

# The Bayesian Learning Rule

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Human Learning at  
the age of 6 months.



Converged at the  
age of 12 months



Transfer  
skills  
at the age  
of 14  
months



# Fail because too slow or quick to adapt



# Adaptation in Machine Learning

- Even a small change may need retraining
- Huge amount of resources are required only few can afford (costly & unsustainable) [1,2, 3]
- Difficult to apply in “dynamic” settings (robotics, medicine, epidemiology, climate science, etc.)
- Our goal is to solve such challenges
  - Help in building safe and trustworthy AI
  - To reduce “magic” in deep learning (DL)

1. Diethe et al. Continual learning in practice, arXiv, 2019.

2. Paleyes et al. Challenges in deploying machine learning: a survey of case studies, arXiv, 2021.

3. <https://www.youtube.com/watch?v=hx7BXih7zx8&t=897s>

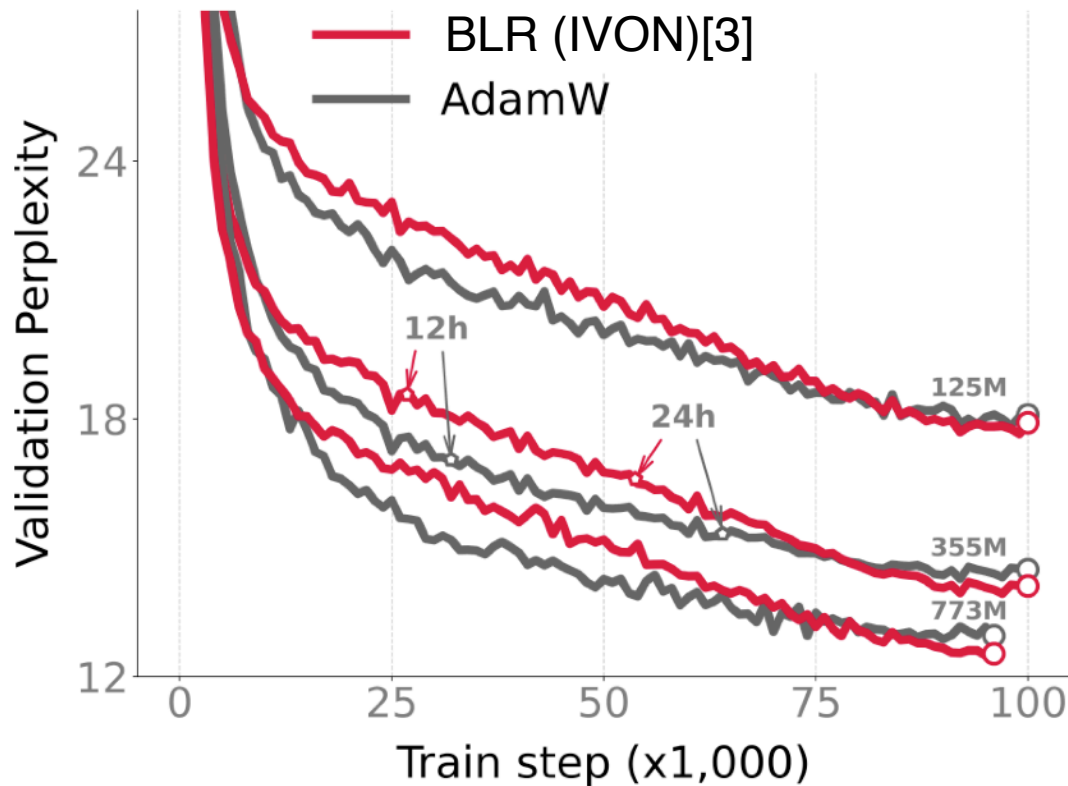
# Bayesian Learning Rule [1]

- Bridge DL & Bayesian learning [2-5]
  - SOTA on GPT-2 and ImageNet [5]
- Improve other aspects of DL [5-7]
  - Calibration, uncertainty, memory etc.
  - Understand and fix model behavior
- Towards human-like quick adaptation

1. Khan and Rue, The Bayesian Learning Rule, JMLR (2023).
2. Khan, et al. Fast and scalable Bayesian deep learning by weight-perturbation in Adam, ICML (2018).
3. Osawa et al. Practical Deep Learning with Bayesian Principles, NeurIPS (2019).
4. Lin et al. Handling the positive-definite constraints in the BLR, ICML (2020).
5. Shen et al. Variational Learning is Effective for Large Deep Networks, Under review.
6. Daheim et al. Model merging by uncertainty-based gradient matching, ICLR (2024).
7. Nickl, Xu, Tailor, Moellenhoff, Khan, The memory-perturbation equation, NeurIPS (2023)

# GPT-2 with Bayes

Better performance & uncertainty at the same cost [5]



Trained on OpenWebText data (49.2B tokens).

On 773M, we get a gain of 0.5 in perplexity.

On 355M, we get a gain of 0.4 in perplexity.

1. Khan, et al. "Fast and scalable Bayesian deep learning by weight-perturbation in Adam." *ICML* (2018).
2. Osawa et al. "Practical Deep Learning with Bayesian Principles." *NeurIPS* (2019).
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# Exponential Family

Natural  
parameters

Sufficient  
Statistics

Expectation  
parameters

$$q(\theta) \propto \exp \left[ \lambda^\top T(\theta) \right]$$

$$\mu := \mathbb{E}_q[T(\theta)]$$

$$\begin{aligned} \mathcal{N}(\theta|m, S^{-1}) &\propto \exp \left[ -\frac{1}{2}(\theta - m)^\top S(\theta - m) \right] \\ &\propto \exp \left[ (Sm)^\top \theta + \text{Tr} \left( -\frac{S}{2} \theta \theta^\top \right) \right] \end{aligned}$$

Gaussian distribution

$$q(\theta) := \mathcal{N}(\theta|m, S^{-1})$$

Natural parameters

$$\lambda := \{Sm, -S/2\}$$

Expectation parameters

$$\mu := \{\mathbb{E}_q(\theta), \mathbb{E}_q(\theta\theta^\top)\}$$

# Bayes and Conjugate Computations [1]

Multiplication of distribution = addition of (natural) params

Bayes rule: posterior  $\propto$  lik  $\times$  prior

$$e^{\lambda_{\text{post}}^\top T(\theta)} \propto e^{\lambda_{\text{lik}}^\top T(\theta)} \times e^{\lambda_{\text{prior}}^\top T(\theta)}$$

log-posterior = log-lik + log-prior

$$\lambda_{\text{post}} = \lambda_{\text{lik}} + \lambda_{\text{prior}}$$

This idea can be generalized through natural-gradients.

$$\lambda_{\text{post}} = \underbrace{\nabla}_{\text{Natural gradient}} \underbrace{\mathbb{E}_q}_{\text{Posterior "approximation"}} [\log\text{-lik} + \log\text{-prior}]$$

# Bayes Rule as (Natural) Gradient Descent

$$\lambda_{\text{post}} \leftarrow \lambda_{\text{lik}} + \lambda_{\text{prior}}$$

Expected log-lik and log-prior are linear in  $\mu$  [1]

$$\mathbb{E}_q[\log\text{-lik}] = \lambda_{\text{lik}}^\top \mathbb{E}_q[T(\theta)] = \lambda_{\text{lik}}^\top \mu$$

Gradient wrt  $\mu$  is simply the natural parameter

$$\nabla_{\mu} \mathbb{E}_q[\log\text{-lik}] = \lambda_{\text{lik}}$$

So Bayes' rule can be written as (for an arbitrary  $q$ )

$$\lambda_{\text{post}} \leftarrow \nabla_{\mu} \mathbb{E}_q[\log\text{-lik} + \log\text{-prior}]$$

As an analogy, think of least-square = 1-step of Newton

# Approximate Bayes

Bayes rule: posterior  $\propto$  lik  $\times$  prior

Bayes as optimization [1], aka variational inference:

$$\min_{q \in \mathcal{Q}} \mathbb{E}_q[\text{log-lik}] + \text{KL}(q \parallel \text{prior})$$

Generalized Approx Bayesian learning:

$$\min_{q \in \mathcal{Q}} \mathbb{E}_{q(\theta)}[\ell(\theta)] - \mathcal{H}(q)$$

log-lik + log-prior  
↓  
Posterior approximation (expo-family)  
↑  
Entropy

# The Bayesian Learning Rule

$$\min_{\theta} \ell(\theta) \quad \text{vs} \quad \min_{q \in \mathcal{Q}} \mathbb{E}_{q(\theta)}[\ell(\theta)] - \mathcal{H}(q)$$

$\uparrow$   
Posterior approximation (expo-family)

Entropy

Bayesian Learning Rule [1,2] (natural-gradient descent)

Natural and Expectation parameters of  $q$

$$\lambda \leftarrow \lambda - \rho \nabla_{\mu} \left\{ \mathbb{E}_q[\ell(\theta)] - \mathcal{H}(q) \right\}$$

Old belief      New information = natural gradients

Exploiting posterior's information geometry to derive existing algorithms as special instances by approximating  $q$  and natural gradients.

