Presentation at ICIAM 2023 Minisymposium on Interaction between Harmonic Analysis and Data Science, Aug 24, 2023

The Bayesian Learning Rule

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http://emtiyaz.github.io

Summary of recent research at https://emtiyaz.github.io/papers/symposium_2022.pdf

Slides available at https://emtiyaz.github.io/

How to make AI that can adapt quickly?

Reasoning is crucial for this!

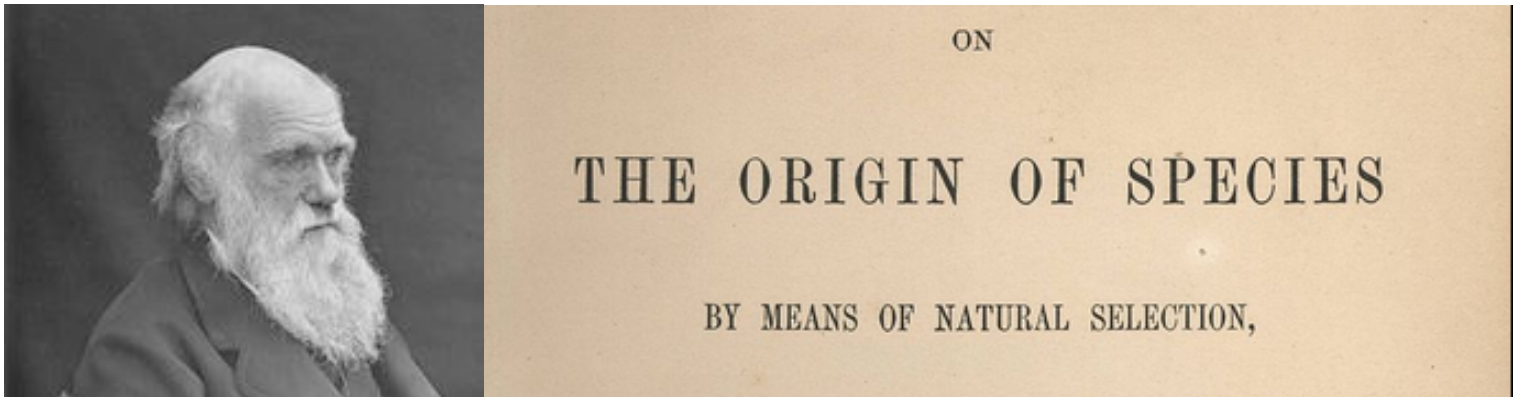
Human Learning at the age of 6 months.

Converged at the age of 12 months

Transfer skills

at the age of 14 months

See Section 6 (discussion) in Khan and Rue, 2021



The Origin of Algorithms

What are the common principles behind popular algorithms?

1. Khan and Rue, The Bayesian Learning Rule, arXiv, https://arxiv.org/abs/2107.04562, 2021

Principles of "good" algorithms?

- Information Geometry of Bayes
  - To unify/generalize/improve learning-algorithms
  - Optimize for "posterior approximations"
- Bayesian Learning rule (BLR)
  - Derive many algorithms from optimization, deep learning, and Bayesian inference
- Natural Gradients are Everywhere!

Khan and Rue, The Bayesian Learning Rule, arXiv, https://arxiv.org/abs/2107.04562, 2021

Bayesian Learning Rule

New information as natural gradients

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

Principle of Trial-and-Error

Frequentist: Empirical Risk Minimization (ERM) or Maximum Likelihood Principle, etc.

$$\min_{\theta} \ \ell(\mathcal{D}, \theta) \quad = \sum_{i=1}^{N} [y_i - f_\theta(x_i)]^2 + \gamma \theta^T \theta$$

Loss

Data

Model Params

Deep Network

Deep Learning Algorithms: $\theta \leftarrow \theta - \rho H_\theta^{-1} \nabla_\theta \ell(\theta)$

We will derive them as special instances of a rule exploiting information geometry of Bayes.

Bayesian Learning

Bayes rule: $\text{posterior} \propto \text{lik} \times \text{prior}$

Bayes as optimization [1]: $\min_{q \in \mathcal{Q}} \mathbb{E}_q[\text{log-lik}] + \text{KL}(q \| \text{prior})$

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

log-lik + log-prior

Entropy

Posterior approximation (expo-family)

