Presentation at the One World Approximate Bayesian Computation Seminar, April 27, 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/papers/Apr27_2023.pdf

AI that learn like humans

Quickly adapt to learn new skills, throughout their lives

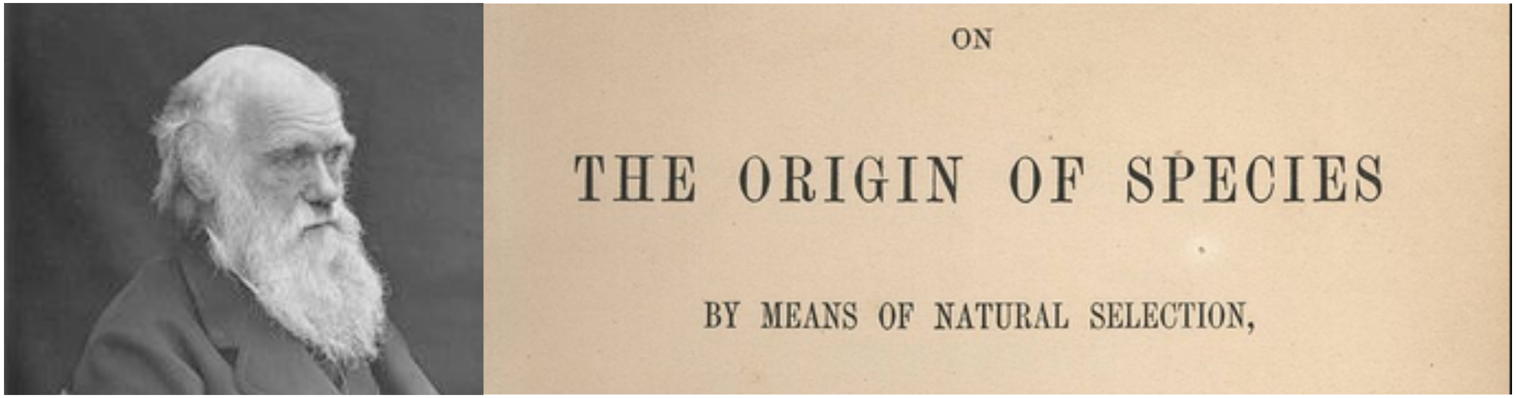
Human Learning at the age of 6 months.

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.

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

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 [1]: $\mathbb{E}_q[\text{log-lik}] + \text{KL}(q\|\text{prior})$

Generalized Approx Bayes:

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

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

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

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

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

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

Entropy

Posterior approximation (expo-family)

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

Natural and Expectation parameters of q

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

$$\lambda \leftarrow (1-\rho)\underbrace{\lambda}_{\text{Old belief}} - \rho \underbrace{\nabla_{\mu} \mathbb{E}_q[\ell(\theta)]}_{\text{New information = natural gradients}}$$

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 might be 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

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

Gradient Descent from Bayesian Learning Rule

(Euclidean) gradients as natural gradients

Bayesian learning rule:

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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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Non-Conjugate VI (New)	Mixture of Exp-family	None	5.4

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).

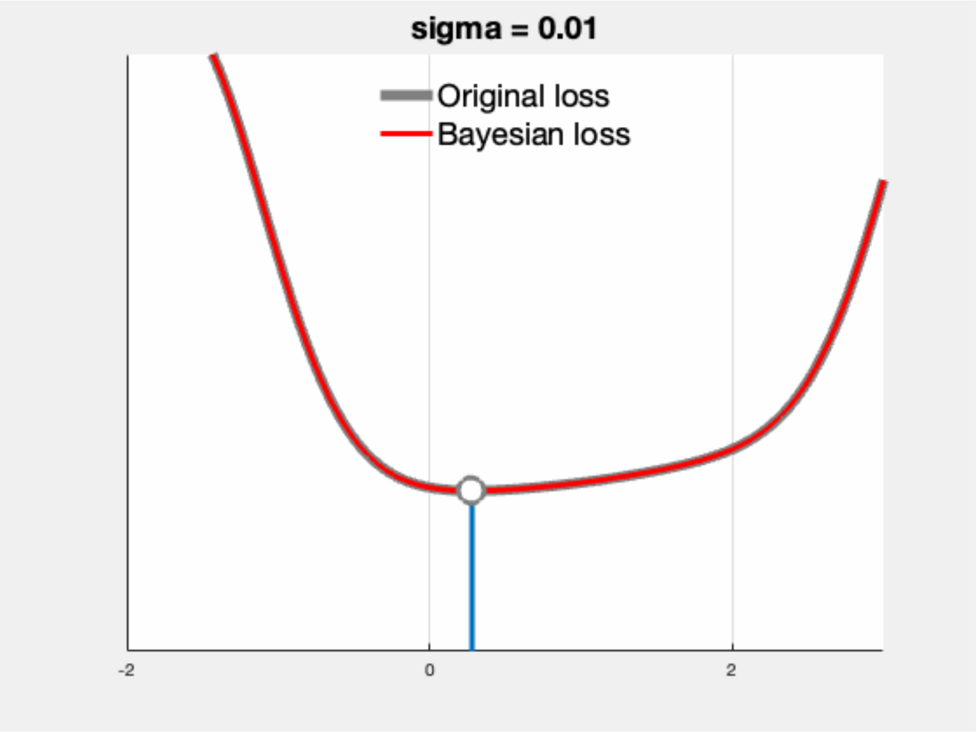
See Eq 25 in Khan and Rue, 2021 (Bonnet's theorem)

