

The Bayesian Learning Rule for Adaptive AI

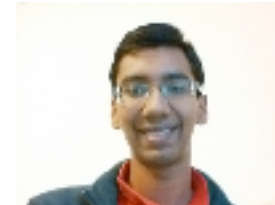
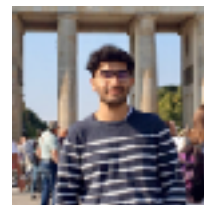
Mohammad **Emtiyaz** Khan

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<http://emtiyaz.github.io>



Thanks to Dharmesh Tailor, Siddharth Swaroop, and Thomas Moellenhoff for their help in the preparation of the talk



EPFL master students in our group

Many thanks to Patricia Genet (Internship program assistant) and Sylviane Dalmas for their help!



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Research Assistant
Jan-Dec 2017

Worked on structured VAEs (coauthor an [ICLR 2018 paper](#)), now working as a data-scientist in Switzerland



Frederik Kunstner
Intern,
Feb-Aug 2018

Worked on natural-gradients and Adam, coauthor on a [NeurIPS 2018 paper](#), now a PhD student at UBC



Ehsan Abedi
Intern,
Mar-Aug 2019

Worked on connections between NN and GPs, coauthor on a [NeurIPS 2019 paper](#), now a PhD student in Switzerland (?)



Alex Immer
Intern,
Mar 2019-
Mar 2020

Worked on linearized DNNs (coauthored [NeurIPS 2019](#), [Alstats 2020](#), and [ICML 2021](#) papers, and a [thesis](#)), now a PhD student in ETH



Roman Bachmann
Intern,
July 2019-
Feb 2020

Worked on Binary Neural Networks (coauthored an [ICML 2021 paper](#)), now a PhD student in EPFL



Lucie Perrotta
Intern,
Sep 2019-
Mar 2020

Worked on model misspecification and tempering (did a [masters thesis](#))

Pattern Classification and Machine Learning CS-433


I designed this course in 2014-2015 (around 200 students back then)

How it started?

Regression

Mohammad Emtiyaz Khan
EPFL

Sep 17, 2015



ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

@Mohammad Emtiyaz Khan 2014

How it's going?


Machine Learning Course - CS-433

Regression

Sept 21, 2021

minor changes by Martin Jaggi 2021,2020,2019,2018,2017,2016;
@Mohammad Emtiyaz Khan 2015

Last updated on: September 20, 2021



AI that learns as quickly as humans and animals

Quickly **adapt** to new situations in the future
by **robustly preserving** & using past knowledge

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 quick to adapt

TayTweets: Microsoft AI bot manipulated into being extreme racist upon release

Posted Fri 25 Mar 2016 at 4:38am, updated Fri 25 Mar 2016 at 9:17am



TayTweets is programmed to converse like a teenage girl who has "zero chill", according to Microsoft. (Twitter/TayTweets)

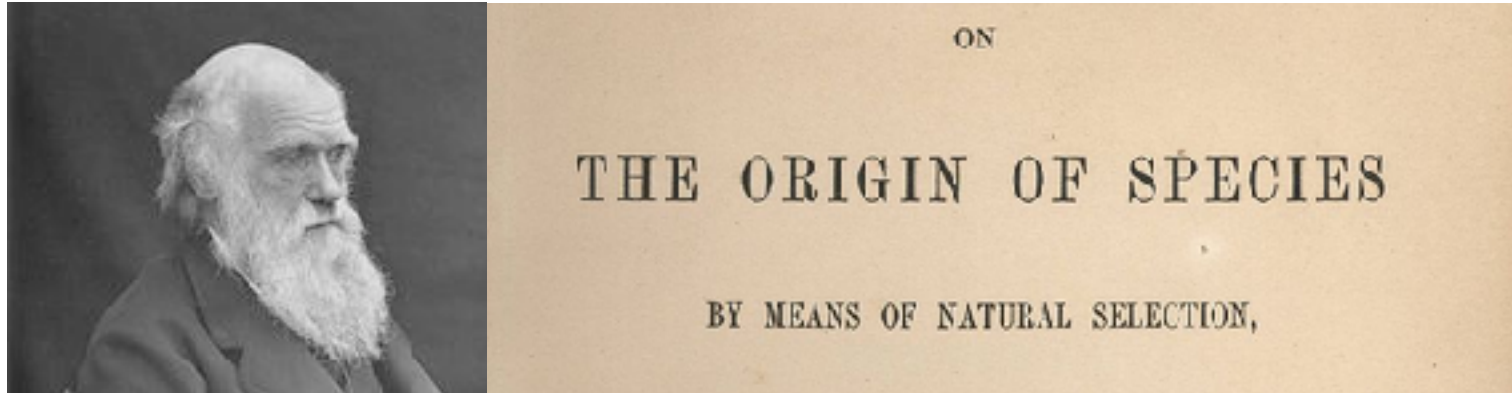
Fail because too slow to adapt



Adaptive & Robust Learning with Bayes

- “Good” algorithms are inherently Bayesian
- Bayesian learning rule [1]
- Robustness: Memorable experiences [2]
- Adaptation: Knowledge-Adaptation Priors [3,4,5]
- Take away: A new perspective of Bayes, essential for adaptive and robust deep learning

1. Khan and Rue, The Bayesian Learning Rule, arXiv, <https://arxiv.org/abs/2107.04562>, 2021
2. Tailor, Chang, Swaroop, Solin, Khan. Memorable experiences of ML models (in preparation)
3. Khan et al. Approximate Inference Turns Deep Networks into Gaussian Process, NeurIPS, 2019
4. Pan et al. Continual Deep Learning by Functional Regularisation of Memorable Past, NeurIPS, 2020
5. Khan and Swaroop. Knowledge-Adaptation Priors, NeurIPS, 2021 (<https://arxiv.org/abs/2106.08769>)



The Origin of Algorithms

A good algorithm must revise its
past beliefs by using useful
future information

Bayesian learning rule

See Table 1 in Khan and Rue, 2021

Learning Algorithm	Posterior Approx.	Natural-Gradient Approx.	Sec.
Optimization Algorithms			
Gradient Descent	Gaussian (fixed cov.)	Delta method	1.3
Newton's method	Gaussian	—"—	1.3
Multimodal optimization _(New)	Mixture of Gaussians	—"—	3.2
Deep-Learning Algorithms			
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 (OGN) _(New)	Gaussian (diagonal cov.)	Gauss-Newton Hessian approx. in Adam & no square-root scaling	4.4
Variational OGN _(New)	—"—	Remove delta method from OGN	4.4
BayesBiNN _(New)	Bernoulli	Remove delta method from STE	4.5
Approximate Bayesian Inference Algorithms			
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 _(New)	Mixture of Exp-family	None	5.4

A Bayesian Origin

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

↑
Entropy
Posterior approximation (expo-family)

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

Natural and Expectation parameters of q

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

↑
Old belief
↑
New information = natural gradients

Using posterior's information geometry to balance new vs old information

1. Khan and Rue, The Bayesian Learning Rule, arXiv, <https://arxiv.org/abs/2107.04562>, 2021
2. Khan and Lin. "Conjugate-computation variational inference: Converting variational inference in non-conjugate models to inferences in conjugate models." Alstats (2017).

