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Stochastic Hessian Projection

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Stochastic Hessian Information

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How do we efficiently collect and apply Hessian information during the course of optimization for machine learning?

Some recent work:

Berahas, Bollapragada, & Nocedal. ***An Investigation of Newton-Sketch and Subsampled Newton Methods. 2017.***

Bollapragada, Byrd, & Nocedal. ***Exact and Inexact Subsampled Newton Methods for Optimization. 2016.***

Byrd, Chin, Neveitt, & Nocedal. ***On the Use of Stochastic Hessian Information in Optimization Methods for Machine Learning. 2011.***

Review - Notation

Sum-like objectives are quite common in optimization for machine learning.

Model parameters: $\theta \in \mathbb{R}^m$

Training samples: $(x_i, y_i) \quad \text{for all} \quad i \in [N]$

(input, desired-output)

Sample index

Sample loss: $j_i(\theta) = j(x_i, y_i|\theta)$

Error between model prediction and desired output.

Goal: $\min_\theta J(\theta) = \frac{1}{N} \sum_i^N j_i(\theta)$

Review - Gradient Descent

Ordinary gradient descent optimization would take the form

Iteration index

This could be generalized to any step-size and descent-direction.

$$\theta^{(j+1)} = \theta^{(j)} - \alpha \nabla J(\theta^{(j)})$$

The gradient of the objective is a **sum over sample gradients**

$$\nabla J(\theta) = \frac{1}{N} \sum_{i}^{N} \nabla j_i(\theta)$$

What if the sum is too big? There could be millions of samples and we'd have to repeat after every iteration.

Review - Stochastic Gradient Descent (SGD)

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It is more feasible to compute updates using sample gradients*.

SGD update: $$\theta^{(j+1)} = \theta^{(j)} - \alpha \nabla j_{s_j}(\theta^{(j)})$$

Randomly select a sample and replace the true gradient with the sample gradient.

The expectation value matches the true gradient. As long as the learning rate is small, the trajectory approaches gradient descent.

$$\mathbb{E}[\nabla j_i(\theta)] = \nabla J(\theta)$$

*Robbins, H. & Monro, S. ***A Stochastic Approximation Method. 1951.***

Review - Batched SGD for Variance Reduction

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The sample gradient, however, may have high variance.
Batched sampling allows one to tune the trade-off between gradient-approximation variance and computational efficiency.

$$J_\Psi(\theta) = \frac{1}{|\Psi|}\sum_{i\in\Psi} j_i(\theta) \qquad \nabla J_\Psi(\theta) = \frac{1}{|\Psi|}\sum_{i\in\Psi} \nabla j_i(\theta)$$

Randomly sample subset with (or without*) replacement.

$$\theta^{(j+1)} = \theta^{(j)} - \alpha \nabla J_{\Psi_j}(\theta^{(j)}) \qquad \mathrm{Var}[\nabla J_\Psi] = \frac{1}{|\Psi|}\mathrm{Var}[\nabla j_i]$$

*Shamir, O. ***Without-Replacement Sampling for Stochastic Gradient Methods***. 2016.*

Related Work by Today's Speakers

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Adaptive batch-sizing:

Bollapragada, Byrd, & Nocedal. ***Adaptive Sampling Strategies for Stochastic Optimization****. 2017.*

Adaptive batch-weighting:

Needell & Ward. ***Batched Stochastic Gradient Descent with Weighted Sampling****. 2017.*

And what if the objective is non-differentiable?

Ryu & Byrd. ***Stochastic Proximal Iteration: A Non-Asymptotic Improvement Upon Stochastic Gradient Descent.*** *2018.*

Low-Rank Hessian Approximation

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Is it possible to use sample gradients to construct a low-rank approximation of the local Hessian?

Key assumption:

$$J(\theta) \approx J(\theta_0) + (\theta - \theta_0)^T g_0 + \frac{1}{2}(\theta - \theta_0)^T H_0 (\theta - \theta_0)$$

Objective at expansion point.

Gradient approximation at expansion point.

Local Hessian approximation.

Parameter Data over an Epoch

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During an SGD epoch, we can track parameters and gradients as columns of a matrix.

Parameter epoch:

$$\Theta = \begin{bmatrix} \theta^{(1)} & \theta^{(2)} & \cdots & \theta^{(n)} \end{bmatrix}$$

We use the **epoch-mean as the expansion point** and express parameters as differences from the mean.

