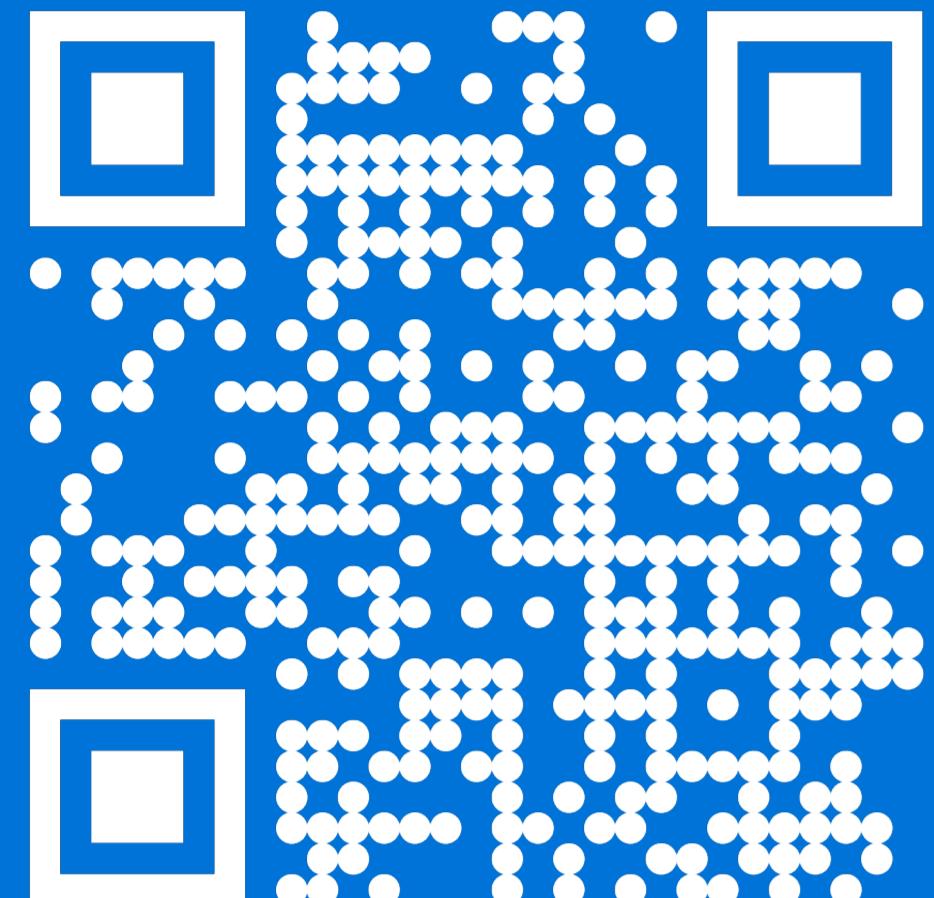


# We perform near-exact inference and hyperparameter optimisation in Bayesian linear models with millions of parameters and observations



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## Sampling-based inference for large linear models, with application to linearised Laplace



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We consider Bayesian Linear Models of the form  $y_i = \phi(x_i)\theta + \eta_i$ , where  $\theta \sim \mathcal{N}(0, A^{-1})$ ,  $\eta_i \sim \mathcal{N}(0, B_i^{-1})$

$$y_i \in \mathbb{R}^m, \quad \phi(x_i) \in \mathbb{R}^{m \times d}, \quad \theta \in \mathbb{R}^d \quad i \in \{1, \dots, n\}$$

1. Posterior is  $\mathcal{N}(\bar{\theta}, \Sigma)$ , where  $\Sigma^{-1} = \Phi^T B \Phi + A$  ← Inversion of  $d \times d$  matrix,  $\mathcal{O}(d^3)$ !
2. Model Evidence can be tuned for hparams, contains  $\log\det(\Sigma^{-1})$  ← Log.det. of  $d \times d$  matrix,  $\mathcal{O}(d^3)$ !