Bayesian learning rule: $\lambda \leftarrow (1 - \rho)\lambda - \rho \nabla_{\mu} \mathbb{E}_q[\ell(\theta)]$

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Non-Conjugate VMP	—"—	—"—	5.3
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Gradient Descent from Bayes

Gradient descent: $\theta \leftarrow \theta - \rho \nabla_{\theta} \ell(\theta)$

Bayes Learn Rule: $m \leftarrow m - \rho \nabla_m \ell(m)$

“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 $\mathcal{H}(q) := \log(2\pi)/2$

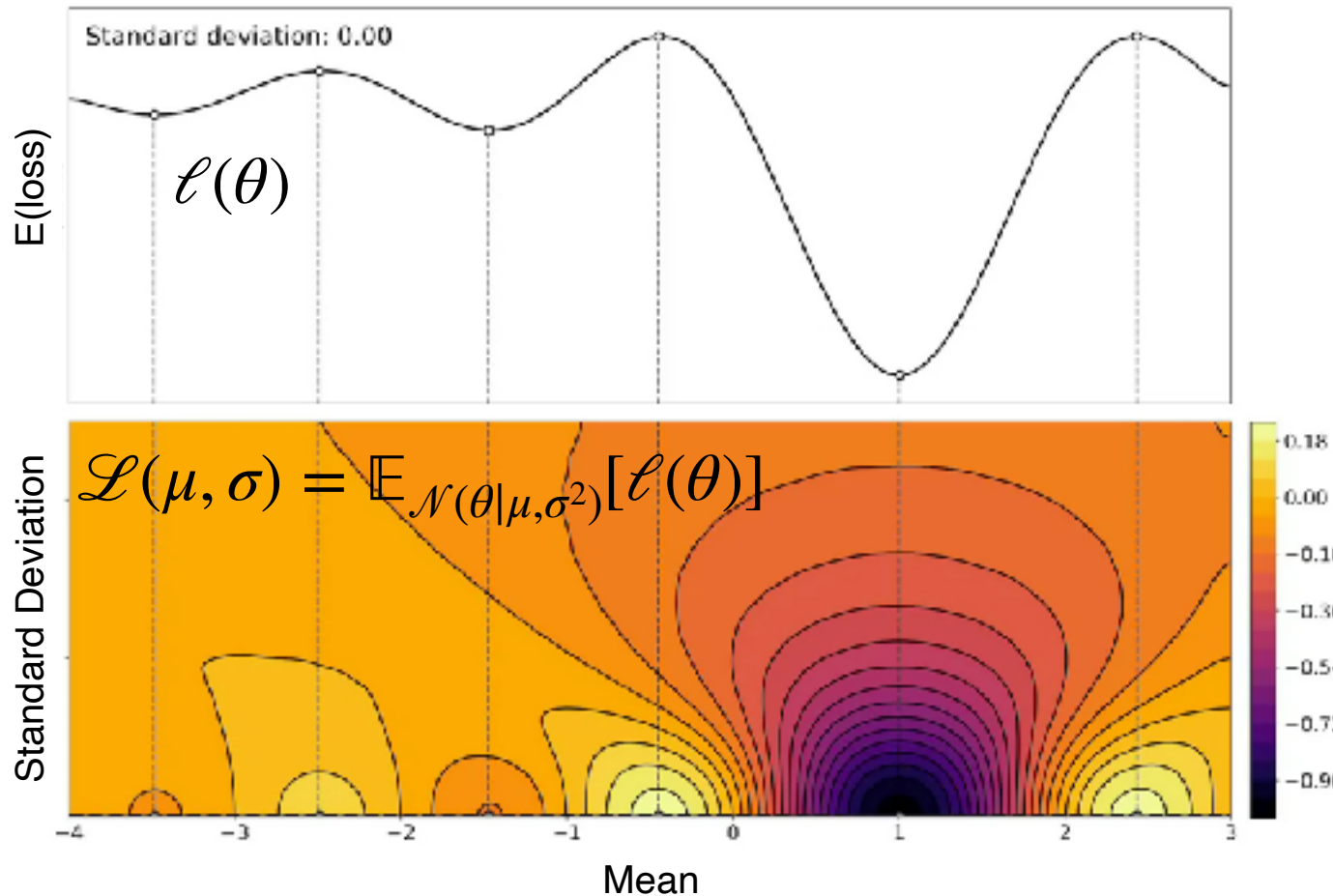
Bayesian learning rule: $\lambda \leftarrow (1 - \rho)\lambda - \rho \nabla_{\mu} \mathbb{E}_q[\ell(\theta)]$

Put the expectation (Bayes) back in!

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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).

Bayes Objective



Instead of the original loss, optimize a different one (Gaussian convolution)

A popular idea of “implicit regularization” in DL [4], but also common in other fields (RL, search, robust optimization)

1. Zellner, A. "Optimal information processing and Bayes's theorem." *The American Statistician* (1988)
2. Many other: Bissiri, et al. (2016), Shawe-Taylor and Williamson (1997), Cesa-Bianchi and Lugosi (2006)
3. Huszar's blog, Evolution Strategies, Variational Optimisation and Natural ES (2017)
4. Smith et al., On the Origin of Implicit Regularization in Stochastic Gradient Descent, ICLR, 2021

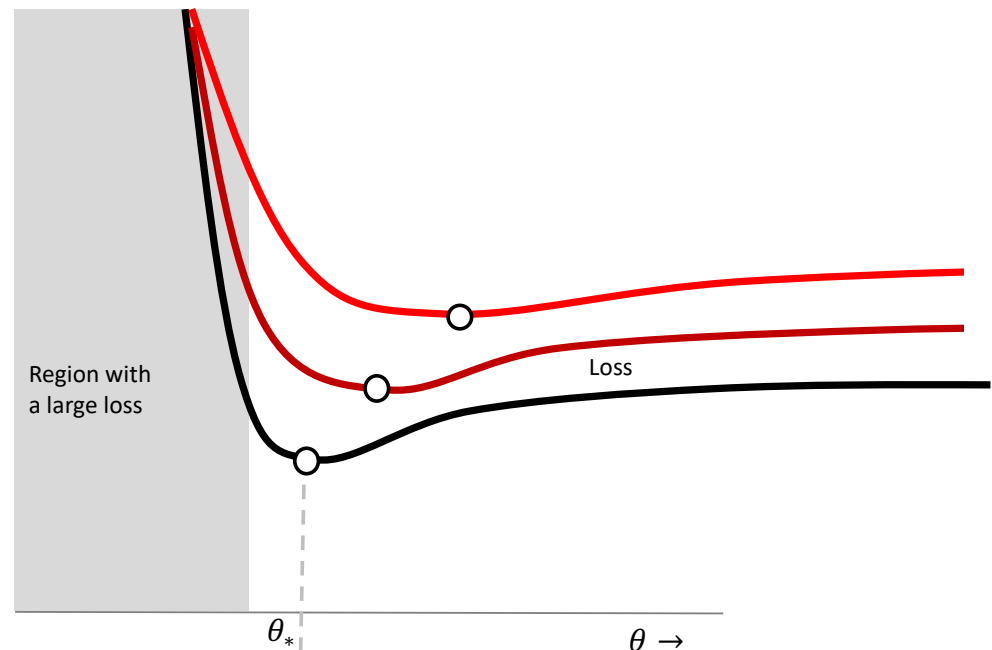
Bayes Prefers Flatter directions

$$\text{GD: } \theta \leftarrow \theta - \rho \nabla_{\theta} \ell(\theta) \quad \implies \nabla_{\theta} \ell(\theta_*) = 0$$

