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Neumann Optimizer

A Practical Optimization Algorithm for Deep Neural Networks

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Training Deep Networks

- Loss function is non-convex
- Finite sample size
- Lower loss doesn't necessarily imply better model performance
- Computational hurdles

Iterative Methods

Create function approximation around the current iterate

Different methods result depending on information used for the approximation

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Cubic reg.: $\nabla \mathcal{F}(w_t)^T (z - w_t) + \frac{1}{2}(z - w_t)^T \nabla^2 \mathcal{F}(w_t)(z - w_t) + \frac{\alpha}{3} \|z - w_t\|^3$

Neumann Optimizer

- Designed for large batch setting
- Incorporates second order information, without explicitly representing the Hessian
- Based on cubic regularized approximation
- Total per step cost is same as Adam

Neumann Optimizer - Results

- Linear speedup with increasing batch size
- 0.8 - 0.9% test accuracy improvements over baseline on image models
- 10-30% faster than current methods for comparable computational resources

Two Loop Algorithm

- For each mini-batch: solve the quadratic problem of the mini-batch to "good" accuracy.

$$\mathcal{G}(z) = \mathcal{F}(w_t) + \nabla \mathcal{F}(w_t)^T (z - w_t) + \frac{1}{2}(z - w_t)^T \nabla^2 \mathcal{F}(w_t)(z - w_t),$$

- Use the solutions of the quadratic problem as updates.

$$w_{t+1} = w_t - \left[\nabla^2 \mathcal{F}(w_t)\right]^{-1} \nabla \mathcal{F}(w_t).$$

- Hypothesis: with very large mini-batches, the cost-benefit is in favour of extracting more information.

Inner loop: solving a quadratic via power series

How to solve the quadratic?

$$Az = b$$

Use the geometric (Neumann) series for inverse, if $A \succ 0, \|A\|_2 < 1$

$$A^{-1} = \sum_{i=0}^{\infty} (I_n - A)^i.$$

This implies the iteration:

$$z_0 = b \qquad \text{and} \qquad z_{t+1} = (I_n - A) z_t + b,$$

Eliminate the Hessian calculation (too expensive)

Back to the mini-batch problem:

$$\nabla^2 \mathcal{F}(w_t)(w - w_t) = -\nabla \mathcal{F}(w_t)$$

This implies an iteration:

$$\begin{aligned} m_{t+1} &= (I_n - \eta \nabla^2 \hat{f}) m_t - \nabla \hat{f}(w_t) \\ &= m_t - (\boldsymbol{\nabla} \hat{\boldsymbol{f}}(\boldsymbol{w_t}) + \boldsymbol{\eta} \boldsymbol{\nabla}^{\mathbf{2}} \hat{\boldsymbol{f}} \boldsymbol{m_t})) \\ &\approx m_t - \boldsymbol{\nabla} \hat{\boldsymbol{f}}(\boldsymbol{w_t} + \boldsymbol{\eta} \boldsymbol{m_t}). \end{aligned}$$

