Stochastic Gradient Descent

Daniil Merkulov

Optimization methods. MIPT

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:

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

- Convergence with constant α or line search.

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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:

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

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 ∇f is Lipschitz continuous then we have:

Assumption	Deterministic Gradient Descent	Stochastic Gradient Descent
PL	$O(\log(1/\varepsilon))$	$O(1/\varepsilon)$
Convex	$O(1/\varepsilon)$	$O(1/\varepsilon^2)$
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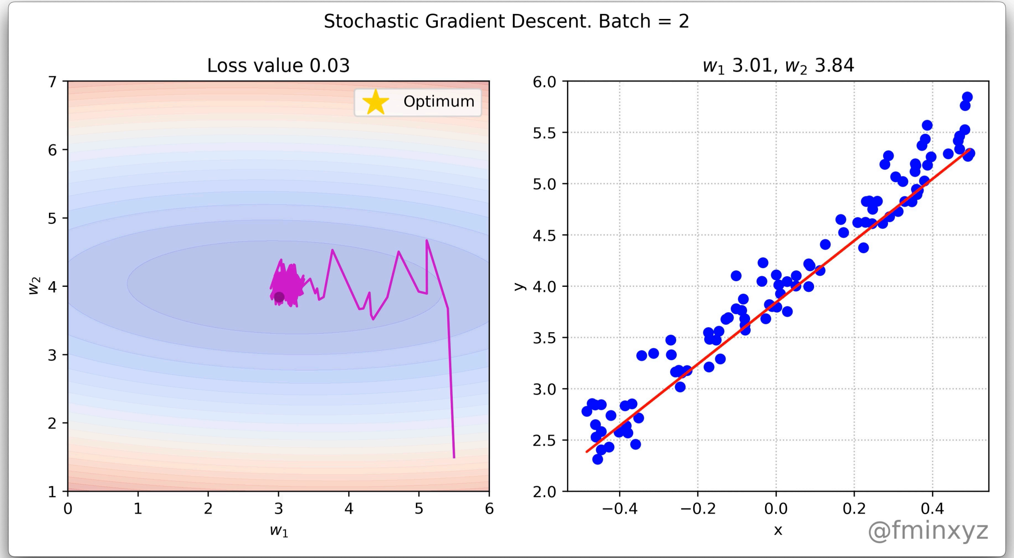
    - Sublinear rate even in strongly-convex case.
    - Bounds are unimprovable under standard assumptions.
    - Oracle returns an unbiased gradient approximation with bounded variance.
- Momentum and Quasi-Newton-like methods do not improve rates in stochastic case. Can only improve constant factors (bottleneck is variance, not condition number).

Stochastic Gradient Descent (SGD)

Typical behaviour



Convergence

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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using (SGD):

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

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Now let's take expectation with respect to i_k:

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

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Using linearity of expectation:

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

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

Convergence. Smooth PL case.

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\frac{1}{2}\|\nabla f(x)\|_2^2 \geq \mu(f(x) - f^*), \forall x \in \mathbb{R}^p \tag{PL}
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This inequality simply requires that the gradient grows faster than a quadratic function as we move away from the optimal function value. Note, that strong convexity implies PL, but not vice versa. Using PL we can write:

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

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Thus, we have

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

Convergence. Smooth PL case.

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

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\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}
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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

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\delta_f(k+1) &\leq \delta_f(k) + \frac{L\sigma^2(2k+1)^2}{8\mu^2(k+1)^2} \\
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where the second line follows from $\frac{2k+1}{k+1} < 2$. Summing up this inequality from $k = 0$ to k and using the fact that $\delta_f(0) = 0$ we get

$$
\delta_f(k+1) \leq \delta_f(0) + \frac{L\sigma^2}{2\mu^2}\sum_{i=0}^{k} 1 \leq \frac{L\sigma^2(k+1)}{2\mu^2} \Rightarrow \quad (k+1)^2\mathbb{E}[f(x_{k+1}) - f^*] \leq \frac{L\sigma^2(k+1)}{2\mu^2}
$$

which gives the stated rate.

Convergence. Smooth PL case.