1. Zellner, Optimal information processing and Bayes's theorem, The American Statistician, 1988.

Geometry of Exponential Family

We will exploit the geometry of "minimal" exp-family

Natural parameters — Sufficient Statistics — Expectation parameters

$$q(\theta) \propto \exp\left[\lambda^\top T(\theta)\right] \qquad \mu := \mathbb{E}_q[T(\theta)]$$

$$\mathcal{N}(\theta|m, S^{-1}) \propto \exp\left[-\frac{1}{2}(\theta - m)^\top S(\theta - m)\right]$$

$$\propto \exp\left[(Sm)^\top \theta + \mathrm{Tr}\left(-\frac{S}{2}\theta\theta^\top\right)\right]$$

Gaussian distribution	$q(\theta) := \mathcal{N}(\theta\|m, S^{-1})$
Natural parameters	$\lambda := \{Sm, -S/2\}$
Expectation parameters	$\mu := \{\mathbb{E}_q(\theta), \mathbb{E}_q(\theta\theta^\top)\}$

1. Wainwright and Jordan, Graphical Models, Exp Fams, and Variational Inference Graphical models 2008
2. Malago et al., Towards the Geometry of Estimation of Distribution Algos based on Exp-Fam, FOGA, 2011

The Bayesian Learning Rule

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

$\mathcal{H}(q)$: Entropy

$\mathcal{Q}$: Posterior approximation (expo-family)

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

Natural and Expectation parameters of q

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

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

$(1-\rho)\lambda$: Old belief

$\nabla_{\mu} \mathbb{E}_q[\ell(\theta)]$: 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, arXiv, https://arxiv.org/abs/2107.04562, 2021
2. Khan and Lin. "Conjugate-computation variational inference…." AIstats (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, 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:

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See Section 1.3.1 in Khan and Rue, 2021

Gradient Descent from BLR

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

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

"Global" to "local" (the delta method)
$\mathbb{E}_q[\ell(\theta)] \approx \ell(m)$

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

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

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:

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Put the expectation (Bayes) back in and use the Bayesian averaging.

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).

Practical DL with Bayes

RMSprop

$$g \leftarrow \hat{\nabla}\ell(\theta)$$
$$s \leftarrow (1-\rho)s + \rho g^2$$
$$\theta \leftarrow \theta - \alpha(\sqrt{s}+\delta)^{-1} g$$

BLR variant called VOGN

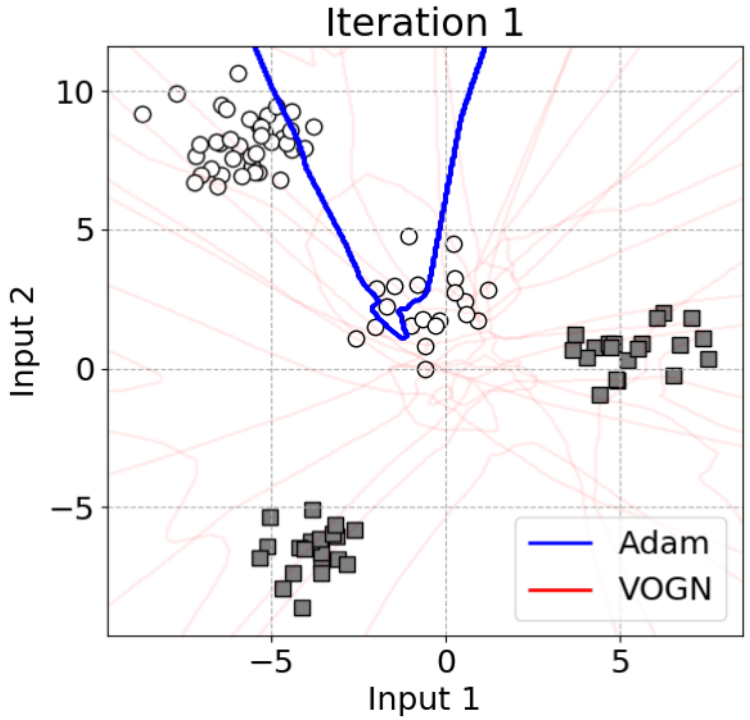
$$g \leftarrow \hat{\nabla}\ell(\theta), \text{ where } \theta \sim \mathcal{N}(m, \sigma^2)$$
$$s \leftarrow (1-\rho)s + \rho(\Sigma_i g_i^2)$$
$$m \leftarrow m - \alpha(s+\gamma)^{-1}\nabla_\theta \ell(\theta)$$
$$\sigma^2 \leftarrow (s+\gamma)^{-1}$$

