Neural Networks Loss Landscape Convergence in Hessian Low-Dimensional Space

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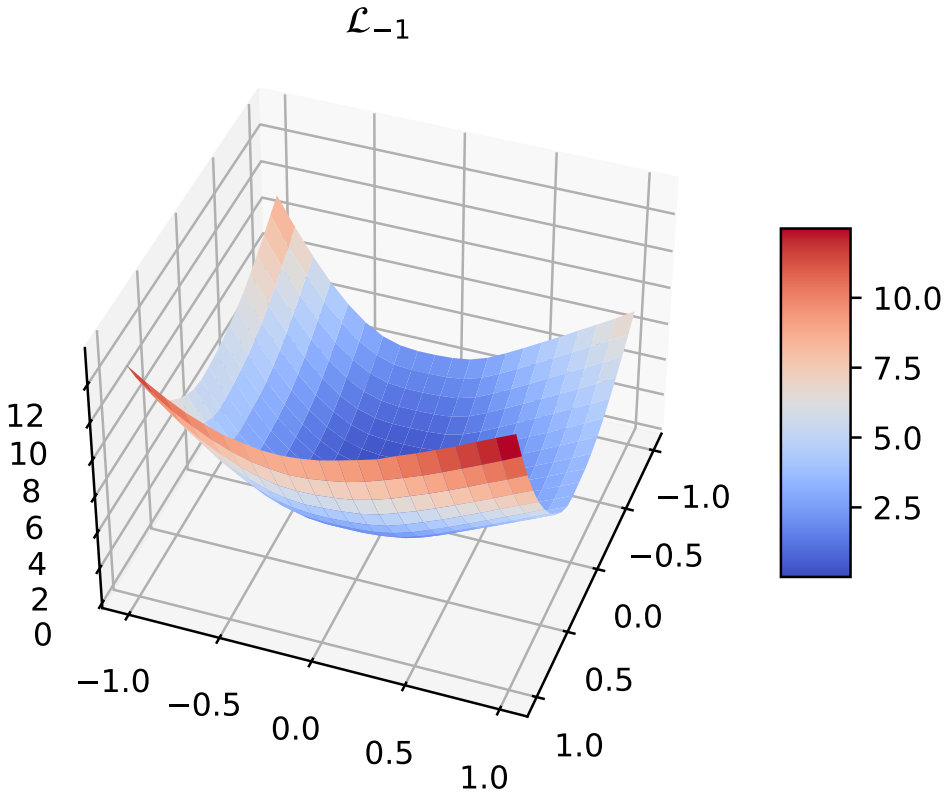
Neural Networks Loss Landscape Convergence in Hessian Low-Dimensional Space

Goals and Tasks

1. Study how neural network loss landscape changes with dataset size
2. Define and measure metrics Δ_k
3. Derive theoretical bound for Δ_k via top-d eigenvalues
4. Propose an algorithm to determine the Δ-sufficient dataset size

Loss landscape stabilizes after sufficient sample size.



Hessian projection onto top-d eigenvectors

Monte Carlo estimate of $\Delta_k^{emp} = \mathbb{E}\Big(\mathcal{L}_{k+1} - \mathcal{L}_k\Big)^2$.

Analytical bound: $\Delta_k^{th} \geq \Delta_k^{emp}$

Detect dataset threshold k^*

Problem Statement

Hypothesis

Beyond some k^*, adding new samples changes the local loss landscape by less than a tolerance Δ_{tol}, i.e. $\forall\, k \geq k^* :\ \Delta_k < \Delta_{tol}$.

Model

MLP with ReLU activations for K-class classification

Empirical loss: $\mathcal{L}_k(\mathbf{w}) = \frac{1}{k} \sum_{i=1}^{k} \ell_i(\mathbf{w})$

Hessian: $\mathbf{H}_k(\mathbf{w}) = \nabla^2_{\mathbf{w}} \mathcal{L}_k(\mathbf{w})$

