

Secant Method: Scalar Case

Finding a root of $r : \mathbb{R} \rightarrow \mathbb{R}$, i.e., find x^* for which $r(x^*) = 0$:

Approximate the derivative: $r'(x^{(k)}) \approx \frac{r(x^{(k)}) - r(x^{(k-1)})}{x^{(k)} - x^{(k-1)}}$

$$x^{(k+1)} = x^{(k)} - \left(\frac{x^{(k)} - x^{(k-1)}}{r(x^{(k)}) - r(x^{(k-1)})} \right) r(x^{(k)}).$$

Local convergence rate is

$$\left| x^{(k+1)} - x^* \right| \leq C \left| x^{(k)} - x^* \right|^{\overbrace{\frac{1 + \sqrt{5}}{2}}^{\text{"Golden Ratio"}}}.$$

In contrast, rate of convergence of Newton is **quadratic**!



L-BFGS [Moritz et al., 2015]

- Combine the ideas of [Byrd et al., 2014] with variance reduction of [Johnson and Zhang, 2013]
 - **Recall SVRG:** For s and k , inner and outer iteration counters, respectively, estimate the gradient as

$$\mathbf{g}^{(s)} = \left(\nabla f_j(\mathbf{x}^{(s)}) - \nabla f_j(\mathbf{x}^{(k)}) + \nabla F(\mathbf{x}^{(k)}) \right)$$

- No need to diminish step-size any more!
- Under strong convexity:

$$\mathbb{E}(f(\mathbf{x}^{(k)}) - f(\mathbf{x}^*)) \leq \rho^k \mathbb{E}(f(\mathbf{x}^{(0)}) - f(\mathbf{x}^*)), \quad \rho < 1$$

- As in SVRG, convergence is with respect to the outer iterations

L-BFGS [Berahas et al., 2016, Berahas and Takáč, 2017]

- **Idea:** Perform QN update on **overlapping** consecutive batches
- Idea: $\mathcal{T}_k = \mathcal{S}_k \cap \mathcal{S}_{k+1} \neq \emptyset$
- $\mathbf{y}_k = \nabla f_{\mathcal{O}_k}(\mathbf{x}^{(k+1)}) - \nabla f_{\mathcal{O}_k}(\mathbf{x}^{(k)})$
- Using constant step-size α

- **Strongly convex:**

$$\mathbb{E}(f(\mathbf{x}^{(k)}) - f(\mathbf{x}^*)) \leq \rho^k \left(f(\mathbf{x}^{(0)}) - f(\mathbf{x}^*) \right) + \mathcal{O}(\alpha)$$

- **Non-convex:** Skip updating $\mathbf{H}^{(k)}$ if $\mathbf{y}_k^T \mathbf{s}_k \leq \epsilon \|\mathbf{s}_k\|^2$

$$\mathbb{E} \left(\frac{1}{T} \sum_{k=0}^{T-1} \left\| \nabla f(\mathbf{x}^{(k)}) \right\|^2 \right) \leq \mathcal{O} \left(\frac{1}{T\alpha} \right) + \mathcal{O}(\alpha)$$

$$\text{If } \alpha \leq \mathcal{O}(1/\sqrt{T}) \implies \min_{k \leq T-1} \mathbb{E} \left\| \nabla f(\mathbf{x}^{(k)}) \right\|^2 \leq \mathcal{O} \sqrt{\frac{1}{T}}$$

Gauss-Newton

Let $\mathbf{J}_h : \mathcal{R}^d \rightarrow \mathcal{R}^p$ be the Jacobian of \mathbf{h} , i.e., $\mathbf{J}_h(\mathbf{x}) \in \mathcal{R}^{p \times d}$.

$$\nabla F(\mathbf{x}) = \mathbf{J}_h^T(\mathbf{x}) \nabla f(\mathbf{h}(\mathbf{x}))$$

$$\nabla^2 F(\mathbf{x}) = \mathbf{J}_h^T(\mathbf{x}) \nabla^2 f(\mathbf{h}(\mathbf{x})) \mathbf{J}_h(\mathbf{x}) + \partial^2 \mathbf{h}(\mathbf{x}) \nabla f(\mathbf{h}(\mathbf{x}))$$

(Generalized) Gauss-Newton Matrix:

$$\nabla^2 F(\mathbf{x}) \approx \underbrace{\mathbf{J}_h^T(\mathbf{x}) \nabla^2 f(\mathbf{h}(\mathbf{x})) \mathbf{J}_h(\mathbf{x})}_{\mathbf{G}(\mathbf{x}) \triangleq \text{Gauss-Newton Matrix}} \succeq 0$$

(Generalized) Gauss-Newton Update:

$$\mathbf{G}(\mathbf{x}^{(k)}) \mathbf{p} \approx -\nabla F(\mathbf{x}^{(k)})$$

Gauss-Newton

(Generalized) Gauss-Newton Matrix

$$\nabla^2 F(\mathbf{x}) \approx \mathbf{J}_h^T(\mathbf{x}) \nabla^2 f(\mathbf{h}(\mathbf{x})) \mathbf{J}_h(\mathbf{x})$$

Properties:

- $\mathbf{G}(\mathbf{x}) \succeq 0, \forall \mathbf{x}$
- In some applications, after computing $\nabla F(\mathbf{x}) = \mathbf{J}_h^T(\mathbf{x}) \nabla f(\mathbf{h}(\mathbf{x}))$, the approximation $\mathbf{G}(\mathbf{x})$ does not involve any additional derivative evaluations
- $\mathbf{G}(\mathbf{x})$ is a good approximation if $\|\partial^2 \mathbf{h}(\mathbf{x}) \nabla f(\mathbf{h}(\mathbf{x}))\|$ is small, i.e.,
 - $\|\nabla f(\mathbf{h}(\mathbf{x}))\|$ is small, or
 - $\|\partial^2 \mathbf{h}(\mathbf{x})\|$ is small, i.e., \mathbf{h} is nearly affine