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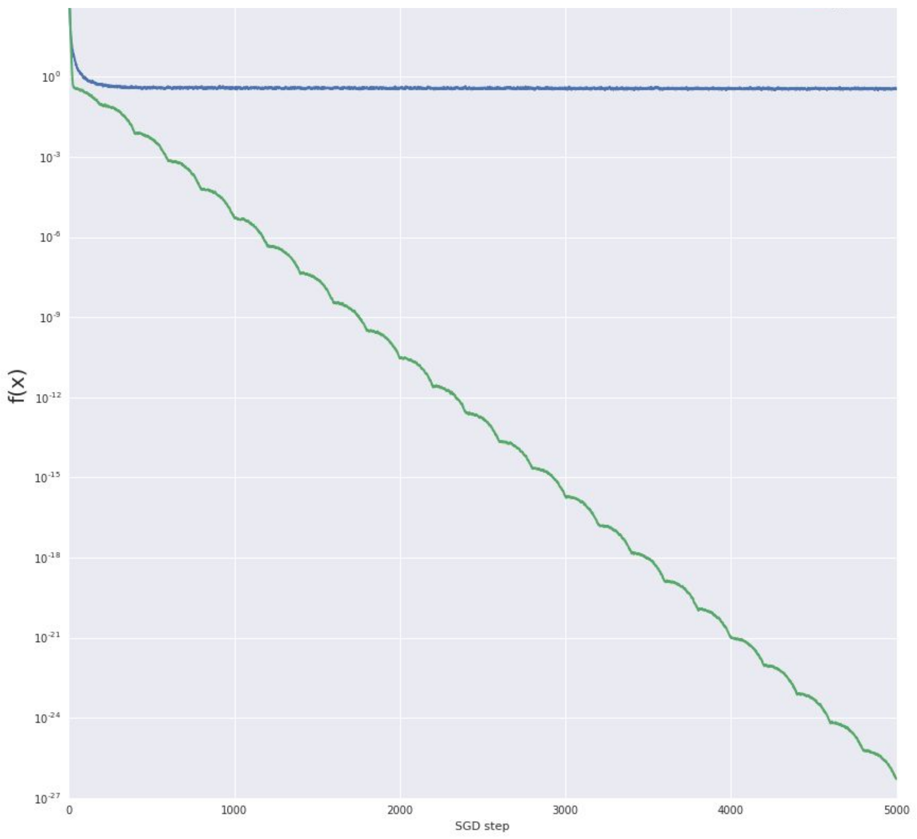
Convex Quadratics



Some tweaks for actual neural networks

Cubic regularizer (convexification of overall problem) + Repulsive regularizer

$$\hat{g}(w) = \hat{f}(w) + \frac{\alpha}{3}\|w - v_t\|^3 + \beta / \|w - v_t\|$$

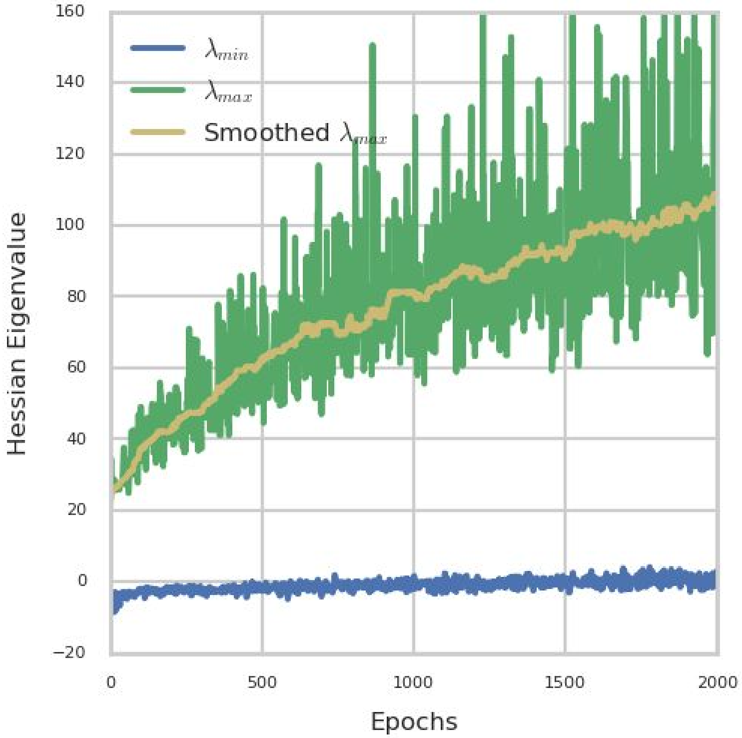
Convexification of each mini-batch.

$$\mu = \frac{\lambda_{\max}}{|\lambda_{\min}| + \lambda_{\max}} \quad \text{and} \quad \eta = \frac{1}{\lambda_{\max}}.$$

$$m_k = \mu m_{k-1} - \eta \nabla \hat{g}(w_t + \mu m_{k-1}).$$

Spectrum of the Hessian

- Studied on various image models
- Lanczos method during optimization
- Similar behavior of extreme eigenvalues
- Consistent with other studies [Sagun ‘16, Chaudhari ‘16, Dauphin ‘14]