1. Khan and Rue, The Bayesian Learning Rule, JMLR, 2023
2. Khan and Lin. "Conjugate-computation variational inference...." Alstats (2017).

# Warning!

- This natural gradient is different from the one what we (often) encounter in machine learning for Maximum-Likelihood
  - In MLE, the loss is the negative log probability distribution

$$\min_{\theta} -\log q(\theta) \Rightarrow F(\theta)^{-1} \nabla \log q(\theta)$$

- Here,  $\theta$  loss and distribution are two different entities, even possible unrelated

$$\min_q \mathbb{E}_q[\ell(\theta)] - \mathcal{H}(q) \Rightarrow F(\lambda)^{-1} \nabla_{\lambda} \mathbb{E}_q[\ell(\theta)]$$

# Gradient Descent from Bayesian Learning Rule

(Euclidean) gradients as natural  
gradients

# Bayesian learning rule:

Learning Algorithm	Posterior Approx.	Natural-Gradient Approx.	Sec.
<b>Optimization Algorithms</b>			
Gradient Descent	Gaussian (fixed cov.)	Delta method	1.3
Newton's method	Gaussian	—"—	1.3
Multimodal optimization <small>(New)</small>	Mixture of Gaussians	—"—	3.2
<b>Deep-Learning Algorithms</b>			
Stochastic Gradient Descent	Gaussian (fixed cov.)	Delta method, stochastic approx.	4.1
RMSprop/Adam	Gaussian (diagonal cov.)	Delta method, stochastic approx., Hessian approx., square-root scaling, slow-moving scale vectors	4.2
Dropout	Mixture of Gaussians	Delta method, stochastic approx., responsibility approx.	4.3
STE	Bernoulli	Delta method, stochastic approx.	4.5
Online Gauss-Newton <small>(New)</small> (OGN)	Gaussian (diagonal cov.)	Gauss-Newton Hessian approx. in Adam & no square-root scaling	4.4
Variational OGN <small>(New)</small>	—"—	Remove delta method from OGN	4.4
BayesBiNN <small>(New)</small>	Bernoulli	Remove delta method from STE	4.5
<b>Approximate Bayesian Inference Algorithms</b>			
Conjugate Bayes	Exp-family	Set learning rate $\rho_t = 1$	5.1
Laplace's method	Gaussian	Delta method	4.4
Expectation-Maximization	Exp-Family + Gaussian	Delta method for the parameters	5.2
Stochastic VI (SVI)	Exp-family (mean-field)	Stochastic approx., local $\rho_t = 1$	5.3
VMP	—"—	$\rho_t = 1$ for all nodes	5.3
Non-Conjugate VMP	—"—	—"—	5.3
Non-Conjugate VI <small>(New)</small>	Mixture of Exp-family	None	5.4



# Gradient Descent from BLR

$$\text{GD: } \theta \leftarrow \theta - \rho \nabla_{\theta} \ell(\theta)$$

$$\text{BLR: } m \leftarrow m - \rho \nabla_m \ell(m)$$

“Global” to “local”  
(the delta method)

$$\mathbb{E}_q[\ell(\theta)] \approx \ell(m)$$

$$m \leftarrow m - \rho \nabla_m \mathbb{E}_q[\ell(\theta)]$$

$$\lambda \leftarrow \lambda - \rho \nabla_{\mu} (\mathbb{E}_q[\ell(\theta)] - \mathcal{H}(q))$$

Derived by choosing **Gaussian with fixed covariance**

Gaussian distribution  $q(\theta) := \mathcal{N}(m, 1)$

Natural parameters  $\lambda := m$

Expectation parameters  $\mu := \mathbb{E}_q[\theta] = m$

Entropy  $\mathcal{H}(q) := \log(2\pi)/2$

# Newton's Method from BLR

Newton's method:  $\theta \leftarrow \theta - H_\theta^{-1} [\nabla_\theta \ell(\theta)]$

$$Sm \leftarrow (1 - \rho)Sm - \rho \nabla_{\mathbb{E}_q(\theta)} \mathbb{E}_q[\ell(\theta)]$$

$$-\frac{1}{2}S \leftarrow (1 - \rho)S - \rho \frac{1}{2} S \nabla_{\mathbb{E}_q(\theta)} \nabla_{\mathbb{E}_q(\theta)} \mathbb{E}_q[\ell(\theta)]$$

$$\lambda \leftarrow (1 - \rho) \nabla_{\mu} \mathcal{H}(q) + \rho \nabla_{\mu} \mathcal{H}(q) \quad -\nabla_{\mu} \mathcal{H}(q) = \lambda$$

Derived by choosing a **multivariate Gaussian**

Gaussian distribution  $q(\theta) := \mathcal{N}(\theta|m, S^{-1})$

Natural parameters  $\lambda := \{Sm, -S/2\}$

Expectation parameters  $\mu := \{\mathbb{E}_q(\theta), \mathbb{E}_q(\theta\theta^\top)\}$

# Newton's Method from BLR

Newton's method:  $\theta \leftarrow \theta - H_{\theta}^{-1} [\nabla_{\theta} \ell(\theta)]$

Set  $\rho=1$  to get  $m \leftarrow m - H_m^{-1} [\nabla_m \ell(m)]$

$$m \leftarrow m - \rho S^{-1} \nabla_m \ell(m)$$

$$S \leftarrow (1 - \rho)S + \rho H_m$$

Delta Method

$$\mathbb{E}_q[\ell(\theta)] \approx \ell(m)$$

Express in terms of gradient and Hessian of loss:

$$\nabla_{\mathbb{E}_q(\theta)} \mathbb{E}_q[\ell(\theta)] = \mathbb{E}_q[\nabla_{\theta} \ell(\theta)] - 2\mathbb{E}_q[H_{\theta}]m$$

$$\nabla_{\mathbb{E}_q(\theta\theta^{\top})} \mathbb{E}_q[\ell(\theta)] = \mathbb{E}_q[H_{\theta}]$$

$$Sm \leftarrow (1 - \rho)Sm - \rho \nabla_{\mathbb{E}_q(\theta)} \mathbb{E}_q[\ell(\theta)]$$

$$S \leftarrow (1 - \rho)S - \rho 2 \nabla_{\mathbb{E}_q(\theta\theta^{\top})} \mathbb{E}_q[\ell(\theta)]$$

# RMSprop/Adam from BLR

RMSprop

$$s \leftarrow (1 - \rho)s + \rho[\hat{\nabla} \ell(\theta)]^2$$

$$\theta \leftarrow \theta - \alpha(\sqrt{s} + \delta)^{-1} \hat{\nabla} \ell(\theta)$$

BLR for Gaussian approx

$$S \leftarrow (1 - \rho)S + \rho(H_\theta)$$

$$m \leftarrow m - \alpha S^{-1} \nabla_\theta \ell(\theta)$$

To get RMSprop, make the following choices

- Restrict covariance to be diagonal
- Replace Hessian by square of gradients
- Add square root for scaling vector

For Adam, use a Heavy-ball term with KL divergence as momentum (Appendix E in [1])

# BLR for large deep networks

RMSprop/Adam

$$\begin{aligned}\hat{g} &\leftarrow \hat{\nabla} \ell(\theta) \\ \hat{h} &\leftarrow \hat{g}^2 \\ h &\leftarrow (1 - \rho)h + \rho \hat{h} \\ \theta &\leftarrow \theta - \alpha(\hat{g} + \delta m) / (\sqrt{h} + \delta)\end{aligned}$$

BLR variant called

Improved Variational Online Newton (IVON)

$$\begin{aligned}\hat{g} &\leftarrow \hat{\nabla} \ell(\theta) \text{ where } \theta \sim \mathcal{N}(m, \sigma^2) \\ \hat{h} &\leftarrow \hat{g} \cdot (\theta - m) / \sigma^2 \\ h &\leftarrow (1 - \rho)h + \rho \hat{h} + \rho^2 (h - \hat{h})^2 / (2(h + \delta)) \\ m &\leftarrow m - \alpha(\hat{g} + \delta m) / (h + \delta) \\ \sigma^2 &\leftarrow 1 / (N(h + \delta))\end{aligned}$$

Code to be released this month!