Bayes Prefers Flatter directions

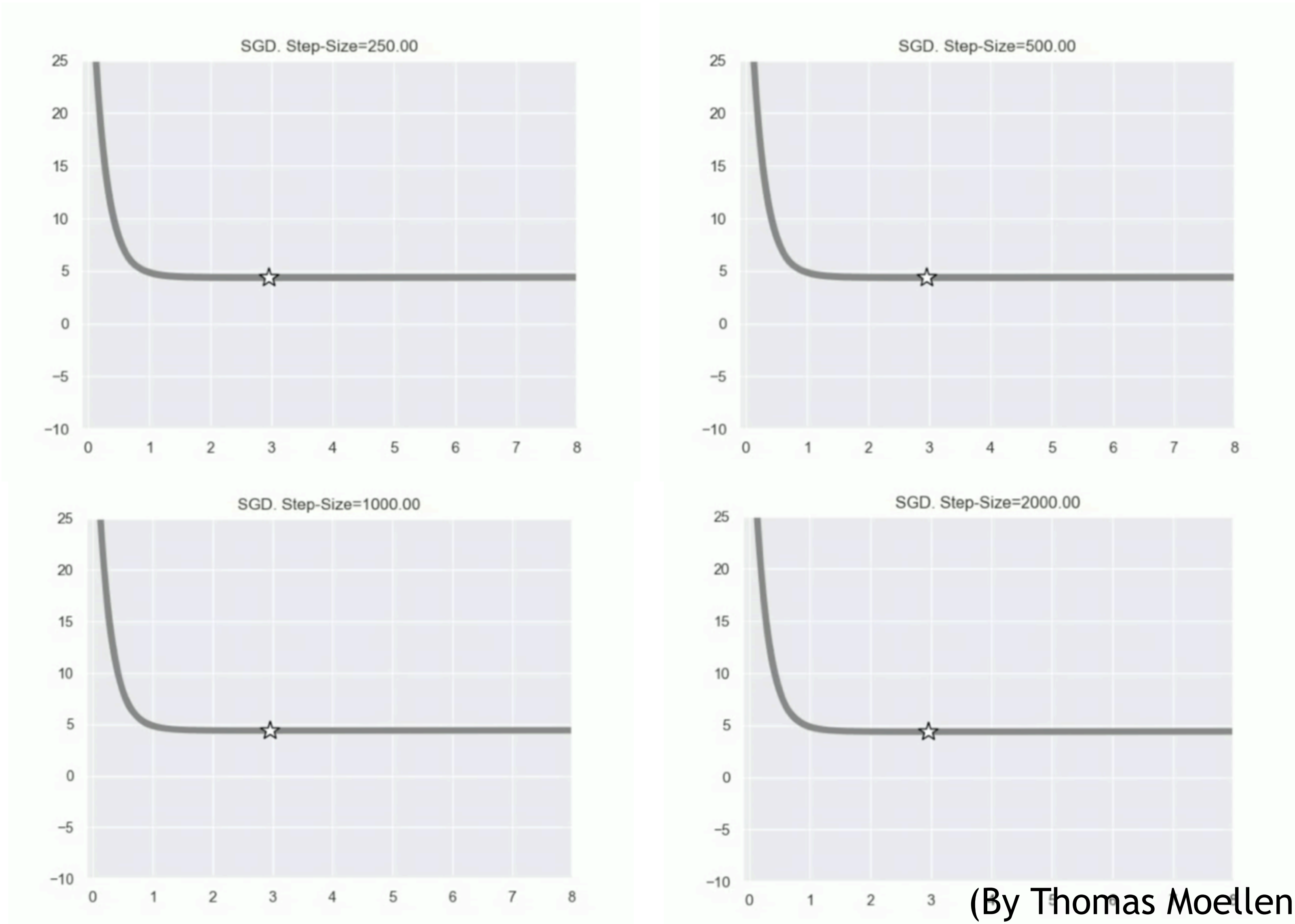
GD: $\theta \leftarrow \theta - \rho \nabla_\theta \ell(\theta) \implies \nabla_\theta \ell(\theta_*) = 0$

