Optimization for Data Science

Mini-batching, sampling, momentum and other tricks

Lecturer: Robert M. Gower & Alexandre Gramfort

Tutorials: Quentin Bertrand, Nidham Gazagnadou

The Stochastic Gradient Method

Solving the *training problem*:

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

Baseline method: Stochastic Gradient Descent (SGD)

$$w^{t+1} = w^t - \gamma \nabla f_j(w^t)$$

Step size/
Learning rate

Sampled i.i.d
$j \in \{1, \ldots, n\}$
$j \sim \frac{1}{n}$

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What about
mini-batching

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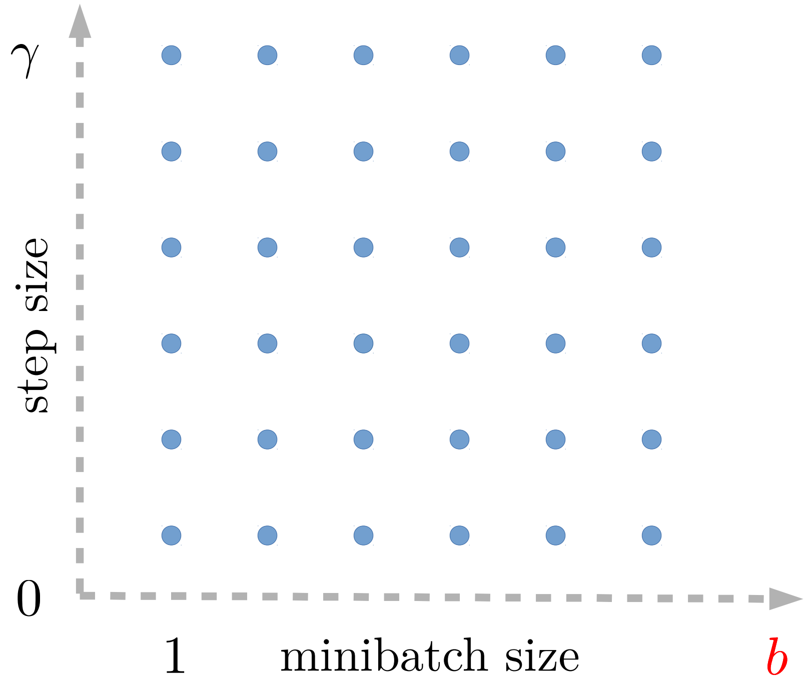
- What should b and γ be?
- How does b influence the stepsize γ ?
- How does the data influence the best mini-batch and stepsize?

How to choose the minibatch size?



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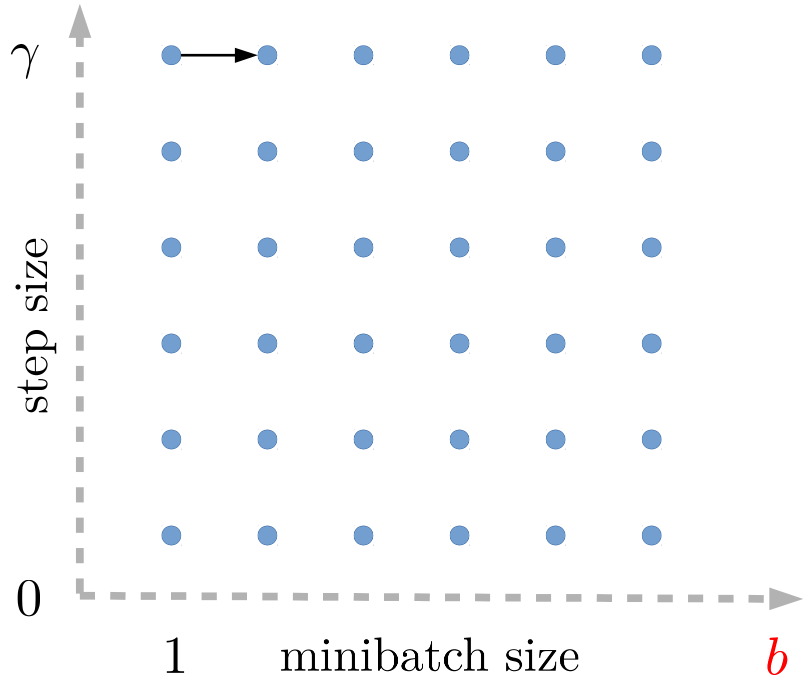

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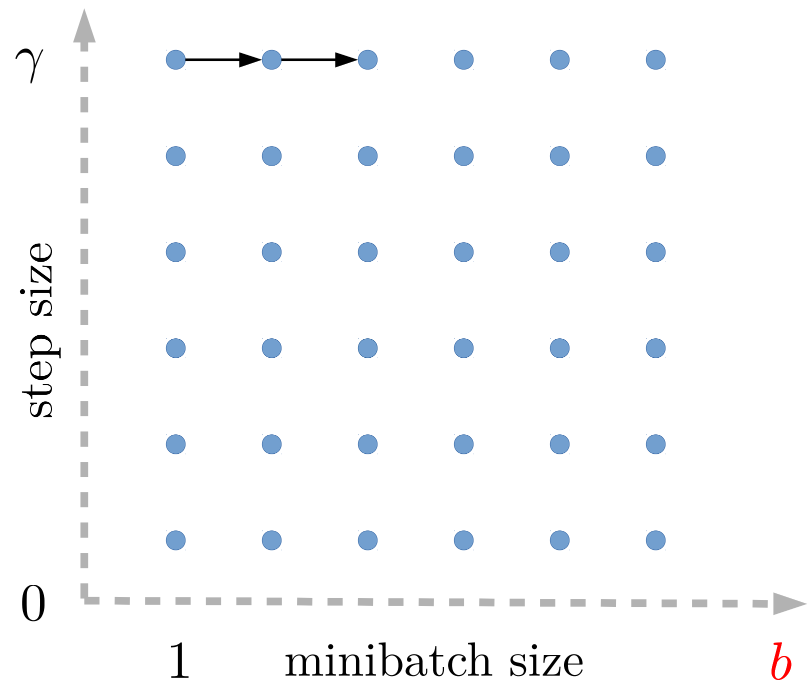

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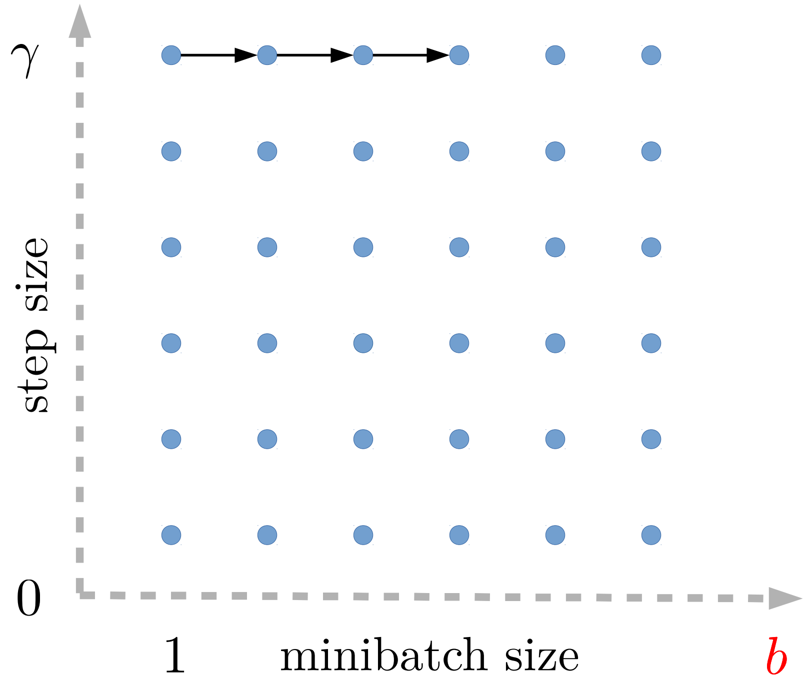

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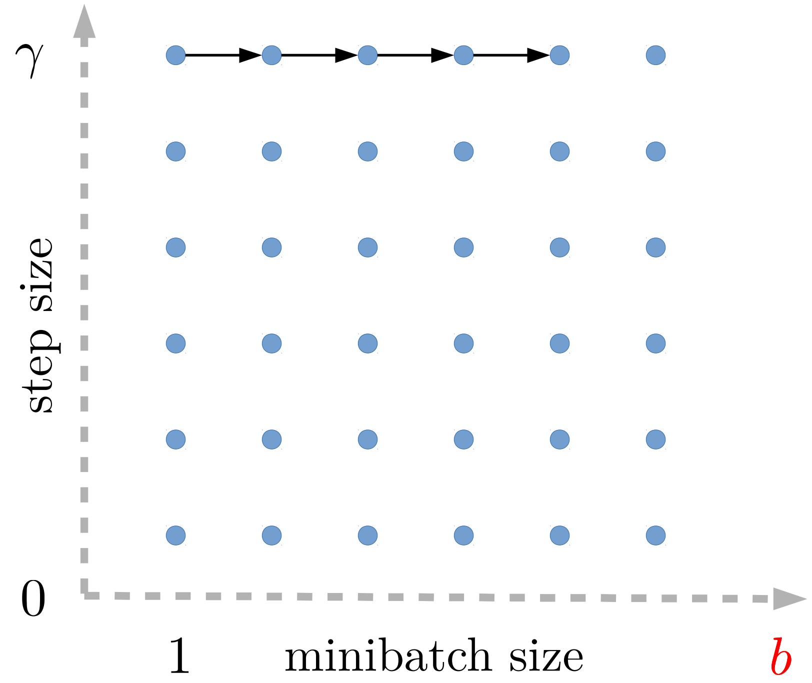

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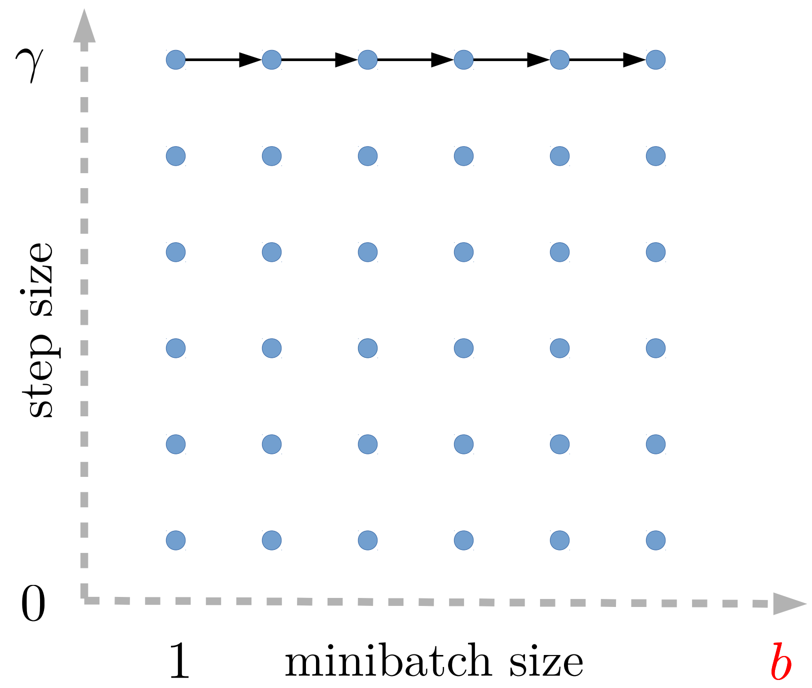

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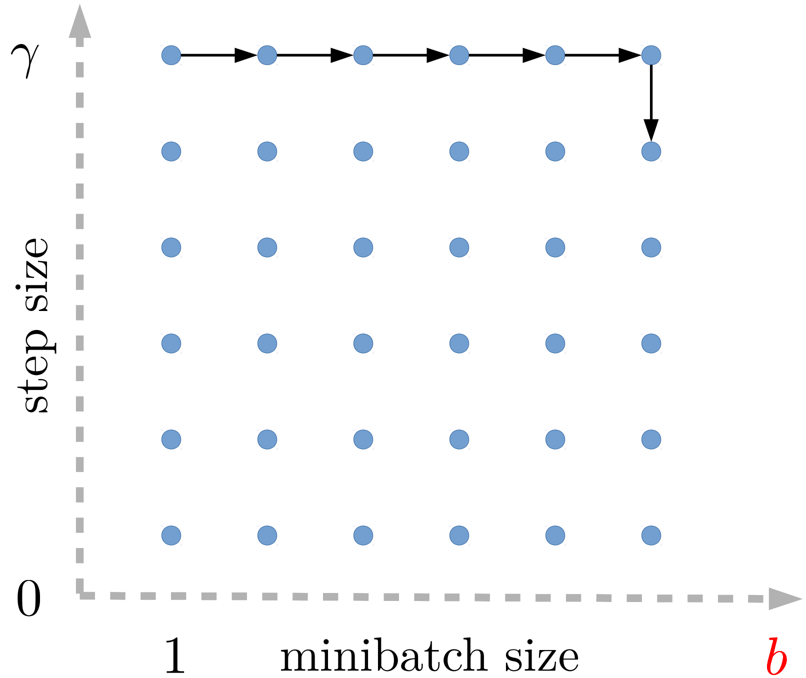

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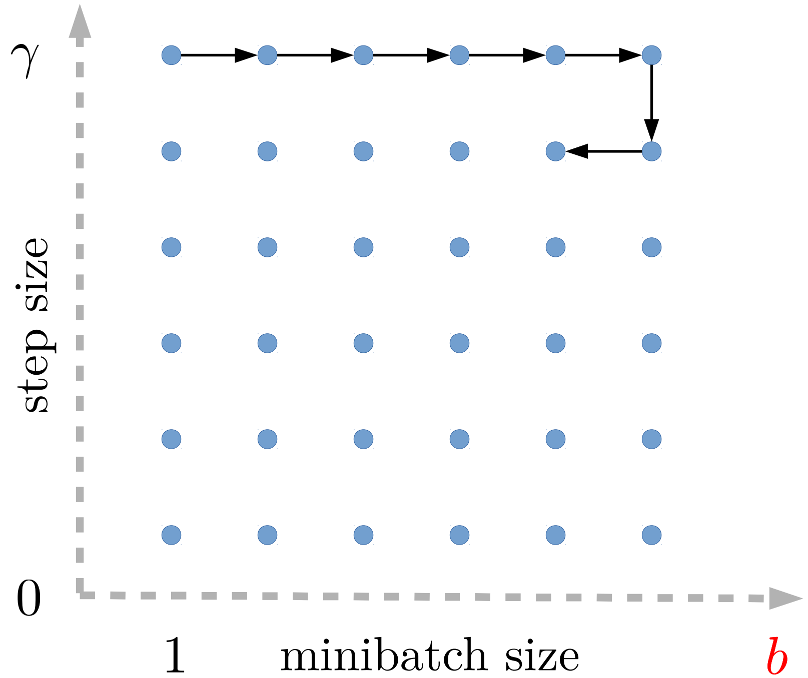

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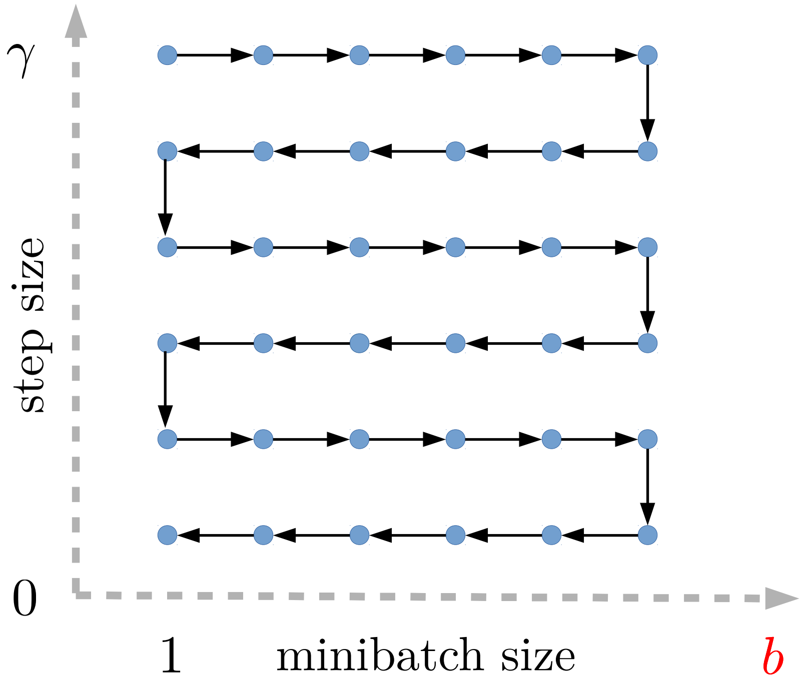

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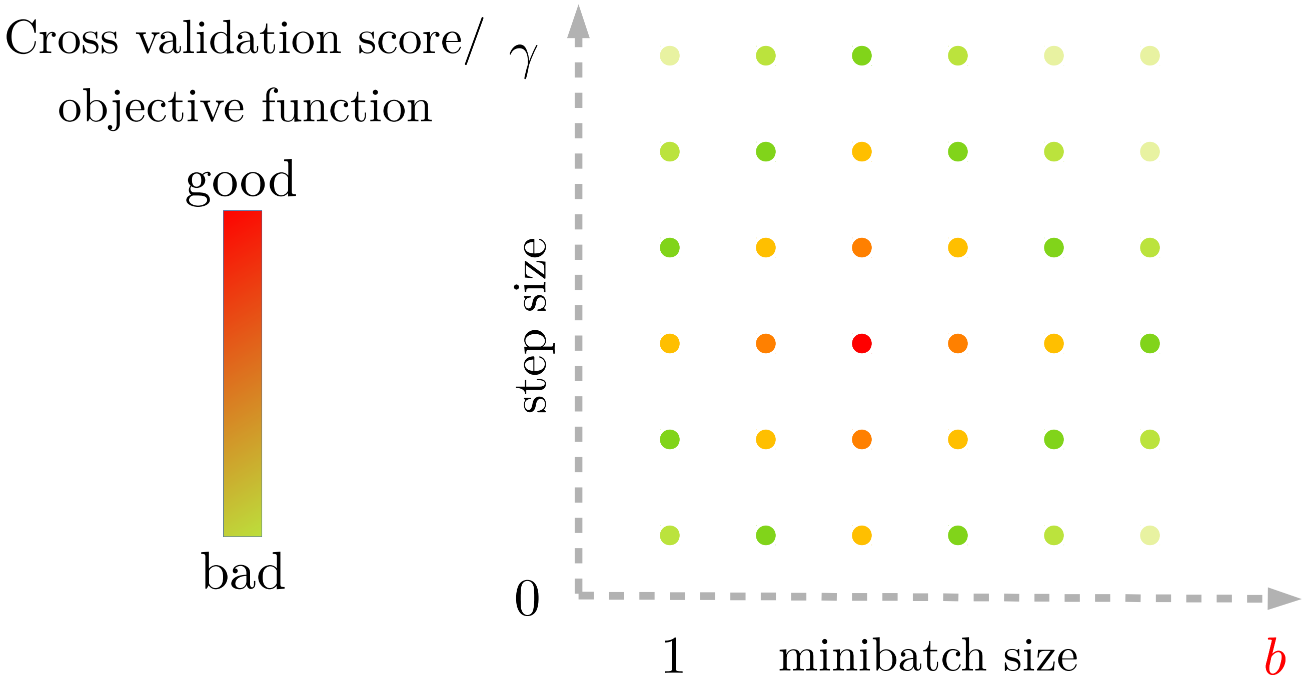