Gauss-Newton

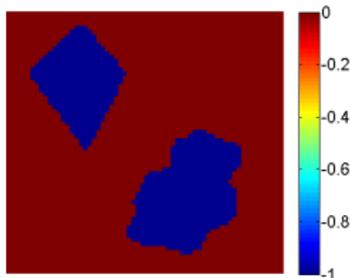
Finite-Sum Problem

$$\min_{\mathbf{x} \in \mathcal{R}^d} F(\mathbf{x}) = \sum_{i=1}^n f_i(\mathbf{h}_i(\mathbf{x}))$$

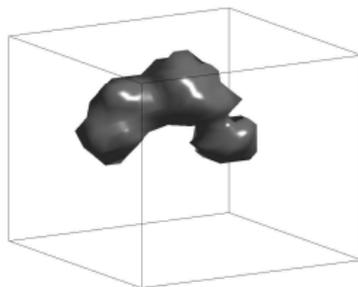
- Machine Learning (e.g., deep/recurrent/reinforcement learning): [Martens, 2010, Martens and Sutskever, 2011, Chapelle and Erhan, 2011, Wu et al., 2017, Botev et al., 2017]... more on this later
- Scientific Computing (e.g., PDE inverse-problems): [Doel and Ascher, 2012, Roosta et al., 2014b, Roosta et al., 2014a, Roosta et al., 2015, Haber et al., 2000, Haber et al., 2012]

PDE Inverse Problems with Many R.H.S

$$\left. \begin{aligned} \nabla \cdot (\mathbf{x}(\mathbf{z}) \nabla u_i(\mathbf{z})) &= q_i(\mathbf{z}), & \mathbf{z} \in \Omega \\ \frac{\partial u_i(\mathbf{z})}{\partial \nu} &= 0, & \mathbf{z} \in \partial\Omega \end{aligned} \right\}, i = 1, \dots, n, \Omega \subset \mathcal{R}^2 \text{ or } \mathcal{R}^3$$



(a) True x : 2D



(b) True x : 3D

A remedy: SAA

$$\mathcal{S} \subset [n] \ \& \ |\mathcal{S}| = s$$

↓

$$F(\mathbf{x}) \approx \hat{F}_s(\mathbf{x}) = \frac{1}{|\mathcal{S}|} \sum_{i \in \mathcal{S}} \|\boldsymbol{\Sigma}_i^{-\frac{1}{2}} (\mathbf{P}_i \mathbf{A}^{-1}(\mathbf{x}) \mathbf{q}_i - \mathbf{v}_i)\|_2^2$$

Trace estimation: [Roosta and Ascher, 2015, Roosta et al., 2015]

Find s such that, for a given ϵ and δ , we get

$$\Pr \left(|\hat{F}_s(\mathbf{x}) - F(\mathbf{x})| \leq \epsilon F(\mathbf{x}) \right) \geq 1 - \delta$$

Natural Gradient

Cross Entropy Minimization

For $p_{\mathbf{x}}(\mathbf{z})$, a density parametrized by \mathbf{x} , the **cross-entropy minimization** with respect to a target density, $p_{\mathbf{x}}(\mathbf{z})$, is

$$\min_{\mathbf{x} \in \mathcal{X}} \mathcal{L}(\mathbf{x}) = -\mathbb{E}_{\mathbf{z}} (\log p_{\mathbf{x}}(\mathbf{z})) = - \int p_{\mathbf{x}}(\mathbf{z}) \log p_{\mathbf{x}}(\mathbf{z}) \, d\mu(\mathbf{z}).$$

NB: $p_{\mathbf{x}}(\mathbf{z})d\mu(\mathbf{z})$ can be the empirical measure over the training data.

Fisher Information Matrix

Suppose $\mathbf{z} \sim p_{\mathbf{x}}$. Under some weak regularity assumptions:

$$\mathbf{F}(\mathbf{x}) \triangleq \mathbb{E}_{\mathbf{z}} \left(\nabla \log p_{\mathbf{x}}(\mathbf{z}) (\nabla \log p_{\mathbf{x}}(\mathbf{z}))^T \right) = -\mathbb{E}_{\mathbf{z}} \left(\nabla^2 \log p_{\mathbf{x}}(\mathbf{z}) \right).$$

Natural Gradient Descent

$$\mathbf{F}(\mathbf{x}^{(k)})\mathbf{p}^{(k)} \approx \mathbf{g}^{(k)} \implies \mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)}\mathbf{p}^{(k)}$$

Natural Gradient

Interpretation III:

KullbackLeibler distance

For given \mathbf{x} and \mathbf{x} , the Kullback-Leibler distance from $p_{\mathbf{x}}$ to $p_{\mathbf{x}}$ is

$$\mathbf{KL}(\mathbf{x} \parallel \mathbf{x}) \triangleq \mathbb{E}_{\mathbf{x}} \left(\log \frac{p_{\mathbf{x}}(\mathbf{z})}{p_{\mathbf{x}}(\mathbf{z})} \right) = \int \left(\log \frac{p_{\mathbf{x}}(\mathbf{z})}{p_{\mathbf{x}}(\mathbf{z})} \right) p_{\mathbf{x}}(\mathbf{z}) \, d\mu(\mathbf{z}).$$

$$\mathbf{F}(\mathbf{x}) = \nabla_{\mathbf{x}}^2 \mathbf{KL}(\mathbf{x} \parallel \mathbf{x})|_{\mathbf{x}=\mathbf{x}}$$

