# Advanced Stochastic Gradient Methods

## Daniil Merkulov

Optimization methods. MIPT

# Finite-sum problem

# Finite-sum problem

We consider classic finite-sample average minimization:

$$\min_{x \in \mathbb{R}^p} f(x) = \min_{x \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} f_i(x)$$

The gradient descent acts like follows:

$$x_{k+1} = x_k - \frac{\alpha_k}{n} \sum_{i=1}^{n} \nabla f_i(x) \tag{GD}$$

- Iteration cost is linear in $n$.

# Finite-sum problem

We consider classic finite-sample average minimization:

$$\min_{x \in \mathbb{R}^p} f(x) = \min_{x \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} f_i(x)$$

The gradient descent acts like follows:

$$x_{k+1} = x_k - \frac{\alpha_k}{n} \sum_{i=1}^{n} \nabla f_i(x) \tag{GD}$$

- Iteration cost is linear in $n$.
- Convergence with constant $\alpha$ or line search.

# Finite-sum problem

We consider classic finite-sample average minimization:

$$\min_{x \in \mathbb{R}^p} f(x) = \min_{x \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} f_i(x)$$

The gradient descent acts like follows:

$$x_{k+1} = x_k - \frac{\alpha_k}{n} \sum_{i=1}^{n} \nabla f_i(x) \tag{GD}$$

- Iteration cost is linear in $n$.
- Convergence with constant $\alpha$ or line search.

# Finite-sum problem

We consider classic finite-sample average minimization:

$$\min_{x \in \mathbb{R}^p} f(x) = \min_{x \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^n f_i(x)$$

The gradient descent acts like follows:

$$x_{k+1} = x_k - \frac{\alpha_k}{n} \sum_{i=1}^n \nabla f_i(x) \tag{GD}$$

- Iteration cost is linear in $n$.
- Convergence with constant $\alpha$ or line search.

Let's/ switch from the full gradient calculation to its unbiased estimator, when we randomly choose $i_k$ index of point at each iteration uniformly:

$$x_{k+1} = x_k - \alpha_k \nabla f_{i_k}(x_k) \tag{SGD}$$

With $p(i_k = i) = \frac{1}{n}$, the stochastic gradient is an unbiased estimate of the gradient, given by:

$$\mathbb{E}[\nabla f_{i_k}(x)] = \sum_{i=1}^n p(i_k = i) \nabla f_i(x) = \sum_{i=1}^n \frac{1}{n} \nabla f_i(x) = \frac{1}{n} \sum_{i=1}^n \nabla f_i(x) = \nabla f(x)$$

This indicates that the expected value of the stochastic gradient is equal to the actual gradient of $f(x)$.

# Results for Gradient Descent

Stochastic iterations are $n$ times faster, but how many iterations are needed?

If $\nabla f$ is Lipschitz continuous then we have:

| Assumption | Deterministic Gradient Descent | Stochastic Gradient Descent |
|---|---|---|
| PL | $O(\log(1/\varepsilon))$ | $O(1/\varepsilon)$ |
| Convex | $O(1/\varepsilon)$ | $O(1/\varepsilon^2)$ |
| Non-Convex | $O(1/\varepsilon)$ | $O(1/\varepsilon^2)$ |

- Stochastic has low iteration cost but slow convergence rate.

# Results for Gradient Descent

Stochastic iterations are $n$ times faster, but how many iterations are needed?

If $\nabla f$ is Lipschitz continuous then we have:

| Assumption | Deterministic Gradient Descent | Stochastic Gradient Descent |
|---|---|---|
| PL | $O(\log(1/\varepsilon))$ | $O(1/\varepsilon)$ |
| Convex | $O(1/\varepsilon)$ | $O(1/\varepsilon^2)$ |
| Non-Convex | $O(1/\varepsilon)$ | $O(1/\varepsilon^2)$ |

- Stochastic has low iteration cost but slow convergence rate.
    - Sublinear rate even in strongly-convex case.

# Results for Gradient Descent

Stochastic iterations are $n$ times faster, but how many iterations are needed?

If $\nabla f$ is Lipschitz continuous then we have:

| Assumption | Deterministic Gradient Descent | Stochastic Gradient Descent |
|---|---|---|
| PL | $O(\log(1/\varepsilon))$ | $O(1/\varepsilon)$ |
| Convex | $O(1/\varepsilon)$ | $O(1/\varepsilon^2)$ |
| Non-Convex | $O(1/\varepsilon)$ | $O(1/\varepsilon^2)$ |

- Stochastic has low iteration cost but slow convergence rate.
    - Sublinear rate even in strongly-convex case.
    - Bounds are unimprovable under standard assumptions.

# Results for Gradient Descent

Stochastic iterations are $n$ times faster, but how many iterations are needed?

If $\nabla f$ is Lipschitz continuous then we have:

| Assumption | Deterministic Gradient Descent | Stochastic Gradient Descent |
|---|---|---|
| PL | $O(\log(1/\varepsilon))$ | $O(1/\varepsilon)$ |
| Convex | $O(1/\varepsilon)$ | $O(1/\varepsilon^2)$ |
| Non-Convex | $O(1/\varepsilon)$ | $O(1/\varepsilon^2)$ |

- Stochastic has low iteration cost but slow convergence rate.
  - Sublinear rate even in strongly-convex case.
  - Bounds are unimprovable under standard assumptions.
  - Oracle returns an unbiased gradient approximation with bounded variance.

# Results for Gradient Descent

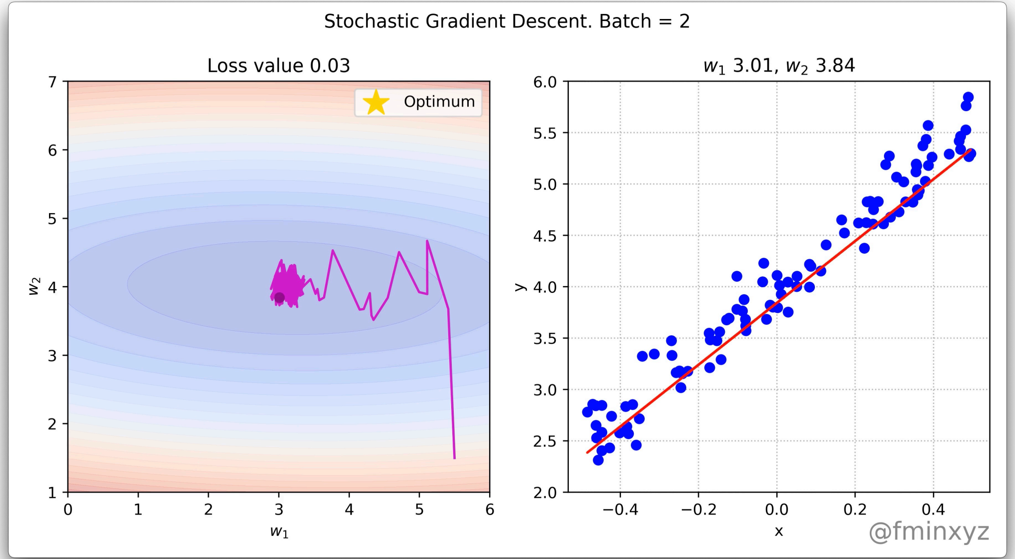
Stochastic iterations are $n$ times faster, but how many iterations are needed?

If $\nabla f$ is Lipschitz continuous then we have:

| Assumption | Deterministic Gradient Descent | Stochastic Gradient Descent |
|---|---|---|
| PL | $O(\log(1/\varepsilon))$ | $O(1/\varepsilon)$ |
| Convex | $O(1/\varepsilon)$ | $O(1/\varepsilon^2)$ |
| Non-Convex | $O(1/\varepsilon)$ | $O(1/\varepsilon^2)$ |

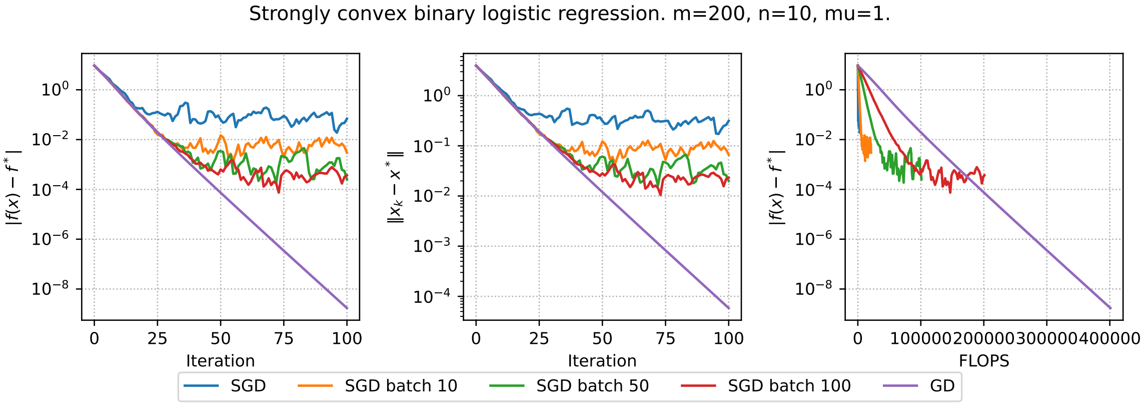
- Stochastic has low iteration cost but slow convergence rate.
    - Sublinear rate even in strongly-convex case.
    - Bounds are unimprovable under standard assumptions.
    - Oracle returns an unbiased gradient approximation with bounded variance.
- Momentum and Quasi-Newton-like methods do not improve rates in stochastic case. Can only improve constant factors (bottleneck is variance, not condition number).

