Faster Algorithms for Deep Learning?

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Motivation: Faster Deep Learning?

- 2006: PhD student Mark goes to CIFAR "deep learning" workshop.

- People seem very excited about this.
  - But they are using the (slow) "SGD" algorithm from 1952.
  - "*I will have a huge impact if I can develop a faster algorithm*".

Stochastic Gradient Descent (SGD)

- For most ML models, we fit parameters by minimizing an expectation:

$$\min_x \{\mathbb{E}[f(x)]\}$$

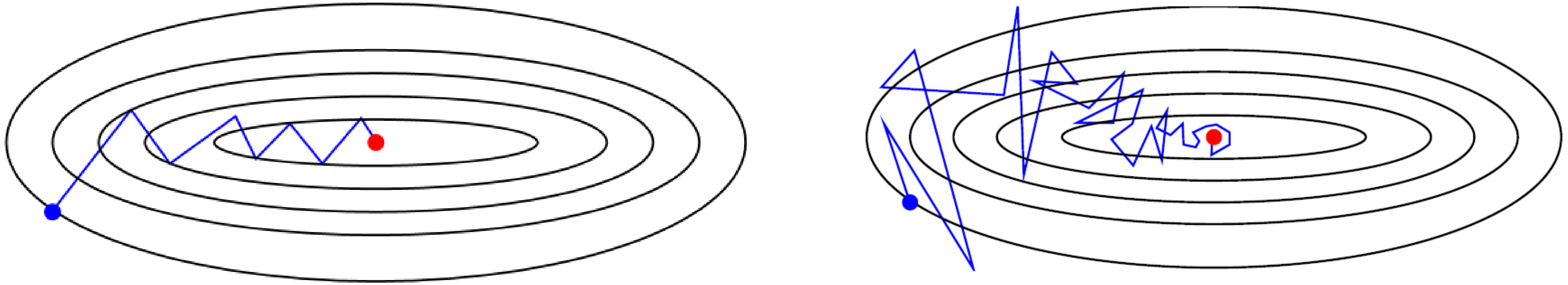
  - Function 'f' measures how well we fit a training example.
  - Fitting a least squares, logistic regression, neural networks, and so on.
- Among most common algorithms is stochastic gradient descent (SGD):

$$x^{k+1} = x^k - \alpha_k g(x^k)$$

  - The iterate x^k is our guess of the parameters on iteration 'k'.
  - The step size α_k is how far we move on iteration 'k'.
  - The direction $g(x_k)$ is an unbiased estimate of the gradient of the expectation.
    - Usually, you get this from taking the gradient of a randomly-chosen example or mini-batch.

Stochastic Gradient Descent (SGD)

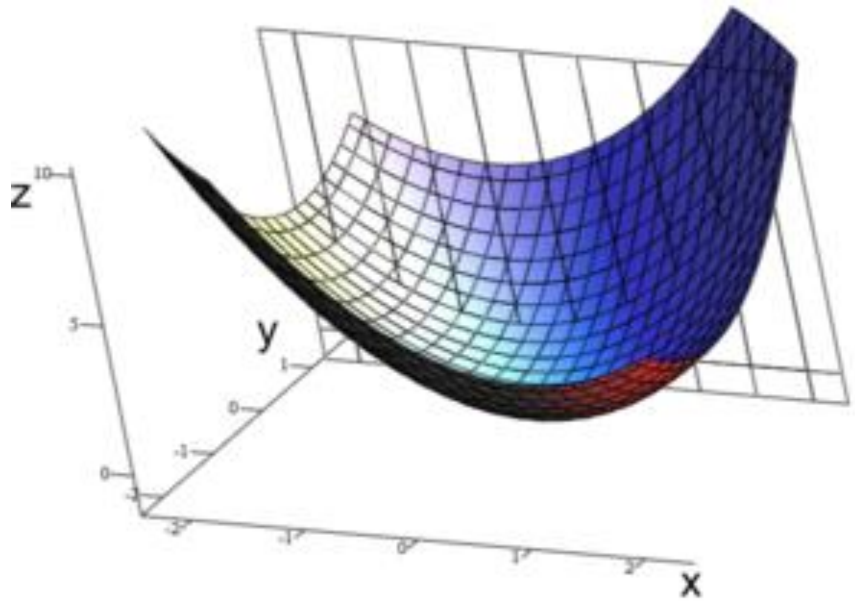
- Deterministic gradient descent vs. stochastic gradient descent:



- Advantage of SGD: iteration cost of O(1) in number of examples.
  - If you have one billion examples, it's 1 billion times faster than gradient descent.
  - Variations of it (often) work for training deep neural networks.
- Disadvantages due to the variance in the gradient approximation:
  - May need a huge number of iterations.
  - May be sensitive to the exact choice of step size.
  - Not obvious when to stop.

Digression: Convex Functions

- Classic work on this problem focuses on convex functions:
  - Where local optima are global optima.



- The (possibly-flawed) reasoning for focusing on convex objectives:
  - It's easier to prove things!
  - *"If it doesn't work for convex, it won't work for non-convex."*
  - Deep learning objectives are convex near solutions.
  - We did not have ways to analyze SGD for non-convex functions at the time.

Impossibility of Faster Methods

- How many iterations of SGD do we need to minimize a convex function?

