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$$\text{(GD)}$$

• Convergence with constant α or line search.

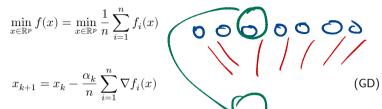
Finite-sum problem

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The gradient descent acts like follows:

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



- Convergence with constant α or line search.
- Iteration cost is linear in n. For ImageNet $n \approx 1.4 \cdot 10^7$, for WikiText $n \approx 10^8$. For FineWeb $n \approx 15 \cdot 10^{12}$ tokens.

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tokens. Let's switch from the full gradient calculation to its unbiased estimator, when we randomly choose i_{ν} index of point

 $x_{k+1} = x_k - \alpha_k^{\text{T}} \nabla f_{i_k}(x_k)$ at each iteration uniformly: (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).

(GD)



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

If ∇f is Lipschitz continuous then we have:

Assumption	Deterministic Gradient Descent	Stochastic Gradient Descent
PL Convex Non-Convex	$egin{array}{c} \mathcal{O}\left(\log(1/arepsilon) ight) \ \mathcal{O}\left(1/arepsilon ight) \ \mathcal{O}\left(1/arepsilon ight) \end{array}$	

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 $f \to \min_{x \in X}$

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- 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).

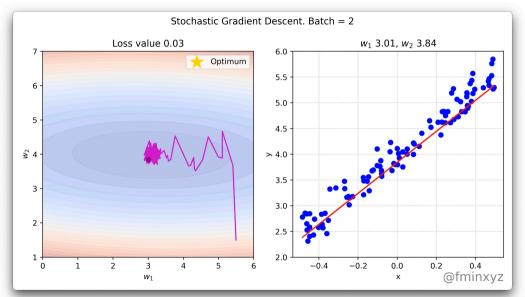


Stochastic Gradient Descent (SGD)





Typical behaviour







Lipschitz continiity implies:

$$f(x_{k+1}) \leq f(x_k) + \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{L}{2} \|x_{k+1} - x_k\|^2$$

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 $X_{k+1} = X_k - J_k \cdot \nabla f_{i_k}(X_k) \xrightarrow{2^{n-k+1}} X_{k+1} - X_k = - d_k \nabla f_{i_k}(X_k)$

 $f(x_{k+1}) \leq f(x_k) - \alpha_k \langle \nabla f(x_k), \nabla f_{i_k}(x_k) \rangle + \alpha_k^2 \frac{L}{2} \|\nabla f_{i_k}(x_k)\|^2$

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using (SGD):

$$f(x_{k+1}) \leq f(x_k) - \alpha_k \langle \nabla f(x_k), \nabla f_{i_k}(x_k) \rangle + \alpha_k^2 \frac{L}{2} \|\nabla f_{i_k}(x_k)\|^2$$

Now let's take expectation with respect to i_k :

$$\mathbb{E}[f(x_{k+1})] \leq \mathbb{E}[f(x_k) - \alpha_k \langle \nabla f(x_k), \nabla f_{i_k}(x_k) \rangle + \alpha_k^2 \frac{L}{2} \|\nabla f_{i_k}(x_k)\|^2]$$

$$\int (\mathbf{x}_k) - \mathbf{d}_k \langle \nabla f(\mathbf{x}_k), \mathbf{E} \nabla f_{i_k}(\mathbf{x}_k) \rangle + \underbrace{\mathbf{d}_k^2 L}_{i_k} \mathbf{E} \|\nabla f_{i_k}(\mathbf{x}_k)\|^2$$

 $f \to \min_{x,y,y}$

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Since uniform sampling implies unbiased estimate of gradient: $\mathbb{E}[\nabla f_{i_k}(x_k)] = \nabla f(x_k)$





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We start from inequality (1):

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Subtract f^*

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Bounded variance: $\mathbb{E}[\|\nabla f_i(x_k)\|^2] \leq \sigma^2$