# SGD with constant stepsize does not converge



# Main problem of SGD

$$f(x) = \frac{\mu}{2}\|x\|_2^2 + \frac{1}{m}\sum_{i=1}^{m} \log(1 + \exp(-y_i\langle a_i, x\rangle)) \to \min_{x \in \mathbb{R}^n}$$



# Variance reduction methods

# Key idea of variance reduction

**Principle:** reducing variance of a sample of $X$ by using a sample from another random variable $Y$ with known expectation:

$$Z_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$$

- $\mathbb{E}[Z_\alpha] = \alpha\mathbb{E}[X] + (1 - \alpha)\mathbb{E}[Y]$

# Key idea of variance reduction

**Principle:** reducing variance of a sample of $X$ by using a sample from another random variable $Y$ with known expectation:

$$Z_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$$

- $\mathbb{E}[Z_\alpha] = \alpha\mathbb{E}[X] + (1-\alpha)\mathbb{E}[Y]$
- $\text{var}(Z_\alpha) = \alpha^2\left(\text{var}(X) + \text{var}(Y) - 2\text{cov}(X,Y)\right)$

# Key idea of variance reduction

**Principle:** reducing variance of a sample of $X$ by using a sample from another random variable $Y$ with known expectation:

$$Z_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$$

- $\mathbb{E}[Z_\alpha] = \alpha \mathbb{E}[X] + (1-\alpha)\mathbb{E}[Y]$
- $\text{var}(Z_\alpha) = \alpha^2 \left(\text{var}(X) + \text{var}(Y) - 2\text{cov}(X, Y)\right)$
    - If $\alpha = 1$: no bias

# Key idea of variance reduction

**Principle:** reducing variance of a sample of $X$ by using a sample from another random variable $Y$ with known expectation:

$$Z_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$$

- $\mathbb{E}[Z_\alpha] = \alpha\mathbb{E}[X] + (1-\alpha)\mathbb{E}[Y]$
- $\text{var}(Z_\alpha) = \alpha^2\left(\text{var}(X) + \text{var}(Y) - 2\text{cov}(X, Y)\right)$
    - If $\alpha = 1$: no bias
    - If $\alpha < 1$: potential bias (but reduced variance).

# Key idea of variance reduction

**Principle:** reducing variance of a sample of $X$ by using a sample from another random variable $Y$ with known expectation:

$$Z_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$$

- $\mathbb{E}[Z_\alpha] = \alpha\mathbb{E}[X] + (1-\alpha)\mathbb{E}[Y]$
- $\text{var}(Z_\alpha) = \alpha^2 \left(\text{var}(X) + \text{var}(Y) - 2\text{cov}(X, Y)\right)$
  - If $\alpha = 1$: no bias
  - If $\alpha < 1$: potential bias (but reduced variance).
- Useful if $Y$ is positively correlated with $X$.

# Key idea of variance reduction

**Principle:** reducing variance of a sample of $X$ by using a sample from another random variable $Y$ with known expectation:

$$Z_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$$

- $\mathbb{E}[Z_\alpha] = \alpha \mathbb{E}[X] + (1 - \alpha)\mathbb{E}[Y]$
- $\text{var}(Z_\alpha) = \alpha^2 \left(\text{var}(X) + \text{var}(Y) - 2\text{cov}(X, Y)\right)$
    - If $\alpha = 1$: no bias
    - If $\alpha < 1$: potential bias (but reduced variance).
- Useful if $Y$ is positively correlated with $X$.

# Key idea of variance reduction

**Principle:** reducing variance of a sample of $X$ by using a sample from another random variable $Y$ with known expectation:

$$Z_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$$

- $\mathbb{E}[Z_\alpha] = \alpha\mathbb{E}[X] + (1-\alpha)\mathbb{E}[Y]$
- $\text{var}(Z_\alpha) = \alpha^2\left(\text{var}(X) + \text{var}(Y) - 2\text{cov}(X, Y)\right)$
    - If $\alpha = 1$: no bias
    - If $\alpha < 1$: potential bias (but reduced variance).
- Useful if $Y$ is positively correlated with $X$.

**Application to gradient estimation ?**

- SVRG: Let $X = \nabla f_{i_k}(x^{(k-1)})$ and $Y = \nabla f_{i_k}(\tilde{x})$, with $\alpha = 1$ and $\tilde{x}$ stored.

# Key idea of variance reduction

**Principle:** reducing variance of a sample of $X$ by using a sample from another random variable $Y$ with known expectation:

$$Z_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$$

- $\mathbb{E}[Z_\alpha] = \alpha\mathbb{E}[X] + (1-\alpha)\mathbb{E}[Y]$
- $\text{var}(Z_\alpha) = \alpha^2\left(\text{var}(X) + \text{var}(Y) - 2\text{cov}(X, Y)\right)$
  - If $\alpha = 1$: no bias
  - If $\alpha < 1$: potential bias (but reduced variance).
- Useful if $Y$ is positively correlated with $X$.

**Application to gradient estimation ?**

- SVRG: Let $X = \nabla f_{i_k}(x^{(k-1)})$ and $Y = \nabla f_{i_k}(\tilde{x})$, with $\alpha = 1$ and $\tilde{x}$ stored.
- $\mathbb{E}[Y] = \frac{1}{n}\sum_{i=1}^n \nabla f_i(\tilde{x})$ full gradient at $\tilde{x}$;

# Key idea of variance reduction

**Principle:** reducing variance of a sample of $X$ by using a sample from another random variable $Y$ with known expectation:

$$Z_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$$

- $\mathbb{E}[Z_\alpha] = \alpha\mathbb{E}[X] + (1-\alpha)\mathbb{E}[Y]$
- $\text{var}(Z_\alpha) = \alpha^2\left(\text{var}(X) + \text{var}(Y) - 2\text{cov}(X,Y)\right)$
  - If $\alpha = 1$: no bias
  - If $\alpha < 1$: potential bias (but reduced variance).
- Useful if $Y$ is positively correlated with $X$.

**Application to gradient estimation ?**

- SVRG: Let $X = \nabla f_{i_k}(x^{(k-1)})$ and $Y = \nabla f_{i_k}(\tilde{x})$, with $\alpha = 1$ and $\tilde{x}$ stored.
- $\mathbb{E}[Y] = \frac{1}{n}\sum_{i=1}^n \nabla f_i(\tilde{x})$ full gradient at $\tilde{x}$;
- $X - Y = \nabla f_{i_k}(x^{(k-1)}) - \nabla f_{i_k}(\tilde{x})$

# SAG (Stochastic average gradient, Schmidt, Le Roux, and Bach 2013)

- Maintain table, containing gradient $g_i$ of $f_i$, $i = 1, \dots, n$

# SAG (Stochastic average gradient, Schmidt, Le Roux, and Bach 2013)

- Maintain table, containing gradient $g_i$ of $f_i$, $i = 1, \dots, n$
- Initialize $x^{(0)}$, and $g_i^{(0)} = \nabla f_i(x^{(0)})$, $i = 1, \dots, n$

# SAG (Stochastic average gradient, Schmidt, Le Roux, and Bach 2013)

- Maintain table, containing gradient $g_i$ of $f_i$, $i = 1, \dots, n$
- Initialize $x^{(0)}$, and $g_i^{(0)} = \nabla f_i(x^{(0)})$, $i = 1, \dots, n$
- At steps $k = 1, 2, 3, \dots$, pick random $i_k \in \{1, \dots, n\}$, then let

$$g_{i_k}^{(k)} = \nabla f_{i_k}(x^{(k-1)}) \quad \text{(most recent gradient of } f_{i_k}\text{)}$$

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

# SAG (Stochastic average gradient, Schmidt, Le Roux, and Bach 2013)

- Maintain table, containing gradient $g_i$ of $f_i$, $i = 1, \dots, n$
- Initialize $x^{(0)}$, and $g_i^{(0)} = \nabla f_i(x^{(0)})$, $i = 1, \dots, n$
- At steps $k = 1, 2, 3, \dots$, pick random $i_k \in \{1, \dots, n\}$, then let

$$g_{i_k}^{(k)} = \nabla f_{i_k}(x^{(k-1)}) \quad \text{(most recent gradient of } f_{i_k}\text{)}$$

  Set all other $g_i^{(k)} = g_i^{(k-1)}$, $i \neq i_k$, i.e., these stay the same
- Update