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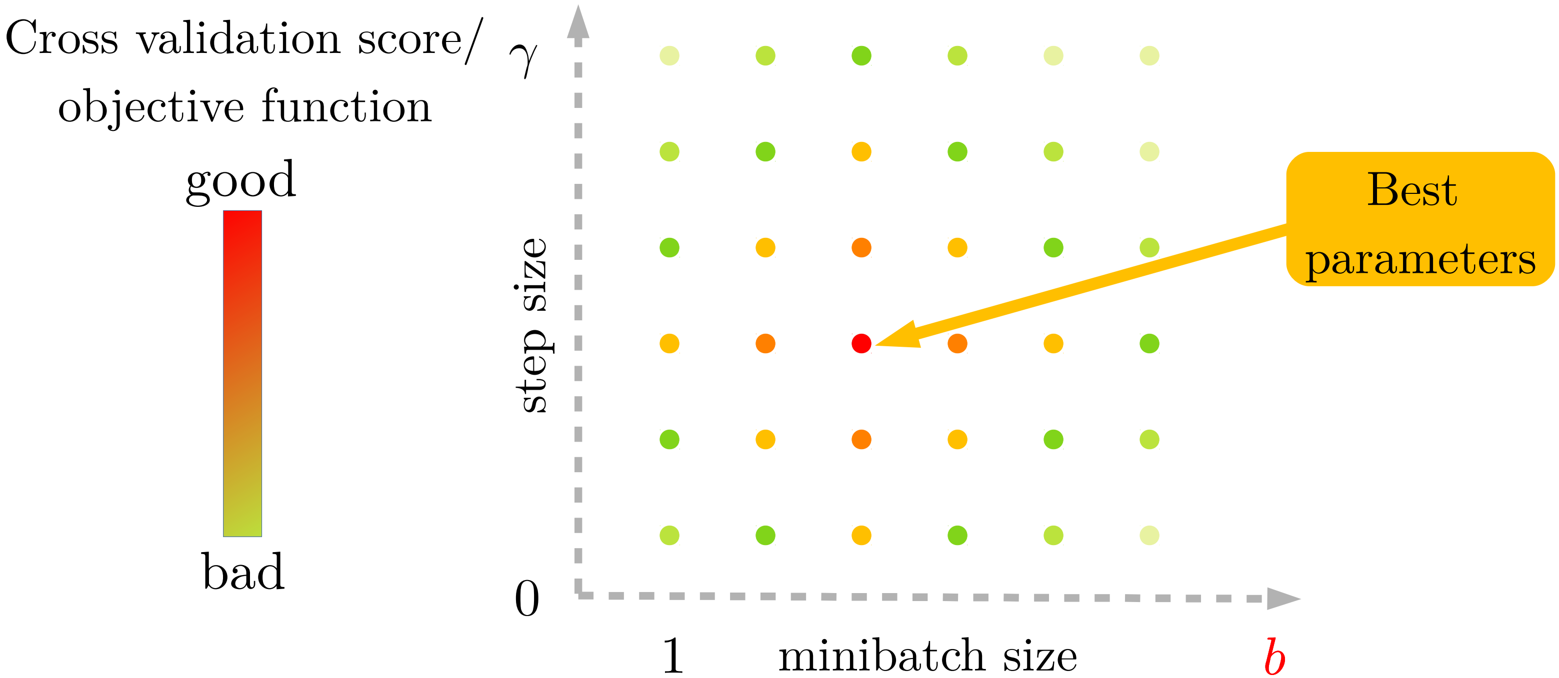

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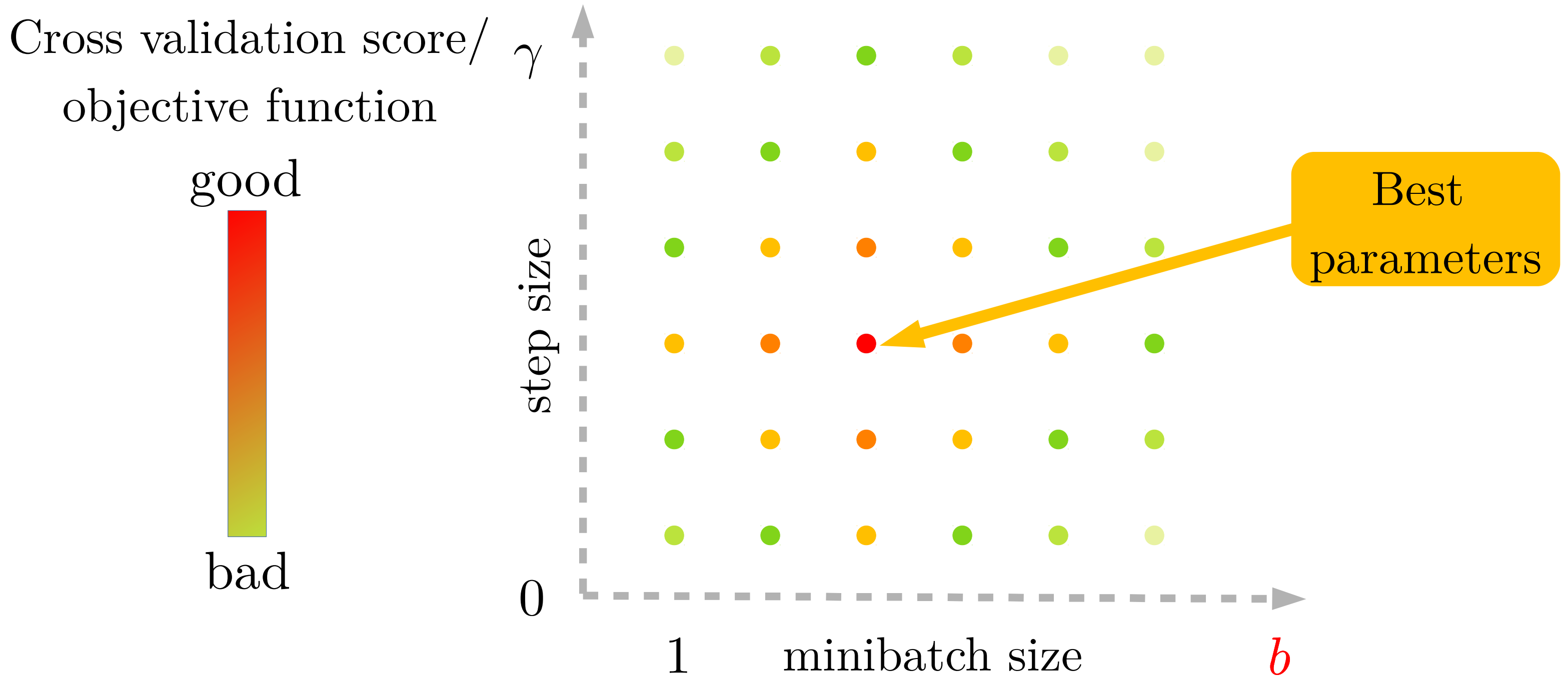

Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour, Goyal et al., CoRR 2017

Linear Scaling Rule: When the minibatch size is multiplied by k, multiply the learning rate by k.

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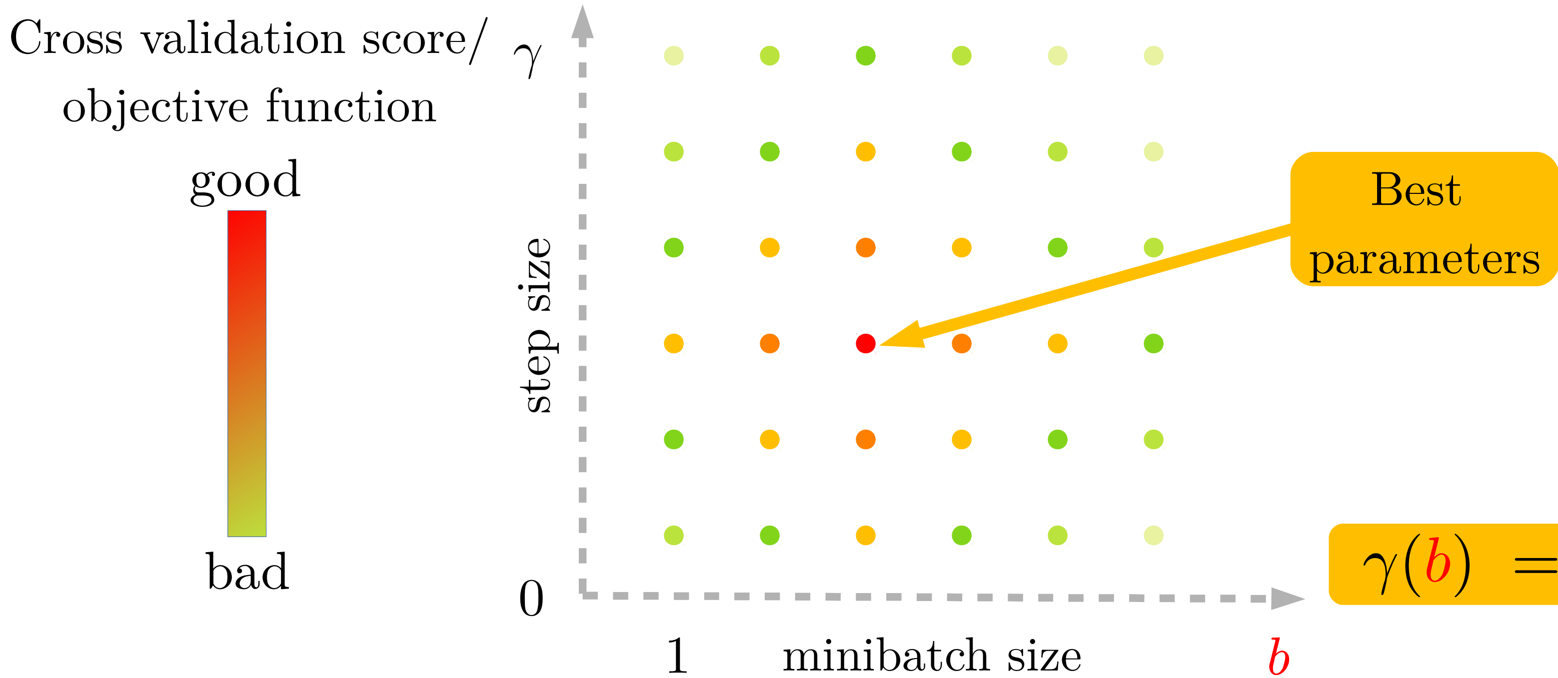

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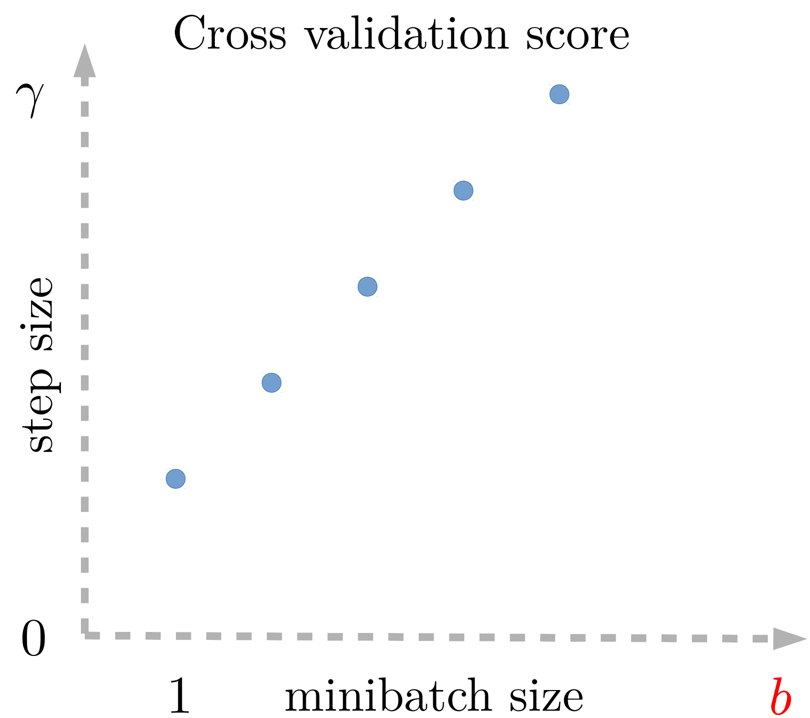

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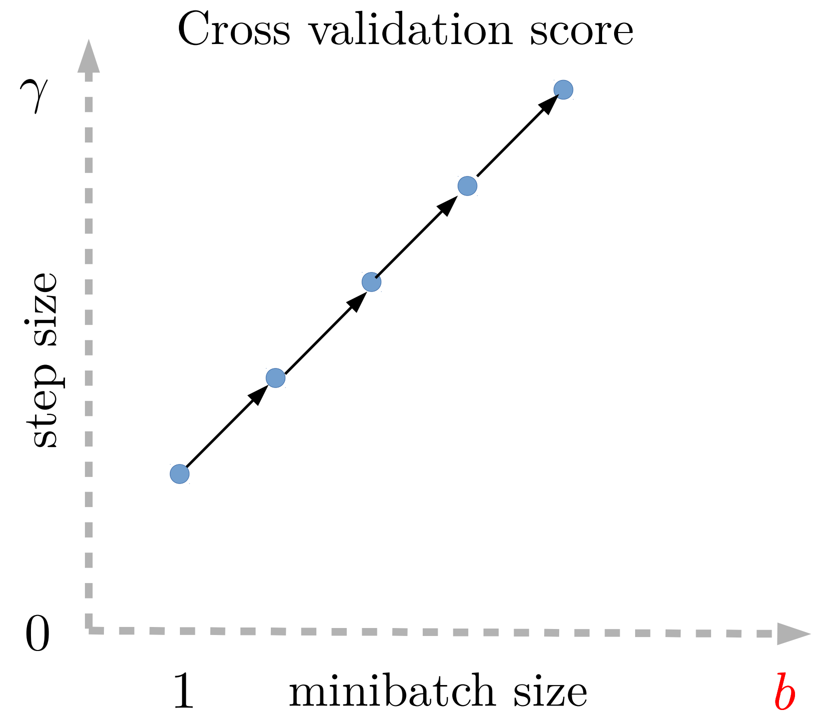

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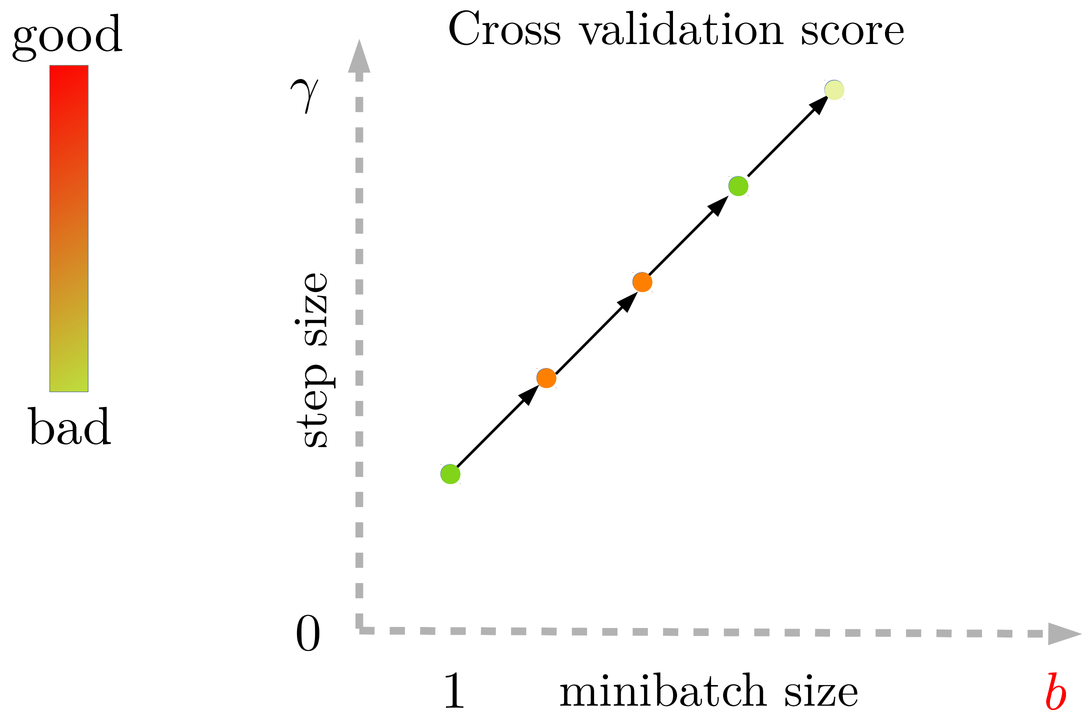

