $\eta_k = \eta d_{k-1}/G$, $m_t = m_{t-1} + \eta_t g_t$, $z_t = z_{t-1} \eta_t g_t$, $\theta_{t+1} = \beta \theta_t + (1-\beta)z_t$, $\hat{d}_t = \frac{2\sum_{i=0}^{t-1} \eta_{i+1} \langle g_{i+1}, m_i \rangle}{\|m_t\|}$, $d_t = \max(d_{t-1}, \hat{d}_t)$.
- Adam version (Based on Adam) $m_t = \beta_1 m_{t-1} + (1-\beta_1) \eta d_{t-1} g_t, \ \theta_{t+1} = \theta_t \frac{m_t}{\sqrt{v_t + \epsilon}}, \ s_t = \sqrt{\beta_2} s_{t-1} + (1-\sqrt{\beta_2}) \eta d_{t-1} g_t, \ r_t = \sqrt{\beta_2} r_{t-1} + (1-\sqrt{\beta_2}) \eta d_{t-1} \left\langle g_t, s_{t-1} \right\rangle_{(\mathrm{diag}(\sqrt{v_t + \epsilon}))^{-1}}, \ \hat{d}_t = \frac{r_t}{(1-\sqrt{\beta_2})\|s_t\|_1}, \ d_t = \max(d_{t-1}, \hat{d}_t)$

Adam++ (Tao et al., 2024) $\eta_t = \max(\eta_{t-1}, \|\theta_t - \theta_0\|/\sqrt{d}), \beta_{1,t} = \beta_1 \lambda^{t-1}, m_t = \beta_{1,t} m_{t-1} + (1-\beta_{1,t})g_t, \theta_{t+1} = \theta_t - \eta_t \cdot \mathbf{H}_t^{-1} m_t$, where $\mathbf{H}_t = \epsilon + \operatorname{diag}(s_t)$, and s_t is calculated by either of the following ways:

• Case I:
$$s_t = \sqrt{\sum_{i=0}^t g_i^2}$$

• Case II:
$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$$
, $s_t = \sqrt{(t+1) \max_{t' \le t} (v_{t'})}$

AdaGrad++ (Tao et al., 2024) Similar to Adam++, but only choose Case I of s_t , and $\lambda = 0$.

7 Randomized Updating

GLD (Gradient Langevin Dynamics) (Durmus & Moulines, 2017; Dalalyan, 2017a,b) $\theta_0 = \mathbf{0}$, $\epsilon_t \sim N(0, I_{d \times d}), \theta_{t+1} = \theta_t - \eta g_t + \sqrt{2\eta/\beta} \epsilon_t$, where g_t is the full gradient.

SGLD (Welling & Teh, 2011) Same as GLD, but g_t is the average gradient over samples in small batch.

SGFS (Ahn et al., 2012) For total number of samples N and batch size $B, \gamma = \frac{B+N}{B}$. For small batch $\{\boldsymbol{\xi}_{t,i}\}_{i=1}^{B}, v_t = (1-\beta)v_{t-1} + \beta\frac{1}{n-1}\sum_{i=1}^{B}(\nabla f(\theta_t,\boldsymbol{\xi}_{t,i}) - g_t)(\nabla f(\theta_t,\boldsymbol{\xi}_{t,i}) - g_t)^{\top}, \epsilon_t \sim \mathcal{N}(0,\frac{4C}{\epsilon}), \theta_{t+1} = \theta_t + 2(\gamma Nv_t + \frac{4C}{\epsilon})^{-1}(g_t + \epsilon_t).$

SVRG-LD (Xu et al., 2018) For each epoch s, first compute the full gradient g_s for θ_s , $\widetilde{g}_{s,t} = g_{s,t} - \nabla f(g_s, \boldsymbol{\xi}_{s,t}) + g_s$, $\epsilon_t \sim N(0, I_{d \times d})$, $\theta_{t+1} = \theta_t - \eta \widetilde{g}_{s,t} + \sqrt{2\eta/\beta}\epsilon_t$. At the last iteration T for each epoch, $g_s = g_{s,T}$.

8 Reconciliation of Optimizers

AdaGraft (Agarwal et al., 2020) For optimizers $\mathcal{M}, \mathcal{D}, \theta_{t,\mathcal{M}} = \mathcal{M}(\theta_t, g_t), \theta_{t,\mathcal{D}} = \mathcal{D}(\theta_t, g_t),$ $\theta_{t+1} = \theta_t + \frac{\|\theta_{t,\mathcal{M}} - \theta_t\|}{\|\theta_{t,\mathcal{D}} - \theta_t\| + \epsilon} \cdot (\theta_{t,\mathcal{D}} - \theta_t)$

9 Architecture-specific Optimizers

GaLore (Zhao et al., 2024a) (Adam for LLM layer weight matrix): $\theta_t \in \mathbb{R}^{m \times n}$, if $t \mod T = 0$ $U, S, V = \text{SVD}(g_t)$, $P_t = U[:,:r]$ (low-rank projection), otherwise $P_t = P_{t-1}$. Then estimate the low-rank gradient $R_t = P_t^{\top} g_t$, and use Adam to optimize: $\theta_{t+1} = \theta_t + \eta \alpha P_t \frac{m_t}{\sqrt{v_t + \epsilon}}$ with scale factor α

Adam-mini (Zhang et al., 2024) (Based on Adam) (For each parameter in parameter blocks) $v_t = \beta_2 v_{t-1} + (1 - \beta_2) * \text{Mean}(g \odot g)$. For Transformers, partition the parameters of embedding and output layers by tokens, partition the parameters of query and key matrices by heads, and partition the parameters of value matrices, attention projection matrices and MLP layers by output neurons.