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

# SAG (Stochastic average gradient, Schmidt, Le Roux, and Bach 2013)

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

$$g_{i_k}^{(k)} = \nabla f_{i_k}(x^{(k-1)}) \quad \text{(most recent gradient of } f_{i_k}\text{)}$$

  Set all other $g_i^{(k)} = g_i^{(k-1)}$, $i \neq i_k$, i.e., these stay the same
- Update

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

- SAG gradient estimates are no longer unbiased, but they have greatly reduced variance

# SAG (Stochastic average gradient, Schmidt, Le Roux, and Bach 2013)

- Maintain table, containing gradient $g_i$ of $f_i$, $i = 1, \dots, n$
- Initialize $x^{(0)}$, and $g_i^{(0)} = \nabla f_i(x^{(0)})$, $i = 1, \dots, n$
- At steps $k = 1, 2, 3, \dots$, pick random $i_k \in \{1, \dots, n\}$, then let

$$g_{i_k}^{(k)} = \nabla f_{i_k}(x^{(k-1)}) \quad \text{(most recent gradient of } f_{i_k}\text{)}$$

  Set all other $g_i^{(k)} = g_i^{(k-1)}$, $i \neq i_k$, i.e., these stay the same
- Update

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

- SAG gradient estimates are no longer unbiased, but they have greatly reduced variance
- Isn't it expensive to average all these gradients? Basically just as efficient as SGD, as long we're clever:

$$x^{(k)} = x^{(k-1)} - \alpha_k \underbrace{\left( \frac{1}{n} g_i^{(k)} - \frac{1}{n} g_i^{(k-1)} + \underbrace{\frac{1}{n} \sum_{i=1}^{n} g_i^{(k-1)}}_{\text{old table average}} \right)}_{\text{new table average}}$$

# SAG convergence

Assume that $f(x) = \frac{1}{n}\sum_{i=1}^{n} f_i(x)$, where each $f_i$ is differentiable, and $\nabla f_i$ is Lipschitz with constant $L$.

Denote $\bar{x}^{(k)} = \frac{1}{k}\sum_{l=0}^{k-1} x^{(l)}$, the average iterate after $k-1$ steps.

Theorem

SAG, with a fixed step size $\alpha = \frac{1}{16L}$, and the initialization

$$g_i^{(0)} = \nabla f_i(x^{(0)}) - \nabla f(x^{(0)}), \quad i = 1, \dots, n$$

satisfies

$$\mathbb{E}[f(\bar{x}^{(k)})] - f^\star \leq \frac{48n}{k}[f(x^{(0)}) - f^\star] + \frac{128L}{k}\|x^{(0)} - x^\star\|^2$$

where the expectation is taken over random choices of indices.

# SAG convergence

- Result stated in terms of the average iterate $\bar{x}^{(k)}$, but also can be shown to hold for the best iterate $x^{(k)}_{best}$ seen so far.

# SAG convergence

- Result stated in terms of the average iterate $\bar{x}^{(k)}$, but also can be shown to hold for the best iterate $x_{best}^{(k)}$ seen so far.
- This is $\mathcal{O}\left(\frac{1}{k}\right)$ convergence rate for SAG. Compare to $\mathcal{O}\left(\frac{1}{k}\right)$ rate for GD, and $\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ rate for SGD.

# SAG convergence

- Result stated in terms of the average iterate $\bar{x}^{(k)}$, but also can be shown to hold for the best iterate $x_{best}^{(k)}$ seen so far.
- This is $\mathcal{O}\left(\frac{1}{k}\right)$ convergence rate for SAG. Compare to $\mathcal{O}\left(\frac{1}{k}\right)$ rate for GD, and $\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ rate for SGD.
- But, the constants are different! Bounds after k steps:

# SAG convergence

- Result stated in terms of the average iterate $\bar{x}^{(k)}$, but also can be shown to hold for the best iterate $x_{best}^{(k)}$ seen so far.
- This is $\mathcal{O}\left(\frac{1}{k}\right)$ convergence rate for SAG. Compare to $\mathcal{O}\left(\frac{1}{k}\right)$ rate for GD, and $\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ rate for SGD.
- But, the constants are different! Bounds after k steps:
  - GD: $\frac{L\|x^{(0)}-x^\star\|^2}{2k}$

# SAG convergence

- Result stated in terms of the average iterate $\bar{x}^{(k)}$, but also can be shown to hold for the best iterate $x^{(k)}_{best}$ seen so far.
- This is $\mathcal{O}\left(\frac{1}{k}\right)$ convergence rate for SAG. Compare to $\mathcal{O}\left(\frac{1}{k}\right)$ rate for GD, and $\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ rate for SGD.
- But, the constants are different! Bounds after k steps:
  - GD: $\frac{L\|x^{(0)}-x^\star\|^2}{2k}$
  - SAG: $\frac{48n[f(x^{(0)})-f^\star]+128L\|x^{(0)}-x^\star\|^2}{k}$

# SAG convergence

- Result stated in terms of the average iterate $\bar{x}^{(k)}$, but also can be shown to hold for the best iterate $x^{(k)}_{best}$ seen so far.
- This is $\mathcal{O}\left(\frac{1}{k}\right)$ convergence rate for SAG. Compare to $\mathcal{O}\left(\frac{1}{k}\right)$ rate for GD, and $\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ rate for SGD.
- But, the constants are different! Bounds after k steps:
  - GD: $\frac{L\|x^{(0)}-x^\star\|^2}{2k}$
  - SAG: $\frac{48n[f(x^{(0)})-f^\star]+128L\|x^{(0)}-x^\star\|^2}{k}$
- So the first term in SAG bound suffers from a factor of $n$; authors suggest smarter initialization to make $f(x^{(0)}) - f^\star$ small (e.g., they suggest using the result of $n$ SGD steps).

# SAG convergence

Assume further that each $f_i$ is strongly convex with parameter $\mu$.

**Theorem**

SAG, with a step size $\alpha = \frac{1}{16L}$ and the same initialization as before, satisfies

$$\mathbb{E}[f(x^{(k)})] - f^\star \leq \left(1 - \min\left(\frac{\mu}{16L}, \frac{1}{8n}\right)\right)^k \left(\frac{3}{2}\left(f(x^{(0)}) - f^\star\right) + \frac{4L}{n}\|x^{(0)} - x^\star\|^2\right)$$

**Notes:**

- This is linear convergence rate $\mathcal{O}(\gamma^k)$ for SAG. Compare this to $\mathcal{O}(\gamma^k)$ for GD, and only $\mathcal{O}\left(\frac{1}{k}\right)$ for SGD.

# SAG convergence

Assume further that each $f_i$ is strongly convex with parameter $\mu$.

ℹ Theorem

SAG, with a step size $\alpha = \frac{1}{16L}$ and the same initialization as before, satisfies

$$\mathbb{E}[f(x^{(k)})] - f^\star \leq \left(1 - \min\left(\frac{\mu}{16L}, \frac{1}{8n}\right)\right)^k \left(\frac{3}{2}\left(f(x^{(0)}) - f^\star\right) + \frac{4L}{n}\|x^{(0)} - x^\star\|^2\right)$$

**Notes:**

- This is linear convergence rate $\mathcal{O}(\gamma^k)$ for SAG. Compare this to $\mathcal{O}(\gamma^k)$ for GD, and only $\mathcal{O}\left(\frac{1}{k}\right)$ for SGD.
- Like GD, we say SAG is adaptive to strong convexity.

# SAG convergence

Assume further that each $f_i$ is strongly convex with parameter $\mu$.

**Theorem**

SAG, with a step size $\alpha = \frac{1}{16L}$ and the same initialization as before, satisfies

$$\mathbb{E}[f(x^{(k)})] - f^\star \leq \left(1 - \min\left(\frac{\mu}{16L}, \frac{1}{8n}\right)\right)^k \left(\frac{3}{2}\left(f(x^{(0)}) - f^\star\right) + \frac{4L}{n}\|x^{(0)} - x^\star\|^2\right)$$

**Notes:**

- This is linear convergence rate $\mathcal{O}(\gamma^k)$ for SAG. Compare this to $\mathcal{O}(\gamma^k)$ for GD, and only $\mathcal{O}\left(\frac{1}{k}\right)$ for SGD.
- Like GD, we say SAG is adaptive to strong convexity.
- Proofs of these results not easy: 15 pages, computed-aided!

# SAG convergence notes

- Note, that the method in vanilla formulation is not applicable to the large neural networks training, due to the memory requirements.

# SAG convergence notes

- Note, that the method in vanilla formulation is not applicable to the large neural networks training, due to the memory requirements.
- In practice you can use backtracking strategy to estimate Lipschitz constant.