- Convergence rate result from (basically) the 1950s:
  - Assume function is "strongly-smooth and strongly-convex".
  - Assume variance of the gradient estimates is bounded.
  - To reach an accuracy of ε, SGD needs O(1/ε) iterations.

- Deterministic gradient descent only needs O(log(1/ε)).
  - "Exponential" vs. "polynomial" number of iterations.

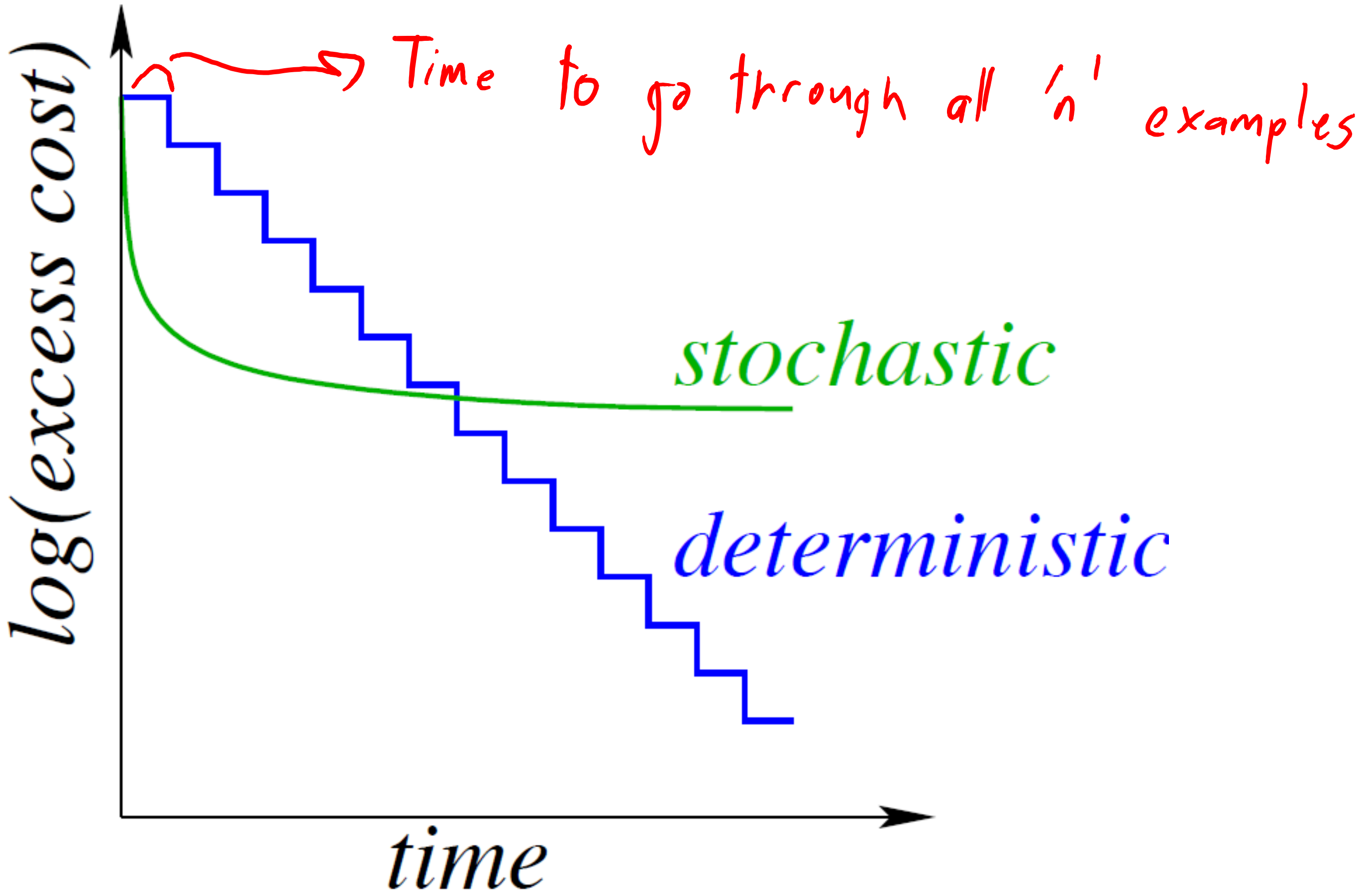
- No method based on unbiased gradients can be faster than O(1/ε).
  - Even if you have a one-dimensional problem (under the assumptions above).
  - Second-derivatives or "acceleration" do not help (no faster "stochastic Newton").
    - The lower bound comes from the variance, not the "condition number".

The Assumptions

- In order to go faster than $O(1/\varepsilon)$, we need stronger assumptions.
  - Otherwise, the lower bound says it's impossible.

