Sampling-based Inference for Large Linear Models, with Application to Linearised Laplace

Cambridge NeurIPS Meetup, Dec. 8 2023 Shreyas Padhy





Bayesian Linear Models are very useful in many fields!

- 1. Uncertainty Estimation in NNs (through linearisation)
- 2. Climate Prediction, Economics, Geology, Computational Biology
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Solution: We cast inference and hyperparameter selection as a sequence of quadratic optimisation problems. We can solve these relatively easily for high dimensional problems with *roughly* linear scaling.

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- Approximate the predictive distribution of the NN as

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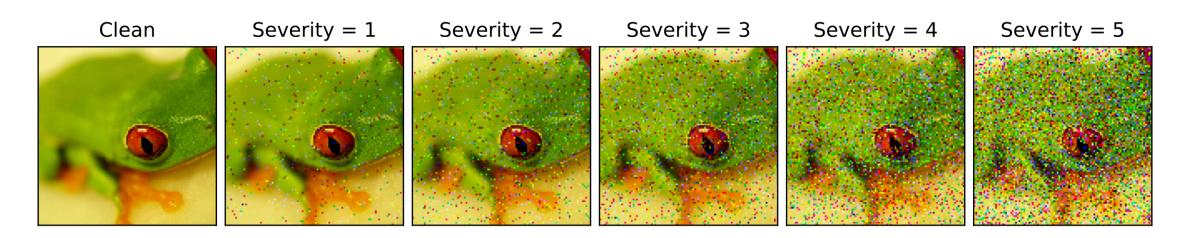
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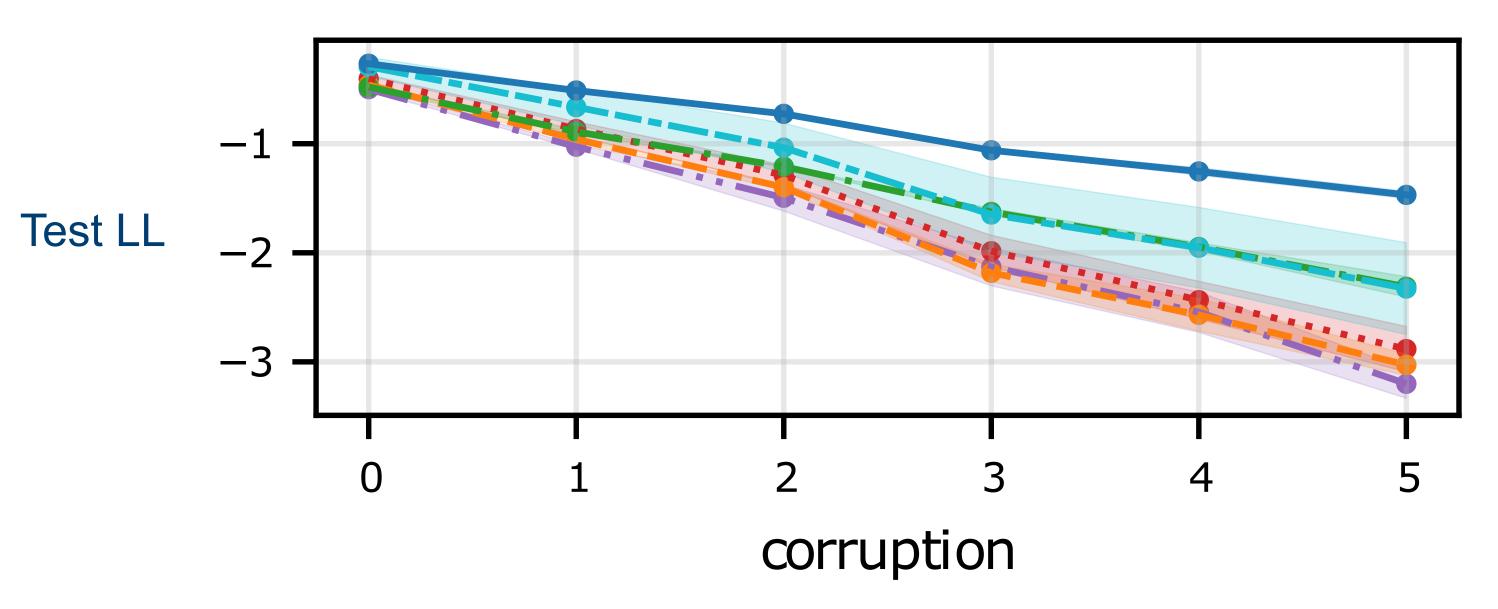
• We can generalise this to non-Gaussian likelihoods (i.e. classification) by 'Gaussianising' with the **Laplace** approximation

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Linearised NNs work well

Corrupted CIFAR10 (Ovadia 2019)