# SAG convergence notes

- Note, that the method in vanilla formulation is not applicable to the large neural networks training, due to the memory requirements.
- In practice you can use backtracking strategy to estimate Lipschitz constant.
    - Choose initial $L_0$

# SAG convergence notes

- Note, that the method in vanilla formulation is not applicable to the large neural networks training, due to the memory requirements.
- In practice you can use backtracking strategy to estimate Lipschitz constant.
  - Choose initial $L_0$
  - Increase $L$, until the following satisfies

$$f_{i_k}(x^{k+1}) \leq f_{i_k}(x^k) + \nabla f_{i_k}(x^k)(x^{k+1} - x^k) + \frac{L}{2}\|x^{k+1} - x^k\|_2^2$$

# SAG convergence notes

- Note, that the method in vanilla formulation is not applicable to the large neural networks training, due to the memory requirements.
- In practice you can use backtracking strategy to estimate Lipschitz constant.
  - Choose initial $L_0$
  - Increase $L$, until the following satisfies

$$f_{i_k}(x^{k+1}) \leq f_{i_k}(x^k) + \nabla f_{i_k}(x^k)(x^{k+1} - x^k) + \frac{L}{2}\|x^{k+1} - x^k\|_2^2$$

  - Decrease $L$ between iterations

# SAG convergence notes

- Note, that the method in vanilla formulation is not applicable to the large neural networks training, due to the memory requirements.
- In practice you can use backtracking strategy to estimate Lipschitz constant.
    - Choose initial $L_0$
    - Increase $L$, until the following satisfies

$$f_{i_k}(x^{k+1}) \leq f_{i_k}(x^k) + \nabla f_{i_k}(x^k)(x^{k+1} - x^k) + \frac{L}{2}\|x^{k+1} - x^k\|_2^2$$

    - Decrease $L$ between iterations
- Since stochastic gradient $g(x^k) \to \nabla f(x^k)$ you can use its norm to track convergence (which is not true for SGD!)

# SAG convergence notes

- Note, that the method in vanilla formulation is not applicable to the large neural networks training, due to the memory requirements.
- In practice you can use backtracking strategy to estimate Lipschitz constant.
  - Choose initial $L_0$
  - Increase $L$, until the following satisfies

$$f_{i_k}(x^{k+1}) \leq f_{i_k}(x^k) + \nabla f_{i_k}(x^k)(x^{k+1} - x^k) + \frac{L}{2}\|x^{k+1} - x^k\|_2^2$$

  - Decrease $L$ between iterations
- Since stochastic gradient $g(x^k) \to \nabla f(x^k)$ you can use its norm to track convergence (which is not true for SGD!)
- For the generalized linear models (this includes LogReg, LLS) you need to store much less memory $\mathcal{O}(n)$ instead of $\mathcal{O}(pn)$.

$$f_i(w) = \varphi(w^T x_i) \leftrightarrow \nabla f_i(w) = \varphi'(w^T x_i) x_i$$

# SAG non-uniform sampling

- The step size $\alpha_k$ and the convergence rate of the method are determined by the constant $L$ for $f(x)$, where $L = \max_{1 \leq i \leq n} L_i$, $L_i$ is the Lipschitz constant for the function $f_i$

# SAG non-uniform sampling

- The step size $\alpha_k$ and the convergence rate of the method are determined by the constant $L$ for $f(x)$, where $L = \max_{1 \le i \le n} L_i$, $L_i$ is the Lipschitz constant for the function $f_i$
- When selecting components with a probability proportional to $L_i$, the constant $L$ can be reduced from $\max_i L_i$ to $\bar{L} = \sum_i L_i / N$:

$$
\begin{aligned}
g(x) &= \frac{1}{n} \sum_{i=1}^{n} f_i(x) \\
&= \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{L_i} \frac{f_i(x)}{L_i} \\
&= \frac{1}{\sum_k L_k} \sum_{i=1}^{n} \sum_{j=1}^{L_i} \left( \sum_k \frac{L_k}{n} \frac{f_i(x)}{L_i} \right)
\end{aligned}
$$

With this approach, the component with a larger value of $L_i$ is selected more often.

# SAG non-uniform sampling

- The step size $\alpha_k$ and the convergence rate of the method are determined by the constant $L$ for $f(x)$, where $L = \max_{1 \le i \le n} L_i$, $L_i$ is the Lipschitz constant for the function $f_i$
- When selecting components with a probability proportional to $L_i$, the constant $L$ can be reduced from $\max_i L_i$ to $\bar{L} = \sum_i L_i / N$:

$$
\begin{aligned}
g(x) &= \frac{1}{n} \sum_{i=1}^{n} f_i(x) \\
&= \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{L_i} \frac{f_i(x)}{L_i} \\
&= \frac{1}{\sum_k L_k} \sum_{i=1}^{n} \sum_{j=1}^{L_i} \left( \sum_k \frac{L_k}{n} \frac{f_i(x)}{L_i} \right)
\end{aligned}
$$

With this approach, the component with a larger value of $L_i$ is selected more often.

- To ensure convergence, component selection should be carried out according to the rule: with probability 0.5, select from a uniform distribution, with probability 0.5, select with probabilities $L_i / \sum_j L_j$.

# SAG non-uniform sampling

- The step size $\alpha_k$ and the convergence rate of the method are determined by the constant $L$ for $f(x)$, where $L = \max_{1\le i\le n} L_i$, $L_i$ is the Lipschitz constant for the function $f_i$
- When selecting components with a probability proportional to $L_i$, the constant $L$ can be reduced from $\max_i L_i$ to $\bar{L} = \sum_i L_i/N$:

$$
\begin{aligned}
g(x) &= \frac{1}{n}\sum_{i=1}^{n} f_i(x) \\
&= \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{L_i} \frac{f_i(x)}{L_i} \\
&= \frac{1}{\sum_k L_k}\sum_{i=1}^{n}\sum_{j=1}^{L_i}\left(\sum_k \frac{L_k}{n}\frac{f_i(x)}{L_i}\right)
\end{aligned}
$$

With this approach, the component with a larger value of $L_i$ is selected more often.

- To ensure convergence, component selection should be carried out according to the rule: with probability 0.5, select from a uniform distribution, with probability 0.5, select with probabilities $L_i/\sum_j L_j$.
- To generate with probabilities $L_i/\sum_j L_j$, there is an algorithm with complexity $O(\log N)$.

# Stochastic Variance Reduced Gradient (SVRG)

- **Initialize:** $\tilde{x} \in \mathbb{R}^d$

# Stochastic Variance Reduced Gradient (SVRG)

- **Initialize:** $\tilde{x} \in \mathbb{R}^d$
- **For** $i_{epoch} = 1$ **to** `# of epochs`

# Stochastic Variance Reduced Gradient (SVRG)

- **Initialize:** $\tilde{x} \in \mathbb{R}^d$
- **For** $i_{epoch} = 1$ **to** `# of epochs`
    - Compute all gradients $\nabla f_i(\tilde{x})$; store $\nabla f(\tilde{x}) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(\tilde{x})$

# Stochastic Variance Reduced Gradient (SVRG)

- **Initialize:** $\tilde{x} \in \mathbb{R}^d$
- **For** $i_{epoch} = 1$ **to** `# of epochs`
  - Compute all gradients $\nabla f_i(\tilde{x})$; store $\nabla f(\tilde{x}) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\tilde{x})$
  - Initialize $x_0 = \tilde{x}$

# Stochastic Variance Reduced Gradient (SVRG)

- **Initialize:** $\tilde{x} \in \mathbb{R}^d$
- **For** $i_{epoch} = 1$ **to** `# of epochs`
    - Compute all gradients $\nabla f_i(\tilde{x})$; store $\nabla f(\tilde{x}) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\tilde{x})$
    - Initialize $x_0 = \tilde{x}$
    - **For** `t = 1` **to** `length of epochs (m)`

# Stochastic Variance Reduced Gradient (SVRG)

- **Initialize:** $\tilde{x} \in \mathbb{R}^d$
- **For** $i_{epoch} = 1$ **to** `# of epochs`
    - Compute all gradients $\nabla f_i(\tilde{x})$; store $\nabla f(\tilde{x}) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(\tilde{x})$
    - Initialize $x_0 = \tilde{x}$
    - **For** `t = 1` **to** `length of epochs (m)`
        - Pick $i_t \in \{1, \dots, n\}$ uniformly at random

# Stochastic Variance Reduced Gradient (SVRG)

- **Initialize:** $\tilde{x} \in \mathbb{R}^d$
- **For** $i_{epoch} = 1$ **to** `# of epochs`
  - Compute all gradients $\nabla f_i(\tilde{x})$; store $\nabla f(\tilde{x}) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(\tilde{x})$
  - Initialize $x_0 = \tilde{x}$
  - **For** `t = 1` **to** `length of epochs (m)`
    - Pick $i_t \in \{1, \dots, n\}$ uniformly at random
    - $x_t = x_{t-1} - \alpha \left[ \nabla f_{i_t}(x_{t-1}) - \nabla f_{i_t}(\tilde{x}) + \nabla f(\tilde{x}) \right]$

