ETH zürich



Ellipsoidal Trust Region Methods for Neural Nets

L. Adolphs*, J. Kohler*, A. Lucchi *Institute for Machine Learning, ETH Zürich*









Finite-sum optimization

$$\min_{\mathbf{w} \in \mathbb{R}^{\mathbf{d}}} \left[\mathcal{L}(\mathbf{w}) := \sum_{i=1}^{\mathbf{n}} \ell(\mathbf{f}(\mathbf{w}, \mathbf{x_i}, \mathbf{y_i}))
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How to optimize?

Stochastic Gradient Descent



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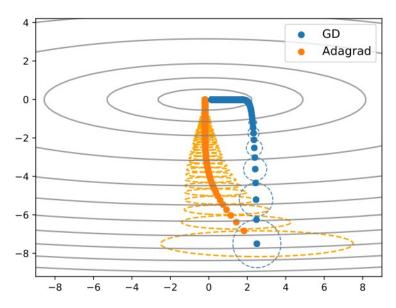
Stochastic Gradient Descent

inadequate for not well-conditioned functions



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Quadratic objective with condition number $\ \kappa=2$

How to optimize?

Stochastic Gradient Descent



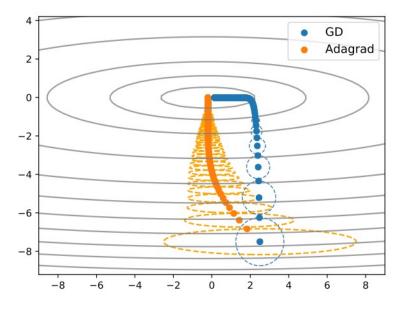
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adaptive 1st-order methods (e.g. RMSProp, Adagrad)

Finite-sum optimization

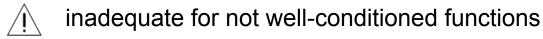
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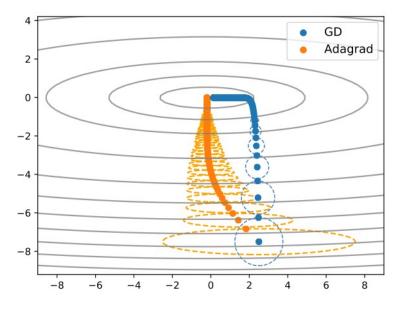


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Newton's Method

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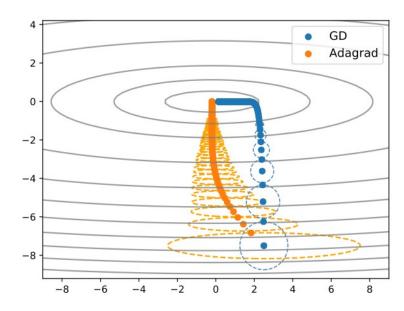
Newton's Method



strong theoretical guarantees

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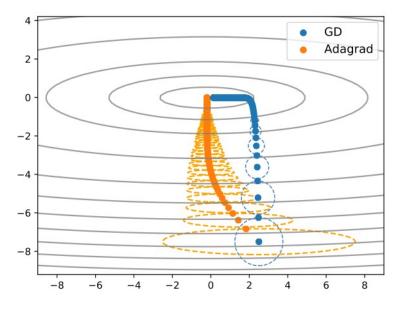




expensive

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Stochastic Hessian-Free Trust Region methods







Gradient Descent methods can be interpreted as first-order TR methods...

$$\mathbf{w_{t+1}} - \mathbf{w_t} = \mathbf{s_t} := -\eta_t \mathbf{A_t^{-1}} \mathbf{g_t}$$
 $| \mathbf{g_t} := \nabla \mathcal{L}(\mathbf{w_t})$



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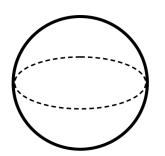
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...with the 'preconditioning' matrix determining the shape of the constraint.