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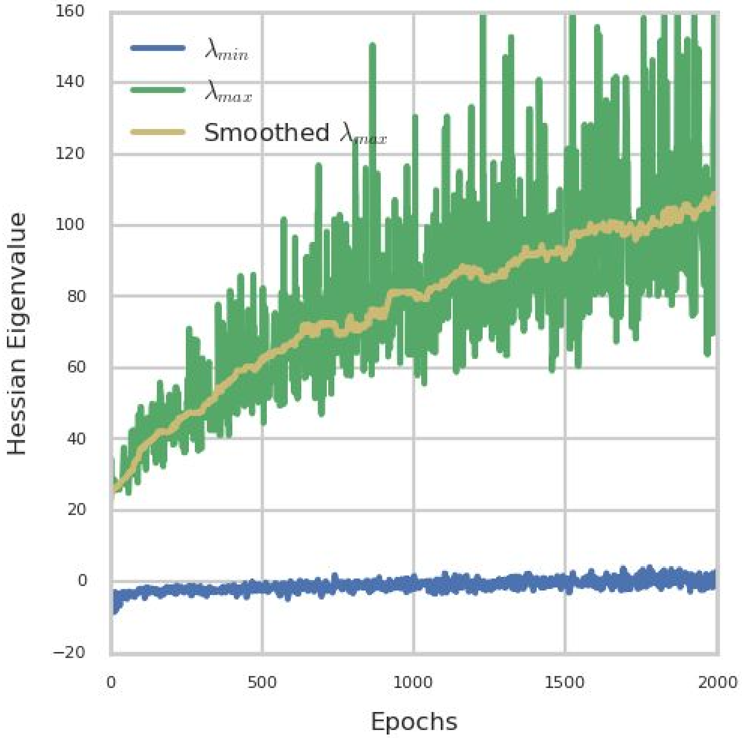
$$\mu \propto 1 - \frac{1}{1+t} \qquad \eta \propto 1/t$$



Our Algorithm

for $t = 1, 2, 3, \ldots, T$ **do**

Draw a sample $(x_{t_1}, y_{t_1}), \ldots, (x_{t_B}, y_{t_B})$.

Compute derivative $\nabla \hat{f} = (1/B) \sum_{i=1}^{B} \nabla \ell(y_{t_i}, g(x_{t_i}, w_t))$

Compute update $d_t = \nabla \hat{f} + \left(\alpha \|w_t - v_t\|^2 - \frac{\beta}{\|w_t - v_t\|^2} \right) \frac{w_t - v_t}{\|w_t - v_t\|}$

Update Neumann iterate: $m_t = \mu(t) m_{t-1} - \eta(t) d_t$.

Update weights: $w_t = w_{t-1} + \mu(t) m_t - \eta(t) d_t$.