Number of updates in epoch.

Parameter differences:

$$\hat{\Theta} = \Theta - \bar{\theta} e^T \quad \text{where} \quad \bar{\theta} = \frac{1}{n} \Theta e$$

Gradient Data over an Epoch

We use corresponding constructions for gradient samples.

Gradient epoch:

$$G = \begin{bmatrix} g^{(1)} & g^{(2)} & \cdots & g^{(n)} \end{bmatrix}$$

$$\text{where} \quad g^{(i)} = \nabla J_{\Psi_i}(\theta^{(i)})$$

Gradient differences:

$$\hat{G} = G - \bar{g}e^T \quad \text{where} \quad \bar{g} = \frac{1}{n}Ge$$

Hind-foresight: this may seem strange now, but it is a good choice.

Second-Order Predictions

If the objective approximation has the form

$$\tilde{J}(\hat{\theta}) = J_0 + \hat{\theta}^T g_0 + \frac{1}{2}\hat{\theta}^T H_0 \hat{\theta}$$

then the gradient would be $\nabla \tilde{J}(\hat{\theta}) = g_0 + H_0\hat{\theta}.$

Gradient predictions for the epoch:

$$\tilde{G} = g_0 e^T + H_0 \hat{\Theta}$$

Recalling $\hat{\Theta} = \Theta - \bar{\theta} e^T.$

Optimizing Gradient Predictions

We seek the gradient g_0 and Hessian H_0 values that **minimize the Frobenius norm of gradient prediction error.**

$$\min_{g_0, H_0} \omega(g_0, H_0) = \left\| \tilde{G} - G \right\|_F^2 \quad \text{subject to} \quad H_0 = H_0^T$$

unpacking definitions so far gives

$$\omega(g_0, H_0) = \left\| g_0 e^T + H_0 \hat{\Theta} - \hat{G} - \bar{g} e^T \right\|_F^2$$

Solving for optimal g_0

A little algebraic manipulation gives

$$\omega(g_0, H_0) = \left\|(g_0 - \bar{g})e^T\right\|_F^2 + \left\|H_0\hat{\Theta} - \hat{G}\right\|_F^2 + 2\,\mathrm{tr}\left((H_0\hat{\Theta} - \hat{G})e(g_0 - \bar{g})^T\right)$$

Unaffected by g_0.

Re: hind-foresight. Since we subtracted means, this is zero.

This term can be reduced to zero by setting $g_0 = \bar{g}$.

Solving for optimal H_0

$$\omega(g_0, H_0) = \left\|(g_0 - \bar{g})e^T\right\|_F^2 + \left\|H_0\hat{\Theta} - \hat{G}\right\|_F^2 + 2\,\mathrm{tr}\left((H_0\hat{\Theta} - \hat{G})(g_0 - \bar{g})^T\right)$$

The intermediate optimization problem is now

$$\min_{H_0} \omega(\bar{g}, H_0) = \left\|H_0\hat{\Theta} - \hat{G}\right\|_F^2$$
$$\text{subject to} \quad H_0 = H_0^T$$

rank-$(n-1)$

rank-m

Unfortunately, the typical epoch duration n will be too short to obtain a full approximation.

Problem: $n \ll m$

Projection onto Active Subspace

We really want to characterize the Hessian in the subspace that is being actively explored.

Orthonormal basis: U $\quad U^T U = I$

Low-rank constraint: $H_0 = U X U^T \quad \text{s.t.} \quad X = X^T$

More hind-foresight: It is always possible to construct the basis to **diagonalize the parameter covariance projection**.

$$\hat{U}^T \hat{\Theta} \hat{\Theta}^T \hat{U} = V \operatorname{diag}(\tau) V^T \quad \text{then} \quad U = \hat{U} V.$$

tentative

adjusted

Stochastic Hessian Projection (SHP)

With the additional projection constraint, we now have

$$\min_X \omega(\bar{g}, UXU^T) = \left\| XU^T\hat{\Theta} - U^T\hat{G} \right\|_F^2$$
$$\text{subject to} \quad X = X^T$$

which, again, we can express using the trace

$$\omega = \text{tr}\left(\left[XU^T\hat{\Theta} - U^T\hat{G} \right] \left[\hat{\Theta}^T UX - \hat{G}^T U \right] \right)$$

Solving for X

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Differentiate and apply variational principle:

$$0 = U^T\hat{\Theta}\left[\hat{\Theta}^T U X - \hat{G}^T U\right] + \left[X U^T\hat{\Theta} - U^T\hat{G}\right]\hat{\Theta}^T U$$

Simple form of continuous Lyapunov equation:

$$\mathrm{diag}(\tau)X + X\mathrm{diag}(\tau) = U^T\hat{\Theta}\hat{G}^T U + U^T\hat{G}\hat{\Theta}^T U$$

This is why diagonalizing parameter covariance was a nice choice.