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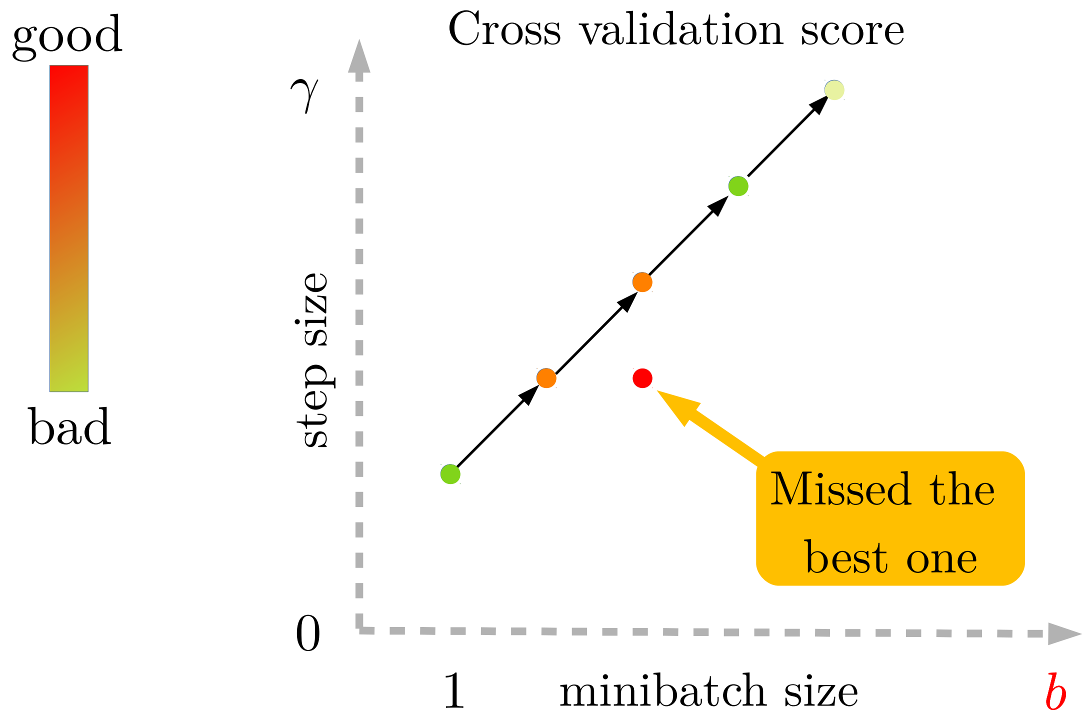

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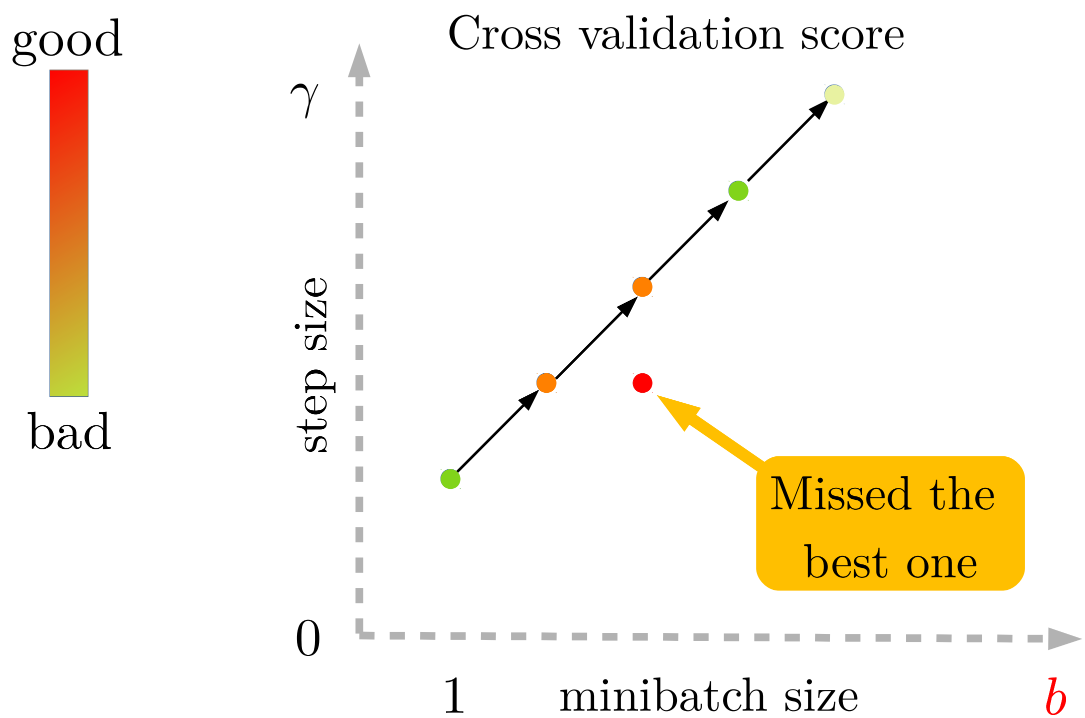

Need to figure out functional relationship between minibatch size and step size

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Stochastic Reformulation of Finite sum problems

Simple Stochastic Reformulation

Random sampling vector $v = (v_1, \ldots, v_n) \sim \mathcal{D}$ with

$$\mathbb{E}[v_i] = 1, \quad \text{for } i = 1, \ldots, n$$

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Original finite sum problem

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

$$\Longleftrightarrow$$

Stochastic Reformulation

$$\min_{w \in \mathbb{R}^d} \mathbb{E}\left[f_v(w)\right]$$

Minimizing the expectation of **random linear combinations** of original function

SGD with arbitrary sampling

$$\min_{w \in \mathbf{R}^d} \mathbb{E}\left[f_{v}(w) := \frac{1}{n} \sum_{i=1}^{n} v_i f_i(w) \right]$$

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Example: Gradient descent

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saves time for theorists: One representation for all forms of sampling

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Examples of arbitrary sampling: uniform single element

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Single element SGD

$$\text{Sample } v^t \sim \mathcal{D}$$

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Examples of arbitrary sampling: uniform mini-batching

Random set $S \subset \{1, \ldots, n\}, \; |S| = b$

$\mathbb{P}[i \in S] = b/n, \quad \text{for } i = 1, \ldots, n$

$$v_i = \begin{cases} \frac{n}{b} & i \in S \\ 0 & i \notin S \end{cases}$$

$\mathbb{E}[v_i] = 1$

$$\nabla f_v(w) = \frac{1}{b} \sum_{i \in S} \nabla f_i(w)$$

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Mini-batch SGD without replacement

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Examples of arbitrary sampling: non-uniform mini-batching

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Richtárik and Takáč (arXiv:1310.3438; Opt Letters 2016)

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Arbitrary sampling SGD

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How to analyse this general SGD?

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Look at the extremes: GD and single element SGD

Assumption and convergence of Gradient Descent and SGD

Reminder: Convergence GD strongly convex + smooth

$$||w^{t+1} - w^*||_2^2 = ||w^t - w^* - \frac{1}{L}\nabla f(w^t)||_2^2$$

$$= ||w^t - w^*||_2^2 + \frac{2}{L}\langle \nabla f(w^t), w^* - w^t \rangle + \frac{1}{L^2}||\nabla f(w^t)||_2^2$$

Now smoothness gives

$$f(w^*) - f(w) \leq -\frac{1}{2L}||\nabla f(w)||_2^2$$

$$\Downarrow$$

$$||\nabla f(w)||_2^2 \leq 2L(f(w) - f(w^*))$$

Assumptions and Convergence of Gradient Descent

quasi strong convexity constant

$$f(w^*) \geq f(w) + \langle \nabla f(w), w^* - w \rangle + \frac{\mu}{2} ||w^* - w||_2^2 \qquad \forall w$$

Smoothness constant

$$||\nabla f(w) - \nabla f(w^*)||_2^2 \leq 2L\,(f(w) - f(w^*)) \qquad \forall w$$

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$w^{t+1} = w^t - \frac{1}{L}\nabla f(w^t), \; v \equiv (1, \ldots, 1)$

$w^* = \arg\min_{w \in \mathbb{R}^d} \frac{1}{n}\sum_{i=1}^n f_i(w)$

Iteration complexity of gradient descent

$$\text{Given } \epsilon > 0 \text{ and } t \geq \frac{L}{\mu}\log\left(\frac{1}{\epsilon}\right) \Rightarrow \frac{\|w^t - w^*\|^2}{\|w^0 - w^*\|^2} \leq \epsilon$$

Assumptions and Convergence of Stochastic Gradient Descent

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Bigger smoothness constant/ stronger assumption

$$\frac{1}{n}\sum_{i=1}^{n} ||\nabla f_i(w) - \nabla f_i(w^*)||_2^2 \;\leq\; 2L_{\max}\left(f(w) - f(w^*)\right) \quad \forall w$$

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Definition $\sigma_*^2 := \frac{1}{n}\sum_{i=1}^{n} \|\nabla f_i(w^*)\|^2$

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Definition $\quad \sigma_*^2 := \frac{1}{n}\sum_{i=1}^{n} ||\nabla f_i(w^*)||^2$

Iteration complexity of SGD

$$t \geq \left(\frac{L_{\max}}{\mu} + \frac{\sigma_*^2}{\epsilon \mu^2}\right) \log\left(\frac{1}{\epsilon}\right) \quad \Rightarrow \quad \frac{\mathbb{E}[||w^t - w^*||^2]}{||w^0 - w^*||^2} \leq \epsilon$$

Needell, Srebro, Ward: Math. Prog, 2016.

Informal comparison between GD and SGD iteration complexity

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SGD

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How do they compare?

In general: $L \leq L_{\max} \leq nL$

Informal comparison between GD and SGD iteration complexity

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SGD

$$t \geq O\left(\frac{L_{\max}}{\mu} + \frac{\sigma_*^2}{\epsilon \mu^2}\right)$$

$$\frac{\mathbb{E}[\|w^t - w^*\|^2]}{\|w^0 - w^*\|^2} \leq \epsilon$$

When n is big $L \ll L_{\max}$

How do they compare?

In general: $L \leq L_{\max} \leq nL$

Informal comparison between GD and SGD iteration complexity

GD

$$t \geq O\left(\frac{L}{\mu}\right)$$

SGD

$$t \geq O\left(\frac{L_{\max}}{\mu} + \frac{\sigma_*^2}{\epsilon \mu^2}\right)$$

$$\frac{\mathbb{E}[\|w^t - w^*\|^2]}{\|w^0 - w^*\|^2} \leq \epsilon$$

When n is big
$L \ll L_{\max}$

How do they compare?

In general: $L \leq L_{\max} \leq nL$

Need new "interpolating" notion of smoothness

$$L \leq \;?\; L(v) \;?\; \leq L_{\max}$$

Key constant: Expected smoothness

Ass: Expected Smoothness. We write $(f, \mathcal{D}) \sim ES(\mathcal{L})$ when

$$\mathbb{E}[||\nabla f_v(w) - \nabla f_v(w^*)||_2^2] \;\leq\; 2\mathcal{L}\left(f(w) - f(w^*)\right) \quad \forall w$$

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Expected smoothness constant

Depends on v and f

RMG, Richtárik and Bach (arXiv:1805.02632, 2018)

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f_i convex and $L_{\max}$–smooth

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(we can do better)

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Generalization of

$$\sigma_*^2 := \frac{1}{n}\sum_{i=1}^n \|\nabla f_i(w^*)\|^2$$

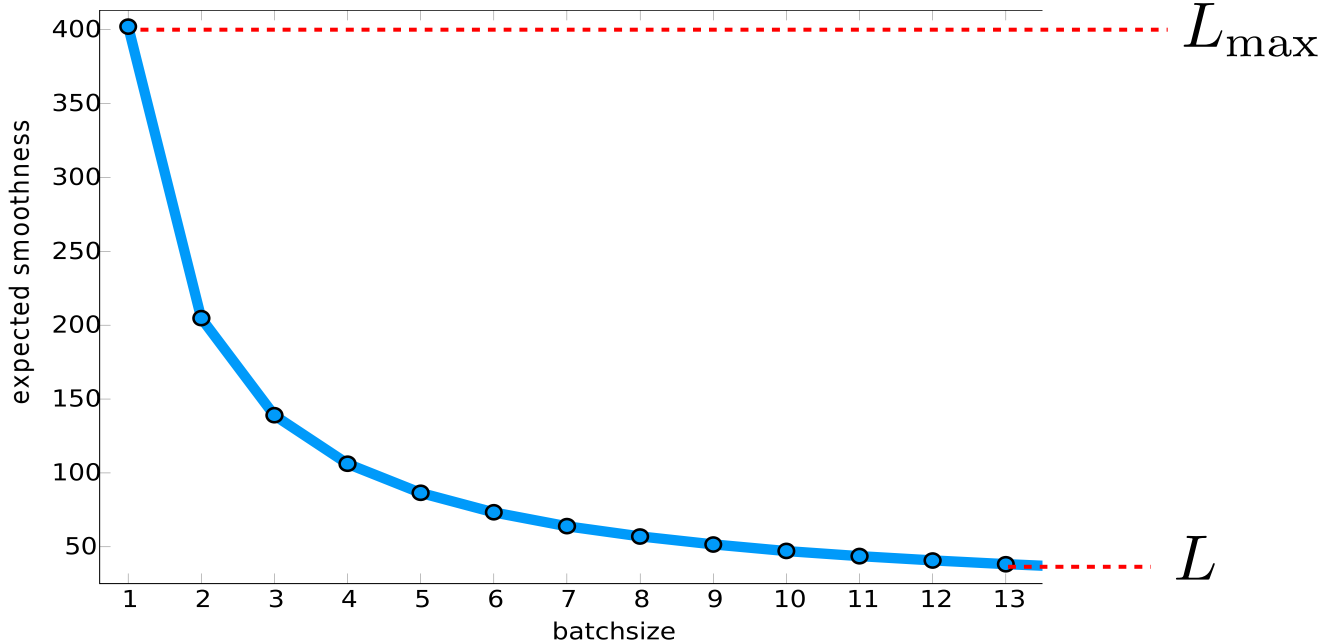
Example of Expected Smoothness

S is chosen uniformly at random from all subsets of size b

$$\mathcal{L}(b) = \frac{n(b-1)}{b(n-1)}L + \frac{n-b}{b(n-1)}L_{\max}$$

$$v_i = \begin{cases} \frac{n}{b} & i \in S \\ 0 & i \notin S \end{cases}$$

EXE: In your list!



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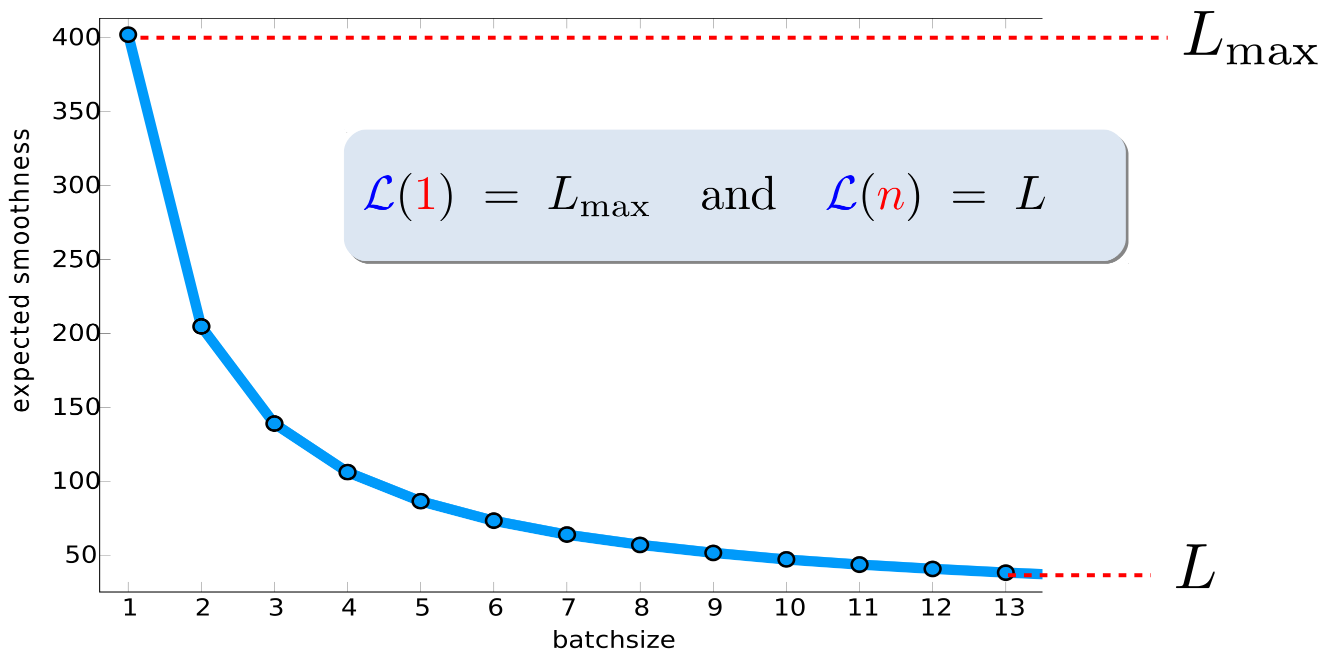

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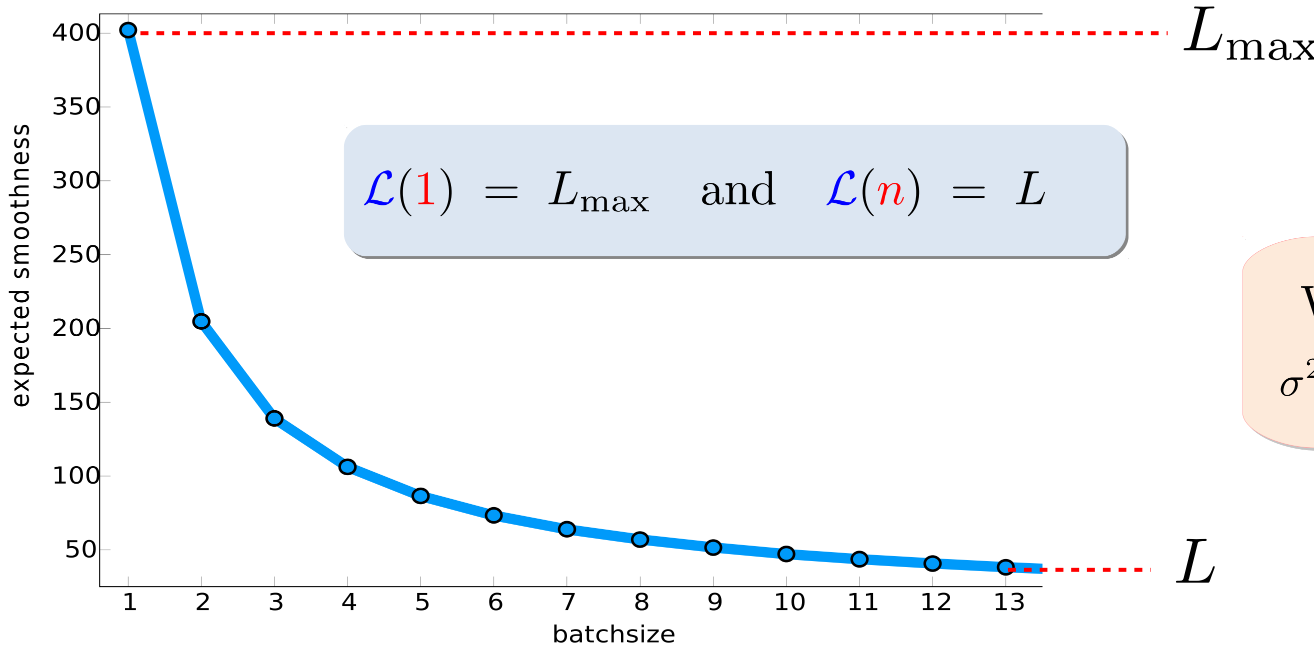