3. **Constant step size**: Choosing $\alpha_k = \alpha$ for any $\alpha < 1/2\mu$ yields

$$
\begin{aligned}
\mathbb{E}[f(x_{k+1}) - f^*] &\leq (1 - 2\alpha\mu)^k [f(x_0) - f^*] + \frac{L\sigma^2\alpha^2}{2} \sum_{i=0}^{k} (1 - 2\alpha\mu)^i \\
&\leq (1 - 2\alpha\mu)^k [f(x_0) - f^*] + \frac{L\sigma^2\alpha^2}{2} \sum_{i=0}^{\infty} (1 - 2\alpha\mu)^i \\
&= (1 - 2\alpha\mu)^k [f(x_0) - f^*] + \frac{L\sigma^2\alpha}{4\mu},
\end{aligned}
$$

where the last line uses that $\alpha < 1/2\mu$ and the limit of the geometric series.

Convergence. Smooth convex case.

Convergence. Non-smooth convex case.

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:

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

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.

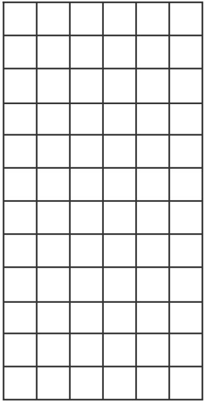
Effect of Error on Convergence Rate

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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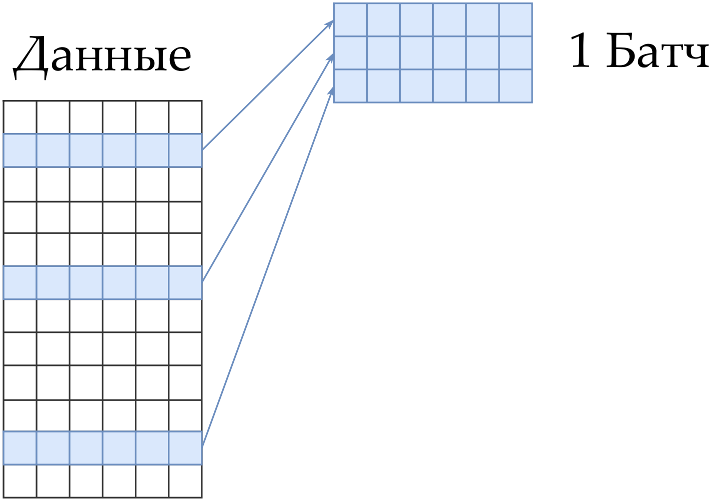

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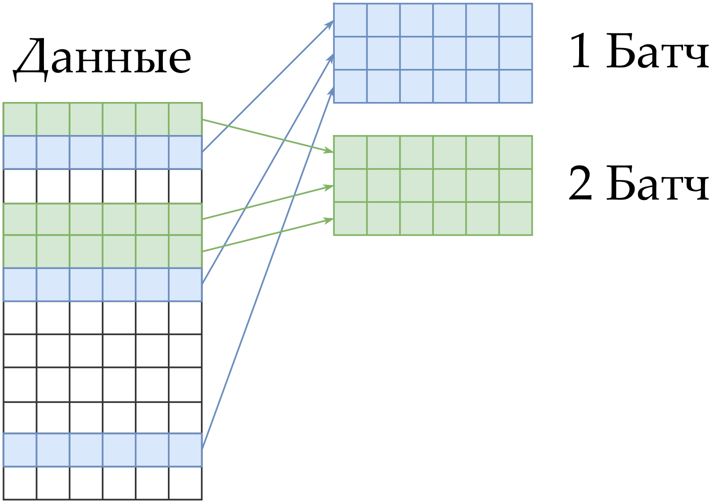