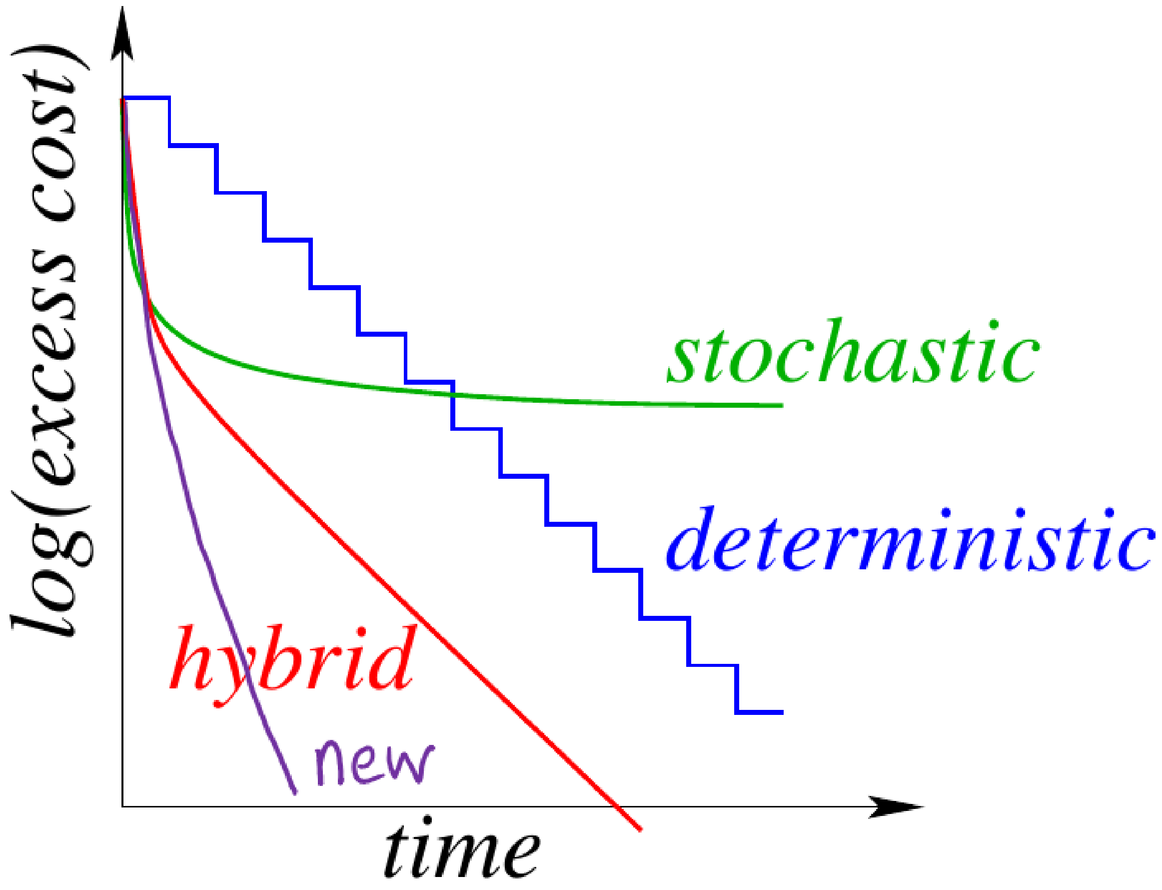
- We explored two possible stronger assumptions to get $O(\log(1/\varepsilon))$:
  1. Assume you only have a finite training set.
     - Usually don't have infinite data, so design an algorithm that exploits this.
  2. Cheat by finding stronger assumptions where plain SGD would go fast.
     - Could explain practical success, and might suggest new methods.

Finite Data Assumption: Deterministic vs. Stochastic



- Gradient descent makes consistent progress with slow iterations.
- Stochastic gradient has fast iterations but decreasing progress.

Finite Data Assumption: Deterministic vs. Stochastic



- You can design hybrids (initialize with SGD, or increase batch sizes).
- Variance reduction methods can be even faster than hybrids.

Variance-Reduction: SAG and SVRG

- Variance reduction methods for finite training sets:
  - Method with cost of stochastic gradient, progress of full gradient.
    - $O(\log(1/\varepsilon))$ iterations to reach accuracy ε with $O(1)$ iteration cost.
  - Key idea: design an estimator of the gradient whose variance goes to zero.

- First general method in 2012: stochastic average gradient (SAG).
  - Keeps a memory of previous gradient value for each example.

