Advanced stochastic methods. Adaptivity and variance reduction.

II I

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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:

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

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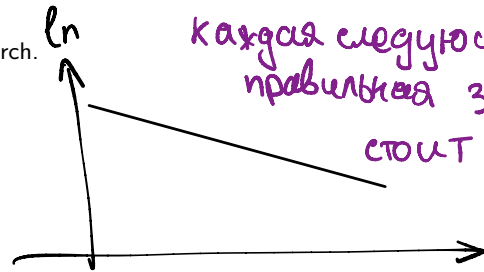
- Convergence with constant α or line search.

$x^* = 1.7245137$

$x^k = 2.6$



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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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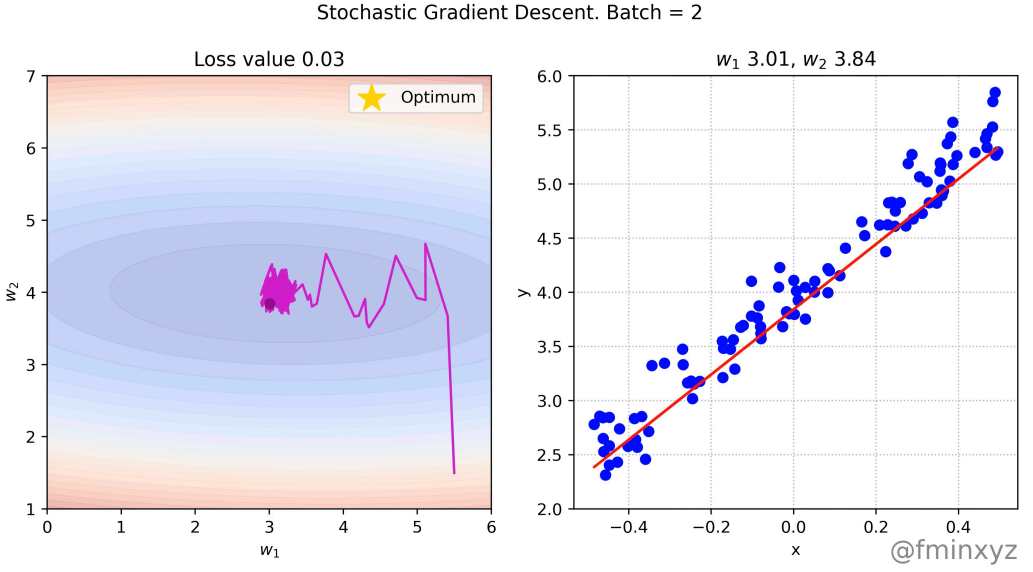
- Momentum and Quasi-Newton-like methods do not improve rates in stochastic case. Can only improve constant factors (bottleneck is variance, not condition number).

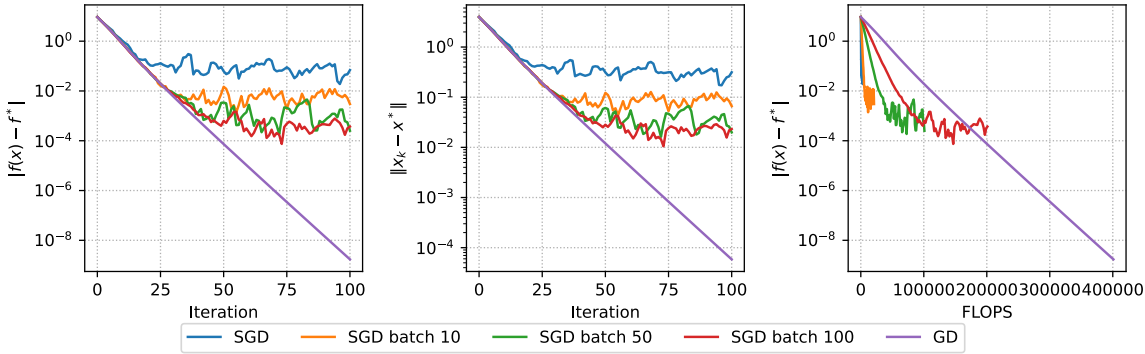
SGD with constant stepsize does not converge



Main problem of SGD

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

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



Key idea of variance reduction

$\mathbb{E}X$, $\mathrm{Var}(X)$

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

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

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

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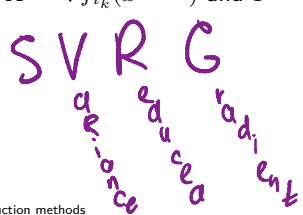
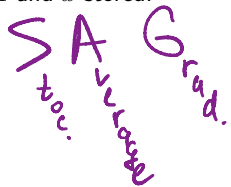
Application to gradient estimation ?