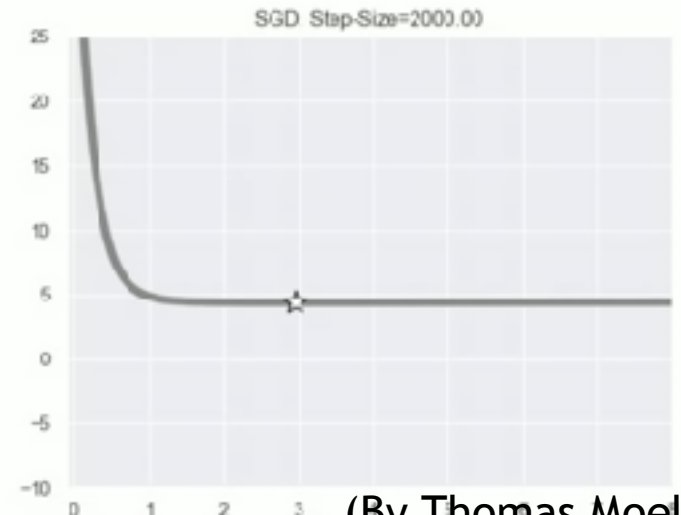
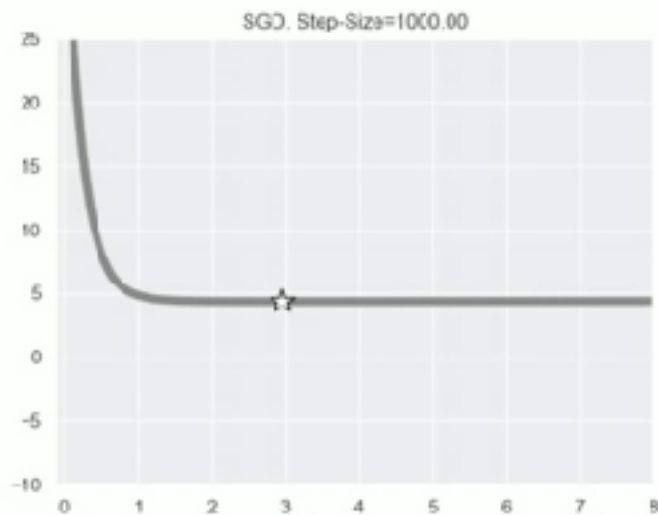
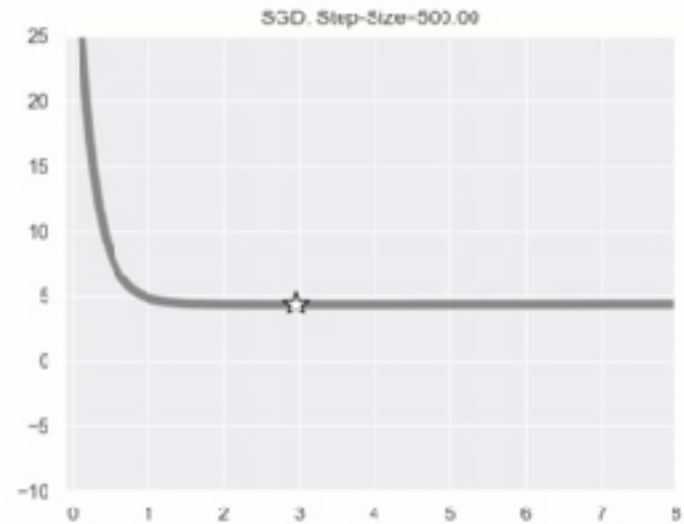
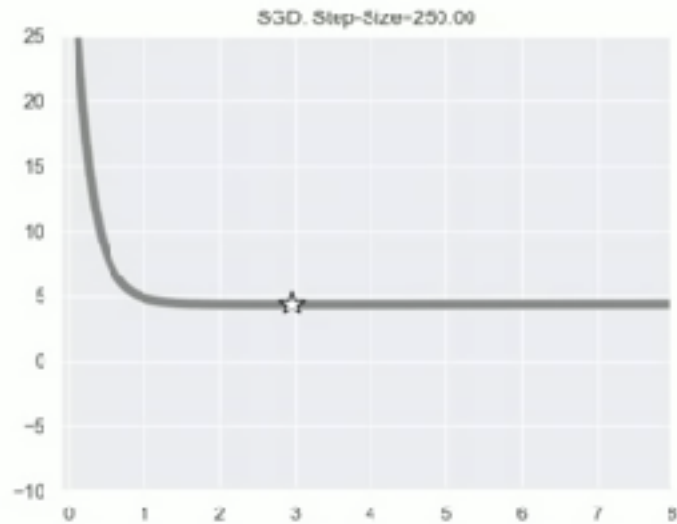
$$\text{BLR: } m \leftarrow m - \rho \nabla_m \mathbb{E}_q[\ell(\theta)] \quad \implies \nabla_m \mathbb{E}_{q_*}[\ell(\theta)] = 0$$

$$\implies \mathbb{E}_{q_*}[\nabla_{\theta} \ell(\theta)] = 0$$

Bayesian solution injects “noise” which has a similar regularization effect to noise in Stochastic GD. It prefers “flatter” directions.



SGD: Implicit Regularization



Bayes: Explicit Regularization

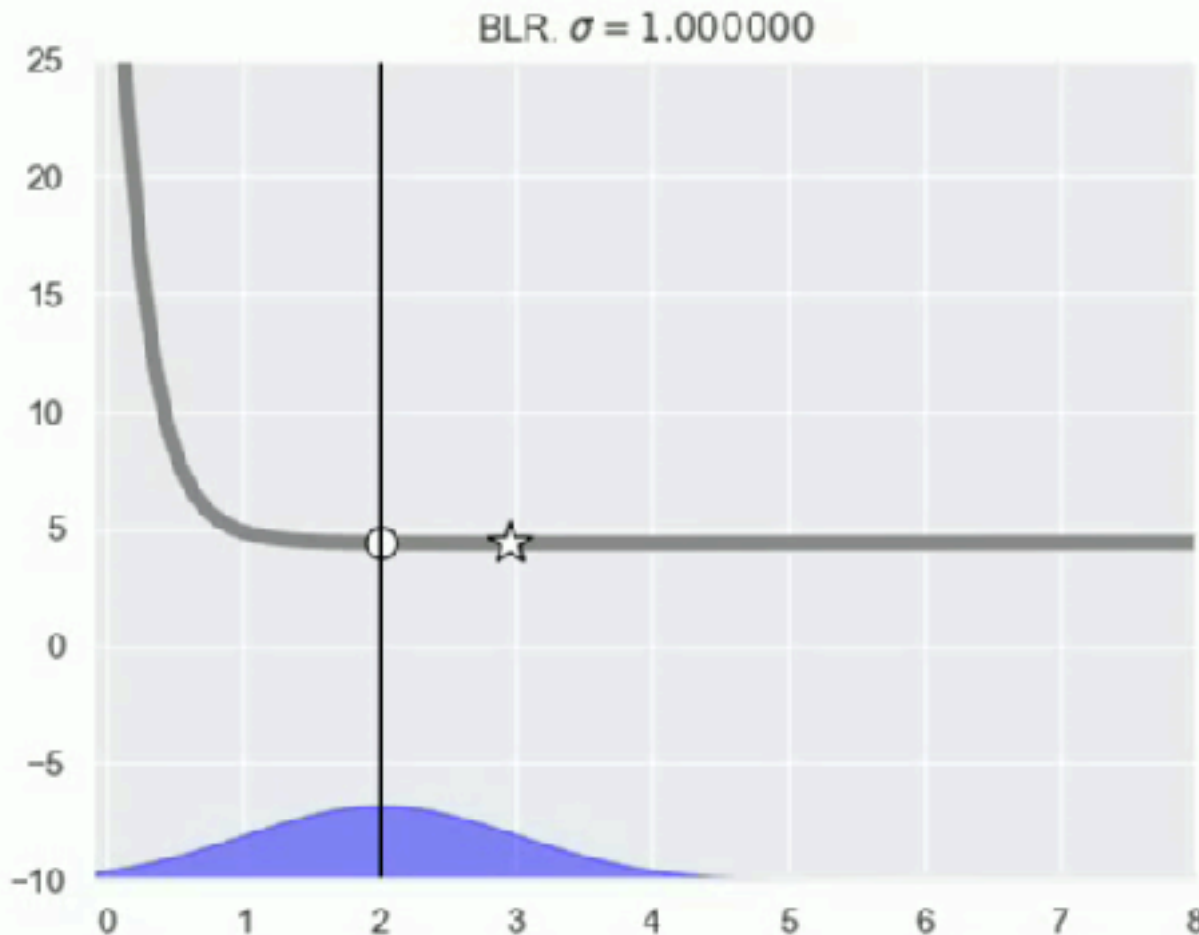
Estimating Gaussian posteriors where the variance is fixed, and only the mean is estimated

$$\mathbb{E}_{q_*}[\nabla_{\theta} \ell(\theta)] = 0$$

By increasing the variance, we can move the mode arbitrarily far.

