COMPUTER SCIENCE
UNIVERSITY OF MARYLAND

Automated Inference with Adaptive Batches

Soham De

Joint work with Abhay Yadav, David Jacobs, Tom Goldstein

University of Maryland

OVERVIEW

Most machine learning models use SGD for training

BUT…**noisy gradients** & **large variance**

↓

Hard to automate stepsize selection & stopping conditions

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Hard to automate stepsize selection & stopping conditions

In this work: **Big Batch SGD**

Adaptively grow batch size based on amount of noise in the gradients

Easy automated stepsize selection

MOST MODEL FITTING PROBLEMS LOOK LIKE THIS

$$\min \ell(x) := \frac{1}{N} \sum_{i=1}^{N} f(x, z_i)$$

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We also consider the more general problem:

$$\min \ell(x) := \mathbb{E}_{z\sim p}[f(x, z)]$$

Applications

SVM

logistic regression

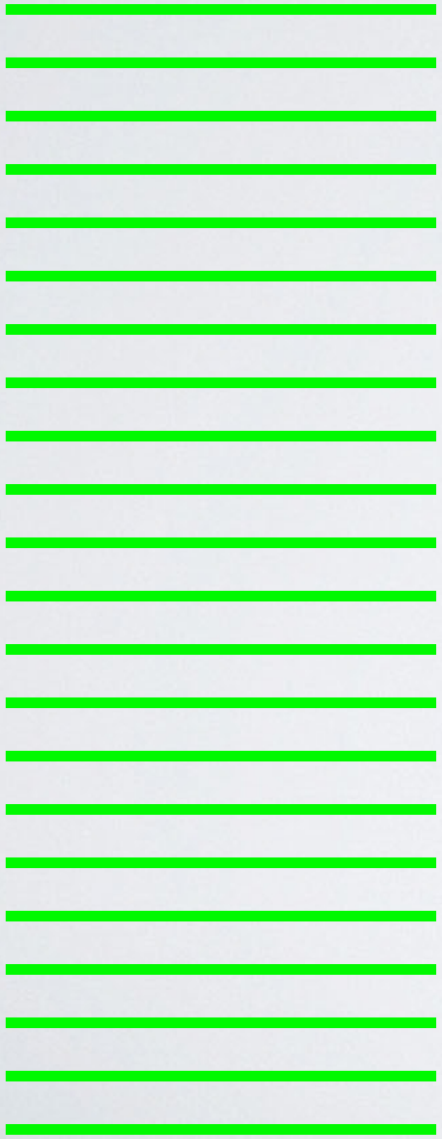
neural nets

matrix factorization

blah blah blah

SGD

select data

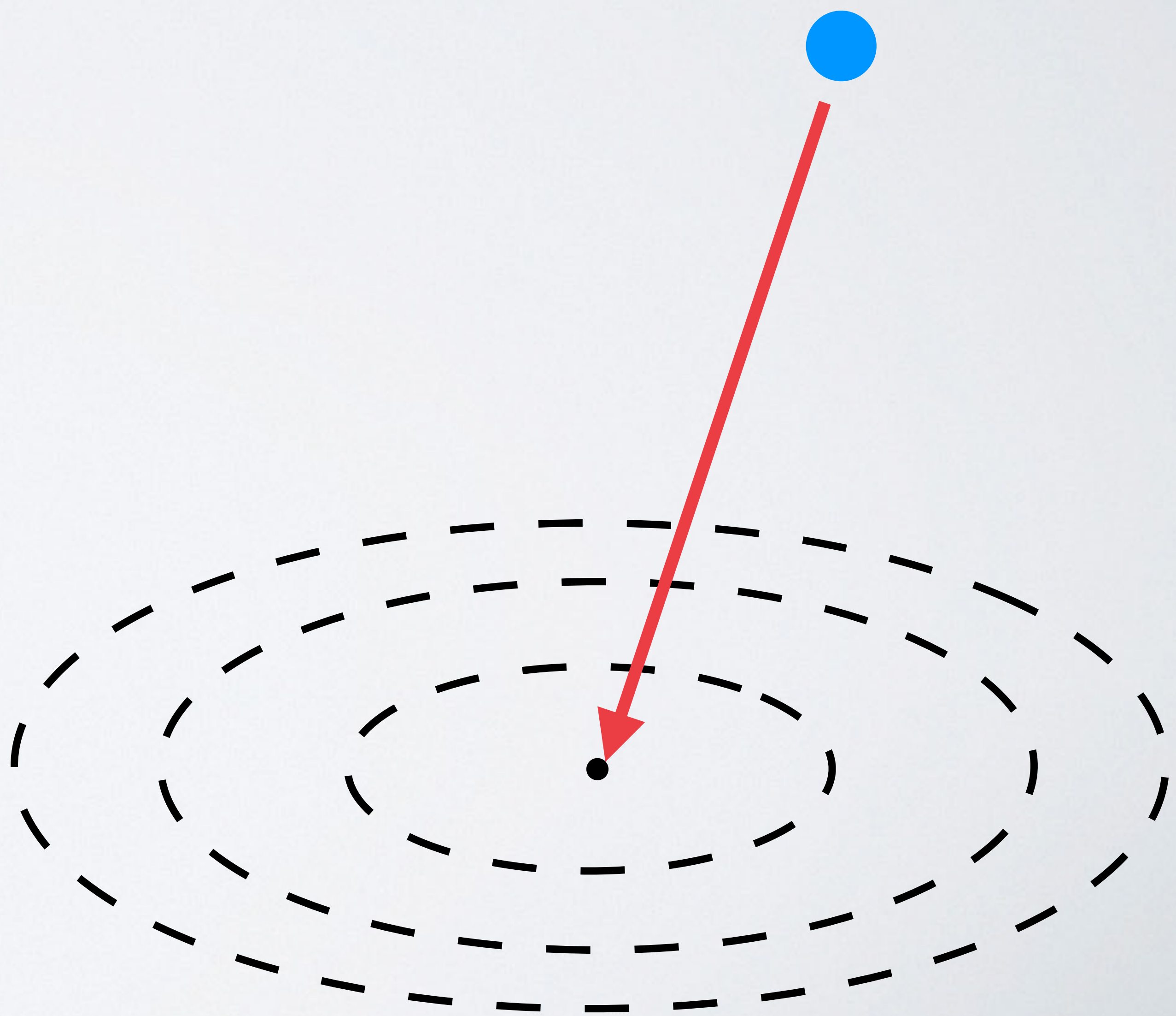


compute gradient

$$g_t = \frac{1}{N}\sum_{i=1}^{N} \nabla f(x_t, z_i)$$

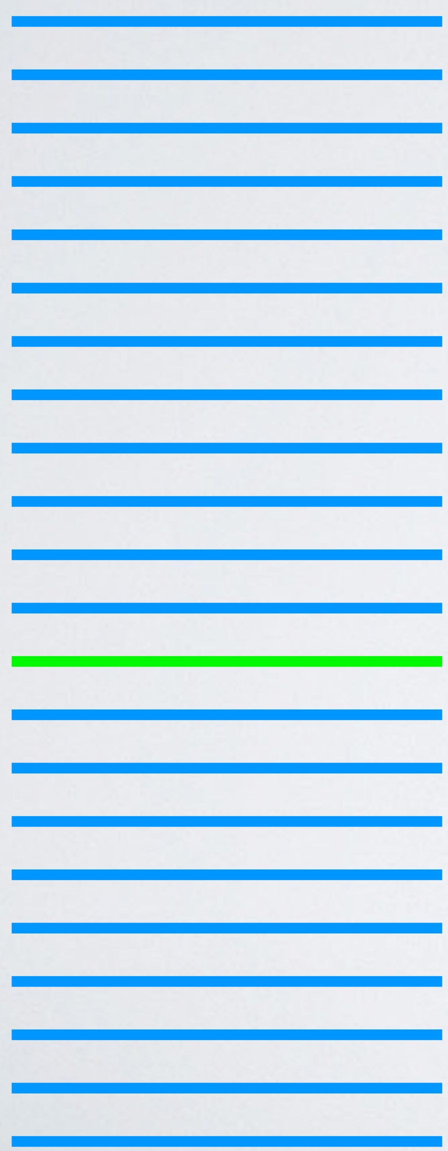
update

$$x_{t+1} = x_t - \alpha_t g_t$$

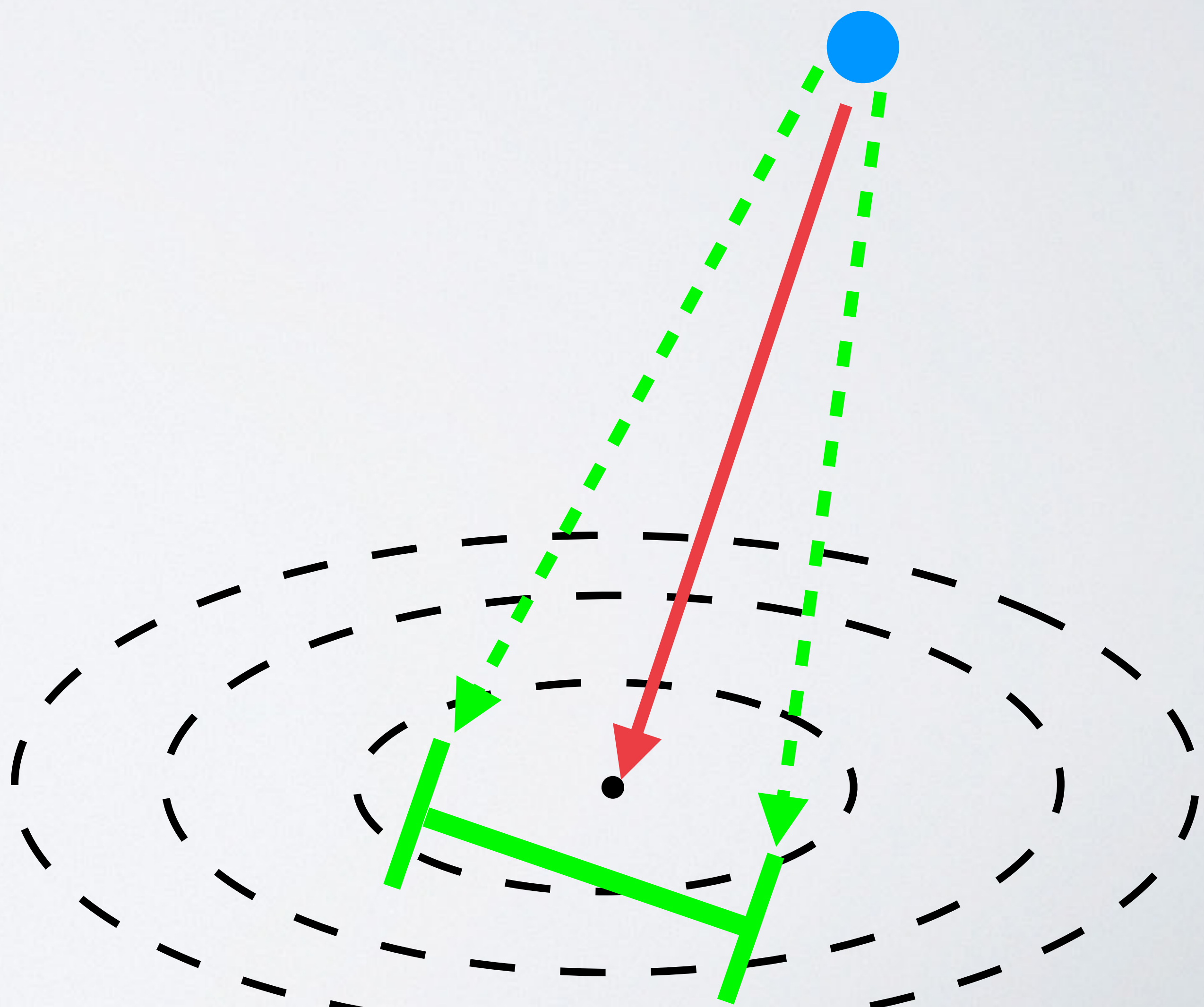


SGD

select data **compute gradient** **update**



$$g_t \approx \nabla f(x_t, z_{12}) \rightarrow x_{t+1} = x_t - \alpha_t g_t$$



SGD

select data

compute gradient

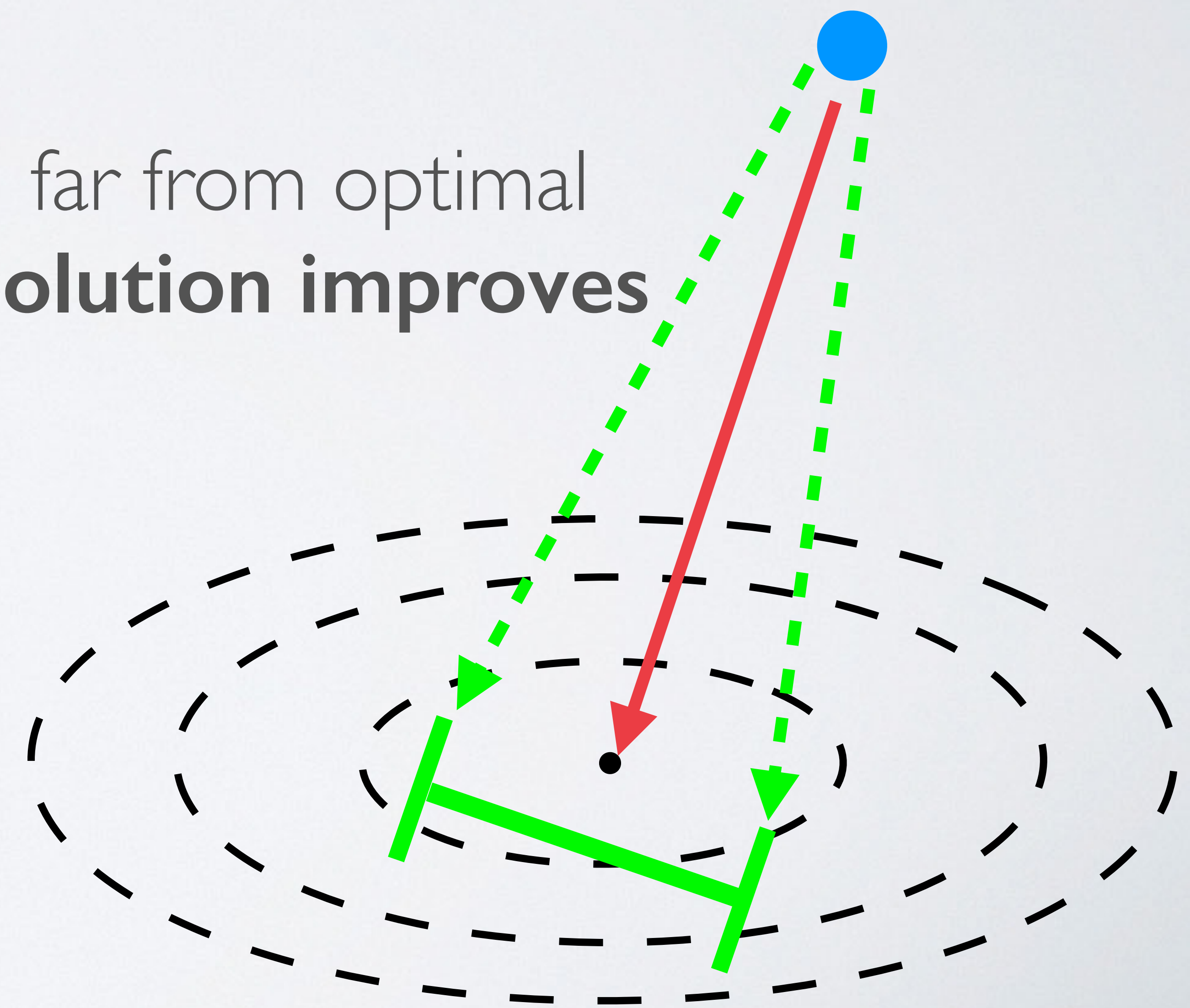
$$g_t \approx \nabla f(x_t, z_8)$$

update

$$x_{t+1} = x_t - \alpha_t g_t$$

far from optimal

solution improves



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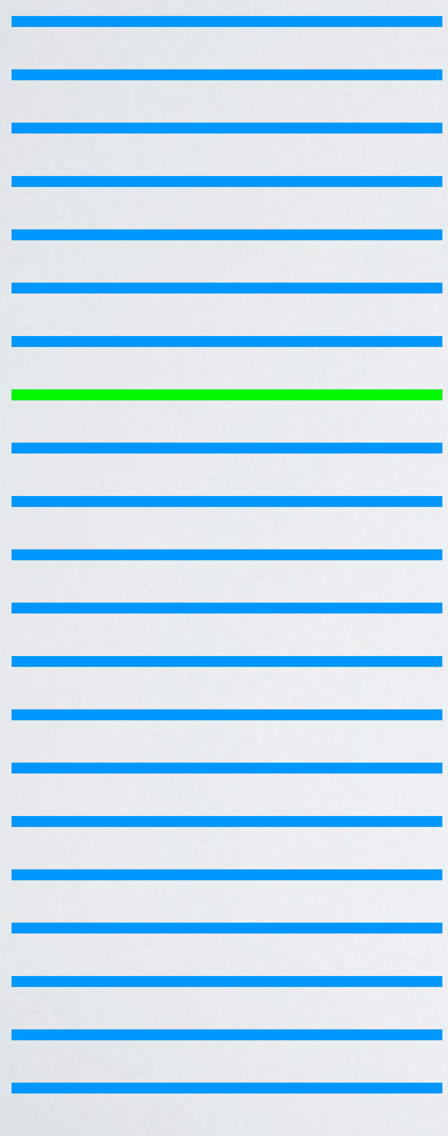

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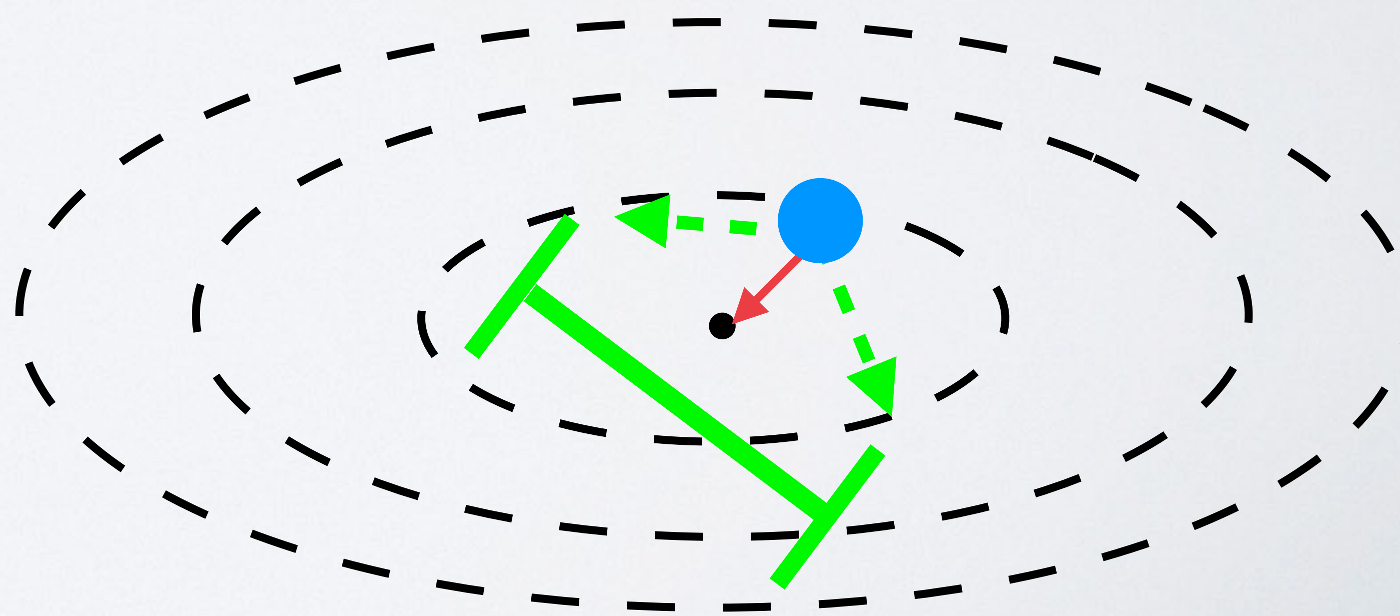
close to optimal

solution gets worse



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Error must **decrease**
as we approach solution

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classical solution

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hard to pick
stepsize schedule

USE BIGGER BATCHES?