Criteria

Convergence rate: $\Delta_k = O(1/k^2)$

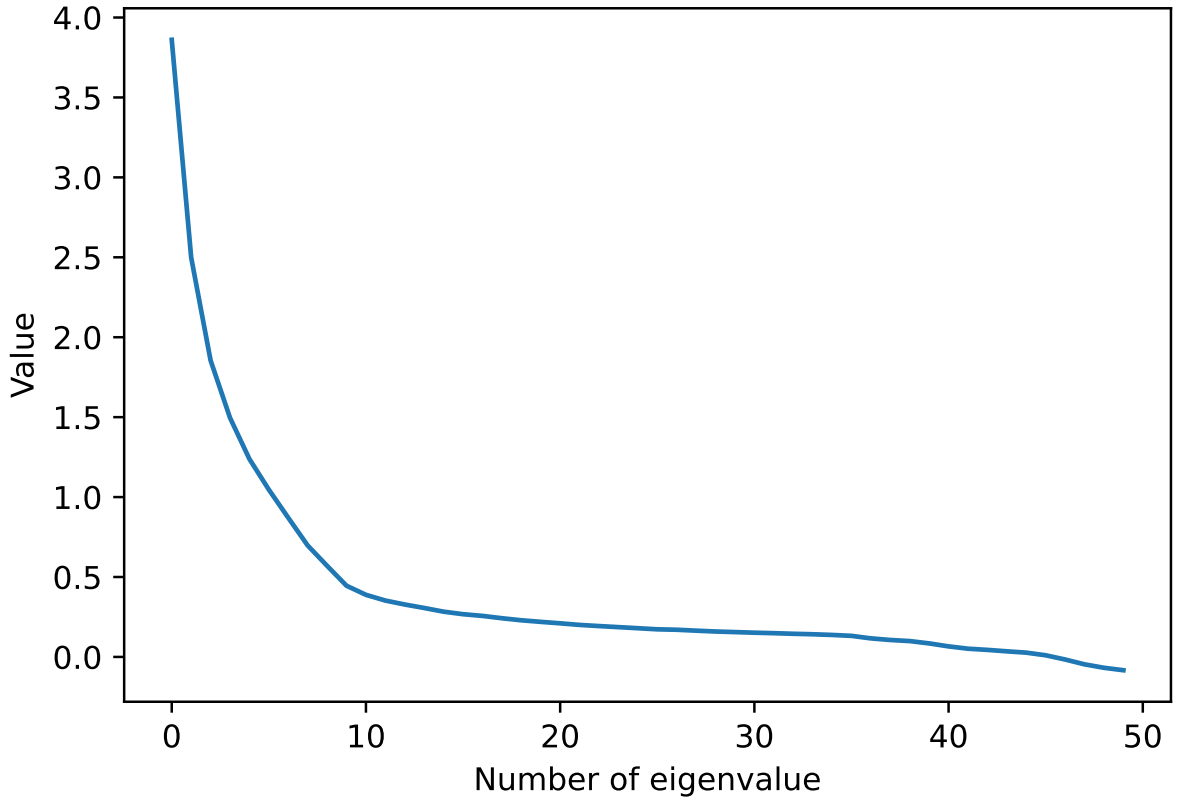
Theoretical bound via top-d eigenvalues upper-bounds empirical Δ_k

Plateau in eigenvalue differences $\lambda_i^{k+1} - \lambda_i^k$ indicates threshold

Theoretical Analysis

Project parameters:
$\mathbf{w} = \mathbf{w}^* + \mathbf{P}\boldsymbol{\theta}$,
$\mathbf{P} = [\mathbf{e}_1, \ldots, \mathbf{e}_d]$

Taylor approx:
$\mathcal{L}_k(\mathbf{w}^* + \mathbf{P}\boldsymbol{\theta}) \approx$
$\mathcal{L}_k(\mathbf{w}^*) + \frac{1}{2}\boldsymbol{\theta}^\top \boldsymbol{\Lambda}_k \boldsymbol{\theta}$



Eigenvalue decay

Bound: $\Delta_k \approx \frac{\sigma^4}{4}\left(2\sum_{i=1}^{d}(\lambda_{k+1}^i - \lambda_k^i)^2 + \left(\sum_{i=1}^{d}(\lambda_{k+1}^i - \lambda_k^i)\right)^2\right)$.

