An Investigation into Neural Net Optimization via Hessian Eigenvalue Density

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(Joint Work with Shankar Krishnan & Ying Xiao from Google Research)

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- We present a scalable algorithm for computing **the full eigenvalue density** of the Hessian for deep neural networks.
- We leverage this algorithm to study the effect of architecture / hyper-parameter choices on the optimization landscape.

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- We focus on estimating the empirical distribution of λ_i as a concrete way to study the loss curvature.

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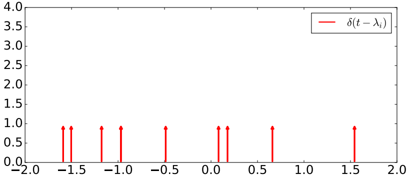

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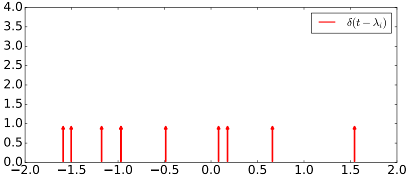

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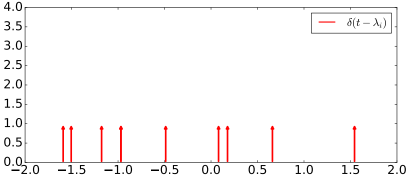

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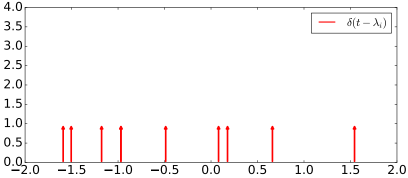

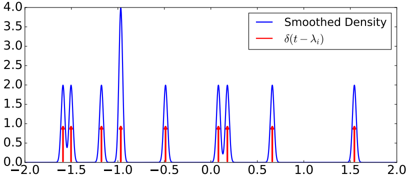

Estimating the Smoothed Density

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- Use $g(x) = f_\sigma(t - x)$:

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Algorithm Sketch

Stochastic Draw $v \sim \mathcal{N}(0, \frac{1}{n} I_n)$

Lanczos

1. Compute a basis for $\{v, Hv, \cdots, H^{m-1} v\}$. Call this basis V.
2. Let $T = V^T H V$

Quadrature

1. Diagonalize $T = UDU^T$.
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- Calculating $(w_i, \ell_i)_{i=1}^m$ takes $O(m \times \text{model size} \times \text{dataset size})$. In practice, $m \approx 100$ is more than enough.
- Explicitly calculating the eigenvalues takes $O(\text{model size}^2 \times \text{dataset size})$.

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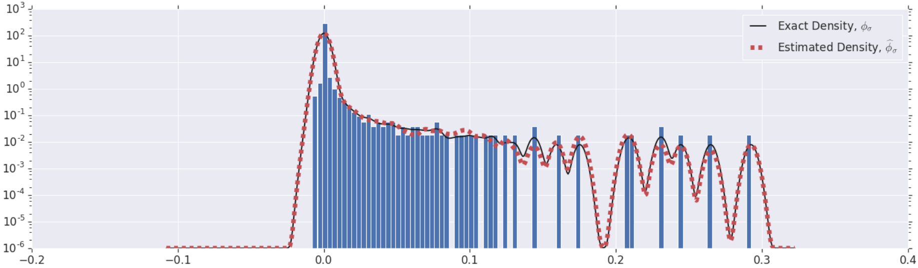

Figure: Comparison of a degree 90 quadrature approximation with the actual Hessian density. The Hessian is calculated from a 2-layer network with 15910 parameters trained on MNIST.

Let's Train a ResNet-32

- 460K parameters.
- Trained on CIFAR-10.
- The network has Batch-Normalization (Ioffe and Szegedy (2015)).