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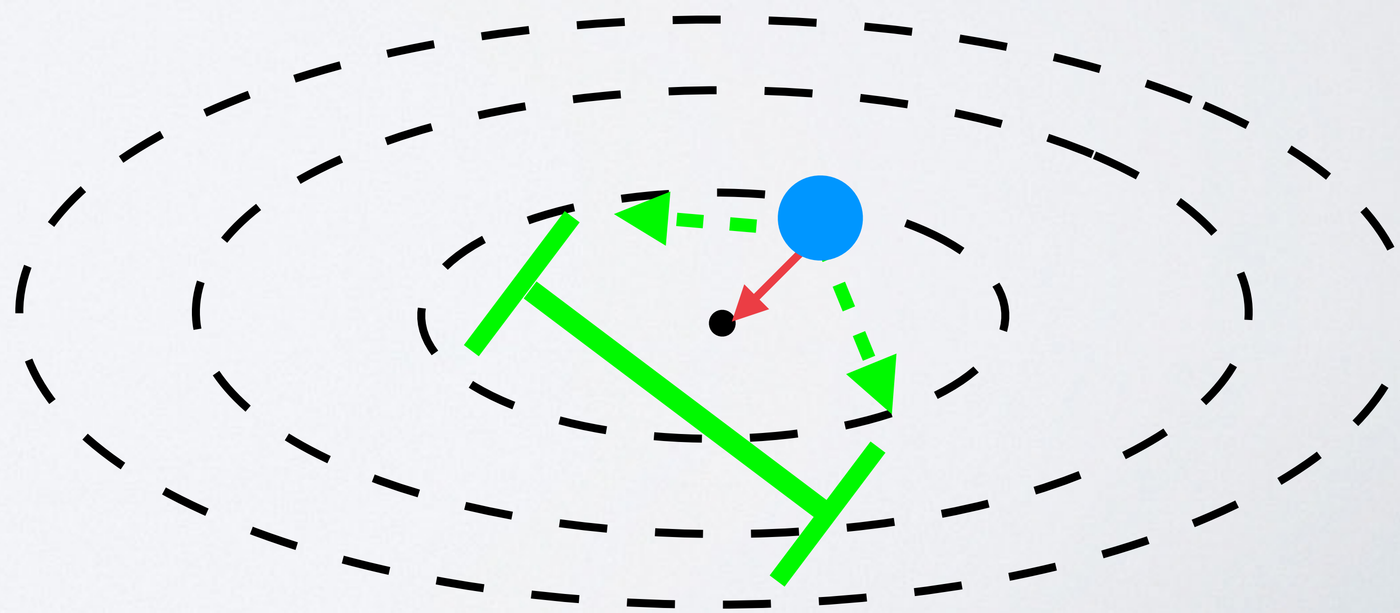

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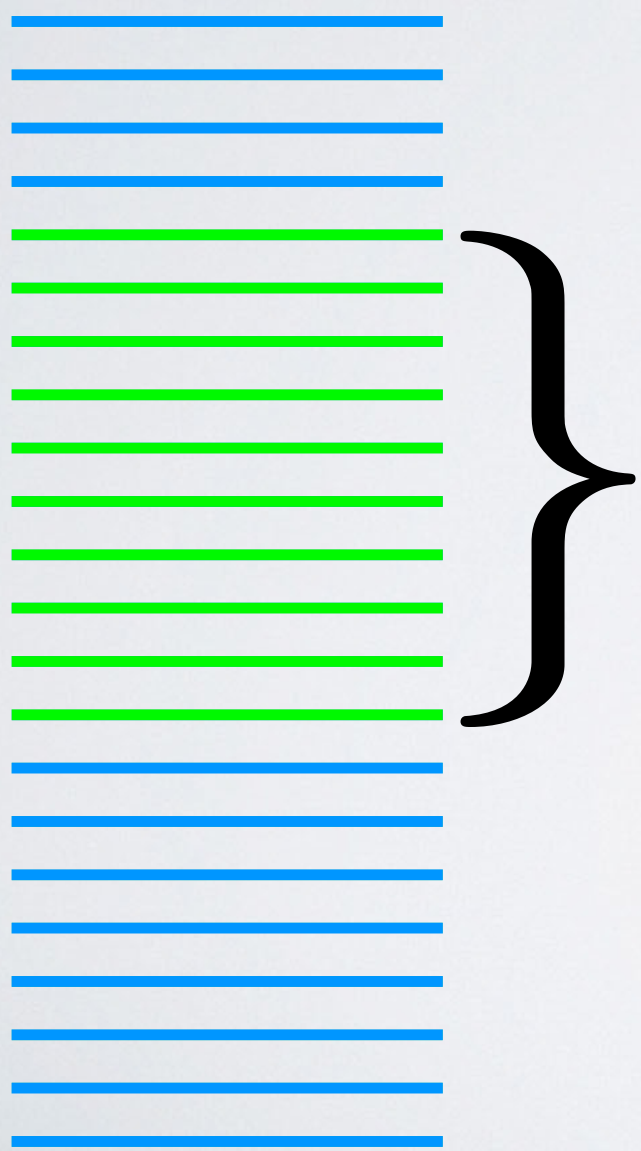

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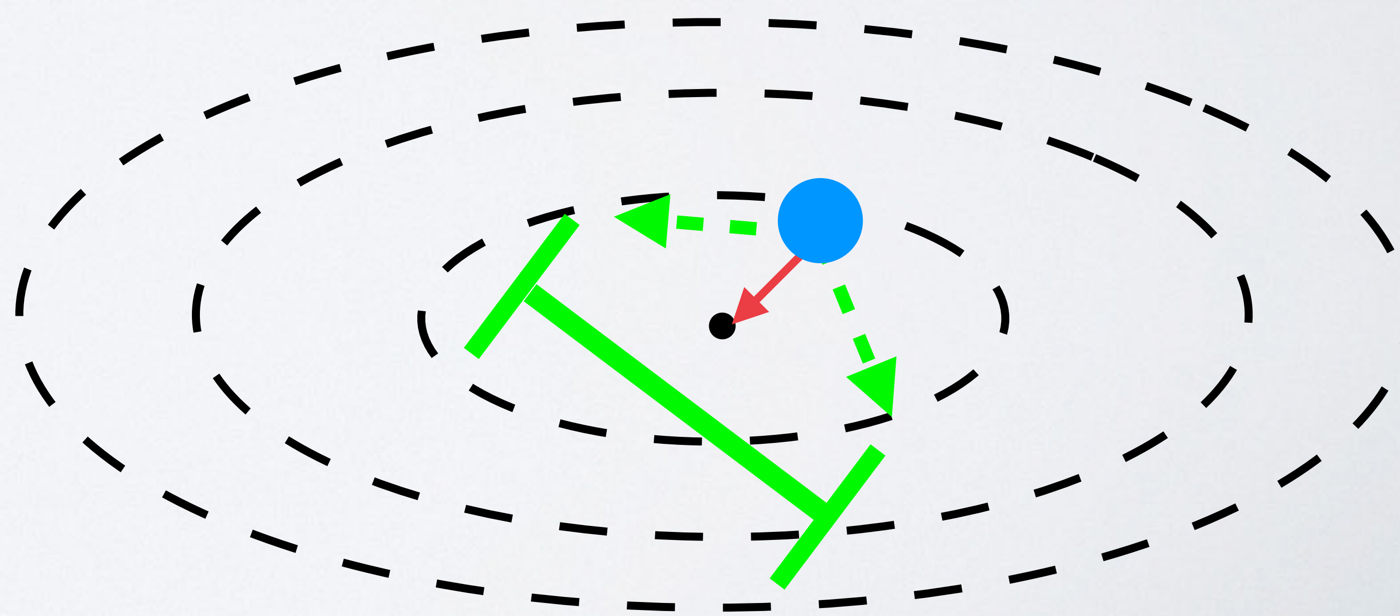
close to optimal

solution gets worse



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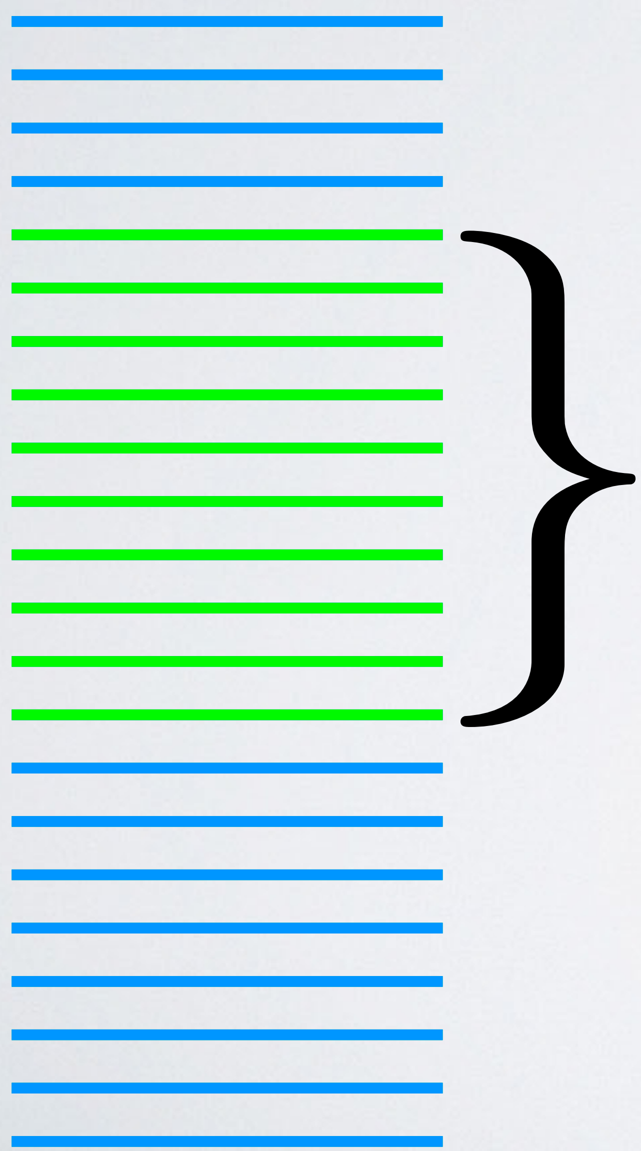

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$$g_t \approx \underline{\nabla \ell_{\mathcal{B}}(x_t)}$$

gradient on batch *B*

update

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close to optimal

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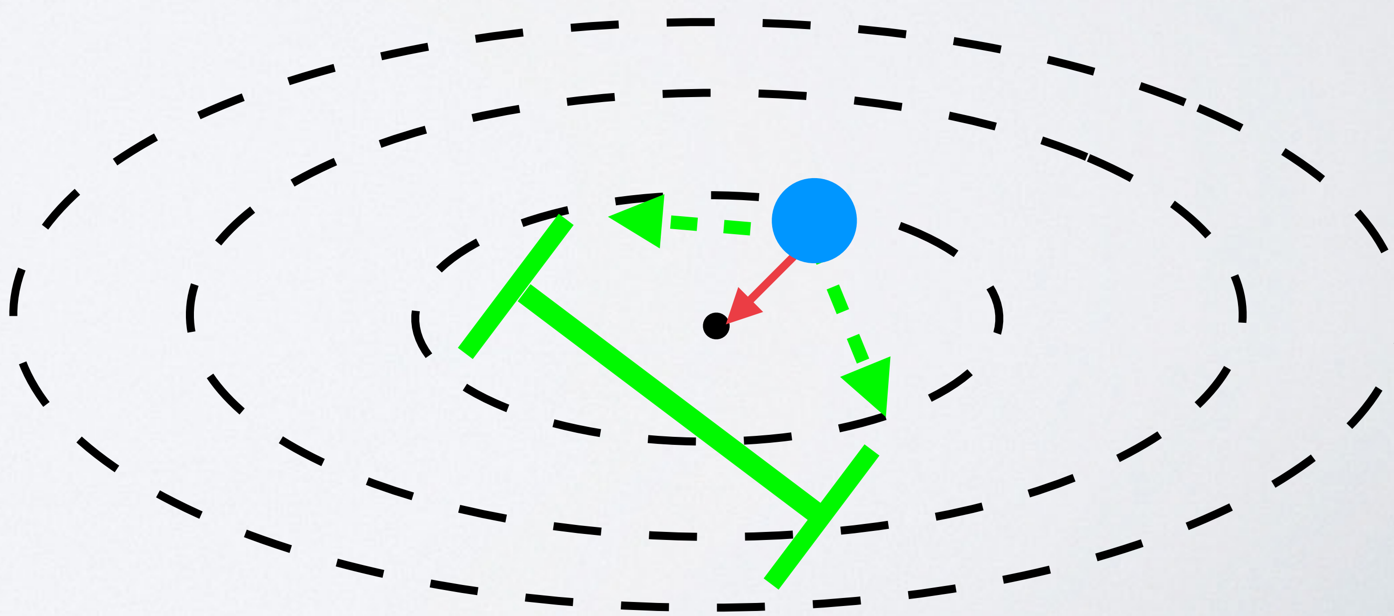

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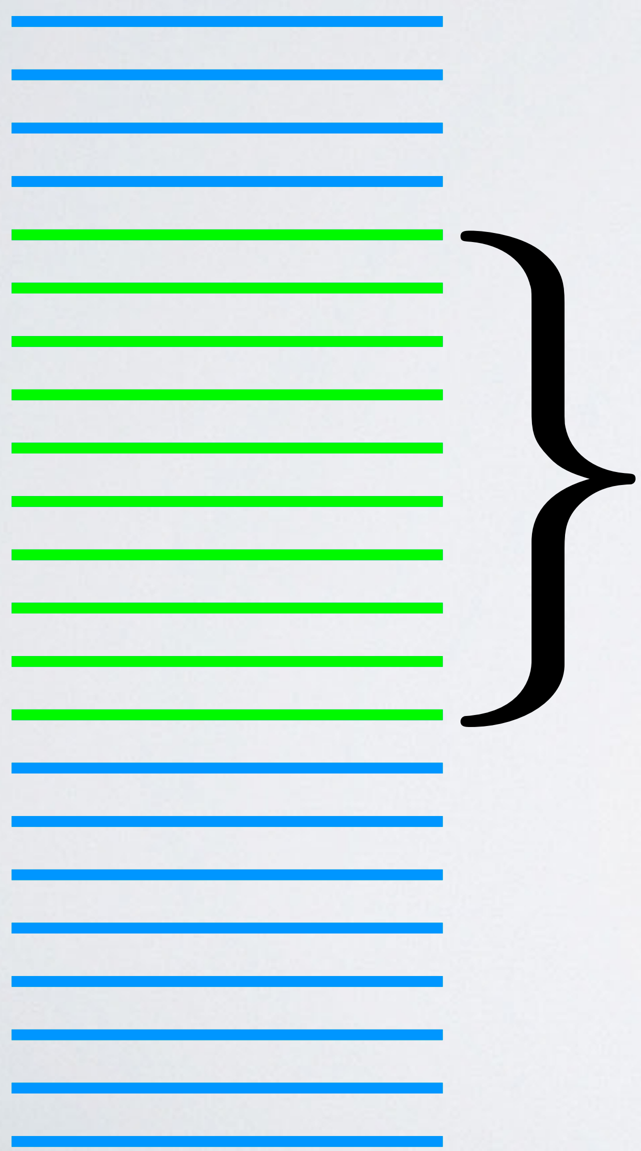