- 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.





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

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

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

$$f'_{i_k}(x) \in \mathbb{R}^p$$

$$n \cdot p$$

Wikitext $n \approx 10^8$

GPT-3 175 B $\approx 10^{11}$

10^{12} fp16

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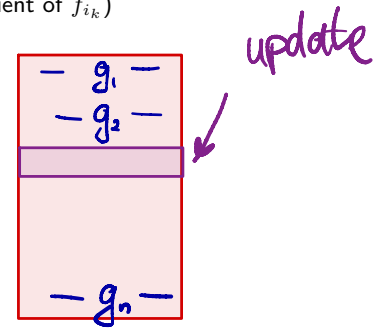
- At steps $k = 1, 2, 3, \ldots$, pick random $i_k \in \{1, \ldots, n\}$, then let

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

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



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- 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 ∇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.

f_i - выпуклые

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.

GD SAG SGD

$\frac{1}{k}$ $\frac{1}{k}$ $\frac{1}{\sqrt{k}}$

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GD $\quad \frac{LR^2}{K}$

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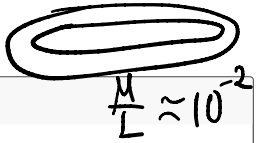
  - SAG: $\frac{48n[f(x^{(0)})-f^\star]+128L\|x^{(0)}-x^\star\|^2}{k}$
- So the first term in SAG bound suffers from a factor of n; authors suggest smarter initialization to make $f(x^{(0)}) - f^\star$ small (e.g., they suggest using the result of n SGD steps).

SAG convergence

Assume further that each f_i is strongly convex with parameter μ.



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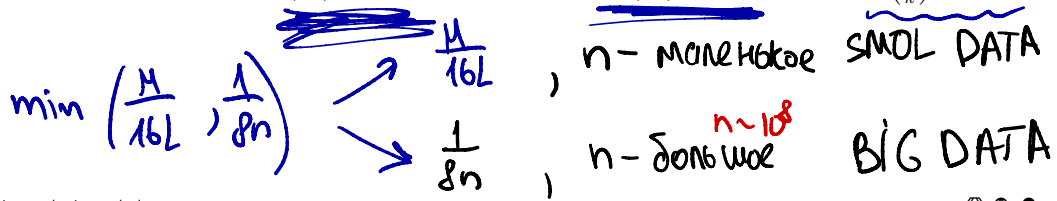
$$\mathbb{E}[f(x^{(k)})] - f^\star \leq \left(1 - \min\left(\frac{\mu}{16L}, \frac{1}{8n}\right)\right)^k \left(\frac{3}{2}\left(f(x^{(0)}) - f^\star\right) + \frac{4L}{n}\|x^{(0)} - x^\star\|^2\right)$$

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.



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- Like GD, we say SAG is adaptive to strong convexity.
- Proofs of these results not easy: 15 pages, computed-aided!

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- In practice you can use backtracking strategy to estimate Lipschitz constant.
  - Choose initial L_0
  - Increase L, until the following satisfies

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

Линейный поиск

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

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

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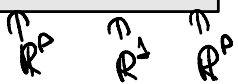
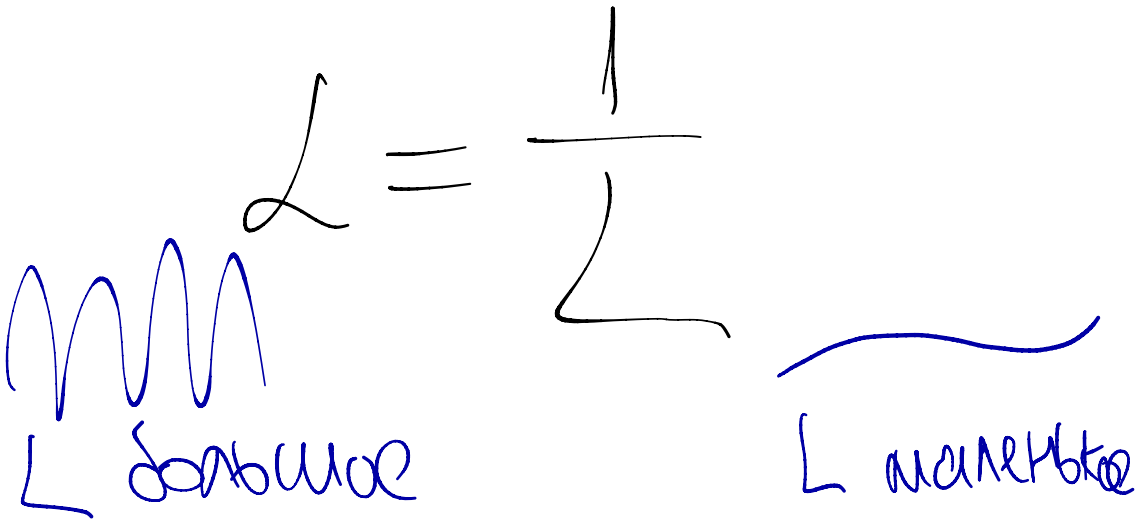
  - Decrease L between iterations
- Since stochastic gradient $g(x^k) \to \nabla f(x^k)$ you can use its norm to track convergence (which is not true for SGD!)
- For the generalized linear models (this includes LogReg, LLS) you need to store much less memory $\mathcal{O}(n)$ instead of $\mathcal{O}(pn)$.