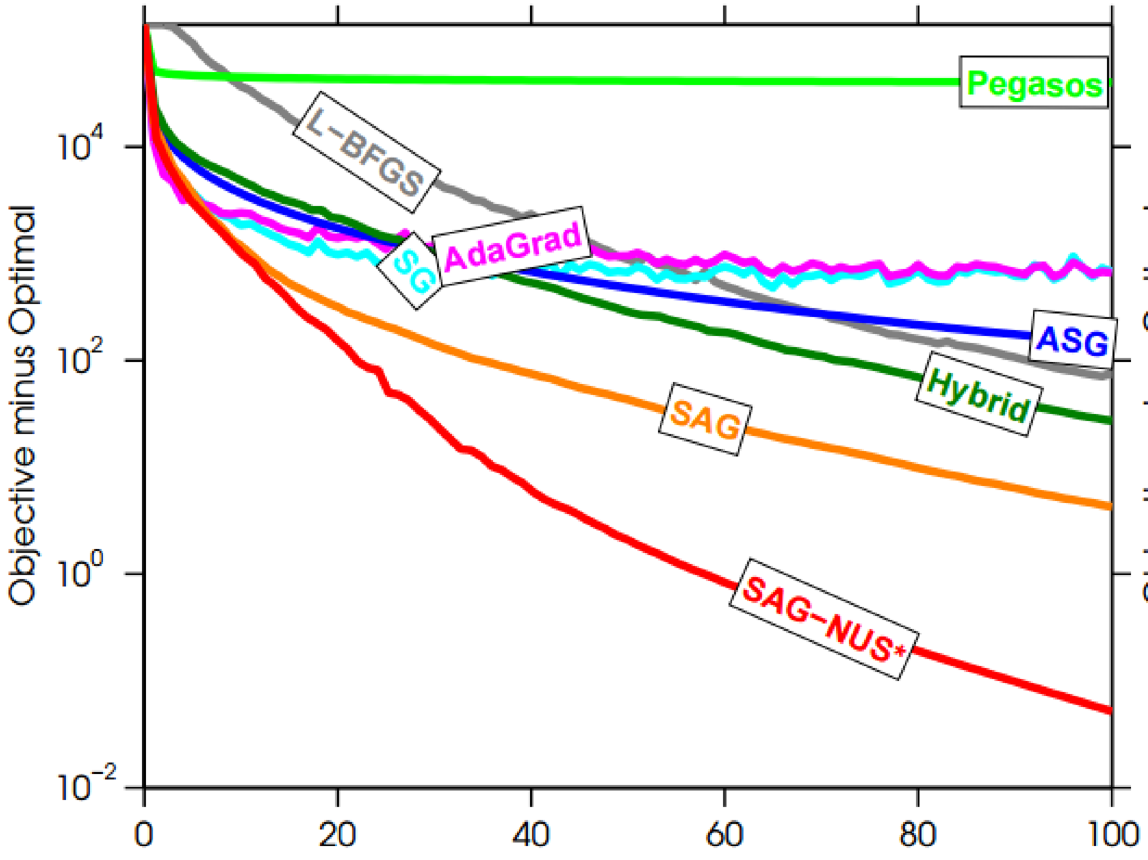
- Memory-free method: stochastic variance-reduced gradient (SVRG):

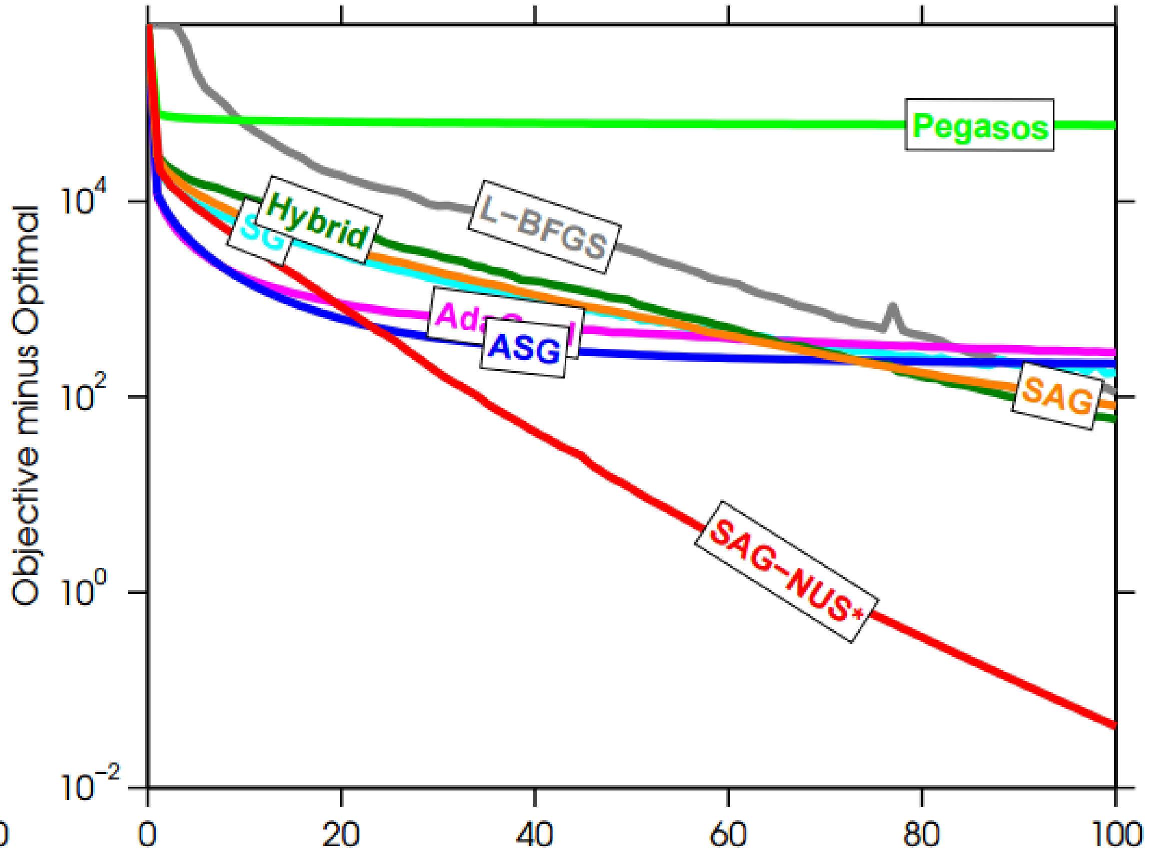
$$x^{k+1} = \underbrace{x^k - \alpha_k(\nabla f_i(x^k)}_{\text{regular SGD}} \underbrace{- \nabla f_i(\tilde{x}^k) + \nabla f(\tilde{x}^k))}_{\text{"control variate" (mean of 0)}}$$

  - The reference point $\tilde{x}_k$ is typically updated every $O(n)$ iterations.