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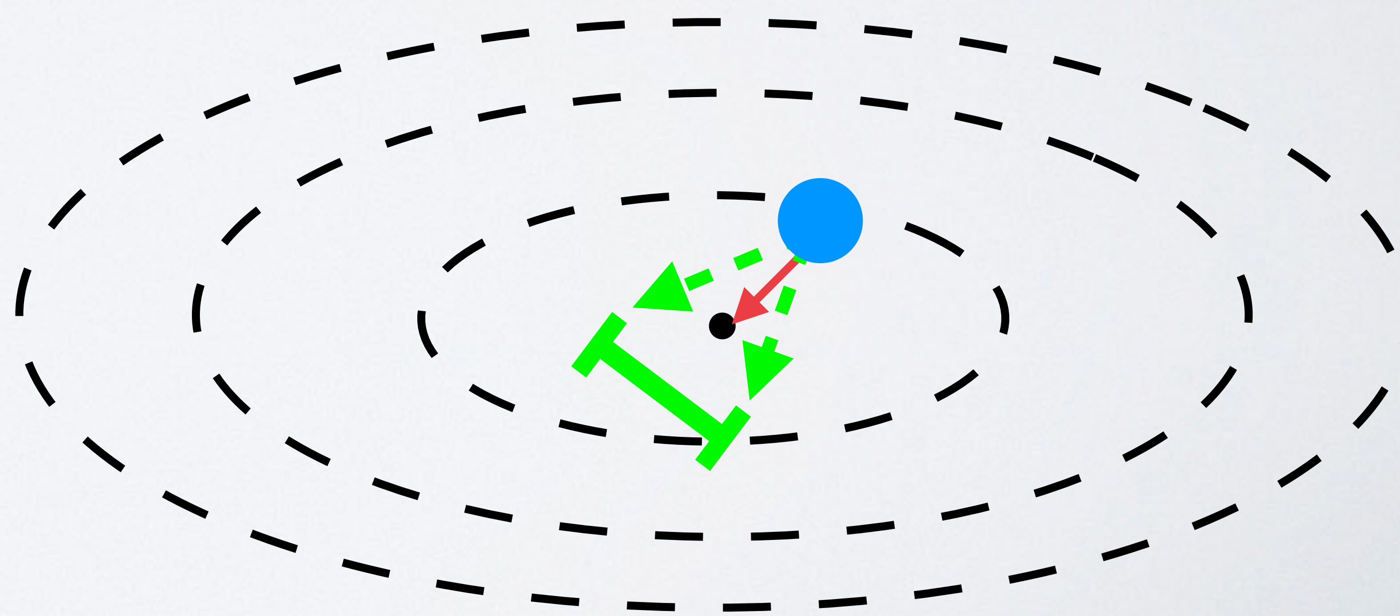

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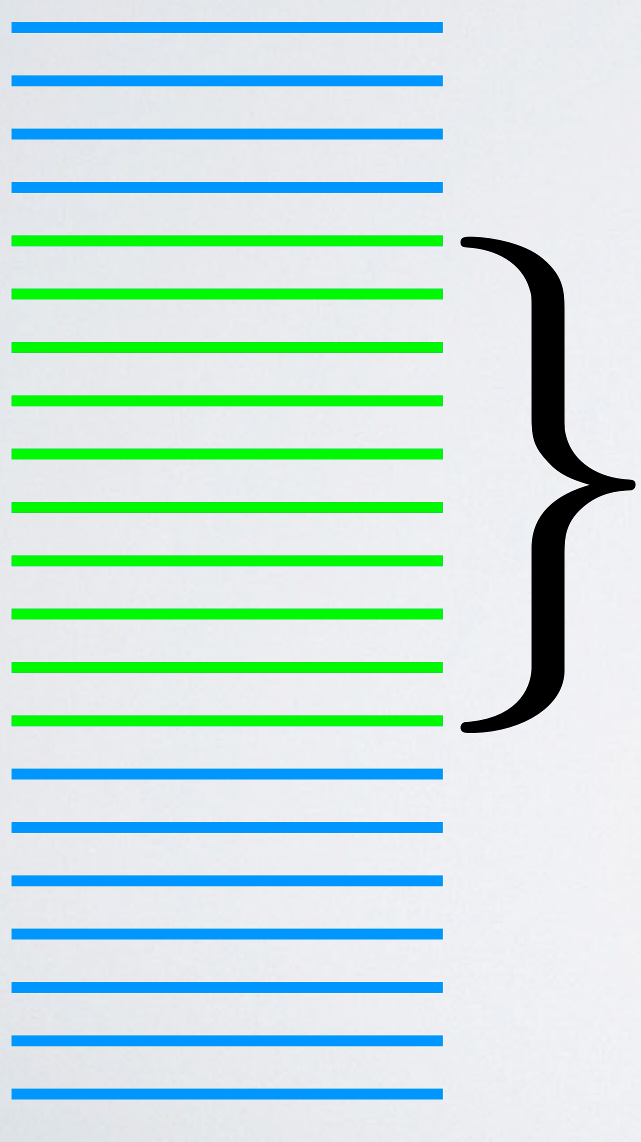

compute gradient

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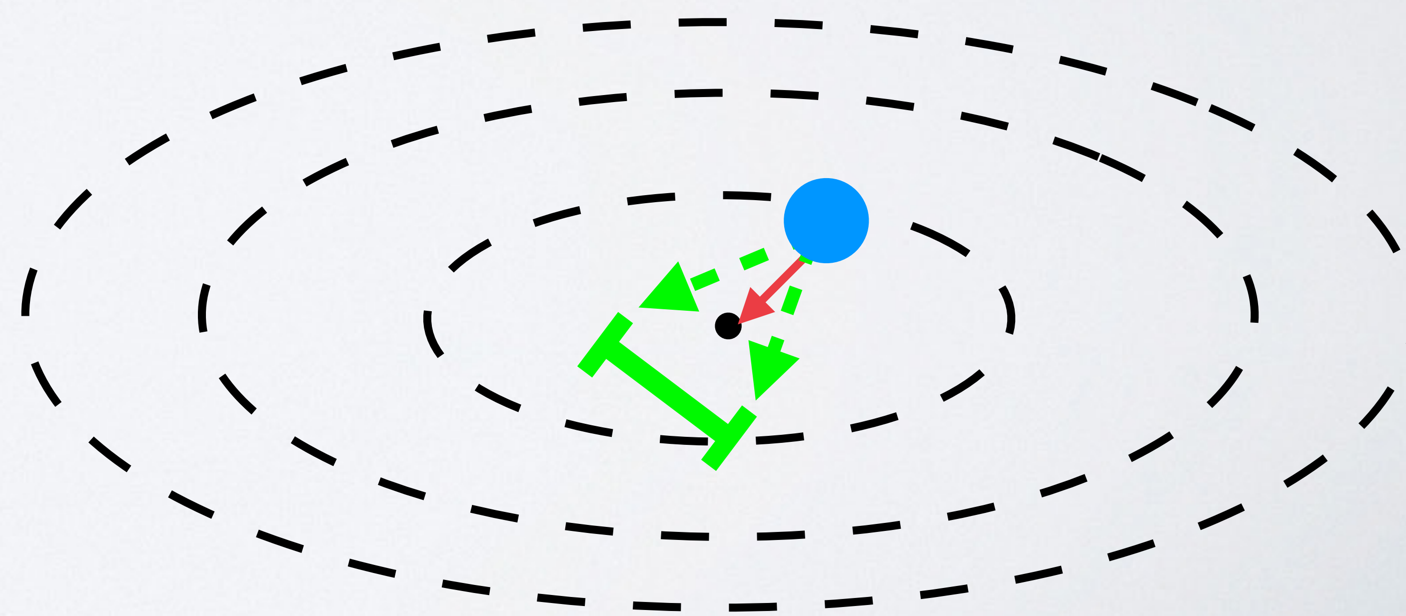
lower variance

solution gets better



GROWING BATCHES

regime 1: far from optimal

regime 2: close to optimal

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Noisy gradients
improve solution

↓

Large batches do
unnecessary work
+
Get stuck in local minima

regime 2: close to optimal

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Adaptively Grow
Batches Over Time!

PRELIMINARIES

Standard result in stochastic optimization:

Lemma
A sufficient condition for $-\nabla \ell_{\mathcal{B}}(x)$ to be a descent direction is:

$$\|\nabla \ell_{\mathcal{B}}(x) - \nabla \ell(x)\|^2 < \|\nabla \ell_{\mathcal{B}}(x)\|^2.$$

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If error is **small** relative to gradient : descent direction

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How big is this error?

How large does the batch need to be to guarantee this?

ERROR BOUND

Theorem

Assume f has L_z - Lipschitz dependence on data z.

Then, expected error is uniformly bounded by:

$$\begin{aligned} \mathbb{E}_{\mathcal{B}}\|\nabla \ell_{\mathcal{B}}(x) - \nabla \ell(x)\|^2 &= \operatorname{Tr}\operatorname{Var}_{\mathcal{B}}(\nabla \ell_{\mathcal{B}}(x)) \\ &\leq \frac{1}{|\mathcal{B}|} \cdot 4L_z^2 \operatorname{Tr}\operatorname{Var}_z(z) \end{aligned}$$

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ERROR BOUND

Theorem

Expected Error (Gradient Variance) < Data Variance

Higher Batch Size → Lower Gradient Variance

data variance

ERROR BOUND

From the previous Lemma and Theorem:
We expect $-\nabla \ell_{\mathcal{B}}(x)$ to be a descent direction reasonably often provided:

$$\theta^2 \mathbb{E}\|\nabla \ell_{\mathcal{B}_t}(x_t)\|^2 \geq \frac{1}{|\mathcal{B}_t|} \operatorname{Tr} \operatorname{Var}_z \nabla f(x_t, z)$$

where $\theta \in (0,1)$

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We use this observation in Big Batch SGD

BIG BATCH SGD

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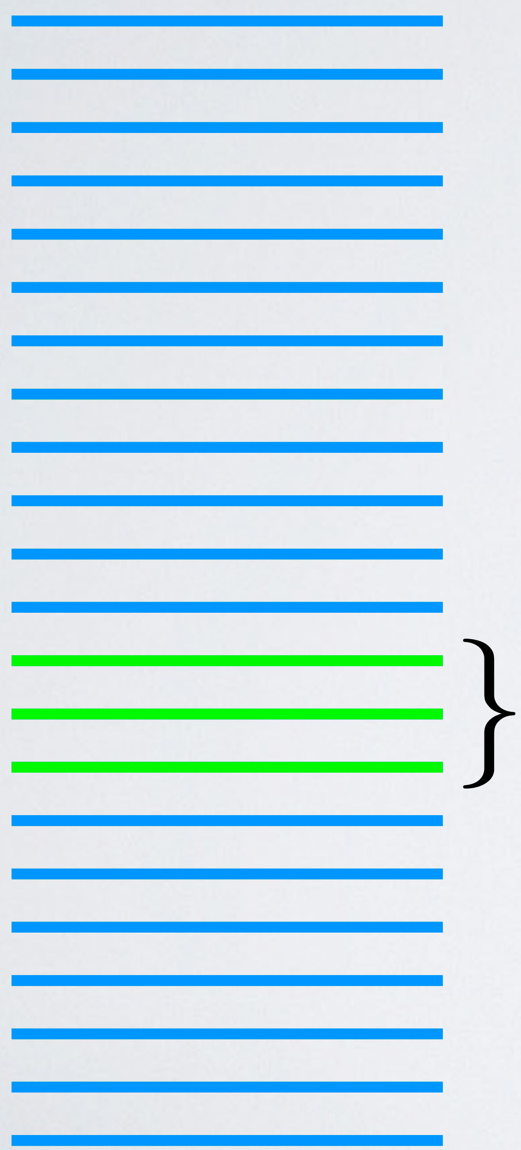
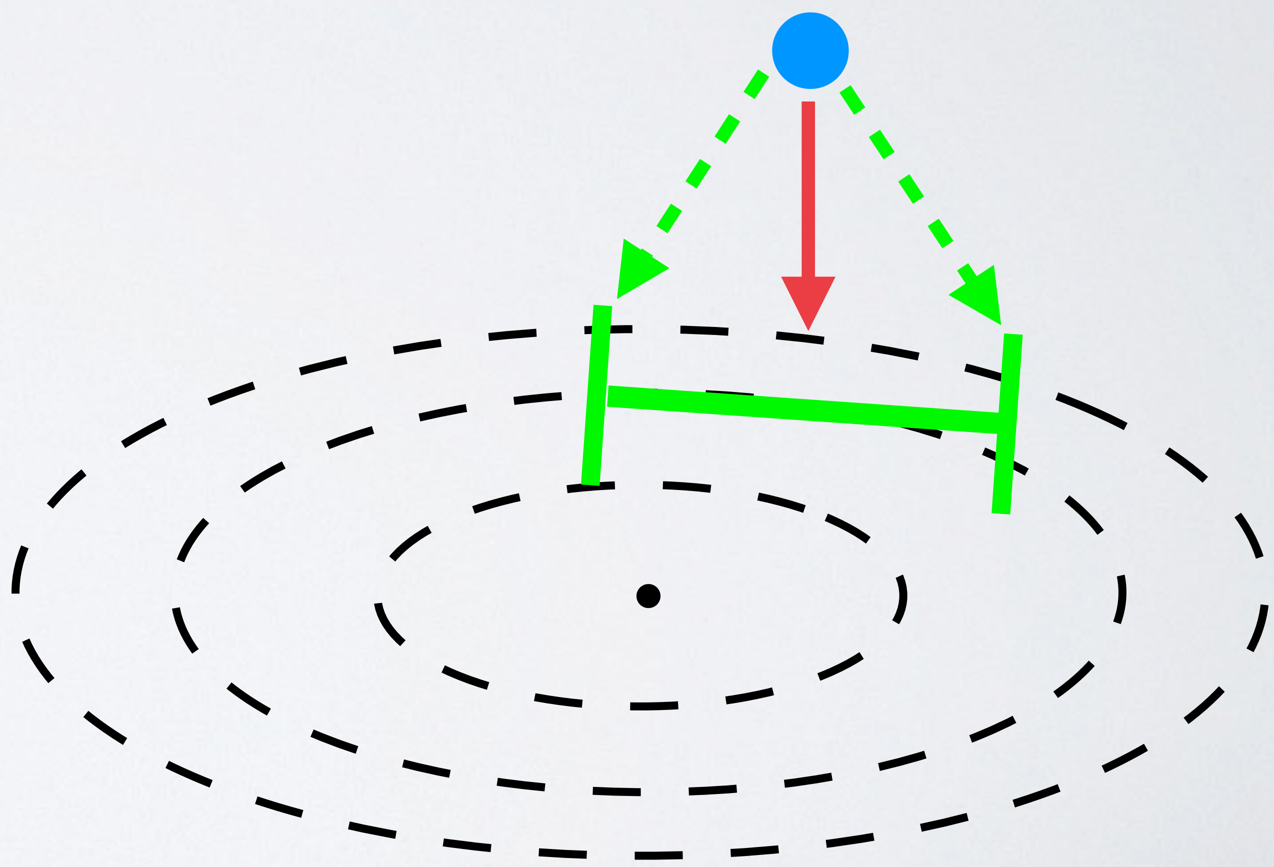
estimate size of error using
variance of batch gradients



pick batch *B*



BIG BATCH SGD

if signal > noise

(gradient) (variance)

update

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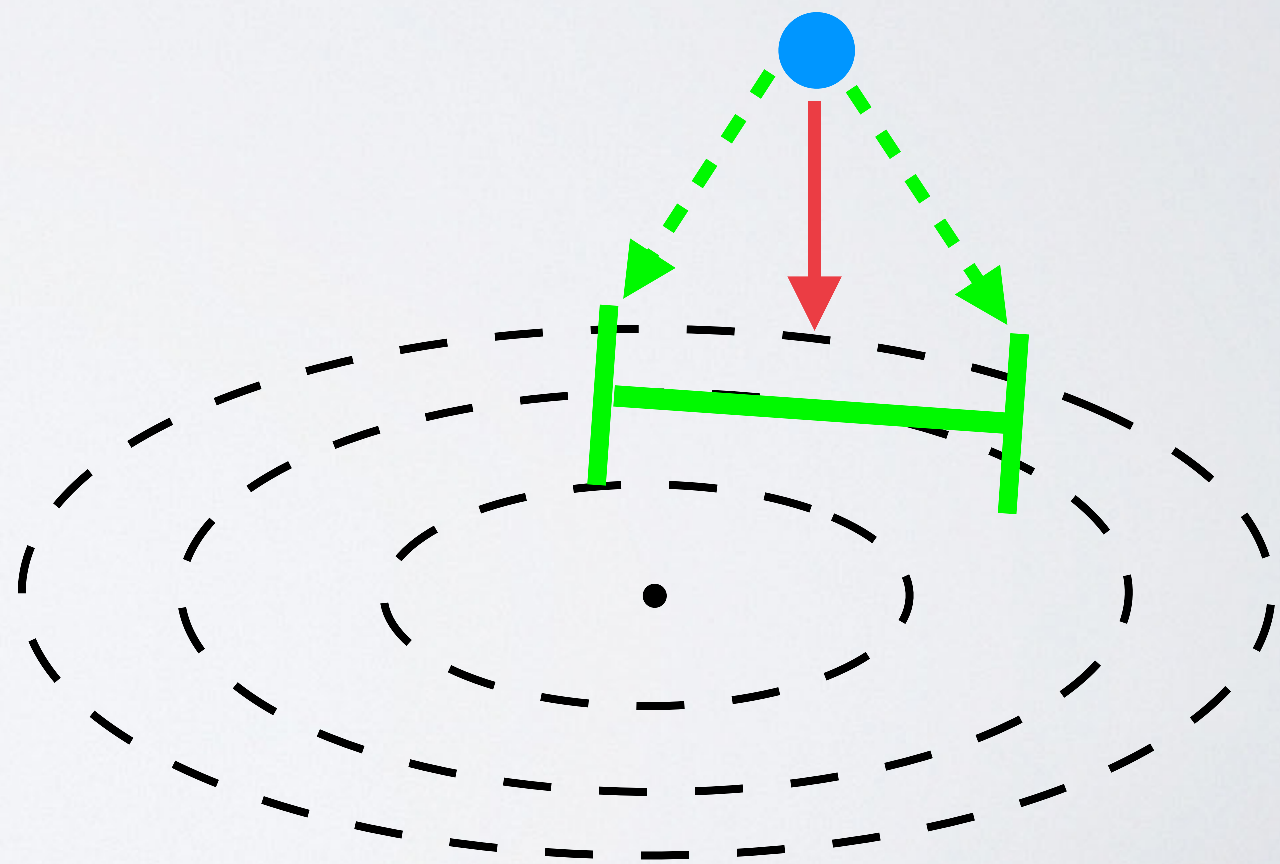

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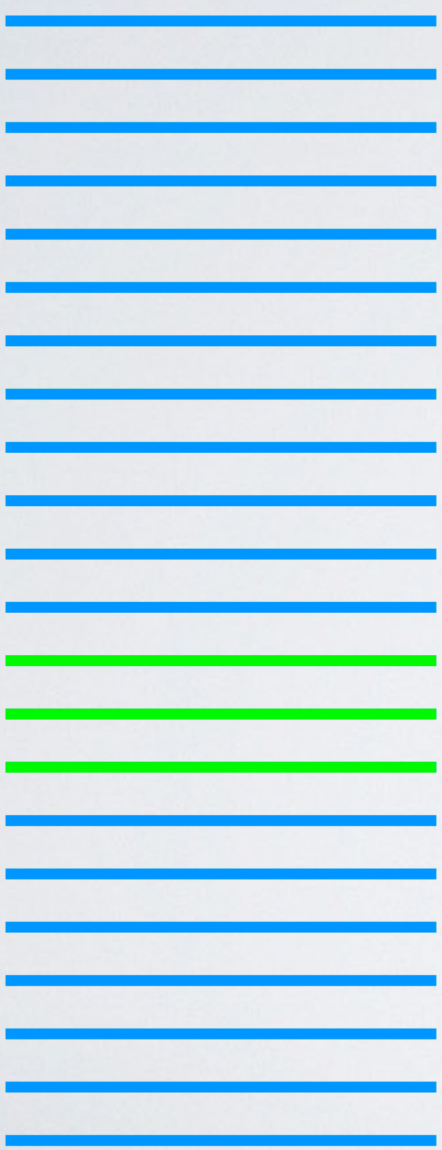