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$$\begin{split} \mathbb{E}[f(x_{k+1})] & \leq f(x_k) - \alpha_k \|\nabla f(x_k)\|^2 + \alpha_k^2 \frac{L}{2} \mathbb{E}[\|\nabla f_{i_k}(x_k)\|^2] \\ & \text{PL: } \|\nabla f(x_k)\|^2 \geq 2\mu(f(x_k) - f^*) & \leq f(x_k) - 2\alpha_k \mu(f(x_k) - f^*) + \alpha_k^2 \frac{L}{2} \mathbb{E}[\|\nabla f_{i_k}(x_k)\|^2] \end{split}$$

$$\text{Subtract } f^* \quad \mathbb{E}[f(x_{k+1})] - f^* \leq (f(x_k) - f^*) - 2\alpha_k \mu(f(x_k) - f^*) + \alpha_k^2 \frac{L}{2} \mathbb{E}[\|\nabla f_{i_k}(x_k)\|^2]$$

$$\text{Rearrange } \leq (1-2\alpha_k\mu)[f(x_k)-f^*] + \alpha_k^2 \frac{L}{2}\mathbb{E}[\|\nabla f_{i_k}(x_k)\|^2]$$

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$$1 - 2\alpha_k \mu = \underbrace{\frac{(k+1)^2}{(k+1)^2}}_{} - \underbrace{\frac{2k+1}{(k+1)^2}}_{} = \underbrace{\frac{k^2}{(k+1)^2}}_{}$$

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$$^{1-2\alpha_k\mu=\frac{(k+1)^2}{(k+1)^2}-\frac{2k+1}{(k+1)^2}=\frac{k^2}{(k+1)^2}}\quad \mathbb{E}[f(x_{k+1})-f^*] \leq \frac{k^2}{(k+1)^2}[f(x_k)-f^*] + \frac{L\sigma^2(2k+1)^2}{8\mu^2(k+1)^4}$$

Пусть f - L-гладкая функция, удовлетворяющая условию Поляка-Лоясиевича (PL) с константой $\mu > 0$, а дисперсия стохастического градиента ограничена: $\mathbb{E}[\|\nabla f_i(x_k)\|^2] \leq \sigma^2$. Тогда стохастический градиентный спуск с убывающим шагом $\alpha_k = \frac{2k+1}{2\mu(k+1)^2}$ гарантирует

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1. Consider decreasing stepsize strategy with $\alpha_k = \frac{2k+1}{2\nu(k+1)^2}$ we obtain

$$\frac{1-2\alpha_{k}\mu = \frac{(k+1)^{2}}{(k+1)^{2}} - \frac{2k+1}{(k+1)^{2}} - \frac{k^{2}}{(k+1)^{2}}}{(k+1)^{2}} \mathbb{E}[f(x_{k+1}) - f^{*}] \leq \frac{k^{2}}{(k+1)^{2}}[f(x_{k}) - f^{*}] + \frac{L\sigma^{2}(2k+1)^{2}}{8\mu^{2}(k+1)^{4}}$$

$$\frac{(2k+1)^{2} < (2k+2)^{2} = 4(k+1)^{2}}{(k+1)^{2}} \leq \frac{k^{2}}{(k+1)^{2}}[f(x_{k}) - f^{*}] + \frac{L\sigma^{2}}{2\mu^{2}(k+1)^{2}}$$

$$^{(2k+1)^2 < (2k+2)^2 = 4(k+1)^2} \ \le \frac{k^2}{(k+1)^2} [f(x_k) - f^*] + \frac{L\sigma^2}{2\mu^2(k+1)^2} \qquad \qquad \boxed{ \text{ (ki)}}$$



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2. Multiplying both sides by $(k+1)^2$ and letting $\delta_f(k) \equiv k^2 \mathbb{E}[f(x_k) - f^*]$ we get

$$\begin{split} (k+1)^2 \mathbb{E}[f(x_{k+1}) - f^*] & \leq k^2 \mathbb{E}[f(x_k) - f^*] + \frac{L\sigma^2}{2\mu^2} \\ \delta_f(k+1) & \leq \delta_f(k) + \frac{L\sigma^2}{2\mu^2}. \end{split}$$

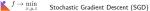


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$$\begin{split} \delta_f(i+1) & \leq \delta_f(i) + \frac{L\sigma^2}{2\mu^2} \\ \sum_{i=0}^k \left[\delta_f(i+1) - \delta_f(i) \right] & \leq \sum_{i=0}^k \frac{L\sigma^2}{2\mu^2} \end{split}$$



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$$\delta_{f}(i+1) \leq \delta_{f}(i) + \frac{L\sigma^{2}}{2\mu^{2}}$$

$$\sum_{i=0}^{k} \left[\delta_{f}(i+1) - \delta_{f}(i)\right] \leq \sum_{i=0}^{k} \frac{L\sigma^{2}}{2\mu^{2}}$$

$$\delta_{f}(k+1) - \delta_{f}(0) \leq \frac{L\sigma^{2}(k+1)}{2\mu^{2}}$$

$$\delta_{F}(0) = 0$$

Convergence. Smooth PL case.