Variance-Reduction: Practical Performance

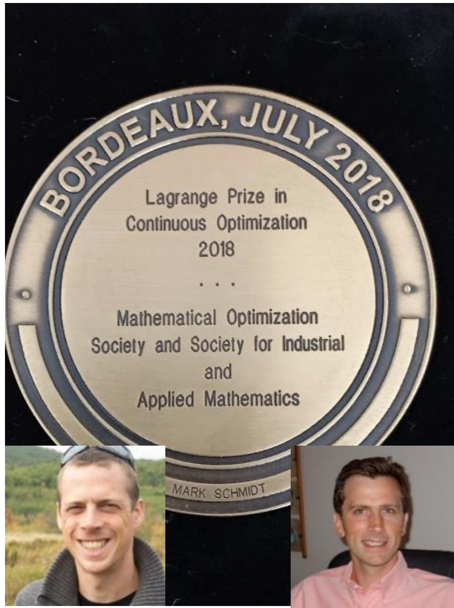
- Variance reduction has led to faster methods in many settings:
  - Least squares, logistic regression, PCA, cryo-EM, conditional random fields, and so on.





Variance Reduction: 8 Years Later.

- Variance reduction has been taken in a wide variety of directions:
  - Memory-free SAG in some settings (like linear and graphical models).
  - Variants giving faster algorithms for some non-smooth problems.
  - Variants giving faster algorithms for some non-convex problems.
    - Including PCA and problems satisfying the "PL inequality".
  - Momentum-like variants that achieve acceleration.
  - Improved test error bounds compared to SGD.
  - Parallel and distributed versions.
  - SAG won 2018 "Lagrange Prize in Continuous Optimization".
  - Does not seem to help with deep learning.



Back to the Assumptions

- In order to go faster than $O(1/\varepsilon)$, we need stronger assumptions.

- We explored two possible stronger assumptions to go faster:
  1. Assume you only have a finite training set (SAG and SVRG).
     - Successful for a lot of problems, but not for deep learning.

  2. Cheat by finding stronger assumptions where plain SGD would go fast.
     - Could explain practical success, and might suggest new methods.

Strong Growth Condition (SGC)

- What conditions would we need for plain SGD to converge fast?
- Consider the strong growth condition (SGC):

$$\mathbb{E}[\|g(x^k)\|^2] \leq \rho \|\nabla f(x^k)\|^2$$

  – Used by Tseng and Solodov in the 90s to analyze SGD on neural networks.
    - Under SGC, they showed that SGD converges with a constant step size.
    - This is possible because it implies variance goes to zero at a solution.

- The SGC is a very-strong assumption:
  – Assumes that gradient is zero at the solution for every training example:

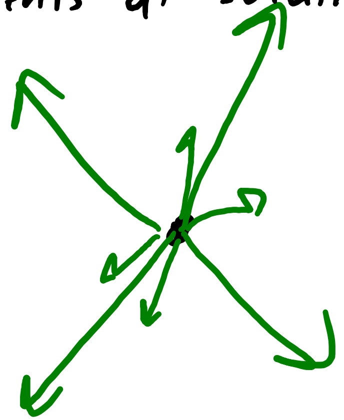
$$\nabla f(x^k) = 0 \Rightarrow \text{every } g(x^k) = 0$$

  – Model is complicated enough to "interpolate" (fit exactly) the data.

Strong Growth Condition (SGC)

- Interpolation changes behaviour of gradients at solution:

Gradients at solution (bounded variance)



point in different directions to cancel out

Gradient at solution (SGC)

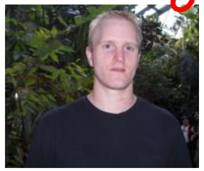
} all zero → no variance

- Under SGC, don't need step size to go to zero to counter variance.

Strong Growth Condition (SGC)

- SGD with constant step-size under SGC requires O(log(1/eps)) iterations.
  - In this setting there is no need to use variance reduction (it would be slower).
  - 2013: we wrote a 5-page paper showing this in 1 day and put in on arXiv.

