

Bayesian Learning Rule

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<http://emtiyaz.github.io>



1. Summary at <https://emtiyaz.github.io/papers/MLfromBayes.pdf>
2. Slides at https://emtiyaz.github.io/papers/Feb22_2022_AI4Sec.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



Failure of AI in “dynamic” setting

Robots need quick adaptation to be deployed
(for example, at homes for elderly care)



Bayesian Principles



Our research

Human learning

≠

Deep learning

Life-long learning from **small** chunks of data in a **non-stationary** world

Bulk learning from a **large** amount of data in a **stationary** world

Our current research focuses on reducing this gap!

1. Parisi, German I., et al. "Continual lifelong learning with neural networks: A review." *Neural Networks* (2019)
2. Geisler, W. S., and Randy L. D. "Bayesian natural selection and the evolution of perceptual systems." *Philosophical Transactions of the Royal Society of London. Biological Sciences* (2002)

Bayesian Learning Rule

- Bayesian principles as a general principle
 - To unify/generalize/improve learning-algorithms
 - By computing “posterior approximations”
- Bayesian Learning rule (BLR)
 - Derive many existing algorithms
 - Deep Learning (SGD, RMSprop, Adam)
 - Design new algorithms for uncertainty in DL
- ~~Dual perspective~~ of BLR for life-long learning
- Impact: Everything with the same principle

The Bayesian Learning Rule



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Abstract

We show that many machine-learning algorithms are specific instances of a single algorithm called the *Bayesian learning rule*. The rule, derived from Bayesian principles, yields a wide-range of algorithms from fields such as optimization, deep learning, and graphical models. This includes classical algorithms such as ridge regression, Newton's method, and Kalman filter, as well as modern deep-learning algorithms such as stochastic-gradient descent, RMSprop, and Dropout. The key idea in deriving such algorithms is to approximate the posterior using candidate distributions estimated by using natural gradients. Different candidate distributions result in different algorithms and further approximations to natural gradients give rise to variants of those algorithms. Our work not only unifies, generalizes, and improves existing algorithms, but also helps us design new ones.

Machine Learning from a Bayesian Perspective

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November 8, 2021

Abstract

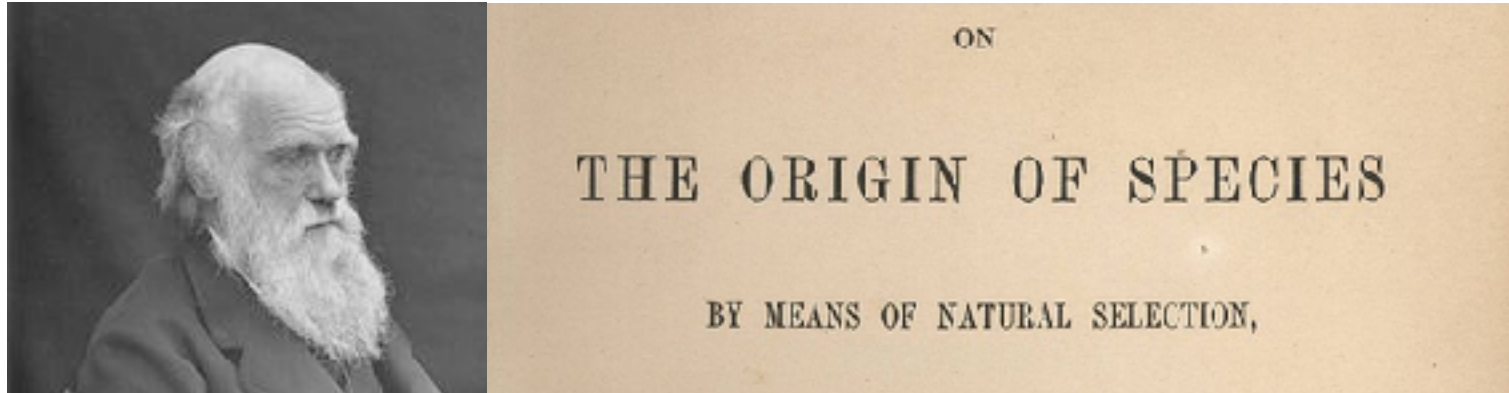
I summarize a Bayesian perspective of machine learning. We view Bayes as an optimization problem whose solutions use the information-geometry of the posterior. Using this perspective, we can show that many machine-learning methods have a (more general) Bayesian side to them. I believe this perspective to be essential for bridging the gap between ‘artificial’ and ‘natural’ learning systems.