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

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

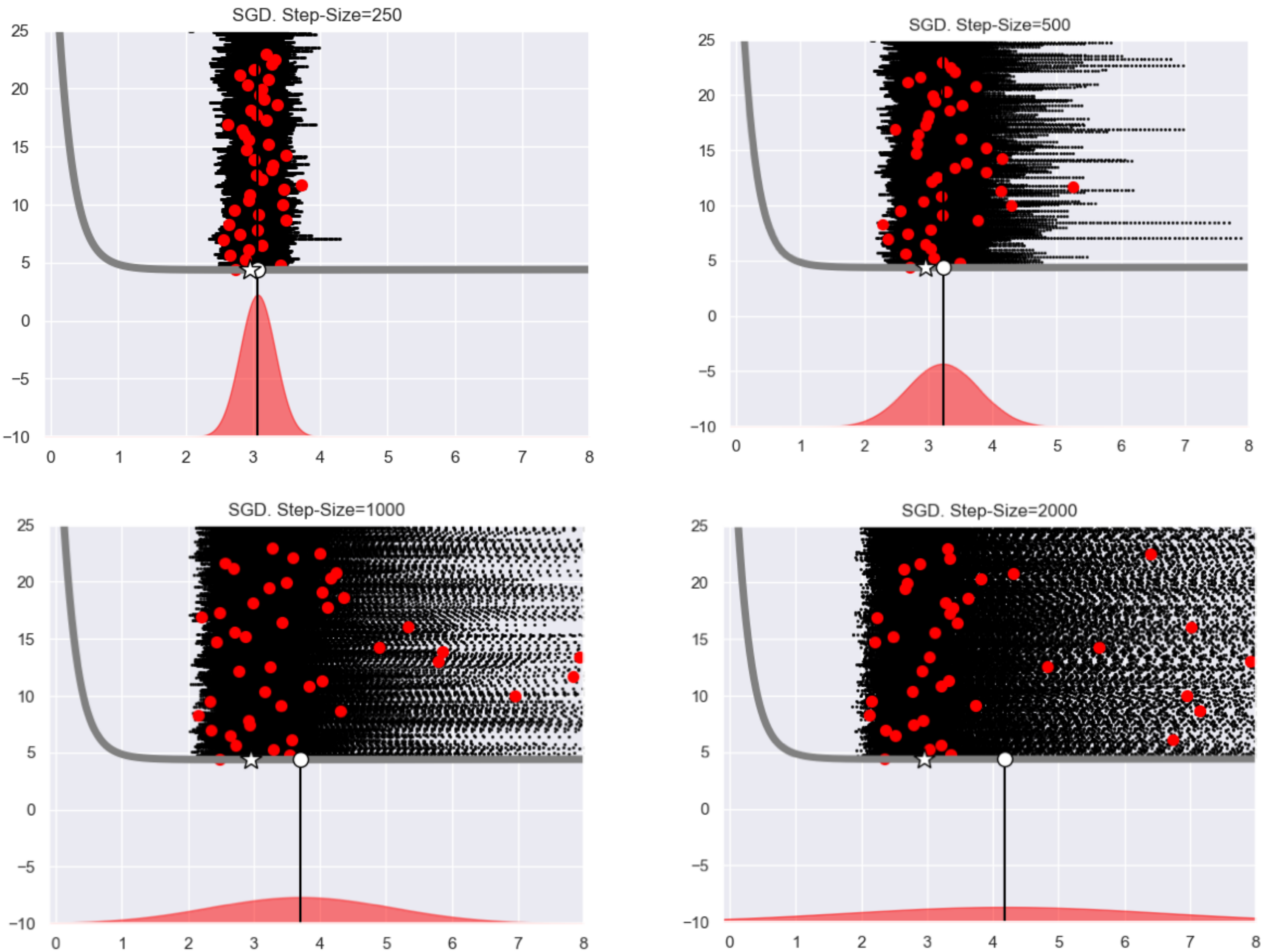


SGD: Implicit Regularization



(By Thomas Moellenhoff)