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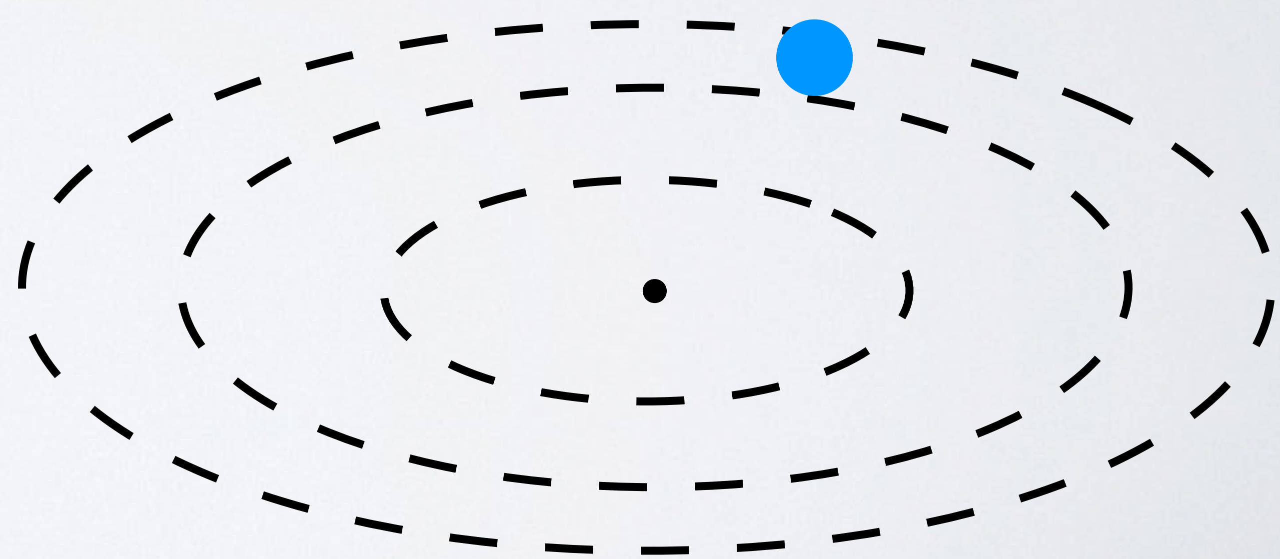

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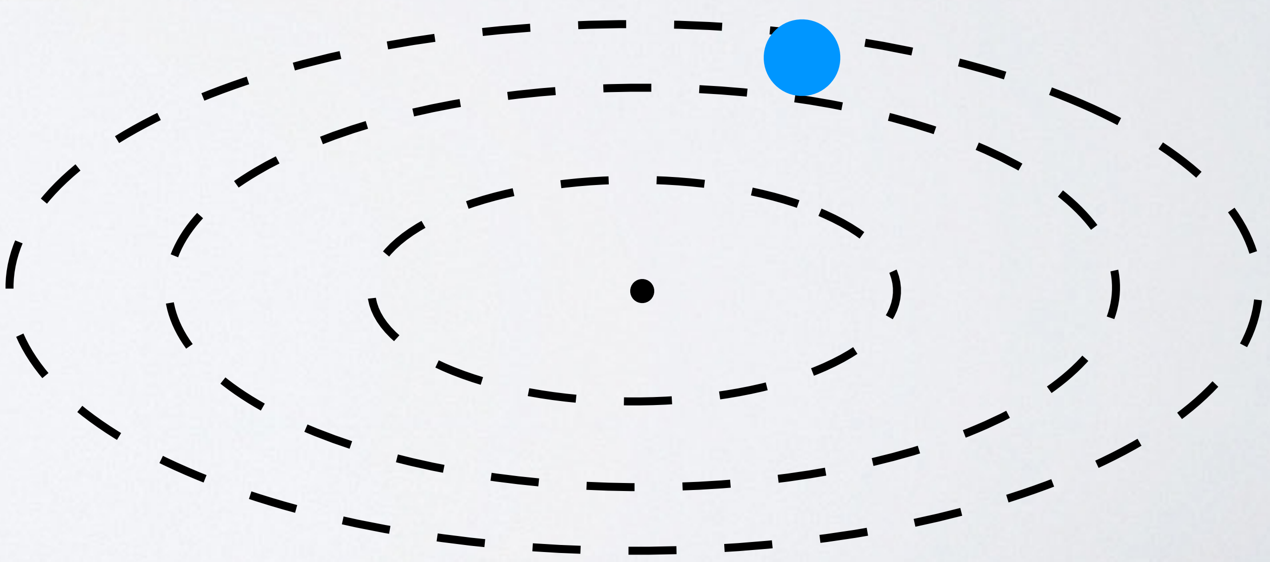

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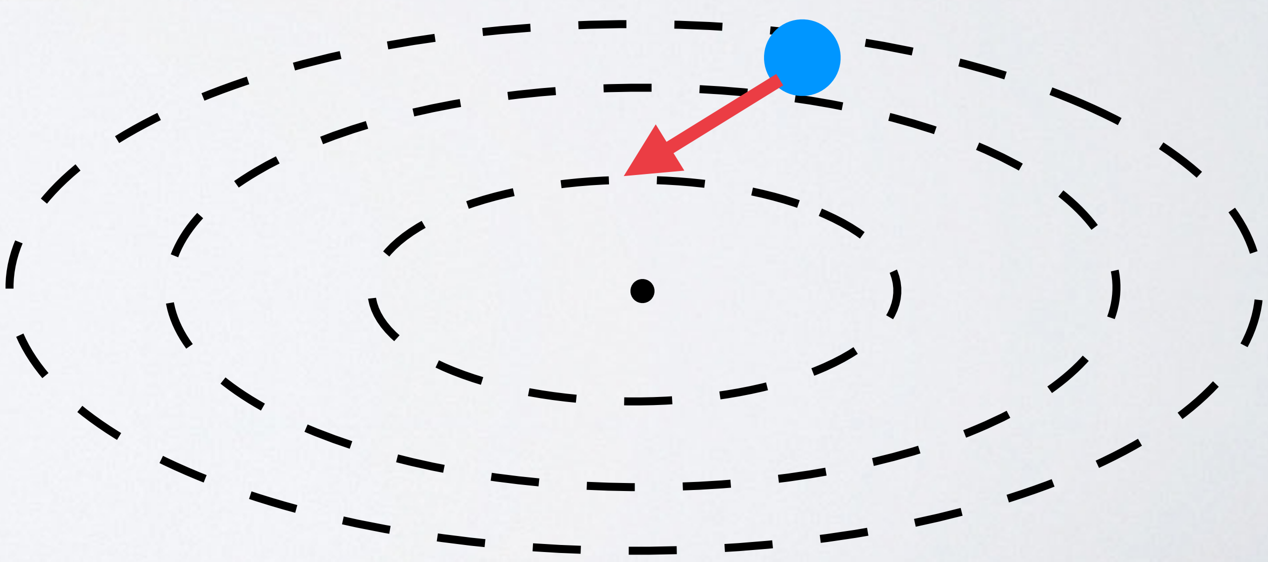

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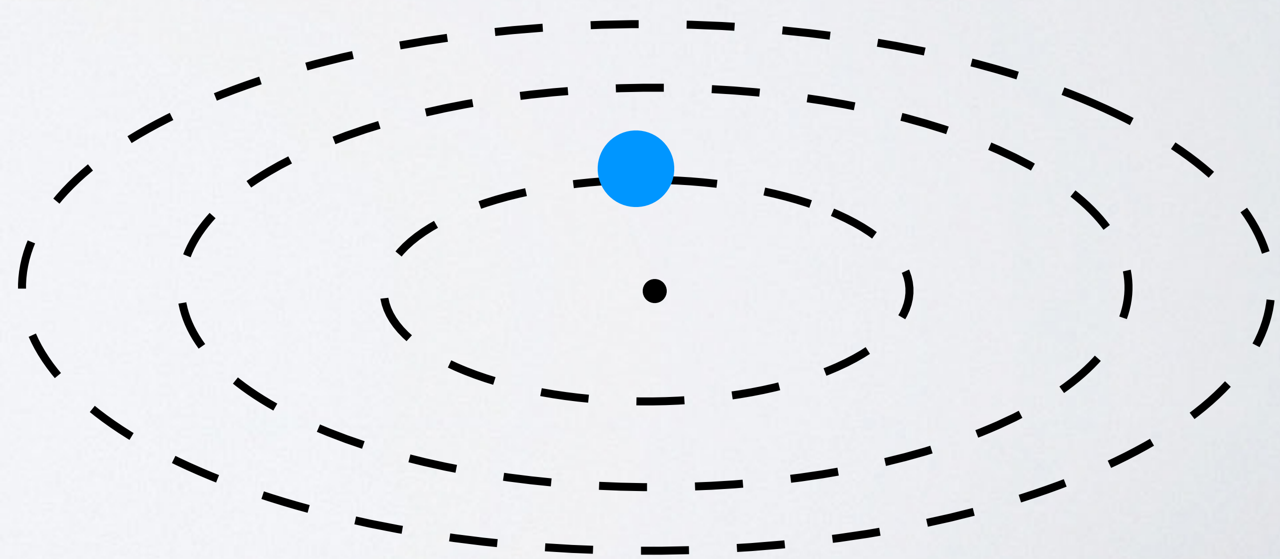

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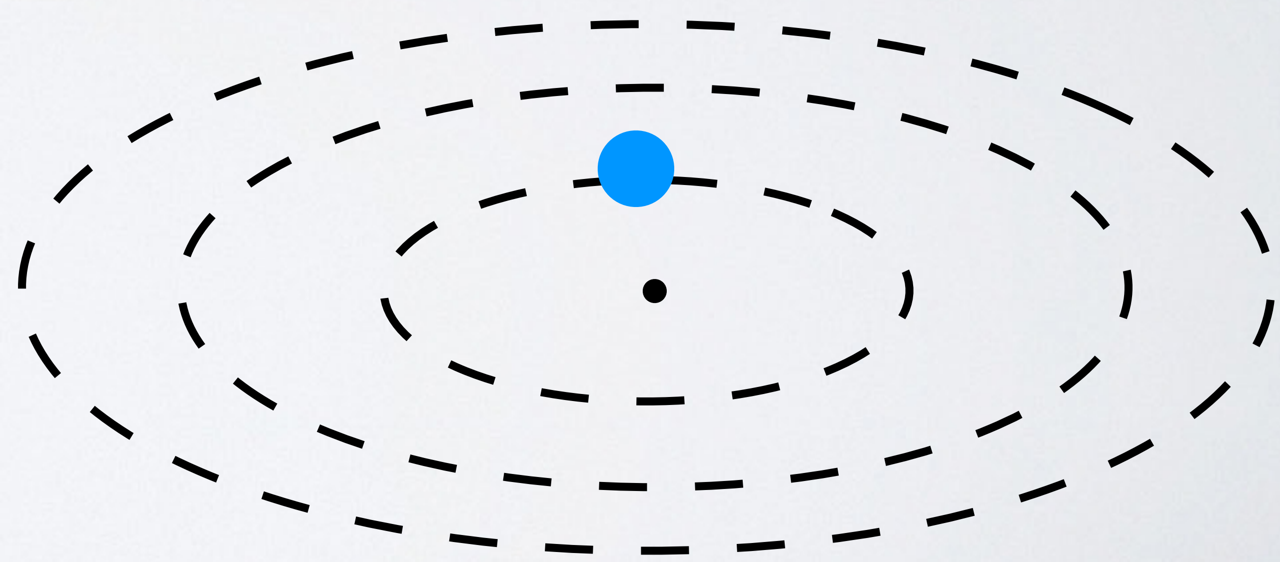

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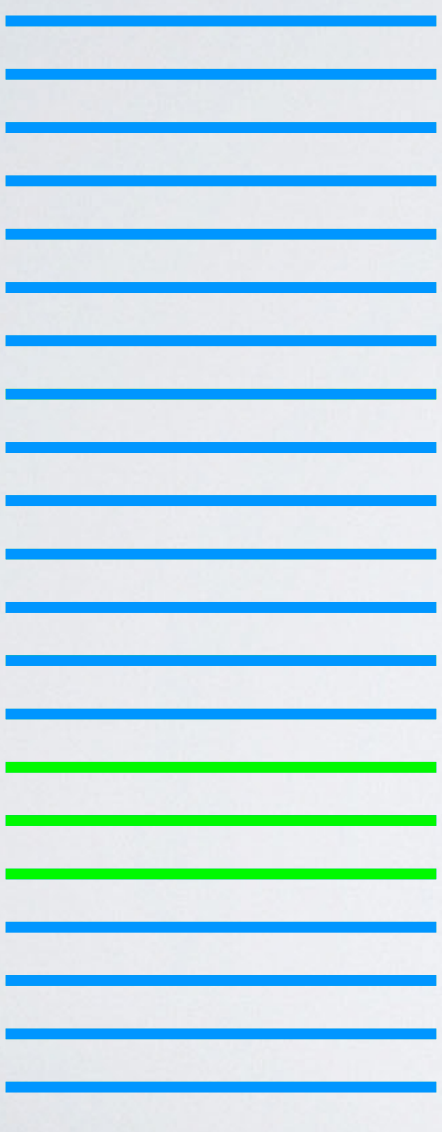

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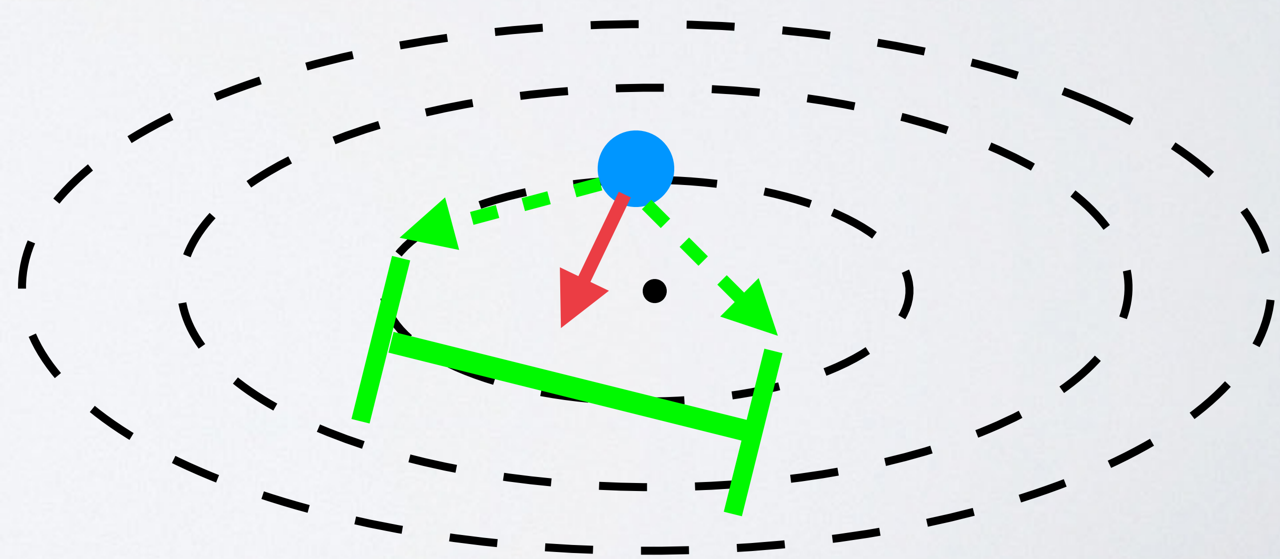

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otherwise
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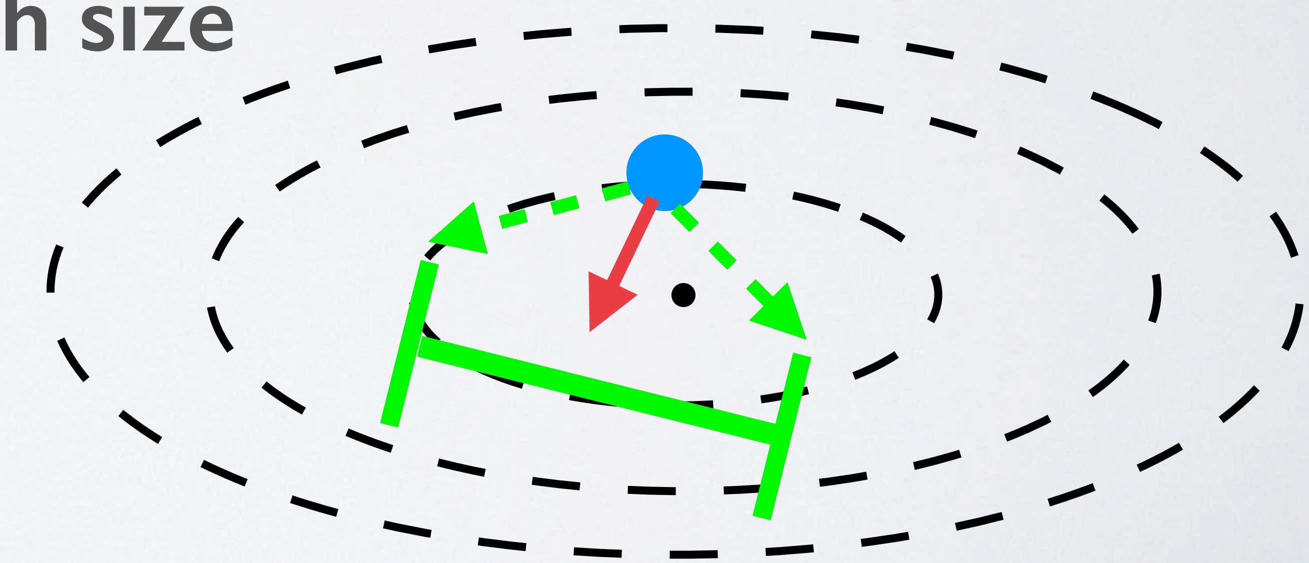