If $\mathbf{F}(\mathbf{x}) \succ 0$, then in a neighborhood of \mathbf{x} , we have $\mathbf{KL}(\mathbf{x} \parallel \mathbf{x}) > 0$, and

$$\mathbf{KL}(\mathbf{x} \parallel \mathbf{x}) \approx \frac{1}{2} (\mathbf{x} - \mathbf{x})^2 \mathbf{F}(\mathbf{x}) (\mathbf{x} - \mathbf{x})$$



- **Trust Region:** [Sorensen, 1982, Conn et al., 2000]

$$\mathbf{s}^{(k)} = \arg \min_{\|\mathbf{s}\| \leq \Delta_k} \left\langle \mathbf{s}, \nabla F(\mathbf{x}^{(k)}) \right\rangle + \frac{1}{2} \left\langle \mathbf{s}, \nabla^2 F(\mathbf{x}^{(k)}) \mathbf{s} \right\rangle$$

- **Cubic Regularization:** [Griewank, 1981, Nesterov et al., 2006, Cartis et al., 2011a, Cartis et al., 2011b]

$$\mathbf{s}^{(k)} = \arg \min_{\mathbf{s} \in \mathbb{R}^d} \left\langle \mathbf{s}, \nabla F(\mathbf{x}^{(k)}) \right\rangle + \frac{1}{2} \left\langle \mathbf{s}, \nabla^2 F(\mathbf{x}^{(k)}) \mathbf{s} \right\rangle + \frac{\sigma_k}{3} \|\mathbf{s}\|^3$$



- Trust Region:

$$\mathbf{s}^{(k)} = \arg \min_{\|\mathbf{s}\| \leq \Delta_k} \left\langle \mathbf{s}, \nabla F(\mathbf{x}^{(k)}) \right\rangle + \frac{1}{2} \left\langle \mathbf{s}, \mathbf{H}^{(k)} \mathbf{s} \right\rangle$$

- Cubic Regularization:

$$\mathbf{s}^{(k)} = \arg \min_{\mathbf{s} \in \mathbb{R}^d} \left\langle \mathbf{s}, \nabla F(\mathbf{x}^{(k)}) \right\rangle + \frac{1}{2} \left\langle \mathbf{s}, \mathbf{H}^{(k)} \mathbf{s} \right\rangle + \frac{\sigma_k}{3} \|\mathbf{s}\|^3$$



$$\|H(\mathbf{x}) - \nabla^2 F(\mathbf{x})\| \leq \epsilon \quad \implies \quad \|(H(\mathbf{x}) - \nabla^2 F(\mathbf{x})) \mathbf{s}\| \leq \epsilon \|\mathbf{s}\|$$

$$H(\mathbf{x}) = \frac{1}{|\mathcal{S}|} \sum_{j \in \mathcal{S}} \nabla^2 f_j(\mathbf{x})$$



Lemma (Uniform Sampling [Xu et al., 2017])

Suppose $\|\nabla^2 f_i(\mathbf{x})\| \leq K_i$, $i = 1, 2, \dots, n$. Let $K = \max_{i=1, \dots, n} K_i$.

Given any $0 < \epsilon < 1$, $0 < \delta < 1$, and $\mathbf{x} \in \mathbb{R}^d$, if

$$|\mathcal{S}| \geq \frac{16K^2}{\epsilon^2} \log \frac{2d}{\delta},$$

then for

$$H(\mathbf{x}) = \frac{1}{|\mathcal{S}|} \sum_{j \in \mathcal{S}} \nabla^2 f_j(\mathbf{x}),$$

we have

$$\Pr\left(\|H(\mathbf{x}) - \nabla^2 F(\mathbf{x})\| \leq \epsilon\right) \geq 1 - \delta.$$

- Only **top** eigenvalues/eigenvectors need to be preserved.



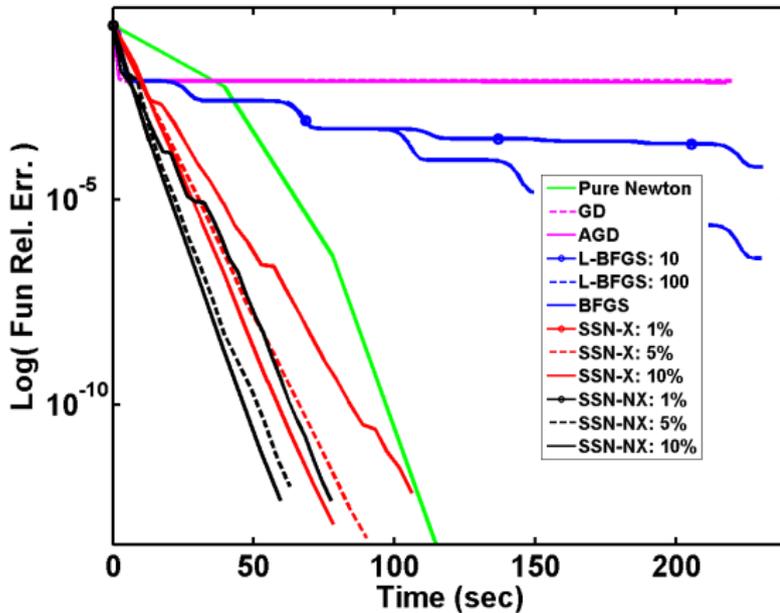
$$\frac{1}{n} \sum_{i=1}^n K_i \leq \max_{i=1, \dots, n} K_i$$



- For $\epsilon_H^2 = \epsilon_g = \epsilon$
 - Stochastic TR: $T \in \mathcal{O}(\epsilon^{-2.5})$
 - Stochastic ARC: $T \in \mathcal{O}(\epsilon^{-1.5})$



