

# Stochastic Gradient Descent

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## Finite-sum problem

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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:

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

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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:

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

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	$\mathcal{O}(\log(1/\varepsilon))$	
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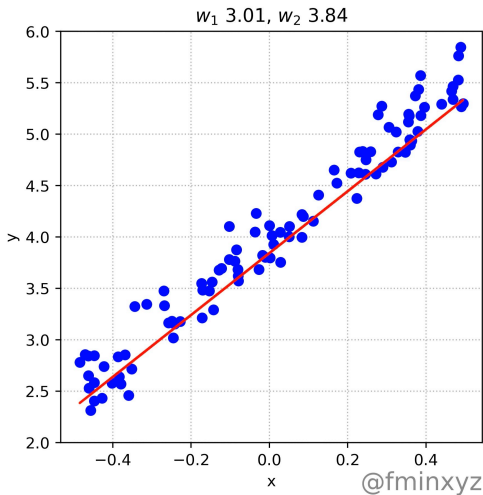
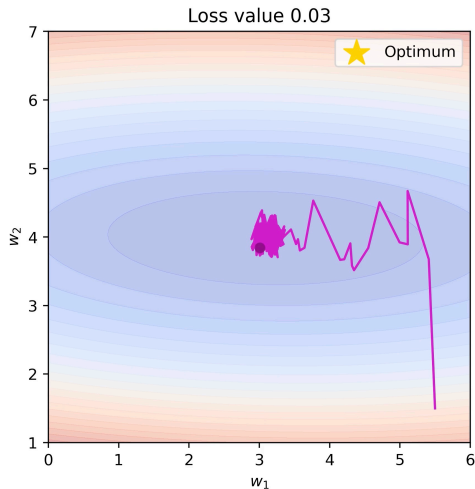
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- Momentum and Quasi-Newton-like methods do not improve rates in stochastic case. Can only improve constant factors (bottleneck is variance, not condition number).

## Stochastic Gradient Descent (SGD)

# Typical behaviour

Stochastic Gradient Descent. Batch = 2



# Convergence

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

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

## Smooth PL case with constant learning rate

**i** 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 постоянным шагом  $\alpha < \frac{1}{2\mu}$  гарантирует

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

We start from inequality (1):

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

## Convergence. Smooth PL case.

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

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

$$\delta_f(k+1) \leq \delta_f(k) + \frac{L\sigma^2}{2\mu^2}.$$



## 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.

## Convergence. Smooth convex case (bounded variance)

### Auxiliary notation

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

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

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

## Smooth convex case with constant learning rate

**i** Пусть  $f$  — выпуклая функция (не обязательно гладкая), а дисперсия стохастического градиента ограничена  $\mathbb{E}[\|\nabla f_{i_k}(x_k)\|^2] \leq \sigma^2 \quad \forall k$ . Если SGD использует постоянный шаг  $\alpha_t \equiv \alpha > 0$ , то для любого  $k \geq 1$

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

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

При выборе постоянного  $\alpha = \frac{\|x_0 - x^*\|}{\sigma\sqrt{k}}$  (зависящего от  $k$ ) имеем

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



## Smooth convex case with constant learning rate

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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2. Берём условное матожидание по  $i_k$  (обозначим  $\mathbb{E}_k[\cdot] = \mathbb{E}[\cdot | x_k]$ ), используем свойство  $\mathbb{E}_k[\nabla f_{i_k}(x_k)] = \nabla f(x_k)$ , ограниченность дисперсии  $\mathbb{E}_k[\|\nabla f_{i_k}(x_k)\|^2] \leq \sigma^2$  и выпуклость  $f$  (которая даёт  $\langle \nabla f(x_k), x_k - x^* \rangle \geq f(x_k) - f^*$ ):

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

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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  $t = 0, \dots, k-1$ :

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

## Smooth convex case with constant learning rate

5. Делим на  $2\alpha k$ :

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

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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:

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

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

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

## Smooth convex case with decreasing learning rate

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

**i** При тех же предположениях, но со спадом шага  $\alpha_k = \frac{\alpha_0}{\sqrt{k+1}}$

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



## 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:

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

A common variant is to use a larger sample  $B_k$  (“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  $|B_k| = 16$  and compute 16 gradients at once.

## 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  $e_k$ .

# Effect of Error on Convergence Rate

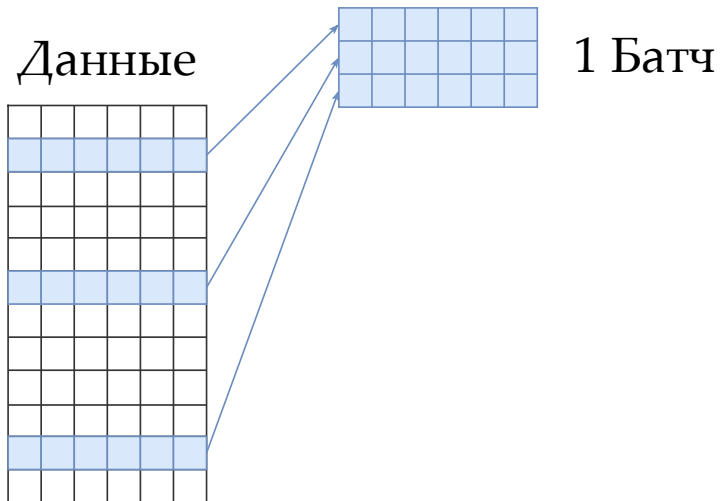
Our progress bound with  $\alpha_k = \frac{1}{L}$  and error in the gradient of  $e_k$  is:

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

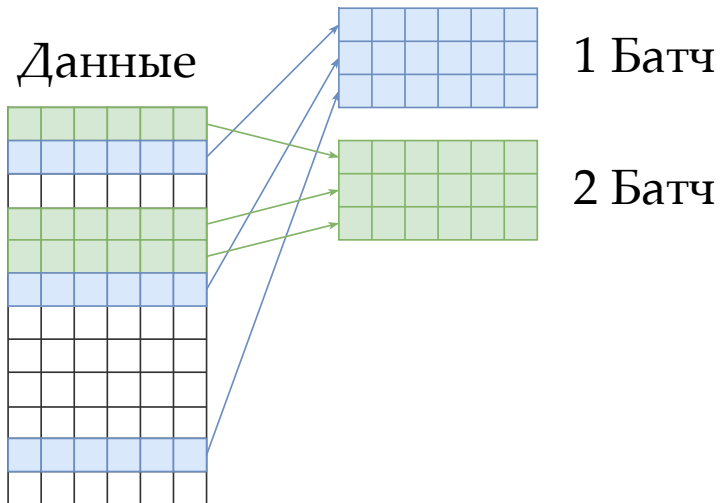
## Идея SGD и батчей

Данные

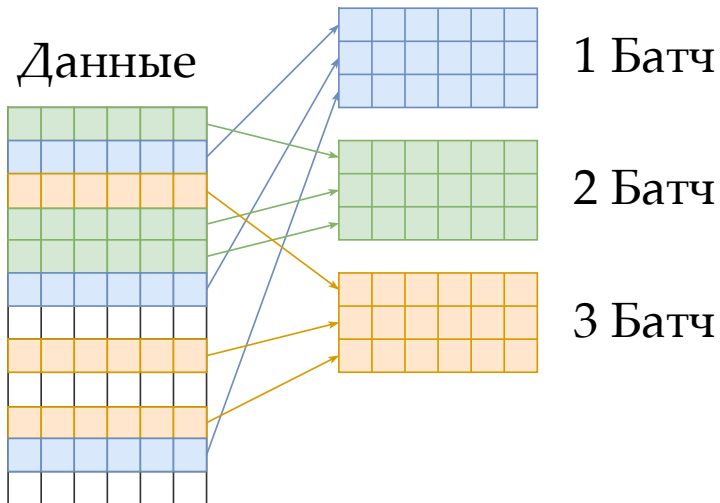

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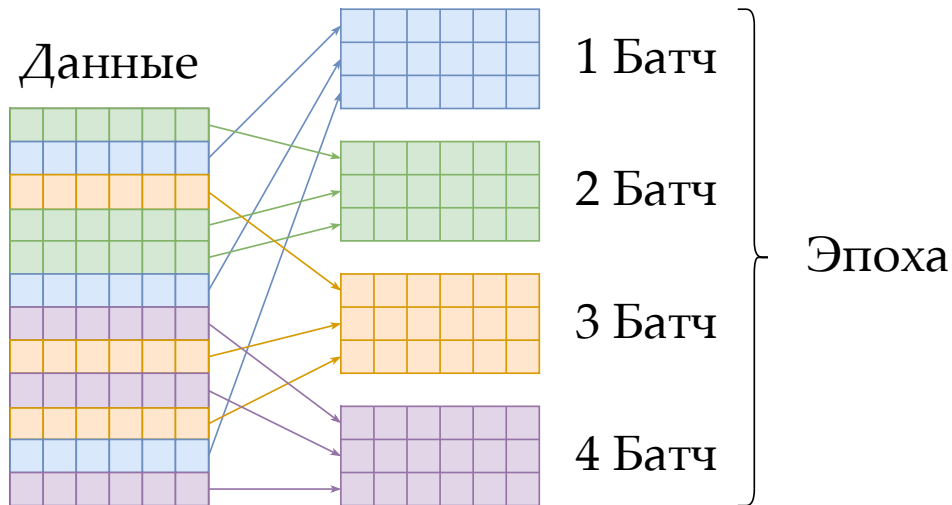


## Идея SGD и батчей





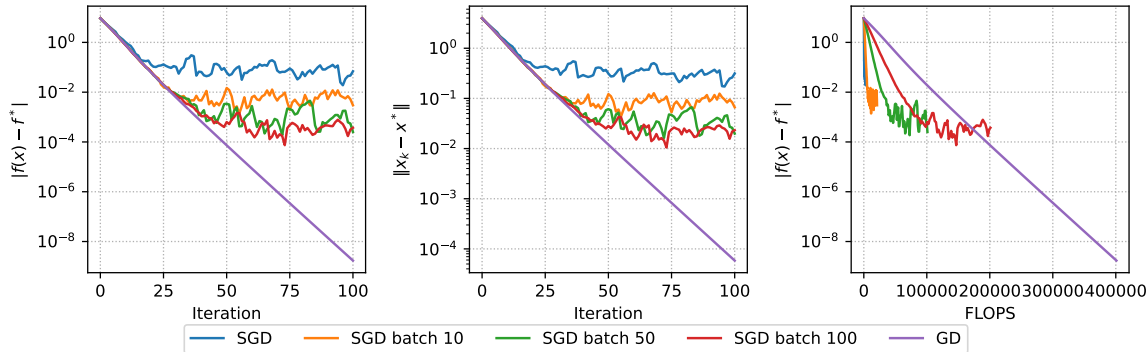
## Идея SGD и батчей



# Main problem of SGD

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

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



# Основные результаты сходимости SGD

**i** Пусть  $f$  -  $L$ -гладкая  $\mu$ -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:

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

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

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- Nesterov/Polyak accelerations do not improve convergence rate

# Conclusions

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