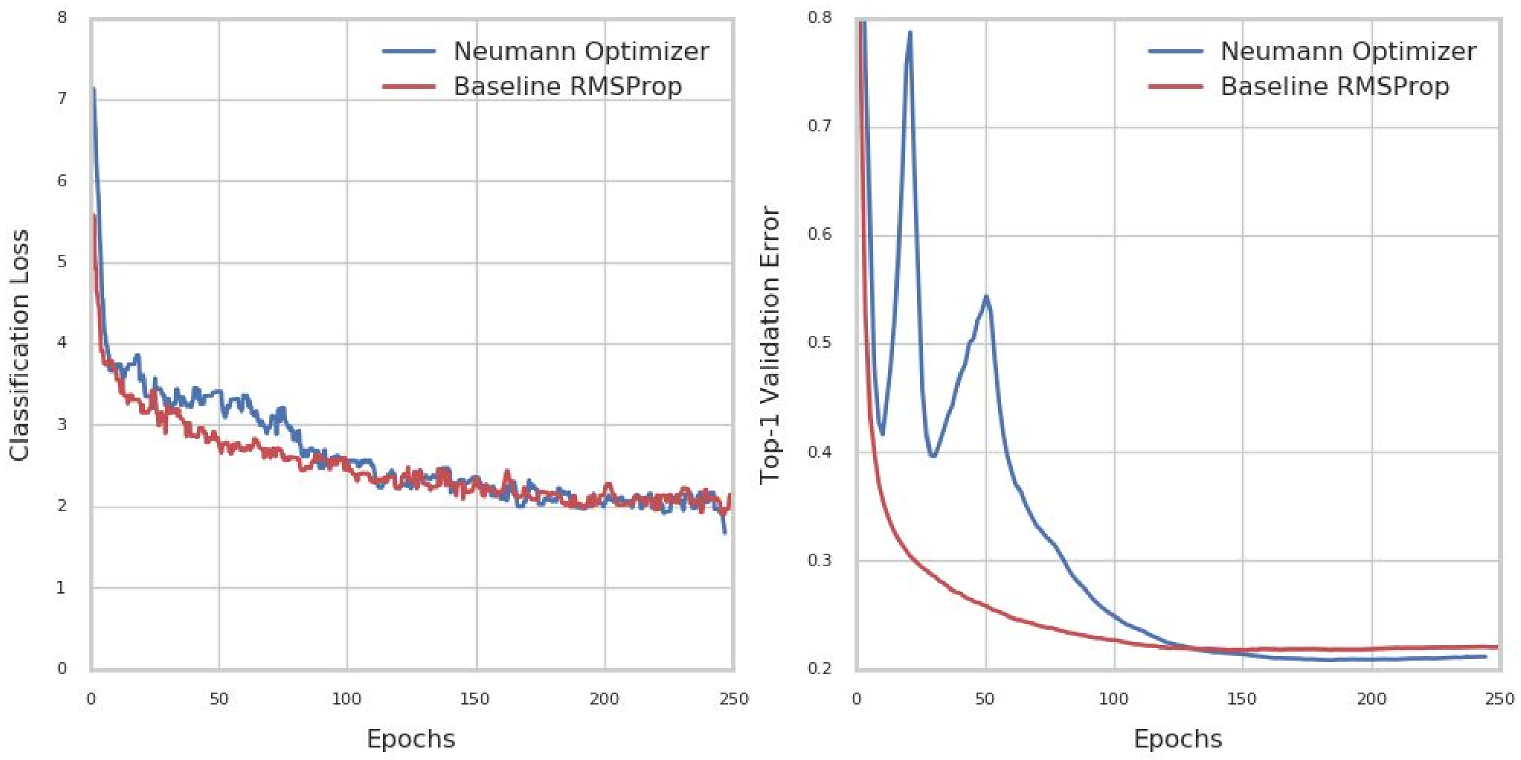
Update moving average of weights: $v_t = w_t + \gamma(v_{t-1} - w_t)$