1 A note about the note

For now, this note deliberately lacks details. One way to read this is to use the accompanying slides. My hope is to add some equations, figures and illustration in the future. Many technical details discussed here can be found in [Khan and Rue \[2021\]](#)

2 Machine learning and Bayes

A main goal of machine-learning is to design AI systems that can learn like us. We humans, and other animals, collect experiences throughout our lives to learn and adapt. Machines currently are extremely bad at this. Majority of successful machine-learning paradigms are the ones that use ‘bulk’ learning in a ‘static’ world, where all the information is assumed to be available at once and the world stands still while we learn about it. This is far from the reality of the world we live in, and it is not surprising to see such systems fail. How can we bridge this gap between machines and living-beings? Taking a Bayesian perspective seems to be one way to go, but we argue that this is perhaps the only way forward.



The Origin of Algorithms

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

Principle of Trial-and-Error

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

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

The diagram illustrates the components of the loss function. A blue arrow points from 'Data' to the \mathcal{D} term in the loss function. Another blue arrow points from 'Model Params' to the θ term. A third blue arrow points from 'Deep Network' to the $f_{\theta}(x_i)$ term in the summation.

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

Scales well to large data and complex model, and very good performance in practice.

Bayes Objective

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

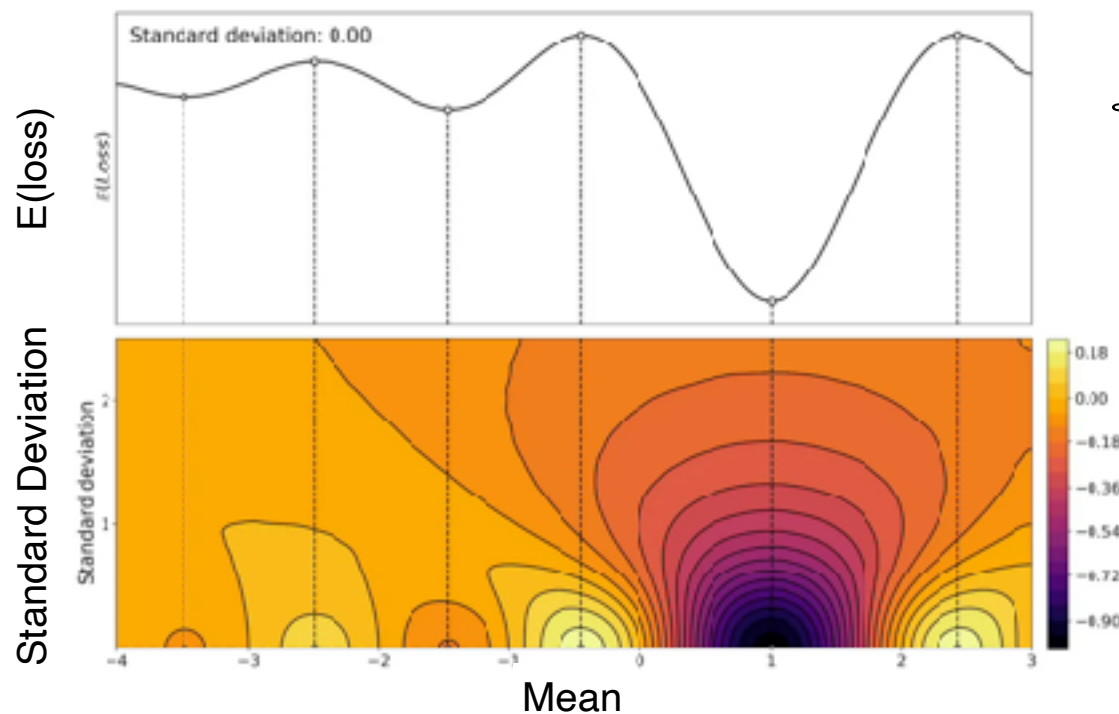
Generalized-Posterior approx.

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 Objective

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

← Generalized-Posterior approx.



$$\mathcal{L}(\mu, \sigma) = \mathbb{E}_{\mathcal{N}(\theta|\mu, \sigma^2)} [\ell(\theta)]$$

Instead of the original loss, optimize a different (smoothed) one.