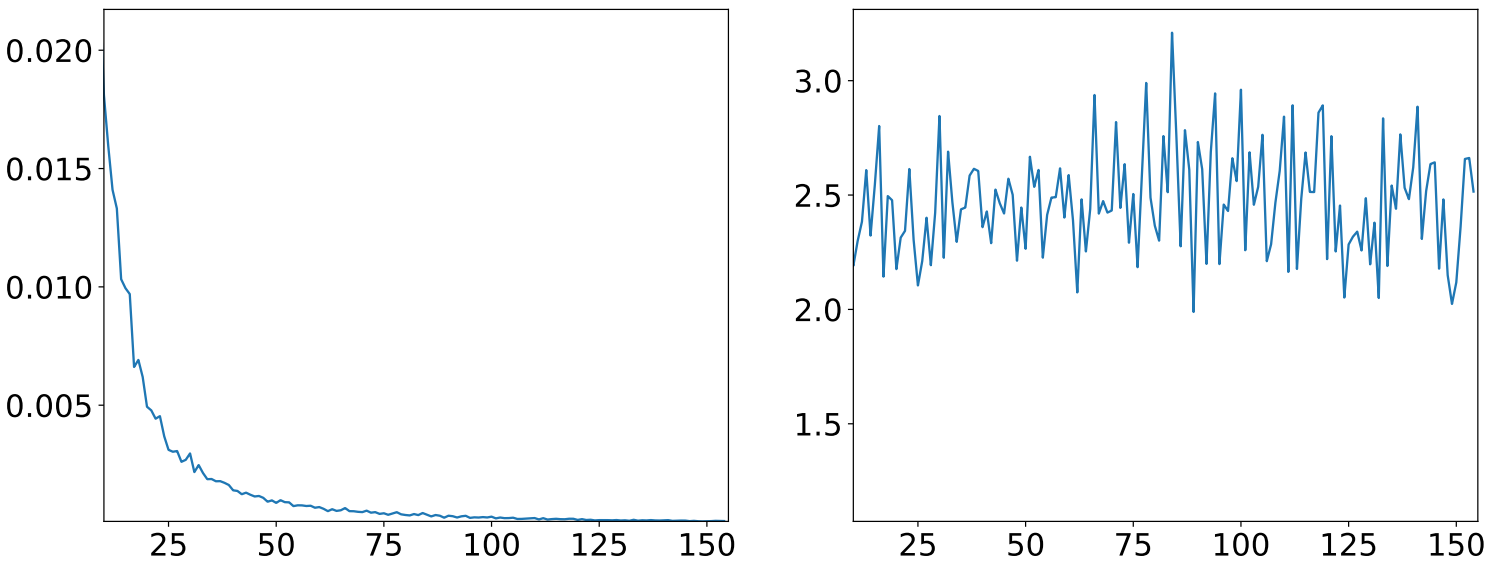
Computational Experiment

Datasets: MNIST, Fashion-MNIST (60k train, 10k test)