Recall $U^T\hat{\Theta}\hat{\Theta}^T U = \mathrm{diag}(\tau)$.

elementwise division

$$X = \left[U^T\hat{\Theta}\hat{G}^T U + U^T\hat{G}\hat{\Theta}^T U\right] \oslash \left[\tau e^T + e\tau^T\right]$$

SHP Summary

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Parameter epoch: $\Theta = \begin{bmatrix} \theta^{(1)} & \theta^{(2)} & \cdots & \theta^{(n)} \end{bmatrix}$

Gradient epoch: $G = \begin{bmatrix} g^{(1)} & g^{(2)} & \cdots & g^{(n)} \end{bmatrix}$

Mean-differences: $\hat{\Theta} = \Theta - \bar{\theta} e^T \quad \hat{G} = G - \bar{g} e^T$

Diag. covariance basis: $U \quad \text{s.t.} \quad U^T \hat{\Theta} \hat{\Theta}^T U = \text{diag}(\tau)$

$$X = \left[U^T \hat{\Theta} \hat{G}^T U + U^T \hat{G} \hat{\Theta}^T U \right] \oslash \left[\tau e^T + e \tau^T \right]$$

Approx. local gradient: $\nabla \tilde{J}(\theta) = \bar{g} + U X U^T (\theta - \bar{\theta})$

How do you choose the basis U?

The upper bound on stable learning rates is controlled by the maximum Hessian eigenvalue. We would like to **maximize the maximum eigenvalue** of

$$X = \left[U^T \hat{\Theta} \hat{G}^T U + U^T \hat{G} \hat{\Theta}^T U\right] \oslash \left[\tau e^T + e \tau^T\right]$$

but we also need to remain in a subspace for which

$U^T \hat{\Theta} \hat{\Theta}^T U$ has been sufficiently explored.

Fast heuristic: $$\max_U \left\| U^T \hat{\Theta} \hat{G}^T U + U^T \hat{G} \hat{\Theta}^T U \right\|_F^2$$

Truncated Symmetric Eigenvalue Decomp.

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We can extract leading eigenpairs from the symmetric matrix

$$\hat{\Theta}\hat{G}^T + \hat{G}\hat{\Theta}^T$$

Challenge: This could easily become a performance bottleneck. We can't afford to form the full m^2 matrix and eigenvalue decomposition ($O(m^3)$ operations).

Randomized QR with Column Pivoting

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We can efficiently approximate maximum eigenpairs using a **minor modification to the randomized truncated SVD***.

Random projection: $$B = (\Omega\hat{\Theta})\hat{G}^T + (\Omega\hat{G})\hat{\Theta}^T$$

Low-rank QRCP: $$QR = BP$$

Candidate basis: $$[U_0, R_0] = \mathrm{qr}\left(\hat{\Theta}(\hat{G}^T P) + \hat{G}(\hat{\Theta}^T P)\right)$$

Concentrate basis: $$[U_1, R_1] = \mathrm{qr}\left(\hat{\Theta}(\hat{G}^T U_0) + \hat{G}(\hat{\Theta}^T U_0)\right)$$

Final extraction with Rayleigh-Ritz:

$$(U_1^T\hat{\Theta})(\hat{G}^T U_1) + (U_1^T\hat{G})(\hat{\Theta}^T U_1) = V\,\mathrm{diag}(\xi)V^T \quad \text{then} \quad U = U_1 V_{\max}.$$

*Duersch & Gu. ***Randomized QR with Column Pivoting***. 2017.