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



SAG non-uniform sampling

- The step size α_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



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- When selecting components with a probability proportional to L_i, the constant L can be reduced from $\max_i L_i$ to $\bar{L} = \sum_i L_i / N$:

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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} \\
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- To generate with probabilities $L_i / \sum_j L_j$, there is an algorithm with complexity $O(\log N)$.

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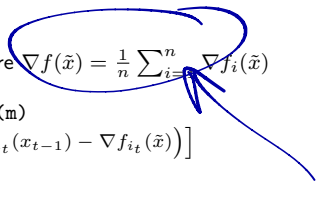

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- Two gradient evaluations per inner step.
- Two parameters: length of epochs + step-size γ.
- Linear convergence rate, simple proof.

Adagrad (Duchi, Hazan, and Singer 2010)

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

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

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- The constant ϵ 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 $j = 1, \ldots, p$:

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

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- 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 α:

сглаженная норма град

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- Often used in deep learning where parameter scales differ significantly across layers.

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

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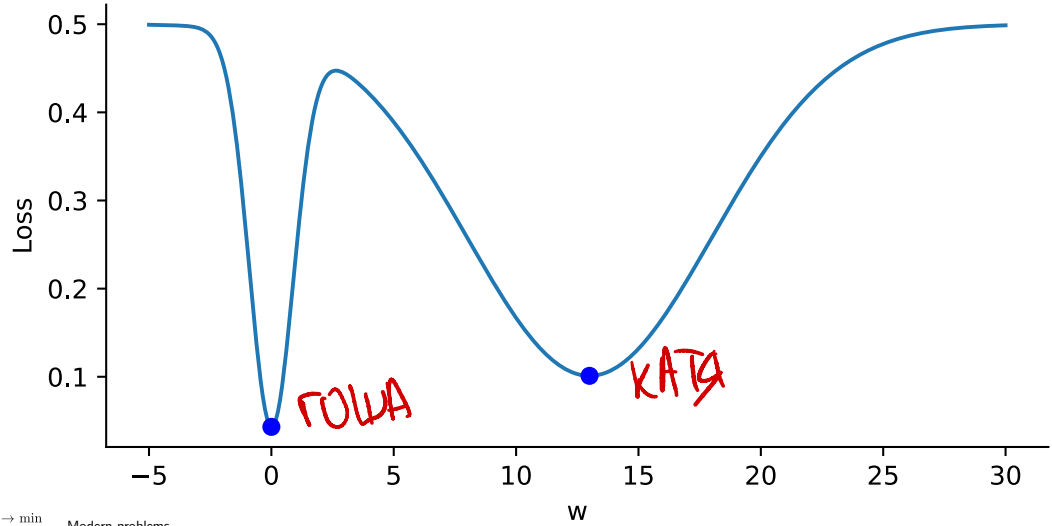
- However, the proposed algorithm in initial version does not converge even in convex setting (later fixes