A popular idea of “implicit regularization” in DL [4] now, but also A common idea in many other fields

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

Bayesian Learning Rule

Unify, generalize, and improve
machine-learning algorithms

A 2-step Bayesian Scheme

Step 1: Choose an approximation (mix-exp-family)

Natural parameters Sufficient statistics Expectation parameters

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

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

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

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

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

A 2-step Bayesian Scheme

Step 2: $\min_{\theta} \ell(\theta)$ vs $\min_{q \in \mathcal{Q}} \mathbb{E}_{q(\theta)}[\ell(\theta)] - \mathcal{H}(q)$
 Exponential-family Approx.

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

Bayes learning rule: $\lambda \leftarrow \lambda - \rho \nabla_{\mu} (\mathbb{E}_q[\ell(\theta)] - \mathcal{H}(q))$
 Natural Gradient

Natural and Expectation parameters of an exponential family distribution q
 (natural-gradient descent & mirror descent)

By changing \mathcal{Q} , we can recover DL algorithms (and more)

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

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 <small>(New)</small>	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 <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
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 <small>(New)</small>	Mixture of Exp-family	None	5.4

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).

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

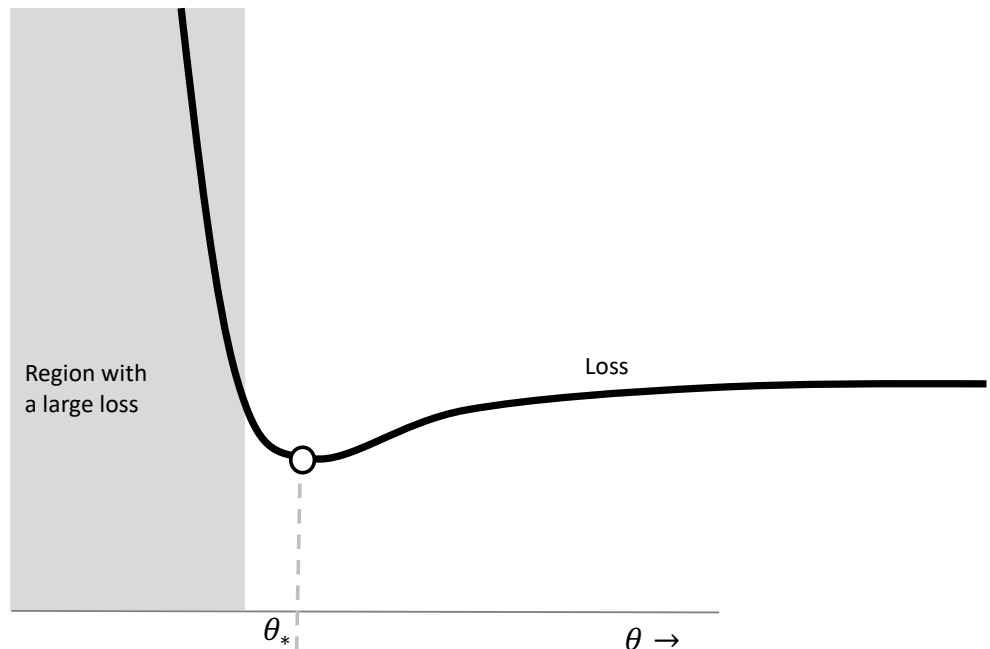
Bayes vs Non-Bayes

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

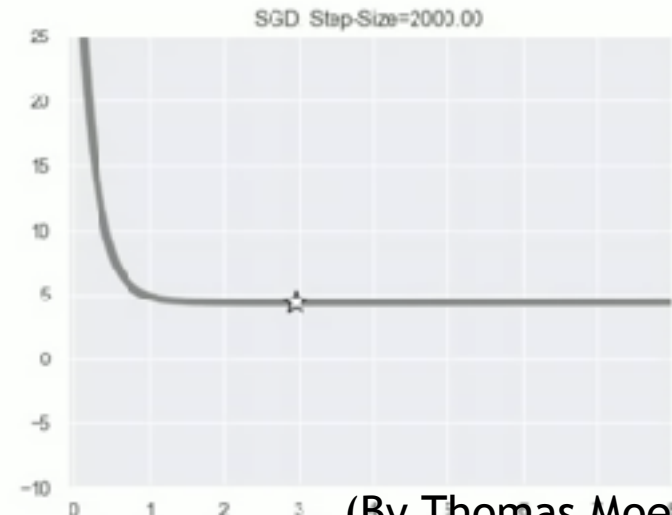
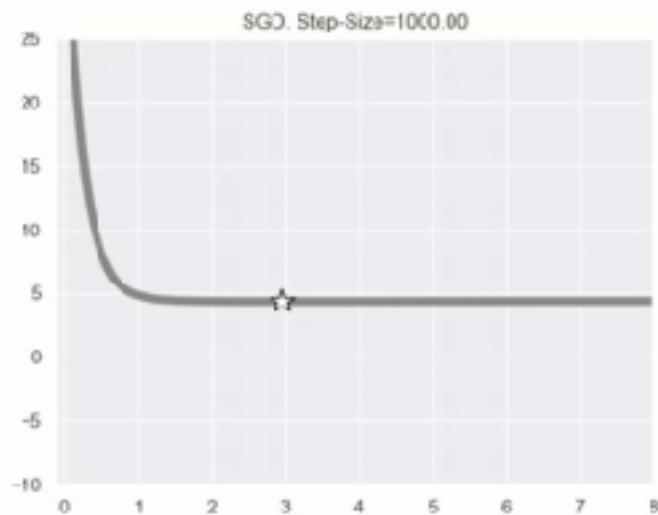
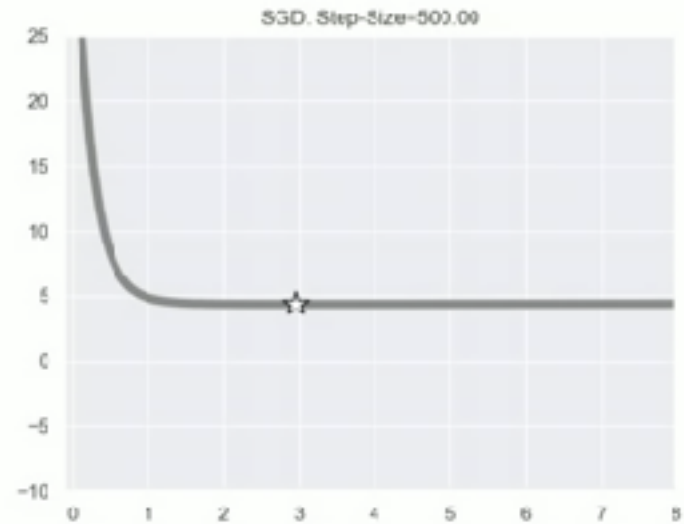
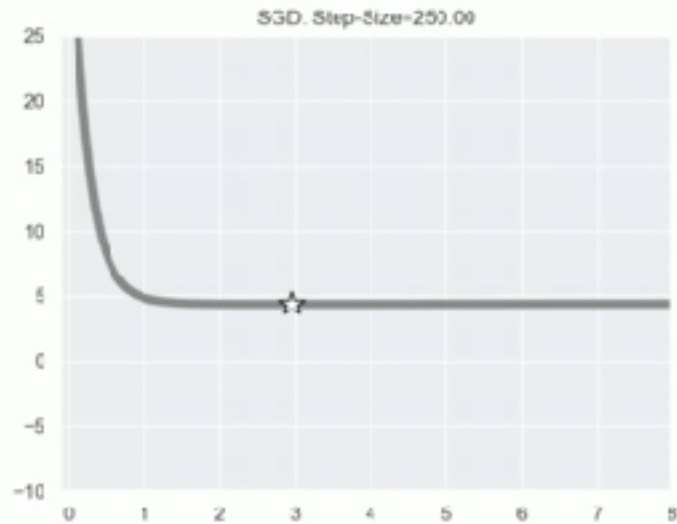
$$\text{BLR: } m \leftarrow m - \rho \nabla_m \mathbb{E}_q[\ell(\theta)]$$