Bayesian “noise” has a similar regularization to the SGD noise.

It prefers “flatter” directions.

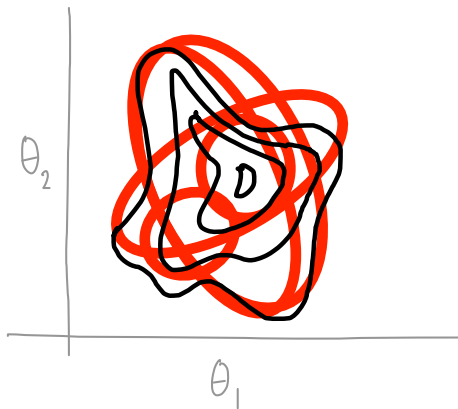


Deriving Learning-Algorithms from the Bayesian Learning Rule

Posterior Approximation \longleftrightarrow Learning-Algorithm

Complex

Simple



Bayes' rule

Mixture
of Newton

Newton

Gradient
Descent

Newton's Method from Bayes

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

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

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

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

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 Bayes

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:

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

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

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

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

BLR Variants

RMSprop

$$g \leftarrow \hat{\nabla} \ell(\theta)$$

$$s \leftarrow (1 - \rho)s + \rho g^2$$

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

Variational Online Gauss-Newton (VOGN)

$$g \leftarrow \hat{\nabla} \ell(\theta), \text{ where } \theta \sim \mathcal{N}(m, \sigma^2)$$

$$s \leftarrow (1 - \rho)s + \rho(\sum_i g_i^2)$$

$$m \leftarrow m - \alpha(s + \gamma)^{-1} \nabla_{\theta} \ell(\theta)$$

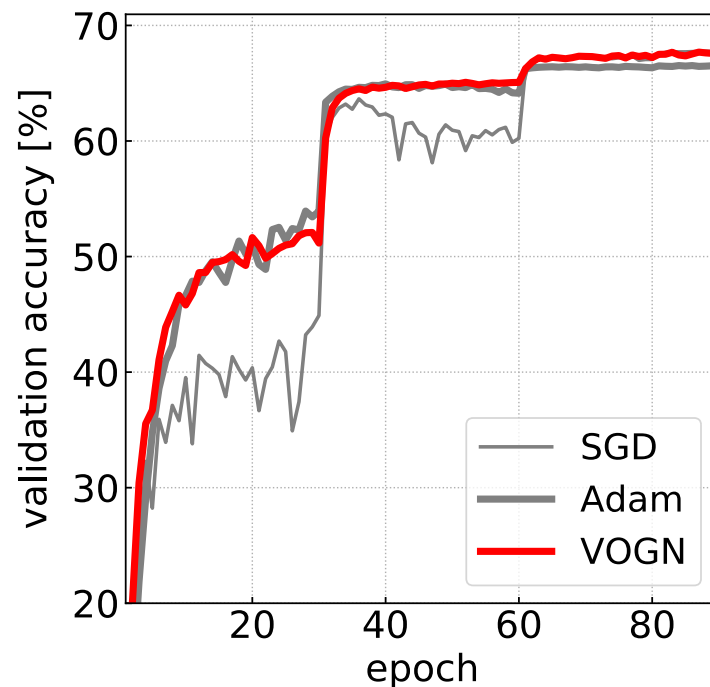
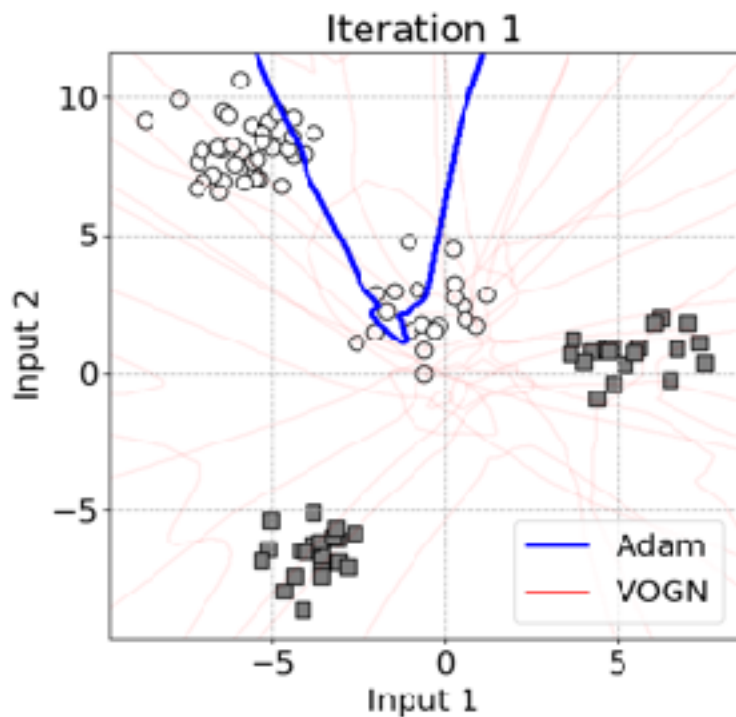
$$\sigma^2 \leftarrow (s + \gamma)^{-1}$$

Available at <https://github.com/team-approx-bayes/dl-with-bayes>

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).

Uncertainty of Deep Nets

VOGN: A modification of Adam but match the performance on ImageNet



Code available at <https://github.com/team-approx-bayes/dl-with-bayes>

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).

BLR variant [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 Möllenhoff¹, Yuesong Shen², Gian Maria Marconi¹
Peter Nickl¹, Mohammad Emtiyaz Khan¹


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).
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).