D_2 , $n = 5 \times 10^4$, $p = 5 \times 10^3$, sparsity : Dense, $\kappa \approx 10^6$

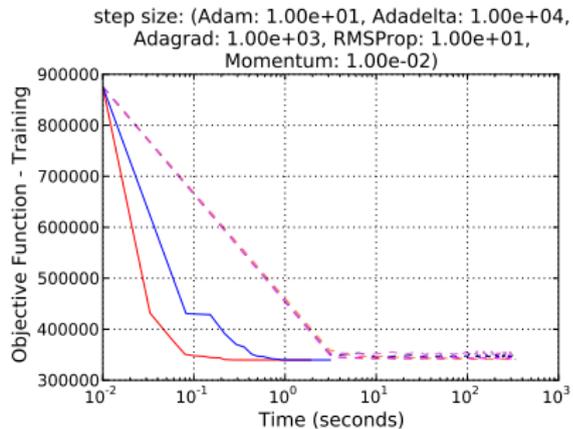
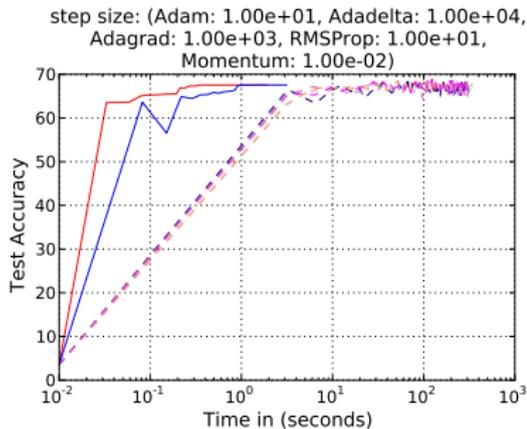