Model: ResNet-18 with **11M** weights

Inference: Lin Laplace Subnetwork (Daxberger et. al. 2021)

"Bayesian Deep Learning via Subnetwork Inference"

Baselines:

- MAP
- Diagonal Laplace
- MC Dropout (Gal 2016)
- Deep Ensembles (Lakshminarayanan 2017)
- SWAG (Maddox 2019)



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d > 1*e*6 Number of parameters is large d > 1e6Observation space is large $n \cdot m > 1e6$

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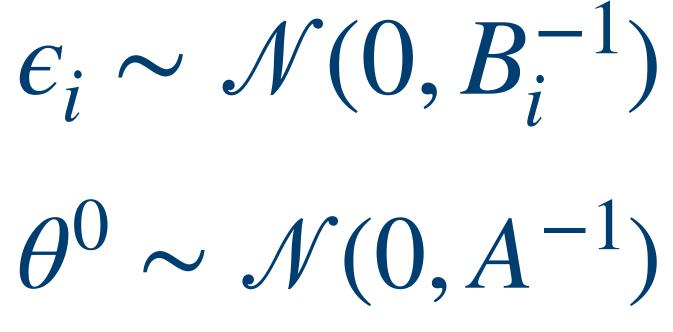
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$$L(z) = \sum_{i=1}^n \|\epsilon_i - \phi(x_i)z\|_{B_i}^2$$

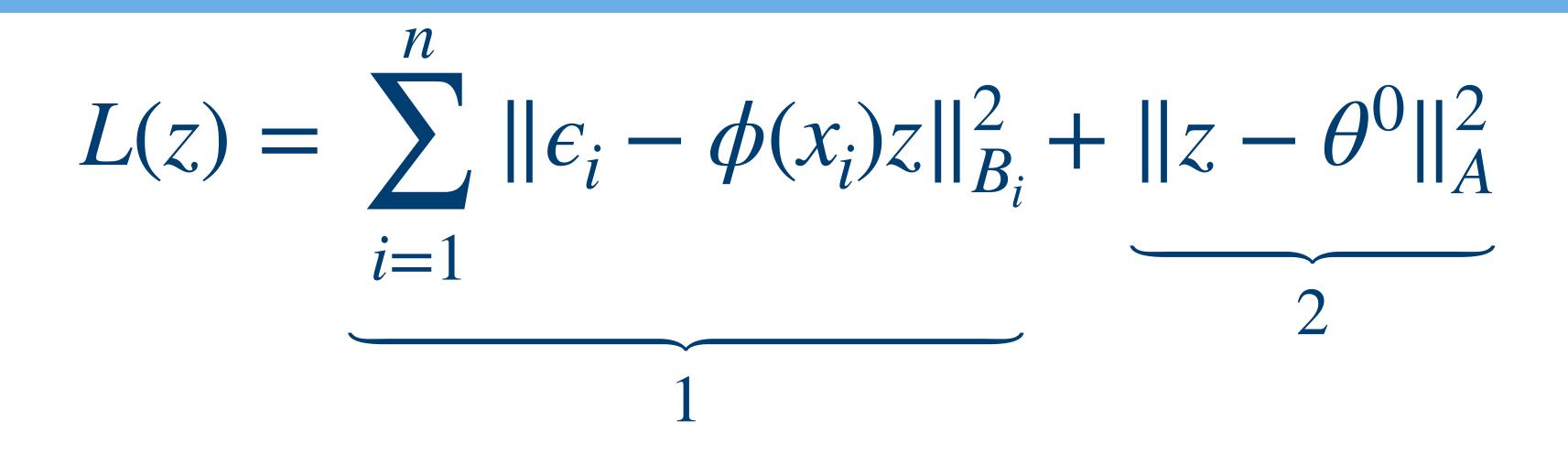
1. Noise-fit term.

- - Very large variance when estimated stochastically.
- 2. Regularisation term.
 - •We can compute its gradient in closed form.