Bayes leads to robust solutions

Avoiding sharp minima

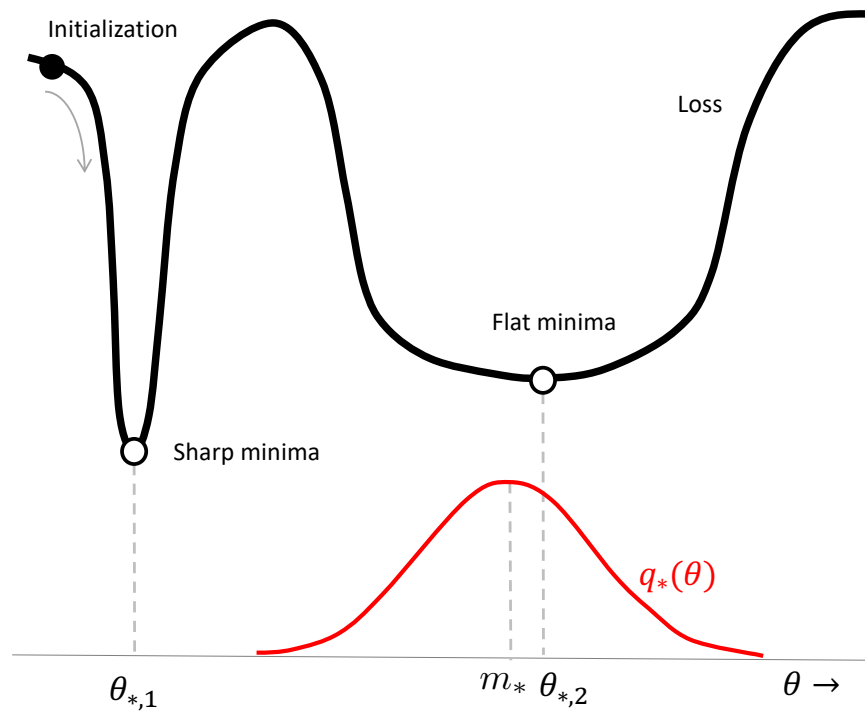
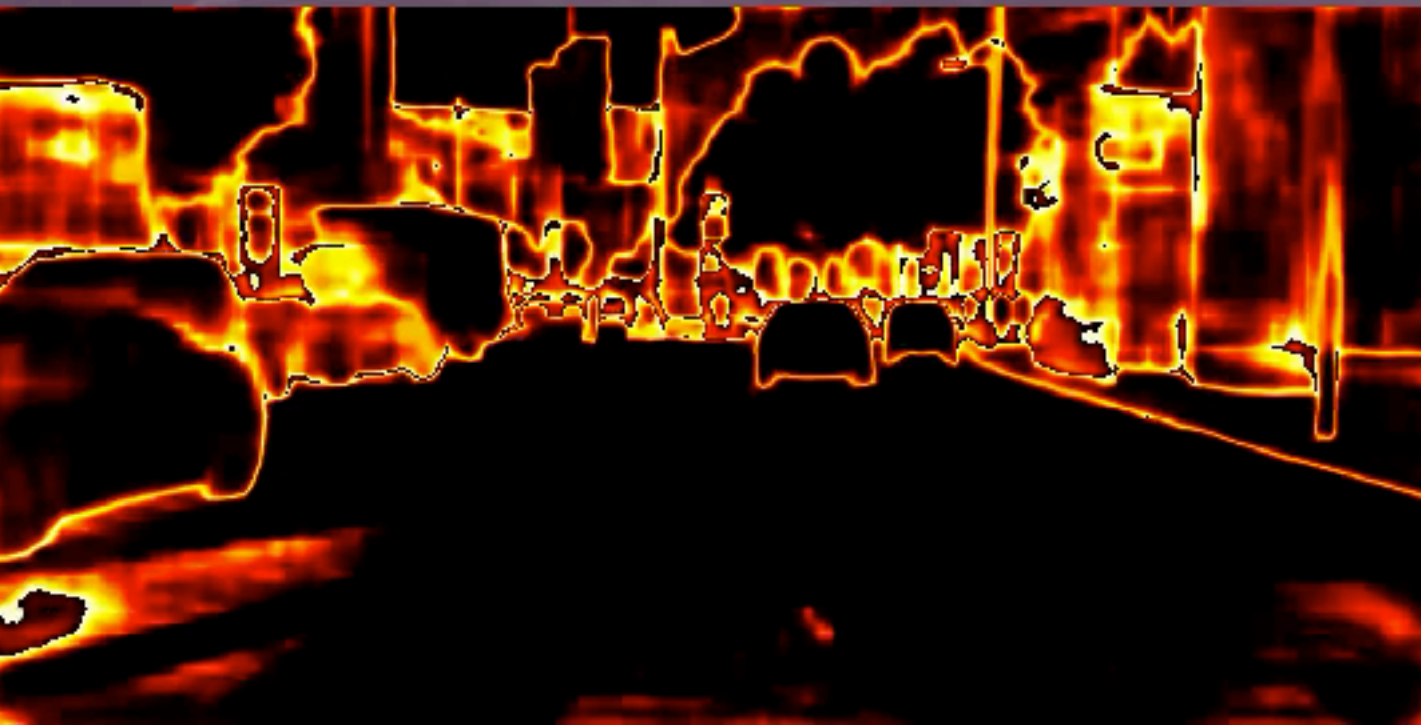


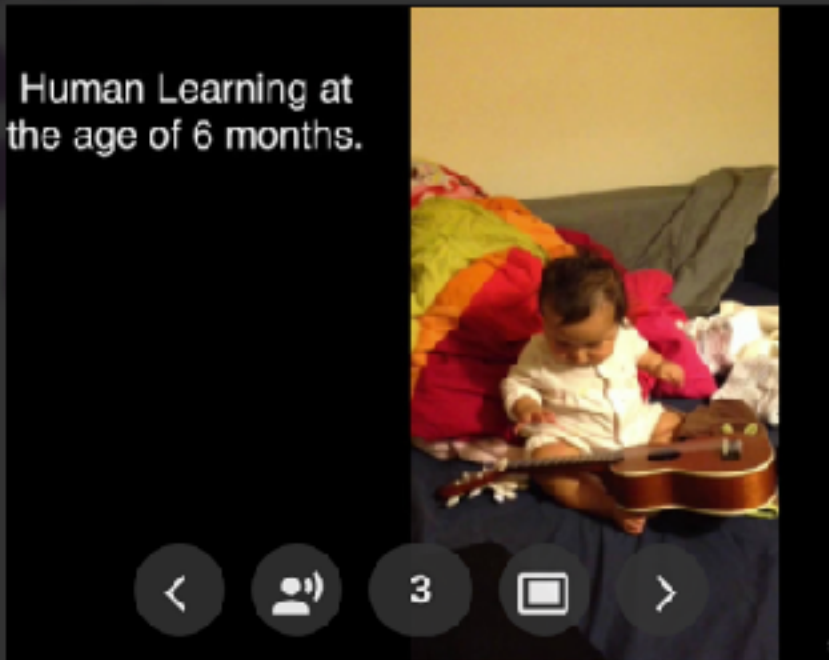
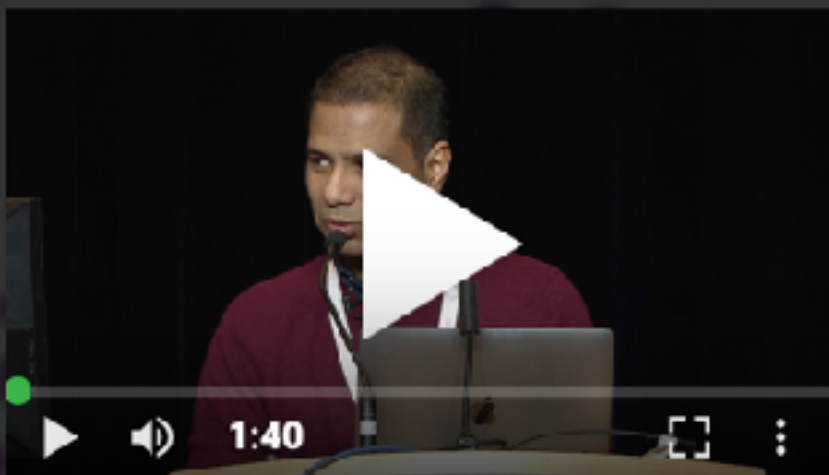


Image
Segmentation



Uncertainty
(entropy of
class probs)