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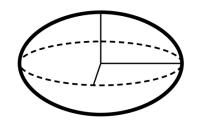
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Gradient Descent

$$\mathbf{A_t} = \mathbb{I}$$

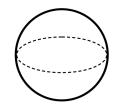


RMSProp Adagrad Adam



$$\min_{\mathbf{s} \in \mathbb{R}^{\mathbf{d}}} \left[m_t(\mathbf{s}) := \mathcal{L}(\mathbf{w_t}) + \mathbf{g_t^\intercal s} + \frac{1}{2} \mathbf{s_t^\intercal B_t s} \right] \quad \text{ s.t. } \|\mathbf{s}\| \leq \mathbf{\Delta_t}$$

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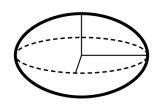






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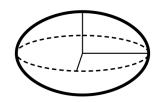








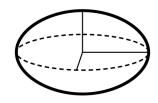
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Why Ellipsoids?

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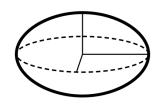
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Many sources for ill-conditioning in Neural Nets

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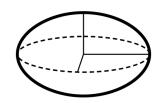
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More flexibility to reshape constraint set to loss landscape

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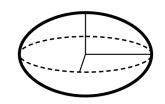
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Why Ellipsoids?



Many sources for ill-conditioning in Neural Nets



More flexibility to reshape constraint set to loss landscape

What Ellipsoid?



Preconditioners from most-common first-order methods, that fulfill *Uniform Equivalence*



RMSProp, Adam, ...

Algorithm 1 Stochastic Ellipsoidal Trust Region Method

- 1: Input: $\mathbf{w}_0 \in \mathbb{R}^d$, $\gamma_1, \gamma_2 > 1, 1 > \eta_2 > \eta_1 > 0, \Delta_0 > 0, T \ge 1, |\mathcal{S}_0|, \mu \ge 1, \epsilon > 0$
- 2: for $t = 0, 1, \ldots$, until convergence do
- Sample \mathcal{L}_t , \mathbf{g}_t and \mathbf{B}_t with batch sizes $|\mathcal{S}_{\mathcal{L},t}|, |\mathcal{S}_{\mathbf{g},t}|, |\mathcal{S}_{\mathbf{B},t}|$
- Compute preconditioner A_t
- Obtain \mathbf{s}_t by solving $m_t(\mathbf{s}_t)$
- Compute actual over predicted decrease on batch 6:

$$\rho_{\mathcal{S},t} = \frac{\mathcal{L}_{\mathcal{S}}(\mathbf{w}_t) - \mathcal{L}_{\mathcal{S}}(\mathbf{w}_t + \mathbf{s}_t)}{m_t(\mathbf{0}) - m_t(\mathbf{s}_t)}$$

7: Set

$$\Delta_{t+1} = \begin{cases} \gamma_1 \Delta_t & \text{if } \rho_{\mathcal{S},t} > \eta_2 \text{ (very successful)} \\ \Delta_t & \text{if } \eta_2 \geq \rho_{\mathcal{S},t} \geq \eta_1 \text{ (successful)}, \mathbf{w}_{t+1} \\ \Delta_t / \gamma_2 & \text{if } \rho_{\mathcal{S},t} < \eta_1 \text{ (unsuccessful)} \end{cases} = \begin{cases} \mathbf{w}_t + \mathbf{s}_t & \text{if } \rho_{\mathcal{S},t} \geq \eta_1 \\ \mathbf{w}_t & \text{otherwise} \end{cases}$$



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8: end for

Loss, Gradient, approx. Hessian

for batch

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 Real loss Model loss

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Adjust TR radius

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> Accept only successful updates $\Delta_{t+1} = \begin{cases} \gamma_1 \Delta_t & \text{if } \rho_{\mathcal{S},t} > \eta_2 \text{ (very successful)} \\ \Delta_t & \text{if } \eta_2 \geq \rho_{\mathcal{S},t} \geq \eta_1 \text{ (successful)}, \mathbf{w}_{t+1} \\ \Delta_t / \gamma_2 & \text{if } \rho_{\mathcal{S},t} < \eta_1 \text{ (unsuccessful)} \end{cases} = \begin{cases} \mathbf{w}_t + \mathbf{s}_t & \text{if } \rho_{\mathcal{S},t} \geq \eta_1 \\ \mathbf{w}_t & \text{otherwise} \end{cases}$