return $w_T - \mu(T) m_T$

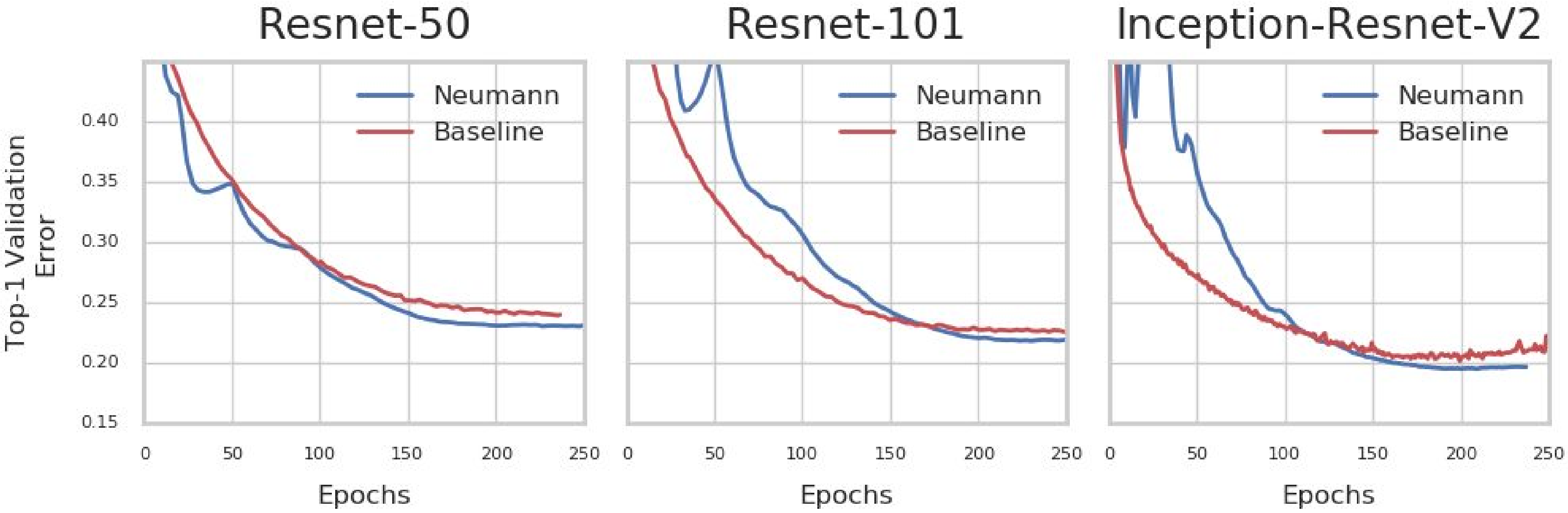
Experimental Results

- Used image models for experimentation
    - Cifar10, Cifar100, Imagenet
- Various network architectures
    - Resnet-V1, Inception-V3, Inception-Resnet-V2
- Training on GPUs (P100, K40)
    - Multiple GPUs in sync mode for large batch training
- Update steps/epochs to measure performance

Experiments on ImageNet (Inception V3)



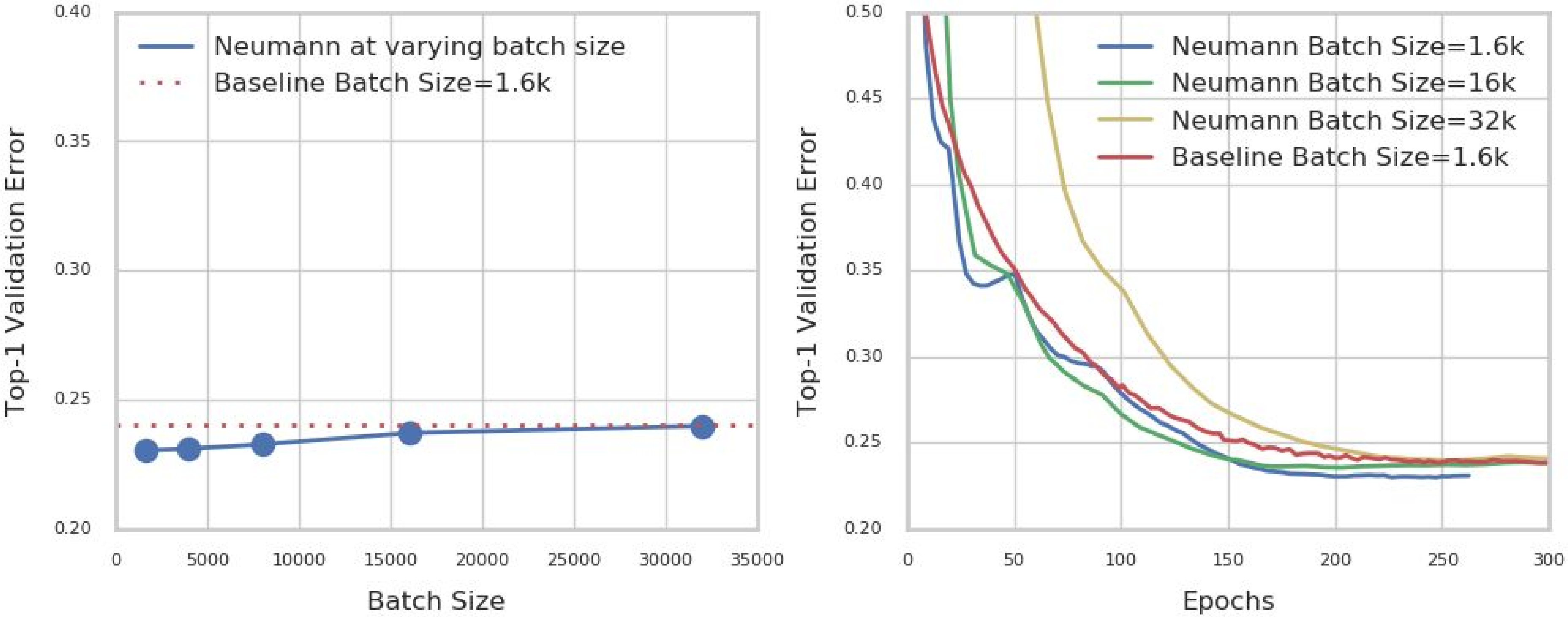
Experiments on ImageNet (Resnet Architectures)