NeurIPS 2019 Tutorial



Deep Learning with Bayesian Principles

by **Mohammad Emtiyaz Khan** · Dec 9, 2019

#NeurIPS 2019

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Robustness

Good algorithms can tell apart
relevant vs irrelevant information

Perturbation, Sensitivity, and Duality



via steampunktendencies.com

BLR Solutions & Their Duality

$$\ell(\theta) = \sum_{i=0}^N \ell_i(\theta) \quad \lambda \leftarrow (1 - \rho)\lambda - \sum_{i=0}^N \rho \nabla_{\mu} \mathbb{E}_q[\ell_i(\theta)]$$

$$\lambda^* = \sum_{i=0}^N \underbrace{\nabla_{\mu^*} \mathbb{E}_{q^*}[-\ell_i(\theta)]}_{\tilde{\lambda}_i^*}$$

Global and local natural parameter

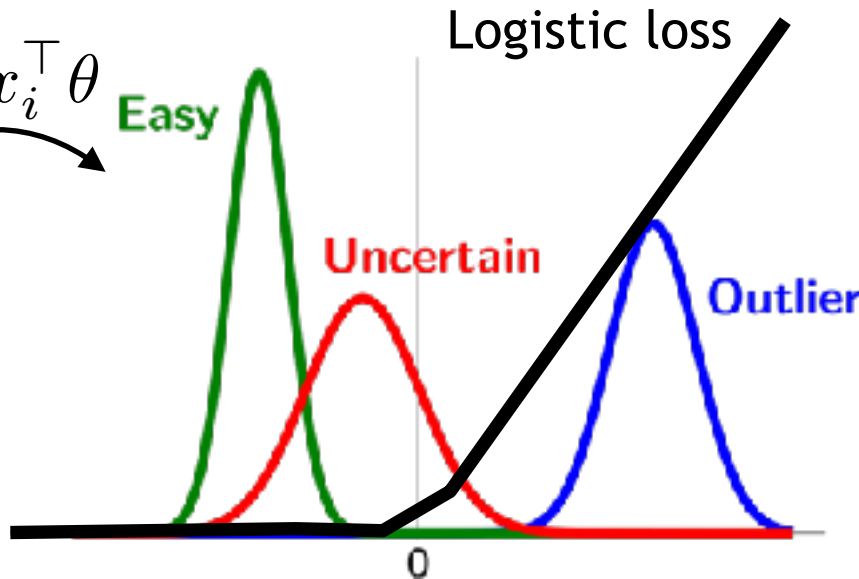
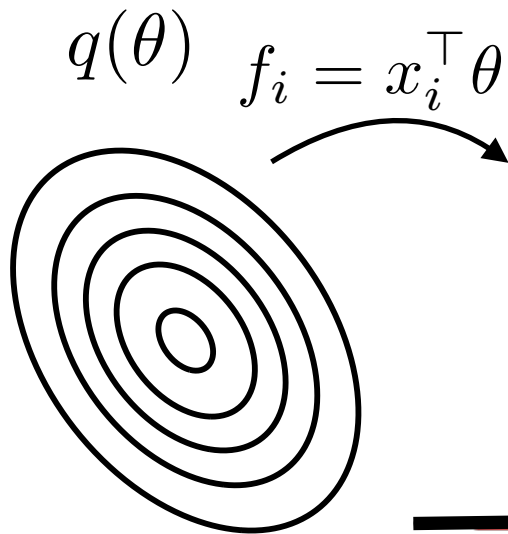
Local parameters are **Lagrange Multipliers**, measuring the sensitivity of BLR solutions to local perturbation [1]. They can be used to tell apart relevant vs irrelevant data.

Memorable Experiences

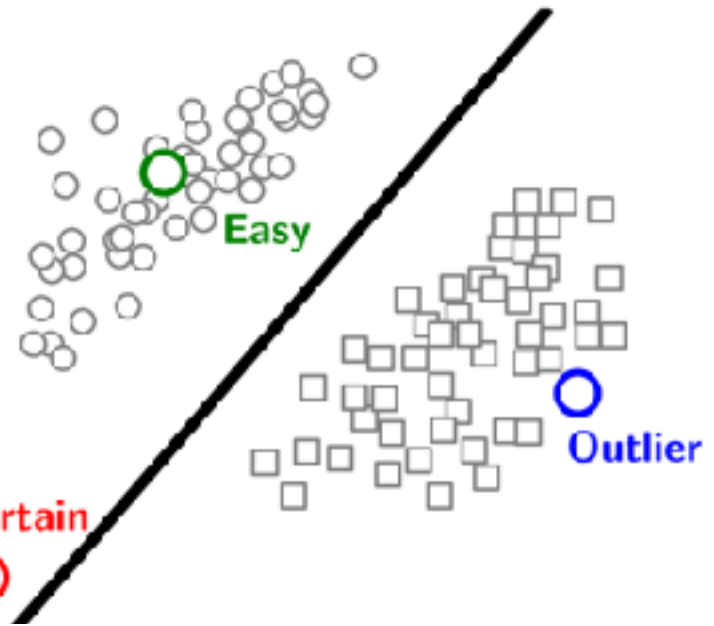
$$\lambda^* = \sum_{i=0}^N \underbrace{\nabla_{\mu^*} \mathbb{E}_{q^*} [-\ell_i(\theta)]}_{\tilde{\lambda}_i^*}$$

“Global”
posterior

Local predictions $q(f_i)$



Uncertain



Lower Sensitivity
to easy example.

Such sensitivity
analysis leads to
memorable
experiences

Memorable Experiences

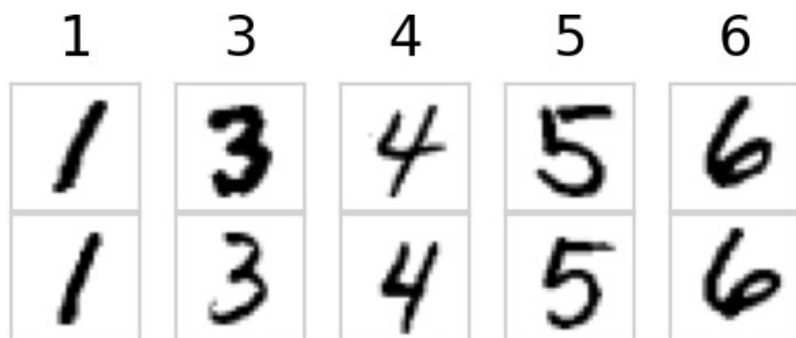
MNIST

FMNIST

Easy

Outliers

Uncertain



T-shirt Pullover Sandal Ankle boot Shirt



Advantages of Memorable Experiences

- Through posterior approximations, the criteria to categorize examples **naturally emerges**
 - Generalizes existing concepts such as support vectors, influence functions, inducing inputs etc
- Local parameters are available for free and applies to almost “any” ML problem
 - Supervised, unsupervised, RL
 - Discrete/continuation loss and model parameters
- The sensitivity of posterior leads to “Bayes Duality”

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
(France side)

Statify-team, Inria
Grenoble Rhône-Alpes



Kenichi Bannai

Co-PI (Japan side)

Math-Science Team at
RIKEN-AIP and Keio
University



Rio Yokota

Co-PI
(Japan side)