Convergence guarantees



$$\exists \mu \geq 1, \quad \frac{1}{\mu} \|\mathbf{w}\|_{\mathbf{A}_t} \leq \|\mathbf{w}\|_2 \leq \mu \|\mathbf{w}\|_{\mathbf{A}_t}, \ \forall t = 1, 2, \dots$$

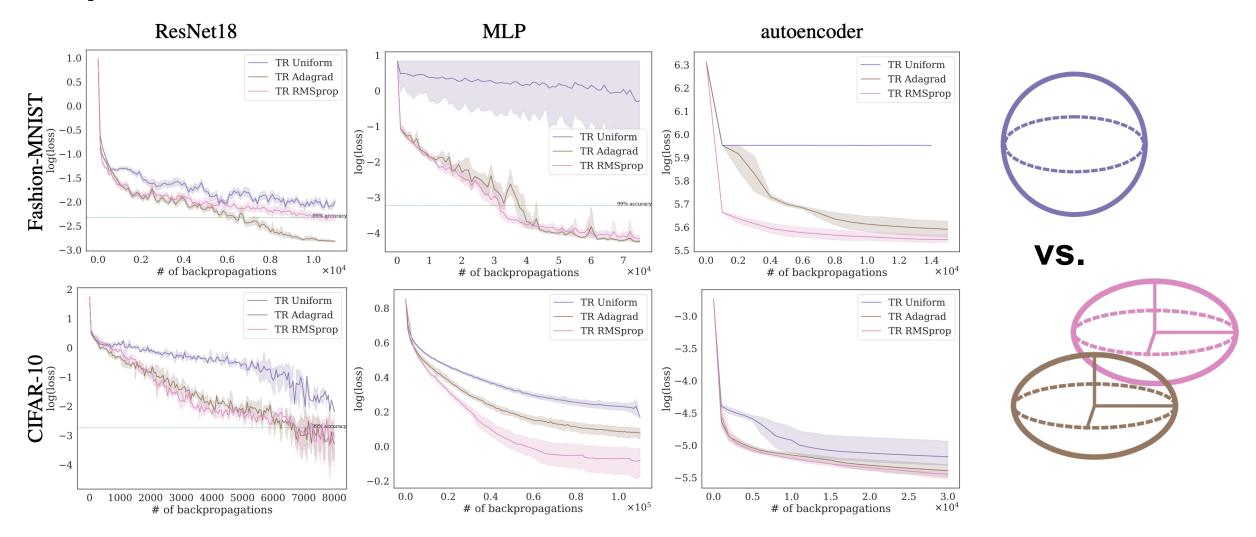
(Conn et al. 2000) prove convergence assuming uniform equivalent norms

We extend this result to prove a convergence **rate** for the semi-stochastic TR framework of (Yao et al. 2018) with ellipsoidal constraints.