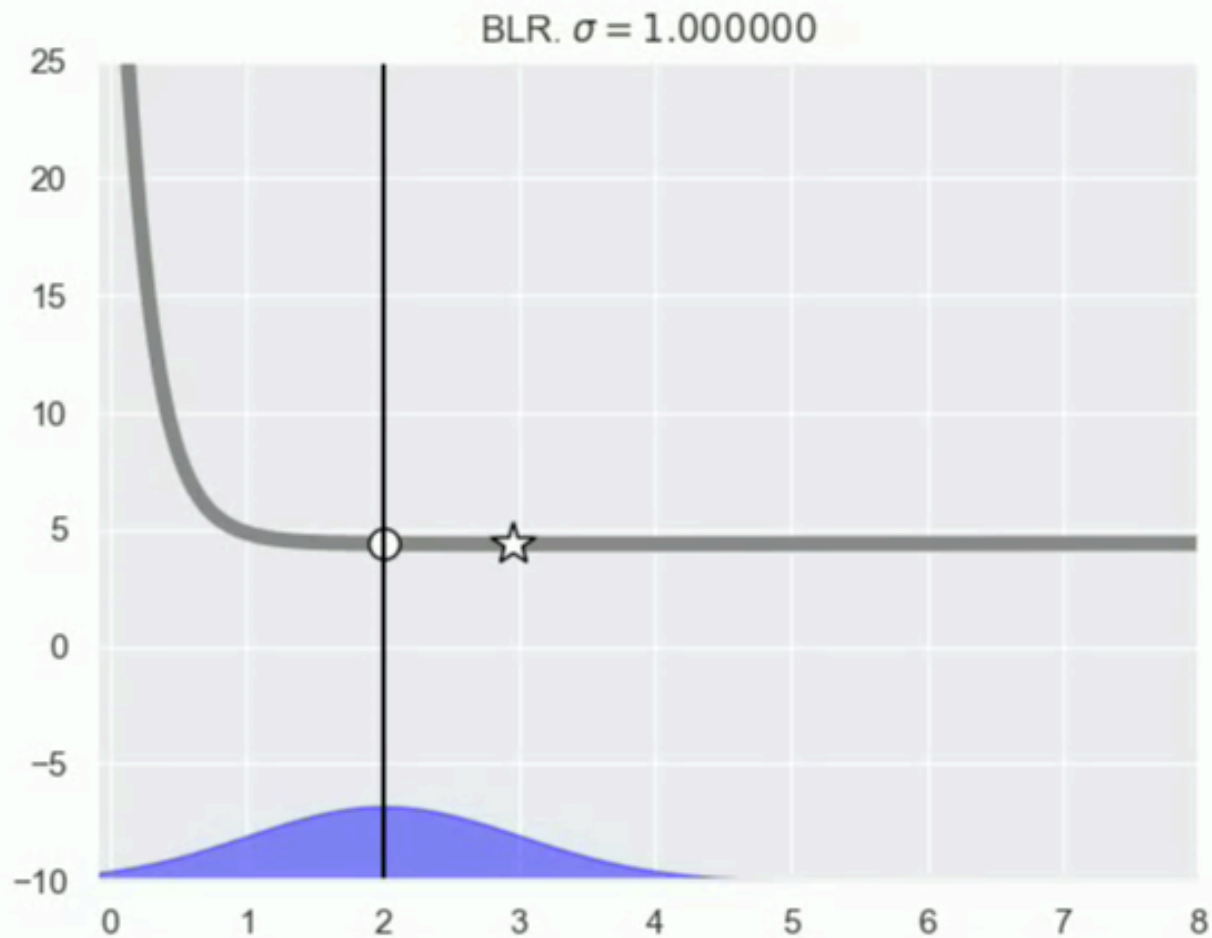
SGD: Implicit Regularization



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.

Newton’s method from Bayesian Learning Rule

(Gradient, Hessian) as natural gradients

See Section 1.3.2 in Khan and Rue, 2021

Newton's Method from BLR

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

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

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

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

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

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

$$\boxed{-\nabla_\mu\mathcal{H}(q) = \lambda}$$

Derived by choosing a multivariate Gaussian

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

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

Newton's Method from BLR

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

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

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

Delta Method

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

Express in terms of gradient and Hessian of loss:

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

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

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

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

See Section 4.2 in Khan and Rue, 2021

RMSprop/Adam from BLR

RMSprop	BLR for Gaussian approx
$s \leftarrow (1-\rho)s + \rho[\hat{\nabla}\ell(\theta)]^2$	$S \leftarrow (1-\rho)S + \rho(H_\theta)$
$\theta \leftarrow \theta - \alpha(\sqrt{s}+\delta)^{-1}\hat{\nabla}\ell(\theta)$	$m \leftarrow m - \alpha S^{-1}\nabla_\theta \ell(\theta)$

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])

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

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).
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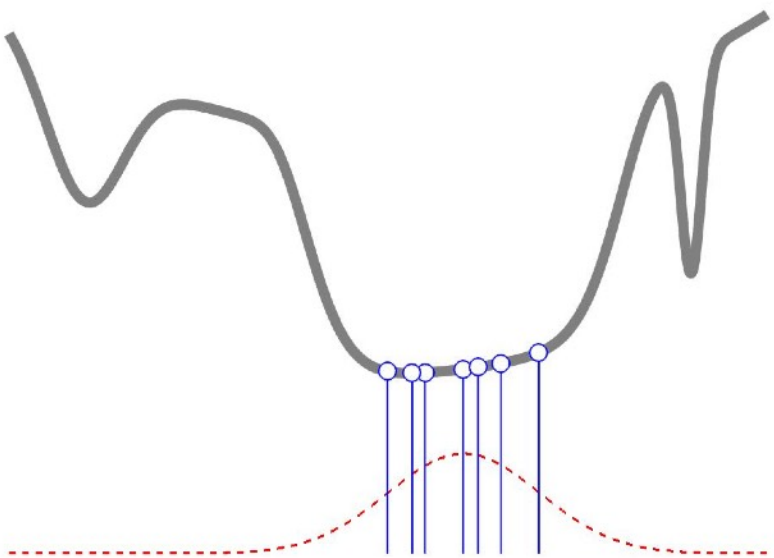
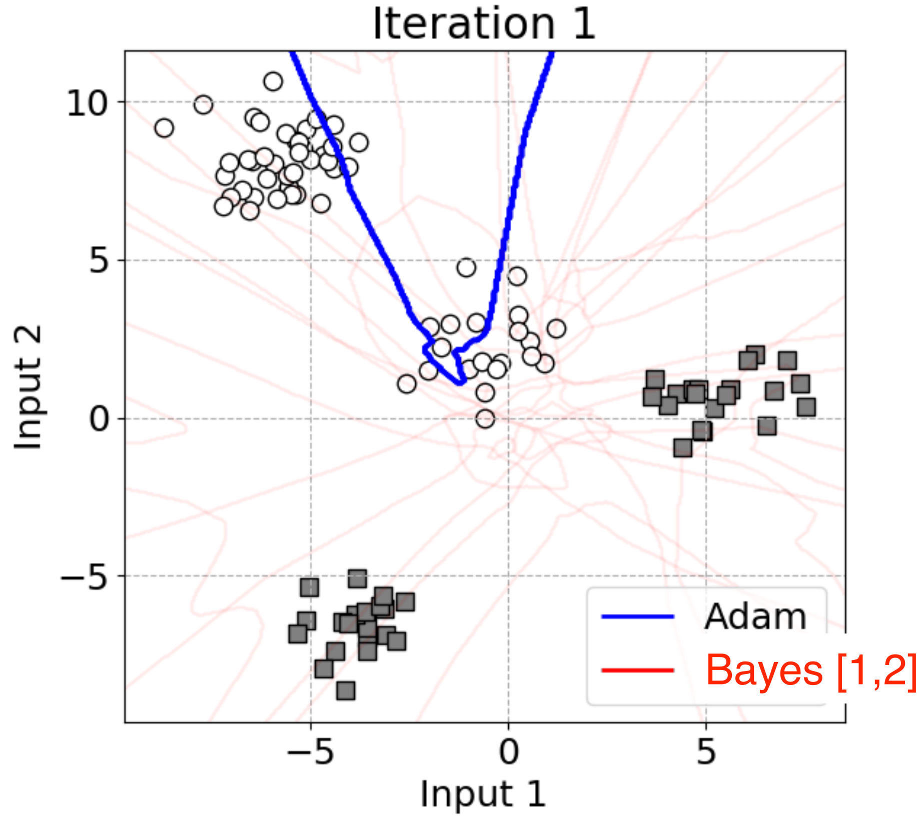
Why use Bayesian averaging?