Wide vs narrow local minima

Узкие и широкие локальные минимумы



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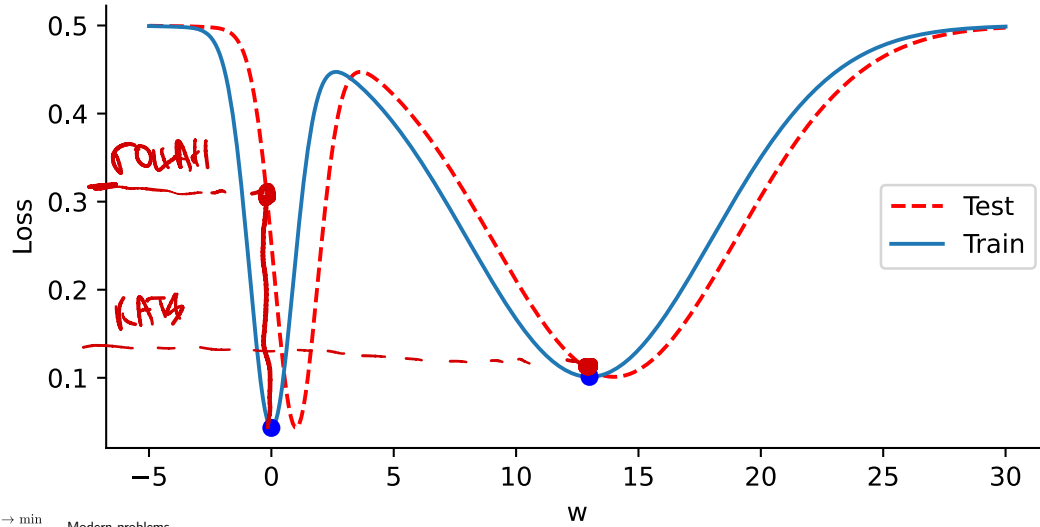

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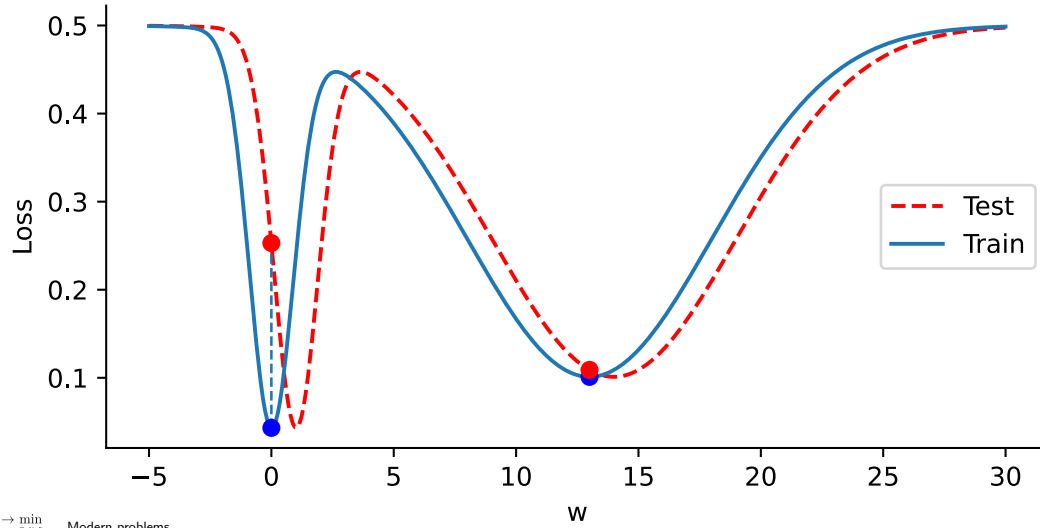
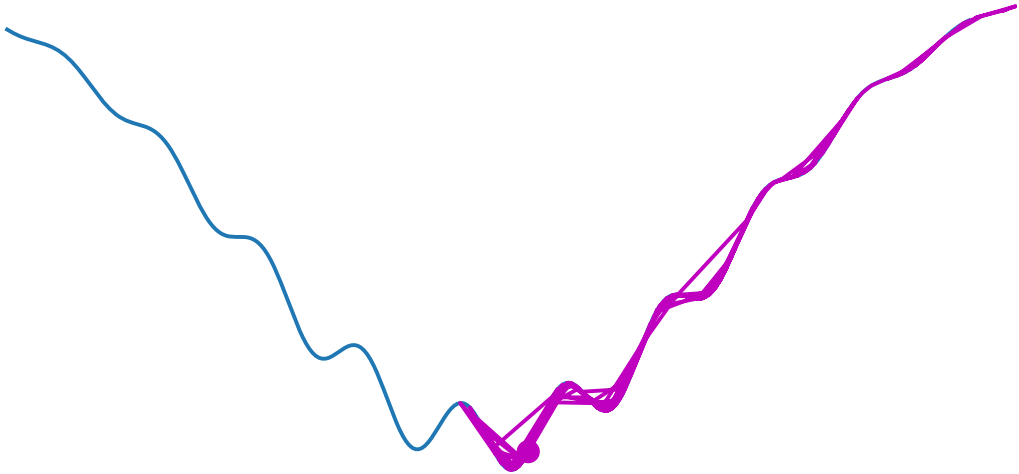


Stochasticity allows to escape local minima

Стохастический градиентный спуск
выпрыгивает из локальных минимумов



Local divergence can also be benefitial

Градиентный спуск с большим шагом
избегает узкого локального минимума