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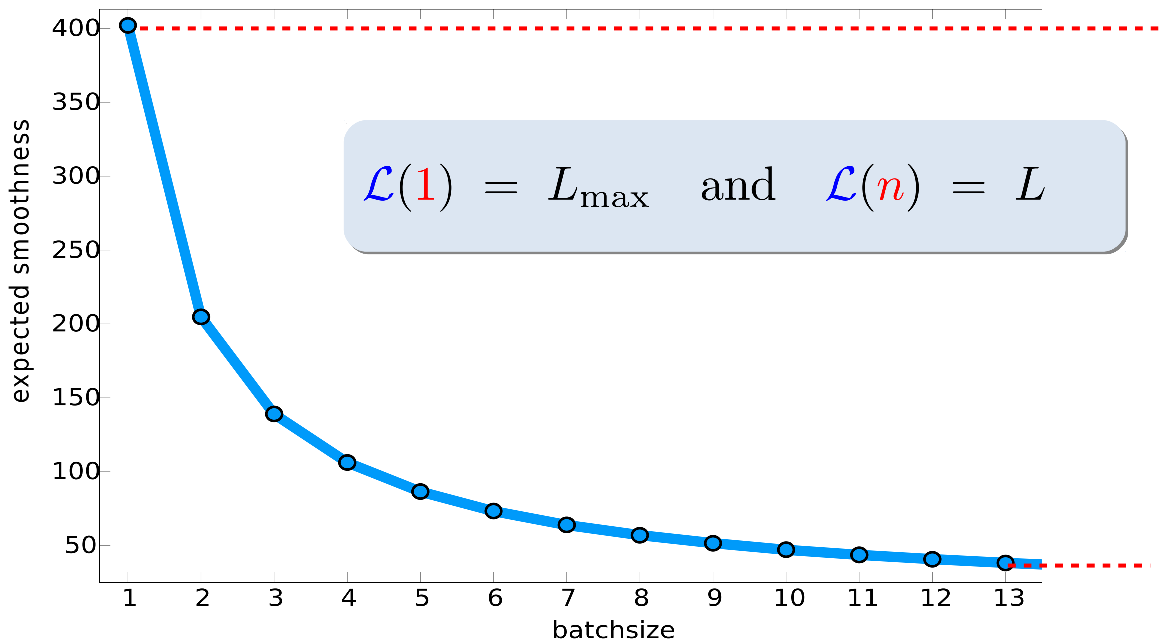
EXE: In your list!

$$\sigma^2(b) = \frac{n-b}{b(n-1)}\sigma_*^2$$

Measures how much model fits data



$L_{\max}$ $\sigma^2 = \sigma_*^2$

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L $\sigma^2 = 0$

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Expected smoothness gives awesome bound on 2nd moment

Normally bound on gradient is an *assumption*

Assumption There exists $B>0$

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informative: with realistic assumptions

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Main Theorem (Linear convergence to a neighborhood)

$f(w^*) \geq f(w) + \langle \nabla f(w), w^* - w \rangle + \frac{\mu}{2}||w^* - w||_2^2$

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saves time for theorists: Includes GD and SGD as special cases. Also tighter!

Proof is SUPER EASY:

$$
\begin{aligned}
||w^{t+1} - w^*||_2^2 &= ||w^t - w^* - \gamma \nabla f_v(w^t)||_2^2 \\
&= ||w^t - w^*||_2^2 - 2\gamma \langle \nabla f_v(w^t), w^t - w^* \rangle + \gamma^2 ||\nabla f_v(w^t)||_2^2.
\end{aligned}
$$

Taking expectation with respect to $v \sim \mathcal{D}$

$\mathbb{E}[\nabla f_v(w)] = \nabla f(w)$

$$
\begin{aligned}
\mathbb{E}_v\left[||w^{t+1} - w^*||_2^2\right] &= ||w^t - w^*||_2^2 - 2\gamma \langle \nabla f(w^t), w^t - w^* \rangle + \gamma^2 \mathbb{E}_v\left[||\nabla f_v(w^t)||_2^2\right] \\
&\leq (1-\gamma\mu)||w^t - w^*||_2^2 - 2\gamma(f(w^t) - f(w^*)) + \gamma^2 \mathbb{E}_v\left[||\nabla f_v(w^t)||_2^2\right] \\
&\leq (1-\gamma\mu)||w^t - w^*||_2^2 + 2\gamma(2\gamma\mathcal{L} - 1)(f(w) - f(w^*)) + 2\gamma^2\sigma^2 \\
&\leq (1-\gamma\mu)||w^t - w^*||_2^2 + 2\gamma^2\sigma^2
\end{aligned}
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quasi strong conv

$\gamma \leq \frac{1}{2\mathcal{L}}$

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Taking total expectation

$$
\begin{aligned}
\mathbb{E}\left[||w^{t+1} - w^*||_2^2\right] &\leq (1-\gamma\mu)\mathbb{E}\left[||w^t - w^*||_2^2\right] + 2\gamma^2\sigma^2 \\
&= (1-\gamma\mu)^{t+1}||w^0 - w^*||_2^2 + 2\sum_{i=0}^t (1-\gamma\mu)^i \gamma^2\sigma^2 \\
&\leq (1-\gamma\mu)^{t+1}||w^0 - w^*||_2^2 + \frac{2\gamma\sigma^2}{\mu}
\end{aligned}
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$$\sum_{i=0}^t (1-\gamma\mu)^i = \frac{1-(1-\gamma\mu)^{t+1}}{\gamma\mu} \leq \frac{1}{\gamma\mu}$$

Exercises on Sampling, Expected Smoothness + gradient noise

Optimal mini-batch sizes

Total complexity for mini-batch SGD

Corollary $\gamma = \max\left\{\frac{1}{\mathcal{L}}, \frac{\epsilon\mu}{4\sigma^2}\right\}$

$$t \geq \max\left\{\frac{2\mathcal{L}}{\mu}, \frac{4\sigma^2}{\epsilon\mu^2}\right\} \log\left(\frac{2}{\epsilon}\right) \quad \Rightarrow \quad \frac{\mathbb{E}[\|w^t - w^*\|]}{\|w^0 - w^*\|} \leq \epsilon$$

Total complexity for mini-batch SGD

$$C(b) := \max\left\{\frac{2\mathcal{L}}{\mu},\ \frac{4\sigma^2}{\epsilon\mu^2}\right\}\log\left(\frac{2}{\epsilon}\right) \times b$$

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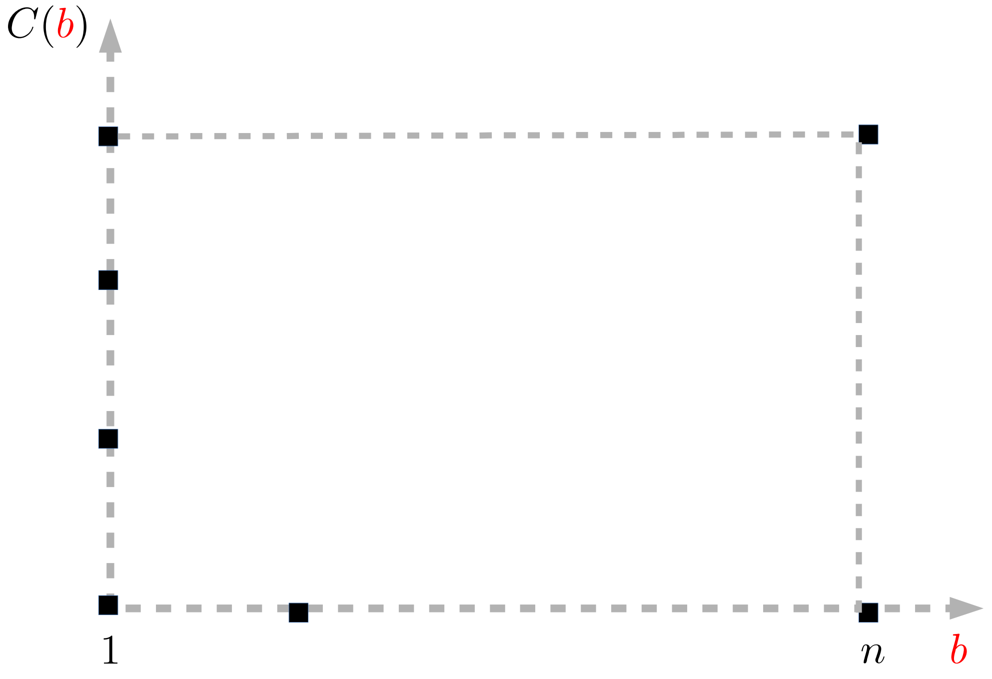
$$\left.\begin{aligned} \mathcal{L} &= \frac{n(b-1)}{b(n-1)}L + \frac{n-b}{b(n-1)}L_{\max} \\ \sigma^2 &= \frac{n-b}{b(n-1)}\sigma_*^2 \end{aligned}\right\} \Rightarrow$$

Total complexity is a simple function of mini-batch size b

Optimal mini-batch size

$$\sigma_1 := \frac{1}{n}\sum_{i=1} \|\nabla f_i(w^*)\|^2$$

$$C(b) := \frac{2}{\mu(n-1)} \max\left\{ n(b-1)L + (n-b)L_{\max},\ \frac{2(n-b)\sigma_*^2}{\epsilon\mu} \right\} \times \log\left(\frac{2}{\epsilon}\right)$$



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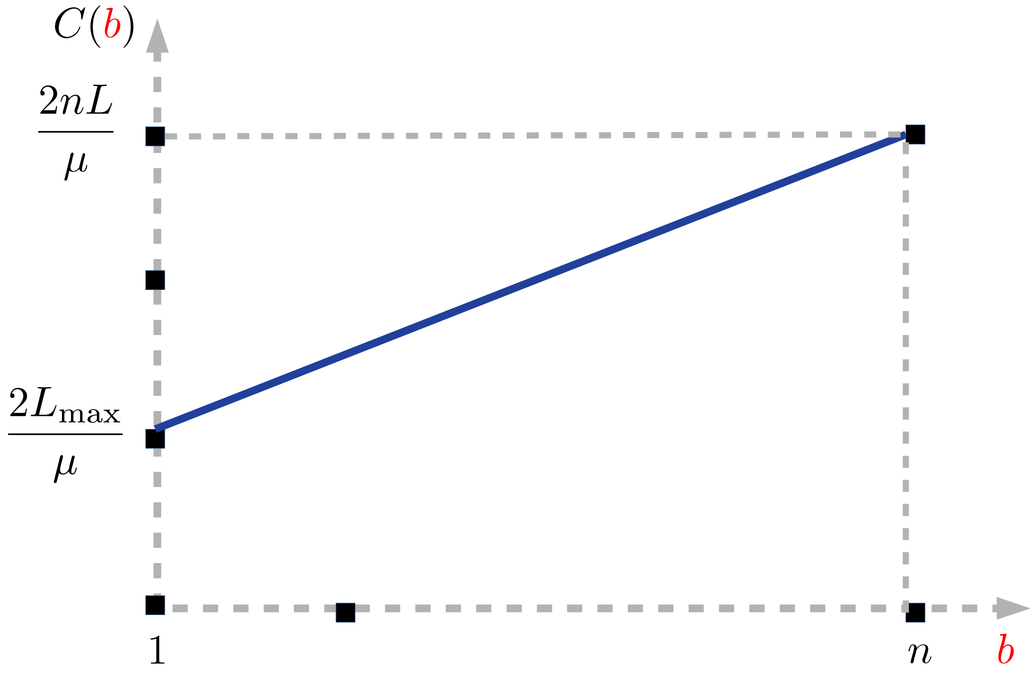

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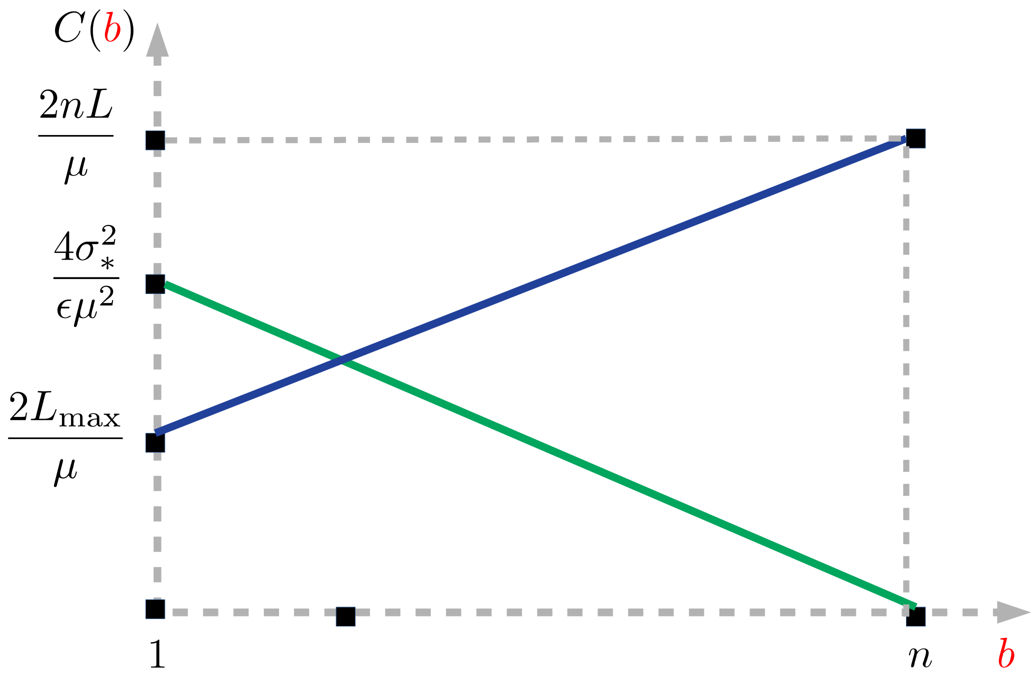

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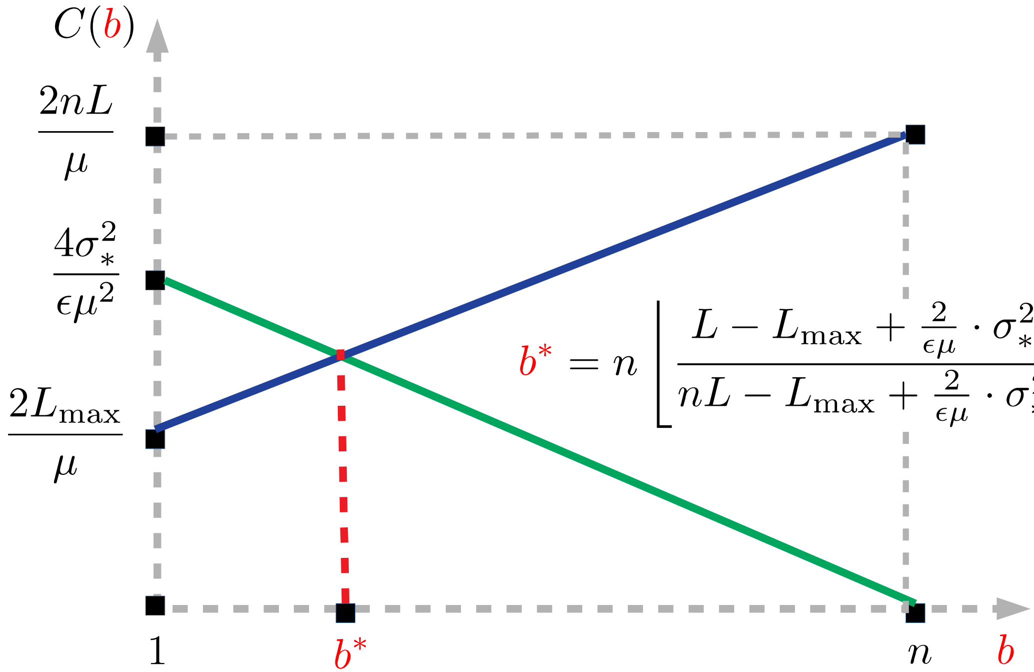

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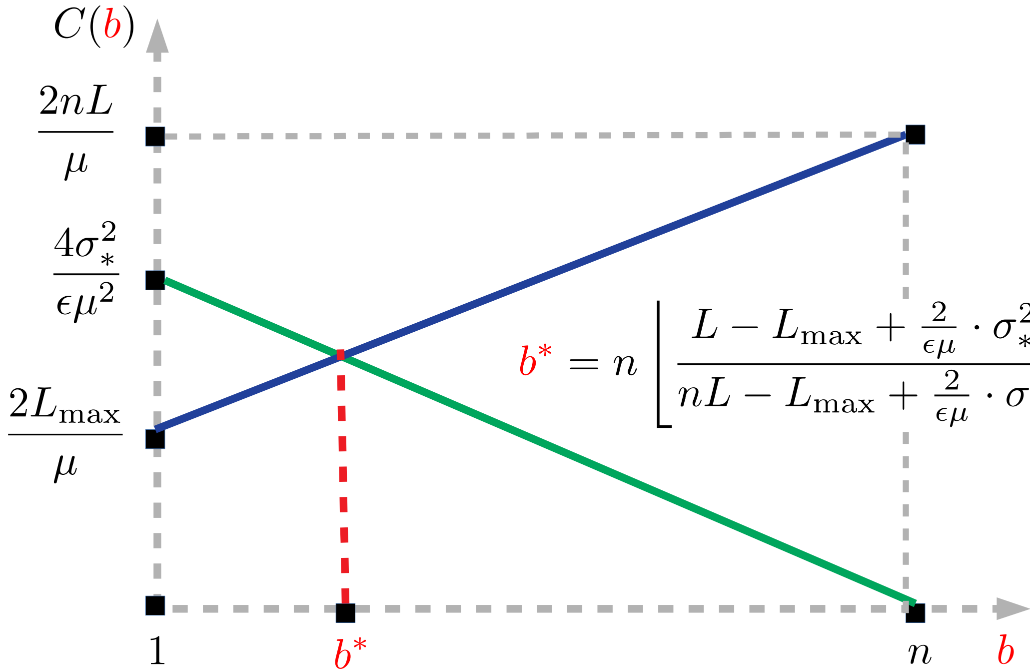
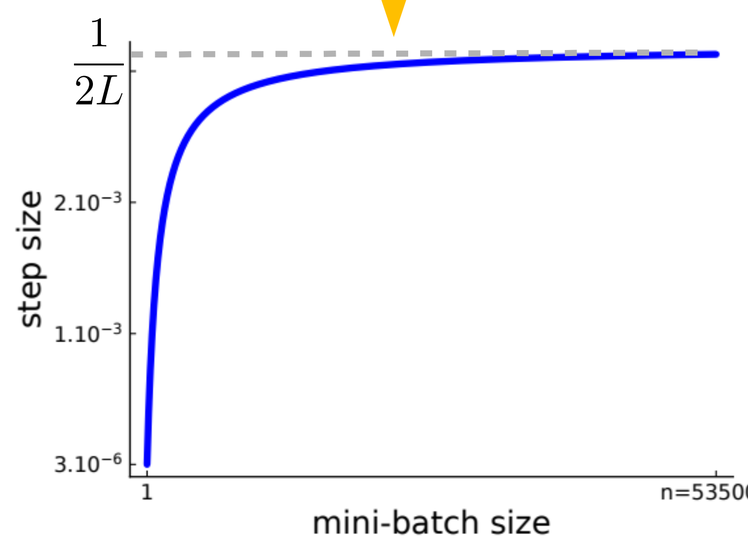
$$\gamma(b) := \frac{n-1}{2} \min\left\{ \frac{b}{n(b-1)L + (n-b)L_{\max}},\ \frac{b\epsilon\mu}{2(n-b)\sigma_*^2} \right\}$$