(i) Function Relative Error



Newton GPU vs. TensorFlow

Data: **Cover Type**, $n = 4.5 \times 10^5$, $d = 378$



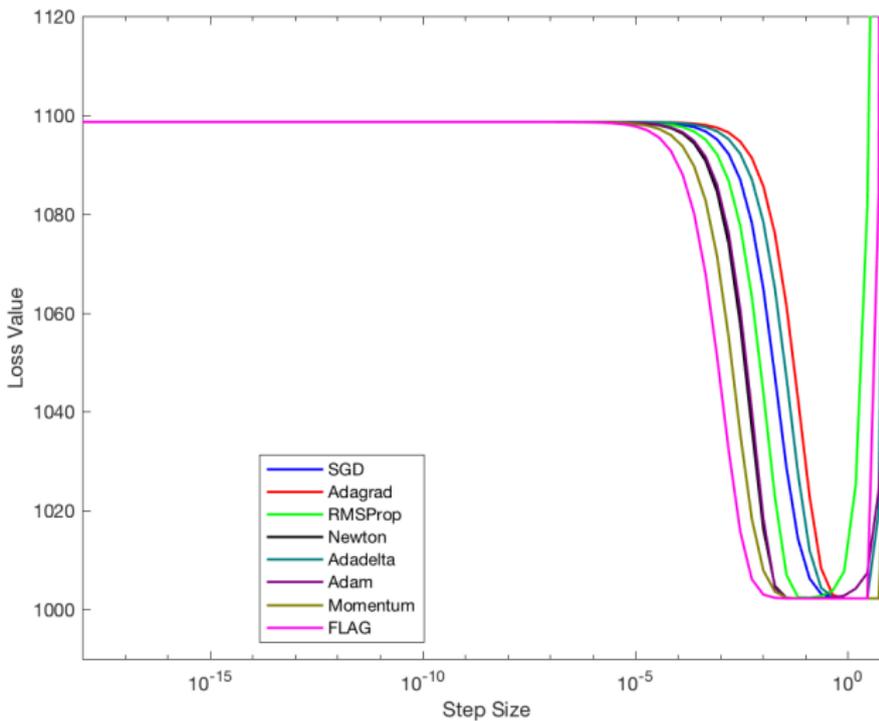


Figure: Skew Param = 0

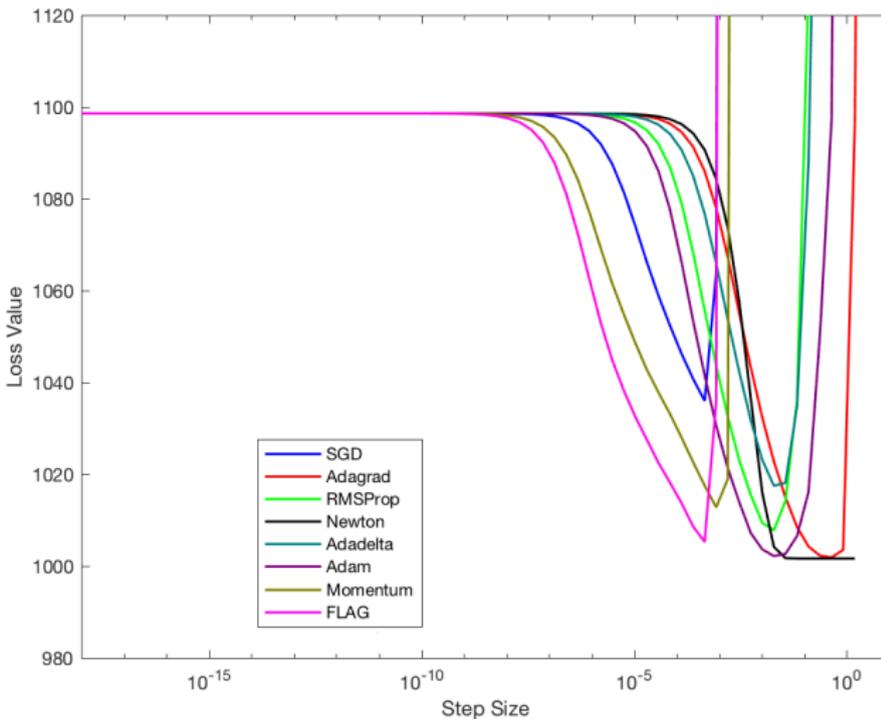


Figure: Skew Param = 2

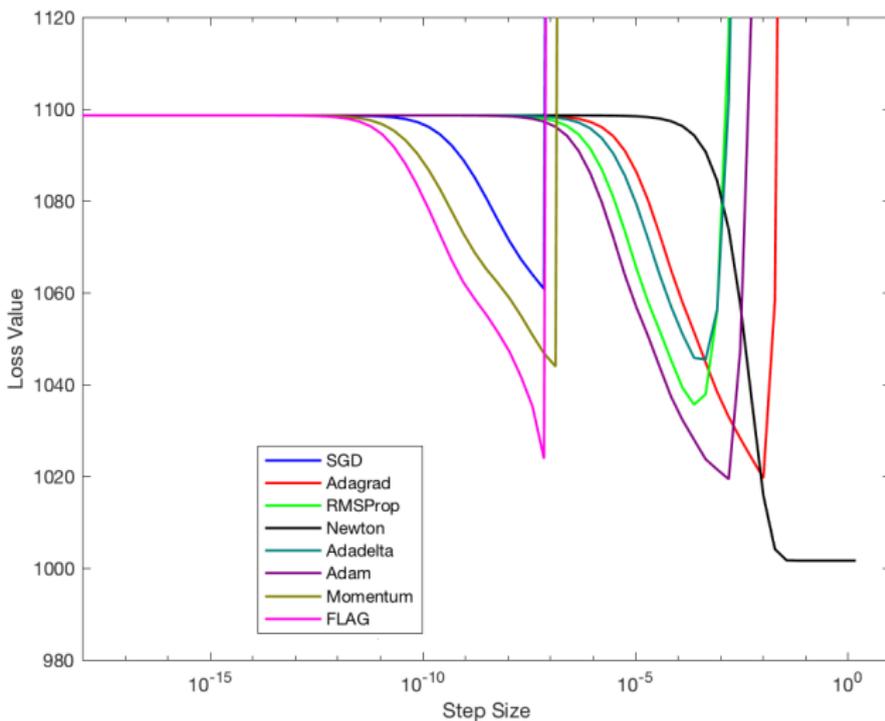


Figure: Skew Param = 4

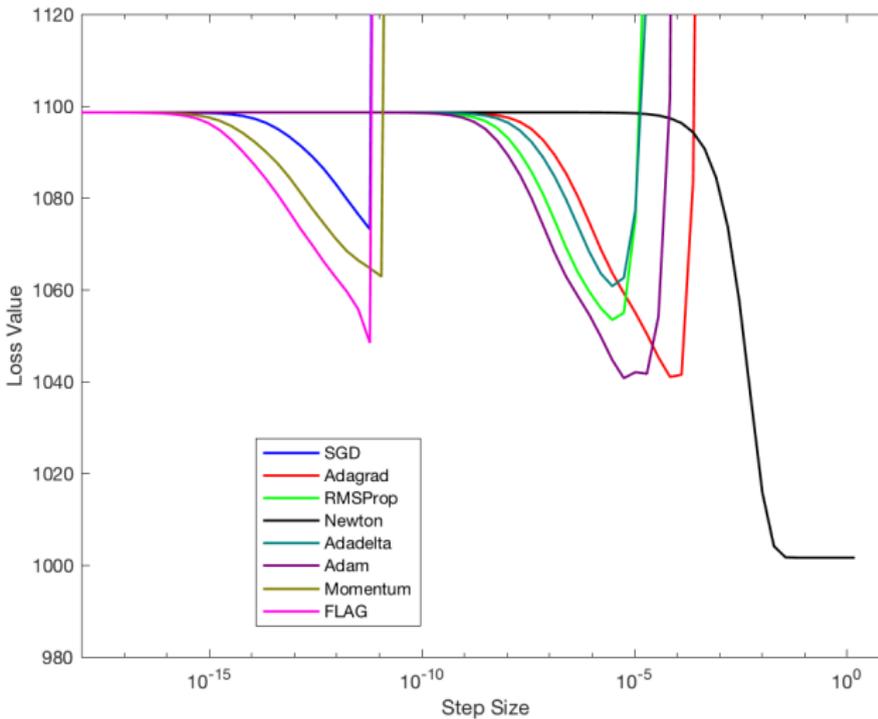