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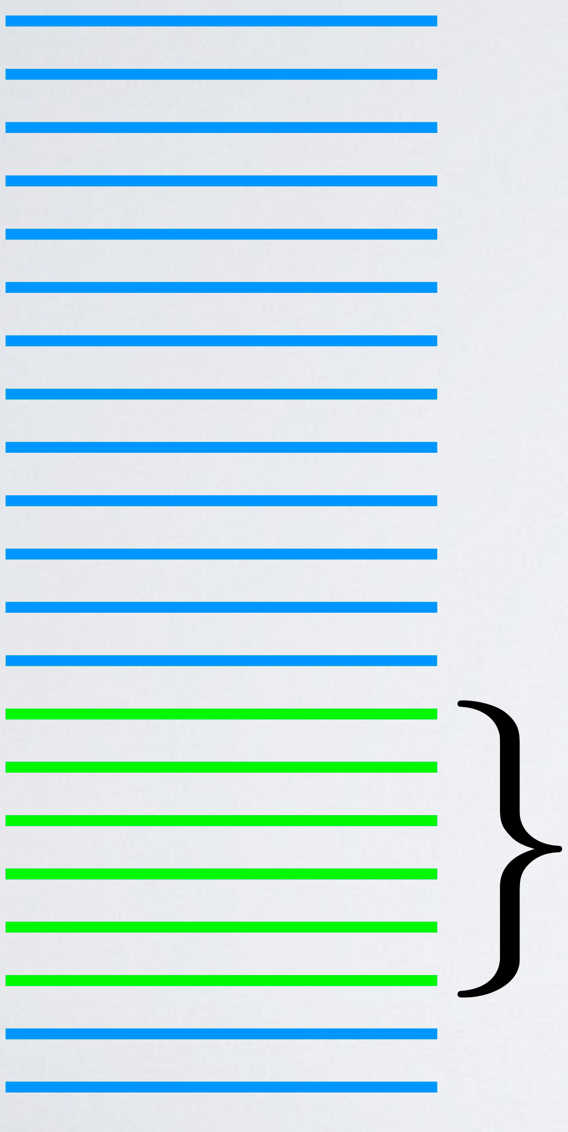

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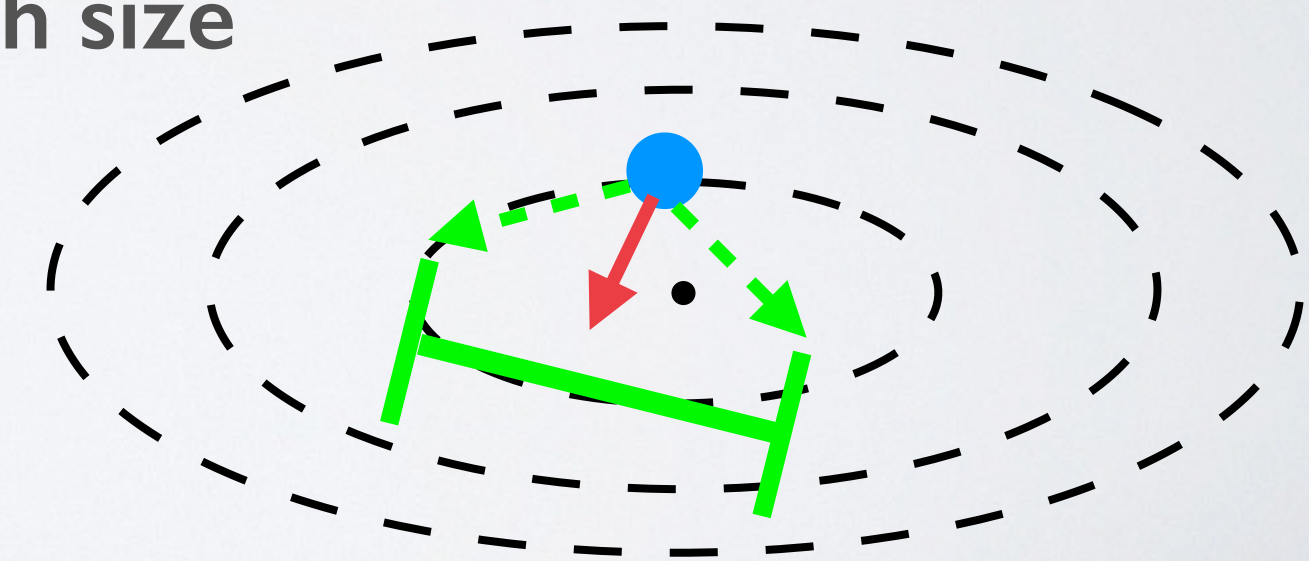

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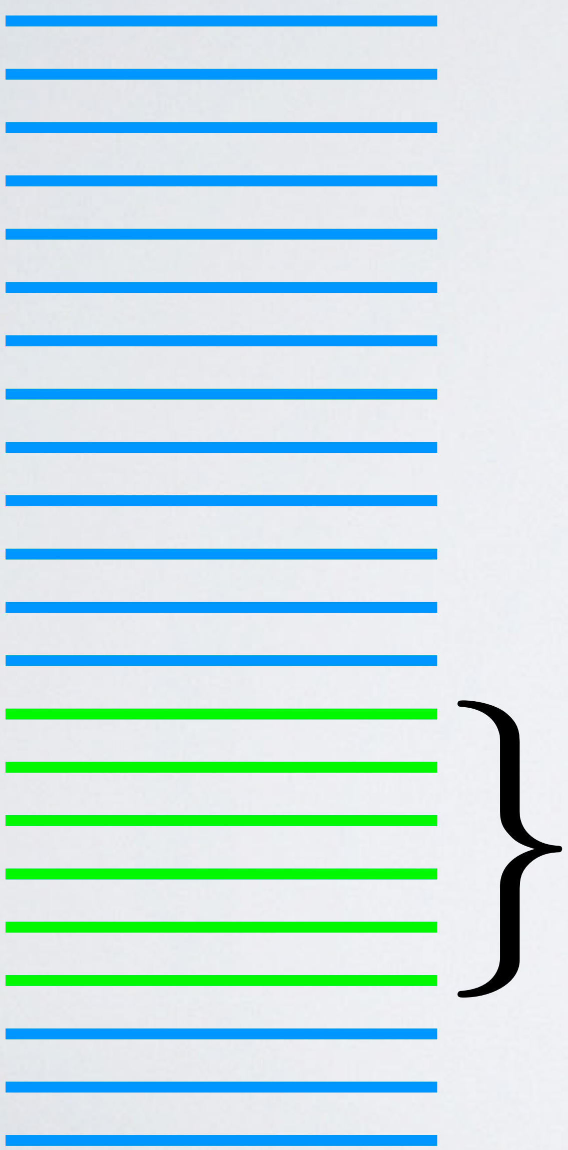

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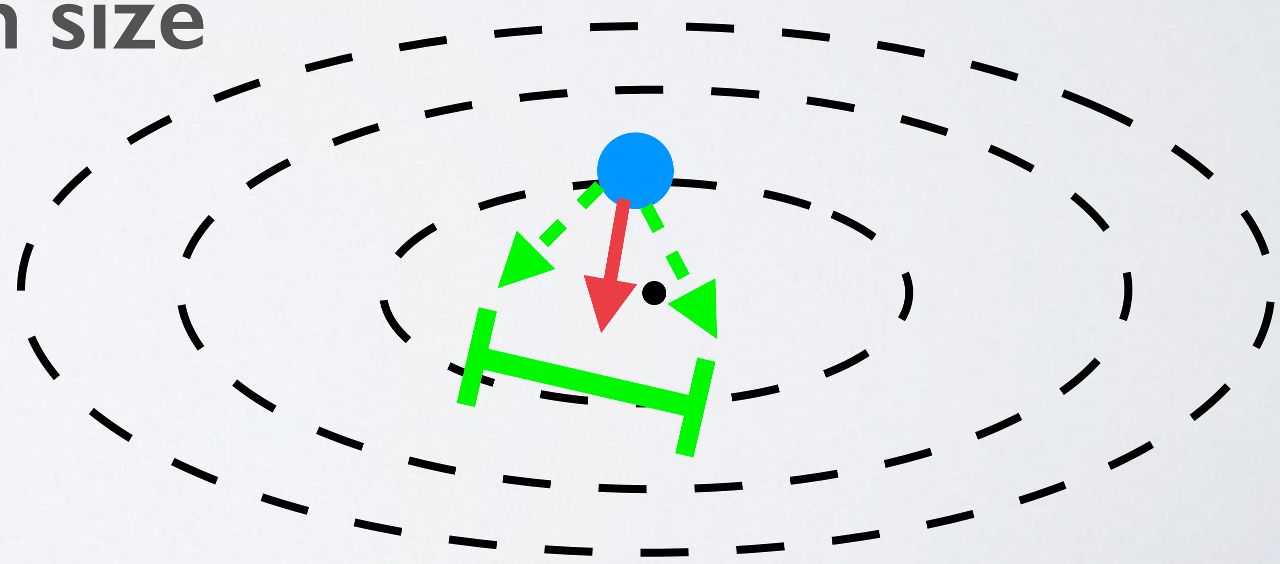

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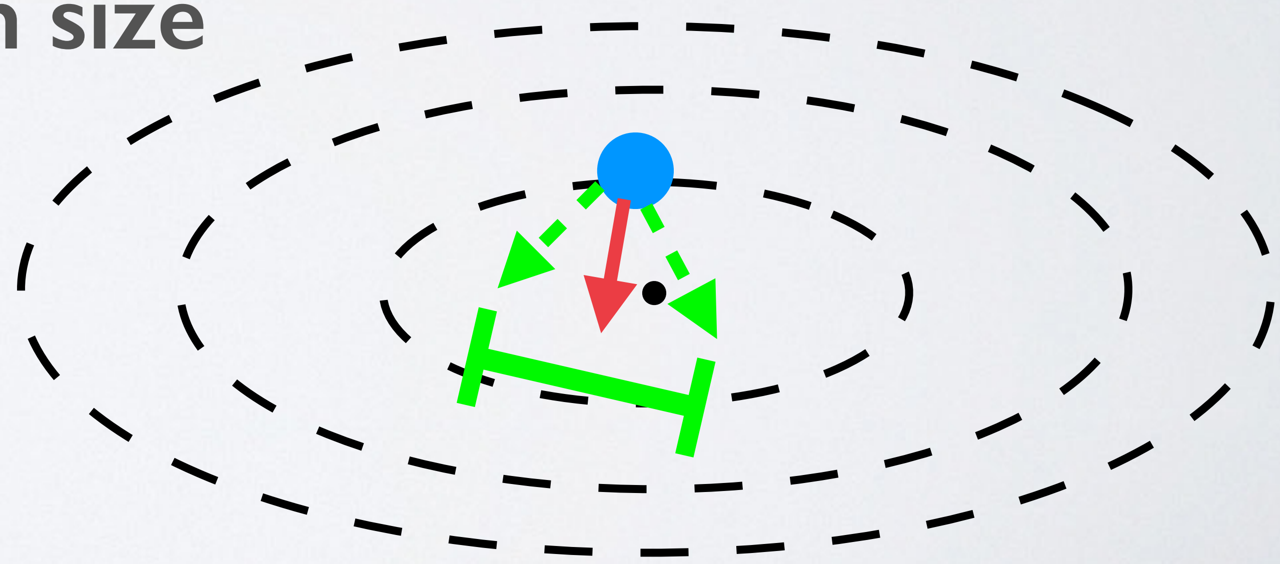

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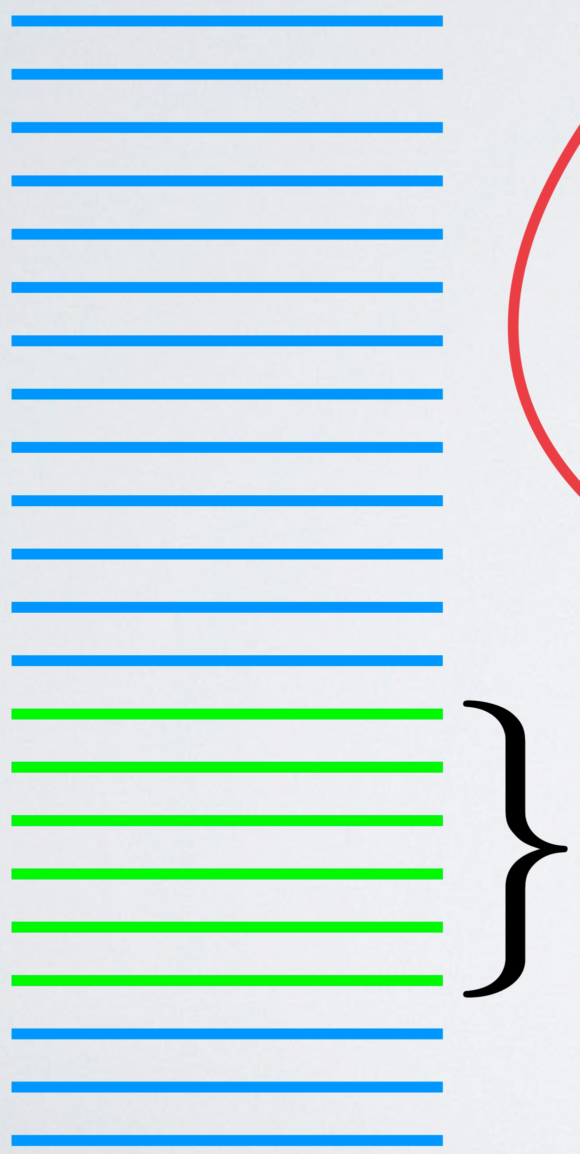

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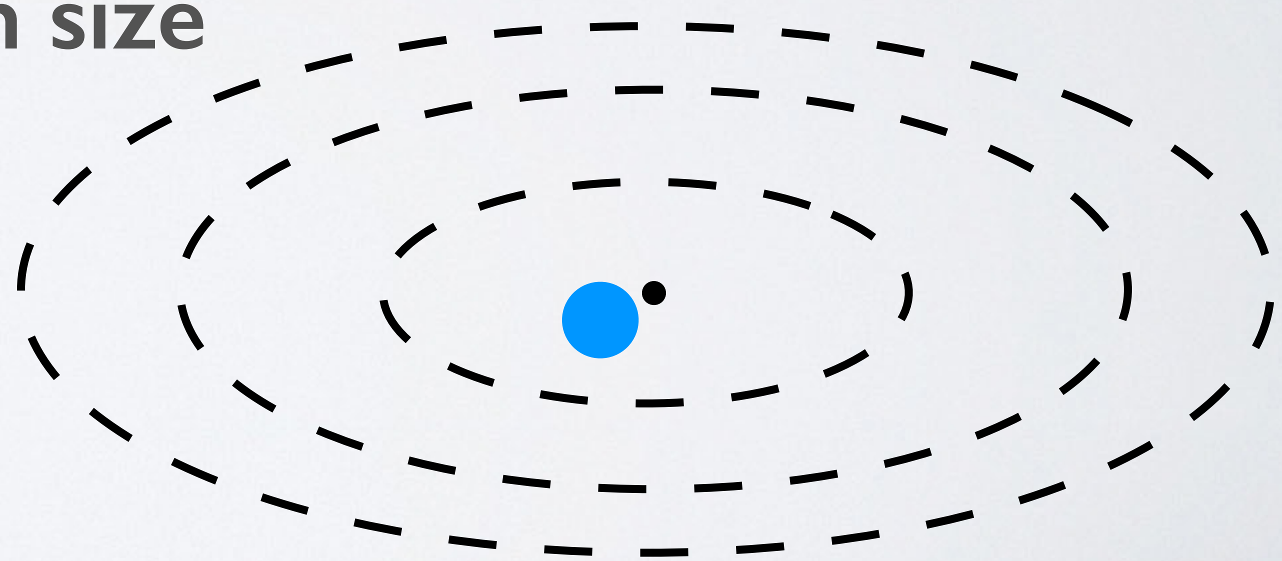

BIG BATCH SGD

On each iteration t

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- Estimate size of gradient error by computing **variance**

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extra step to SGD

- Choose stepsize α_t
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Can be estimated using the batch *B*

- Choose stepsize α_t
- Update

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CONVERGENCE

Assumption: ℓ has L-Lipschitz gradients

$$\ell(x) \leq \ell(y) + \nabla \ell(y)^T (x - y) + \frac{L}{2}\|x - y\|^2$$

Assumption: ℓ satisfies the Polyak-Lojasiewicz (PL) Inequality

$$\|\nabla \ell(x)\|^2 \geq 2\mu(\ell(x) - \ell(x^\star))$$

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Theorem

Big Batch SGD converges linearly:

$$\mathbb{E}[\ell(x_{t+1}) - \ell(x^\star)] \leq \left(1 - \frac{\mu}{\beta L}\right) \cdot \mathbb{E}[\ell(x_t) - \ell(x^\star)]$$

with optimal step size $\alpha = \dfrac{1}{\beta L}$ where $\beta = \dfrac{\theta^2 + (1-\theta)^2}{(1-\theta)^2}$

CONVERGENCE RESULTS

Theorem

Big Batch SGD converges linearly:

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with optimal step size $\alpha = \dfrac{1}{\beta L}$ where $\beta = \dfrac{\theta^2 + (1-\theta)^2}{(1-\theta)^2}$

Per-iteration convergence rate

CONVERGENCE RESULTS

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$\downarrow$

Per-iteration convergence rate

We show: $\boxed{|\mathcal{B}| > \mathcal{O}(1/\epsilon) \longrightarrow \text{Error} < \epsilon}$

optimal convergence in the infinite data case

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- More accurate gradients enable **automatic stopping conditions**
- Bigger batches are **better in parallel/distributed settings**

BACKTRACKING LINE SEARCH

Also referred to as **Armijo Line Search**

Measures **sufficient decrease condition** of objective function

For regular (deterministic) gradient descent:

$$\ell(x_{t+1}) \quad \leq \quad \ell(x_t) \quad - \quad c\alpha_t \|\nabla \ell(x_t)\|^2$$