# Stochastic Variance Reduced Gradient (SVRG)

- **Initialize:** $\tilde{x} \in \mathbb{R}^d$
- **For** $i_{epoch} = 1$ **to** `# of epochs`
  - Compute all gradients $\nabla f_i(\tilde{x})$; store $\nabla f(\tilde{x}) = \frac{1}{n} \sum_{i=1}^n \nabla f_i(\tilde{x})$
  - Initialize $x_0 = \tilde{x}$
  - **For** `t = 1` **to** `length of epochs (m)`
    - Pick $i_t \in \{1, \dots, n\}$ uniformly at random
    - $x_t = x_{t-1} - \alpha \left[ \nabla f_{i_t}(x_{t-1}) - \nabla f_{i_t}(\tilde{x}) + \nabla f(\tilde{x}) \right]$
  - Update $\tilde{x} = x_m$

# Stochastic Variance Reduced Gradient (SVRG)

```
- Initialize: $\tilde{x} \in \mathbb{R}^d$
- For $i_{epoch} = 1$ to # of epochs
    - Compute all gradients $\nabla f_i(\tilde{x})$; store $\nabla f(\tilde{x}) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(\tilde{x})$
    - Initialize $x_0 = \tilde{x}$
    - For t = 1 to length of epochs (m)
        - Pick $i_t \in \{1, \dots, n\}$ uniformly at random
        - $x_t = x_{t-1} - \alpha \left[\nabla f_{i_t}(x_{t-1}) - \nabla f_{i_t}(\tilde{x}) + \nabla f(\tilde{x})\right]$
    - Update $\tilde{x} = x_m$
```

# Stochastic Variance Reduced Gradient (SVRG)

- **Initialize:** $\tilde{x} \in \mathbb{R}^d$
- **For** $i_{epoch} = 1$ **to** `# of epochs`
    - Compute all gradients $\nabla f_i(\tilde{x})$; store $\nabla f(\tilde{x}) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\tilde{x})$
    - Initialize $x_0 = \tilde{x}$
    - **For** `t = 1` **to** `length of epochs (m)`
        - Pick $i_t \in \{1, \dots, n\}$ uniformly at random
        - $x_t = x_{t-1} - \alpha \left[\nabla f_{i_t}(x_{t-1}) - \nabla f_{i_t}(\tilde{x}) + \nabla f(\tilde{x})\right]$
    - Update $\tilde{x} = x_m$

**Notes:**

- Two gradient evaluations per inner step.

# Stochastic Variance Reduced Gradient (SVRG)

- **Initialize:** $\tilde{x} \in \mathbb{R}^d$
- **For** $i_{epoch} = 1$ **to** `# of epochs`
    - Compute all gradients $\nabla f_i(\tilde{x})$; store $\nabla f(\tilde{x}) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\tilde{x})$
    - Initialize $x_0 = \tilde{x}$
    - **For** `t = 1` **to** `length of epochs (m)`
        - Pick $i_t \in \{1, \dots, n\}$ uniformly at random
        - $x_t = x_{t-1} - \alpha \left[\nabla f_{i_t}(x_{t-1}) - \nabla f_{i_t}(\tilde{x}) + \nabla f(\tilde{x})\right]$
    - Update $\tilde{x} = x_m$

**Notes:**

- Two gradient evaluations per inner step.
- Two parameters: length of epochs + step-size $\alpha$.

# Stochastic Variance Reduced Gradient (SVRG)

- **Initialize:** $\tilde{x} \in \mathbb{R}^d$
- **For** $i_{epoch} = 1$ **to** `# of epochs`
  - Compute all gradients $\nabla f_i(\tilde{x})$; store $\nabla f(\tilde{x}) = \frac{1}{n} \sum_{i=1}^n \nabla f_i(\tilde{x})$
  - Initialize $x_0 = \tilde{x}$
  - **For** `t = 1` **to** `length of epochs (m)`
    - Pick $i_t \in \{1, \dots, n\}$ uniformly at random
    - $x_t = x_{t-1} - \alpha \left[ \nabla f_{i_t}(x_{t-1}) - \nabla f_{i_t}(\tilde{x}) + \nabla f(\tilde{x}) \right]$
  - Update $\tilde{x} = x_m$

**Notes:**

- Two gradient evaluations per inner step.
- Two parameters: length of epochs + step-size $\alpha$.
- Linear convergence rate, simple proof.

# Adaptivity or scaling

# Adagrad (Duchi, Hazan, and Singer 2010)

Very popular adaptive method. Let $g^{(k)} = \nabla f_{i_k}(x^{(k-1)})$, and update for $j = 1, \dots, p$:

$$
\begin{aligned}
v_j^{(k)} &= v_j^{k-1} + (g_j^{(k)})^2 \\
x_j^{(k)} &= x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}
\end{aligned}
$$

**Notes:**

- AdaGrad does not require tuning the learning rate: $\alpha > 0$ is a fixed constant, and the learning rate decreases naturally over iterations.

# Adagrad (Duchi, Hazan, and Singer 2010)

Very popular adaptive method. Let $g^{(k)} = \nabla f_{i_k}(x^{(k-1)})$, and update for $j = 1, \dots, p$:

$$
v_j^{(k)} = v_j^{k-1} + (g_j^{(k)})^2
$$

$$
x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}
$$

**Notes:**

- AdaGrad does not require tuning the learning rate: $\alpha > 0$ is a fixed constant, and the learning rate decreases naturally over iterations.
- The learning rate of rare informative features diminishes slowly.

# Adagrad (Duchi, Hazan, and Singer 2010)

Very popular adaptive method. Let $g^{(k)} = \nabla f_{i_k}(x^{(k-1)})$, and update for $j = 1, \ldots, p$:

$$v_j^{(k)} = v_j^{k-1} + (g_j^{(k)})^2$$

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}$$

**Notes:**

- AdaGrad does not require tuning the learning rate: $\alpha > 0$ is a fixed constant, and the learning rate decreases naturally over iterations.
- The learning rate of rare informative features diminishes slowly.
- Can drastically improve over SGD in sparse problems.

# Adagrad (Duchi, Hazan, and Singer 2010)

Very popular adaptive method. Let $g^{(k)} = \nabla f_{i_k}(x^{(k-1)})$, and update for $j = 1, \dots, p$:

$$
v_j^{(k)} = v_j^{k-1} + (g_j^{(k)})^2
$$

$$
x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}
$$

**Notes:**

- AdaGrad does not require tuning the learning rate: $\alpha > 0$ is a fixed constant, and the learning rate decreases naturally over iterations.
- The learning rate of rare informative features diminishes slowly.
- Can drastically improve over SGD in sparse problems.
- Main weakness is the monotonic accumulation of gradients in the denominator. AdaDelta, Adam, AMSGrad, etc. improve on this, popular in training deep neural networks.

# Adagrad (Duchi, Hazan, and Singer 2010)

Very popular adaptive method. Let $g^{(k)} = \nabla f_{i_k}(x^{(k-1)})$, and update for $j = 1, \ldots, p$:

$$
v_j^{(k)} = v_j^{k-1} + (g_j^{(k)})^2
$$

$$
x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}
$$

**Notes:**

- AdaGrad does not require tuning the learning rate: $\alpha > 0$ is a fixed constant, and the learning rate decreases naturally over iterations.
- The learning rate of rare informative features diminishes slowly.
- Can drastically improve over SGD in sparse problems.
- Main weakness is the monotonic accumulation of gradients in the denominator. AdaDelta, Adam, AMSGrad, etc. improve on this, popular in training deep neural networks.
- The constant $\epsilon$ is typically set to $10^{-6}$ to ensure that we do not suffer from division by zero or overly large step sizes.

# RMSProp (Tieleman and Hinton, 2012)

An enhancement of AdaGrad that addresses its aggressive, monotonically decreasing learning rate. Uses a moving average of squared gradients to adjust the learning rate for each weight. Let $g^{(k)} = \nabla f_{i_k}(x^{(k-1)})$ and update rule for $j = 1, \dots, p$:

$$v_j^{(k)} = \gamma v_j^{(k-1)} + (1-\gamma)(g_j^{(k)})^2$$

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}$$

**Notes:**

- RMSProp divides the learning rate for a weight by a running average of the magnitudes of recent gradients for that weight.

# RMSProp (Tieleman and Hinton, 2012)

An enhancement of AdaGrad that addresses its aggressive, monotonically decreasing learning rate. Uses a moving average of squared gradients to adjust the learning rate for each weight. Let $g^{(k)} = \nabla f_{i_k}(x^{(k-1)})$ and update rule for $j = 1, \dots, p$:

$$v_j^{(k)} = \gamma v_j^{(k-1)} + (1-\gamma)(g_j^{(k)})^2$$

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}$$

**Notes:**

- RMSProp divides the learning rate for a weight by a running average of the magnitudes of recent gradients for that weight.
- Allows for a more nuanced adjustment of learning rates than AdaGrad, making it suitable for non-stationary problems.