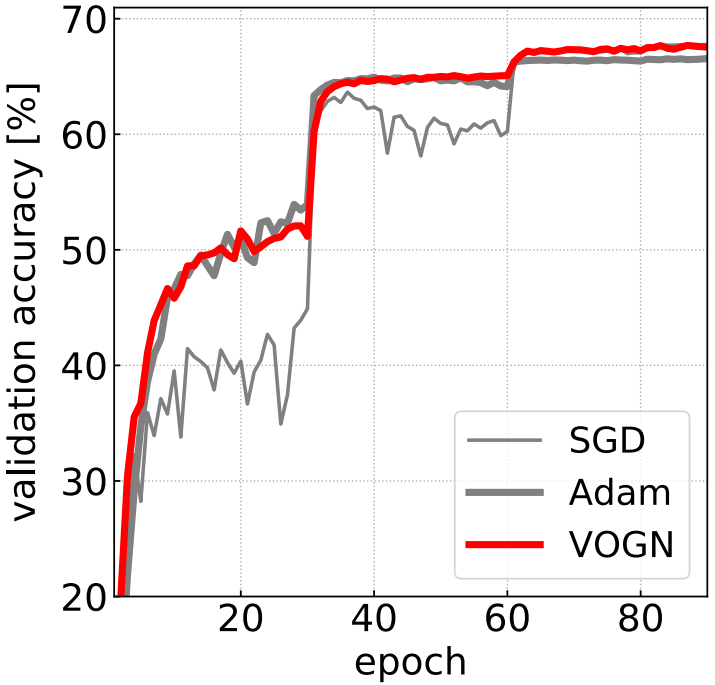
Available at https://github.com/team-approx-bayes/dl-with-bayes

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 with similar performance on ImageNet, but better uncertainty





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=LQInlN5EU7E.

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

Thomas Möllenhoff[1], Yuesong Shen[2], Gian Maria Marconi[1]
Peter Nickl[1], Mohammad Emtiyaz Khan[1]

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).

Image Segmentation

Uncertainty (entropy of class probs)

(By Roman Bachmann)

Summary

- Gradient descent is derived using a Gaussian with fixed covariance, and estimating the mean
- Newton's method is derived using multivariate Gaussian
- RMSprop is derived using diagonal covariance
- Adam is derived by adding heavy-ball momentum term
- For "ensemble of Newton", use Mixture of Gaussians [1]
- To derive DL algorithms, we need to use the Delta method (a local approximation) $\mathbb{E}_q[\ell(\theta)] \approx \ell(m)$
- Then, to improve DL algorithms, we just need to add some "global" touch by relaxing the local approximation

1. Lin, Wu, Mohammad Emtiyaz Khan, and Mark Schmidt. "Fast and Simple Natural-Gradient Variational Inference with Mixture of Exponential-family Approximations." *ICML* (2019).

See Section 1.2 in Khan and Rue, 2021

Our use of natural-gradients here is not a matter of choice. In fact, natural-gradients are inherently present in *all solutions of the Bayesian objective* in Eq. 2. For example, a solution of Eq. 2 or equivalently a fixed point of Eq. 3, satisfies the following,

$$\nabla_{\boldsymbol{\mu}} \mathbb{E}_{q_*}[\bar{\ell}(\boldsymbol{\theta})] = \nabla_{\boldsymbol{\mu}} \mathcal{H}(q_*), \text{ which implies } \widetilde{\nabla}_{\boldsymbol{\lambda}} \mathbb{E}_{q_*}[-\bar{\ell}(\boldsymbol{\theta})] = \boldsymbol{\lambda}_*, \tag{5}$$

for candidates with constant base-measure. This is obtained by setting the gradient of Eq. 2 to 0, then noting that $\nabla_{\boldsymbol{\mu}} \mathcal{H}(q) = -\boldsymbol{\lambda}$ (App. B), and then interchanging $\nabla_{\boldsymbol{\mu}}$ by $\widetilde{\nabla}_{\boldsymbol{\lambda}}$ (because of Eq. 4). In other words, natural parameter of the best $q_*(\boldsymbol{\theta})$ is equal to the natural gradient of the expected negative-loss. The importance of natural-gradients is entirely missed in the Bayesian/variational inference literature, including textbooks, reviews, tutorials on this topic [Bishop, 2006, Murphy, 2012, Blei et al., 2017, Zhang et al., 2018a] where natural-gradients are often put in a special category.

We will show that natural gradients retrieve essential higher-order information about the loss landscape which are then assigned to appropriate natural parameters using Eq. 5. The information-matching is due to the presence of the entropy term there, which is an important quantity for the optimality of Bayes in general [Jaynes, 1982, Zellner, 1988, Littlestone and Warmuth, 1994, Vovk, 1990], and which is generally absent in non-Bayesian formulations (Eq. 1). The entropy term in general leads to exponential-weighting in Bayes' rule. In our context, it gives rise to natural-gradients and, as we will soon see, automatically determines the complexity of the derived algorithm through the complexity of the class of distributions $\mathcal{Q}$, yielding a principled way to develop new algorithms.