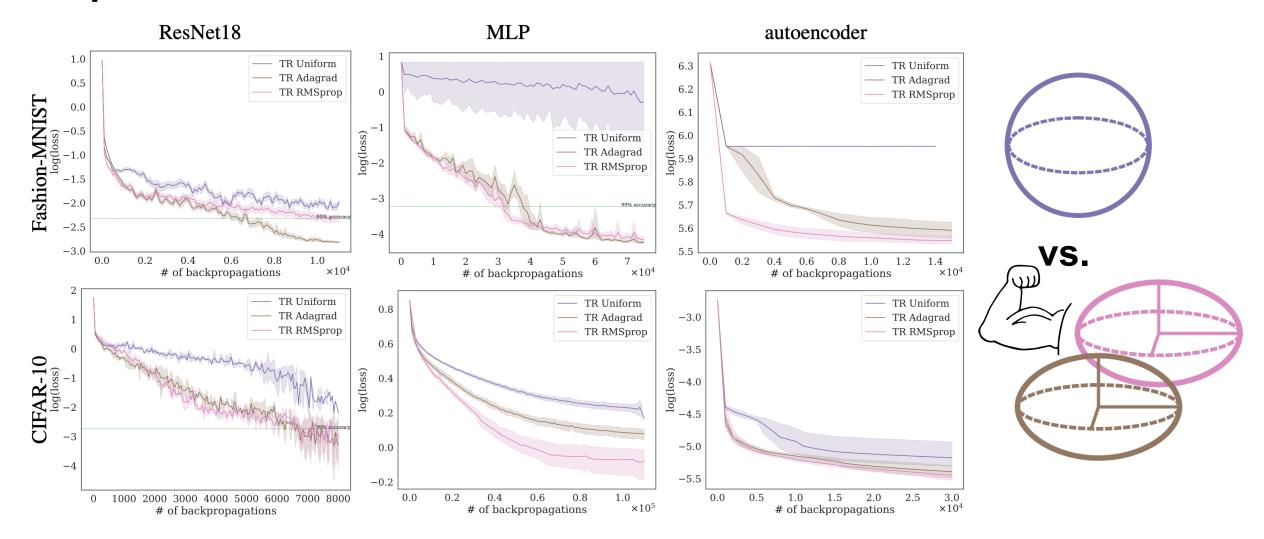
full function - but inexact derivative information

Theorem 2 (Convergence rate of Algorithm 1). Assume that $\mathcal{L}(\mathbf{w})$ is second-order smooth with Lipschitz constants L_g and L_H . Furthermore, let Assumption 1 and 2 hold. Then Algorithm 1 finds an $\mathcal{O}(\epsilon_g, \epsilon_H)$ first- and second-order stationary point in at most $\mathcal{O}(\max\{\epsilon_g^{-2}\epsilon_H^{-1}, \epsilon_H^{-3}\})$ iterations.

Experiments



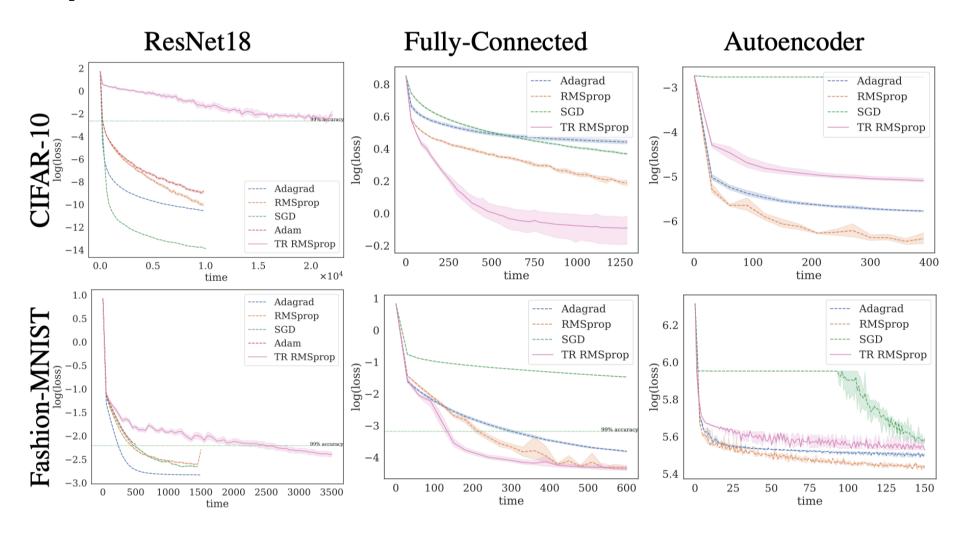
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Experiments



Comparison against 1st-order methods in wall-clock-time



Thank you! Any Questions?