# RMSProp (Tieleman and Hinton, 2012)

An enhancement of AdaGrad that addresses its aggressive, monotonically decreasing learning rate. Uses a moving average of squared gradients to adjust the learning rate for each weight. Let $g^{(k)} = \nabla f_{i_k}(x^{(k-1)})$ and update rule for $j = 1, \dots, p$:

$$v_j^{(k)} = \gamma v_j^{(k-1)} + (1 - \gamma)(g_j^{(k)})^2$$

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}$$

**Notes:**

- RMSProp divides the learning rate for a weight by a running average of the magnitudes of recent gradients for that weight.
- Allows for a more nuanced adjustment of learning rates than AdaGrad, making it suitable for non-stationary problems.
- Commonly used in training neural networks, particularly in recurrent neural networks.

# Adadelta (Zeiler, 2012)

An extension of RMSProp that seeks to reduce its dependence on a manually set global learning rate. Instead of accumulating all past squared gradients, Adadelta limits the window of accumulated past gradients to some fixed size $w$. Update mechanism does not require learning rate $\alpha$:

$$
\begin{aligned}
v_j^{(k)} &= \gamma v_j^{(k-1)} + (1-\gamma)(g_j^{(k)})^2 \\
\tilde{g}_j^{(k)} &= \frac{\sqrt{\Delta x_j^{(k-1)} + \epsilon}}{\sqrt{v_j^{(k)} + \epsilon}} g_j^{(k)} \\
x_j^{(k)} &= x_j^{(k-1)} - \tilde{g}_j^{(k)} \\
\Delta x_j^{(k)} &= \rho \Delta x_j^{(k-1)} + (1-\rho)(\tilde{g}_j^{(k)})^2
\end{aligned}
$$

**Notes:**

- Adadelta adapts learning rates based on a moving window of gradient updates, rather than accumulating all past gradients. This way, learning rates adjusted are more robust to changes in model's dynamics.

# Adadelta (Zeiler, 2012)

An extension of RMSProp that seeks to reduce its dependence on a manually set global learning rate. Instead of accumulating all past squared gradients, Adadelta limits the window of accumulated past gradients to some fixed size $w$. Update mechanism does not require learning rate $\alpha$:

$$
\begin{aligned}
v_j^{(k)} &= \gamma v_j^{(k-1)} + (1-\gamma)(g_j^{(k)})^2 \\
\tilde{g}_j^{(k)} &= \frac{\sqrt{\Delta x_j^{(k-1)} + \epsilon}}{\sqrt{v_j^{(k)} + \epsilon}} g_j^{(k)} \\
x_j^{(k)} &= x_j^{(k-1)} - \tilde{g}_j^{(k)} \\
\Delta x_j^{(k)} &= \rho \Delta x_j^{(k-1)} + (1-\rho)(\tilde{g}_j^{(k)})^2
\end{aligned}
$$

**Notes:**

- Adadelta adapts learning rates based on a moving window of gradient updates, rather than accumulating all past gradients. This way, learning rates adjusted are more robust to changes in model's dynamics.
- The method does not require an initial learning rate setting, making it easier to configure.

# Adadelta (Zeiler, 2012)

An extension of RMSProp that seeks to reduce its dependence on a manually set global learning rate. Instead of accumulating all past squared gradients, Adadelta limits the window of accumulated past gradients to some fixed size $w$. Update mechanism does not require learning rate $\alpha$:

$$v_j^{(k)} = \gamma v_j^{(k-1)} + (1-\gamma)(g_j^{(k)})^2$$

$$\tilde{g}_j^{(k)} = \frac{\sqrt{\Delta x_j^{(k-1)} + \epsilon}}{\sqrt{v_j^{(k)} + \epsilon}} g_j^{(k)}$$

$$x_j^{(k)} = x_j^{(k-1)} - \tilde{g}_j^{(k)}$$

$$\Delta x_j^{(k)} = \rho \Delta x_j^{(k-1)} + (1-\rho)(\tilde{g}_j^{(k)})^2$$

**Notes:**

- Adadelta adapts learning rates based on a moving window of gradient updates, rather than accumulating all past gradients. This way, learning rates adjusted are more robust to changes in model's dynamics.
- The method does not require an initial learning rate setting, making it easier to configure.
- Often used in deep learning where parameter scales differ significantly across layers.

# Adam (Kingma and Ba, 2014) [1] [2]

Combines elements from both AdaGrad and RMSProp. It considers an exponentially decaying average of past gradients and squared gradients.

EMA:

$$m_j^{(k)} = \beta_1 m_j^{(k-1)} + (1-\beta_1) g_j^{(k)}$$

$$v_j^{(k)} = \beta_2 v_j^{(k-1)} + (1-\beta_2) \left(g_j^{(k)}\right)^2$$

Bias correction:

$$\hat{m}_j = \frac{m_j^{(k)}}{1-\beta_1^k}$$

$$\hat{v}_j = \frac{v_j^{(k)}}{1-\beta_2^k}$$

Update:

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{\hat{m}_j}{\sqrt{\hat{v}_j} + \epsilon}$$

**Notes:**

- It corrects the bias towards zero in the initial moments seen in other methods like RMSProp, making the estimates more accurate.

# Adam (Kingma and Ba, 2014) [1] [2]

Combines elements from both AdaGrad and RMSProp. It considers an exponentially decaying average of past gradients and squared gradients.

EMA:

$$m_j^{(k)} = \beta_1 m_j^{(k-1)} + (1-\beta_1) g_j^{(k)}$$

$$v_j^{(k)} = \beta_2 v_j^{(k-1)} + (1-\beta_2)\left(g_j^{(k)}\right)^2$$

Bias correction:

$$\hat{m}_j = \frac{m_j^{(k)}}{1-\beta_1^k}$$

$$\hat{v}_j = \frac{v_j^{(k)}}{1-\beta_2^k}$$

Update:

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{\hat{m}_j}{\sqrt{\hat{v}_j + \epsilon}}$$

**Notes:**

- It corrects the bias towards zero in the initial moments seen in other methods like RMSProp, making the estimates more accurate.
- Одна из самых цитируемых научных работ в мире

# Adam (Kingma and Ba, 2014) [1] [2]

Combines elements from both AdaGrad and RMSProp. It considers an exponentially decaying average of past gradients and squared gradients.

EMA:

$$m_j^{(k)} = \beta_1 m_j^{(k-1)} + (1 - \beta_1) g_j^{(k)}$$

$$v_j^{(k)} = \beta_2 v_j^{(k-1)} + (1 - \beta_2) \left(g_j^{(k)}\right)^2$$

Bias correction:

$$\hat{m}_j = \frac{m_j^{(k)}}{1 - \beta_1^k}$$

$$\hat{v}_j = \frac{v_j^{(k)}}{1 - \beta_2^k}$$

Update:

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{\hat{m}_j}{\sqrt{\hat{v}_j} + \epsilon}$$

**Notes:**

- It corrects the bias towards zero in the initial moments seen in other methods like RMSProp, making the estimates more accurate.
- Одна из самых цитируемых научных работ в мире
- В 2018-2019 годах вышли статьи, указывающие на ошибку в оригинальной статье

# Adam (Kingma and Ba, 2014) [1] [2]

Combines elements from both AdaGrad and RMSProp. It considers an exponentially decaying average of past gradients and squared gradients.

EMA:

$$m_j^{(k)} = \beta_1 m_j^{(k-1)} + (1 - \beta_1) g_j^{(k)}$$

$$v_j^{(k)} = \beta_2 v_j^{(k-1)} + (1 - \beta_2) \left(g_j^{(k)}\right)^2$$

Bias correction:

$$\hat{m}_j = \frac{m_j^{(k)}}{1 - \beta_1^k}$$

$$\hat{v}_j = \frac{v_j^{(k)}}{1 - \beta_2^k}$$

Update:

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{\hat{m}_j}{\sqrt{\hat{v}_j} + \epsilon}$$

**Notes:**

- It corrects the bias towards zero in the initial moments seen in other methods like RMSProp, making the estimates more accurate.
- Одна из самых цитируемых научных работ в мире
- В 2018-2019 годах вышли статьи, указывающие на ошибку в оригинальной статье
- Не сходится для некоторых простых задач (даже выпуклых)

# Adam (Kingma and Ba, 2014) [1] [2]

Combines elements from both AdaGrad and RMSProp. It considers an exponentially decaying average of past gradients and squared gradients.

EMA:

$$m_j^{(k)} = \beta_1 m_j^{(k-1)} + (1-\beta_1) g_j^{(k)}$$

$$v_j^{(k)} = \beta_2 v_j^{(k-1)} + (1-\beta_2) \left(g_j^{(k)}\right)^2$$

Bias correction:

$$\hat{m}_j = \frac{m_j^{(k)}}{1-\beta_1^k}$$

$$\hat{v}_j = \frac{v_j^{(k)}}{1-\beta_2^k}$$

Update:

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{\hat{m}_j}{\sqrt{\hat{v}_j} + \epsilon}$$

**Notes:**

- It corrects the bias towards zero in the initial moments seen in other methods like RMSProp, making the estimates more accurate.
- Одна из самых цитируемых научных работ в мире
- В 2018-2019 годах вышли статьи, указывающие на ошибку в оригинальной статье
- Не сходится для некоторых простых задач (даже выпуклых)
- Почему-то очень хорошо работает для некоторых сложных задач

# Adam (Kingma and Ba, 2014) [1] [2]

Combines elements from both AdaGrad and RMSProp. It considers an exponentially decaying average of past gradients and squared gradients.