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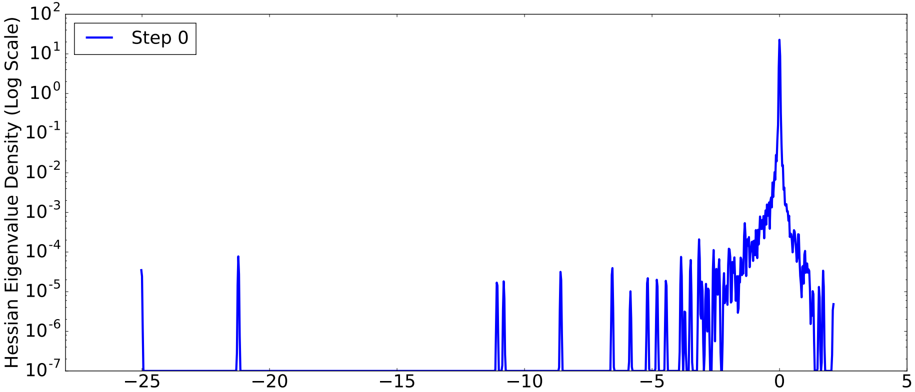

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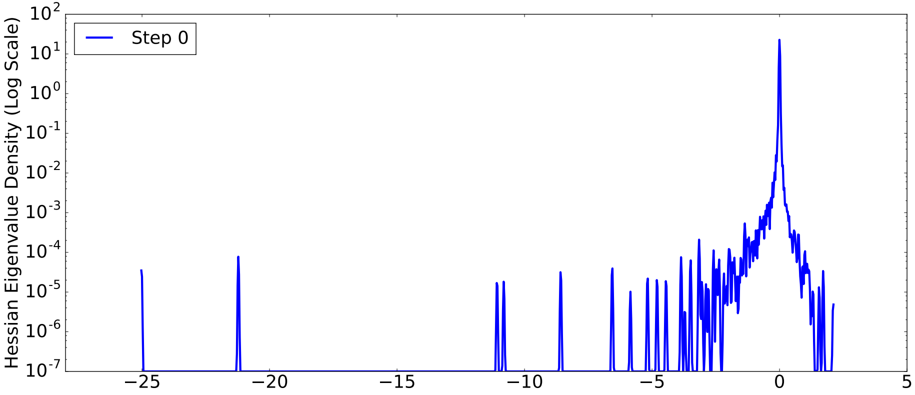

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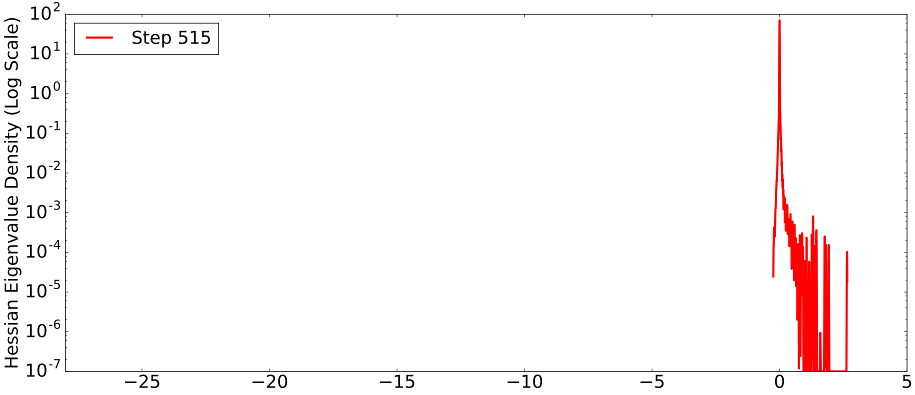