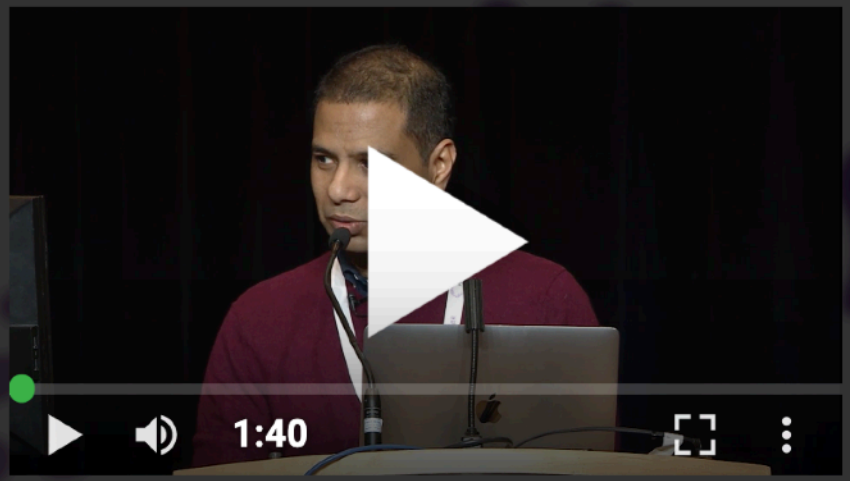
Overall, our work demonstrates the importance of natural-gradients and information geometry for algorithm design in ML. This is similar in spirit to Information Geometric Optimization [Ollivier et al., 2017], which focuses on the optimization of black-box, deterministic functions. In contrast, we derive generic learning algorithms by using the same Bayesian principles. The BLR we use is a generalization of the method proposed in Khan and Lin [2017], Khan and Nielsen [2018] specifically for approximate Bayesian inference. Here, we establish it as a general learning rule to derive many old and new learning algorithms, which include both Bayesian and non-Bayesian ones, way beyond its original proposal. We do not claim that these successful algorithms work well because they are derived from the BLR. Rather, we use the BLR to simply unravels the inherent Bayesian nature of these "good" algorithms. In this sense, the BLR can be seen as a variant of Bayes' rule, useful for generic algorithm design.

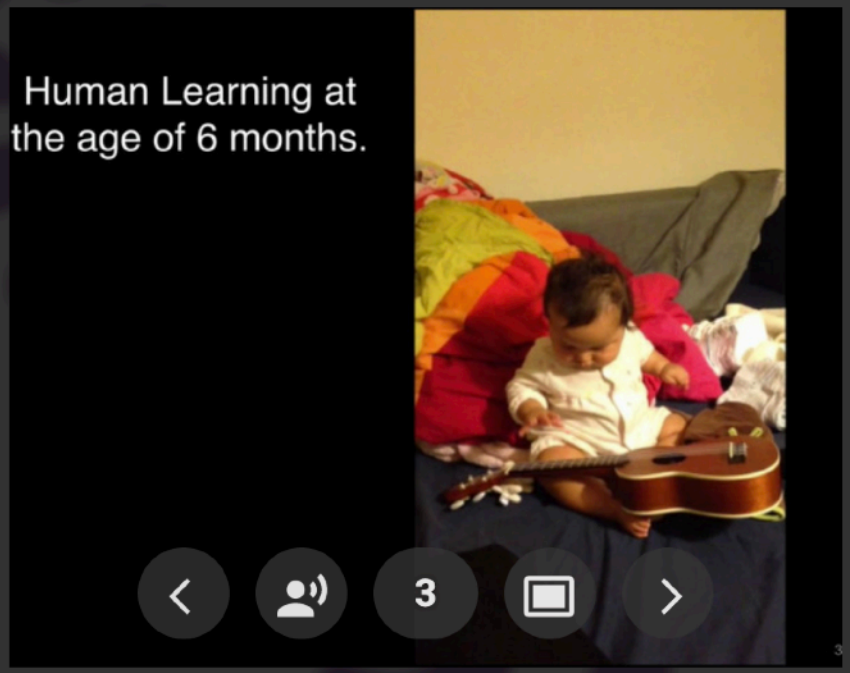
Principles of "good" algorithms?

- Information Geometry of Bayes
  - To unify/generalize/improve learning-algorithms
  - Optimize for "posterior approximations"
- Bayesian Learning rule (BLR)
  - Derive many algorithms from optimization, deep learning, and Bayesian inference
- Natural Gradients are Everywhere!