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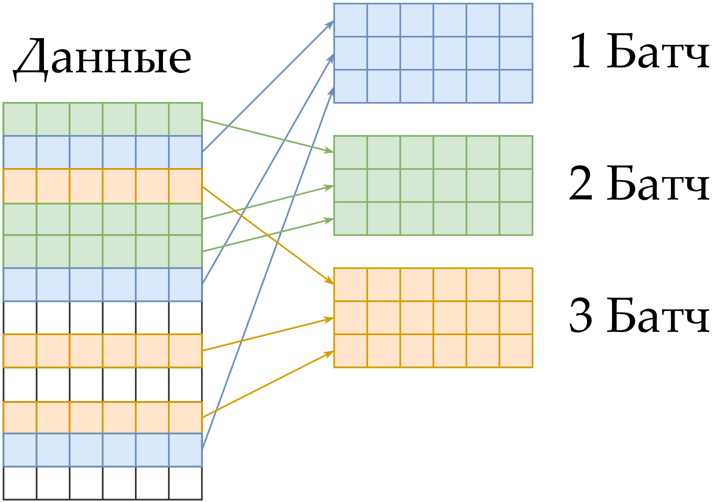

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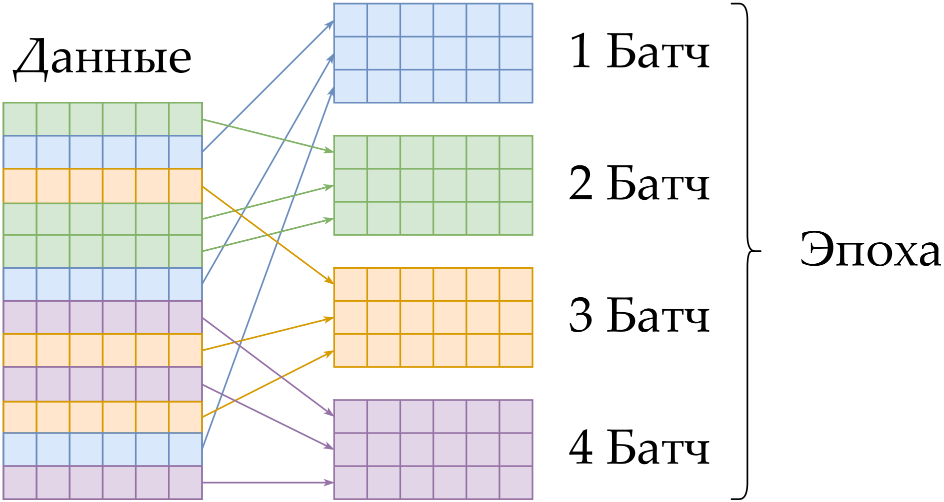
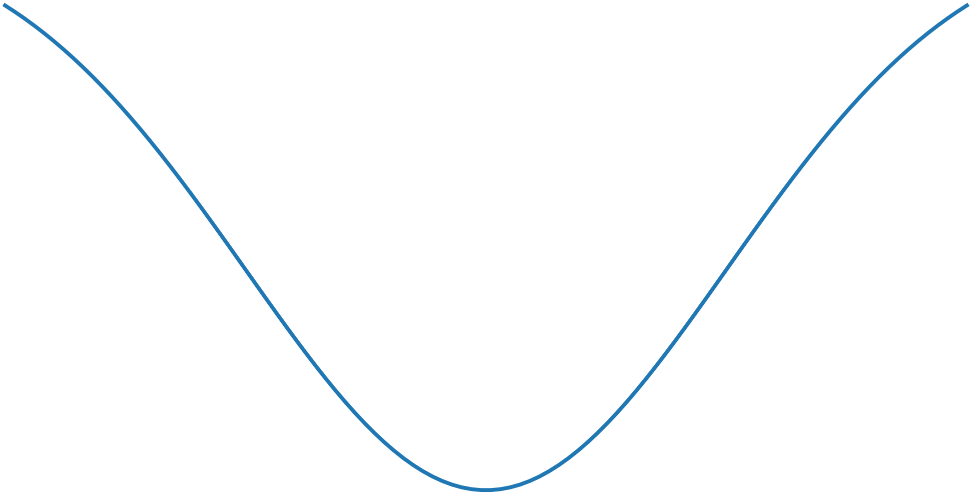