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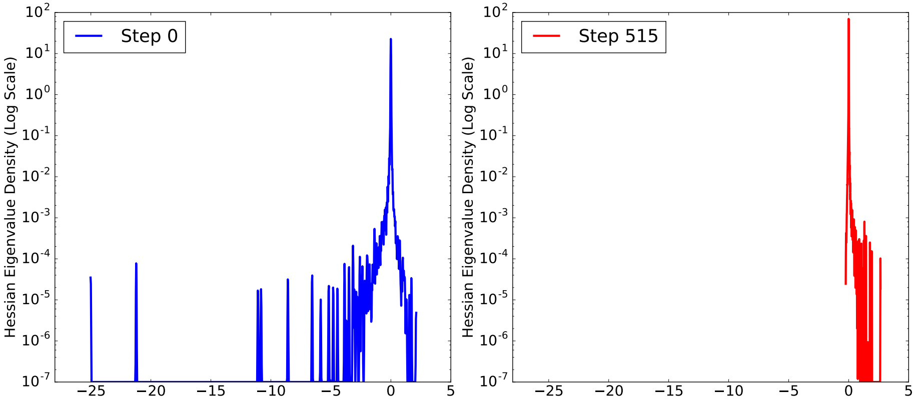
- For small datasets such as CIFAR-10 / MNIST, negative directions disappear extremely fast.



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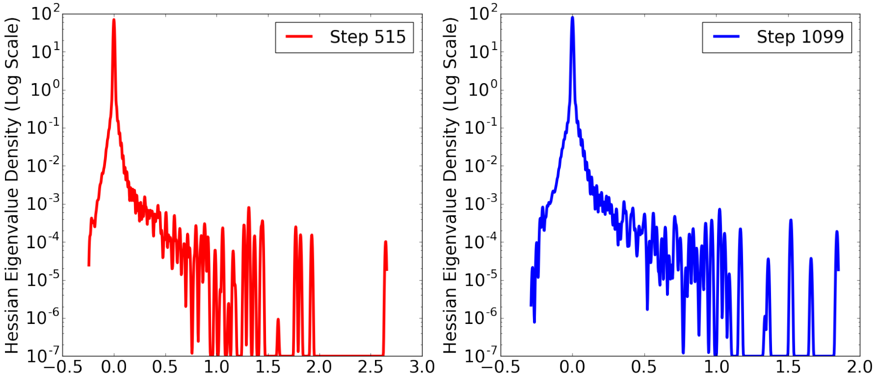

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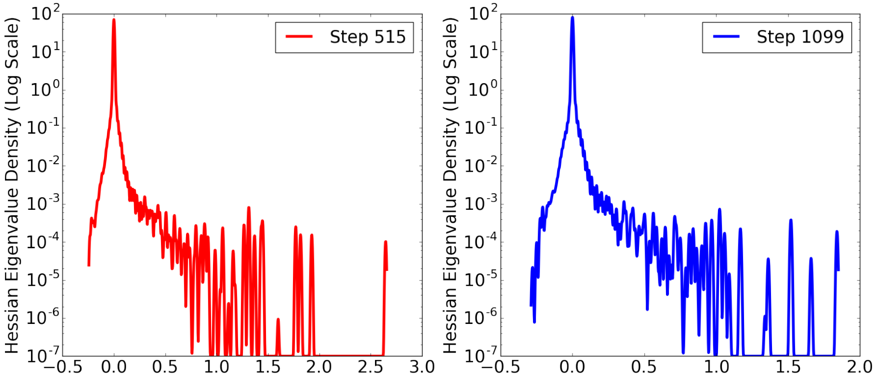

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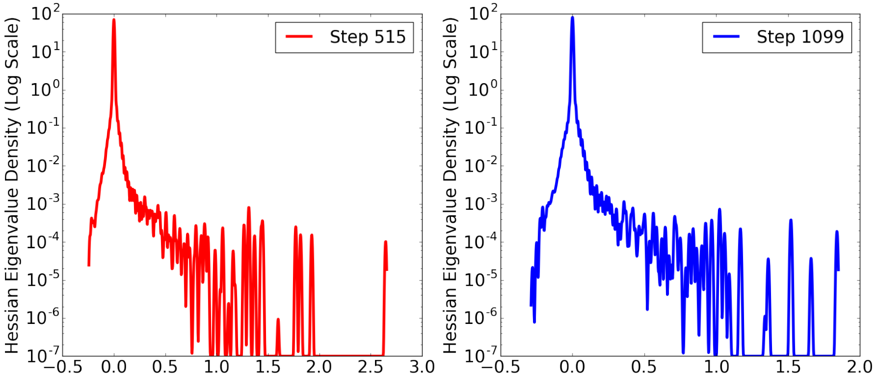