Related Work

Efficient randomized matrix decomposition:

Xiao, Gu, & Langou. ***Fast Parallel Randomized QR with Column Pivoting Algorithms for Reliable Low-rank Matrix Approximation****. 2017.*

Feng, Xiao, & Gu. ***Low-Rank Matrix Approximations with Flip-Flop Spectrum-Revealing QR Factorization****. 2018.*

Efficient symmetric eigen-decomposition:

Duersch, Shao, Yang, & Gu. ***A Robust and Efficient Implementation of LOBPCG****. 2017.*

Stationary Distribution

We also solved the stationary distribution of fixed-rate SGD with a **quadratic objective** assuming **gradient noise is Gaussian**.

$$J(\theta) \approx J_0 + \frac{1}{2}(\theta - \bar{\theta})^T H (\theta - \bar{\theta})$$

Sample gradient covariance: $\Gamma = \mathrm{Cov}(\nabla j_{\Psi_i})$

Parameters also follow a Gaussian distribution

Parameter covariance: $\Delta = \mathrm{Cov}(\theta^{(i)})$

Requires $\alpha < 2\, h_{max}^{-1}$

$$\Delta = \alpha V \left(\Gamma \oslash \left[he^T + eh^T - \alpha hh^T\right]\right) V^T$$

where $H = V \mathrm{diag}(h) V^T$

learning rate

Validating Approximations

Another (*very expensive*) way to approximate the maximum Hessian eigenvalue uses **symmetric finite differences**.

Second-order finite difference:

$$\frac{\partial}{\partial \theta_i} \nabla J_\Psi(\theta) \approx \eta_i = \frac{1}{2\delta} \left(\nabla J_\Psi(\theta + \delta e_i) - \nabla J_\Psi(\theta - \delta e_i) \right)$$

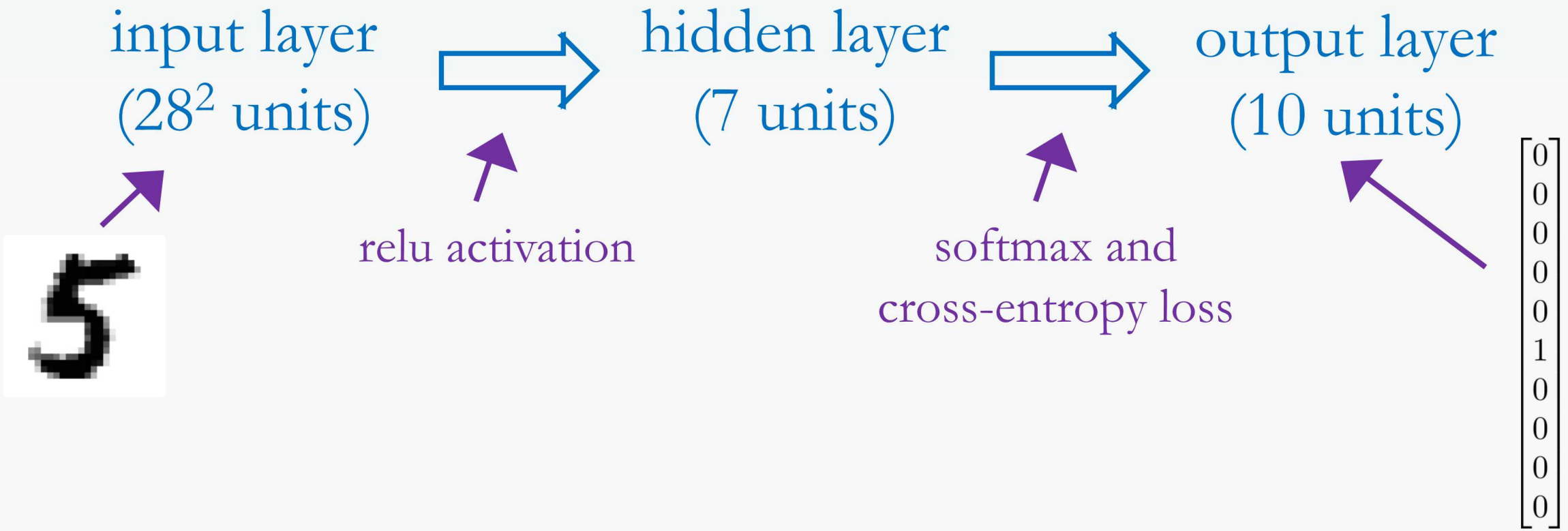
Evaluate for **all** parameters:

$$H \approx \begin{bmatrix} \eta_1 & \eta_2 & \cdots & \eta_m \end{bmatrix}$$

Then simply use the full symmetric eigenvalue decomposition.