Initialization of h (& scaling with N) matter.

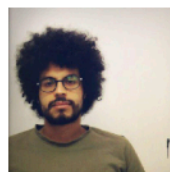
1. Khan, et al. "Fast and scalable Bayesian deep learning by weight-perturbation in Adam." *ICML* (2018).
2. Osawa et al. "Practical Deep Learning with Bayesian Principles." *NeurIPS* (2019).
3. Lin et al. "Handling the positive-definite constraints in the BLR." *ICML* (2020).
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# IVON [3] got 1st prize in NeurIPS 2021 Approximate Inference Challenge

Watch **Thomas Moellenhoff's** talk at  
<https://www.youtube.com/watch?v=LQInIN5EU7E>.

## Mixture-of-Gaussian Posteriors with an Improved Bayesian Learning Rule

Thomas Möllenhoff<sup>1</sup>, Yuesong Shen<sup>2</sup>, Gian Maria Marconi<sup>1</sup>  
Peter Nickl<sup>1</sup>, Mohammad Emtiyaz Khan<sup>1</sup>



1 Approximate Bayesian Inference Team  
RIKEN Center for AI Project, Tokyo, Japan

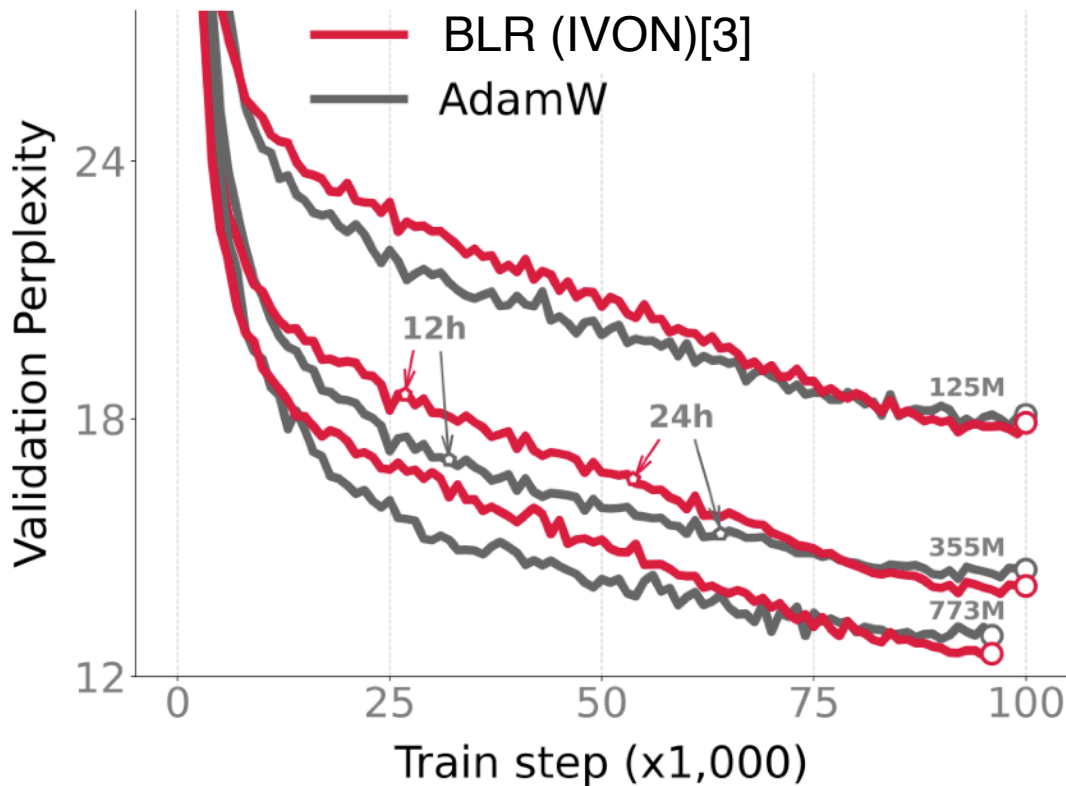
2 Computer Vision Group  
Technical University of Munich, Germany

Dec 14th, 2021 — NeurIPS Workshop on Bayesian Deep Learning

1. Khan, et al. "Fast and scalable Bayesian deep learning by weight-perturbation in Adam." *ICML* (2018).
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# GPT-2 with Bayes

Better performance and uncertainty at the same cost



Trained on OpenWebText data (49.2B tokens).

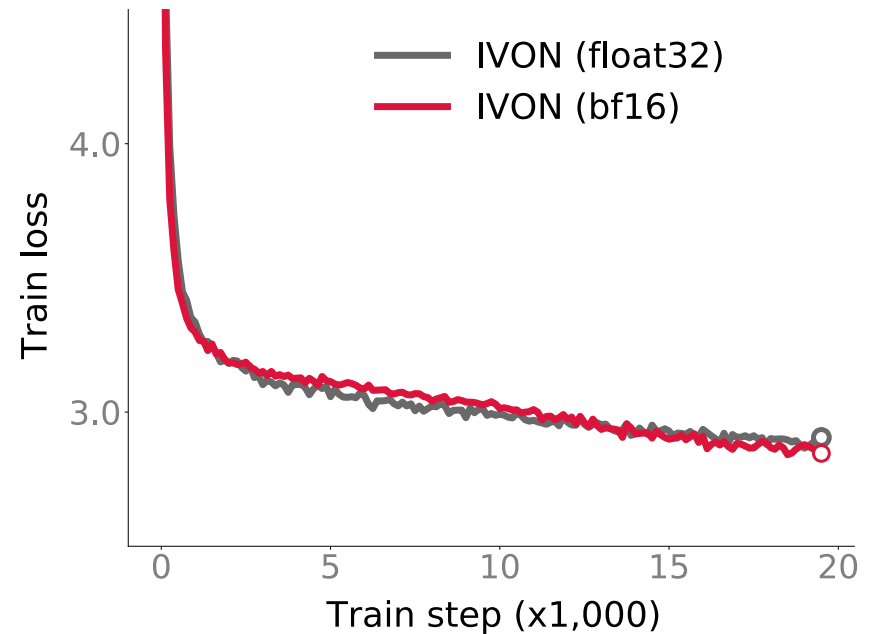
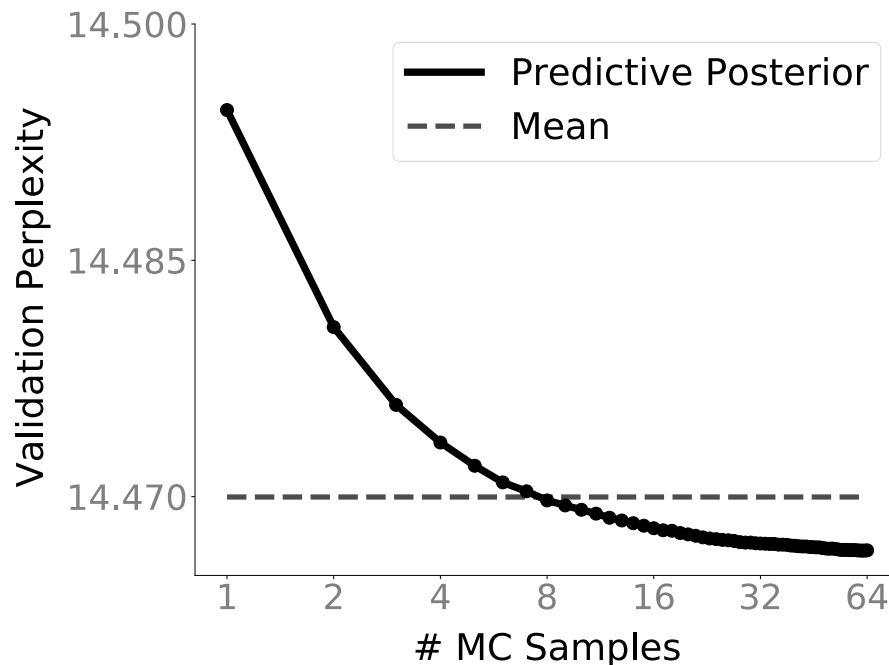
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# GPT-2 with Bayes

Posterior averaging improve the result. Can also train on low-precision (a stable optimizer)