Stepsize increases with b



$$b^* = n\left\lfloor \frac{L - L_{\max} + \frac{2}{\epsilon\mu}\cdot\sigma_*^2}{nL - L_{\max} + \frac{2}{\epsilon\mu}\cdot\sigma_*^2} \right\rfloor$$



Optimal mini-batch size for models that interpolate data

$$\nabla f_i(w^*) = 0, \ \forall i$$

$$\times \log\left(\frac{2}{\epsilon}\right)$$

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Optimal mini-batch size for models that interpolate data

$\boxed{\nabla f_i(w^*) = 0, \; \forall i}$

0

$\times \log\left(\frac{2}{\epsilon}\right)$

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increases with b

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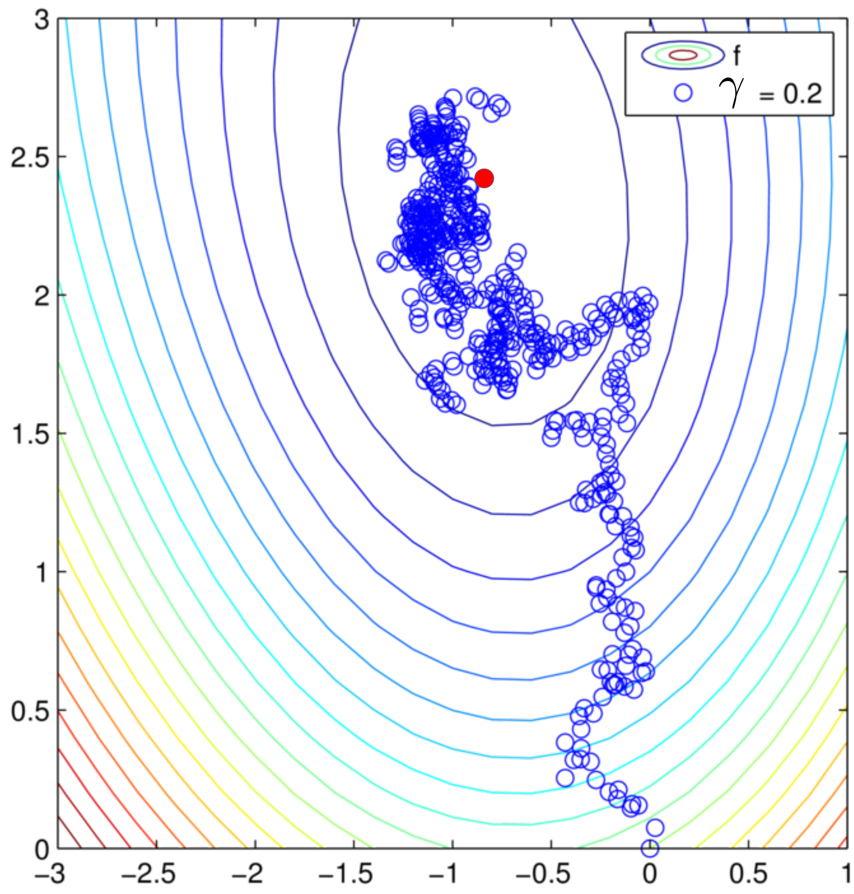
increases with b

$$b^* = 1$$

All gains in mini-batching are due to multi-threading and cache memory?

Stochastic Gradient Descent

$\gamma = 0.2$



Learning schedule: Constant & decreasing step sizes

Theorem $(f, \mathcal{D}) \sim ES(\mathcal{L})$ and μ–quasi strongly convex

Learning rate with switch point

$$\gamma_t = \begin{cases} \dfrac{1}{2\mathcal{L}} & \text{for} \quad t \leq 4\lceil \mathcal{L}/\mu \rceil \\ \dfrac{2t+1}{(t+1)^2\mu} & \text{for} \quad t > 4\lceil \mathcal{L}/\mu \rceil \end{cases}$$

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A stochastic condition number

Learning schedule: Constant & decreasing step sizes

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A stochastic condition number

$\sigma^2 := \mathbb{E}[\|\nabla f_v(w^*)\|^2]$

$$\mathbb{E}\|w^t - w^*\|^2 \leq \frac{\sigma^2}{\mu^2}\frac{8}{t} + \frac{16\lceil \mathcal{L}/\mu \rceil^2}{e^2 t^2}\|w^0 - w^*\|^2$$

for $t > 4\lceil \mathcal{L}/\mu \rceil$

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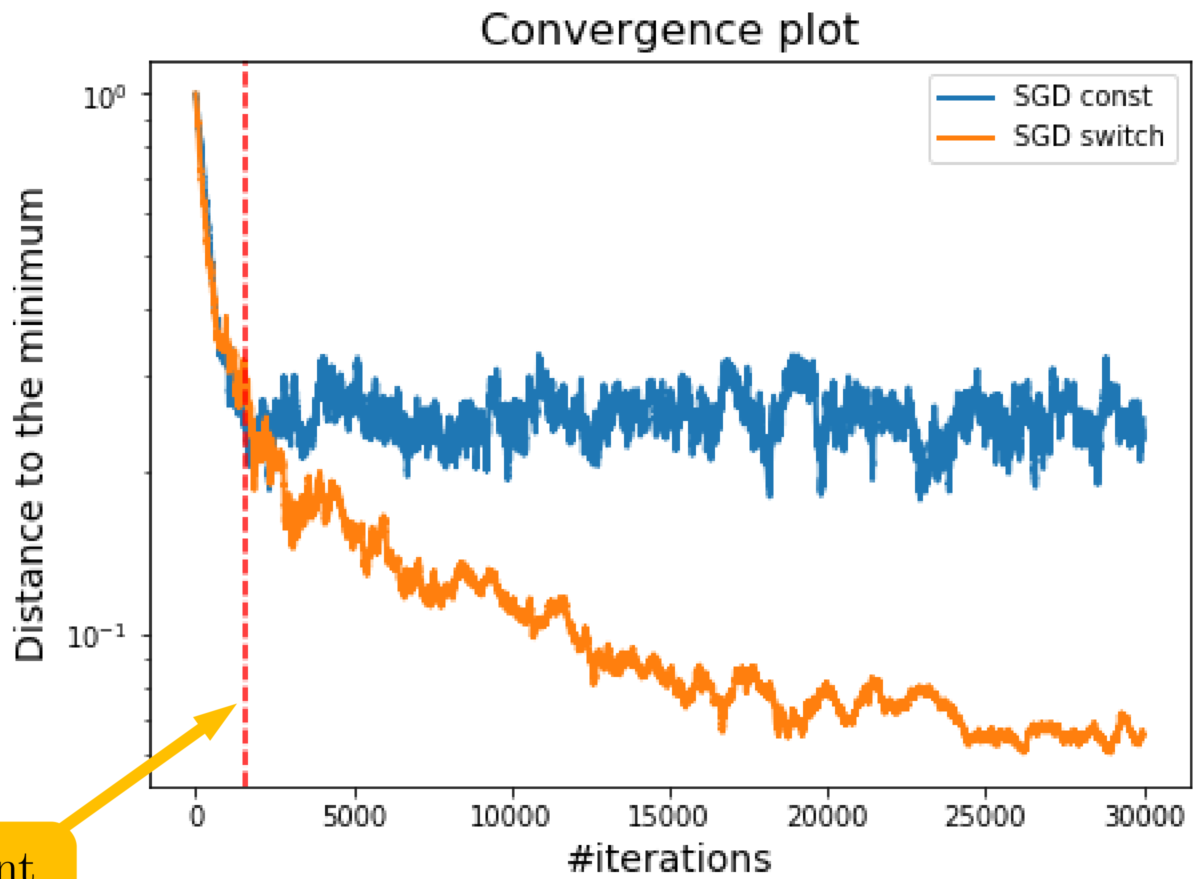
$\nabla f_i(w^*) = 0, \ \forall i$

$$\mathbb{E}\|w^t - w^*\|^2 \leq O\left(\frac{1}{t^2}\right)$$

Stochastic Gradient Descent with switch to decreasing stepsizes



Switch point
$t = 4\lceil \mathcal{L}/\mu \rceil$

Stochastic variance reduced methods

Simple Stochastic Reformulation

Random sampling vector $v = (v_1, \ldots, v_n) \in \mathbb{R}^n$ with

$$\mathbb{E}[v_i] = 1, \quad \text{for } i = 1, \ldots, n$$

$$f(w) := \frac{1}{n}\sum_{i=1}^{n} f_i(w) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}[v_i] f_i(w) = \mathbb{E}\left[\underbrace{\frac{1}{n}\sum_{i=1}^{n} v_i f_i(w)}_{=:\, f_v(w)}\right]$$

What to do about the variance?

Original finite sum problem

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

Stochastic Reformulation

$$\min_{w \in \mathbb{R}^d} \mathbb{E}\left[f_v(w)\right]$$

Minimizing the expectation of **random linear combinations** of original function

Controlled Stochastic Reformulation

$$\frac{1}{n}\sum_{i=1}^{n} f_i(w) \;=\; \mathbb{E}[f_{\color{red}{v}}(w)] \;=\; \mathbb{E}[f_{\color{red}{v}}(w)] - \mathbb{E}[z_{\color{red}{v}}(w)] + \mathbb{E}[z_{\color{red}{v}}(w)]$$

Controlled Stochastic Reformulation

covariate $z_{v}(w) \in \mathbb{R}$

Cancel out

$$\frac{1}{n}\sum_{i=1}^{n} f_i(w) \;=\; \mathbb{E}[f_{v}(w)] \;=\; \mathbb{E}[f_{v}(w)] - \mathbb{E}[z_{v}(w)] + \mathbb{E}[z_{v}(w)]$$

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$$= \mathbb{E}\left[f_{v}(w) - z_{v}(w) + \mathbb{E}[z_{v}(w)]\right]$$

Controlled Stochastic Reformulation

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$\Longleftrightarrow$

Controlled Stochastic Reformulation

$$\min_{w \in \mathbb{R}^d} \mathbb{E}\big[f_v(w) - z_v(w) + \mathbb{E}[z_v(w)]\big]$$

Use covariates to **control the variance**

Variance reduction with arbitrary sampling

$$\min_{w \in \mathbb{R}^d} \mathbb{E}\left[f_{v}(w) - z_{v}(w) + \mathbb{E}[z_{v}(w)] \right]$$

Variance reduction with arbitrary sampling

$$\min_{w \in \mathbb{R}^d} \mathbb{E}\Big[f_{v}(w) - z_{v}(w) + \mathbb{E}[z_{v}(w)]\Big]$$

$$\Downarrow$$

Sample $v^t \sim \mathcal{D}$

$$w^{t+1} = w^t - \gamma_t g_{v^t}(w^t)$$

Variance reduction with arbitrary sampling

$$\min_{w\in\mathbb{R}^d} \mathbb{E}\left[f_v(w) - z_v(w) + \mathbb{E}[z_v(w)]\right]$$

$$\text{Sample } v^t \sim \mathcal{D}$$

$$w^{t+1} = w^t - \gamma_t g_{v^t}(w^t)$$

$$g_v(w) := \nabla f_v(w) - \nabla z_v(w) + \mathbb{E}[\nabla z_v(w)]$$

Variance reduction with arbitrary sampling

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Sample $v^t \sim \mathcal{D}$

$$w^{t+1} = w^t - \gamma_t g_{v^t}(w^t)$$

By design we have that
$\mathbb{E}[g_{v^t}(w^t)] = \nabla f(w^t)$

$$g_v(w) := \nabla f_v(w) - \nabla z_v(w) + \mathbb{E}[\nabla z_v(w)]$$

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$$w^{t+1} = w^t - \gamma_t g_{v^t}(w^t)$$

How to choose $z_v(w)$?

$$g_v(w) := \nabla f_v(w) - \nabla z_v(w) + \mathbb{E}[\nabla z_v(w)]$$

Choosing the covariate

$$\text{Sample } v^t \sim \mathcal{D}$$

$$w^{t+1} = w^t - \gamma_t g_{v^t}(w^t)$$

$$:= \nabla f_v(w) - \nabla z_v(w) + \mathbb{E}[\nabla z_v(w)]$$

Choosing the covariate

Sample $v^t \sim \mathcal{D}$

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We would like:

$$g_v(w) \approx \nabla f(w)$$

Choosing the covariate

Sample $v^t \sim \mathcal{D}$

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We would like:

$$g_v(w) \approx \nabla f(w) \quad \Rightarrow \quad \nabla z_v(w) \approx \nabla f_v(w)$$

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We would like:

$$g_v(w) \approx \nabla f(w)$$

$$\nabla z_v(w) \approx \nabla f_v(w)$$

Linear approximation

$$z_v(w) = f_v(\tilde{w}) + \langle \nabla f_v(\tilde{w}), w - \tilde{w} \rangle$$

A reference point/ snap shot

SVRG: Stochastic Variance Reduced Gradients

Johnson & Zhang, 2013 NIPS

$$w^{t+1} = w^t - \gamma_t g_{v^t}(w^t)$$

Reference point: $\tilde{w} \in \mathbb{R}^d$

Sample: $\nabla f_{v^t}(w^t), \quad v^t \sim \mathcal{D}$ Sampled i.i.d

Grad. estimate: $g_{v^t}(w^t) = \nabla f_{v^t}(w^t) - \nabla f_{v^t}(\tilde{w}) + \nabla f(\tilde{w})$

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$$z_{v^t}(w) = f_{v^t}(\tilde{w}) + \langle \nabla f_{v^t}(\tilde{w}), w - \tilde{w} \rangle \Leftarrow \nabla z_{v^t}(w^t) = \nabla f_{v^t}(\tilde{w}) \Rightarrow \mathbb{E}[\nabla z_{v^t}(w^t)] = \nabla f(\tilde{w})$$

Iteration complexity for SVRG and SAGA for arbitrary sampling

Theorem for SVRG $(f, \mathcal{D}) \sim ES(\mathcal{L})$ and μ–strongly convex

stepsize $\gamma \leq \frac{1}{6\mathcal{L}}$ $\Rightarrow$ Iteration complexity $\approx O\left(\frac{\mathcal{L}}{\mu}\log\left(\frac{1}{\epsilon}\right)\right)$

PDF Adobe Sebbouh, Gazagnadou, Jelassi, Bach, G., 2019

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Sebbouh, Gazagnadou, Jelassi, Bach, G., 2019

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G., Bach, Richtarik, 2018

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Sebbouh, Gazagnadou, Jelassi, Bach, G., 2019

Missing details due to extra definitions

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Total Complexity of mini-batch SVRG

Sebbouh, Gazagnadou, Jelassi, Bach, G, 2019

$$\times \log\left(\frac{2}{\epsilon}\right)$$

$$C(b) \;=\; 2\left(\frac{n}{m}+2b\right)\max\left\{\frac{3}{b}\frac{n-b}{n-1}\frac{L_{\max}}{\mu}+\frac{3n}{b}\frac{b-1}{n-1}\frac{L}{\mu}, m\right\}$$

$$\gamma = \frac{1}{6}\frac{b(n-1)}{(n-b)L_{\max}+n(b-1)L}$$

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Linearly decreasing

$$C(b) = 2\left(\frac{n}{m} + 2b\right) \max\left\{\frac{3}{b}\frac{n-b}{n-1}\frac{L_{\max}}{\mu} + \frac{3n}{b}\frac{b-1}{n-1}\frac{L}{\mu}, m\right\} \times \log\left(\frac{2}{\epsilon}\right)$$

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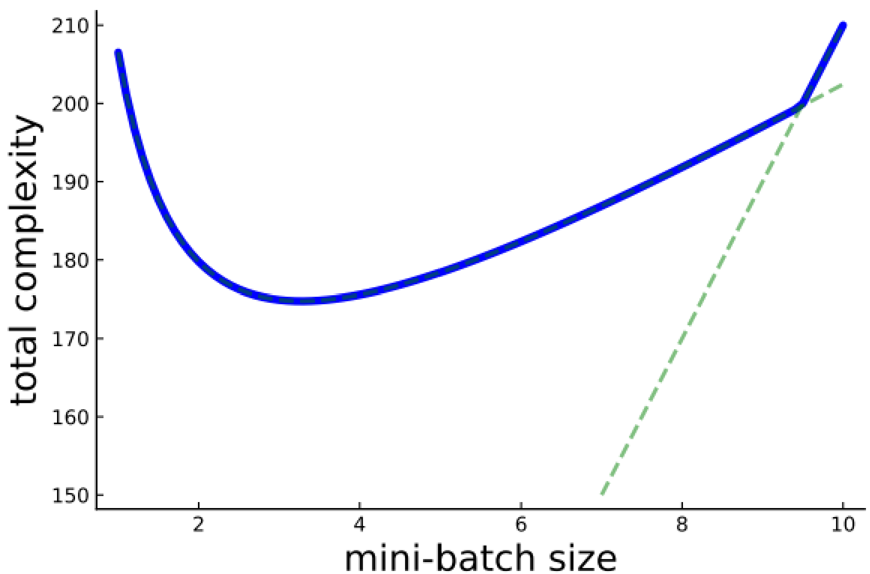