MNIST Experiment Setup

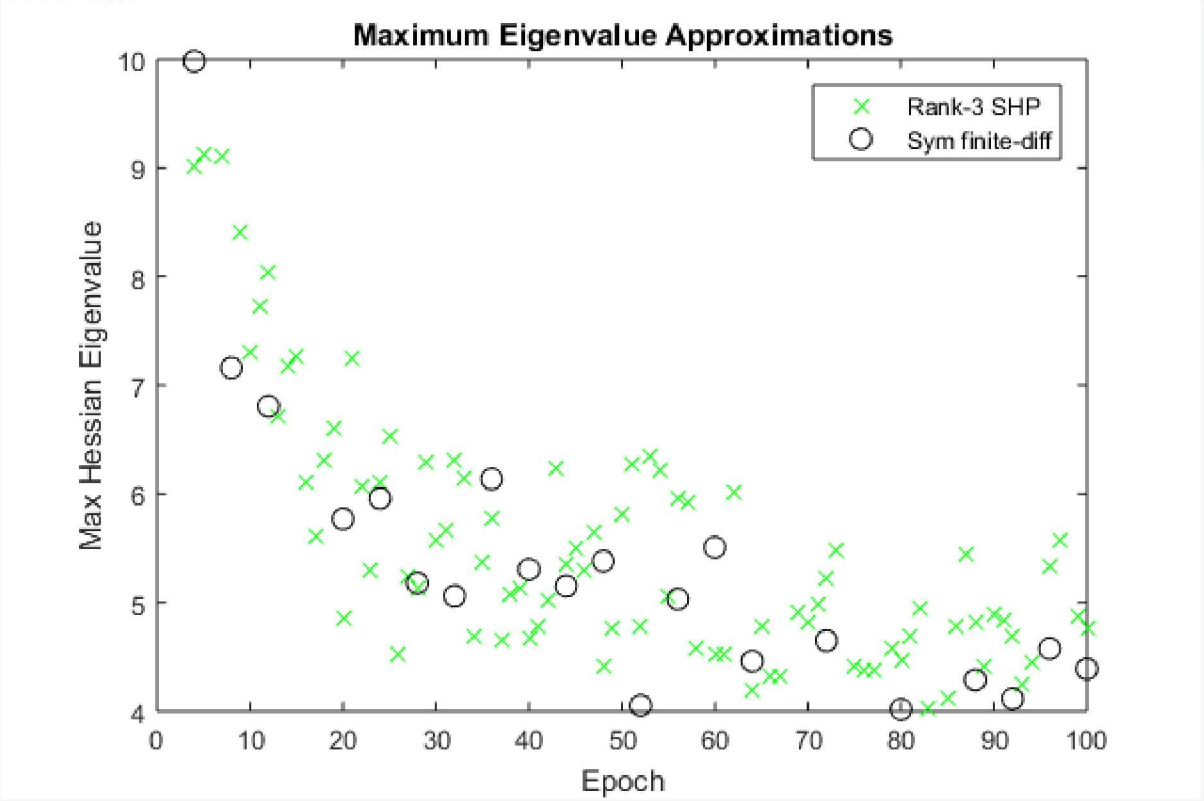
We checked SHP predictions on a simple MNIST digit classifier.



MNIST Hessian Comparison

Every 4 epochs we compute the finite-difference approximation using the same expansion point as SHP (parameter mean). We observe the same trend and spread.