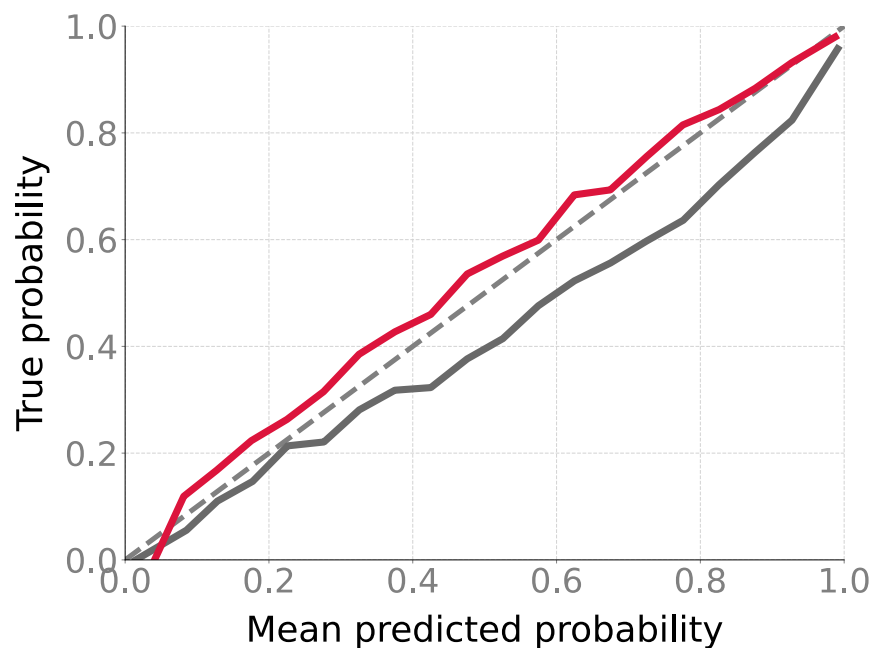
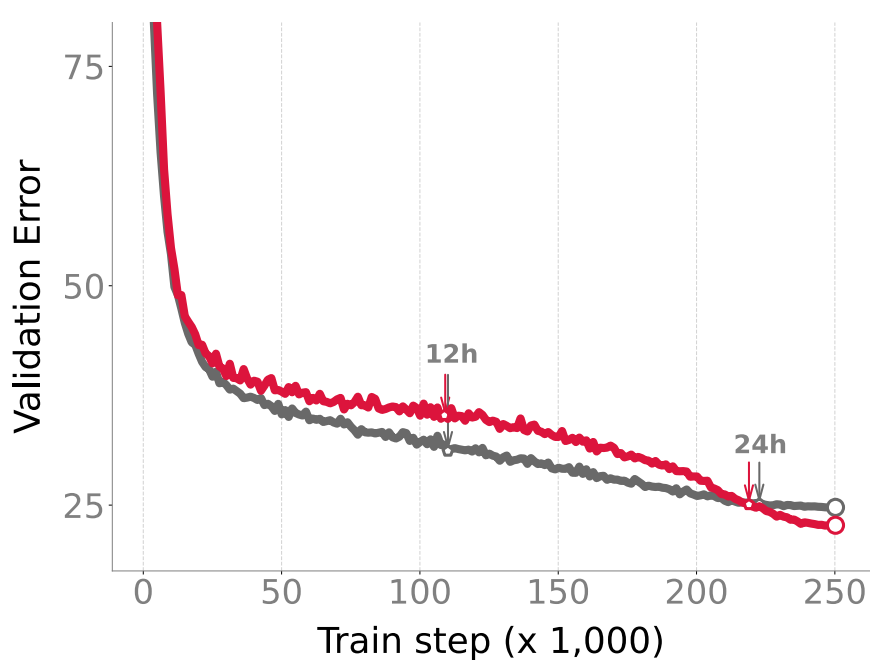


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# ImageNet on ResNet-50 (25.6M)

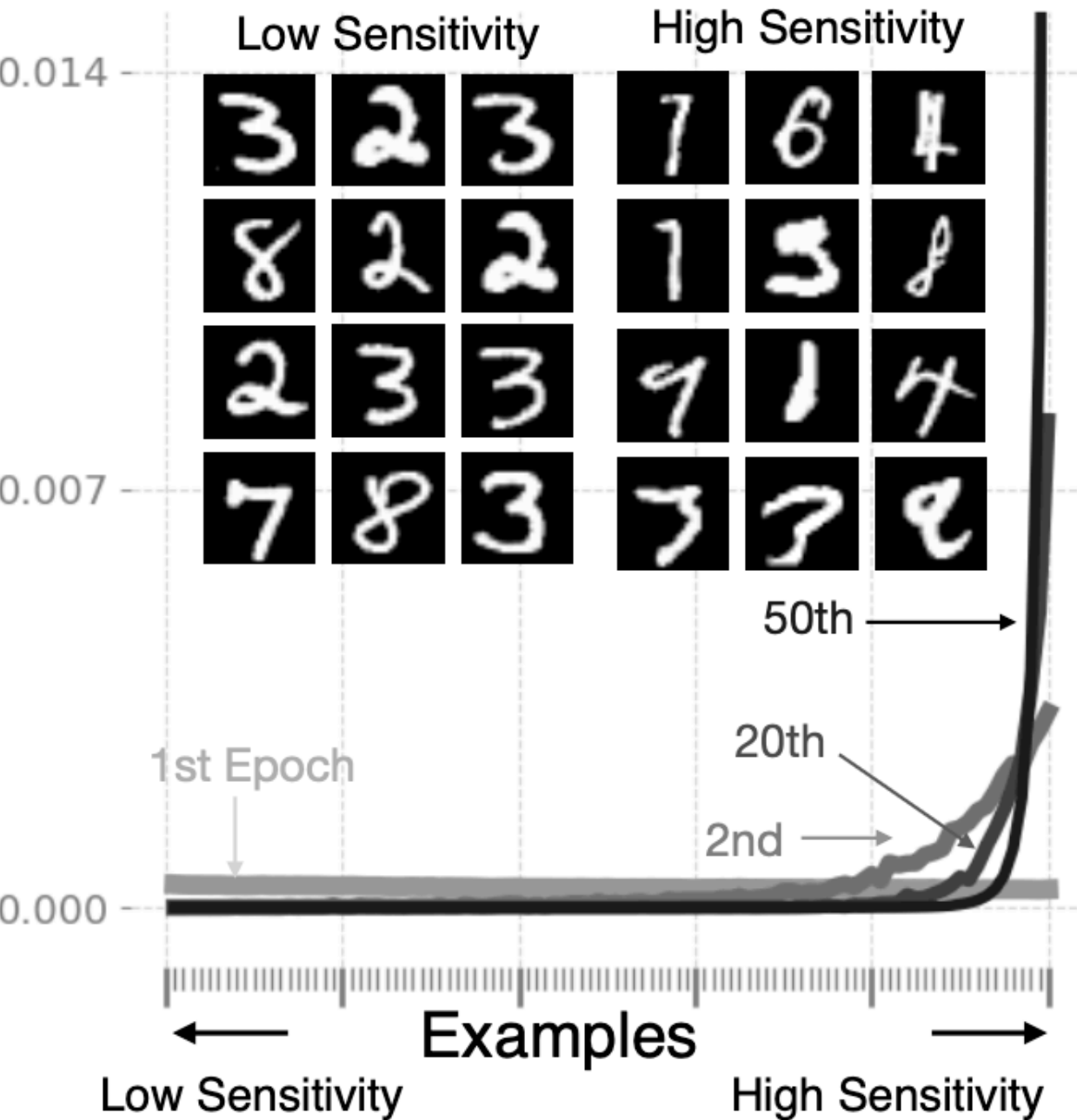
2% better accuracy over AdamW and 1% over SGD. Better calibration (ECE of 0.022 vs 0.066)



# ImageNet on ResNet-50 (25.6M)

No severe overfitting like AdamW while improving accuracy over SGD consistently & better uncertainty