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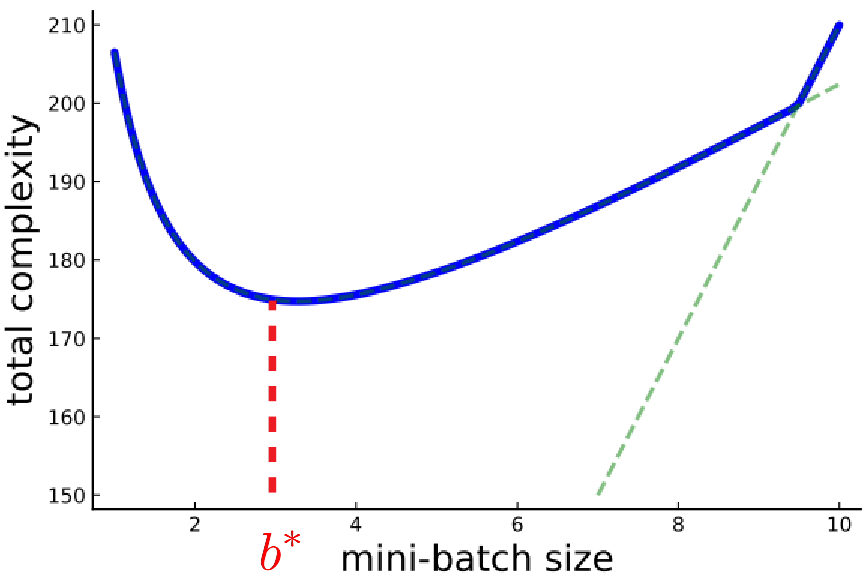

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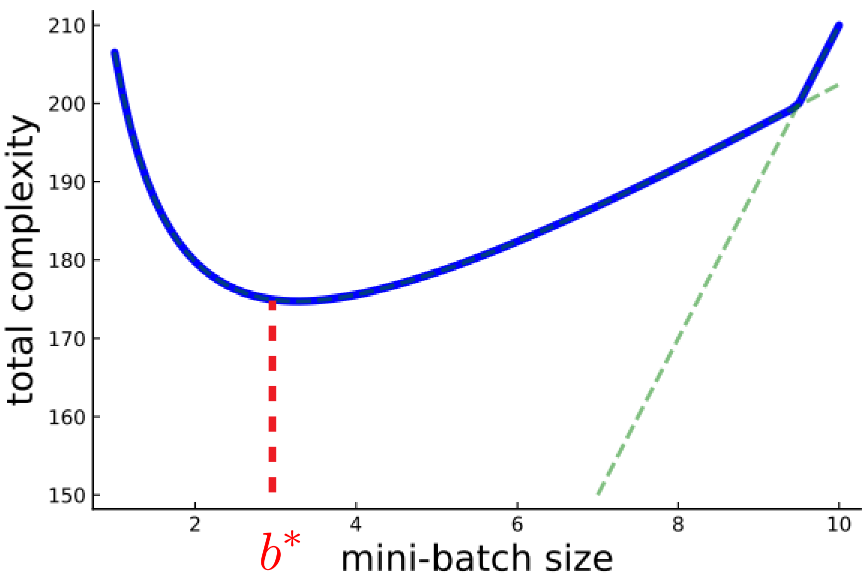
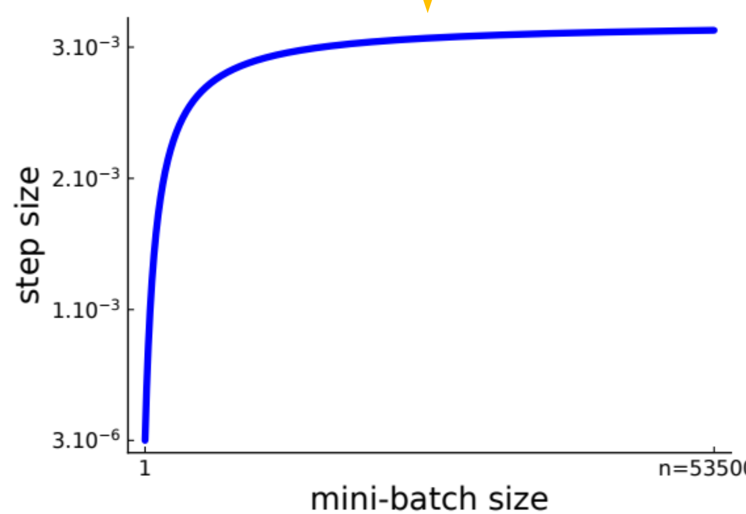
Stepsize increasing with b





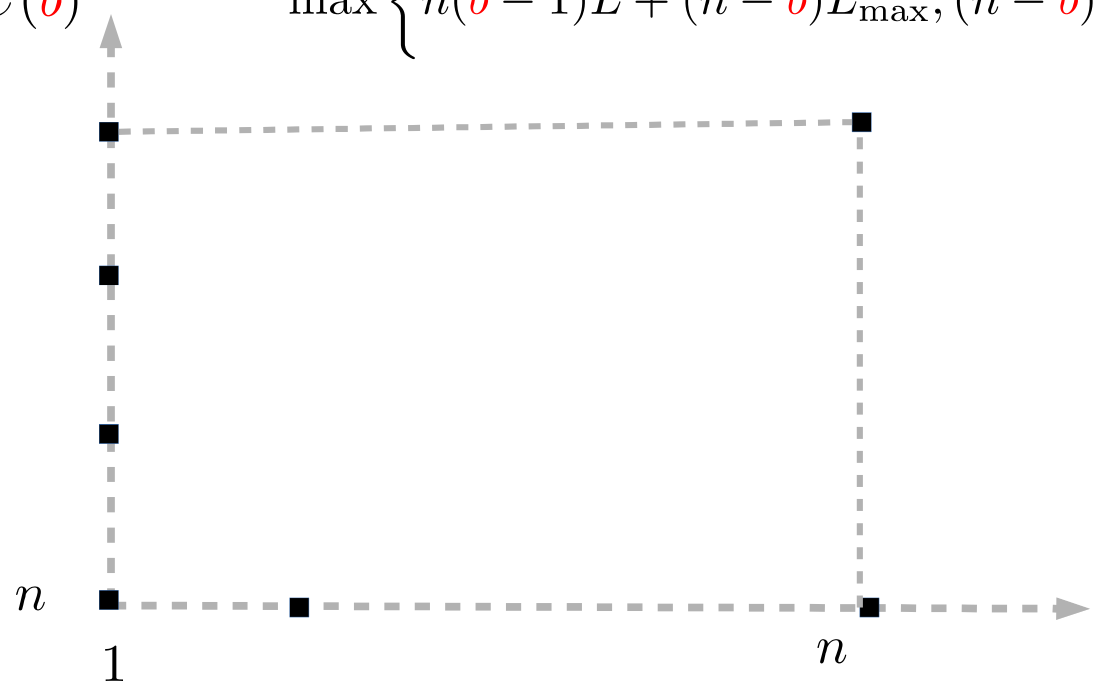
Total Complexity of mini-batch SAGA

Gazagnadou, G & Salmon, ICML 2019

$$C(b) = \max\left\{ n\frac{b-1}{n-1}\frac{4L}{\mu} + \frac{n-b}{n-1}\frac{4L_{\max}}{\mu},\; n + \frac{n-b}{n-1}\frac{4L_{\max}}{\mu} \right\}_{\times \log\left(\frac{2}{\epsilon}\right)}$$

$$\gamma = \frac{1}{4}\frac{b(n-1)}{\max\left\{ n(b-1)L + (n-b)L_{\max},\, (n-b)L_{\max} + \frac{n(n-1)\mu}{4} \right\}}$$

$C(b)$



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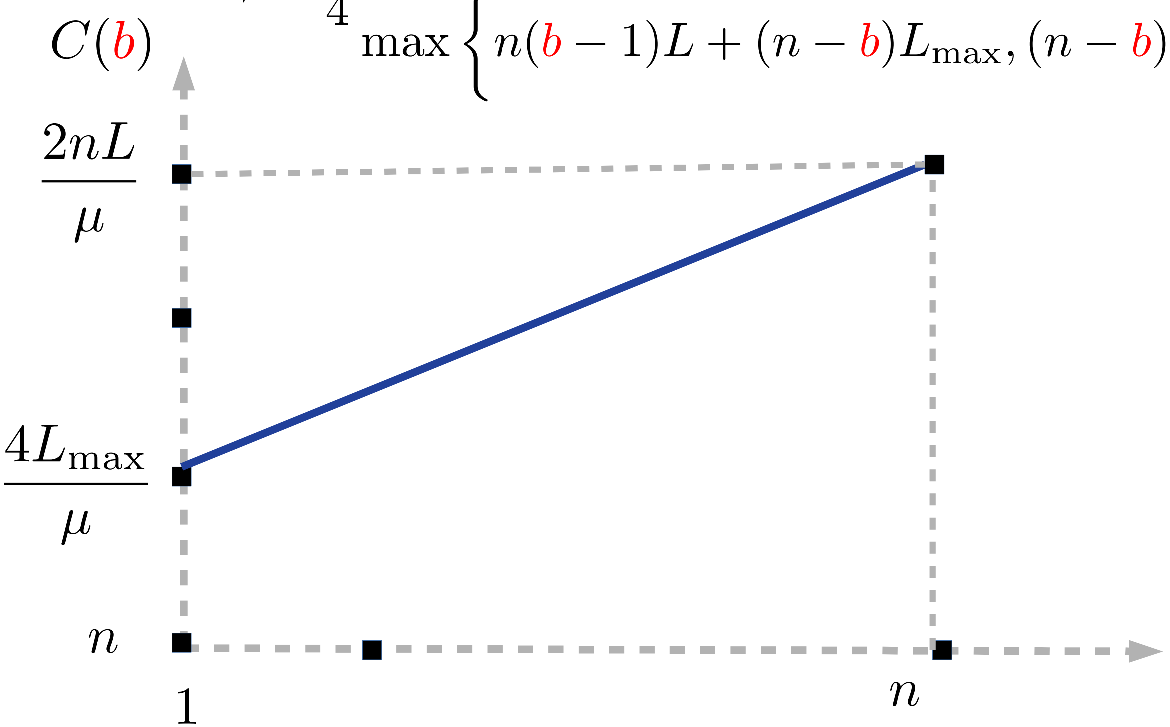

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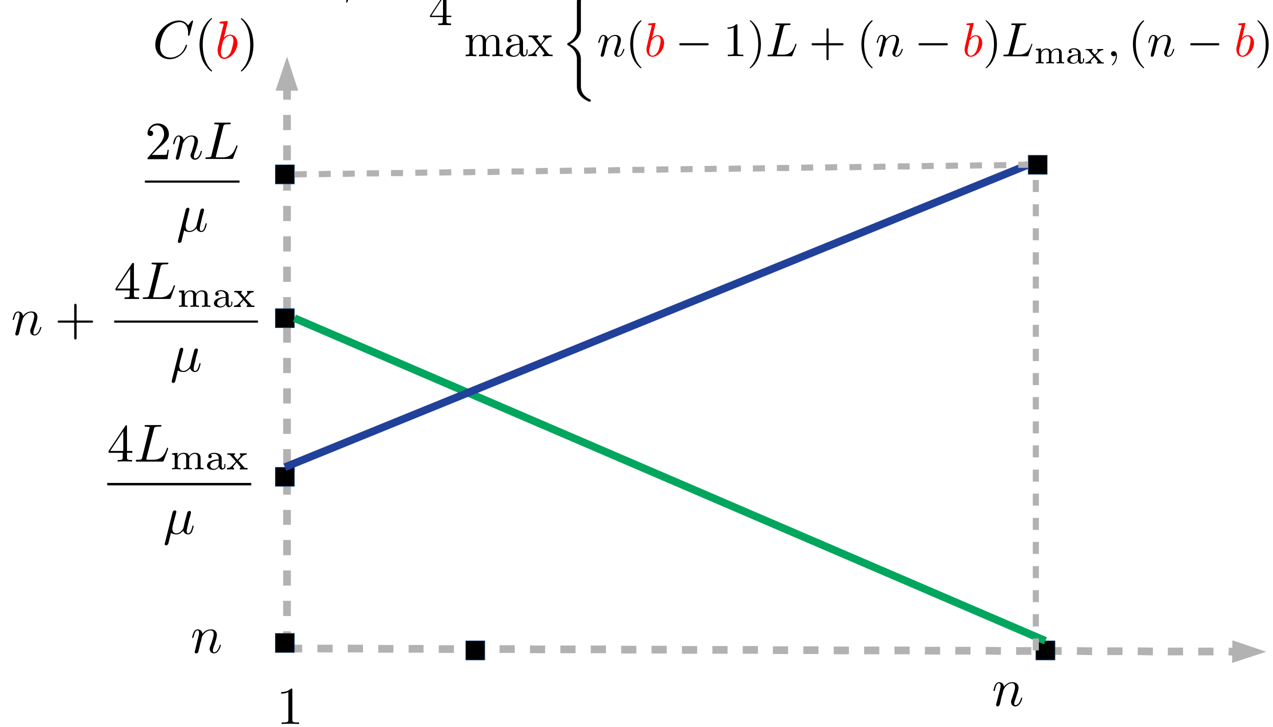

Total Complexity of mini-batch SAGA

Gazagnadou, G & Salmon, ICML 2019

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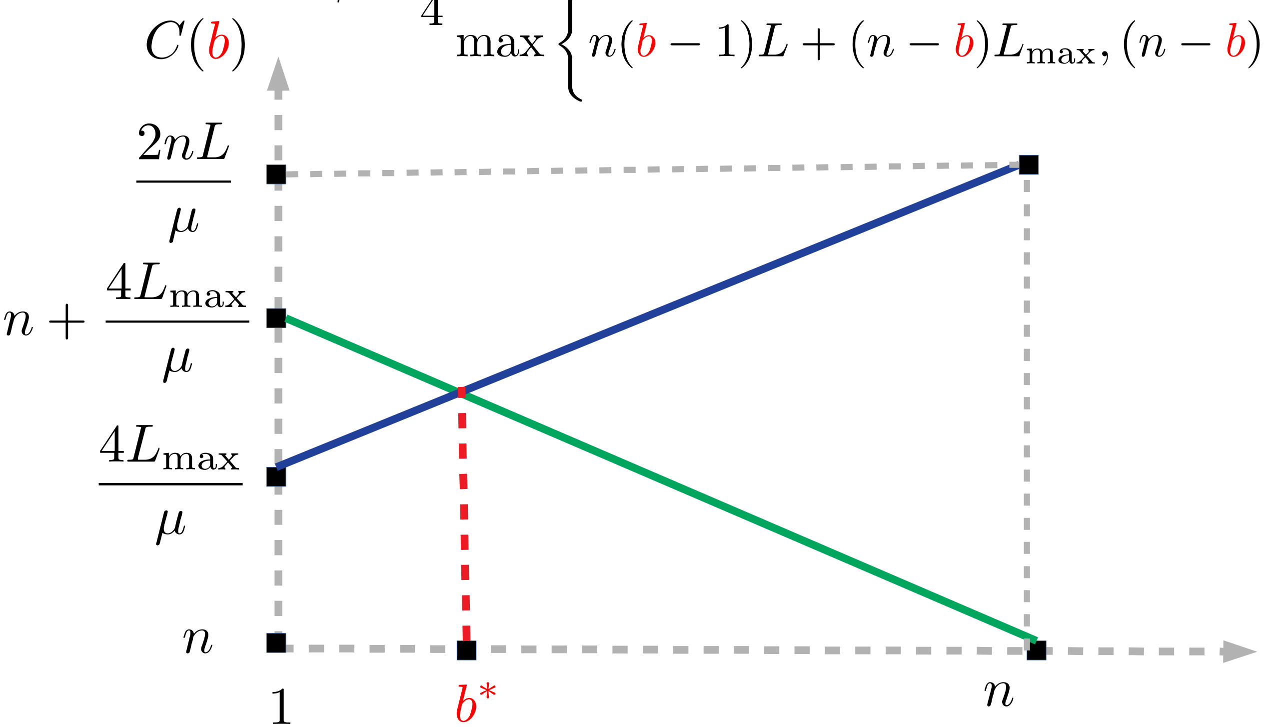

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Total Complexity of mini-batch SAGA

Gazagnadou, G & Salmon, ICML 2019

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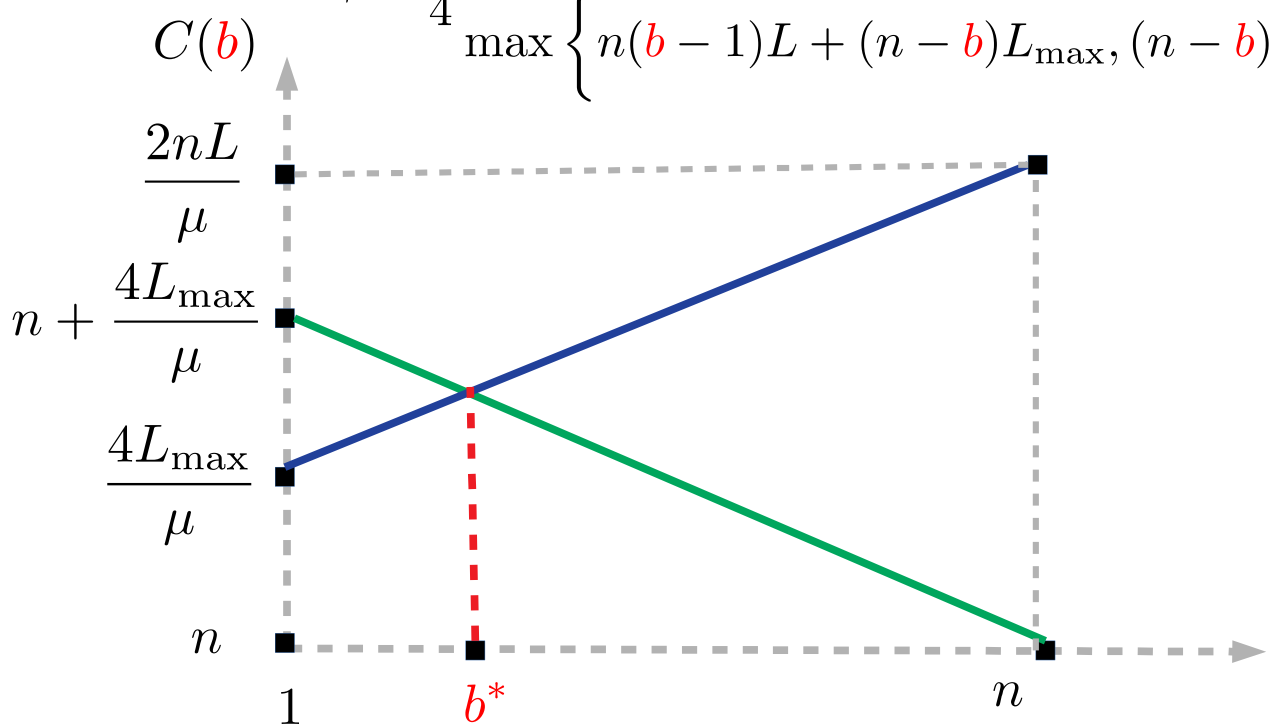