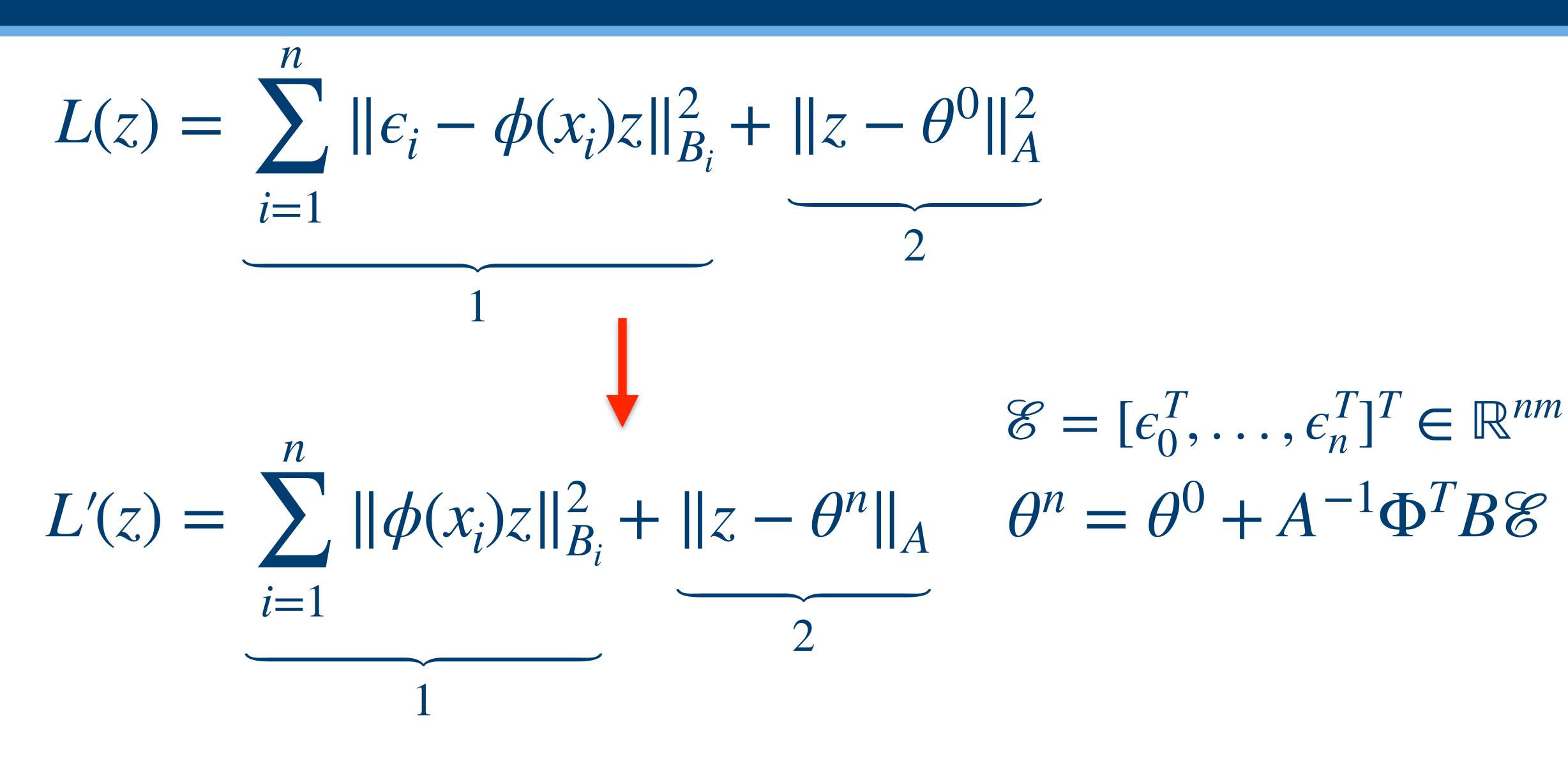
$\operatorname{rgmin}_{7} L(z)$ $\epsilon_i \sim \mathcal{N}(0, B_i^{-1})$ $+ \|z - \theta^0\|_A^2$ $\theta^0 \sim \mathcal{N}(0, A^{-1})$ 2

Depends on each observation's feature expansion so it needs to be minibatched.