Choose an “ensemble” of almost equally good models (similar to sampling in SGD trajectories)





1. Khan, et al. "Fast and scalable Bayesian deep learning by weight-perturbation in Adam." *ICML* (2018).
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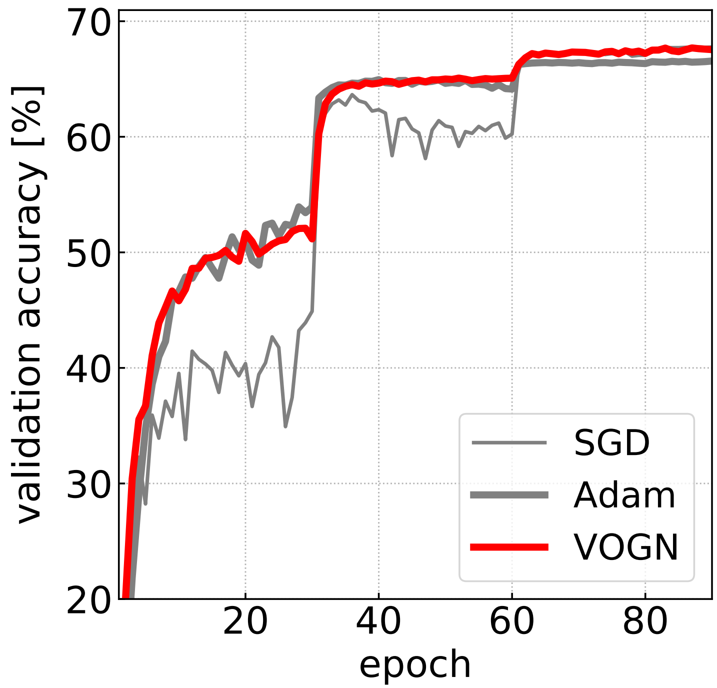
Uncertainty of Deep Nets

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]

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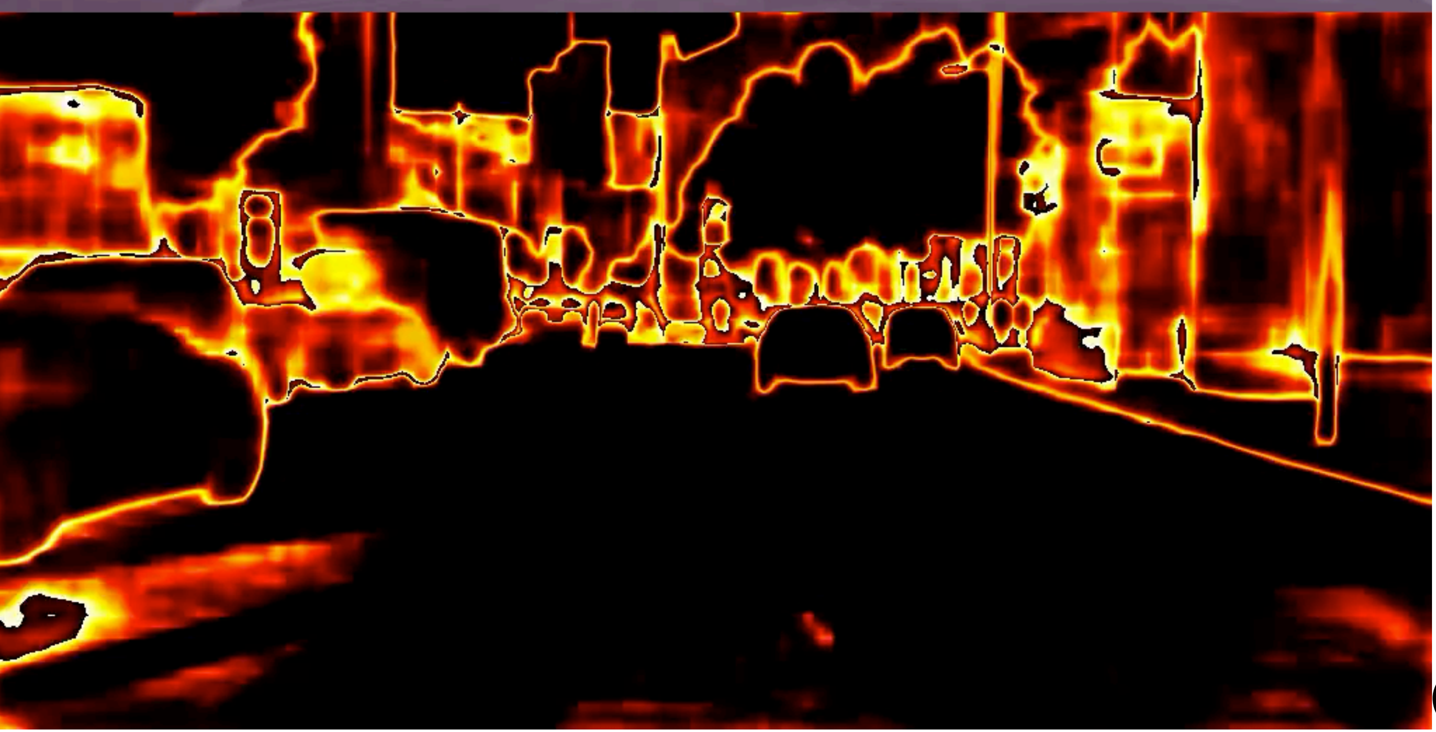
Dec 14th, 2021 — NeurIPS Workshop on Bayesian Deep Learning