Figure: Skew Param = 6

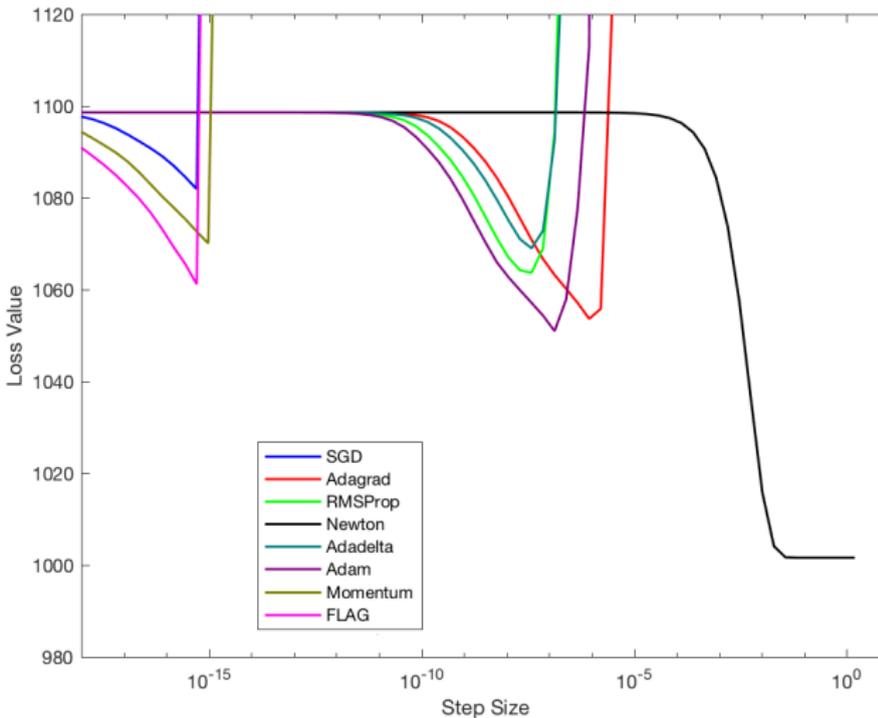


Figure: Skew Param = 8

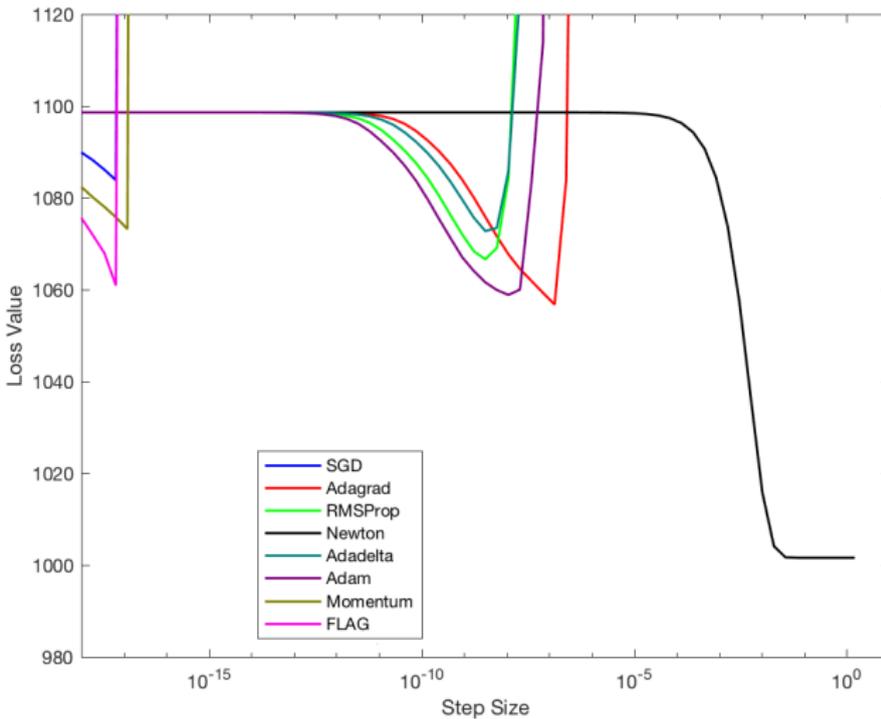


Figure: Skew Param = 9

Deep Auto-Encoder

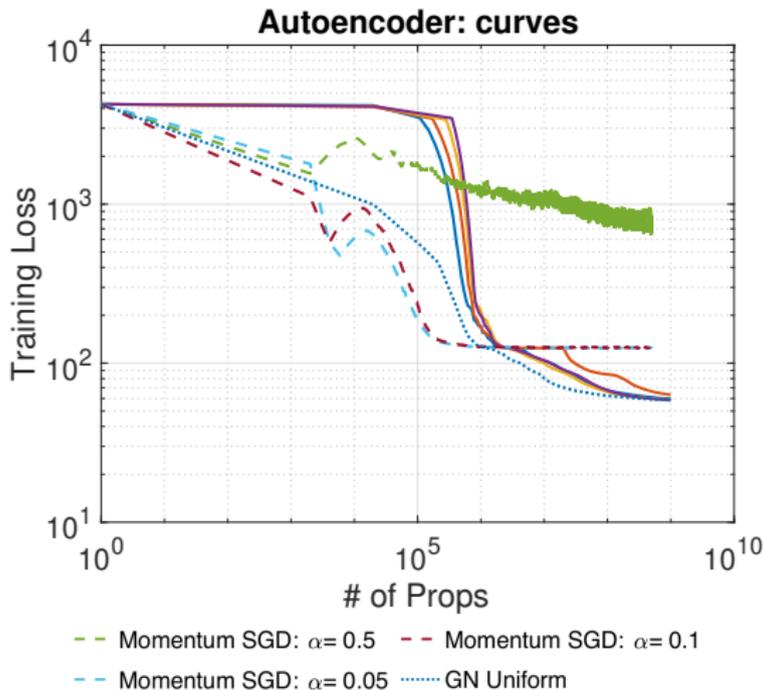


Figure: Random Initialization

Deep Auto-Encoder

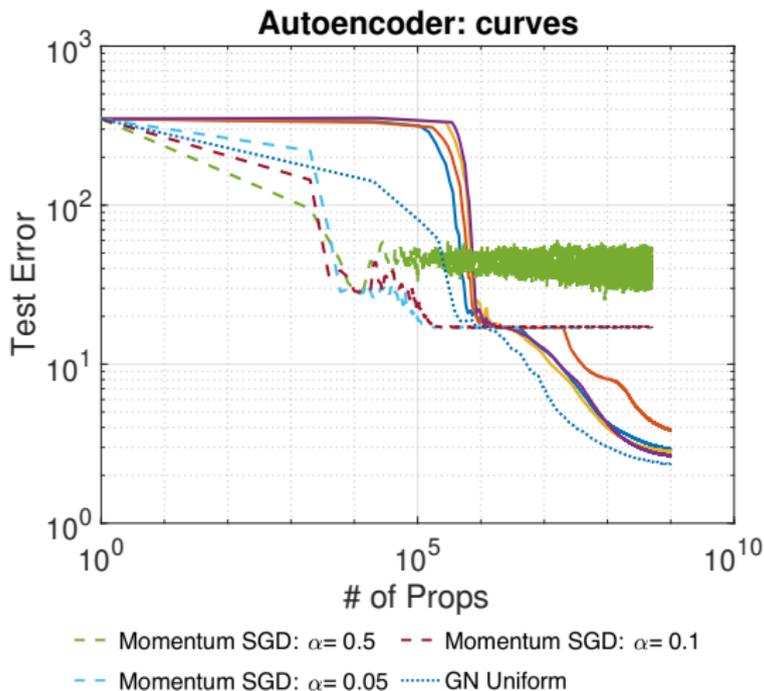


Figure: Random Initialization

Deep Auto-Encoder