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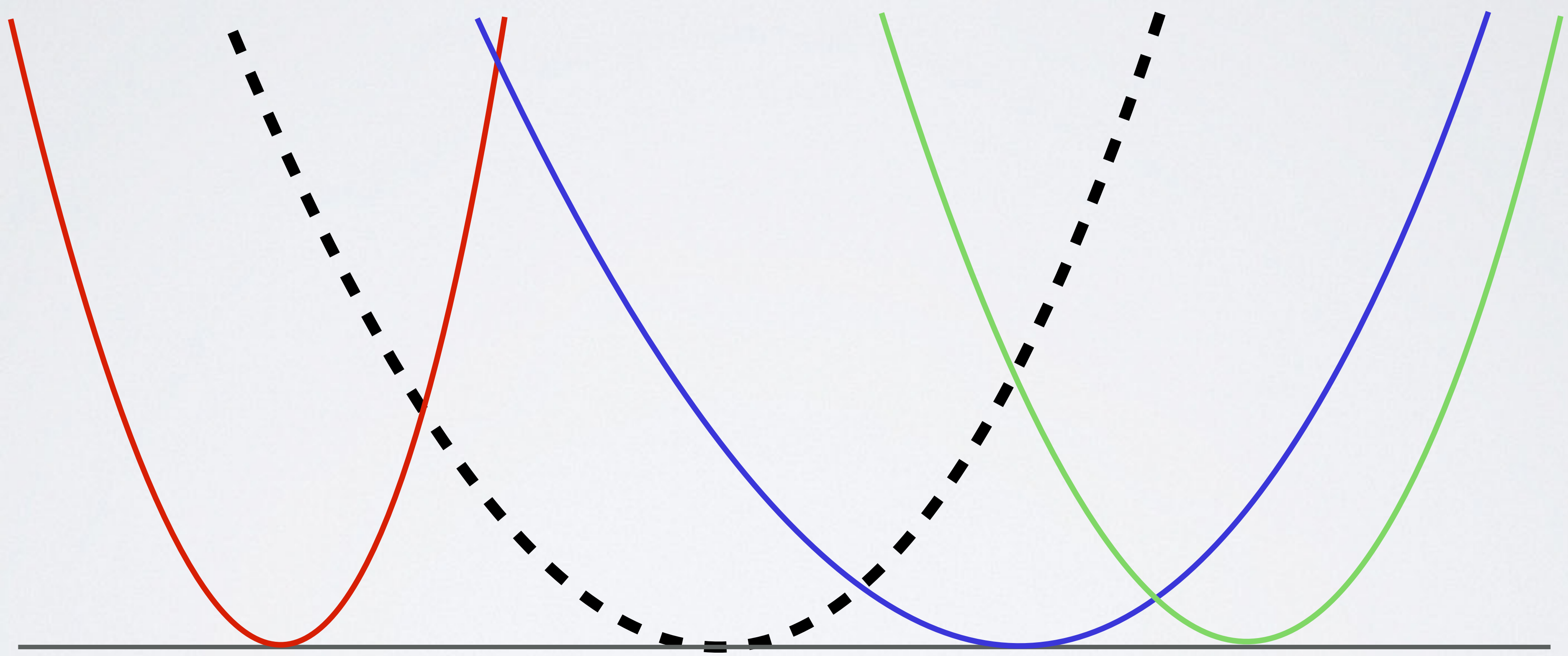
If this fails, **decrease stepsize** and check again

BACKTRACKING WITH SGD

Measures sufficient decrease condition on **individual functions**



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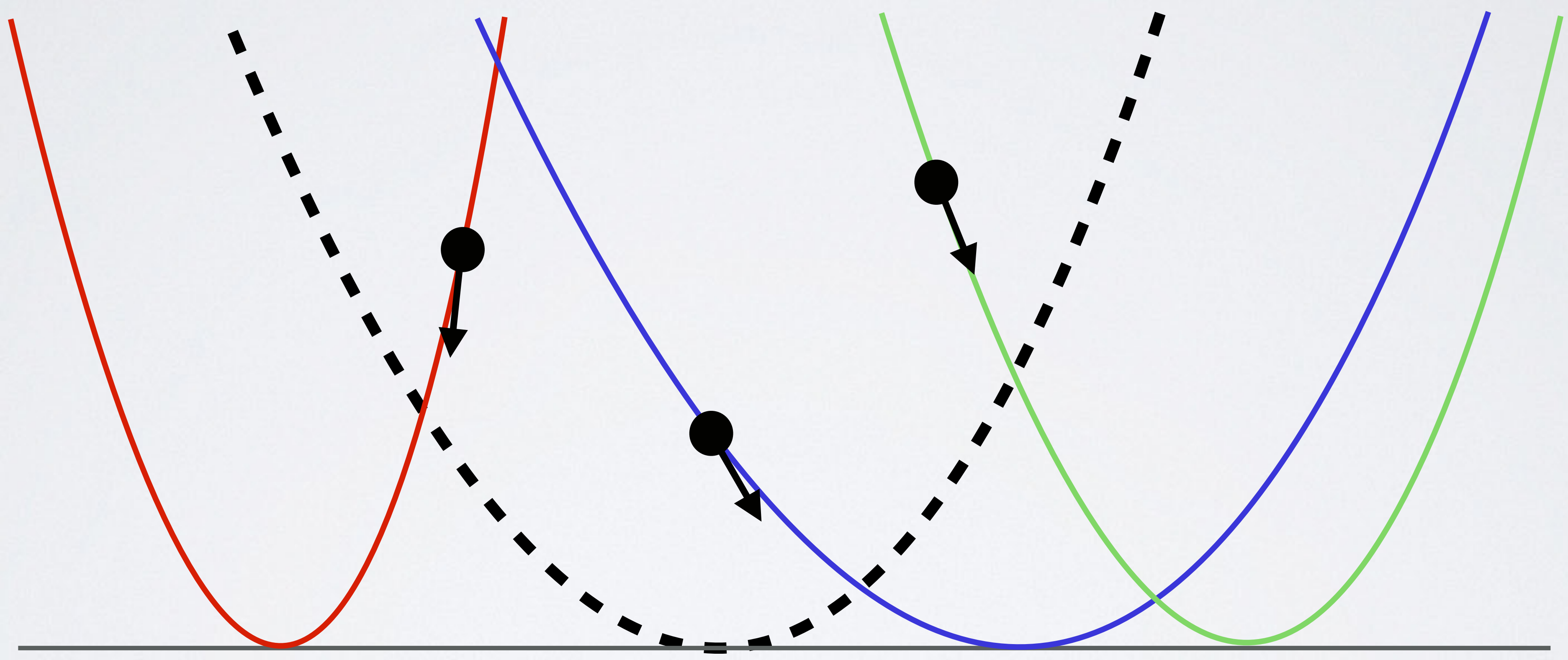

Moves to the optimum of individual functions, not the global average

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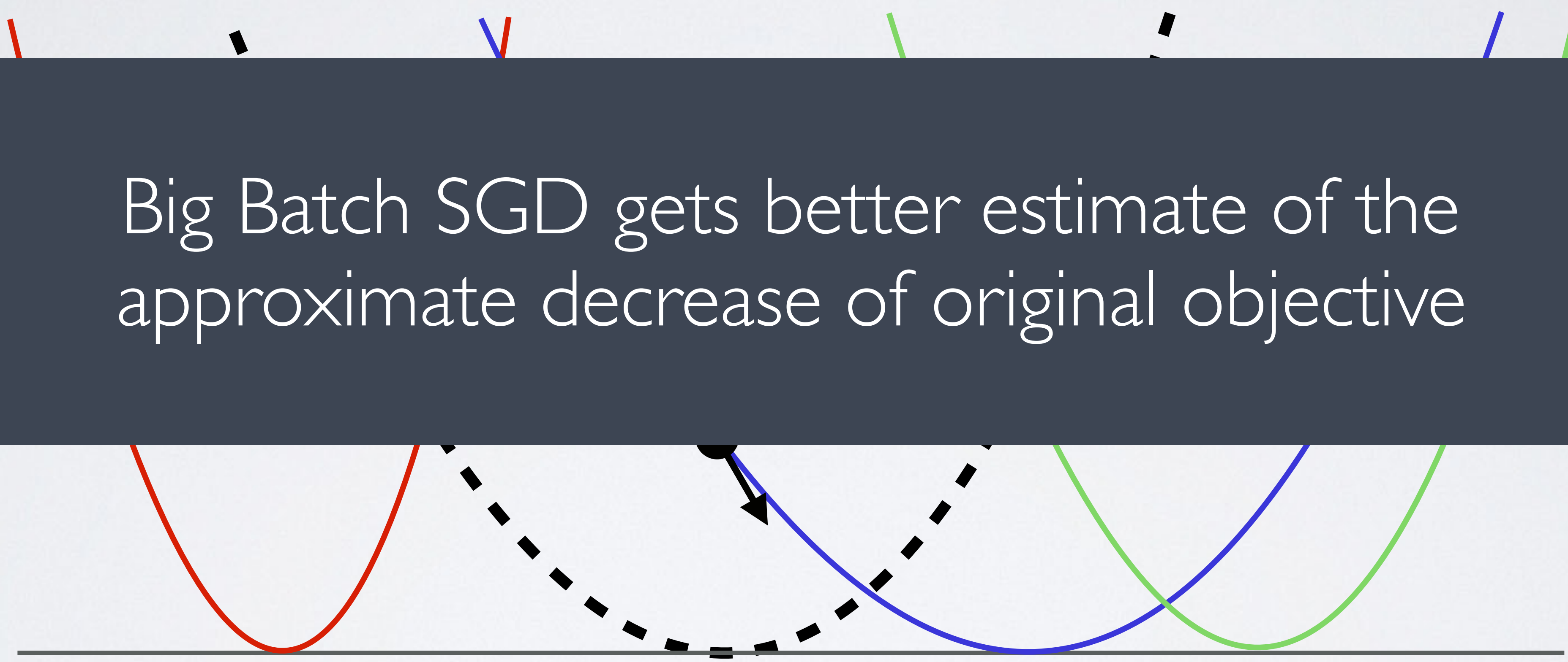

Big Batch SGD gets better estimate of the approximate decrease of original objective

Moves to the optimum of individual functions, not the global average

BACKTRACKING WORKS WITH BIG BATCH SGD

Decrease stepsize until:

$$\ell_{\mathcal{B}}(x_{t+1}) \leq \ell_{\mathcal{B}}(x_t) - c\alpha_t \|\nabla \ell_{\mathcal{B}}(x_t)\|^2$$

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Measures a condition of **sufficient decrease** using batch *B*

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Big Batch SGD with backtracking line search converges linearly:

$$\mathbb{E}[\ell(x_{t+1}) - \ell(x^\star)] \leq \left(1 - \frac{c\mu}{\beta L}\right)\mathbb{E}[\ell(x_t) - \ell(x^\star)]$$

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We also derive optimal stepsizes for Big Batch SGD using Barzilai-Borwein (BB) curvature estimates, with provable guarantees. Check paper for details.

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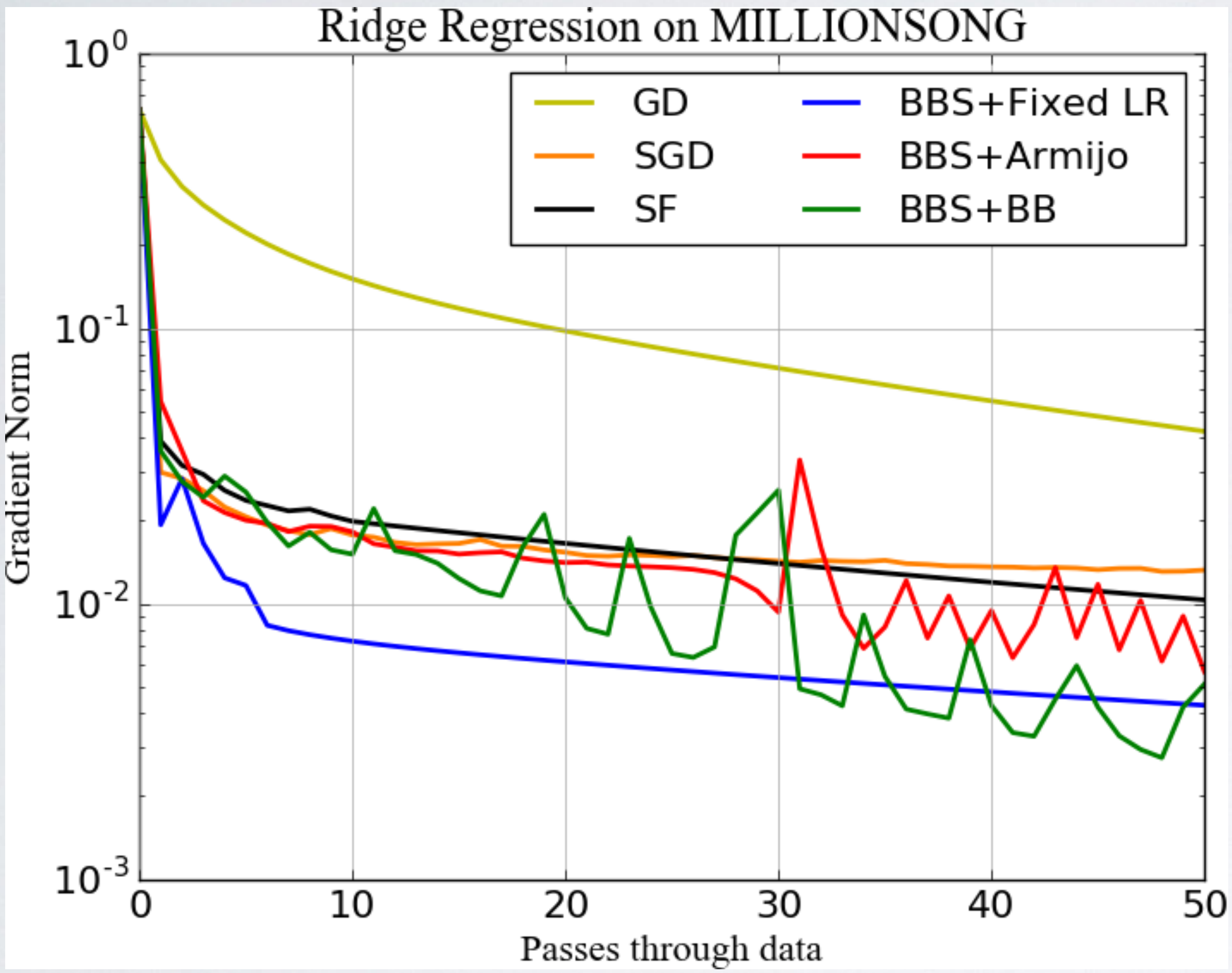
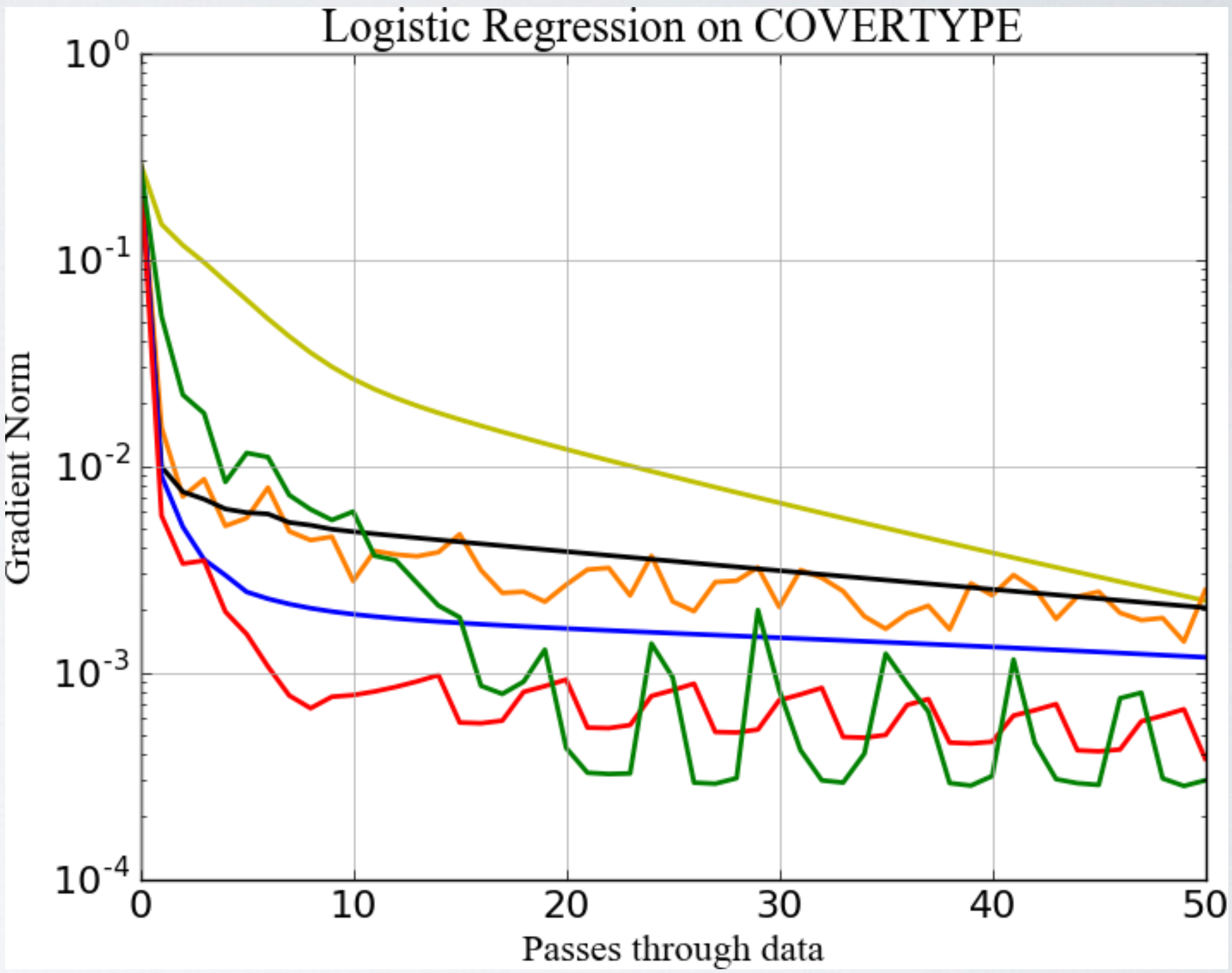
CONVEX EXPERIMENTS

Model: Ridge Regression & Logistic Regression





BBS: Big Batch SGD

Proposed methods: **Blue** (Fixed stepsize), **Red** (Backtracking), **Green** (Optimal stepsizes using curvature estimates) curves