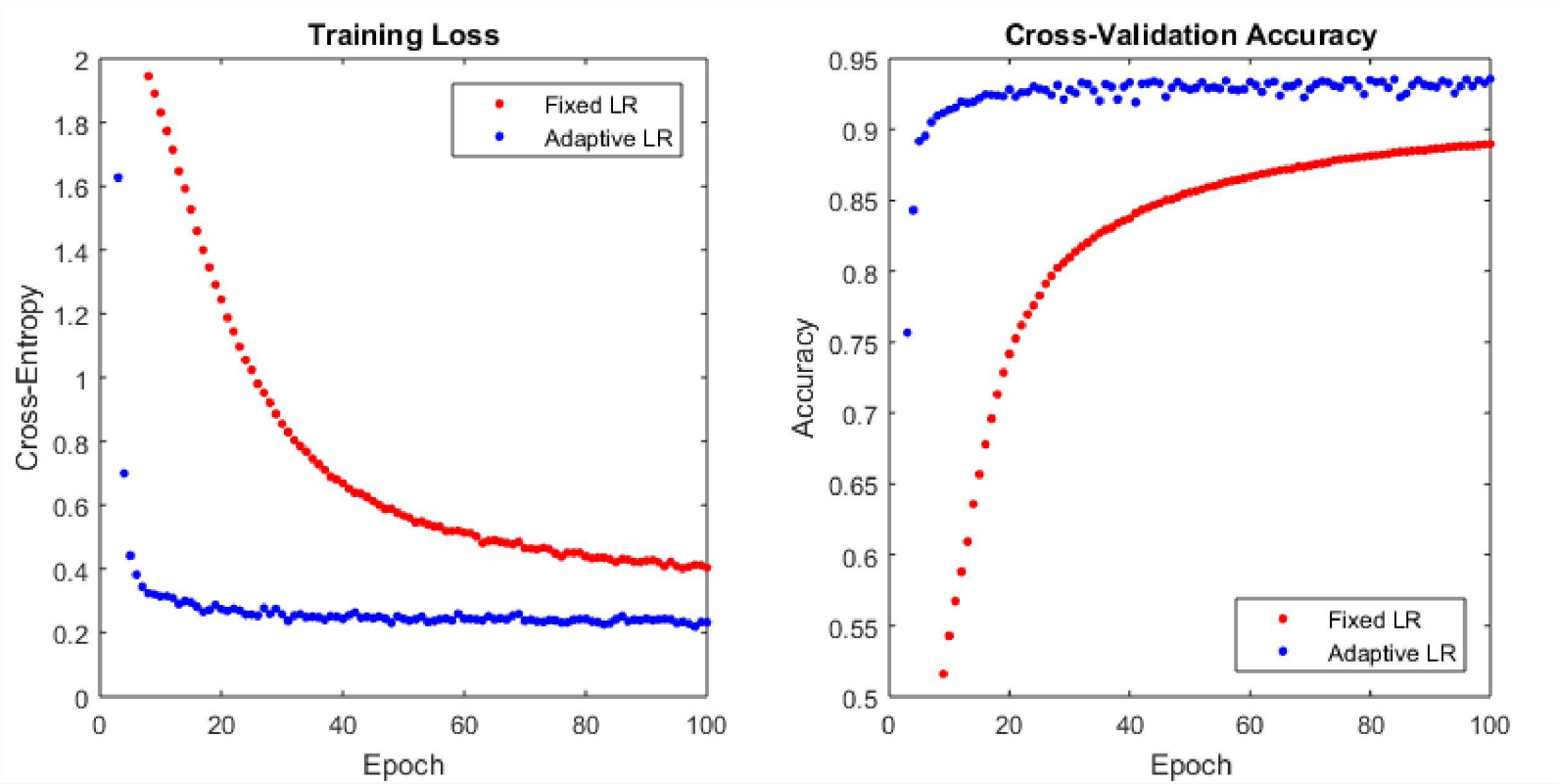
Batch size: 60
Epoch duration: 240
Initial learning rate: 0.001
Adaptive rate: $\frac{1}{2h_{max}}$
SHP rank: 3
Finite-difference samples: 800



MNIST Adaptive Learning Rate

Red points:
Fixed rate = 0.001

Blue points:
Initial rate = 0.001
Adapt target = $\frac{1}{2\,h_{max}}$



Adjusting the learning rate with SHP clearly improves convergence.

Conclusion

Stochastic Hessian Projection provides a feasible means of extracting Hessian information during optimization.

- **Negligible additional cost** over standard SGD.
- Max eigenvalue allows **dynamic learning rate** adjustment.

Questions for continuing research:

- Is there a principled way to **determine the extraction rank**?
- How do we dynamically **adjust the epoch duration**?
- Can we accelerate descent using small eigenvalues in a similar fashion to Newton-Sketch methods?

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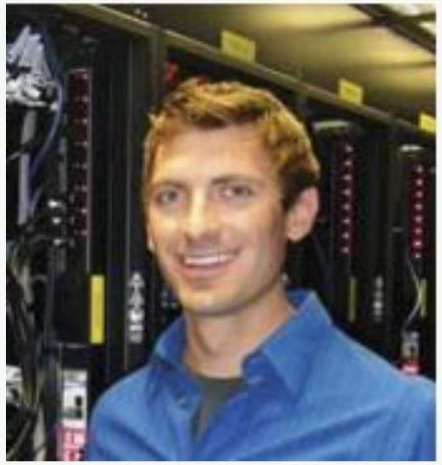

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