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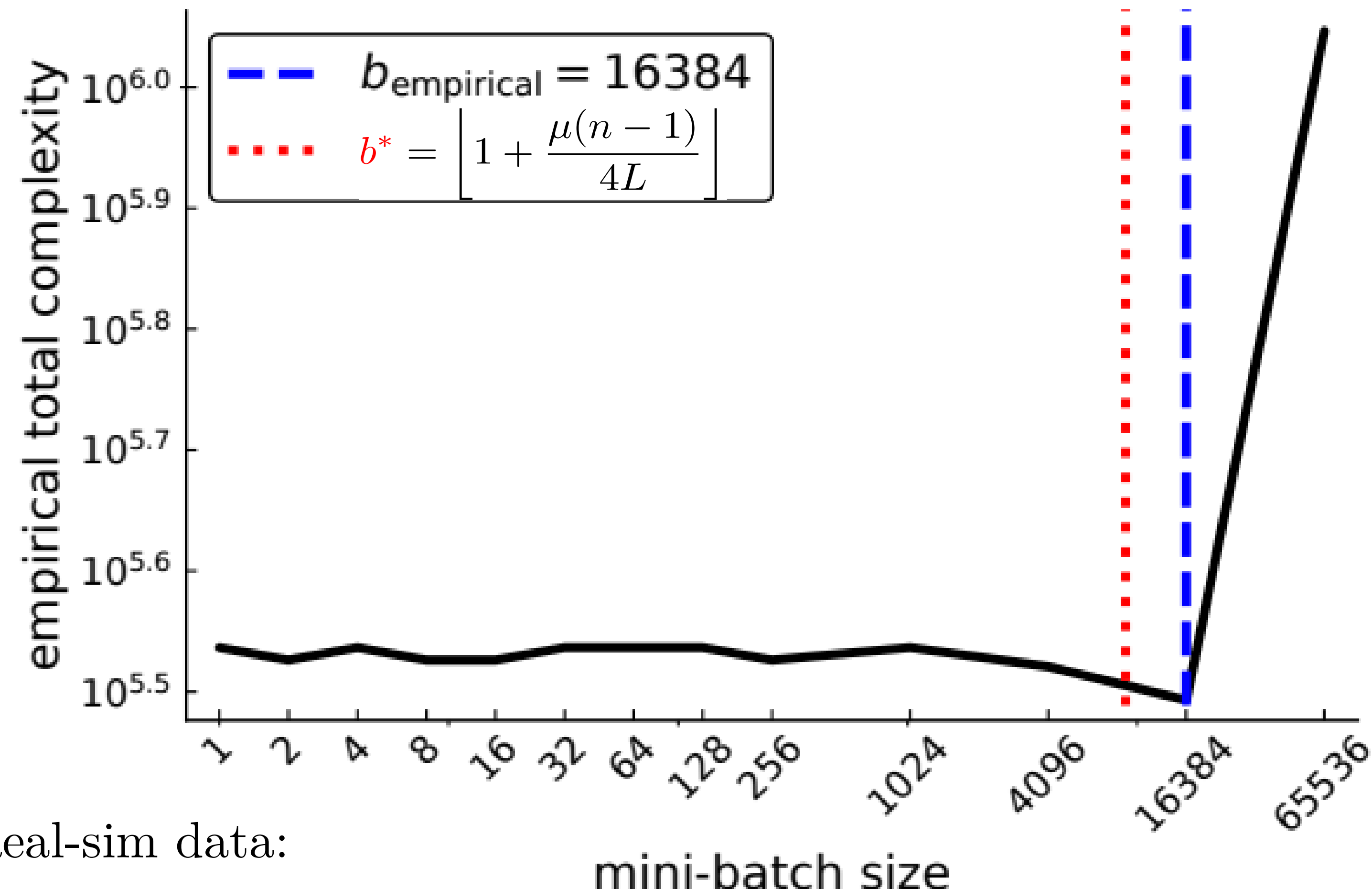
Always smaller than 25% of data

Total Complexity of mini-batch SAGA

Predicts good total complexity

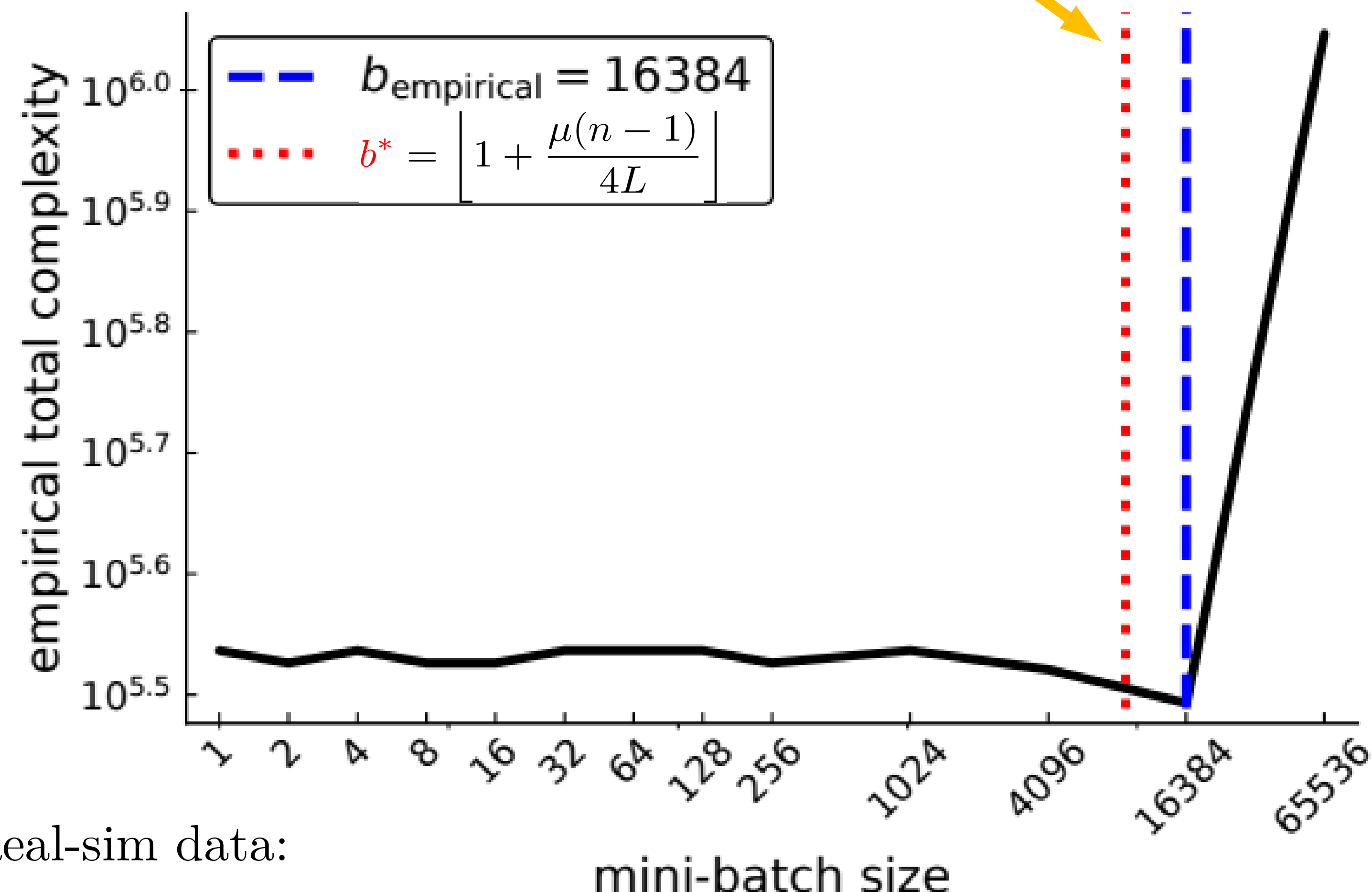


Real-sim data:

(n,d) = (72'309, 20'958)

Total Complexity of mini-batch SAGA

Predicts good total complexity



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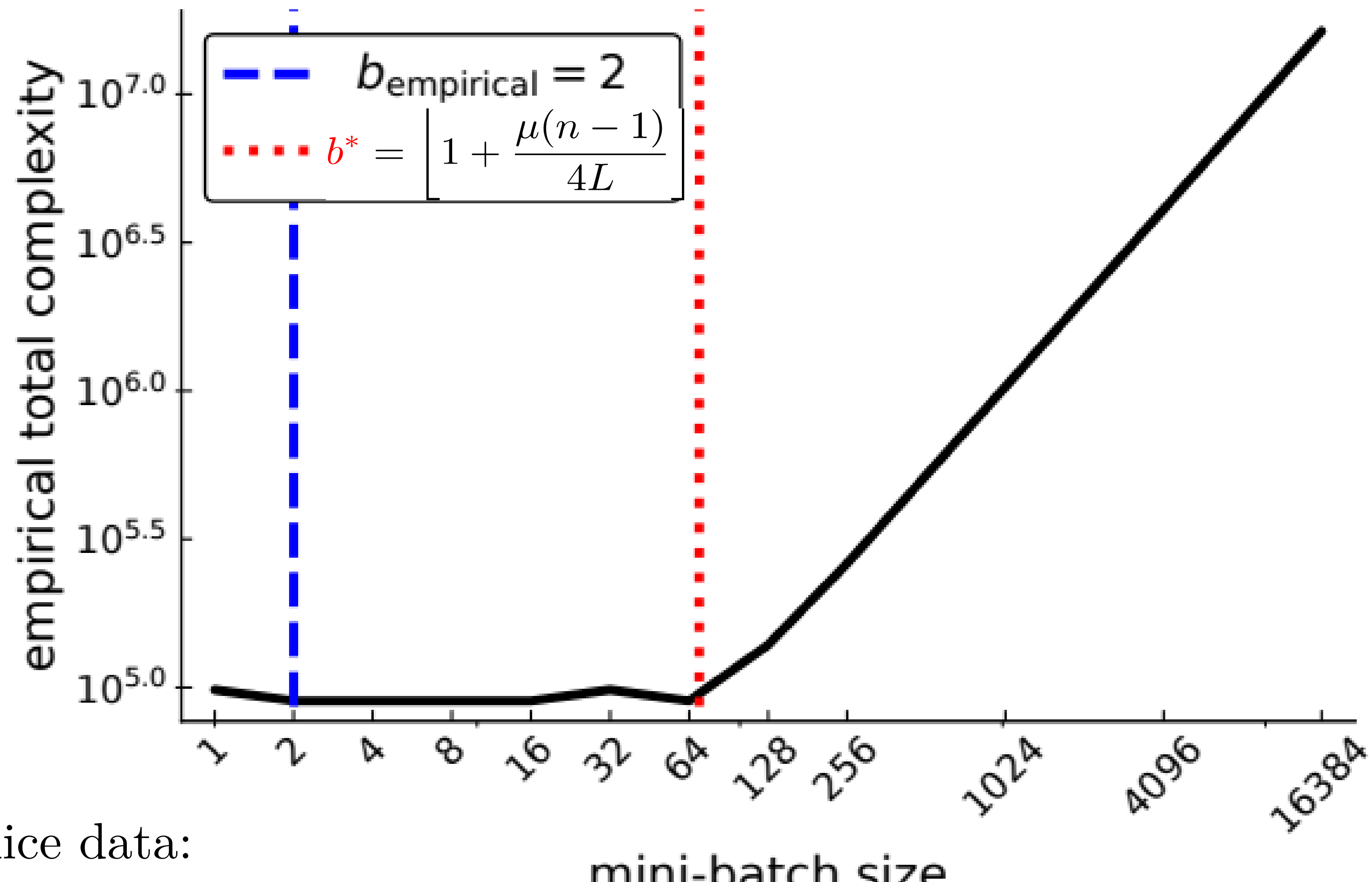
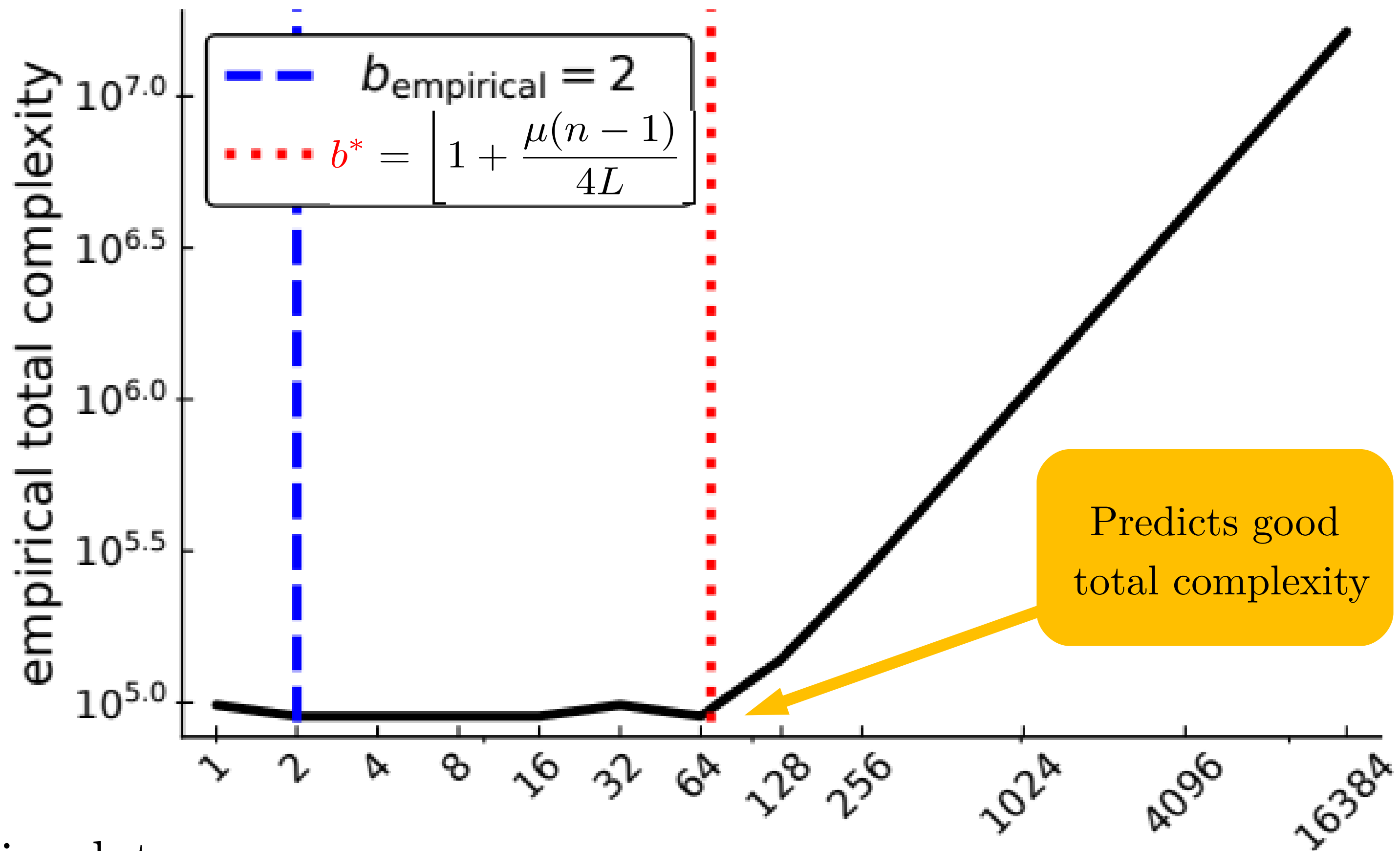


Slice data:

$(n,d) = (53'500,\ 386)$

Total Complexity of mini-batch SAGA



Slice data:

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Take home message so far

Stochastic reformulations allow to view all variants as simple SGD

$$\min_{w \in \mathbf{R}^d} \mathbb{E}\left[f_v(w) := \frac{1}{n} \sum_{i=1}^{n} v_i f_i(w) \right]$$

To analyse all forms of sampling used through expected smooth

$$\mathbb{E}[||\nabla f_v(w) - \nabla f_v(w^*)||_2^2] \leq \mathcal{L} \left(f(w) - f(w^*) \right)$$

$$(f, \mathcal{D}) \sim ES(\mathcal{L})$$

How to calculate optimal mini-batch size of SGD, SAGA and SVRG

Stepsize increase by orders when mini-batch size increases

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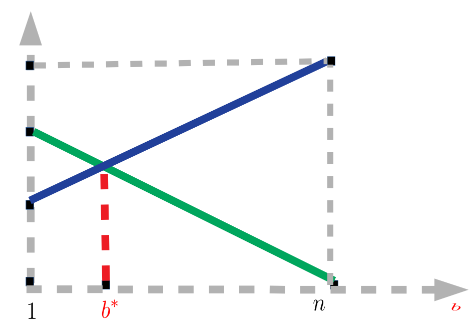

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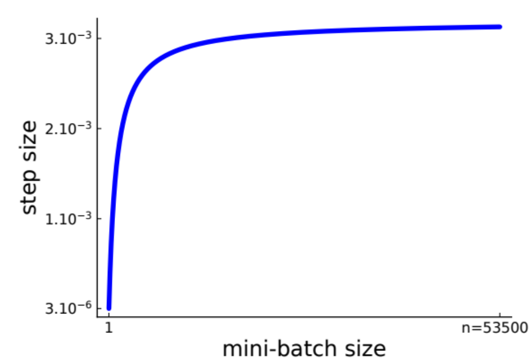


Momentum

Issue with Gradient Descent

Solving the *training problem*: $\min_{w\in\mathbb{R}^d} \frac{1}{n}\sum_{i=1}^{n} f_i(w) =: f(w)$