Dataset & Model	Epochs	Method	Top-1 Acc. $\uparrow$	Top-5 Acc. $\uparrow$	NLL $\downarrow$	ECE $\downarrow$	Brier $\downarrow$
ImageNet-1k ResNet-50 (25.6M params)	100	AdamW	74.56 $\pm$ 0.24	92.05 $\pm$ 0.17	1.018 $\pm$ 0.012	0.043 $\pm$ 0.001	0.352 $\pm$ 0.003
		SGD	<b>76.18</b> $\pm$ 0.09	<b>92.94</b> $\pm$ 0.05	<b>0.928</b> $\pm$ 0.003	0.019 $\pm$ 0.001	<b>0.330</b> $\pm$ 0.001
		IVON@mean	<b>76.14</b> $\pm$ 0.11	92.83 $\pm$ 0.04	0.934 $\pm$ 0.002	0.025 $\pm$ 0.001	<b>0.330</b> $\pm$ 0.001
		IVON	<b>76.24</b> $\pm$ 0.09	<b>92.90</b> $\pm$ 0.04	<b>0.925</b> $\pm$ 0.002	<b>0.015</b> $\pm$ 0.001	<b>0.330</b> $\pm$ 0.001
	200	AdamW	+2% 75.16 $\pm$ 0.14	92.37 $\pm$ 0.03	1.018 $\pm$ 0.003	0.066 $\pm$ 0.002	0.349 $\pm$ 0.002
		SGD	+1% 76.63 $\pm$ 0.45	93.21 $\pm$ 0.25	0.917 $\pm$ 0.026	0.038 $\pm$ 0.009	0.326 $\pm$ 0.006
		IVON@mean	77.30 $\pm$ 0.08	93.58 $\pm$ 0.05	0.884 $\pm$ 0.002	0.035 $\pm$ 0.002	<b>0.316</b> $\pm$ 0.001
		IVON	<b>77.46</b> $\pm$ 0.07	<b>93.68</b> $\pm$ 0.04	<b>0.869</b> $\pm$ 0.002	<b>0.022</b> $\pm$ 0.002	<b>0.315</b> $\pm$ 0.001
TinyImageNet ResNet-18 (11M params, wide)	200	AdamW	+15% 47.33 $\pm$ 0.90	71.54 $\pm$ 0.95	6.823 $\pm$ 0.235	0.421 $\pm$ 0.008	0.913 $\pm$ 0.018
		SGD	+1% 61.39 $\pm$ 0.18	82.30 $\pm$ 0.22	1.811 $\pm$ 0.010	0.138 $\pm$ 0.002	0.536 $\pm$ 0.002
		IVON@mean	<b>62.41</b> $\pm$ 0.15	<b>83.77</b> $\pm$ 0.18	1.776 $\pm$ 0.018	0.150 $\pm$ 0.005	0.532 $\pm$ 0.002
		IVON	<b>62.68</b> $\pm$ 0.16	<b>84.12</b> $\pm$ 0.24	<b>1.528</b> $\pm$ 0.010	<b>0.019</b> $\pm$ 0.004	<b>0.491</b> $\pm$ 0.001
TinyImageNet PreResNet-110 (4M params, deep)	200	AdamW	+10% 50.65 $\pm$ 0.0*	74.94 $\pm$ 0.0*	4.487 $\pm$ 0.0*	0.357 $\pm$ 0.0*	0.812 $\pm$ 0.0*
		AdaHessian	55.03 $\pm$ 0.53	78.49 $\pm$ 0.34	2.971 $\pm$ 0.064	0.272 $\pm$ 0.005	0.690 $\pm$ 0.008
		SGD	+2% 59.39 $\pm$ 0.50	81.34 $\pm$ 0.30	2.040 $\pm$ 0.040	0.176 $\pm$ 0.006	0.577 $\pm$ 0.007
		IVON @mean	<b>60.85</b> $\pm$ 0.39	<b>83.89</b> $\pm$ 0.14	1.584 $\pm$ 0.009	0.053 $\pm$ 0.002	<b>0.514</b> $\pm$ 0.003
		IVON	<b>61.25</b> $\pm$ 0.48	<b>84.13</b> $\pm$ 0.17	<b>1.550</b> $\pm$ 0.009	<b>0.049</b> $\pm$ 0.002	<b>0.511</b> $\pm$ 0.003
CIFAR-100 ResNet-18 (11M params, wide)	200	AdamW	+11% 64.12 $\pm$ 0.43	86.85 $\pm$ 0.51	3.357 $\pm$ 0.071	0.278 $\pm$ 0.005	0.615 $\pm$ 0.008
		SGD	+7% 74.46 $\pm$ 0.17	92.66 $\pm$ 0.06	1.083 $\pm$ 0.007	0.113 $\pm$ 0.001	0.376 $\pm$ 0.001
		IVON@mean	74.51 $\pm$ 0.24	92.74 $\pm$ 0.19	1.284 $\pm$ 0.013	0.152 $\pm$ 0.003	0.399 $\pm$ 0.002
		IVON	<b>75.14</b> $\pm$ 0.34	<b>93.30</b> $\pm$ 0.19	<b>0.912</b> $\pm$ 0.009	<b>0.021</b> $\pm$ 0.003	<b>0.344</b> $\pm$ 0.003

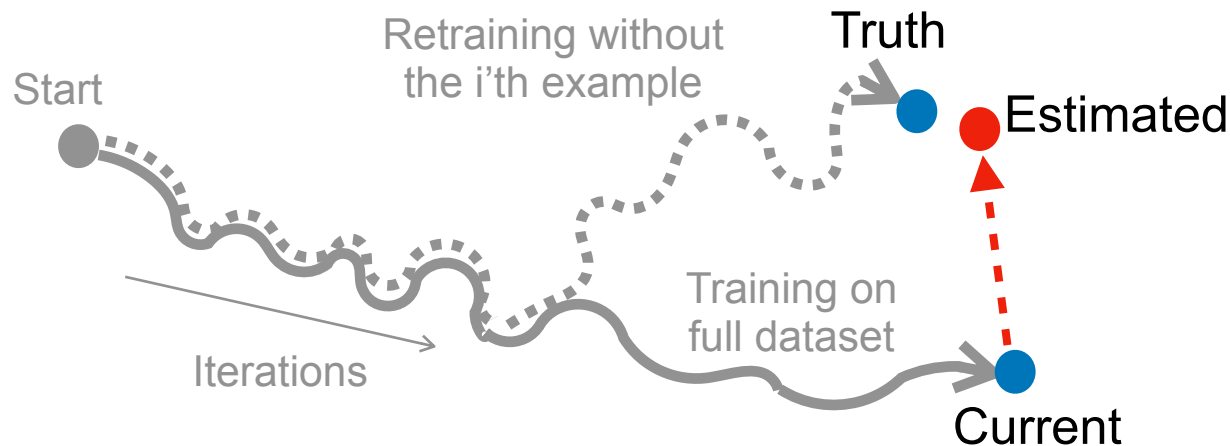


Sensitivity to data is easy to compute “during” training.

MNIST on MLP. Also work at large scale (ImageNet)

# Sensitivity to Training Data

Past information with most influence on the present

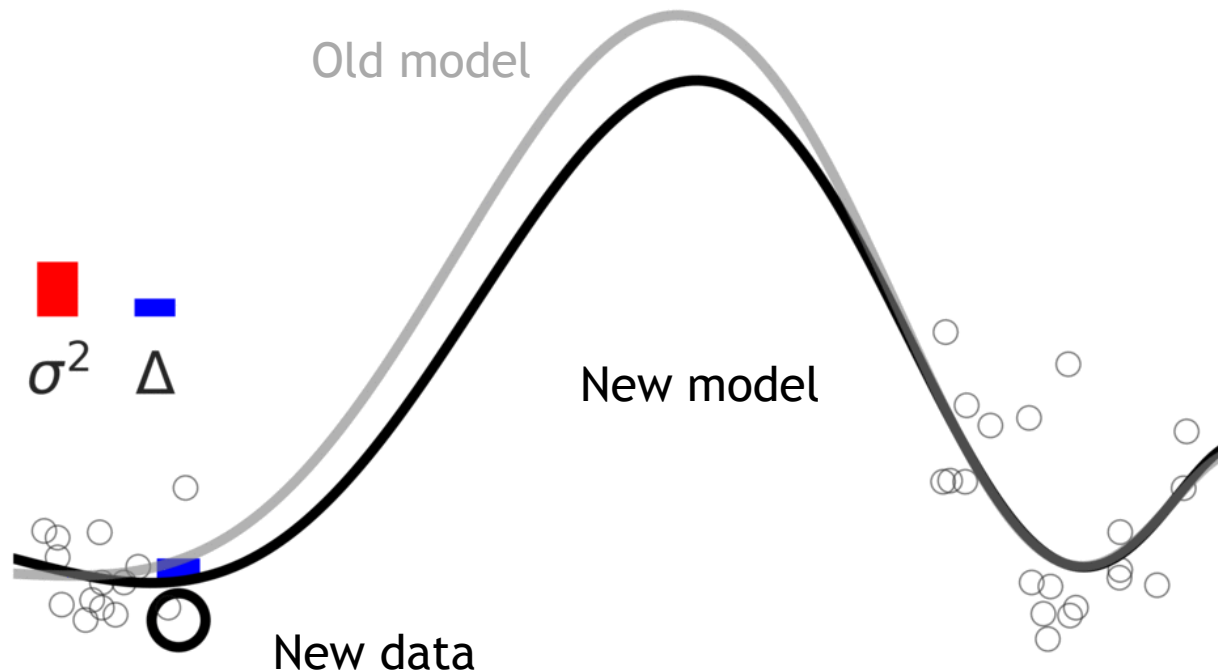


Estimating it without retraining: Using the BLR, we can recover all sorts of influence criteria used in literature.

