Measurements of Three-Level Hierarchical Structure in the Outliers in the Spectrum of Deepnet Hessians

Vardan Papyan

Department of Statistics
Stanford University

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- Hessian:

$$\mathrm{Hess}(\theta) = \mathrm{Ave}_{i,c}\left\{\frac{\partial^2 \ell(f(x_{i,c};\theta); y_c)}{\partial\theta^2}\right\}$$

- Gauss-Newton decomposition:

$$\mathrm{Hess} = G + H$$

Previous work: LeCun et al. (1998)

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  - Bulk+outliers
  - Number of outliers number of classes

This work

What is causing the outliers in the spectrum?

G is a second moment of gradients with structure on ind

- De ne the gradient:

$$ {}_{i;c;c'}{}^{T} = \sqrt{p_{c'}(x_{i;c}; \ )}\,(y_{c'} \quad p(x_{i;c}; \ ))^{T} \frac{\partial f(x_{i;c}; \ )}{\partial} $$

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$$ {}_{i;c;c^0}{}^T = \sqrt{p_{c^0}(x_{i;c};\ )}\,(y_{c^0} \quad p(x_{i;c};\ ))^T \frac{@f(x_{i;c};\ )}{@} $$

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- These gradients can be indexed by three numbers:

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- Define the gradient:

$$\psi_{i,c,c'}^T = \sqrt{p_{c'}(x_{i,c};\theta)}\,(y_{c'} - p(x_{i,c};\theta))^T \frac{\partial f(x_{i,c};\theta)}{\partial \theta}$$

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- These gradients can be indexed by three numbers:
  - i: observation
  - c: true class
  - c^0: potential class
- G is a second moment (not Covariance) of these gradients:

$$G = \mathrm{Ave}_{i,c,c^0} \left\{ {}_{i,c,c^0} \; {}^T_{i,c,c^0} \right\}$$

Three-level hierarchical structure in gradients

- Averaging over the index i

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- Averaging over the index i
- Averaging over the index x^0

Three-level hierarchical structure in gradients

- Averaging over the index i
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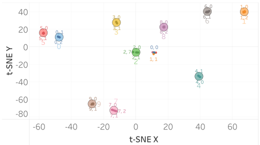
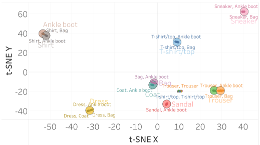
Visualization of three-level hierarchical structure in grad

Figure: ResNet50 trained on ImageNet. Large circles: c. Small circles: $c;c^0$.

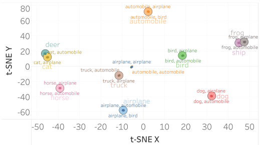
Visualization of three-level hierarchical structure in gradients



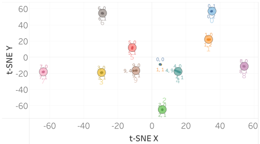
MNIST, 13 examples per class



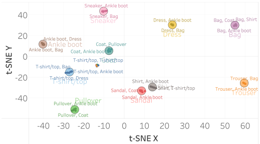
Fashion, 13 examples per class



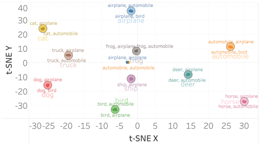
CIFAR10, 13 examples per class



MNIST, 702 examples per class



Fashion, 702 examples per class



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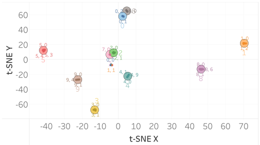
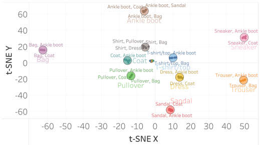
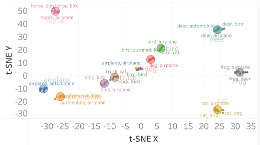


MNIST, 5000 examples per class



Fashion, 5000 examples per class



CIFAR10, 5000 examples per class

Ave$_c$ $_c$ ^T_c causes outliers in $\boldsymbol{G}$

Figure: ResNet18 trained on CIFAR10, 1351 examples per class. Orange: eigenvalues of Ave$_c$ $_c$ ^T_c .