Baseline method: Gradient Descent (GD)

$$w^{t+1} = w^t - \gamma \nabla f(w^t)$$

Step size/
Learning rate

Issue with Gradient Descent

Local rate of change

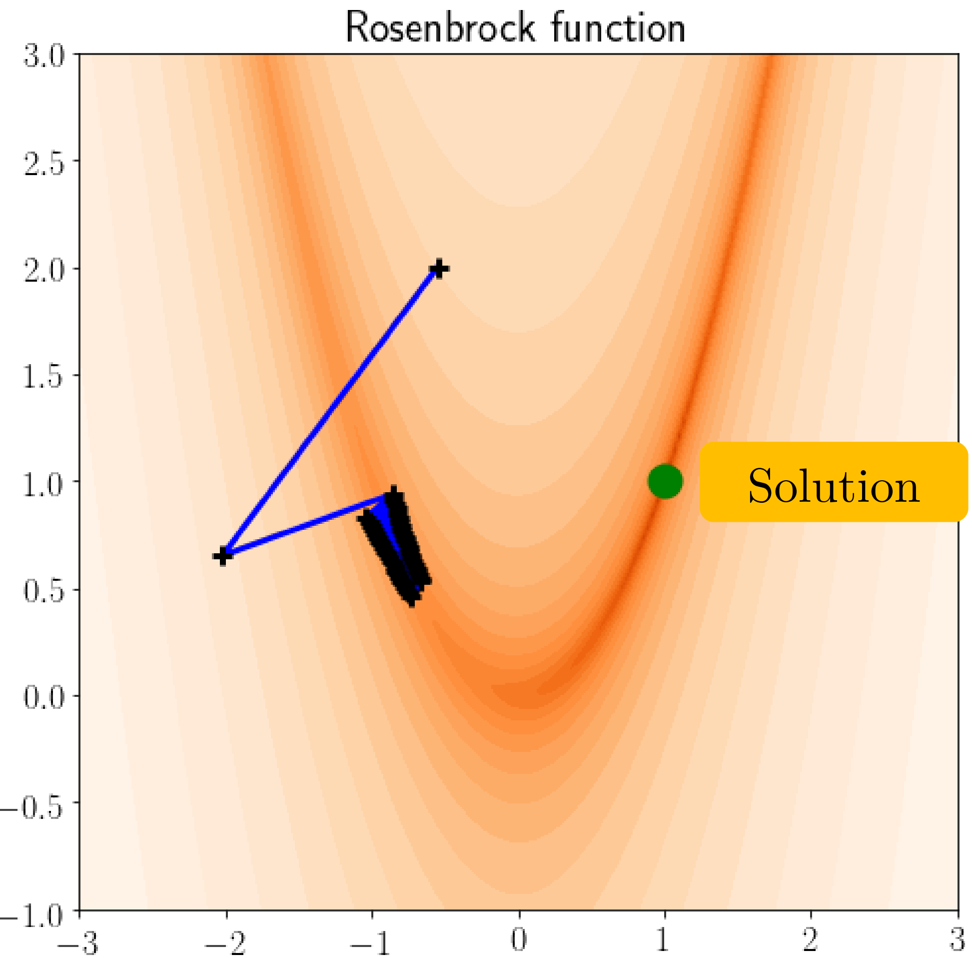
$$\Delta(d) \;:=\; \lim_{s \to 0^+} \frac{f(x+ds) - f(x)}{s}$$

Max local rate

$$\frac{\nabla f(w^t)}{\|\nabla f(w^t)\|} \;:=\; \max_{w \in \mathbb{R}^d} \Delta(d) \quad \text{subject to} \quad \|d\| = 1$$

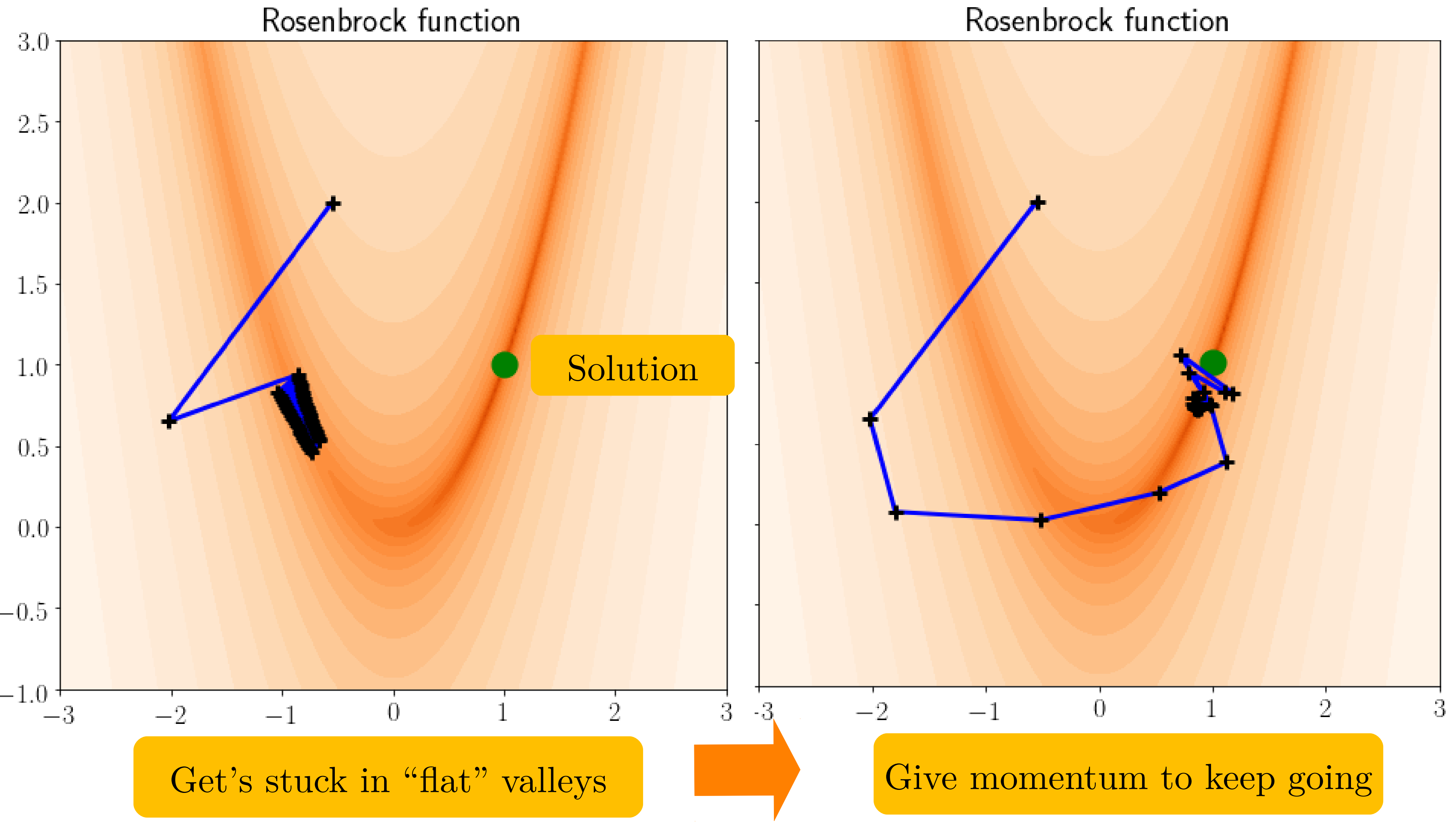
GD is the "steepest descent"

Issue with Gradient Descent



Get's stuck in "flat" valleys

Issue with Gradient Descent



Adding some Momentum to GD

Heavey Ball Method:

$$w^{t+1} = w^t - \gamma \nabla f(w^t) + \underbrace{\beta(w^t - w^{t-1})}_{\text{Adds ``Inertia'' to update}}$$

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GD with momentum (GDm):

Adds "Momentum" to update

$$m^t = \beta\, m^{t-1} + \nabla f(w^t)$$

$$w^{t+1} = w^t - \gamma\, m^t$$

GDm and Heavy Ball Equivalence

GD with momentum:

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Convergence of Gradient Descent with Momentum

Polyak 1964

Theorem Let f be μ–strongly convex and L–smooth, that is

stepsize

$$\mu I \quad \preceq \quad \nabla^2 f(w) \quad \preceq \quad LI, \quad \forall w \in \mathbb{R}^d$$

If $\gamma = \dfrac{4}{(\sqrt{L}+\sqrt{\mu})^2}$ and $\beta = \dfrac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}}$ then SGDm converges

momentum parameter

$$\Rightarrow \quad \|w^t - w^*\| \;\leq\; \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^t \|w^0 - w^*\|$$

$\kappa := L/\mu$

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Corollary $t \geq \dfrac{1}{\sqrt{\kappa}+1}\log\left(\dfrac{1}{\epsilon}\right) \quad \Rightarrow \quad \dfrac{\|w^t - w^*\|}{\|w^0 - w^*\|} \leq \epsilon$

Proof sketch: GDm convergence

Fundamental Theorem of Calculus

$$\int_{s=0}^{1} \nabla^2 f(\underbrace{w_s}_{w_s := w^* + s(w^t - w^*)})ds(w^t - w^*) = \nabla f(w^t) - \nabla f(w^*) = \nabla f(w^t)$$

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Depends on past. Difficult recurrence

Proof: Convergence of Heavy Ball

$$z^{t+1} = \begin{bmatrix} w^{t+1} - w^* \\ w^t - w^* \end{bmatrix} \in \mathbb{R}^{2d}$$

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Adding Momentum to SGD

Rumelhart, Hinton, Geoffrey, Ronald, 1986, Nature

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Sampled i.i.d
$j \in \{1, \ldots, n\}$
$j \sim \frac{1}{n}$

SGDm and Averaging

$$
\begin{aligned}
m^t &= \beta\, m^{t-1} + \nabla f_{j_t}(w^t) \\
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http://fa.bianp.net/teaching/2018/COMP-652/stochastic_gradient.html

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$$\sum_{i=1}^{t} \beta^i \nabla f_{j_{t-i}}(w^{t-i}) \approx \sum_{i=1}^{n} \frac{1}{n} \nabla f_i(w^t)$$

http://fa.bianp.net/teaching/2018/COMP-652/stochastic_gradient.html

RMG, Nicolas Loizou, Xun Qian, Alibek Sailanbayev, Egor Shulgin and Peter Richtárik (2019), ICML
SGD: general analysis and improved rates

RMG, P. Richtarik, F. Bach (2018), preprint online
Stochastic quasi-gradient methods: Variance reduction via Jacobian sketching

N. Gazagnadou, RMG, J. Salmon (2019) , ICML 2019.
Optimal mini-batch and step sizes for SAGA

O. Sebbouh, N. Gazagnadou, S. Jelassi, F. Bach, RMG Neurips 2019, preprint online. **Towards closing the gap between the theory and practice of SVRG**

Stochastic variance reduced methods in detail

SVRG: Stochastic Variance Reduced Gradients

Johnson & Zhang, 2013 NIPS

$$w^{t+1} = w^t - \gamma_t g_{v^t}(w^t)$$

Reference point	$\tilde{w} \in \mathbb{R}^d$
Sample	$\nabla f_i(w^t), \quad i \in \{1, \ldots, n\}$ uniformly
Grad. estimate	$g_{v^t}(w^t) = \nabla f_i(w^t) - \nabla f_i(\tilde{w}) + \nabla f(\tilde{w})$

SVRG: Stochastic Variance Reduced Gradients

Johnson & Zhang, 2013 NIPS

$$w^{t+1} = w^t - \gamma_t g_{v^t}(w^t)$$

Single element sampling

$$v_j = \begin{cases} n & j = i \\ 0 & j \neq i \end{cases}$$

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Grad. estimate: $g_{v^t}(w^t) = \nabla f_i(w^t) - \nabla f_i(\tilde{w}) + \nabla f(\tilde{w})$

$$\nabla z_{v^t}(w^t) = \nabla f_i(\tilde{w})$$

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Grad. estimate	$g_{v^t}(w^t) = \nabla f_i(w^t) - \nabla f_i(\tilde{w}) + \nabla f(\tilde{w})$

$$z_{v^t}(w) = f_i(\tilde{w}) + \langle \nabla f_i(\tilde{w}), w - \tilde{w} \rangle$$

$$\nabla z_{v^t}(w^t) = \nabla f_i(\tilde{w})$$

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Grad. estimate	$g_{v^t}(w^t) = \nabla f_i(w^t) - \nabla f_i(\tilde{w}) + \nabla f(\tilde{w})$

$z_{v^t}(w) = f_i(\tilde{w}) + \langle \nabla f_i(\tilde{w}), w - \tilde{w} \rangle$ ⇐ $\nabla z_{v^t}(w^t) = \nabla f_i(\tilde{w})$ ⇒ $\mathbb{E}[\nabla z_{v^t}(w^t)] = \nabla f(\tilde{w})$

SVRG: Stochastic Variance Reduced Gradients

Jonhson & Zhang, NIPS 2013

Set $w^0 = 0$, choose $\gamma > 0, m \in \mathbb{N}$,

$\quad \alpha_k > 0$ for $k = 0, \ldots, m-1$

$\tilde{w}^0 = w^0$

for $t = 0, 1, 2, \ldots, T-1$

$\quad$ calculate $\nabla f(\tilde{w}^t)$

$\quad$ for $k = 0, 1, 2, \ldots, m-1$

$\quad\quad$ sample $i \in \{1, \ldots, n\}$

$\quad\quad$ $g^k = \nabla f_i(w^k) - \nabla f_i(\tilde{w}^t) + \nabla f(\tilde{w}^t)$

$\quad\quad$ $w^{k+1} = w^k - \gamma g^k$

$\quad$ $\tilde{w}^{t+1} = \frac{1}{m} \sum_{k=0}^{m-1} \alpha_k w^k$

Output $\tilde{w}^T$

Sebbouh, Gazagnadou, Jelassi, Bach, Gower, 2019

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Jonhson & Zhang, NIPS 2013

Set $w^0 = 0$, choose $\gamma > 0, m \in \mathbb{N}$,

$\alpha_k > 0$ for $k = 0, \ldots, m-1$

$\tilde{w}^0 = w^0$

for $t = 0, 1, 2, \ldots, T-1$

calculate $\nabla f(\tilde{w}^t)$

for $k = 0, 1, 2, \ldots, m-1$

sample $i \in \{1, \ldots, n\}$

$g^k = \nabla f_i(w^k) - \nabla f_i(\tilde{w}^t) + \nabla f(\tilde{w}^t)$

$w^{k+1} = w^k - \gamma g^k$

$\tilde{w}^{t+1} = \frac{1}{m} \sum_{k=0}^{m-1} \alpha_k w^k$

Output $\tilde{w}^T$

Freeze reference point for m iterations

Sebbouh, Gazagnadou, Jelassi, Bach, Gower, 2019

SVRG: Stochastic Variance Reduced Gradients

Jonhson & Zhang, NIPS 2013

Set $w^0 = 0$, choose $\gamma > 0, m \in \mathbb{N}$,

$\alpha_k > 0$ for $k = 0, \ldots, m-1$

$\tilde{w}^0 = w^0$

for $t = 0, 1, 2, \ldots, T-1$

calculate $\nabla f(\tilde{w}^t)$

Freeze reference point for m iterations

for $k = 0, 1, 2, \ldots, m-1$

sample $i \in \{1, \ldots, n\}$

$g^k = \nabla f_i(w^k) - \nabla f_i(\tilde{w}^t) + \nabla f(\tilde{w}^t)$

$w^{k+1} = w^k - \gamma g^k$

$\tilde{w}^{t+1} = \frac{1}{m} \sum_{k=0}^{m-1} \alpha_k w^k$

Weighted average of inner iterates

Output $\tilde{w}^T$

Sebbouh, Gazagnadou, Jelassi, Bach, Gower, 2019

SAGA: Stochastic Average Gradient

Defazio, Bach, & Lacoste-Julien, 2014 NIPs

Single element sampling

$$v_j = \begin{cases} n & j = i \\ 0 & j \neq i \end{cases}$$

$$w^{t+1} = w^t - \gamma_t g_{v^t}(w^t)$$

Sample: $\nabla f_i(w^t), \quad i \in \{1, \ldots, n\}$ uniformly

Grad. estimate:

$$g_{v^t}(w^t) = \nabla f_i(w^t) - \nabla f_i(w^{t_i}) + \frac{1}{n}\sum_{j=1}^{n} \nabla f_j(w^{t_j})$$

Store grad.: $\nabla f_i(w^{t_i}) = \nabla f_i(w^t)$

SAGA: Stochastic Average Gradient

Defazio, Bach, & Lacoste-Julien, 2014 NIPs

Single element sampling

$$v_j = \begin{cases} n & j = i \\ 0 & j \neq i \end{cases}$$

$$w^{t+1} = w^t - \gamma_t g_{v^t}(w^t)$$

Sample

$$\nabla f_i(w^t), \quad i \in \{1, \ldots, n\} \text{ uniformly}$$

Grad. estimate

$$g_{v^t}(w^t) = \nabla f_i(w^t) - \nabla f_i(w^{t_i}) + \frac{1}{n}\sum_{j=1}^{n} \nabla f_j(w^{t_j})$$

$$\nabla z_{v^t}(w^t) = \nabla f_i(w^{t_i})$$

Store grad.

$$\nabla f_i(w^{t_i}) = \nabla f_i(w^t)$$

SAGA: Stochastic Average Gradient

Defazio, Bach, & Lacoste-Julien, 2014 NIPs

$$w^{t+1} = w^t - \gamma_t g_{v^t}(w^t)$$

Single element sampling

$$v_j = \begin{cases} n & j = i \\ 0 & j \neq i \end{cases}$$

Sample $\nabla f_i(w^t), \quad i \in \{1, \ldots, n\}$ uniformly

Grad. estimate

$$g_{v^t}(w^t) = \nabla f_i(w^t) - \nabla f_i(w^{t_i}) + \frac{1}{n}\sum_{j=1}^{n} \nabla f_j(w^{t_j})$$

$$z_{v^t}(w) = f_i(w^{t_i}) + \langle \nabla f_i(w^{t_i}), w - w^{t_i} \rangle \quad \nabla z_{v^t}(w^t) = \nabla f_i(w^{t_i})$$

Store grad. $\nabla f_i(w^{t_i}) = \nabla f_i(w^t)$

SAGA: Stochastic Average Gradient

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Single element sampling

$$v_j = \begin{cases} n & j = i \\ 0 & j \neq i \end{cases}$$

Sample: $\nabla f_i(w^t), \quad i \in \{1, \ldots, n\}$ uniformly

Grad. estimate: $$g_{v^t}(w^t) = \nabla f_i(w^t) - \nabla f_i(w^{t_i}) + \frac{1}{n}\sum_{j=1}^{n} \nabla f_j(w^{t_j})$$

$$z_{v^t}(w) = f_i(w^{t_i}) + \langle \nabla f_i(w^{t_i}), w - w^{t_i} \rangle$$

$\nabla z_{v^t}(w^t) = \nabla f_i(w^{t_i})$

$\mathbb{E}[\nabla z_{v^t}(w^t)]$

Store grad.: $$\nabla f_i(w^{t_i}) = \nabla f_i(w^t)$$

SAGA: Stochastic Average Gradient

Set $w^0 = 0, g_i = \nabla f_i(w^0),$ for $i = 1 \ldots, n$
Choose $\gamma > 0$
for $t = 0, 1, 2, \ldots, T-1$
    sample $i \in \{1, \ldots, n\}$
    $g^t = \nabla f_i(w^t) - g_i + \frac{1}{n}\sum_{j=1}^n g_j$
    $w^{t+1} = w^t - \gamma g^t$
    $g_i = \nabla f_i(w^t)$
Output w^T

No inner loop, rolling update

Stores a $d \times n$ matrix

Additional Experiments

Optimal mini-batch size