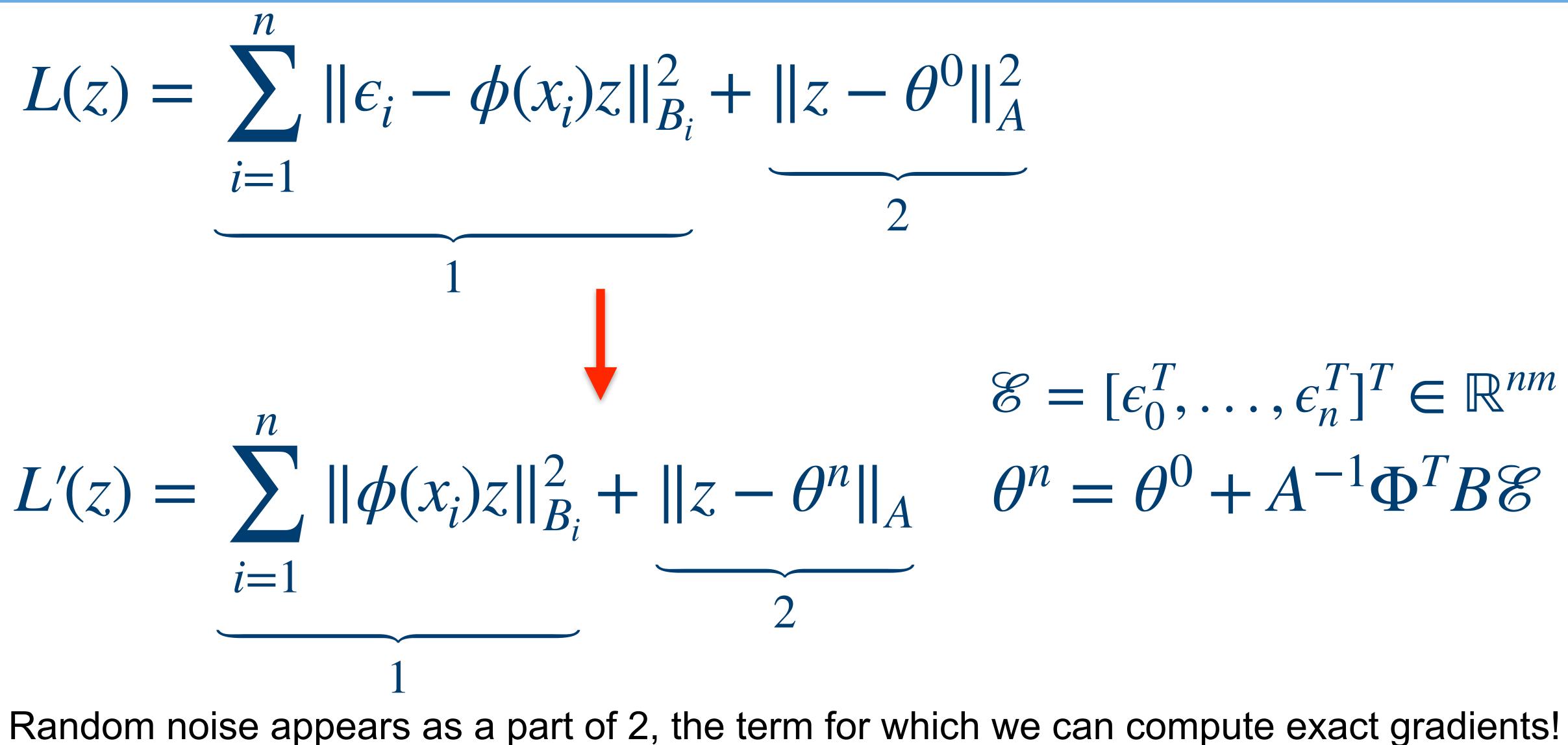










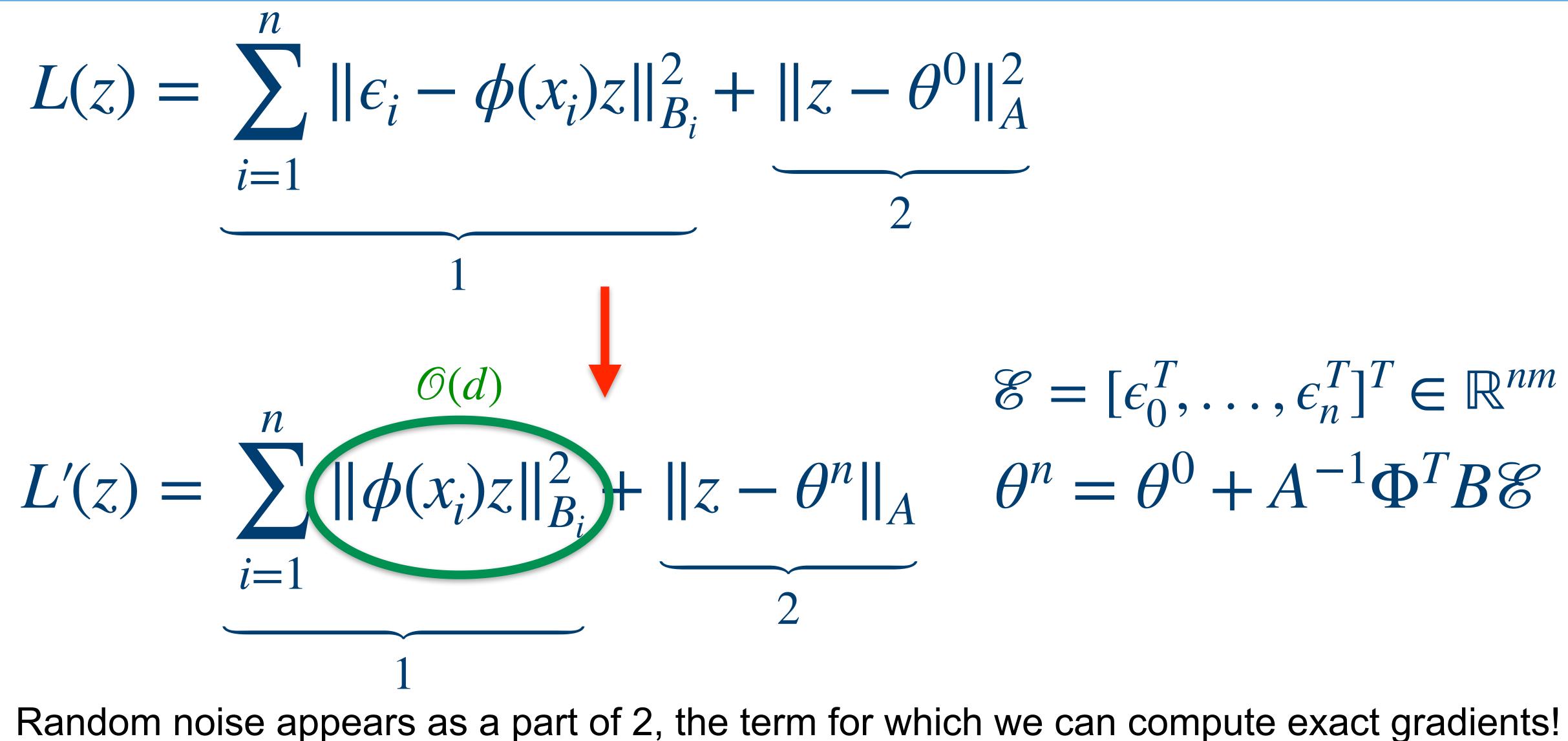
















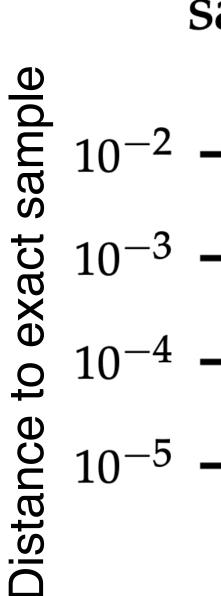




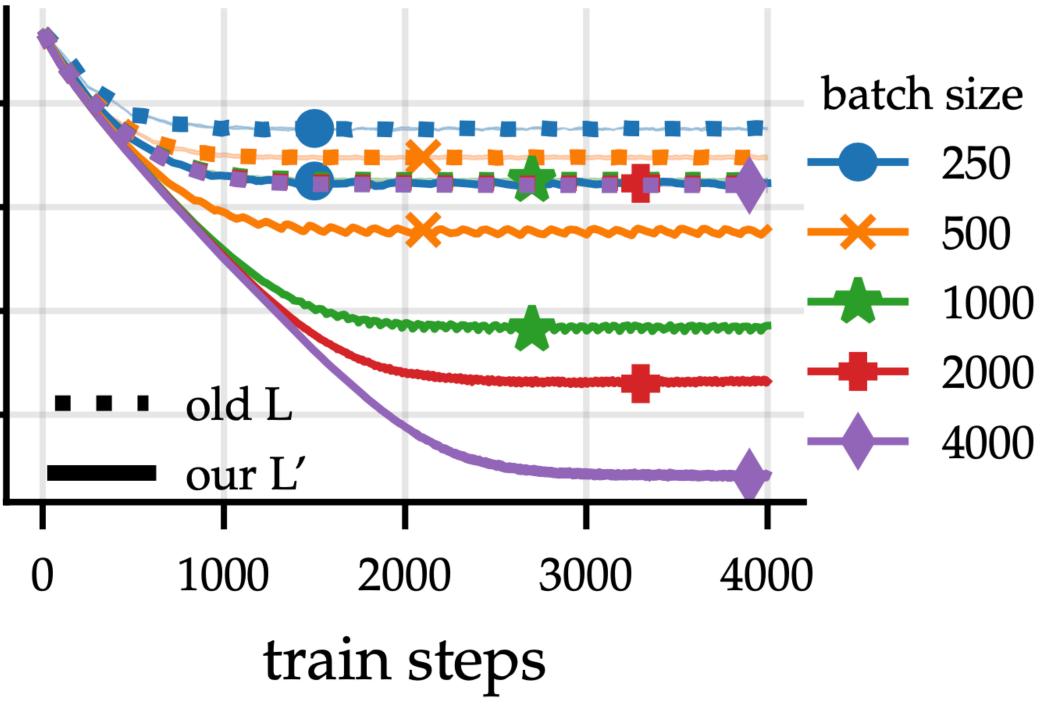


$$L(z) = \sum_{i=1}^{n} \|e_i - \phi(x_i)z\|_{B_i}^2 + \|z - \theta^0\|_A \qquad L'(z) = \sum_{i=1}^{n} \|\phi(x_i)z\|_{B_i}^2 + \|z - \theta^n\|_A$$

Both objectives are equal (L(z) = L'(z)) but their mini-batch estimators have different variances!