### Idea 1: Sample from Posterior with Stochastic Optimisation

$$z^* \sim \mathcal{N}(0, H^{-1}) \text{ if } z^* = \operatorname{argmin}_z L(z)$$

$$\text{Where } L(z) = \underbrace{\sum_{i=1}^n \|\epsilon_i - \phi(x_i)z\|_{B_i}^2}_{1} + \underbrace{\frac{1}{2} \|z - \theta^0\|_A^2}_{2}$$

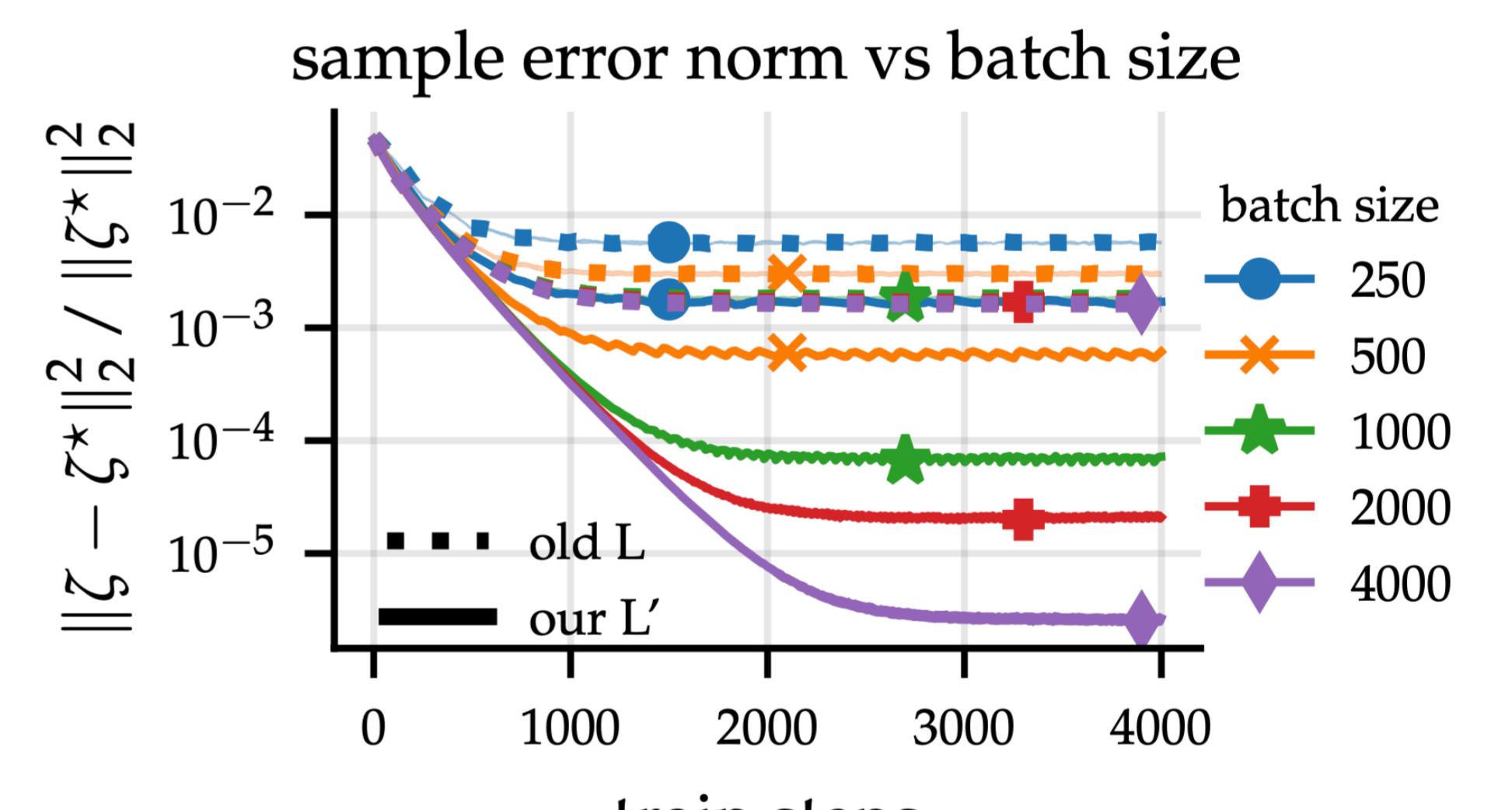
$$\epsilon_i \sim \mathcal{N}(0, B_i^{-1})$$