3. Summing up previous inequality from i=0 to k and using the fact that $\delta_f(0)=0$ we get

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which gives the stated rate.

Stochastic Gradient Descent (SGD)

[(K+1) - Pe | 5 2/18/10-1

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which gives the stated rate.

Convergence. Smooth convex case (bounded variance)

Auxiliary notation

For a (possibly) non-constant stepsize sequence $(\alpha_t)_{t>0}$ define the stepsize-weighted average

$$\bar{x}_k \stackrel{\text{def}}{=} \frac{1}{\sum_{t=0}^{k-1} \alpha_t} \sum_{t=0}^{k-1} \alpha_t x_t, \qquad k \ge 1.$$

Everywhere below $f^* \equiv \min_x f(x)$ and $x^* \in \arg\min_x f(x)$.



Пусть f — выпуклая функция (не обязательно гладкая), а дисперсия стохастического градиента ограничена $\mathbb{E} ig[\|
abla f_{i_k}(x_k) \|^2 ig] \, \leq \, \sigma^2 \quad orall k.$ Если SGD использует постоянный шаг $lpha_t \equiv \, lpha \, > \, 0$, то для любого k > 1

$$\mathbb{E}[f(\bar{x}_k)-f^*] \leq \frac{\|x_0-x^*\|^2}{2\alpha\,k} + \frac{\alpha\,\sigma^2}{2}$$

где $\bar{x}_k = \frac{1}{k} \sum_{t=0}^{k-1} x_t$.

При выборе постоянного $\mu = \frac{k_0 + k_1}{k_1 + k_2}$ (зависящего от k) имеем

$$\mathbb{E}[f(\bar{x}_k) - f^*] \leq \frac{\|x_0 - x^*\|\sigma}{\sqrt{k}} = \mathcal{O}\!\!\left(\frac{1}{\sqrt{k}}\right)\!.$$



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1. Начнём с разложения квадрата расстояния до минимума:

$$\|x_{k+1} - x^*\|^2 = \|x_k - \alpha \nabla f_{i_k}(x_k) - x^*\|^2 = \|x_k - x^*\|^2 - 2\alpha \langle \nabla f_{i_k}(x_k), x_k - x^* \rangle + \alpha^2 \|\nabla f_{i_k}(x_k)\|^2.$$

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$$\begin{split} \mathbb{E}_{k}[\|x_{k+1} - x^*\|^2] &= \|x_k - x^*\|^2 - 2\alpha \langle \nabla f(x_k), x_k - x^* \rangle + \alpha^2 \mathbb{E}_{k}[\|\nabla f_{i_k}(x_k)\|^2] \\ \mathbf{f}^* \mathbf{f}(\mathbf{x}_k) + \langle \nabla \mathbf{f}(\mathbf{x}_k), \mathbf{x}_k^* - \mathbf{x}^*\|^2 - 2\alpha (f(x_k) - f^*) + \alpha^2 \sigma^2. \\ - \langle \nabla \mathbf{f}(\mathbf{x}_k), \mathbf{x}_k - \mathbf{x}^* \rangle &\leq \mathbf{f}^* - \mathbf{f}(\mathbf{x}_k) \\ &\leq - \left(\mathbf{f}(\mathbf{x}_k) - \mathbf{f}^*\right) \end{split}$$





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3. Переносим член с $f(x_k)$ влево и берём полное матожидание:

$$2\alpha \mathbb{E}[f(x_k) - f^*] \leq \mathbb{E}[\|x_k - x^*\|^2] - \mathbb{E}[\|x_{k+1} - x^*\|^2] + \alpha^2 \sigma^2.$$