Final Top-1 Validation Error

	Baseline	Neumann	Improvement
Inception-V3	21.7 %	20.8 %	**0.91%**
Resnet-50	23.9 %	23.0 %	**0.94 %**
Resnet-101	22.6 %	21.7%	**0.86 %**
Inception-Resnet-V2	20.3 %	19.5 %	**0.84 %**

Large batch training



Scaling Performance on Resnet-50

Batch Size	Top-1 Validation Error	# Epochs
1600	23.0 %	**226**
4000	23.0 %	**230**
8000	23.1 %	**258**
16000	23.5 %	**210**
32000	24.0 %	**237**

Mini-batch Training

Stochastic methods use unbiased estimates to carry out optimization

For first order methods with batch size B, $\hat{f}(w) = \frac{1}{B} \sum_{i=1}^{B} f_{t_i}(w)$

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$$B \approx O\left(\frac{\sigma^2 T}{LD}\right)$$

Conclusion and Future Work

- Stochastic optimization algorithm for training deep nets
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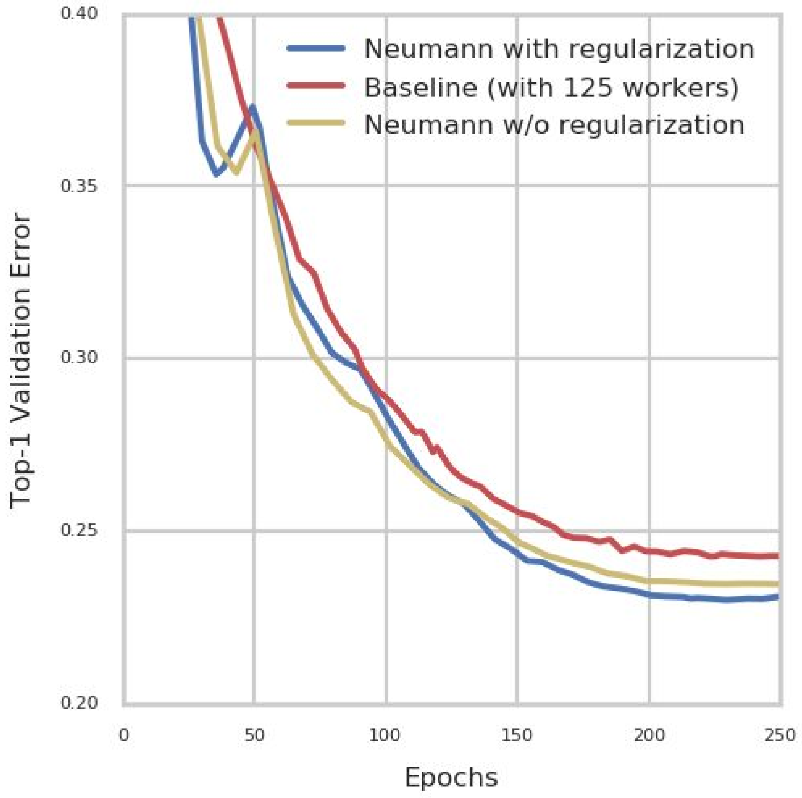
- Other model architectures and models
  - Preconditioned Neumann
- Experiment on TPUs

Thank you!

Paper: https://goo.gl/7M9Avr

Code: Tensorflow implementation coming soon

Ablation Experiment



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