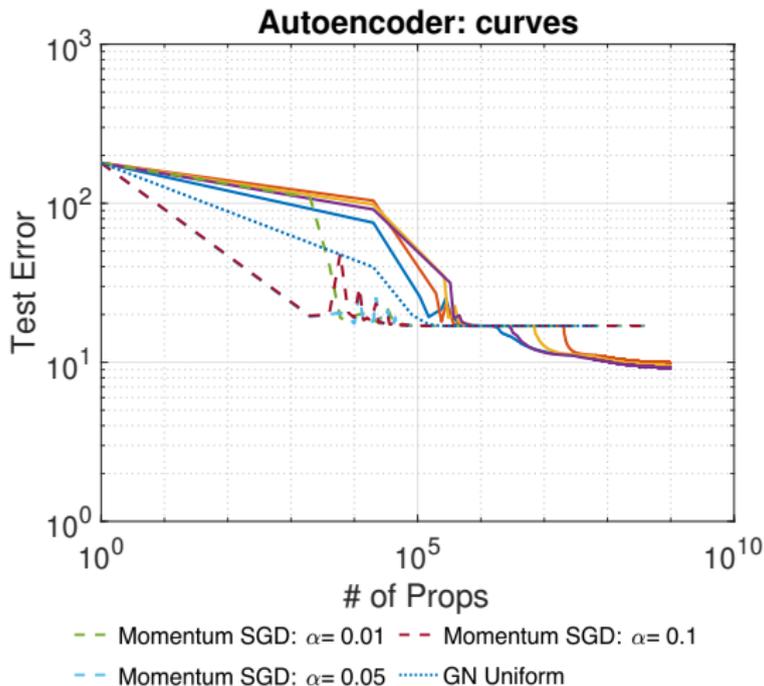
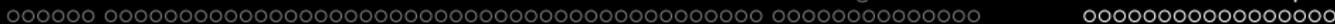


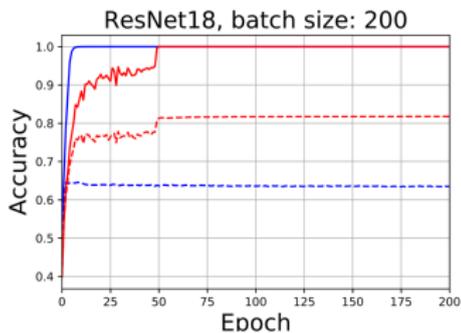
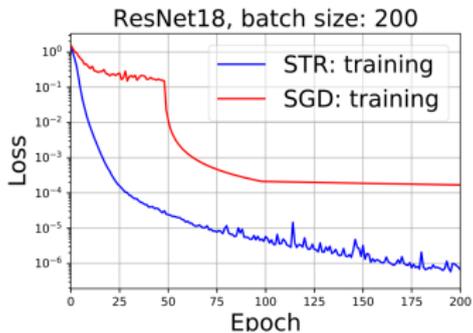
Figure: Zero Initialization



Is it all rosie?



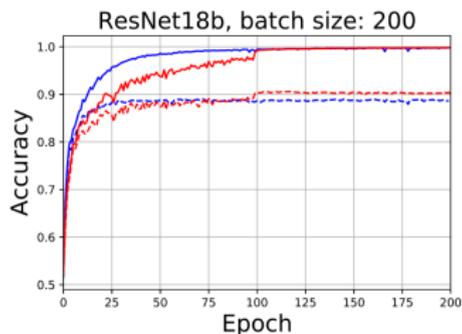
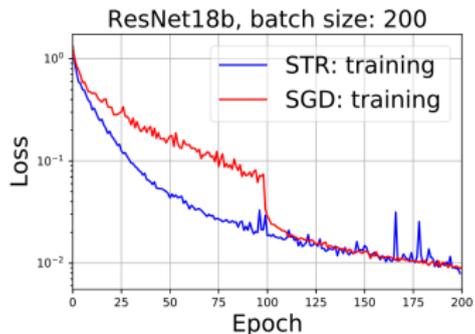
ResNet18



No Batch Normalization + No data augmentation.