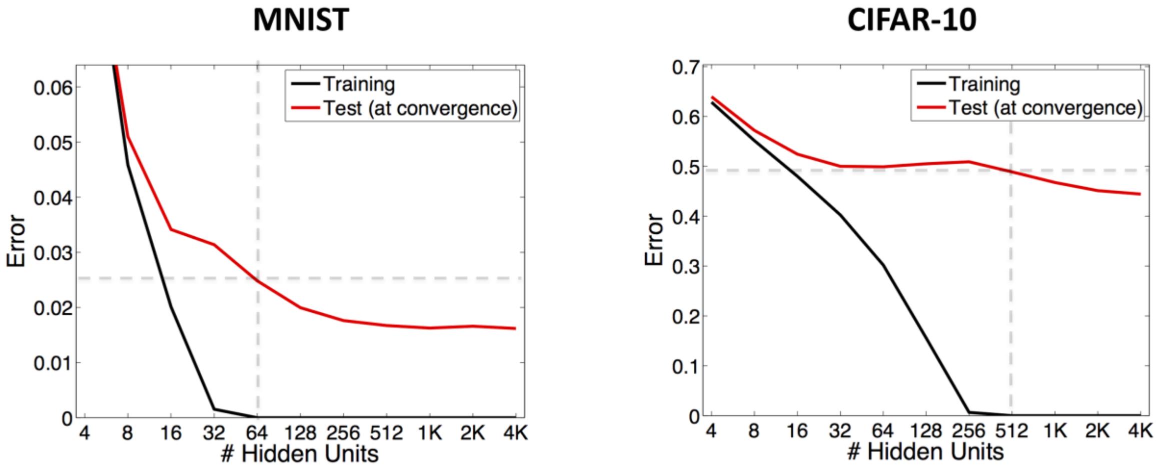
  - Moved on with life, *"this assumption is clearly ridiculous"*.



  - You would probably excessively overfit if this was true anyways?

Interpolation and Deep Learning?

- 2014: Adam optimizer.
  - Became wildly-popular for training deep models.
    - Poor performance for optimizing some convex functions.
    - ??????????!!!!!??????????????????????!!!!!!?????????????!!!!???????
- Several groups observed that deep networks can drive error to 0.



  - Without excessive overfitting.
  - Maybe interpolation isn’t such a ridiculous assumption?

https://www.neyshabur.net/papers/inductive_bias_poster.pdf

Over-Parameterization and Interpolation

- Ma, Bassily, and Belkin [ICML, 2018]:
  - Show that SGD under interpolation has linear convergence rate.
  - Provided theoretical justification (and limits) for "linear scaling rule".
  - Discussed connection between interpolation and over-parameterization.

- "Over-parameterization":
  - You have so many parameters that you can drive the loss to 0.
  - True for many modern deep neural networks.
  - Also true for linear models with a sufficiently-expressive basis.
    - You can make it true by making model more complicated (more features = fast SGD).
    - Several groups explored implicit regularization of SGD (may not ridiculously ovefit).

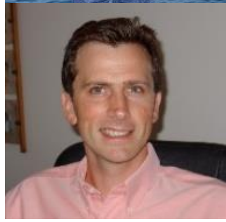
Back to the SGC?

- Connection to 2013: assumptions of Ma et al. imply the SGC.
  - Maybe the SGC assumption is relevant in applications?

- Does SGC/interpolation explain SGD behaviour for deep learning?
  - Would explain why variance reduction does not help.
  - Would explain success of Adam and constant step size regimes.

- Suggests opportunities to develop better deep learning algorithms.
  - We have "fast", "faster", "painless", and "furious" algorithms under SGC.

“Fast” SGD under the SGC (AI/Stats 2019)



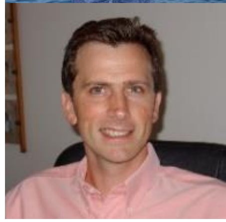
- Previous analyses under the SGC assumed convexity.
- We showed the following non-convex result for plain-old SGD:

Theorem 3 (Non-Convex). *Under L-smoothness, if f satisfies SGC with constant ρ, then SGD with a constant step-size $\eta = \frac{1}{\rho L}$ attains the following convergence rate:*

$$\min_{i=0,1,\ldots k-1} \mathbb{E}\left[\|\nabla f(w_i)\|^2\right] \leq \left(\frac{2\rho L}{k}\right)[f(w_0) - f^*].$$

  - We analyze norm of gradient due to non-convexity.
- This is faster than all previous general non-convex stochastic results.
  - Even for fancier methods.
  - Gives justification for things like constant step-size regimes and Adam.
  - Bassily et al. [2018] later gave a result under “PL inequality”.
    - Much faster but this assumption is much stronger (implies all minima are global minima).

"Faster" SGD under the SGC (AI/Stats 2019)

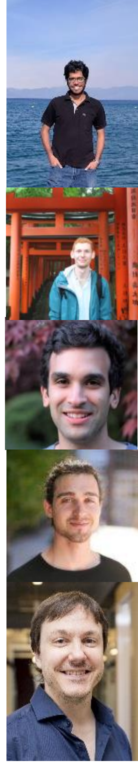


- Sutskever, Martens, Dahl, Hinton [2013]:
  - Nesterov acceleration improves practical performance in some settings.
  - Acceleration is closely-related to momentum, which also helps in practice.
- Existing stochastic analyses only achieved partial acceleration.

