

Stochastic Gradient Descent

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Методы Оптимизации в Машинном Обучении. ФКН ВШЭ

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 ∇f is Lipschitz continuous then we have:

Assumption	Deterministic Gradient Descent	Stochastic Gradient Descent
PL	$\mathcal{O}(\log(1/\varepsilon))$	
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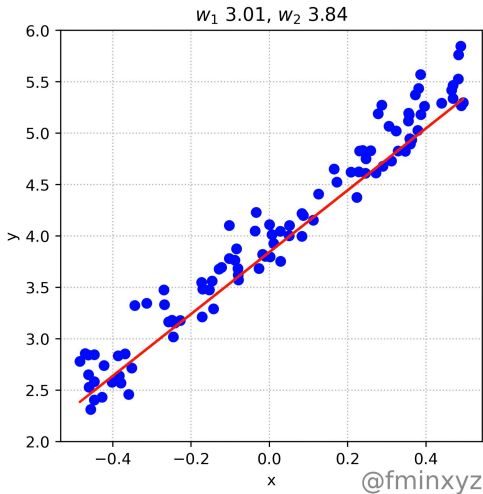
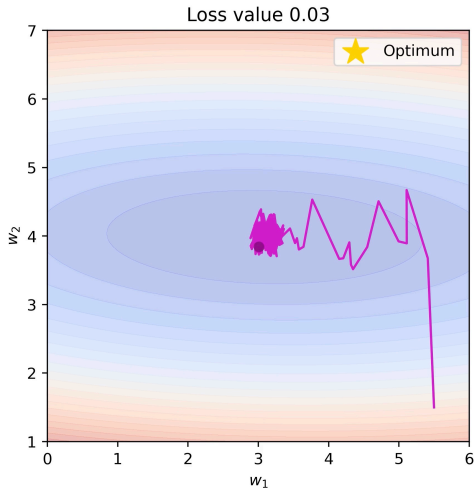
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 - Oracle returns an unbiased gradient approximation with bounded variance.
- Momentum and Quasi-Newton-like methods do not improve rates in stochastic case. Can only improve constant factors (bottleneck is variance, not condition number).

Stochastic Gradient Descent (SGD)

Typical behaviour

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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using (SGD):

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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

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

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Convergence. Smooth PL case.

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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

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

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

which gives the stated rate.

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Convergence. Smooth PL case.

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

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

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

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

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 $2\alpha k$:

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

Smooth convex case with constant learning rate

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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:

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

Smooth convex case with constant learning rate

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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

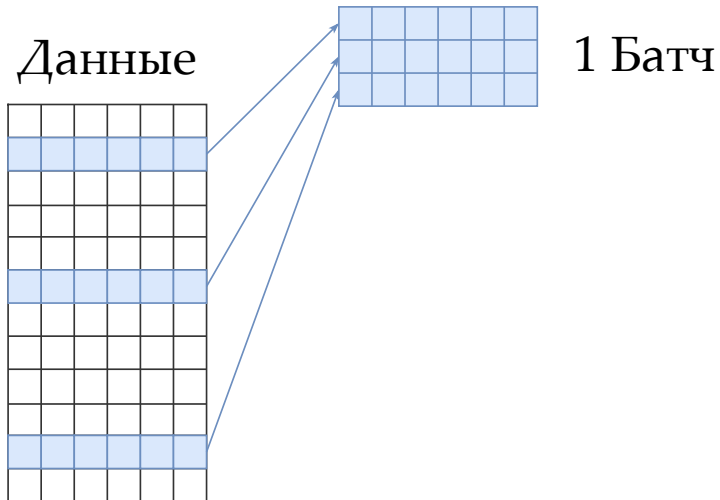
Our progress bound with $\alpha_k = \frac{1}{L}$ and error in the gradient of e_k is:

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

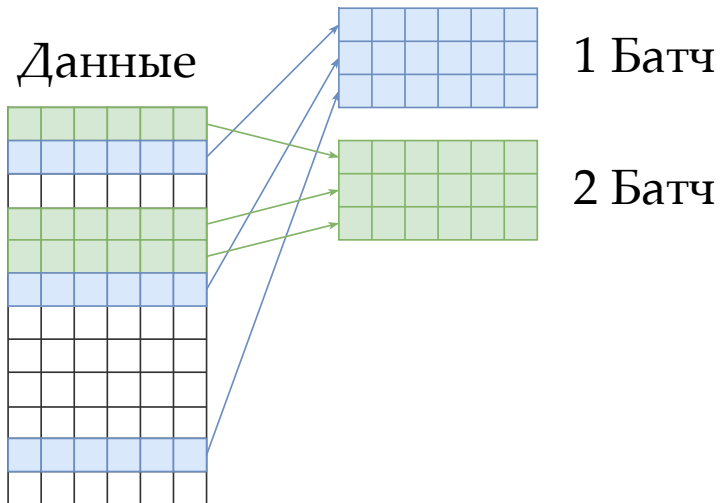
Идея SGD и батчей

Данные

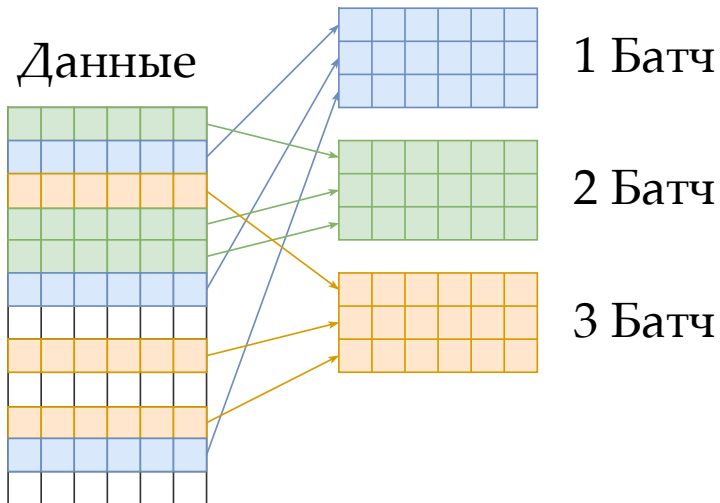
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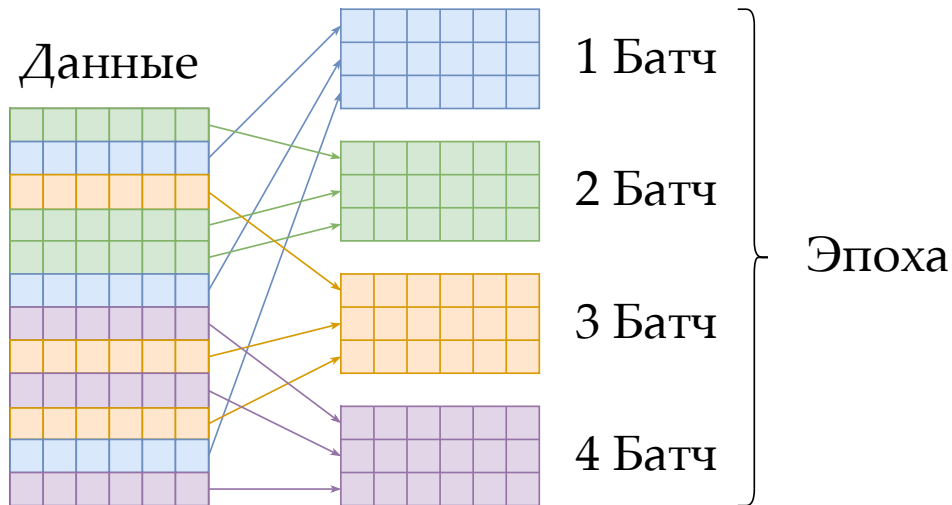
Идея SGD и батчей



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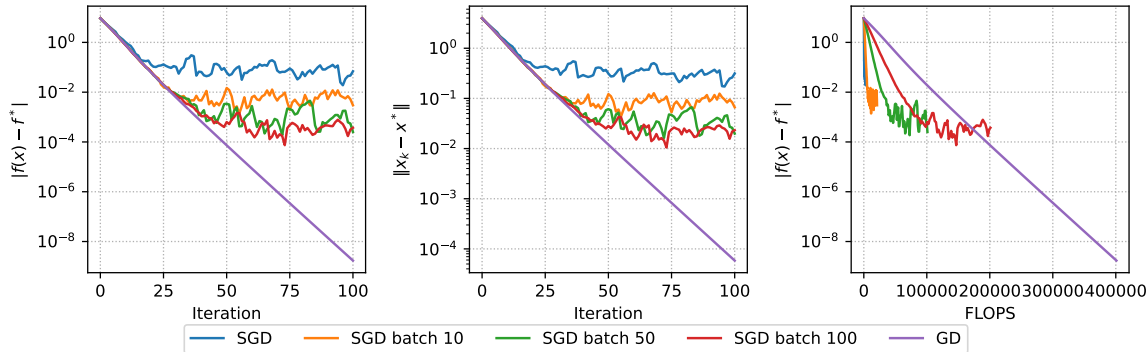
Идея SGD и батчей



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 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:

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

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- i** 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 стохастический градиентный шум с уменьшающимся шагом $\alpha_k = \frac{2k+1}{2\mu(k+1)^2}$ будет сходиться сублинейно:

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

Conclusions

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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.