Khan and Rue, The Bayesian Learning Rule, arXiv, https://arxiv.org/abs/2107.04562, 2021
Lin et al., Tractable structured natural gradient descent using local parameterizations, ICML 2021

NeurIPS 2019 Tutorial





Deep Learning with Bayesian Principles

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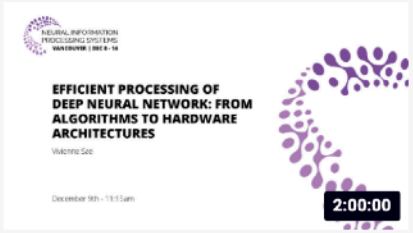

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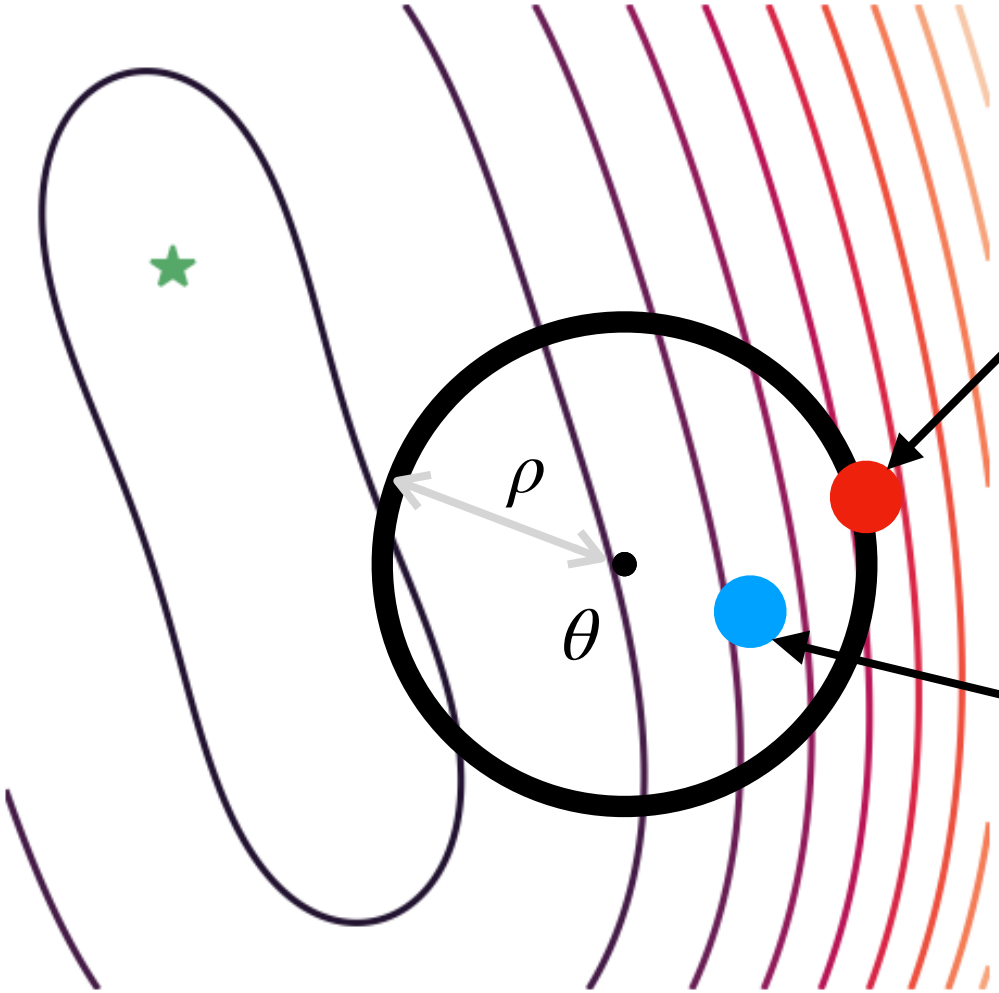
SAM as an Optimal relaxation of Bayes



SAM: $\sup_{|\epsilon|<\rho} \ell(\theta+\epsilon)$

Our work: Fenchel Biconjugate

Bayes: $\mathbb{E}_{\epsilon\sim\mathcal{N}(0,\sigma^2)}[\ell(\theta+\epsilon)]$

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

What's Next

- Bayesian "Duality" Principle
  - The BLR unravels a duality perspective of good algorithms
  - Unifies many results from many fields
    - convex duality, Kernel methods, Bayesian nonparametric methods, Deep Learning, Robust statistics, and Information Geometry
  - Helps to solve the Adaptation problem

The webpage is available at https://bayesduality.github.io/, and Twitter account @BayesDuality

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

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

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