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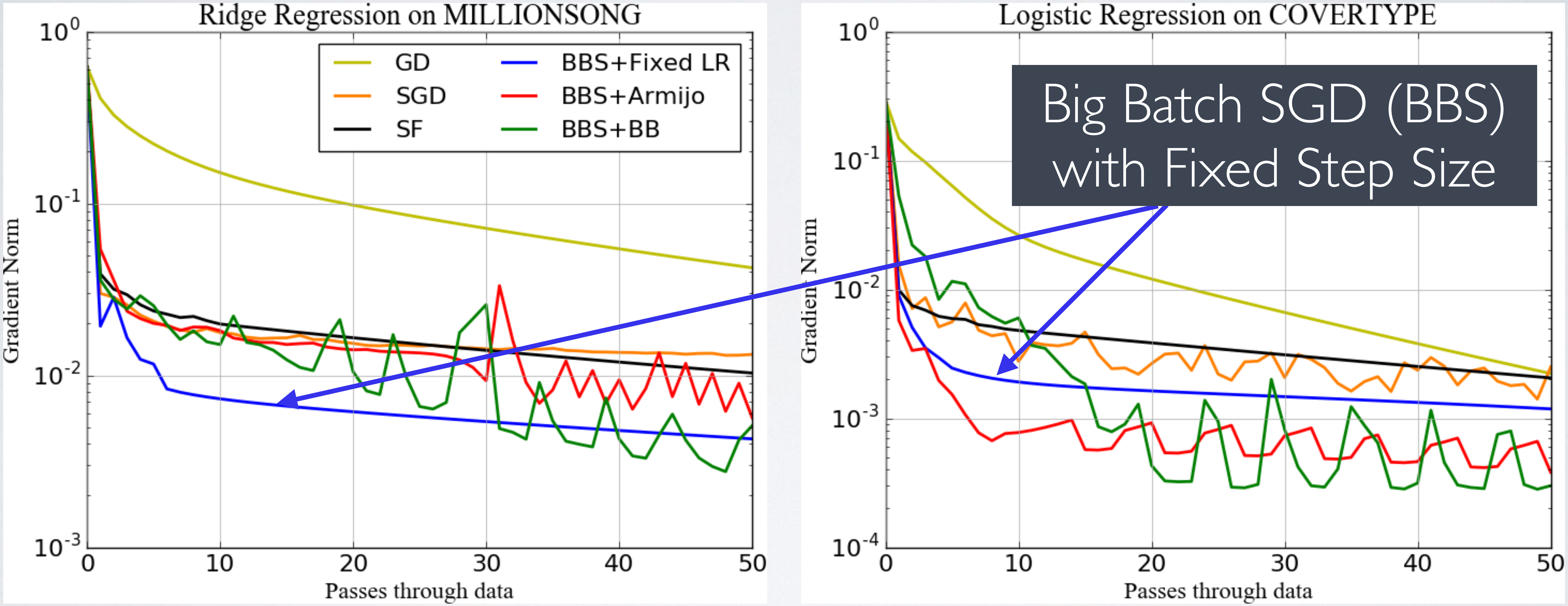

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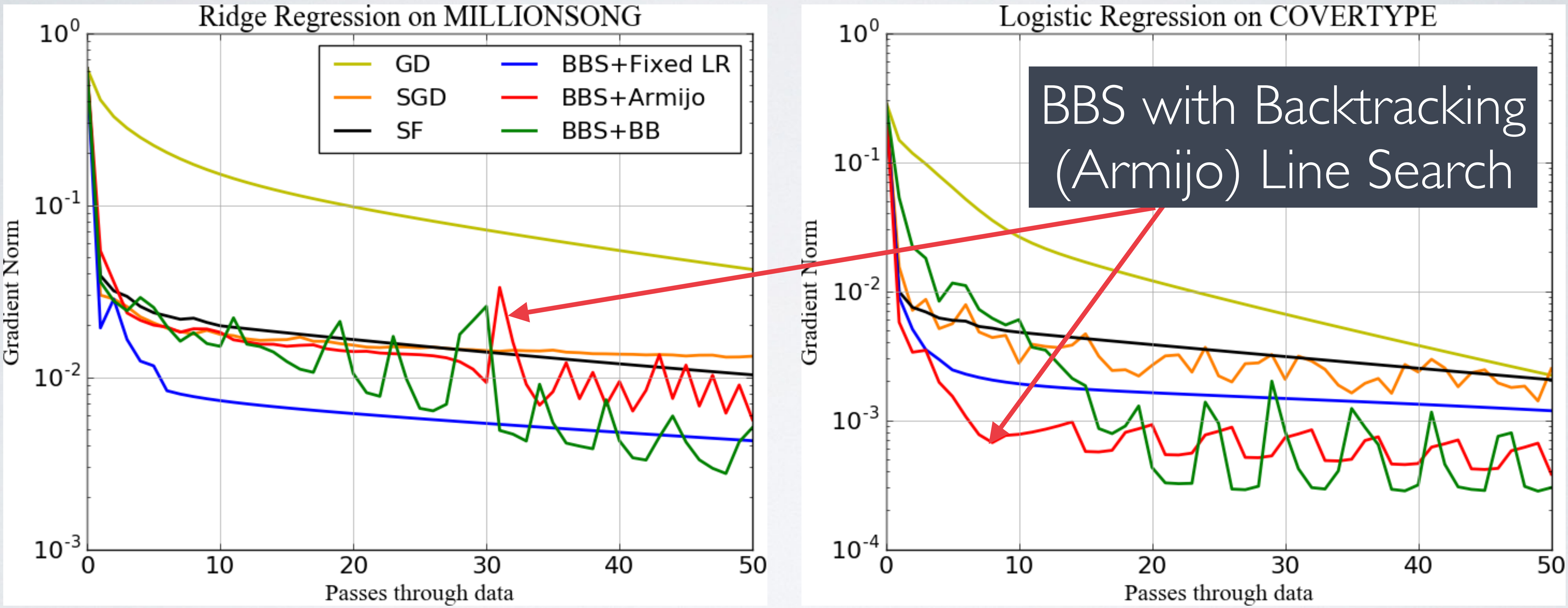

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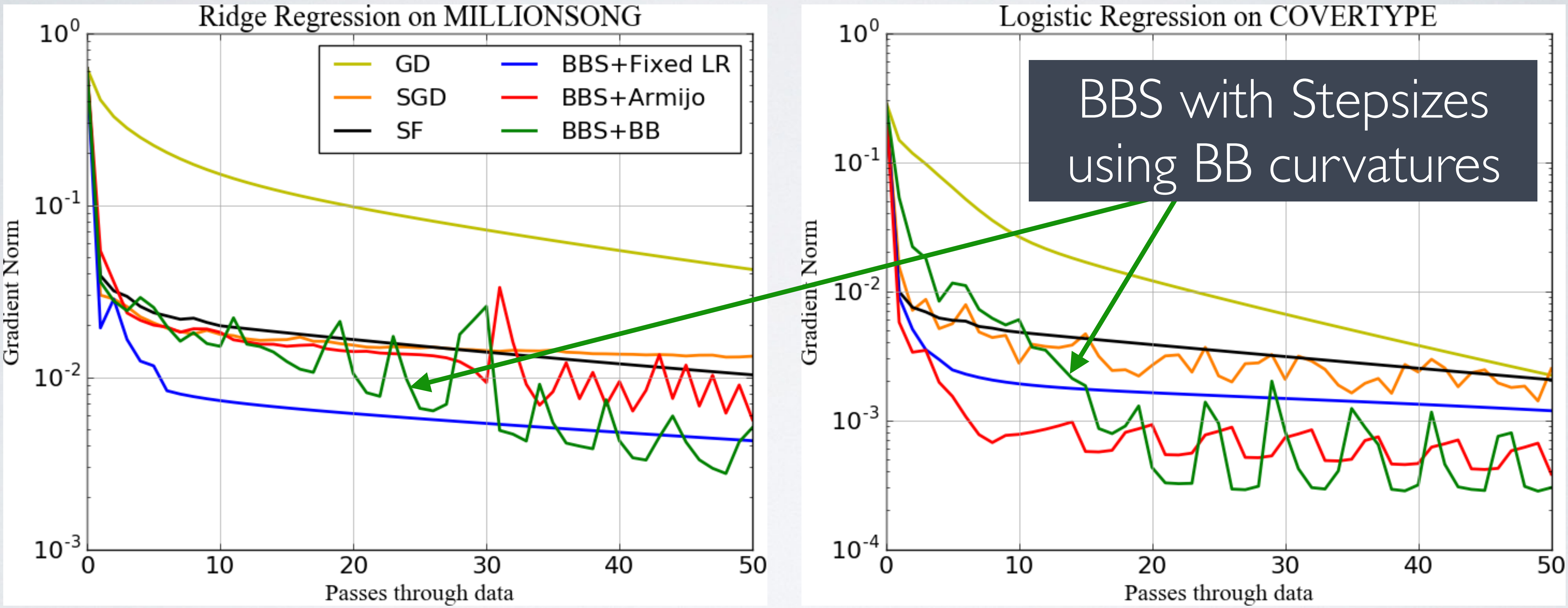

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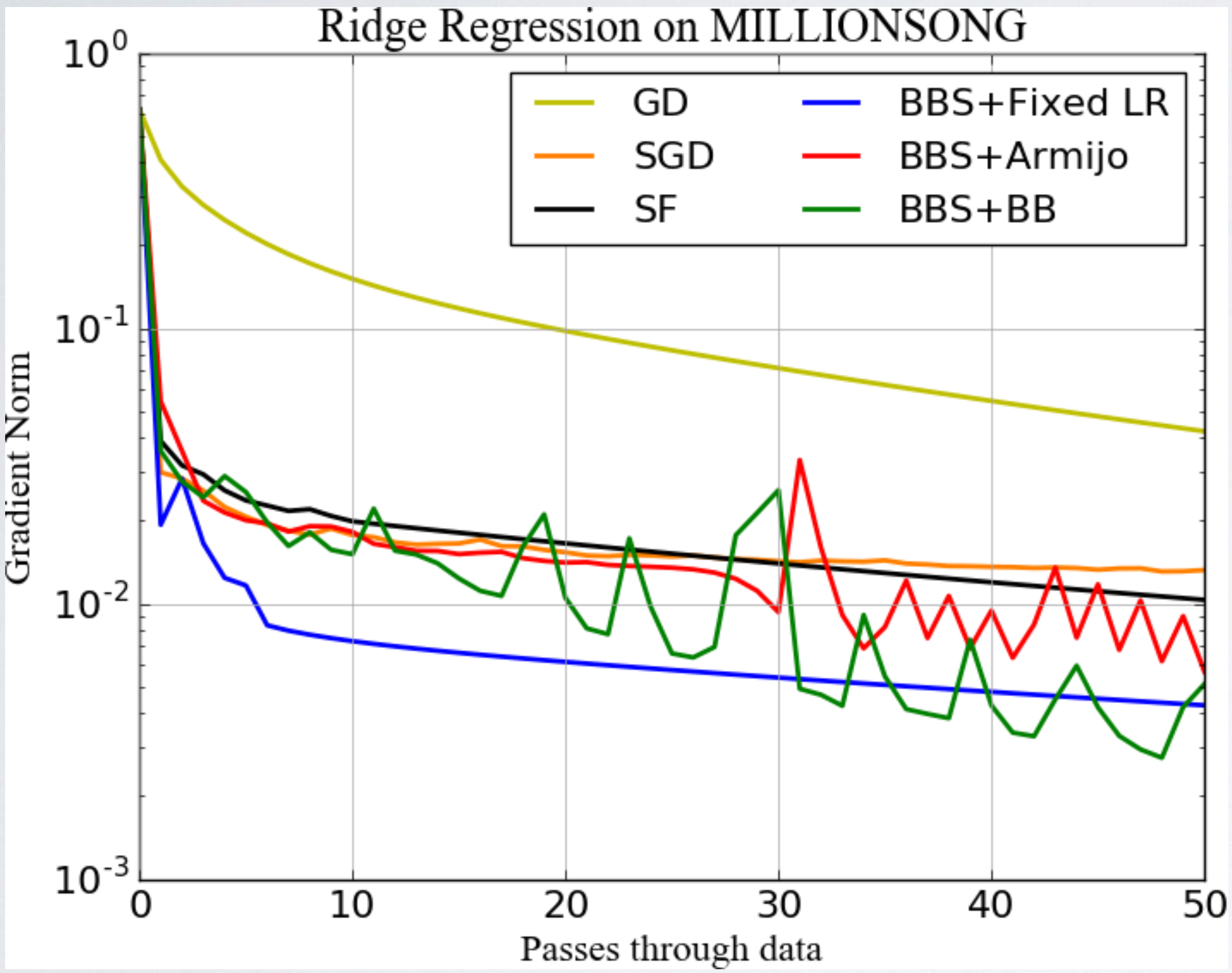