- sample error norm vs batch size

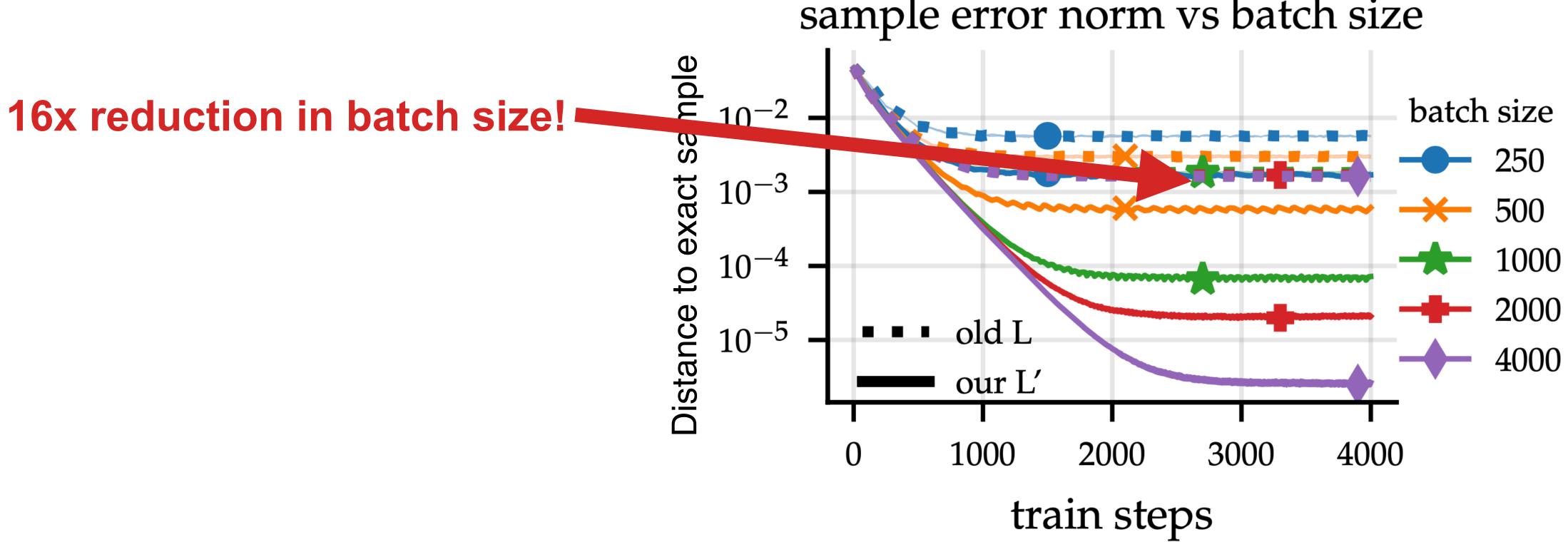






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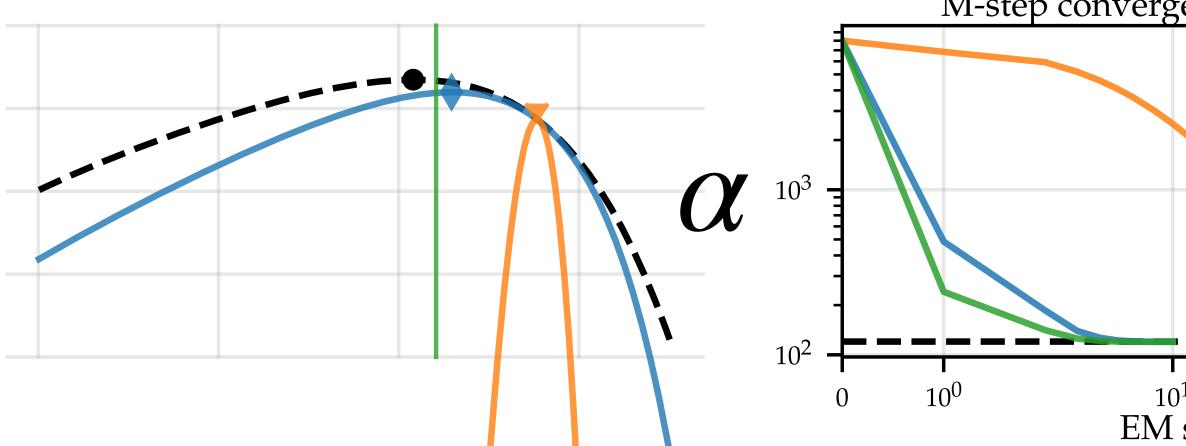
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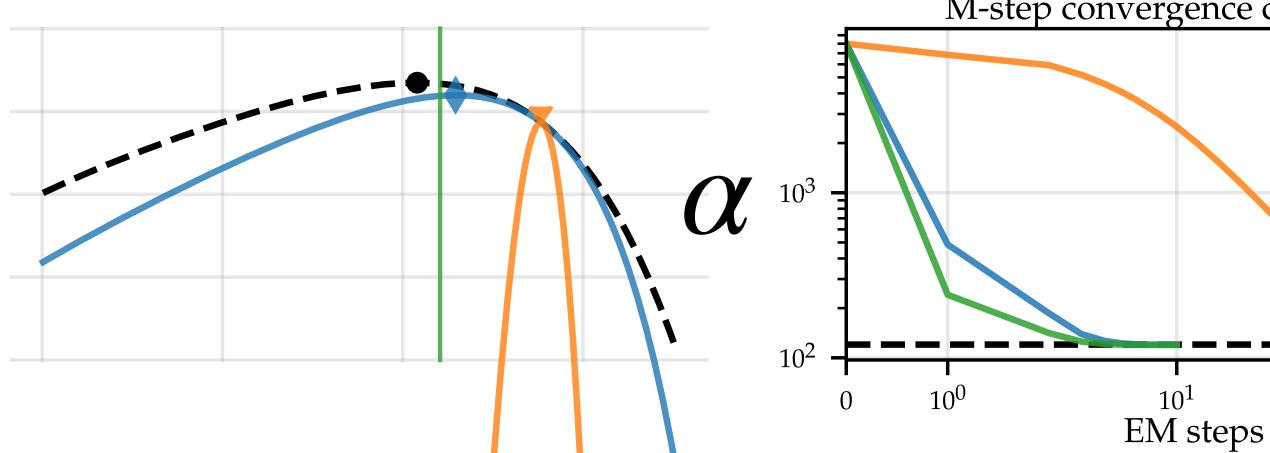