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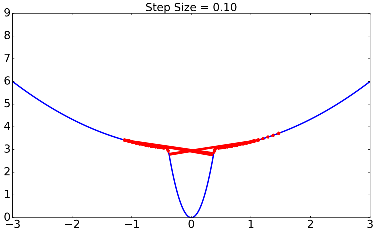

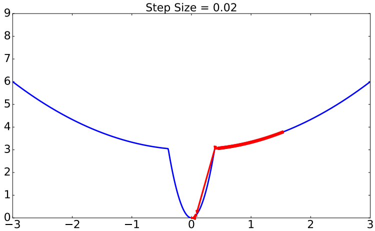

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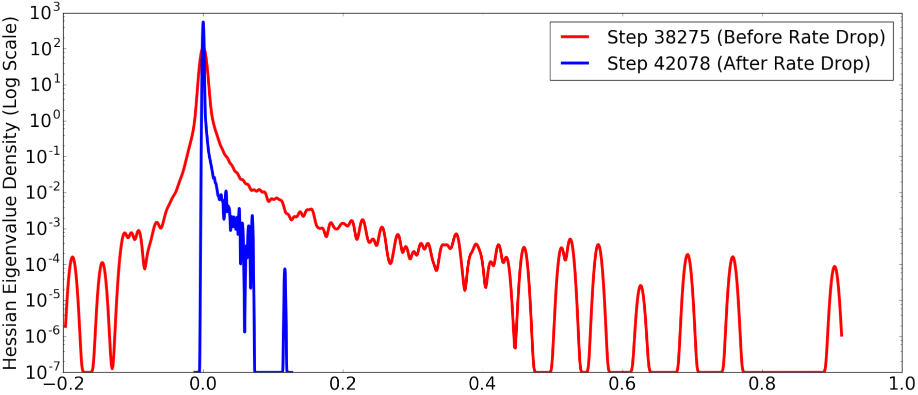

Figure: Learning rate is reduced by a factor of 10 at step 40k. Surprisingly, the top eigenvalue also decreases.

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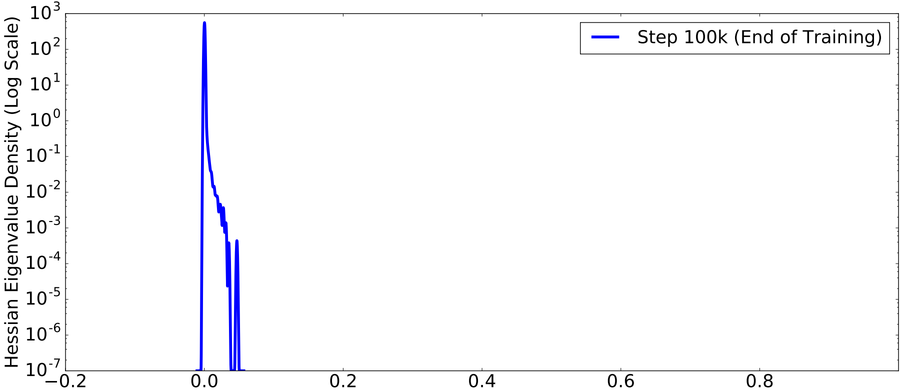

Figure: Spectrum of the Hessian after $100k$ steps of training. The smallest eigenvalue is ≈ -0.0006.