# Memory Perturbation

How sensitive is a model to its training data?

Deviation ( $\Delta$ ) = predictionError \* predictionVariance

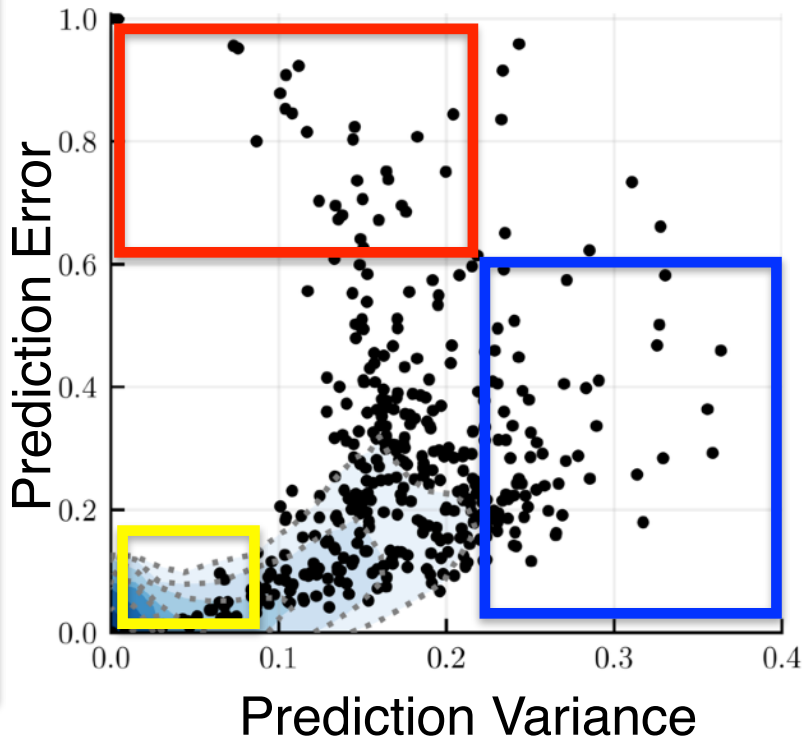
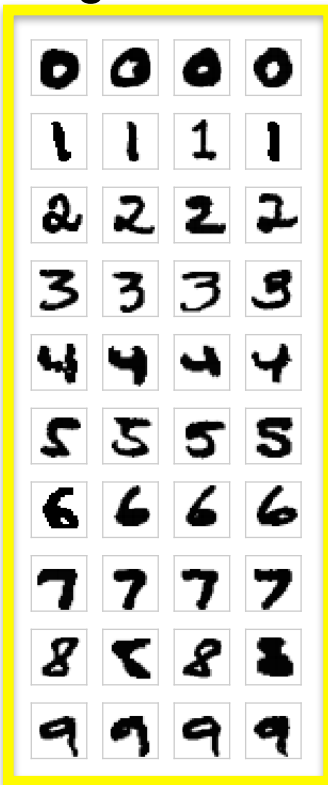


1. Cook. Detection of Influential Observations in Linear Regression. Technometrics. ASA 1977
2. Nickl, Xu, Tailor, Moellenhoff, Khan, The memory-perturbation equation, NeurIPS, 2023

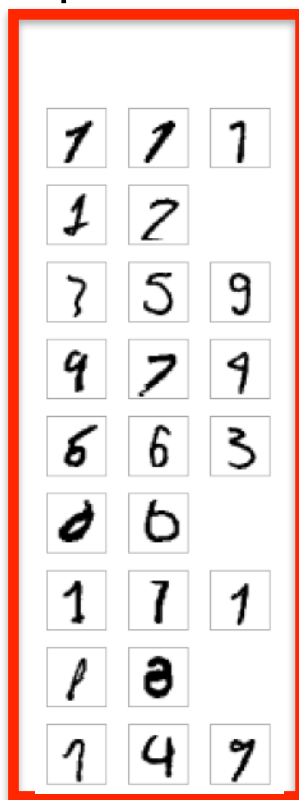
# Memory Maps using the BLR

Understand generic ML models and algorithms.