MLP: 2 hidden layers, $\sim 10^5$ parameters

Subspace dimension $d = 10$, Monte Carlo samples $K = 64$, $\sigma = 1$

Compare empirical Δ_k vs theoretical bound across k



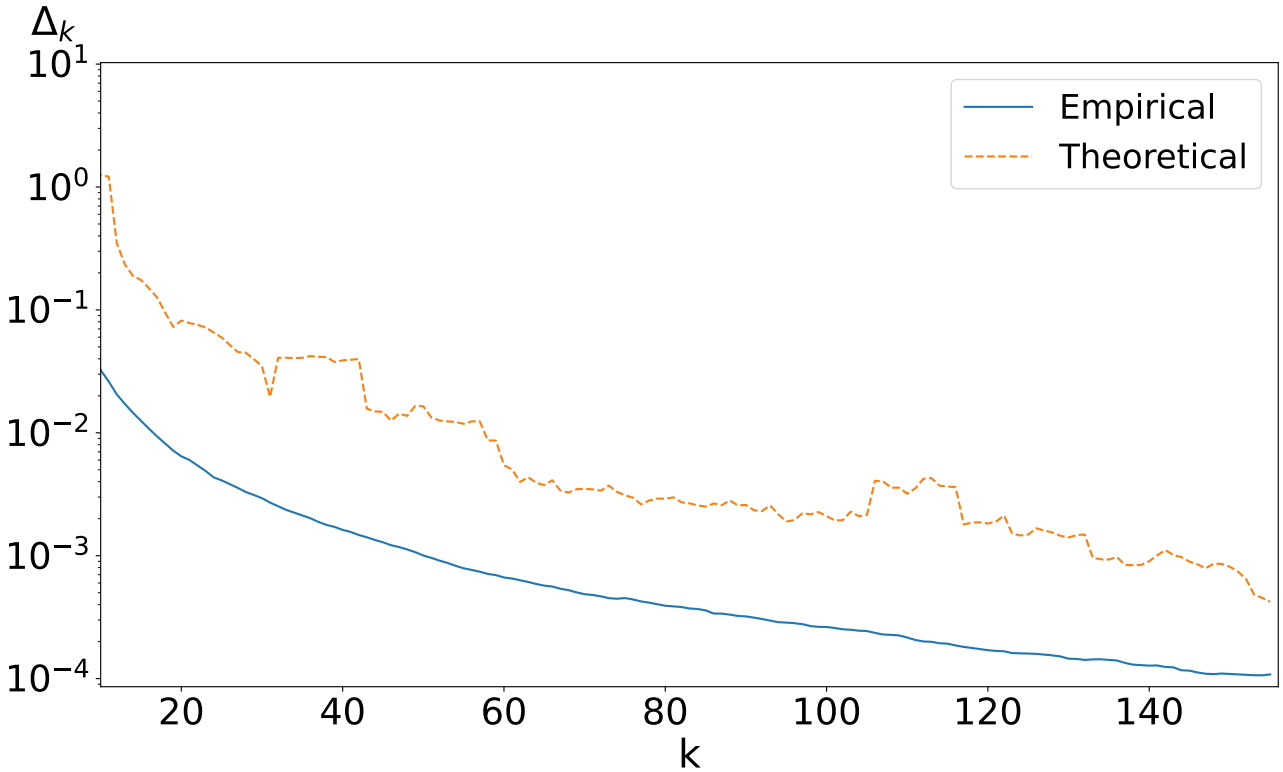
Monte Carlo Δ_k vs k and $\Delta_k \cdot k^2$

Combining results

Empirical Δ_k consistently below theoretical estimate

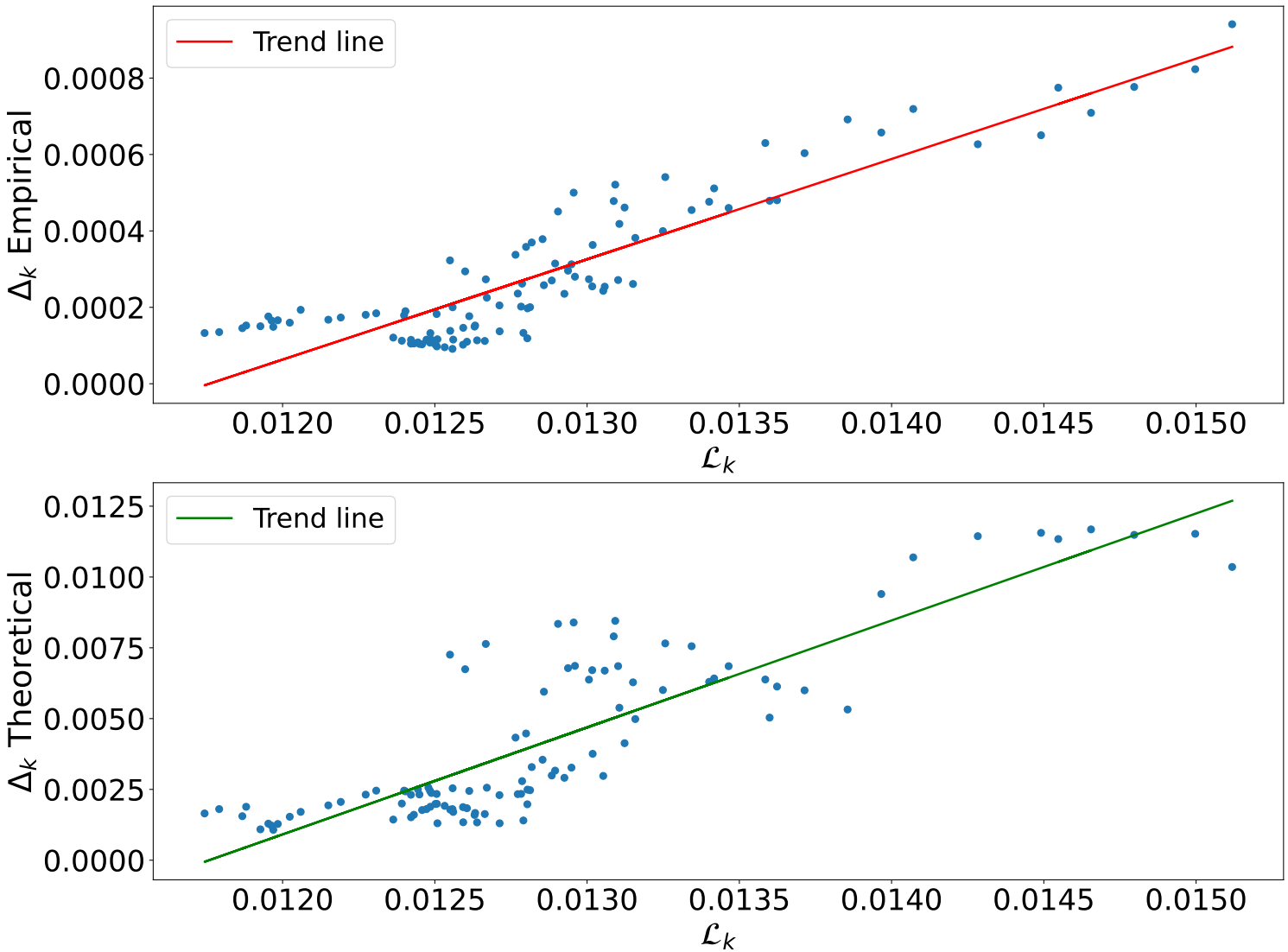
Gap due to neglected eigen-modes beyond top-d