Method	Regular	Accelerated	Comment
Deterministic	$\tilde{O}(n\kappa)$	$\tilde{O}(n\sqrt{\kappa})$	Unconditional acceleration
SGD + (var < σ^2)	$O\left(\frac{\sigma^2}{\epsilon}+\frac{\kappa}{\epsilon}\right)$	$O\left(\frac{\sigma^2}{\epsilon}+\sqrt{\frac{\kappa}{\epsilon}}\right)$	Faster if $\kappa > \sigma^2$
Variance Reduction	$\tilde{O}(n+\kappa)$	$\tilde{O}(n+\sqrt{n\kappa})$	Faster if $\kappa > n$
SGC + SGC	$\tilde{O}(\kappa)$	$\tilde{O}(\sqrt{\kappa})$	Unconditional acceleration

- Under SGC we show full acceleration (convex, appropriate parameters).
  - Special cases also shown by Liu and Belkin [2018], Jain et al. [2018]

“Painless” SGD under the SGC (NeurIPS 2019)



- Previous SGC/interpolation results relied on particular step-sizes.
  - Depending on values we don’t know, like eigenvalues of Hessian.
- Existing methods to set step-size don’t guarantee fast convergence.
  - Meta-learning, heuristics, adaptive, online learning, prob line-search.
- Under SGC, we showed you can can set the step-size as you go.
- Achieved (basically) optimal rate in a variety of settings:

Theorem 1 (Strongly-Convex). *Assuming interpolation, L-smoothness and μ strong-convexity of f, and convexity of the f_i, SGD with Armijo line-search with $c = 1/2$ in Equation 1 achieves the rate:*

$$\mathbb{E}\left[\|w_T - w^*\|^2\right] \leq \left(\max\left\{\left(1 - \frac{\mu}{L}\right), (1 - \eta_{max}\,\mu)\right\}\right)^T \|w_0 - w^*\|^2 .$$

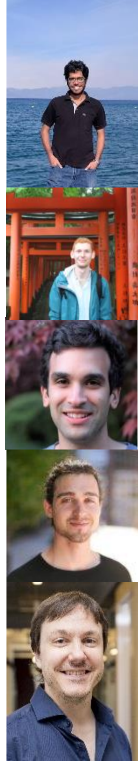
Theorem 2 (Convex). *Assuming interpolation and under L_i-smoothness and convexity of f_i's, SGD with Armijo line-search for all $c \geq 1/2$ in Equation 1 and iterate averaging achieves the rate:*

$$\mathbb{E}\left[f(\bar{w}_T) - f(w^*)\right] \leq \frac{c \cdot \max\left\{\frac{L_{max}}{2\,(1-c)}, \frac{1}{\eta_{max}}\right\}}{(2c-1)\,T} \|w_0 - w^*\|^2 .$$

Theorem 3 (Non-Convex). *Assuming the SGC with constant ρ and under L_i-smoothness of f_i's, SGD with Armijo line-search in Equation 1 with $c = \rho\, L_{max}$ and setting $\eta_{max} = 1$ achieves the rate:*

$$\min_{k=0,\ldots,T-1} \mathbb{E}\,\|\nabla f(w_k)\|^2 \leq \frac{\max\left\{\frac{L_{max}}{1-\rho\, L_{max}}, 2\right\} + 1}{T} \left[f(w_0) - f^*\right] .$$

“Painless” SGD under the SGC (NeurIPS 2019)



- Key idea: Armijo line-search on the batch.
  - “Backtrack if you don’t improve cost on the batch relative to the norm of the batch’s gradient.”

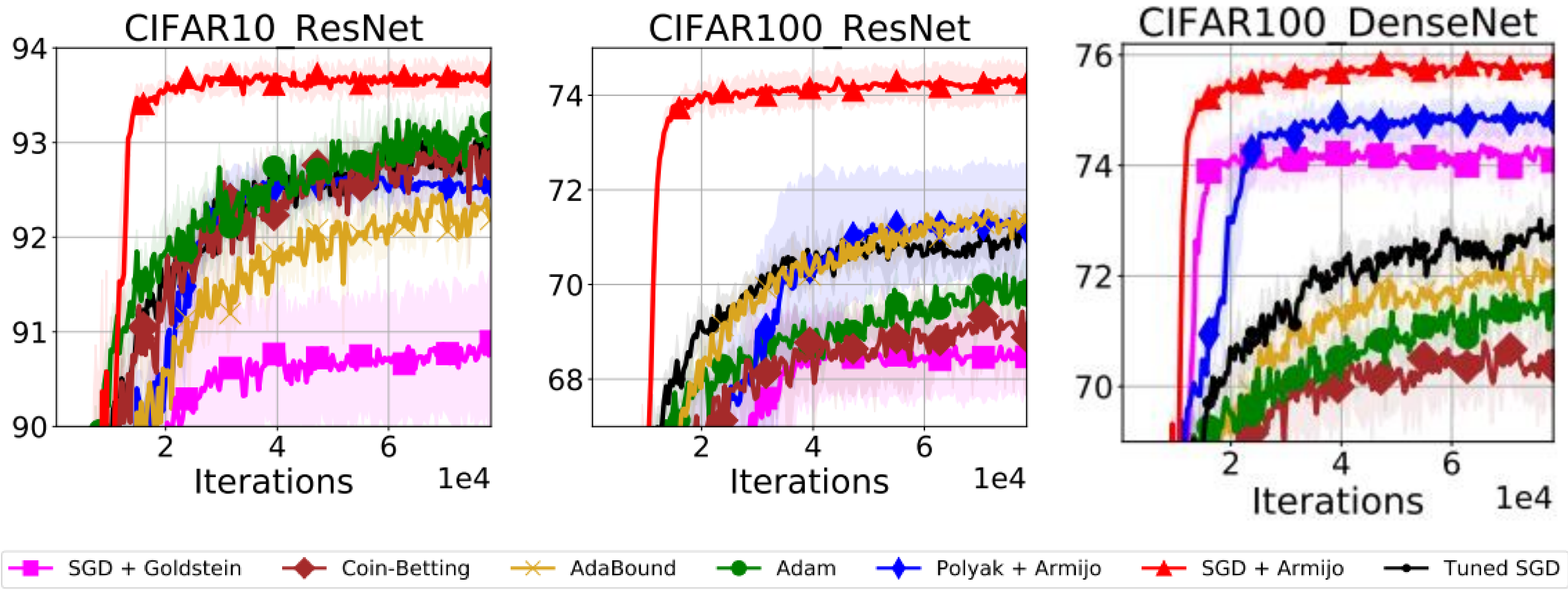
Algorithm 1 SGD+Armijo($f, w_0, \eta_{\max}, b, c, \beta, \gamma$, opt)