EMA:

$$m_j^{(k)} = \beta_1 m_j^{(k-1)} + (1-\beta_1) g_j^{(k)}$$

$$v_j^{(k)} = \beta_2 v_j^{(k-1)} + (1-\beta_2) \left(g_j^{(k)}\right)^2$$

Bias correction:

$$\hat{m}_j = \frac{m_j^{(k)}}{1-\beta_1^k}$$

$$\hat{v}_j = \frac{v_j^{(k)}}{1-\beta_2^k}$$

Update:

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{\hat{m}_j}{\sqrt{\hat{v}_j} + \epsilon}$$

**Notes:**

- It corrects the bias towards zero in the initial moments seen in other methods like RMSProp, making the estimates more accurate.
- Одна из самых цитируемых научных работ в мире
- В 2018-2019 годах вышли статьи, указывающие на ошибку в оригинальной статье
- Не сходится для некоторых простых задач (даже выпуклых)
- Почему-то очень хорошо работает для некоторых сложных задач
- Гораздо лучше работает для языковых моделей, чем для задач компьютерного зрения - почему?

[1] Adam: A Method for Stochastic Optimization

[2] On the Convergence of Adam and Beyond

# AdamW (Loshchilov & Hutter, 2017)

Addresses a common issue with $\ell_2$ regularization in adaptive optimizers like Adam. Standard $\ell_2$ regularization adds $\lambda\|x\|^2$ to the loss, resulting in a gradient term $\lambda x$. In Adam, this term gets scaled by the adaptive learning rate $\left(\sqrt{\hat{v}_j} + \epsilon\right)$, coupling the weight decay to the gradient magnitudes.

AdamW decouples weight decay from the gradient adaptation step.

Update rule:

$$m_j^{(k)} = \beta_1 m_j^{(k-1)} + (1-\beta_1) g_j^{(k)}$$

$$v_j^{(k)} = \beta_2 v_j^{(k-1)} + (1-\beta_2)(g_j^{(k)})^2$$

$$\hat{m}_j = \frac{m_j^{(k)}}{1-\beta_1^k}, \quad \hat{v}_j = \frac{v_j^{(k)}}{1-\beta_2^k}$$

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \left( \frac{\hat{m}_j}{\sqrt{\hat{v}_j} + \epsilon} + \lambda x_j^{(k-1)} \right)$$

**Notes:**

- The weight decay term $\lambda x_j^{(k-1)}$ is added *after* the adaptive gradient step.

# AdamW (Loshchilov & Hutter, 2017)

Addresses a common issue with $\ell_2$ regularization in adaptive optimizers like Adam. Standard $\ell_2$ regularization adds $\lambda\|x\|^2$ to the loss, resulting in a gradient term $\lambda x$. In Adam, this term gets scaled by the adaptive learning rate $\left(\sqrt{\hat{v}_j} + \epsilon\right)$, coupling the weight decay to the gradient magnitudes.

AdamW decouples weight decay from the gradient adaptation step.

Update rule:

$$m_j^{(k)} = \beta_1 m_j^{(k-1)} + (1-\beta_1) g_j^{(k)}$$

$$v_j^{(k)} = \beta_2 v_j^{(k-1)} + (1-\beta_2) (g_j^{(k)})^2$$

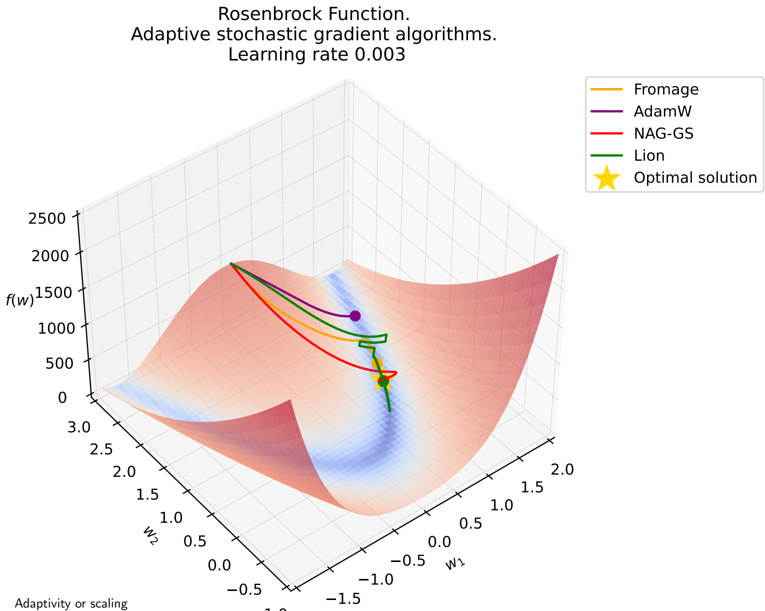
$$\hat{m}_j = \frac{m_j^{(k)}}{1-\beta_1^k}, \quad \hat{v}_j = \frac{v_j^{(k)}}{1-\beta_2^k}$$

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \left( \frac{\hat{m}_j}{\sqrt{\hat{v}_j} + \epsilon} + \lambda x_j^{(k-1)} \right)$$

**Notes:**

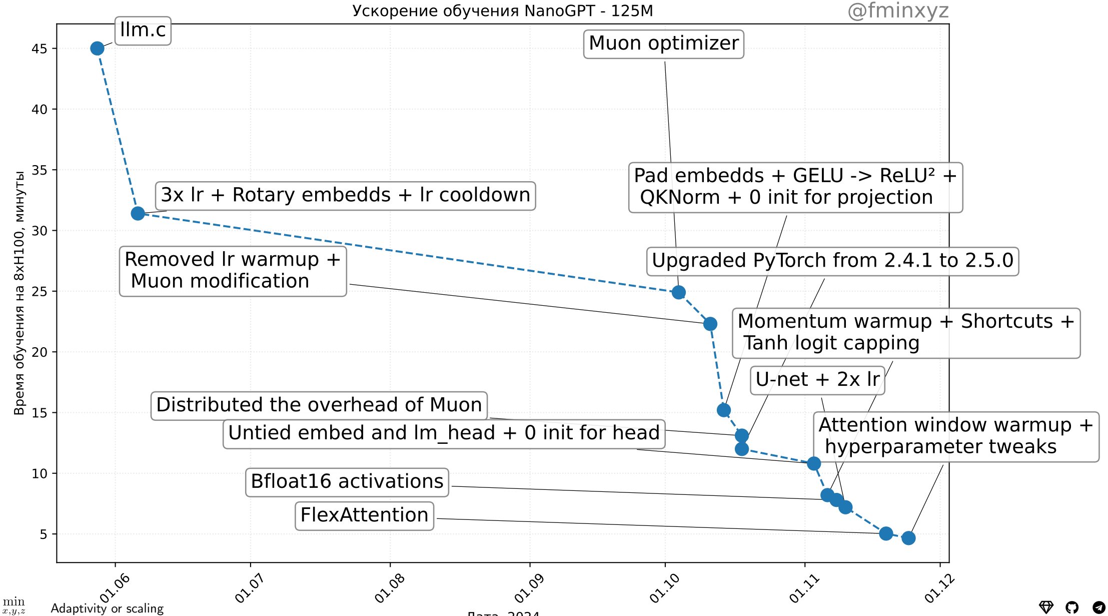
- The weight decay term $\lambda x_j^{(k-1)}$ is added *after* the adaptive gradient step.
- Widely adopted in training transformers and other large models. Default choice for huggingface trainer.

# A lot of them


Rosenbrock Function.
Adaptive stochastic gradient algorithms.
Learning rate 0.003
Fromage
AdamW
NAG-GS
Lion
Optimal solution
$f(w)$
2500
2000
1500
1000
500
0
$w_2$
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
$w_1$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5

# How to compare them? AlgoPerf benchmark

# NanoGPT speedrun



# Shampoo (Gupta, Anil, et al., 2018; Anil et al., 2020)

Stands for **S**tochastic **H**essian-**A**pproximation **M**atrix **P**reconditioning for **O**ptimization **O**f deep networks. It's a method inspired by second-order optimization designed for large-scale deep learning.

**Core Idea:** Approximates the full-matrix AdaGrad pre conditioner using efficient matrix structures, specifically Kronecker products.

For a weight matrix $W \in \mathbb{R}^{m\times n}$, the update involves preconditioning using approximations of the statistics matrices $L \approx \sum_k G_k G_k^T$ and $R \approx \sum_k G_k^T G_k$, where $G_k$ are the gradients.

Simplified concept:

1. Compute gradient $G_k$.

**Notes:**

# Shampoo (Gupta, Anil, et al., 2018; Anil et al., 2020)

Stands for **S**tochastic **H**essian-**A**pproximation **M**atrix **P**reconditioning for **O**ptimization **O**f deep networks. It's a method inspired by second-order optimization designed for large-scale deep learning.