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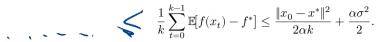
4. Суммируем (телескопируем) по t = 0, ..., k - 1:

$$\begin{split} \sum_{t=0}^{k-1} 2\alpha \, \mathbb{E}[f(x_t) - f^*] &\leq \sum_{t=0}^{k-1} \left(\mathbb{E}[\|x_t - x^*\|^2] - \mathbb{E}[\|x_{t+1} - x^*\|^2] \right) + \sum_{t=0}^{k-1} \alpha^2 \sigma^2 \\ &= \mathbb{E}[\|x_0 - x^*\|^2] - \mathbb{E}[\|x_k - x^*\|^2] + k \, \alpha^2 \sigma^2 \\ &\leq \|x_0 - x^*\|^2 + k \, \alpha^2 \sigma^2. \end{split}$$

5. Делим на $2\alpha k$:



$$\frac{1}{k} \sum_{t=0}^{k-1} \mathbb{E}[$$



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$$\frac{1}{k} \sum_{t=0}^{k-1} \mathbb{E} \big[f(x_t) - f^* \big] \leq \frac{\|x_0 - x^*\|^2}{2\alpha k} + \frac{\alpha \sigma^2}{2}.$$

6. Используя выпуклость f и неравенство Йенсена для усреднённой точки $\bar{x}_k = \frac{1}{k} \sum_{t=0}^{k-1} x_t$:

$$\mathbb{E}[f(\bar{x}_k)] \leq \mathbb{E}\left[\frac{1}{k}\sum_{t=0}^{k-1}f(x_t)\right] = \frac{1}{k}\sum_{t=0}^{k-1}\mathbb{E}[f(x_t)].$$

Вычитая f^* из обеих частей, получаем:

$$\mathbb{E}[f(\bar{x}_k) - f^*] \leq \frac{1}{k} \sum_{t=0}^{k-1} \mathbb{E}[f(x_t) - f^*]. \leq \frac{R^2}{2dk} + \frac{26^2}{2}$$

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7. Объединяя (5) и (6), получаем искомую оценку:

$$\mathbb{E}[f(\bar{x}_k) - f^*] \le \frac{\|x_0 - x^*\|^2}{2\alpha k} + \frac{\alpha \sigma^2}{2}.$$

Smooth convex case with decreasing learning rate

$$\alpha_k = \frac{\alpha_0}{\sqrt{k+1}}, \quad 0 < \alpha_0 \le \frac{1}{4L}$$

 $oldsymbol{i}$ При тех же предположениях, но со спадом шаг $oldsymbol{lpha}_k = rac{lpha_0}{\sqrt{k+1}}$

$$\mathbb{E}[f(\bar{x}_k) - f^*] \ \leq \ \frac{5\|x_0 - x^*\|^2}{4\alpha_0\sqrt{k}} \ + \ 5\alpha_0\sigma^2 \, \frac{\log(k+1)}{\sqrt{k}} \ = \ \mathcal{O}\Big(\frac{\log k}{\sqrt{k}}\Big).$$





Mini-batch SGD



Mini-batch SGD



Mini-batch SGD

Approach 1: Control the sample size

The deterministic method uses all n gradients:

$$\nabla f(x_k) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(x_k).$$

The stochastic method approximates this using just 1 sample:

$$\Pr \left\{ \nabla f_{ik}(x_k) \approx \frac{1}{n} \sum_{i=1}^n \nabla f_i(x_k) \right\}. \qquad \Pr \left\{ \text{ci How} \right\}$$

A common variant is to use a larger sample ${\cal B}_k$ ("mini-batch"):

$$\frac{1}{|B_k|} \sum_{i \in B_k} \nabla f_i(x_k) \approx \frac{1}{n} \sum_{i=1}^n \nabla f_i(x_k),$$

particularly useful for vectorization and parallelization.

For example, with 16 cores set $\left|B_k\right|=16$ and compute 16 gradients at once.

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Mini-Batching as Gradient Descent with Error

The SG method with a sample B_k ("mini-batch") uses iterations:

$$x_{k+1} = x_k - \alpha_k \left(\frac{1}{|B_k|} \sum_{i \in B_k} \nabla f_i(x_k) \right).$$

Let's view this as a "gradient method with error":

$$x_{k+1} = x_k - \alpha_k (\nabla f(x_k) + e_k),$$

where e_k is the difference between the approximate and true gradient.