Градиентный спуск сходится к локальному минимуму



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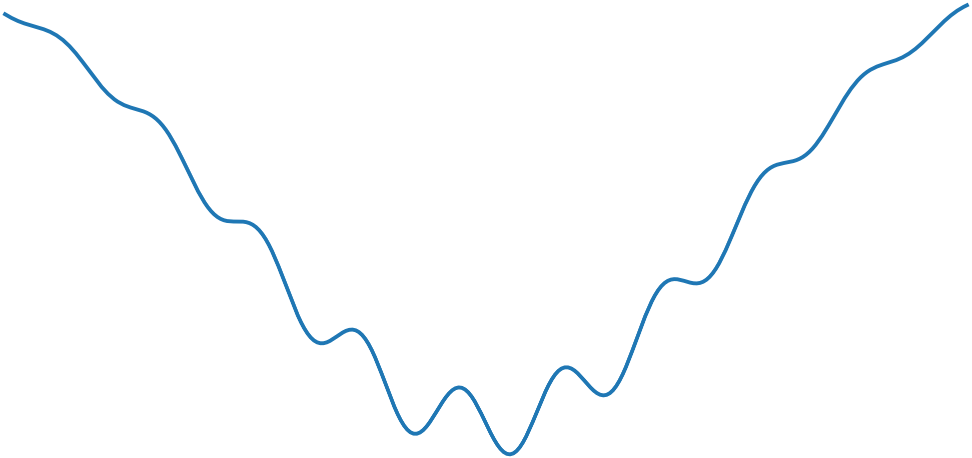
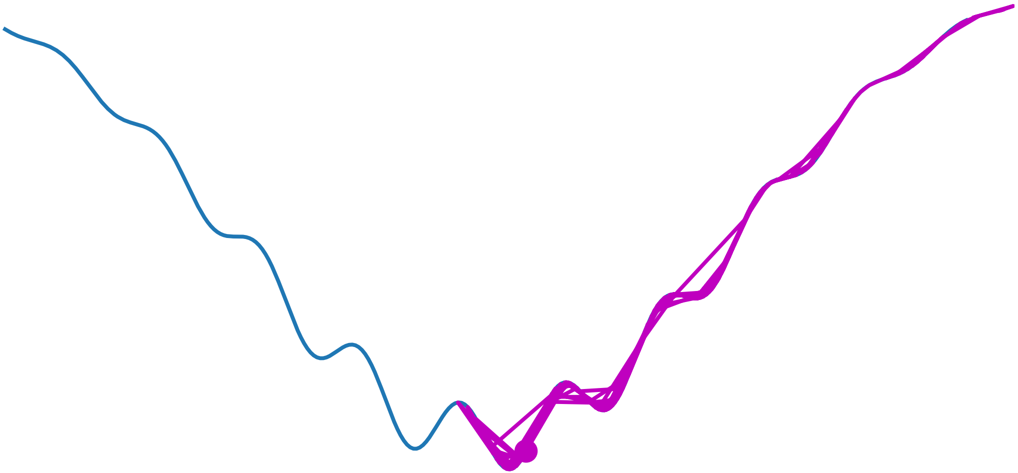
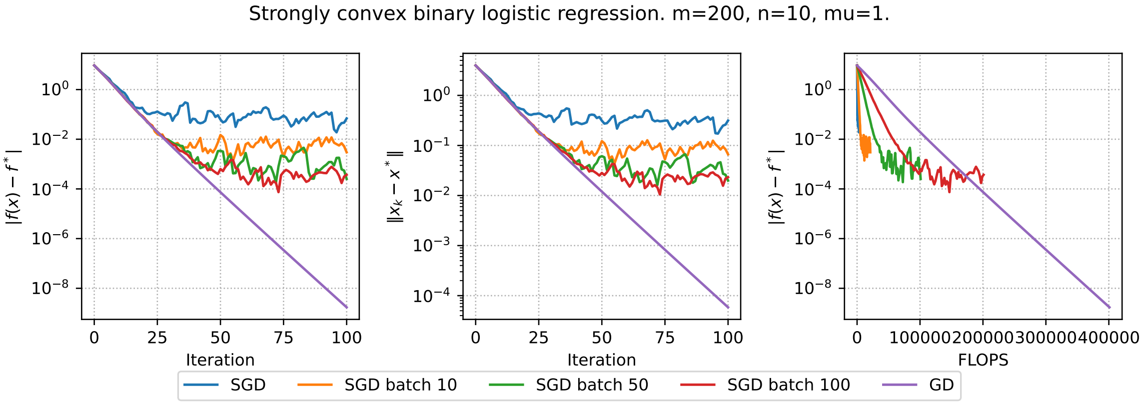