Regular examples



Unpredictable

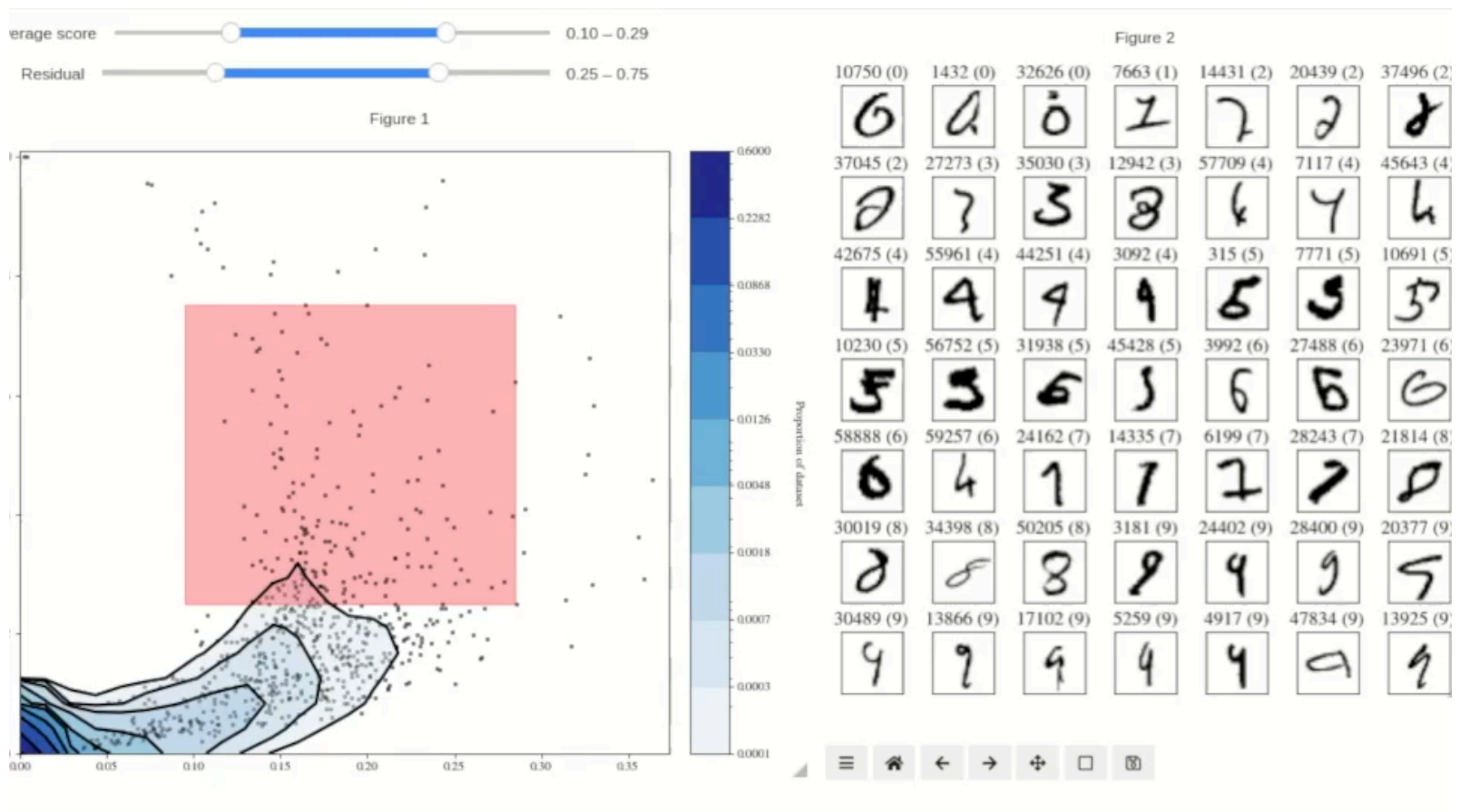


Uncertain



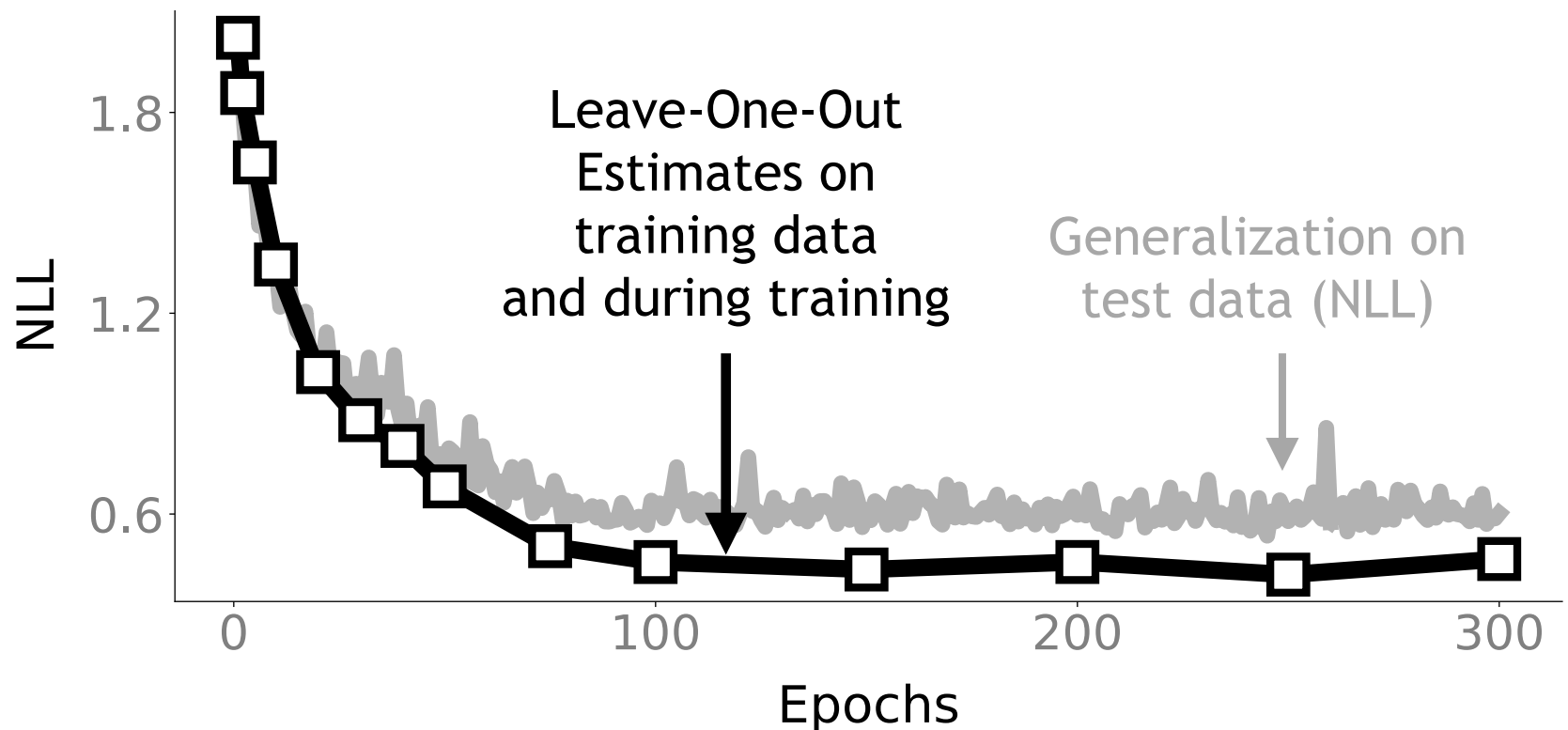
# A Tool for Data-Scientists

Understand the memory of a model.



# Predict Generalization during Training

CIFAR10 on ResNet-20 using IVON. SGD or Adam do not work as well.

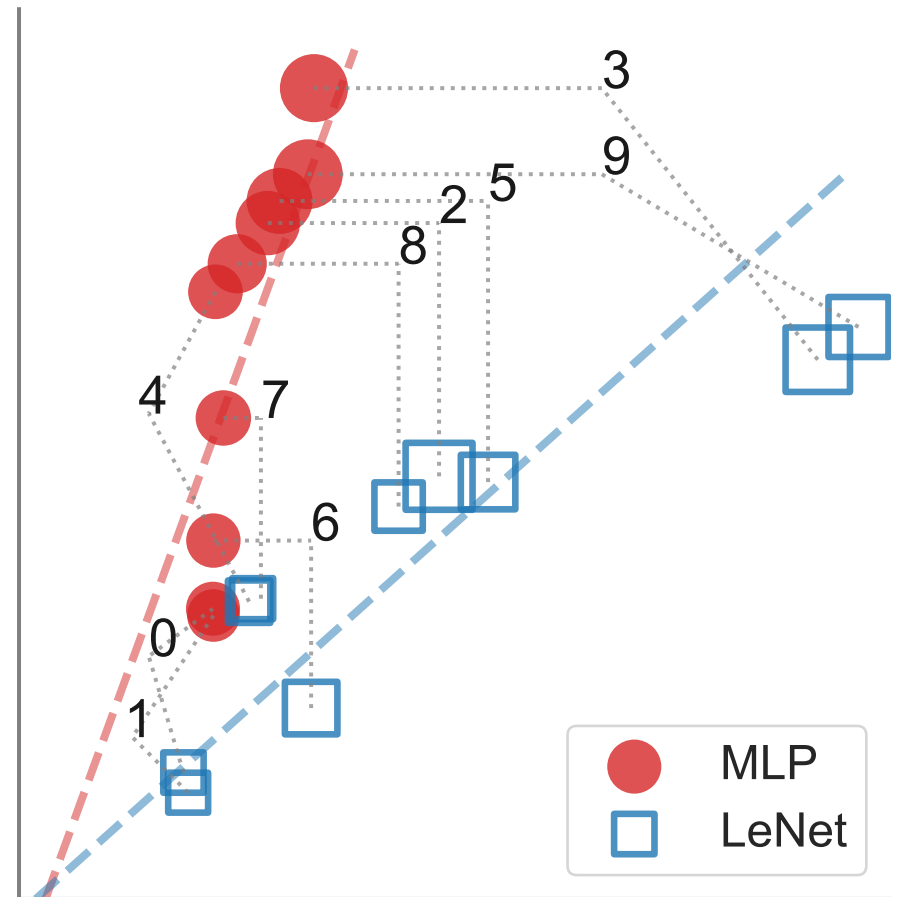




# Answering “What-If” Questions

What if we removed a class from MNIST?