If you use $\alpha_k = \frac{1}{L}$, then using the descent lemma, this algorithm has:

$$f(x_{k+1}) \leq f(x_k) - \frac{1}{2L} \|\nabla f(x_k)\|^2 + \frac{1}{2L} \|e_k\|^2,$$

for any error e_k .

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Effect of Error on Convergence Rate

Our progress bound with $\alpha_k = \frac{1}{L}$ and error in the gradient of e_k is:

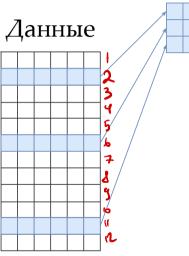
$$f(x_{k+1}) \leq f(x_k) - \frac{1}{2L} \|\nabla f(x_k)\|^2 + \frac{1}{2L} \|e_k\|^2.$$

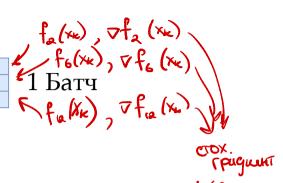




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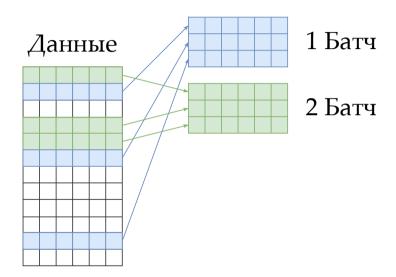
Mini-batch SGD



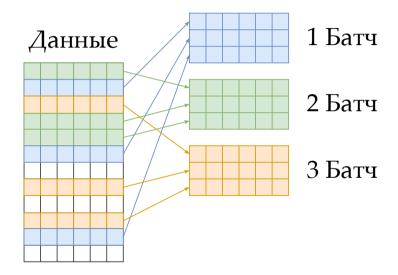


 $X_{k+1} = X_k - d_k g_k$

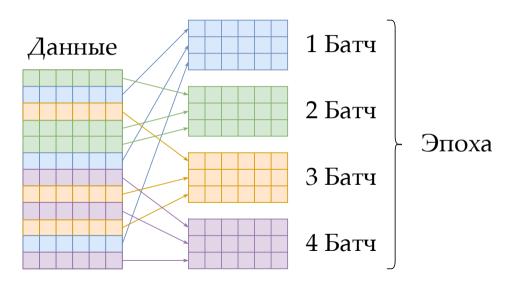
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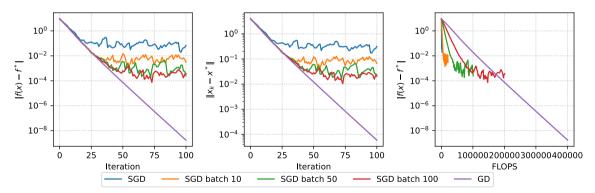
Mini-batch SGD ♥ ೧ •



Main problem of SGD

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

Strongly convex binary logistic regression. m=200, n=10, mu=1.



Основные результаты сходимости SGD

Пусть f - L-гладкая μ -сильно выпуклая функция, а дисперсия стохастического градиента конечна $(\mathbb{E}[\|\nabla f_i(x_k)\|^2] \leq \sigma^2)$. Тогда траектория стохастического градиентного спуска с постоянным шагом $\alpha < \frac{1}{2\mu}$ будет гарантировать:

$$\mathbb{E}[f(x_{k+1}) - f^*] \le (1 - 2\alpha\mu)^k [f(x_0) - f^*] + \frac{L\sigma^2\alpha}{4\mu}.$$

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$$\mathbb{E}[f(x_{k+1}) - f^*] \le \frac{L\sigma^2}{2\mu^2(k+1)}$$

 $f o \min_{x,y,z}$

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• SGD with fixed learning rate does not converge even for PL (strongly convex) case



Mini-batch SGD



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- SGD achieves sublinear convergence with rate $\mathcal{O}\left(\frac{1}{k}\right)$ for PL-case.

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- SGD with fixed learning rate does not converge even for PL (strongly convex) case
- SGD achieves sublinear convergence with rate $\mathcal{O}\left(\frac{1}{L}\right)$ for PL-case.
- Nesterov/Polyak accelerations do not improve convergence rate
- Two-phase Newton-like method achieves $\mathcal{O}\left(\frac{1}{h}\right)$ without strong convexity.