Monte Carlo variance decreases with sample size K



Theoretical (dashed) vs empirical (solid) Δ_k

Theoretical vs. Empirical Δ_k



Practical Measurements

Dataset	**Model**	Δ	k	L_k	**Time (s)**
MNIST	Single-layer MLP	0.025	100	0.013	2000
	Multi-layer MLP	0.025	40	0.010	3500
	Convolutional CNN	0.025	60	0.024	1800
Fashion-MNIST	Single-layer MLP	0.030	120	0.020	2100
	Multi-layer MLP	0.030	90	0.017	4400
	Convolutional CNN	0.030	70	0.015	2400

Algorithm: Δ-sufficient Dataset Size

Algorithm 1: Determine Δ-sufficient dataset size

1. Initialize dataset $D \leftarrow \emptyset$ and batch counter $k \leftarrow 0$.
2. **Repeat:**

   $k \leftarrow k + 1$.
   Sample a new batch of data and append to D.
   Train or update model on D.
   Compute top-d Hessian eigenvalues $\{\lambda_k^{(i)}\}_{i=1}^{d}$ and $\{\lambda_{k+1}^{(i)}\}$.
   Estimate

$$\Delta_k \approx \frac{\sigma^4}{4}\left(2\sum_{i=1}^{d}(\lambda_{k+1}^{(i)} - \lambda_k^{(i)})^2 + \left(\sum_{i=1}^{d}(\lambda_{k+1}^{(i)} - \lambda_k^{(i)})\right)^2\right).$$

3. **Until** $\Delta_k < \Delta_{\text{tol}}$.
4. **Return** $|D|$, the Δ-sufficient sample size.

Summary

Results

1. Loss landscape stabilizes.
2. Hessian-based bound provides a reliable upper-bound for Δ_k.
3. Proposed a practical algorithm for Δ-sufficient dataset sizing.
4. Offers guidelines for dataset collection and early stopping.

Future work

1. Test the method on additional architectures.
2. Evaluate the approach on other datasets.
3. Incorporate automatic selection of the optimal number of Hessian eigenvalues.

Literature

1. Wu *et al.* (2017): loss landscapes vs dataset size
2. Sagun *et al.* (2018): Hessian low effective rank
3. Li *et al.* (2018): visualizing loss surfaces
4. Ghorbani *et al.* (2019): eigenvalue density analysis
5. Bousquet & Elisseeff (2002): stability and generalization bounds