Стохастический градиентный спуск выпрыгивает из локальных минимумов



Main problem of SGD

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



Ширина локальных минимумов

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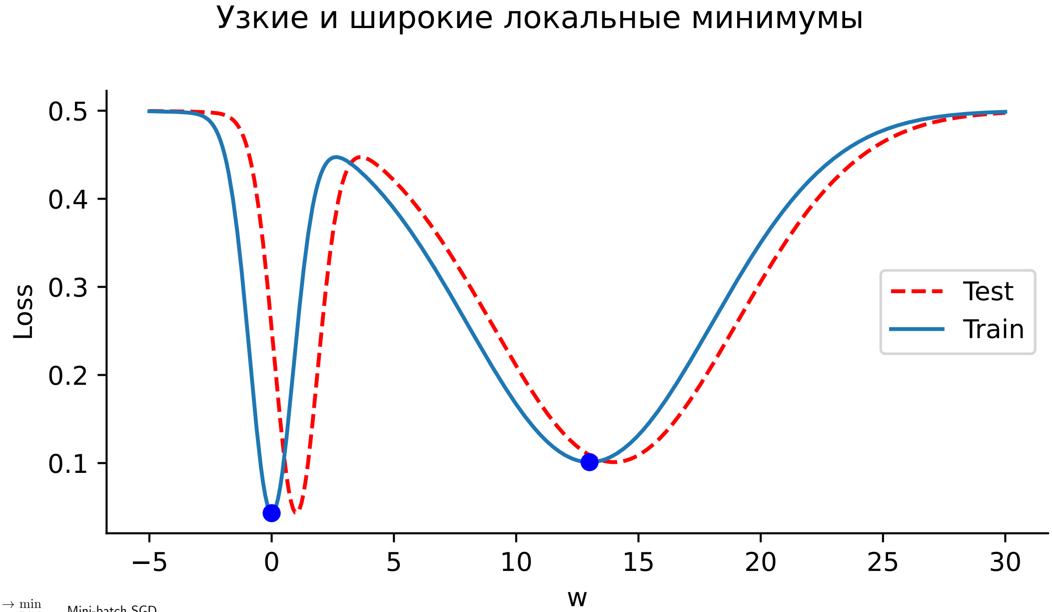