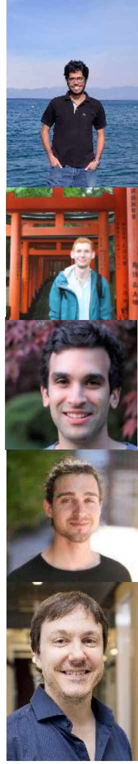
for $k = 1, \dots, T$ **do**
  $i_k \leftarrow$ sample mini-batch of size b
  $\eta \leftarrow \texttt{reset}(\eta, \eta_{\max}, \gamma, b, k, \texttt{opt})/\beta$
  repeat
    $\eta \leftarrow \beta \cdot \eta$
    $w'_k \leftarrow w_k - \eta \nabla f_{ik}(w_k)$
  until $f_{ik}(w'_k) \le f_{ik}(w_k) - c \cdot \eta \left\|\nabla f_{ik}(w_k)\right\|^2$
  $w_{k+1} \leftarrow w'_k$
end for
return w_{k+1}

- Backtracking guarantees steps are “not too big”.
- With appropriate initialization, guarantees steps are “not too small”.
  - Theory says that it’s at least as good as the best constant step-size.
- Requires an extra forward pass per iteration, and forward pass for each backtrack.
- We proposed a procedure to propose trial step sizes that works well in practice:
  - Slowly increases the step size, but median number of backtracking steps per iteration is 0.

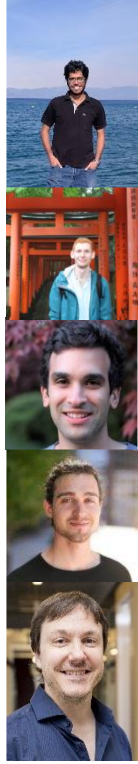
"Painless" SGD under the SGC (NeurIPS 2019)

- We did a variety of experiments, including training CNNs on standard problems.
  - Better in practice than any fixed step size, adaptive methods, alternative adaptive step sizes.





Discussion: Sensitivity to Assumptions



- To ease some of your anxiety/skepticism:
  - You don't need to run it to the point of interpolating the data, it just needs to be possible.
  - Results can be modified to handle case of being "close" to interpolation.
    - You get an extra term depending on your step-size and how "close" you are.
  - We ran synthetic experiments where we controlled the degree of over-parameterization:
    - If it's over-parameterized, the stochastic line search works great.
    - If it's close to being over-parameterized, it still works really well.
    - If it's far from being over-parameterized, it catastrophically fails.
  - Another group [Berrada, Zisserman, Pawan Kumar] proposed a similar method a few days later.
  - We've compared to a wide variety of existing methods to set the step size.

- To add some anxiety/skepticism:
  - My students said all the neural network experiments were done with batch norm.
  - They had more difficulty getting it to work for LSTMs ("first thing we tried" didn't work here).
  - Some of the line-search results have extra "sneaky" assumptions I would like to remove.

“Furious” SGD under the SGC (AI/Stats 2020)




- The reason “stochastic Newton” can’t improve rate is the variance.
- SGC gets rid of the variance, so stochastic Newton makes sense.
- Under SGC:
  - Stochastic Newton gets “linear” convergence with constant batch size.
    - Previous works required fininte-sum assumption or exponentially-growing batch size.
  - Stochastic Newton gets “quadratic” with exponentially-growing batch.
    - Previous works required faster-than-exponential growing batch size for “superlinear”.

- The paper gives a variety of other results and experiments.
  - Self-concordant analysis, L-BFGS analysis, Hessian-free implementation.

Take-Home Messages

- For under-parameterized models, use variance reduction.
- For over-parameterized models, don’t use variance reduction.

- New algorithms and/or analyses for over-parameterized models:
  - “Fast” non-convex convergence rates for plain SGD.
  - “Faster” SGD using acceleration.
  - “Painless” SGD using line-search.
  - “Furious” SGD using second-order information.

- Try out the line-search, we want to make it a black box code.
  - It will helpful to know cases where it does and doesn’t work.
- Variance-reduction might still be relevant for deep learning:
  - Reducing Noise in GAN Training with Variance Reduced Extragradient. T. Chavdarova, G. Gidel, F. Fleuret, S. Lacoste-Julien [NeurIPS, 2019].