Tokyo Institute of
Technology

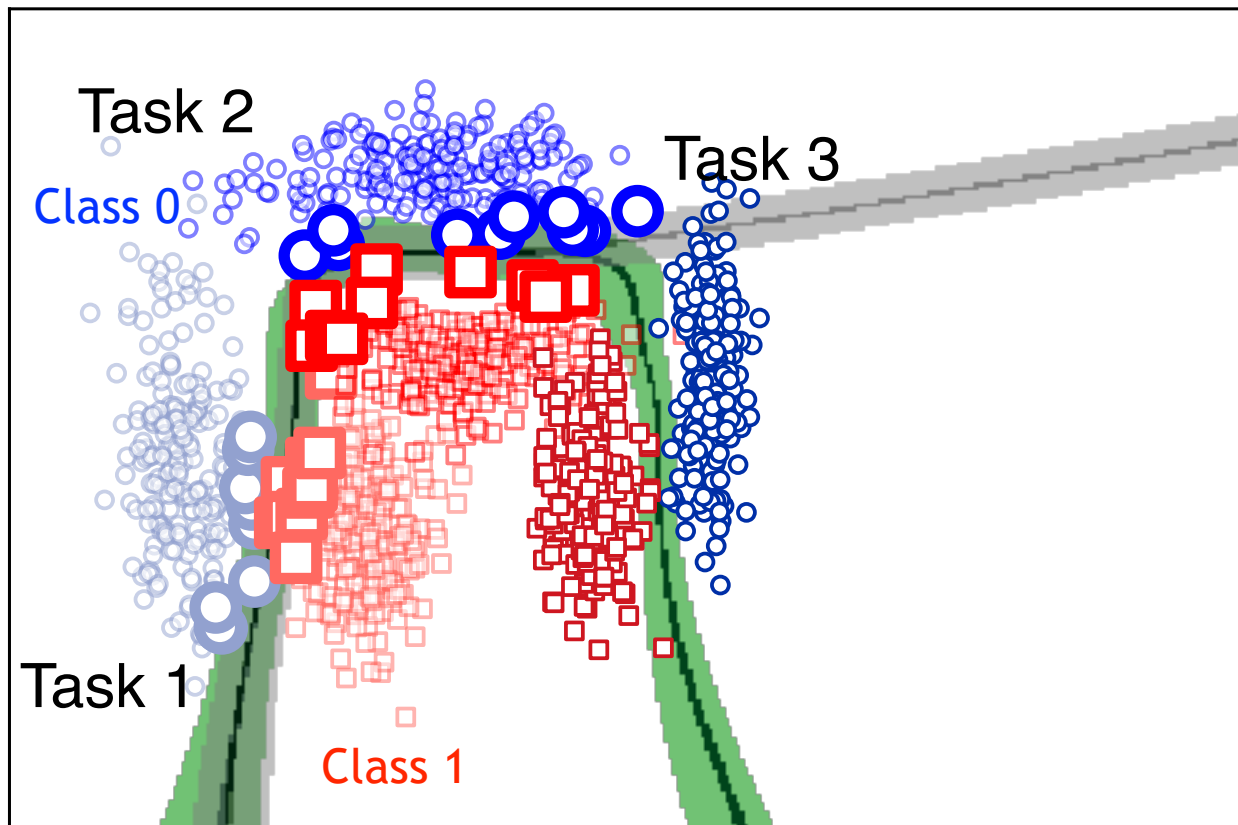
Received total funding of around **USD 3 million** through JST's CREST-ANR and Kakenhi Grants.

Adaptation

Continual Learning without forgetting the past (by using memorable examples)

Continual Learning

Avoid forgetting by using memorable examples [1,2]



1. Khan et al. Approximate Inference Turns Deep Networks into Gaussian Process, NeurIPS, 2019
2. Pan et al. Continual Deep Learning by Functional Regularisation of Memorable Past, NeurIPS, 2020

Functional Regularization of Memorable Past (FROMP) [4]

Previous approaches used weight-regularization [1,2]

$$q_{new}(\theta) = \min_{q \in \mathcal{Q}} \underbrace{\mathbb{E}_{q(\theta)}[\ell_{new}(\theta)]}_{\text{New data}} - \mathcal{H}(q) - \underbrace{\mathbb{E}_{q(\theta)}[\log q_{old}(\theta)]}_{\text{Weight-regularizer}}$$

We replace it by a functional regularizer using a “Gaussian Process view” of DNNs [2]

$$\underbrace{[\sigma(\mathbf{f}(\theta)) - \sigma(\mathbf{f}_{old})]^\top K_{old}^{-1} [\sigma(\mathbf{f}(\theta)) - \sigma(\mathbf{f}_{old})]}_{\substack{\text{Kernels weighs examples} \\ \text{according to their memorability}}} \underbrace{\mathbb{E}_{\tilde{q}_\theta(\mathbf{f})}[\log \tilde{q}_{\theta_{old}}(\mathbf{f})]}_{\substack{\text{Forces network-outputs} \\ \text{to be similar}}}$$

1. Kirkpatrick, James, et al. "Overcoming catastrophic forgetting in neural networks." *PNAS* 2017
2. Nguyen et al., Variational Continual Learning, ICLR, 2018
3. Khan et al. Approximate Inference Turns Deep Networks into Gaussian Process, NeurIPS, 2019
4. Pan et al. Continual Deep Learning by Functional Regularisation of Memorable Past, NeurIPS, 2020

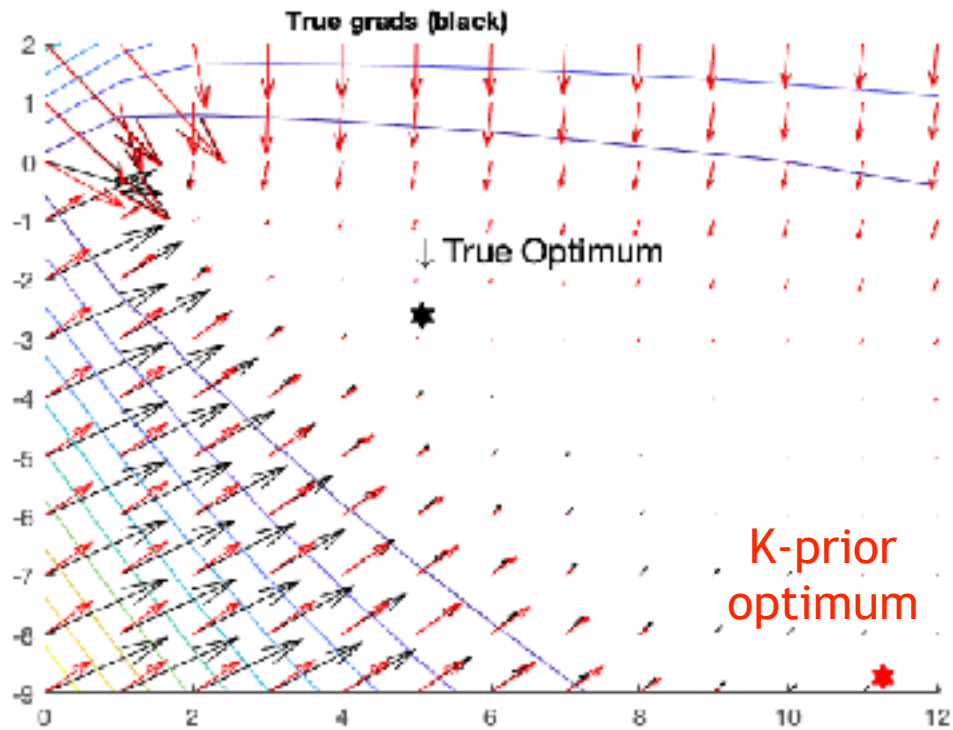
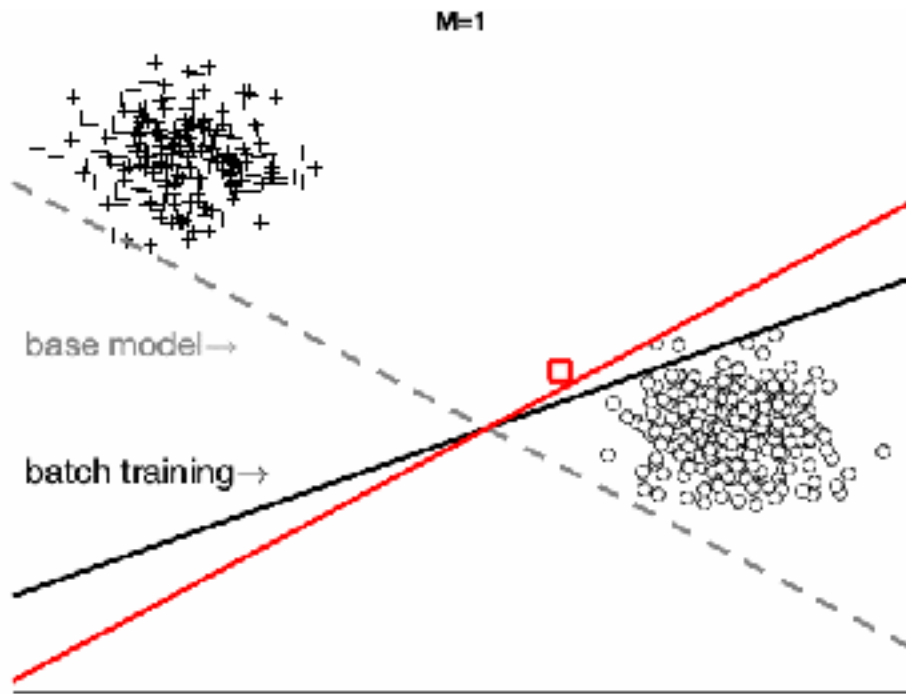
K-Priors and Bayes-Duality