$$\theta^0 \sim \mathcal{N}(0, A^{-1})$$

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

$$\theta^n = \theta^0 + A^{-1}\Phi^T B \mathcal{E}$$

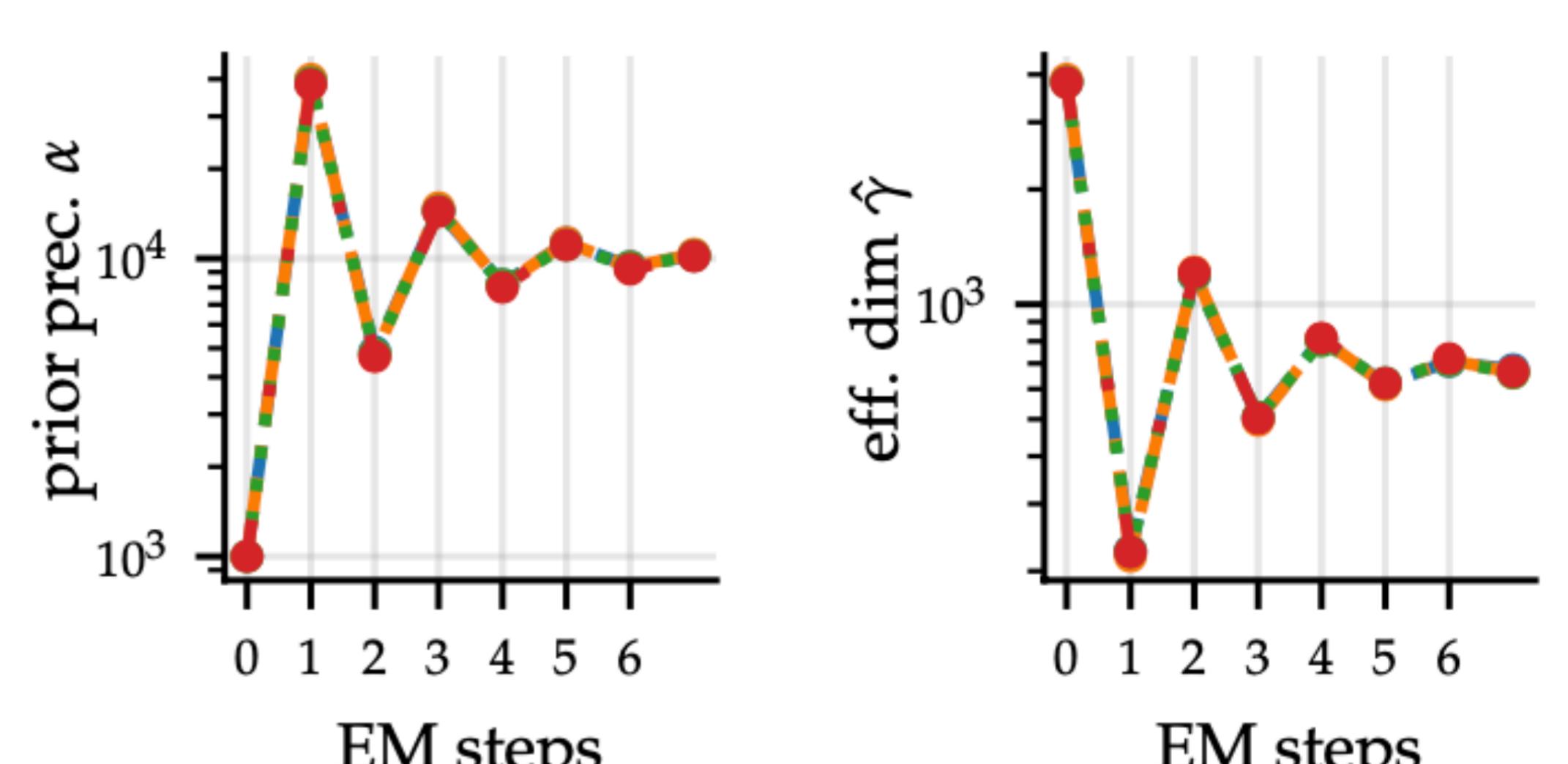
$$\mathcal{E} = [\epsilon_0^T, \dots, \epsilon_n^T]^T \in \mathbb{R}^{nm}$$



### Idea 2: Optimise the model evidence using only samples

$$\text{MacKay proposed update for prior precision } A = \alpha I, \quad \alpha = \frac{\operatorname{Tr}(\Sigma \Phi^T B \Phi)}{\|\bar{\theta}\|^2}$$

$$\operatorname{Tr}\{\Sigma M\} = \operatorname{Tr}\left\{\Sigma^{\frac{1}{2}} M \Sigma^{\frac{1}{2}}\right\} = \mathbb{E}[z_1^T M z_1] \approx \frac{1}{k} \sum_{j=1}^k z_j^T \Phi^T B \Phi z_j$$



### Application: Uncertainty Quantification with very large NNs

Linearised NNs + Laplace Approximation = Bayesian Linear Models

Largest scale exact Laplace inference with ResNet-18 + CIFAR100

$$d = 11M \text{ and } nm = 5M$$