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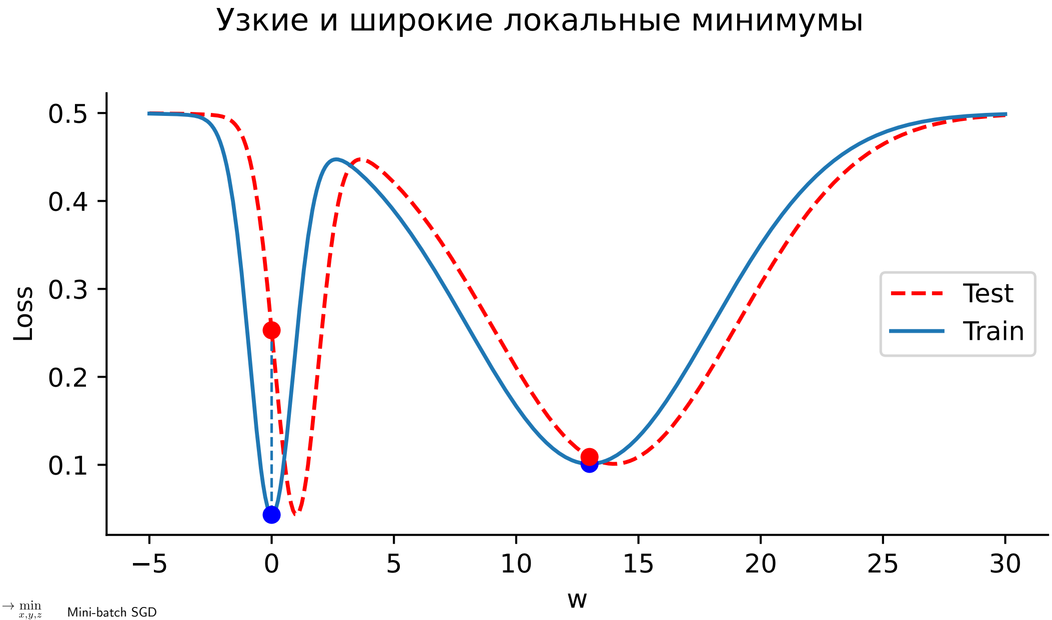
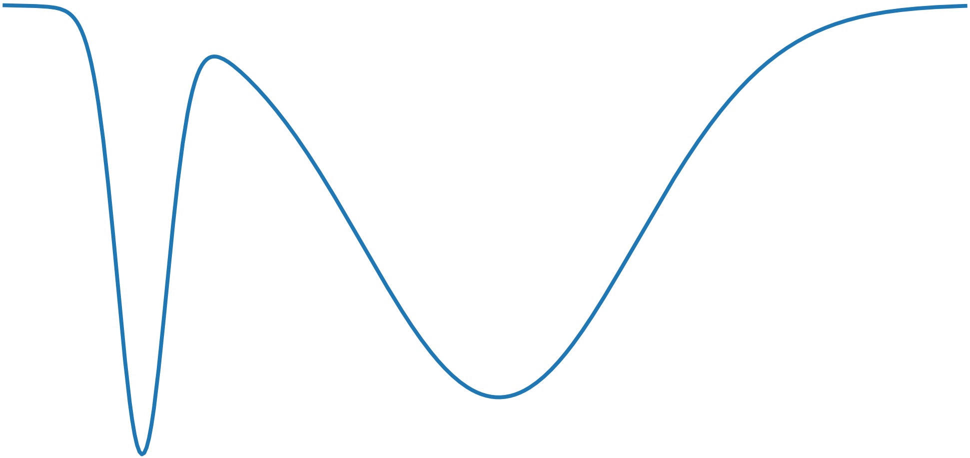
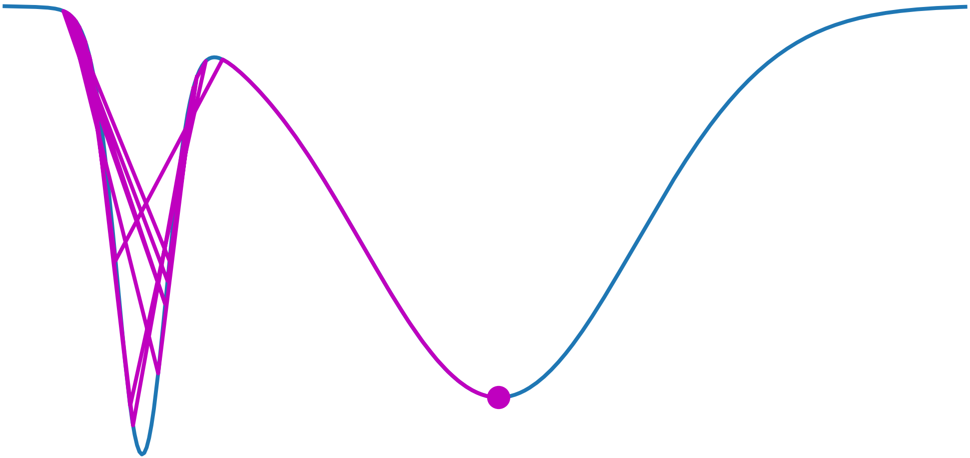


Градиентный спуск с маленьким шагом сходится в узкий локальный минимум



Градиентный спуск с большим шагом избегает узкого локального минимума



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:

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

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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
- Two-phase Newton-like method achieves $\mathcal{O}\left(\frac{1}{k}\right)$ without strong convexity.