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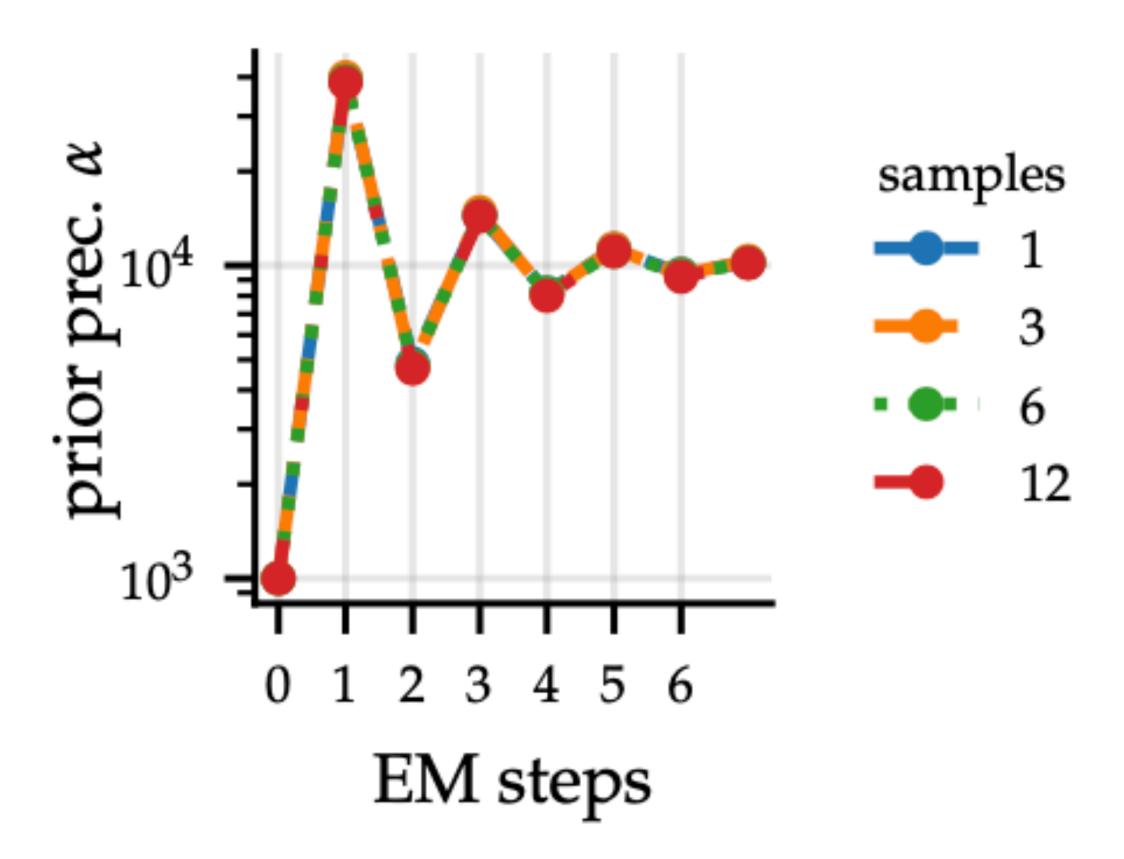
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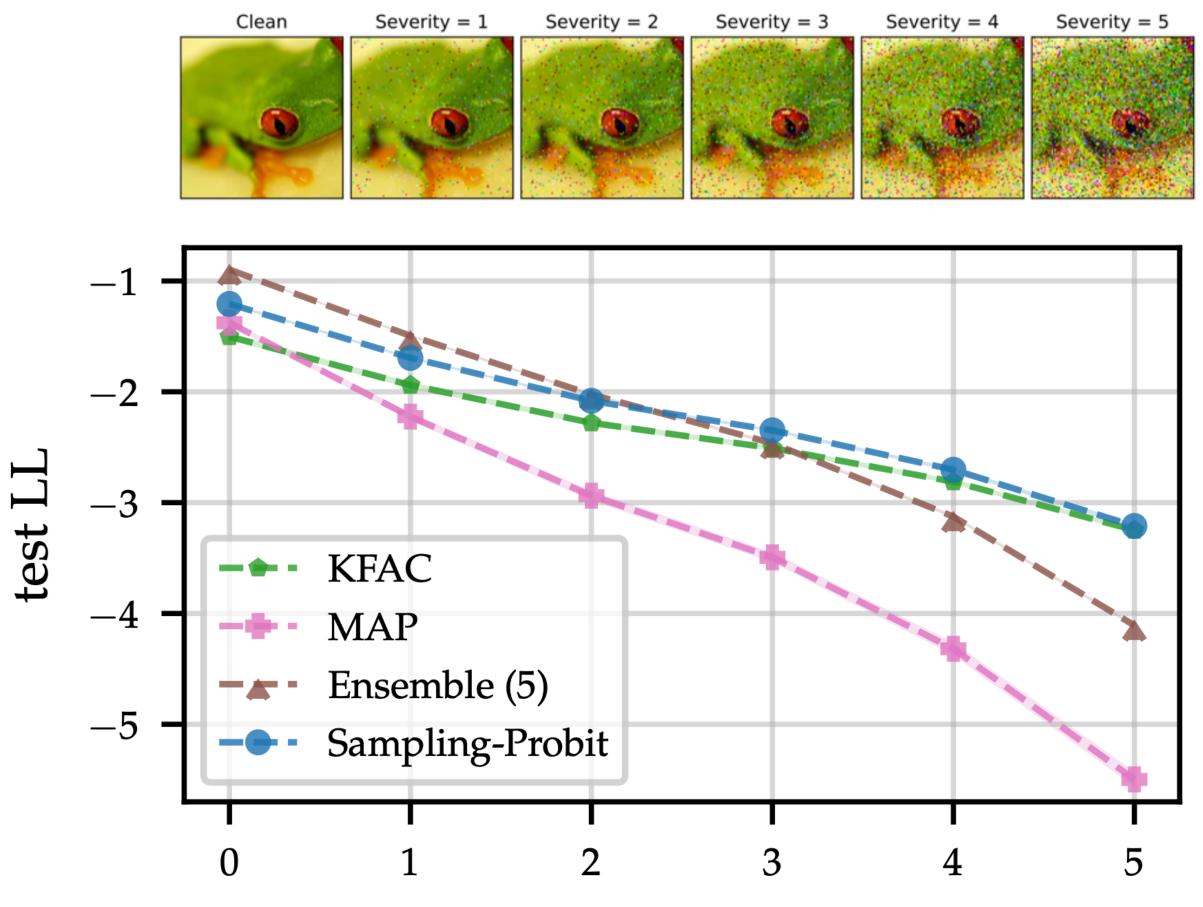
Stability of estimator: 1 sample is enough

ResNet-18 (d = 11M) on CIFAR-100 (nm = 5M)



Demonstration: Scalable Uncertainty Estimation in NNs

ResNet-18 (d = 11M) on CIFAR-100 (nm = 5M)



corruption severity

Thank you to my collaborators!

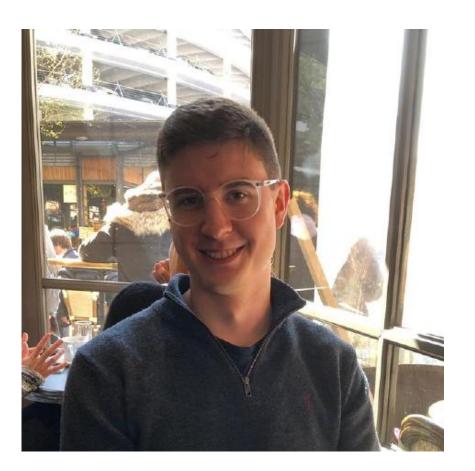
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