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).

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!

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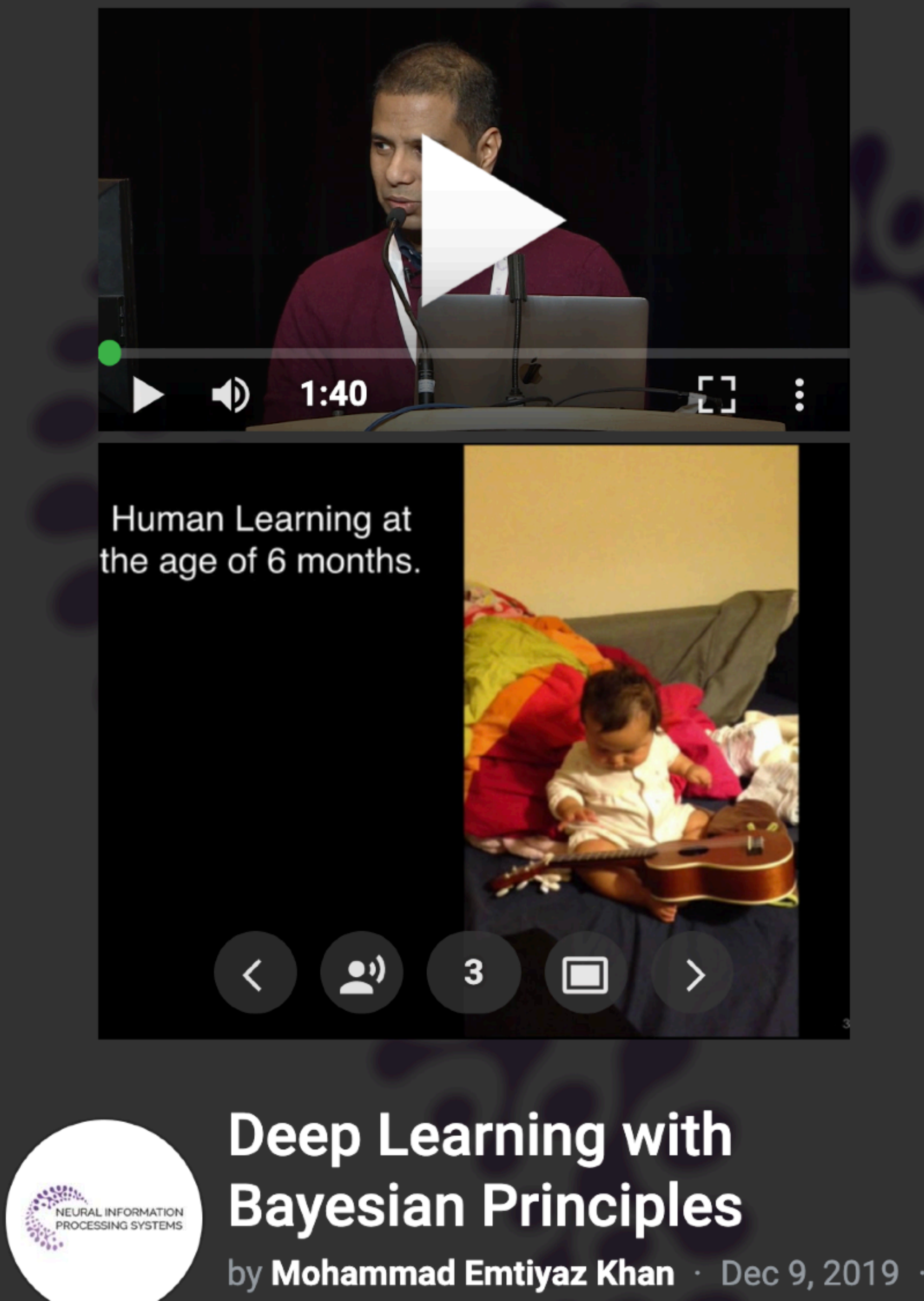
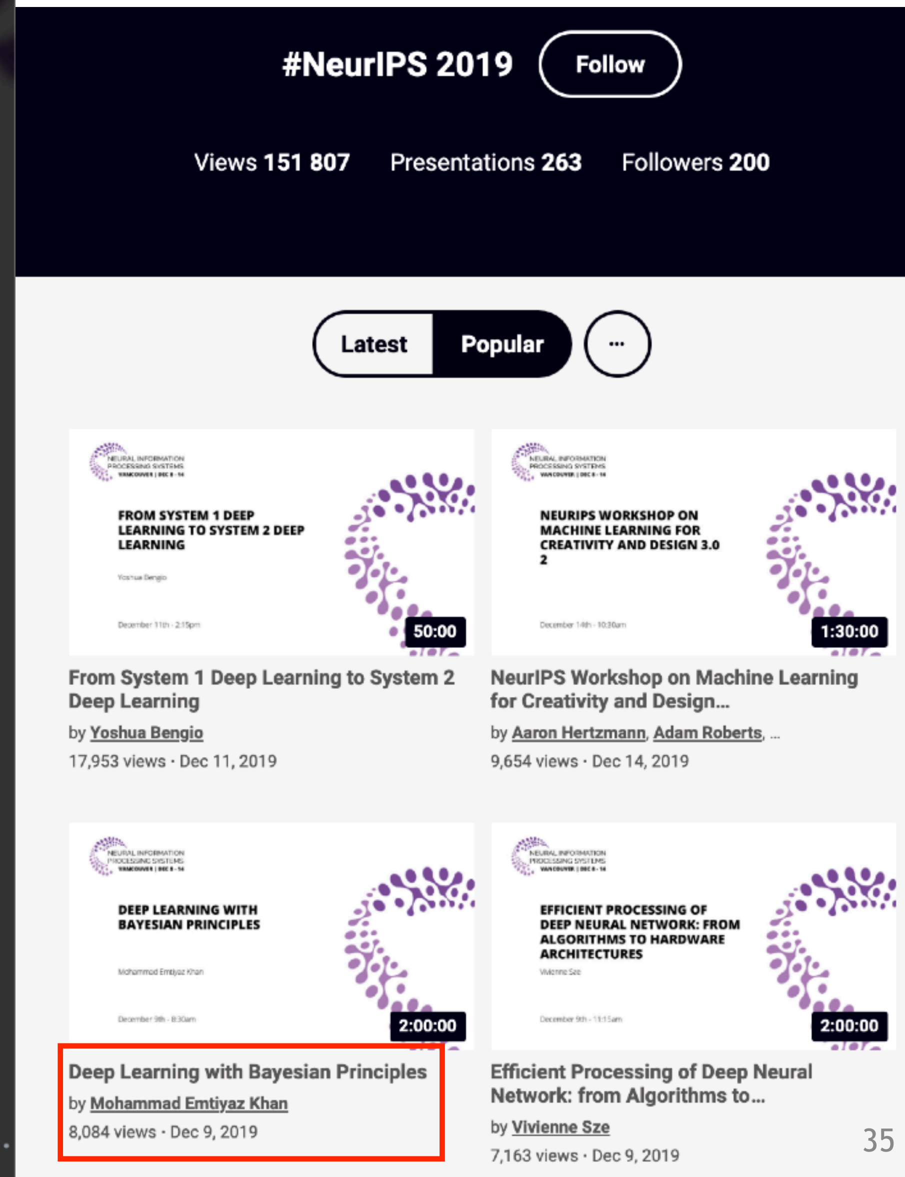
Lin et al., Tractable structured natural gradient descent using local parameterizations, ICML 2021



NeurIPS 2019 Tutorial



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

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Research director
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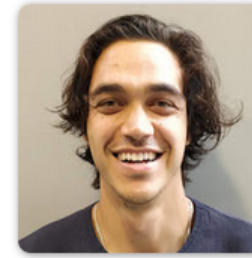
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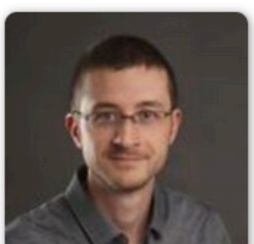
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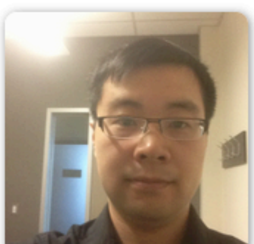
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