Adalayer (Zhao et al., 2024b) (Based on Adam, for language model) For each layer: $v_t = \beta_2 v_{t-1} + (1-\beta_2) \|g_t\|_2^2 / \sqrt{p}$ with p the number of parameters in each layer, $\theta_{t+1} = \theta_t - \eta \frac{m_t}{\sqrt{v_t} + \epsilon}$

STORM-PG (Yuan et al., 2020) (Based on Reinforce Learning tasks) $\theta_{t+1} = \theta_t + \eta \widehat{g}_t$, $\widehat{g}_{t+1} = (1-\gamma)g_t' + g_t$, where $g_t = \frac{1}{B}\sum_{i\in\mathcal{B}}d_i(\theta_{t+1})$, $g_t' = \frac{1}{B}\sum_{i\in\mathcal{B}}[\widehat{g}_t - d_i^{\theta_{t+1}}(\theta_t)]$ is the gradient estimation with different parameters on small batch of trajectories $\{\tau_i\}_{i\in\mathcal{B}}$ with size B, and $d_i(\theta) = \sum_{h=0}^{H-1}d_{i,h}(\theta)$, $d_i^{\theta'}(\theta) = \sum_{h=0}^{H-1}\frac{p(\tau_{i,h}|\theta)}{p(\tau_{i,h}|\theta')}d_{i,h}(\theta)$, where $d_{i,h}(\theta) = (\sum_{t=0}^h \nabla \log \pi_{\theta}(a_t|s_t))(\gamma^h r(s_h,a_h) - b_h)$.

SPPO (Wu et al., 2024) (Based on Reinforce Learning tasks)

$$\theta_{t+1} = \arg\min_{\theta} \mathbb{E}_{(\boldsymbol{\xi}_t, y_t, \widehat{P}(y_t \succ \pi_t | \boldsymbol{\xi}_t))} \left(\log \left(\frac{\pi_{\theta}(y_t | \boldsymbol{\xi}_t)}{\pi_t(y_t | \boldsymbol{\xi}_t)} \right) - \eta (\widehat{P}(y_t \succ \pi_t | \boldsymbol{\xi}_t) - \frac{1}{2}) \right)^2,$$

where $\pi_t = \pi_{\theta_t}$ is the policy model with the parameter θ_t .

10 Something Beyond Optimizers

In the previous sections, I did not emphasize the changing of the learning rate η . In this section, I collected some interesting research related to the changing rule of learning rate (Scheduler).

10.1 Scheduler

Warmup-Stable-Decay (WSD) Scheduler (Hu et al., 2024) Different from the Cosine Learning Rate Scheduler, in MiniCPM, the researchers utilized WSD scheduler (linear warmup-stable learning rate-decay). It is widely used in industry because it can support continual training, and decaying schedule in the end is also compatible for downstream tasks fine-tuning.

For intermediate checkpoints, WSD performs decay schedule and starts from the state before decay when continuing training. However, in WSD-S (Wen et al., 2024), the researchers find that the dispose of training in decay phase is not necessary, and just starts from the state after decay with the max learning rate is fine.

10.2 Schedule Refinement

Schedule Refinement (Defazio et al., 2023) The researchers perform comprehensive evaluation of learning rate schedules, give proofs on the convergence of some common optimization approaches, and proposed some important conclusions and algorithms:

- Warm-up followed by linear decay is the best overall non-adaptive schedule, outperforming cosine decay.
- Schedule Refinement for SGD $\widehat{g}_t = \text{Median-filter}(\|g_t\|, \text{width} = \tau T, \text{pad} = (\text{nearest, reflect})), w_t = \widehat{g}_t^{-2}, \eta_t' = w_t \sum_{p=t+1}^T w_p, \eta_t = \eta_t' / \max_p(\eta_p').$
- Schedule Refinement for SGD $\widehat{g}_t = \text{Median-filter}(\|\sum_{i=1}^d \frac{g_{t,i}^2}{\sqrt{v_{t,i}}}\|, \text{width} = \tau T, \text{pad} = (\text{nearest, reflect})), w_t = \widehat{g}_t^{-1}, \eta_t' = w_t \sum_{p=t+1}^T w_p, \eta_t = \eta_t' / \max_p(\eta_p').$

10.3 "Scaling Law" of Learning Rate

 μ P and Tensor Program series (Yang et al., 2022) In Tensor Program series, the researchers led by Greg Yang² provides theoretical foundation for the "Scaling Law" of hyper-parameter to the model size. In Tensor Program V (μ P), they researched how the best hyper-parameters (including initialization variances and learning rates for different optimizers of different components in deep learning models) change with respect to the size of these components.

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