**Core Idea:** Approximates the full-matrix AdaGrad pre conditioner using efficient matrix structures, specifically Kronecker products.

For a weight matrix $W \in \mathbb{R}^{m \times n}$, the update involves preconditioning using approximations of the statistics matrices $L \approx \sum_k G_k G_k^T$ and $R \approx \sum_k G_k^T G_k$, where $G_k$ are the gradients.

Simplified concept:

1. Compute gradient $G_k$.
2. Update statistics $L_k = \beta L_{k-1} + (1-\beta) G_k G_k^T$ and $R_k = \beta R_{k-1} + (1-\beta) G_k^T G_k$.

**Notes:**

# Shampoo (Gupta, Anil, et al., 2018; Anil et al., 2020)

Stands for **S**tochastic **H**essian-**A**pproximation **M**atrix **P**reconditioning for **O**ptimization **O**f deep networks. It's a method inspired by second-order optimization designed for large-scale deep learning.

**Core Idea:** Approximates the full-matrix AdaGrad pre conditioner using efficient matrix structures, specifically Kronecker products.

For a weight matrix $W \in \mathbb{R}^{m \times n}$, the update involves preconditioning using approximations of the statistics matrices $L \approx \sum_k G_k G_k^T$ and $R \approx \sum_k G_k^T G_k$, where $G_k$ are the gradients.

Simplified concept:

1. Compute gradient $G_k$.
2. Update statistics $L_k = \beta L_{k-1} + (1-\beta) G_k G_k^T$ and $R_k = \beta R_{k-1} + (1-\beta) G_k^T G_k$.
3. Compute preconditioners $P_L = L_k^{-1/4}$ and $P_R = R_k^{-1/4}$. (Inverse matrix root)

**Notes:**

# Shampoo (Gupta, Anil, et al., 2018; Anil et al., 2020)

Stands for **S**tochastic **H**essian-**A**pproximation **M**atrix **P**reconditioning for **O**ptimization **O**f deep networks. It's a method inspired by second-order optimization designed for large-scale deep learning.

**Core Idea:** Approximates the full-matrix AdaGrad pre conditioner using efficient matrix structures, specifically Kronecker products.

For a weight matrix $W \in \mathbb{R}^{m \times n}$, the update involves preconditioning using approximations of the statistics matrices $L \approx \sum_k G_k G_k^T$ and $R \approx \sum_k G_k^T G_k$, where $G_k$ are the gradients.

Simplified concept:

1. Compute gradient $G_k$.
2. Update statistics $L_k = \beta L_{k-1} + (1-\beta) G_k G_k^T$ and $R_k = \beta R_{k-1} + (1-\beta) G_k^T G_k$.
3. Compute preconditioners $P_L = L_k^{-1/4}$ and $P_R = R_k^{-1/4}$. (Inverse matrix root)
4. Update: $W_{k+1} = W_k - \alpha P_L G_k P_R$.

**Notes:**

# Shampoo (Gupta, Anil, et al., 2018; Anil et al., 2020)

Stands for **S**tochastic **H**essian-**A**pproximation **M**atrix **P**reconditioning for **O**ptimization **O**f deep networks. It's a method inspired by second-order optimization designed for large-scale deep learning.

**Core Idea:** Approximates the full-matrix AdaGrad pre conditioner using efficient matrix structures, specifically Kronecker products.

For a weight matrix $W \in \mathbb{R}^{m\times n}$, the update involves preconditioning using approximations of the statistics matrices $L \approx \sum_k G_k G_k^T$ and $R \approx \sum_k G_k^T G_k$, where $G_k$ are the gradients.

Simplified concept:

1. Compute gradient $G_k$.
2. Update statistics $L_k = \beta L_{k-1} + (1-\beta) G_k G_k^T$ and $R_k = \beta R_{k-1} + (1-\beta) G_k^T G_k$.
3. Compute preconditioners $P_L = L_k^{-1/4}$ and $P_R = R_k^{-1/4}$. (Inverse matrix root)
4. Update: $W_{k+1} = W_k - \alpha P_L G_k P_R$.

**Notes:**

- Aims to capture curvature information more effectively than first-order methods.

# Shampoo (Gupta, Anil, et al., 2018; Anil et al., 2020)

Stands for **S**tochastic **H**essian-**A**pproximation **M**atrix **P**reconditioning for **O**ptimization **O**f deep networks. It's a method inspired by second-order optimization designed for large-scale deep learning.

**Core Idea:** Approximates the full-matrix AdaGrad pre conditioner using efficient matrix structures, specifically Kronecker products.

For a weight matrix $W \in \mathbb{R}^{m \times n}$, the update involves preconditioning using approximations of the statistics matrices $L \approx \sum_k G_k G_k^T$ and $R \approx \sum_k G_k^T G_k$, where $G_k$ are the gradients.

Simplified concept:

1. Compute gradient $G_k$.
2. Update statistics $L_k = \beta L_{k-1} + (1-\beta) G_k G_k^T$ and $R_k = \beta R_{k-1} + (1-\beta) G_k^T G_k$.
3. Compute preconditioners $P_L = L_k^{-1/4}$ and $P_R = R_k^{-1/4}$. (Inverse matrix root)
4. Update: $W_{k+1} = W_k - \alpha P_L G_k P_R$.

**Notes:**

- Aims to capture curvature information more effectively than first-order methods.
- Computationally more expensive than Adam but can converge faster or to better solutions in terms of steps.

# Shampoo (Gupta, Anil, et al., 2018; Anil et al., 2020)

Stands for **S**tochastic **H**essian-**A**pproximation **M**atrix **P**reconditioning for **O**ptimization **O**f deep networks. It's a method inspired by second-order optimization designed for large-scale deep learning.

**Core Idea:** Approximates the full-matrix AdaGrad pre conditioner using efficient matrix structures, specifically Kronecker products.

For a weight matrix $W \in \mathbb{R}^{m \times n}$, the update involves preconditioning using approximations of the statistics matrices $L \approx \sum_k G_k G_k^T$ and $R \approx \sum_k G_k^T G_k$, where $G_k$ are the gradients.

Simplified concept:

1. Compute gradient $G_k$.
2. Update statistics $L_k = \beta L_{k-1} + (1-\beta) G_k G_k^T$ and $R_k = \beta R_{k-1} + (1-\beta) G_k^T G_k$.
3. Compute preconditioners $P_L = L_k^{-1/4}$ and $P_R = R_k^{-1/4}$. (Inverse matrix root)
4. Update: $W_{k+1} = W_k - \alpha P_L G_k P_R$.

**Notes:**

- Aims to capture curvature information more effectively than first-order methods.
- Computationally more expensive than Adam but can converge faster or to better solutions in terms of steps.
- Requires careful implementation for efficiency (e.g., efficient computation of inverse matrix roots, handling large matrices).

# Shampoo (Gupta, Anil, et al., 2018; Anil et al., 2020)

Stands for **S**tochastic **H**essian-**A**pproximation **M**atrix **P**reconditioning for **O**ptimization **O**f deep networks. It's a method inspired by second-order optimization designed for large-scale deep learning.

**Core Idea:** Approximates the full-matrix AdaGrad pre conditioner using efficient matrix structures, specifically Kronecker products.

For a weight matrix $W \in \mathbb{R}^{m \times n}$, the update involves preconditioning using approximations of the statistics matrices $L \approx \sum_k G_k G_k^T$ and $R \approx \sum_k G_k^T G_k$, where $G_k$ are the gradients.

Simplified concept:

1. Compute gradient $G_k$.
2. Update statistics $L_k = \beta L_{k-1} + (1-\beta) G_k G_k^T$ and $R_k = \beta R_{k-1} + (1-\beta) G_k^T G_k$.
3. Compute preconditioners $P_L = L_k^{-1/4}$ and $P_R = R_k^{-1/4}$. (Inverse matrix root)
4. Update: $W_{k+1} = W_k - \alpha P_L G_k P_R$.

**Notes:**

- Aims to capture curvature information more effectively than first-order methods.
- Computationally more expensive than Adam but can converge faster or to better solutions in terms of steps.
- Requires careful implementation for efficiency (e.g., efficient computation of inverse matrix roots, handling large matrices).
- Variants exist for different tensor shapes (e.g., convolutional layers).

# Muon [3]

$$
\begin{aligned}
W_{t+1} &= W_t - \eta (G_t G_t^\top)^{-1/4} G_t (G_t^\top G_t)^{-1/4} \\
&= W_t - \eta (U S^2 U^\top)^{-1/4} (U S V^\top)(V S^2 V^\top)^{-1/4} \\
&= W_t - \eta (U S^{-1/2} U^\top)(U S V^\top)(V S^{-1/2} V^\top) \\
&= W_t - \eta U S^{-1/2} S S^{-1/2} V^\top \\
&= W_t - \eta U V^\top
\end{aligned}
$$

[3] Deriving Muon