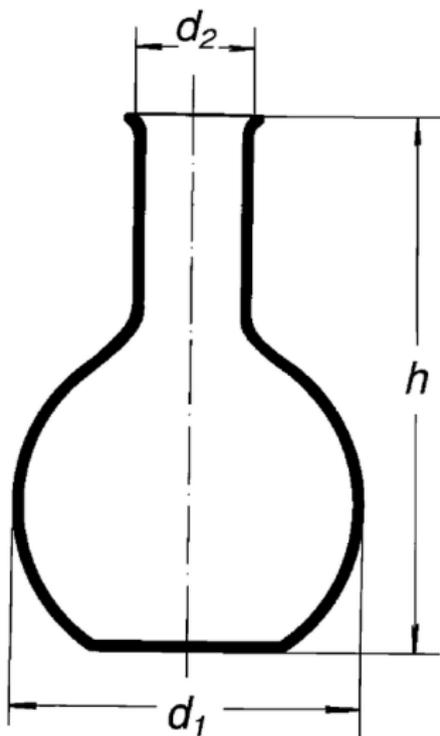
ResNet18



Batch Normalization + Data augmentation.

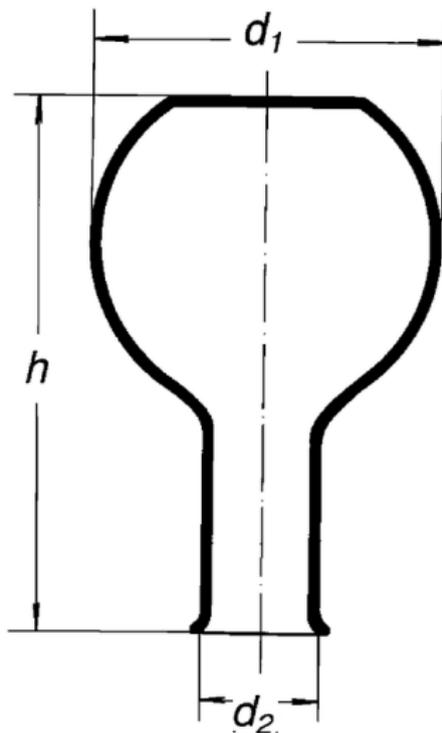


Worst Case Complexity

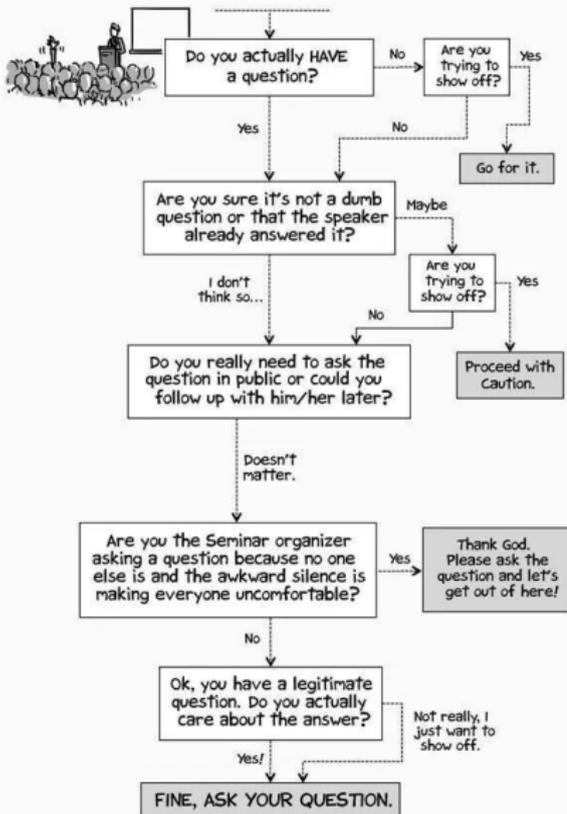




Worst Case Complexity



Should you ask a Question during Seminar?



THANK YOU!



Amari, S.-I. (1998).

Natural gradient works efficiently in learning.

Neural computation, 10(2):251–276.



Berahas, A. S., Nocedal, J., and Takáč, M. (2016).

A multi-batch l-bfgs method for machine learning.

In *Advances in Neural Information Processing Systems*, pages 1055–1063.



Berahas, A. S. and Takáč, M. (2017).

A Robust Multi-Batch L-BFGS Method for Machine Learning.

arXiv preprint arXiv:1707.08552.



Botev, A., Ritter, H., and Barber, D. (2017).

Practical Gauss-Newton optimisation for deep learning.

arXiv preprint arXiv:1706.03662.



Byrd, R. H., Hansen, S., Nocedal, J., and Singer, Y. (2014).

A stochastic quasi-Newton method for large-scale optimization.

arXiv preprint arXiv:1401.7020.



Cartis, C., Gould, N. I., and Toint, P. L. (2012).
Complexity bounds for second-order optimality in
unconstrained optimization.

Journal of Complexity, 28(1):93–108.



Chapelle, O. and Erhan, D. (2011).
Improved preconditioner for Hessian free optimization.
In *NIPS Workshop on Deep Learning and Unsupervised
Feature Learning*, volume 201.



Dai, Y.-H. (2002).
Convergence properties of the bfgs algorithm.
SIAM Journal on Optimization, 13(3):693–701.



Doel, K. v. d. and Ascher, U. (2012).
Adaptive and stochastic algorithms for EIT and DC resistivity
problems with piecewise constant solutions and many
measurements.

Improved bounds on sample size for implicit matrix trace estimators.

Foundations of Computational Mathematics, 15(5):1187–1212.



Roosta, F., Székely, G. J., and Ascher, U. (2015).

Assessing stochastic algorithms for large scale nonlinear least squares problems using extremal probabilities of linear combinations of gamma random variables.

SIAM/ASA Journal on Uncertainty Quantification, 3(1):61–90.



Roosta, F., van den Doel, K., and Ascher, U. (2014a).

Data completion and stochastic algorithms for PDE inversion problems with many measurements.

Electronic Transactions on Numerical Analysis, 42:177–196.



Roosta, F., van den Doel, K., and Ascher, U. (2014b).

Stochastic algorithms for inverse problems involving PDEs and many measurements.

SIAM J. Scientific Computing, 36(5):S3–S22.