- Dual parameterization of DNNs
 - expressed as Gaussian Process [1]
 - Found using the Bayesian learning rule
- The functional regularizer can provably reconstruct the gradient of the past faithfully [2]
 - Knowledge-Adaptation priors (K-priors)
 - There is a strong evidence that “good” adaptive algorithms must use K-priors

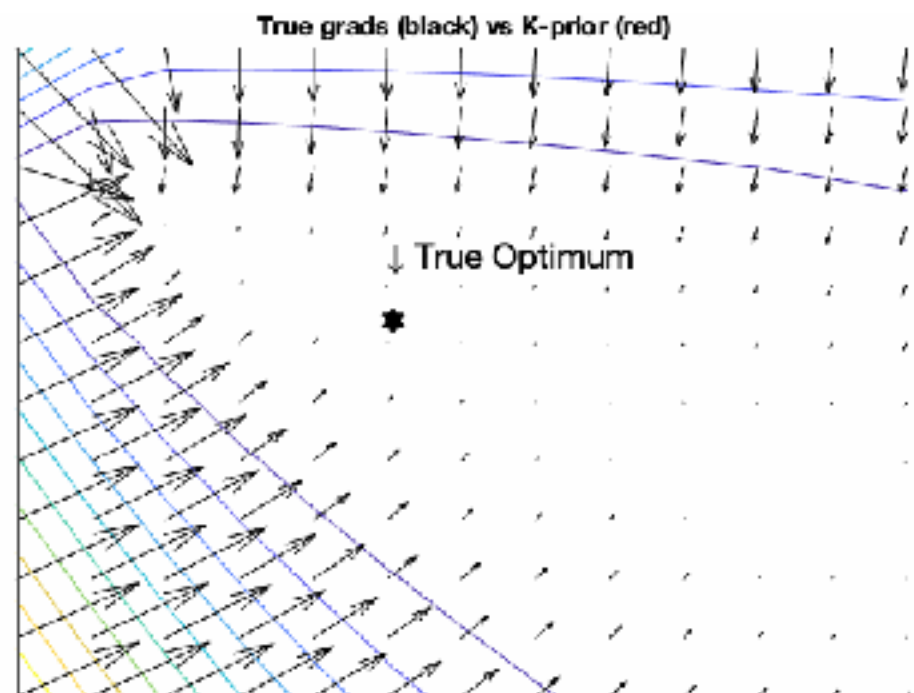
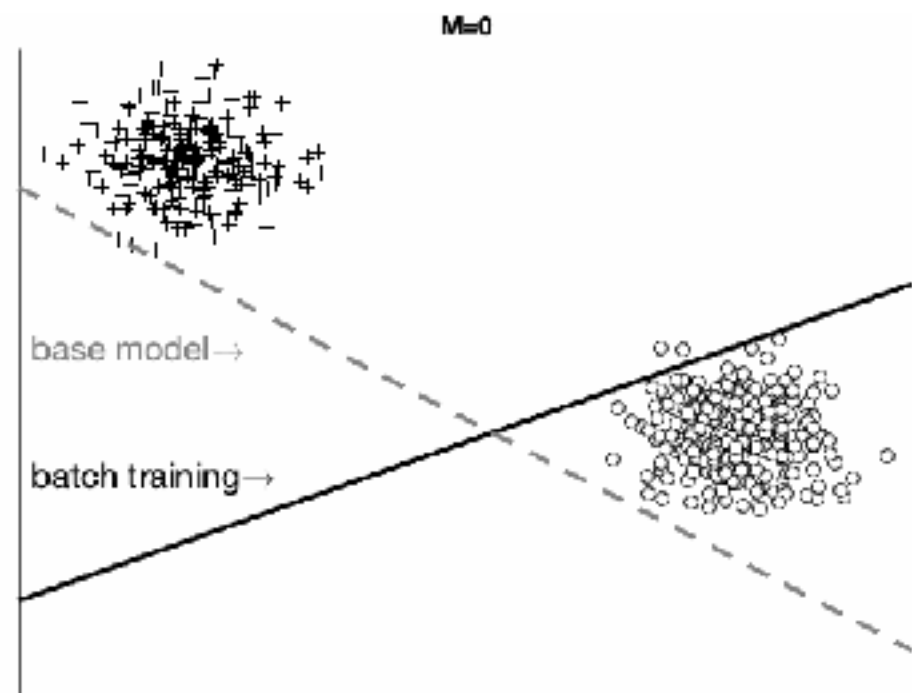
1. Khan et al. Approximate Inference Turns Deep Networks into Gaussian Process, NeurIPS, 2019

2. Khan and Swaroop. Knowledge-Adaptation Priors, NeurIPS, 2021 (<https://arxiv.org/abs/2106.08769>)

Faithful Gradient Reconstruction



Faithful Gradient Reconstruction



No labels required, so \mathcal{M} can include any inputs!

Summary

- A new perspective of Bayes, essential for adaptive and robust deep learning
- Approximate posteriors are crucial
 - Bayesian learning rule [1]
 - Robustness: Memorable experiences [2]
 - Adaptation: K-Priors [3,4,5]
- Bayes-duality for AI that learns like humans

1. Khan and Rue, The Bayesian Learning Rule, arXiv, <https://arxiv.org/abs/2107.04562>, 2021
2. Tailor, Chang, Swaroop, Tangkaratt, Solin, Khan. Memorable experiences of ML models (in preparation)
3. Khan et al. Approximate Inference Turns Deep Networks into Gaussian Process, NeurIPS, 2019
4. Pan et al. Continual Deep Learning by Functional Regularisation of Memorable Past, NeurIPS, 2020
5. Khan and Swaroop. Knowledge-Adaptation Priors, NeurIPS, 2021 (<https://arxiv.org/abs/2106.08769>)

Approximate Bayesian Inference Team

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

We have many open positions!
Come, join us.



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Team Leader



Pierre Alquier
Research Scientist



Gian Maria Marconi
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Thomas Möllenhoff
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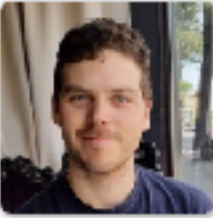
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