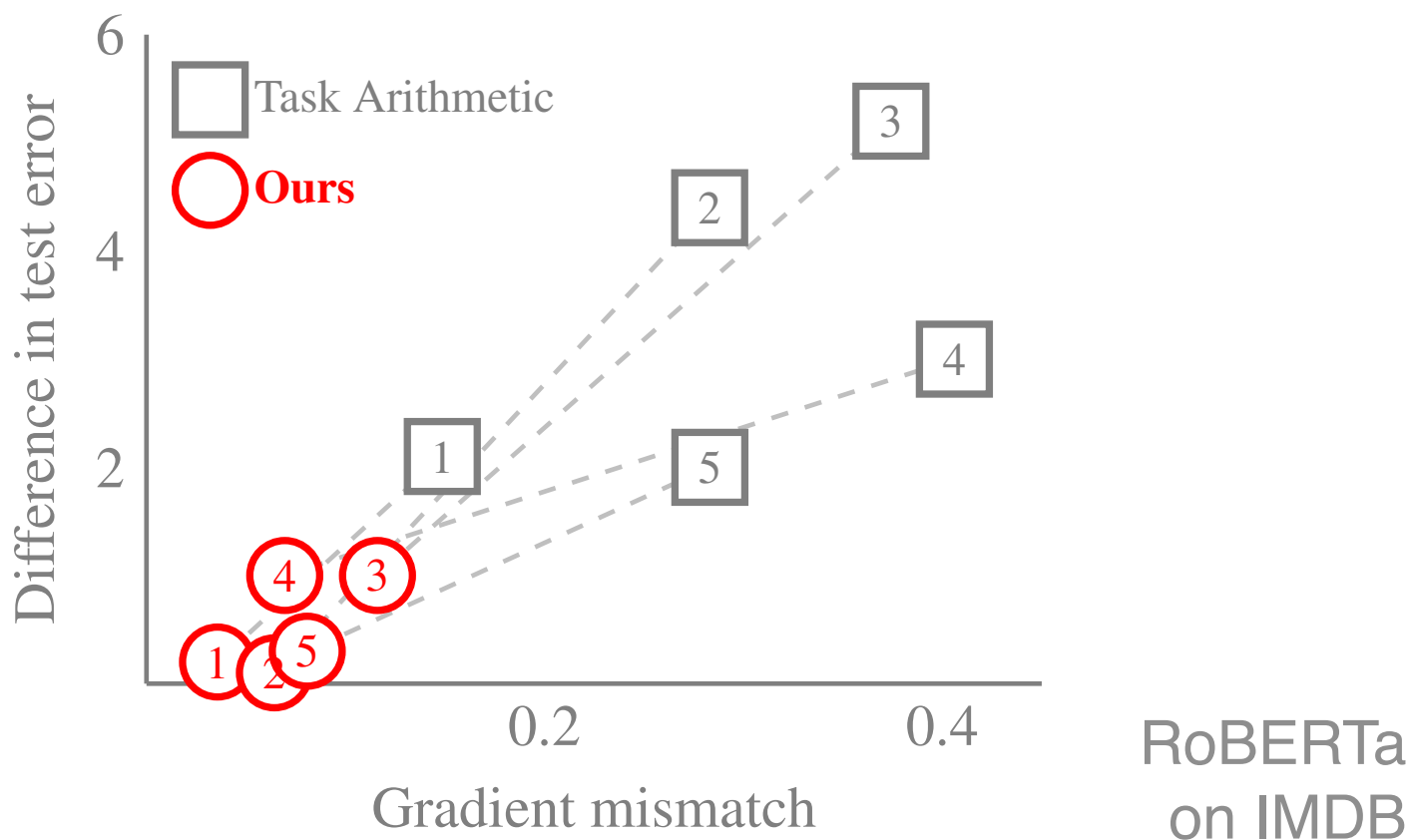
Estimates on training data (no retraining)



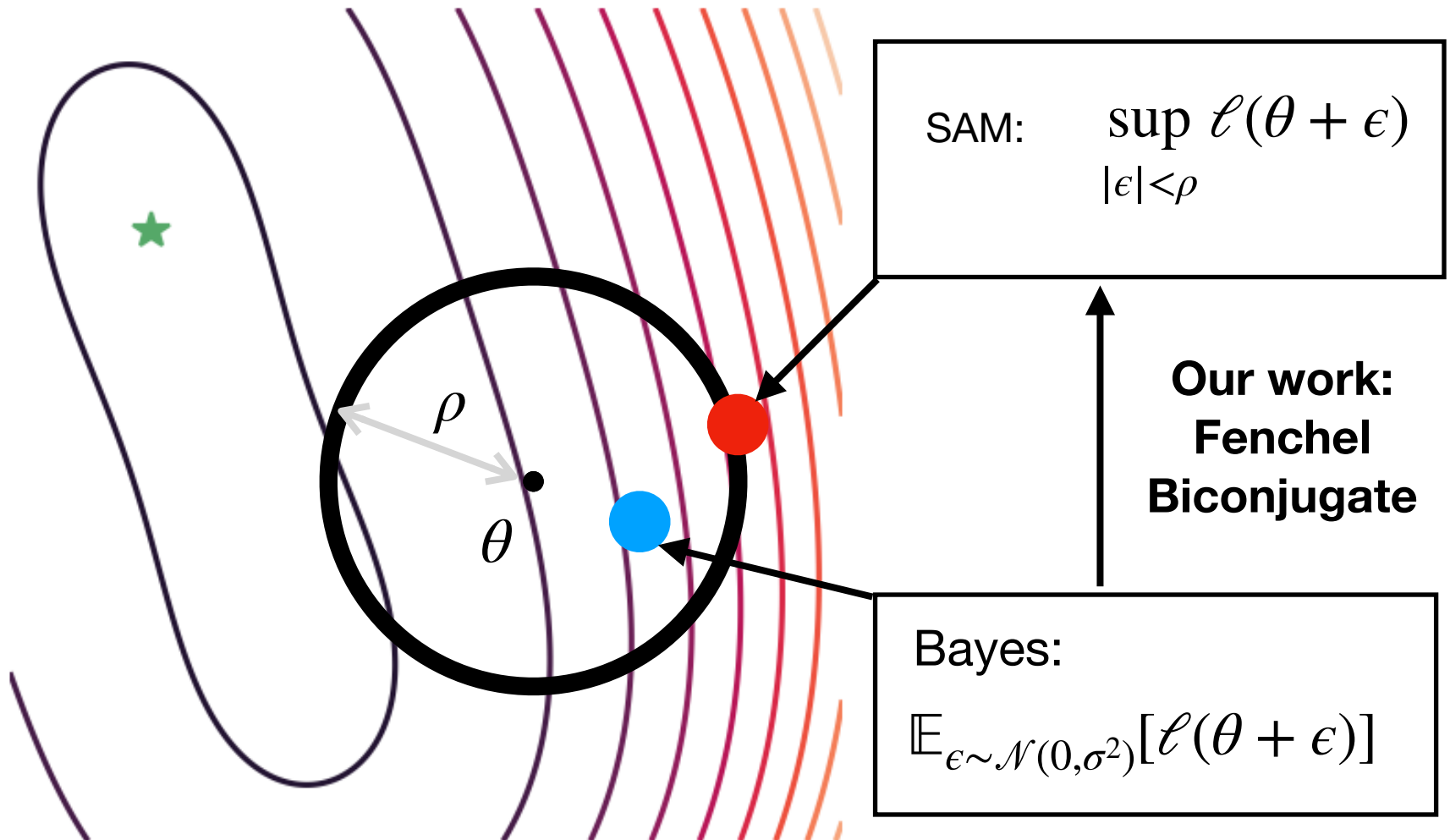
Test Performance (NLL) by  
brute-force retraining

# Answering “What-If” Questions

What if we merge fine-tuned large-language models?



# SAM as an Optimal relaxation of Bayes



1. Foret et al. Sharpness-Aware Minimization for Efficiently Improving Generalization, ICLR, 2021
2. Moellenhoff and Khan, SAM as an Optimal Relaxation of Bayes, Under review, 2022

# Bayesian Learning Rule [1]

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2. Khan, et al. Fast and scalable Bayesian deep learning by weight-perturbation in Adam, ICML (2018).
3. Osawa et al. Practical Deep Learning with Bayesian Principles, NeurIPS (2019).
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# The Bayes-Duality Project

Toward AI that learns adaptively, robustly, and continuously, like humans



**Emtiyaz Khan**

Research director  
(Japan side)

Approx-Bayes team at  
RIKEN-AIP and OIST



**Julyan Arbel**

Research director  
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Statify-team, Inria  
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Co-PI  
(Japan side)

Tokyo Institute of  
Technology

Received total funding of around **USD 3 million** through JST's CREST-ANR (2021-2027) and Kakenhi Grants (2019-2021).

# Team Approx-Bayes

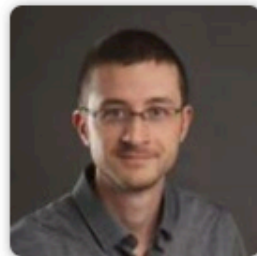
<https://team-approx-bayes.github.io/>



**Emtiyaz Khan**  
Team Leader



**Thomas Möllenhoff**  
Research Scientist



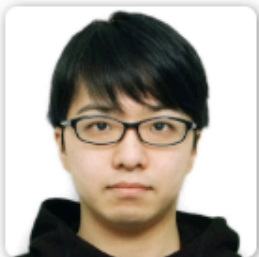
**Geoffrey Wolfer**  
Special  
Postdoctoral  
Resesarcher



**Hugo Monzón Maldonado**  
Postdoctoral  
Researcher

Many thanks to our group members and collaborators (many not on this slide).

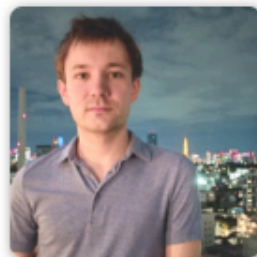
We are always looking for new collaborations.



**Keigo Nishida**  
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**Zhedong Liu**  
Postdoctoral  
Researcher



**Peter Nickl**  
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