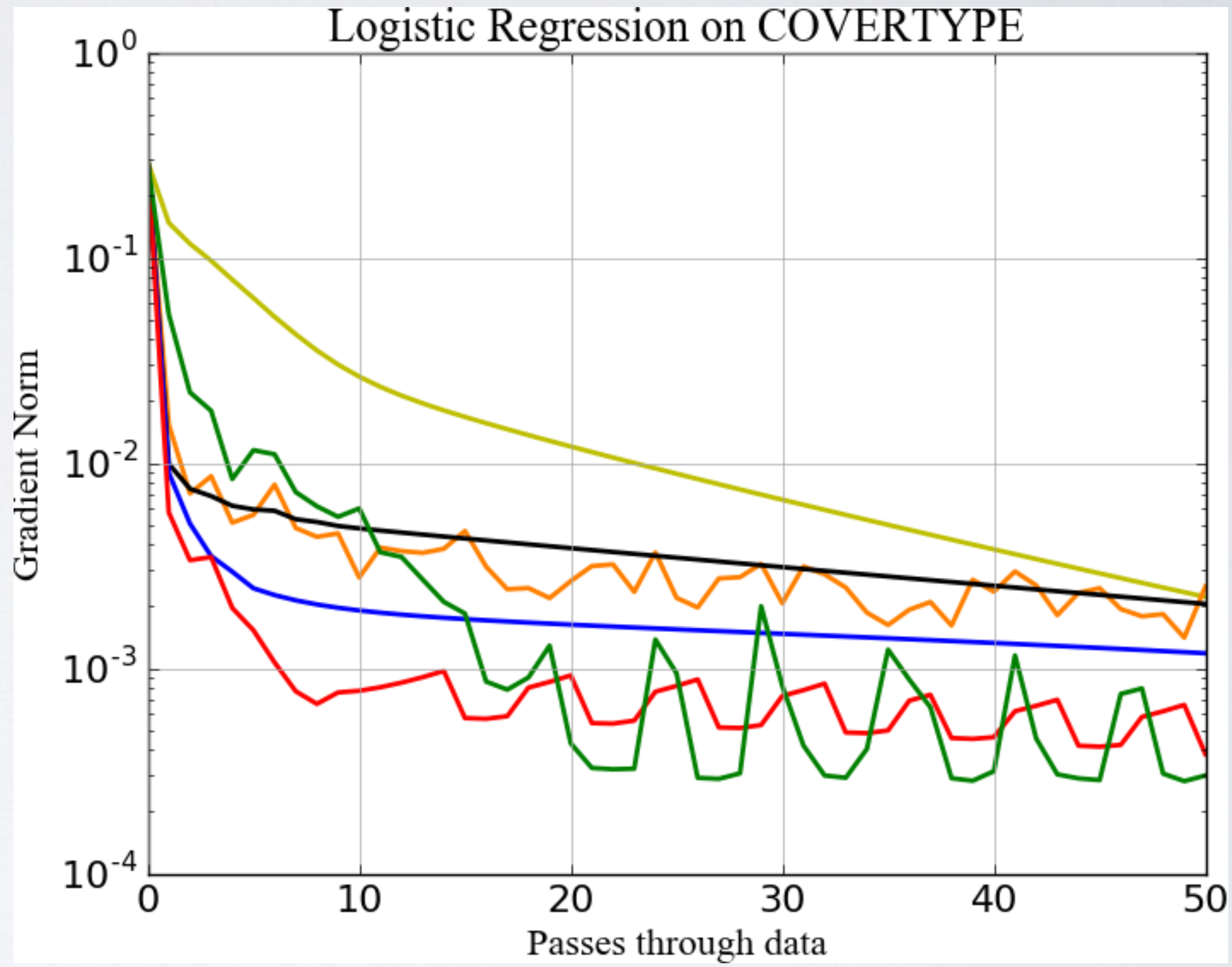

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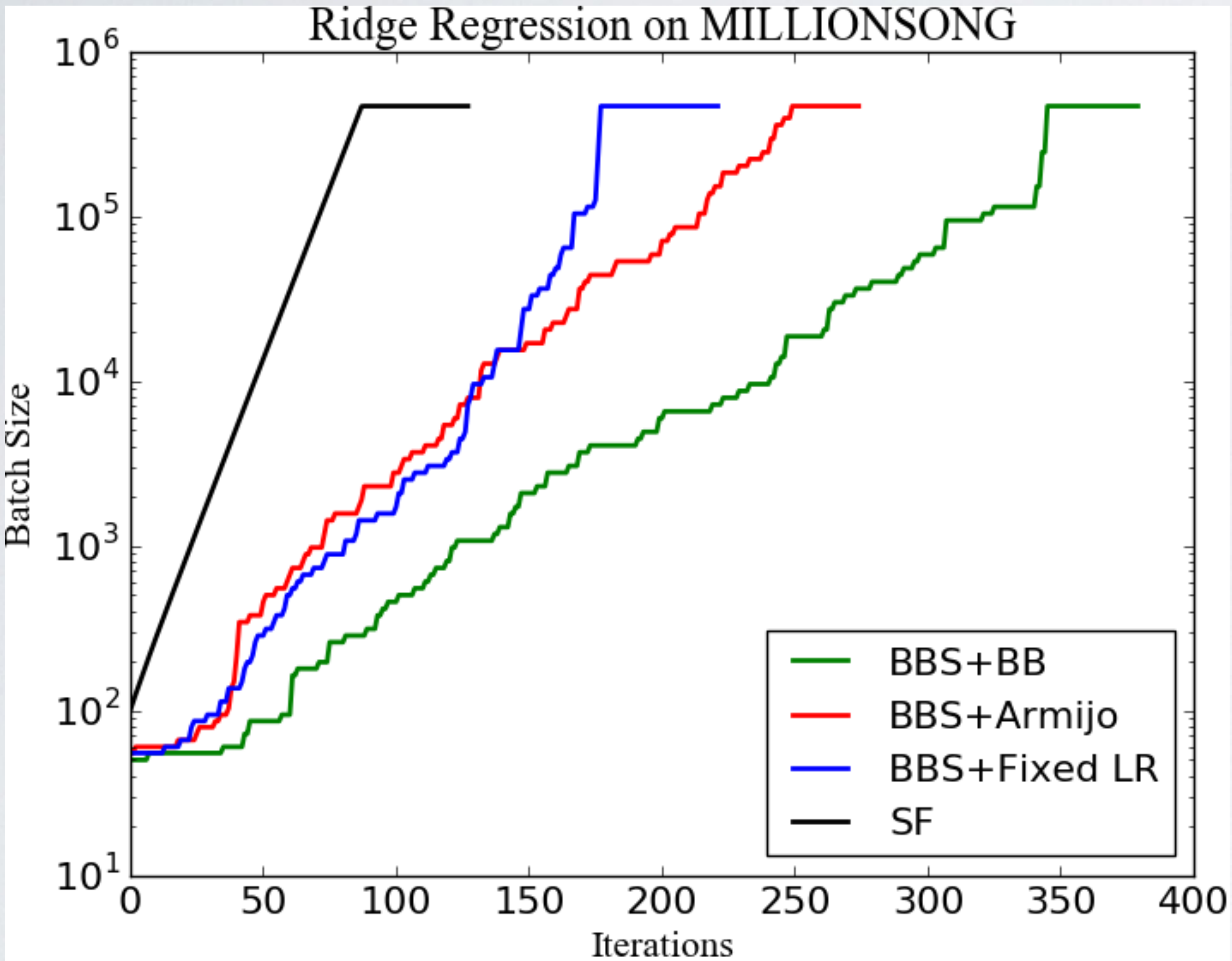
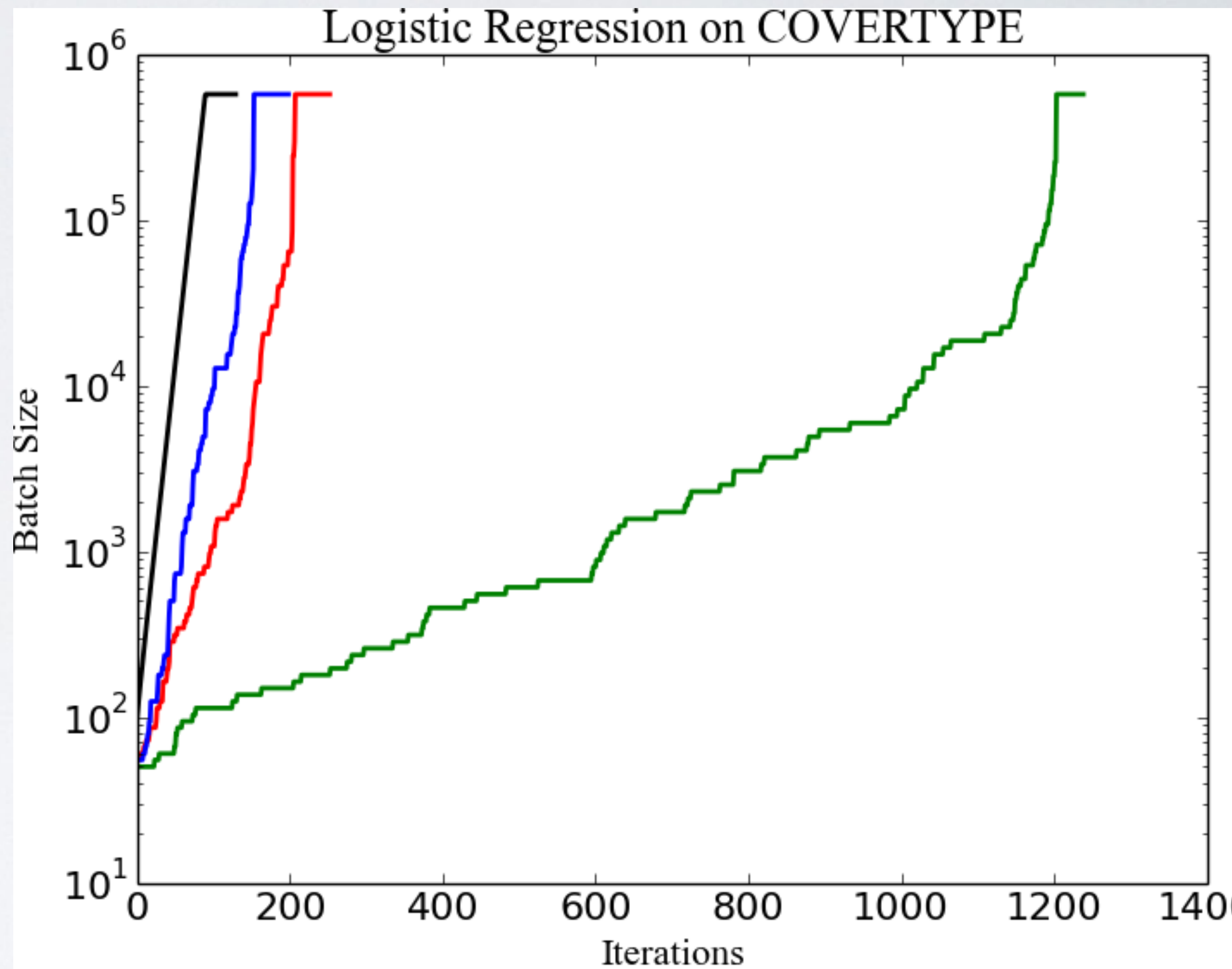
CONVEX EXPERIMENTS

Batch Size Increase





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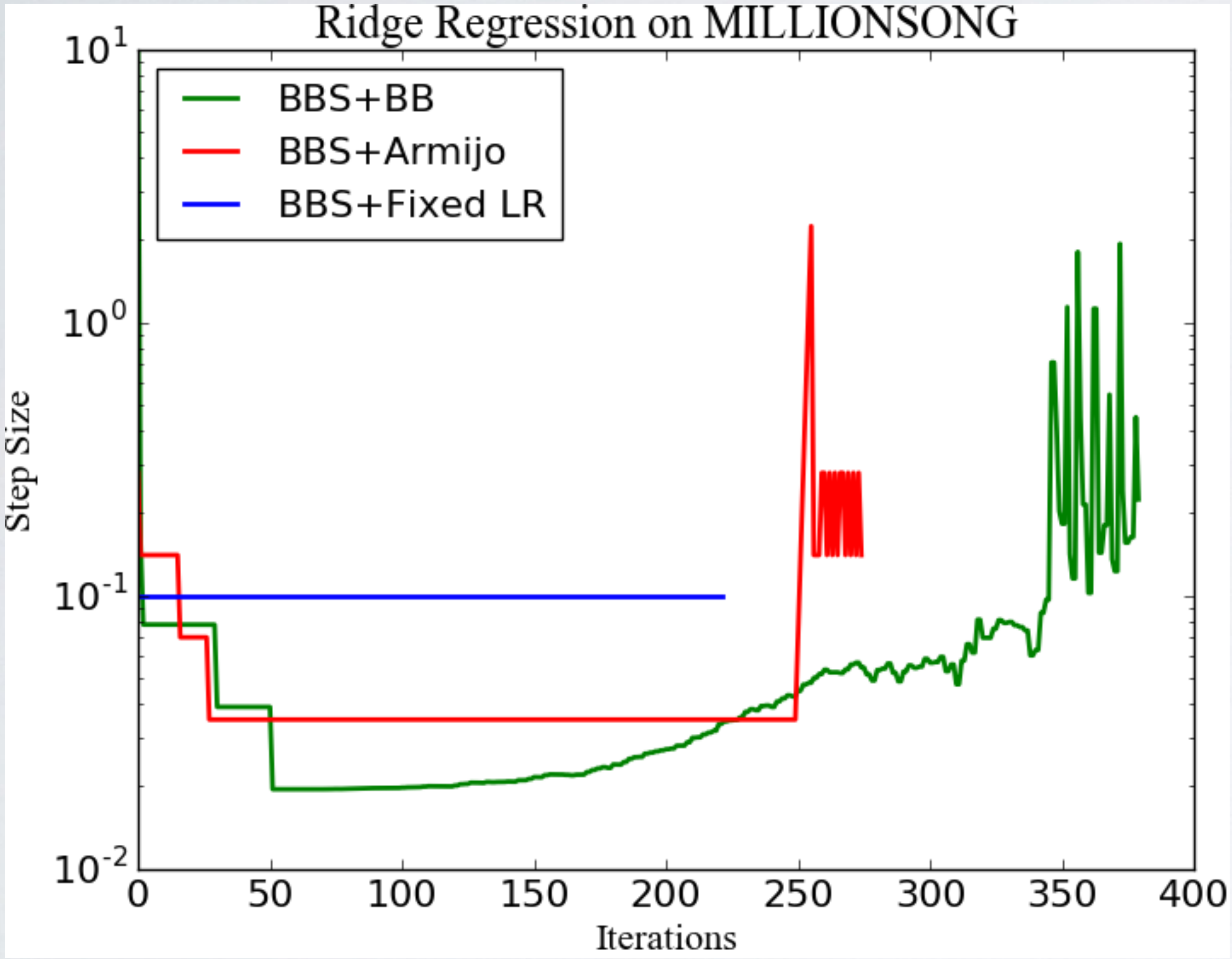
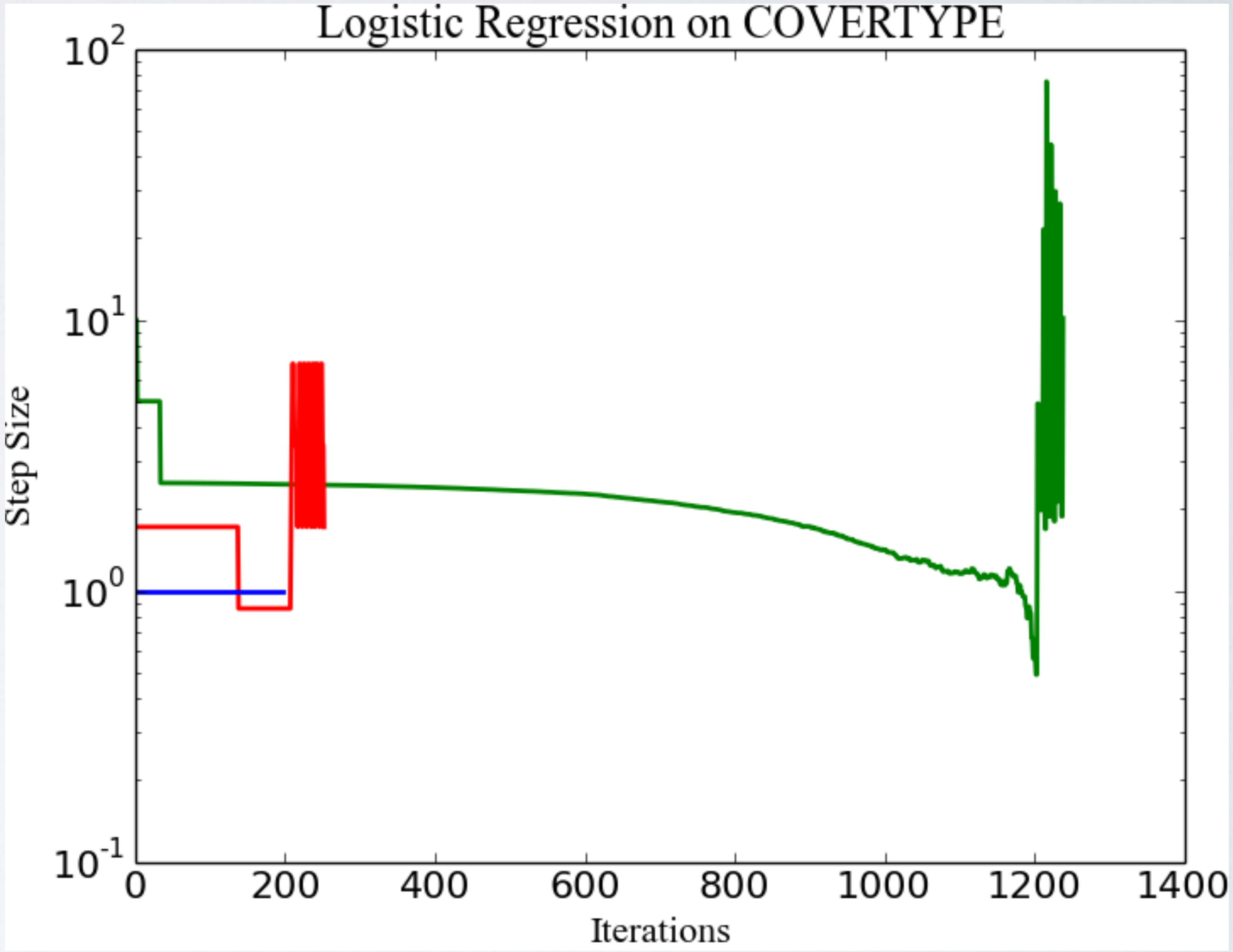
CONVEX EXPERIMENTS

Stepsizes Used





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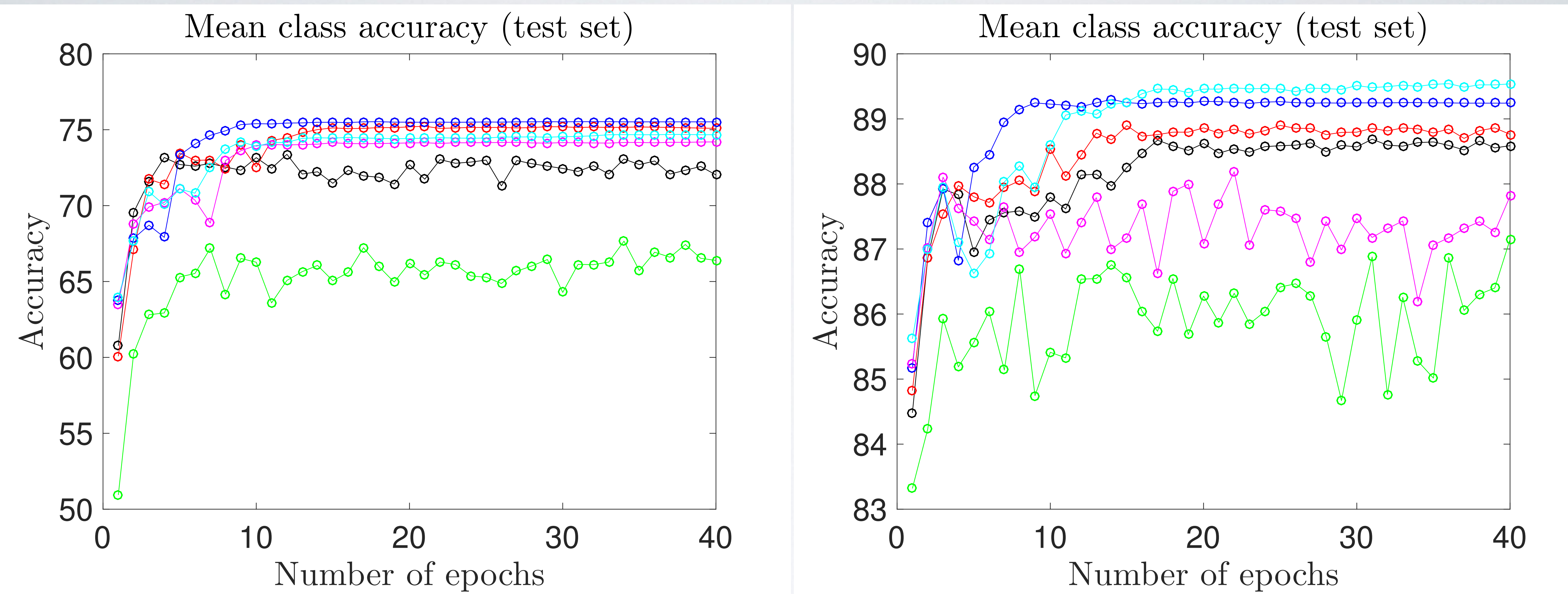
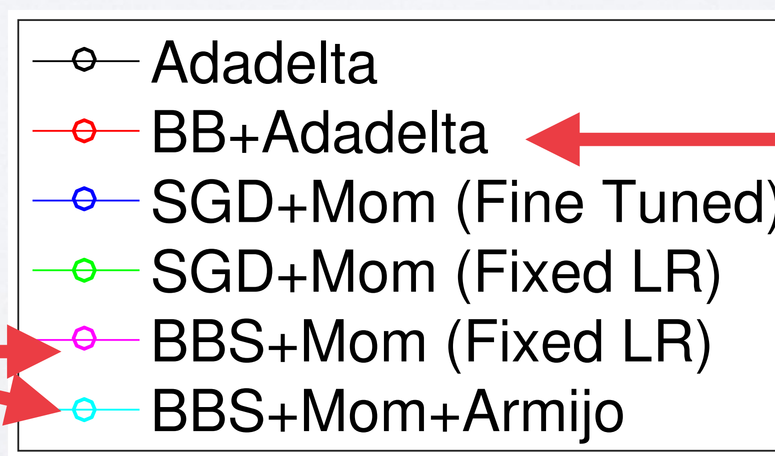
4-LAYER CNN

CIFAR-10 (left) & SVHN (right)





Big Batch SGD can also be used with AdaGrad, AdaDelta…

Proposed Methods

TAKEAWAYS

We introduce: **Big Batch SGD**

Adaptively grows batch size over time to maintain a nearly constant signal-to-noise ratio in the gradients

Better control of the noise makes it **easy to automate**

Adaptive stepsize methods work well with this method

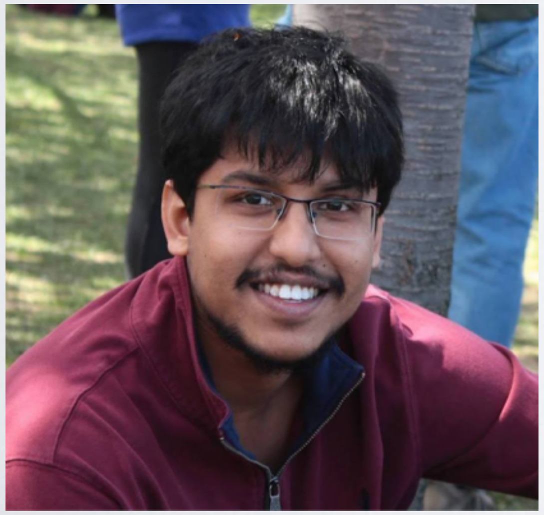
Better for **parallel/distributed settings**

THANKS!

Feel free to get in touch!

Extended version on arXiv:
"Big Batch SGD: Automated Inference using Adaptive Batch Sizes"
https://arxiv.org/abs/1610.05792

email: sohamde@cs.umd.edu
website: https://cs.umd.edu/~sohamde/



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