Examining the Role of Architecture

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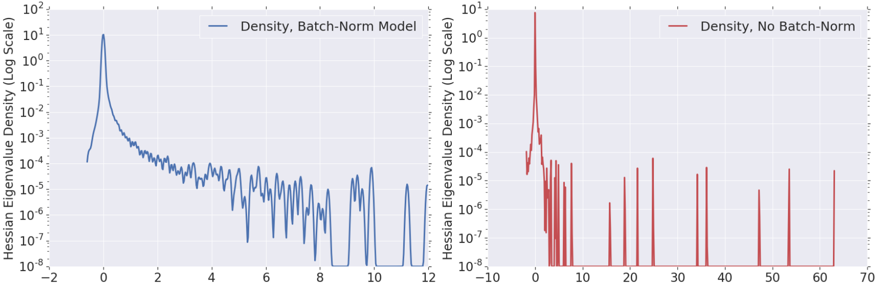

Figure: Spectrum of the Hessian after $7k$ steps of training. Outlier eigenvalues appear when BN is removed from the network.

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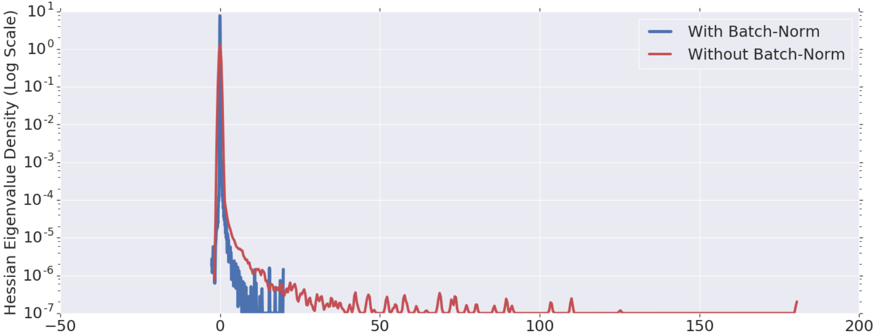

Figure: The eigenvalue comparison of the Hessian of Resnet-18 trained on ImageNet dataset. Model with BN is shown in blue and the model without BN in red. The Hessians are computed at the end of training.

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- Let's test this assertion!

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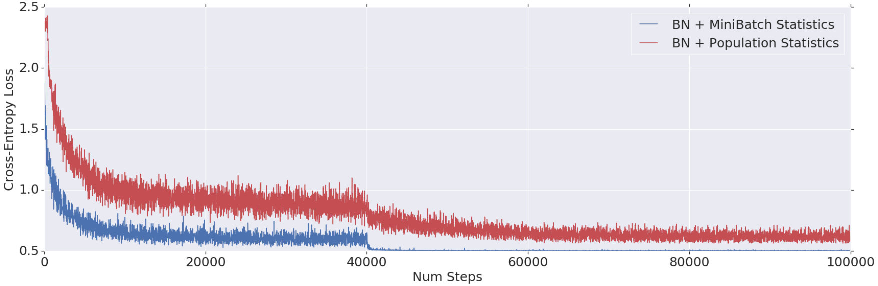

Figure: Optimization progress (in terms of loss) of batch normalization with mini-batch statistics and population statistics.

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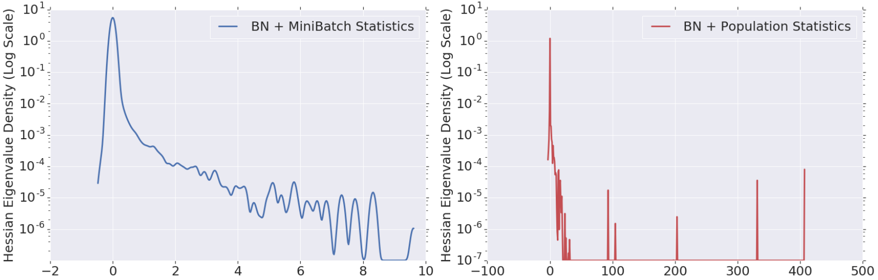

Figure: The Hessian spectrum for a Resnet-32 after 15k steps. On the left BN is using mini-batch statistics. The network on the right is using population statistics.

Any Questions?

Hope to see you at our poster session today (06:30 to 09:00 at Pacific Ballroom #51)

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