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

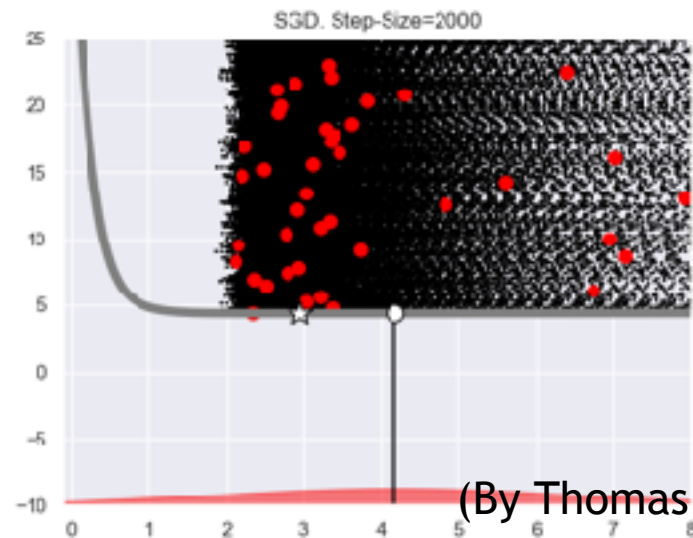
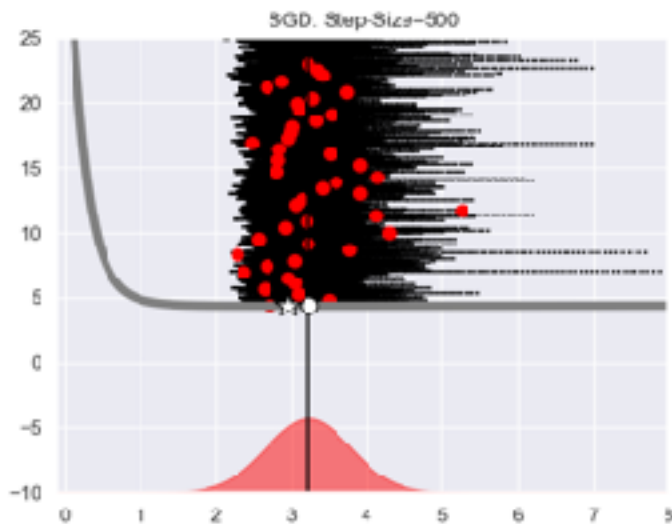
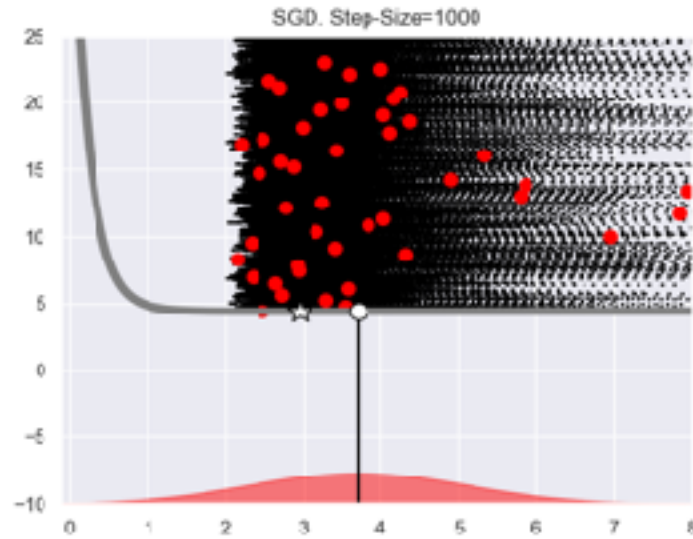
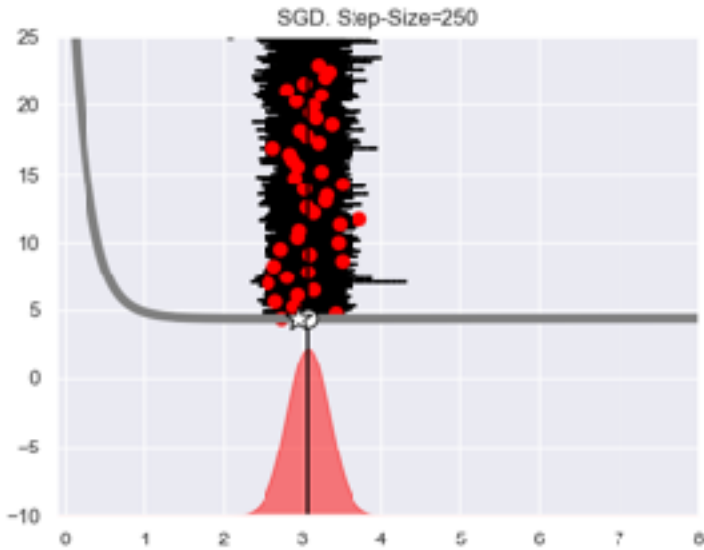
Bayesian solution injects “noise” which has a similar regularization effect to noise in Stochastic GD. It prefers “flatter” directions.



SGD: Implicit Regularization

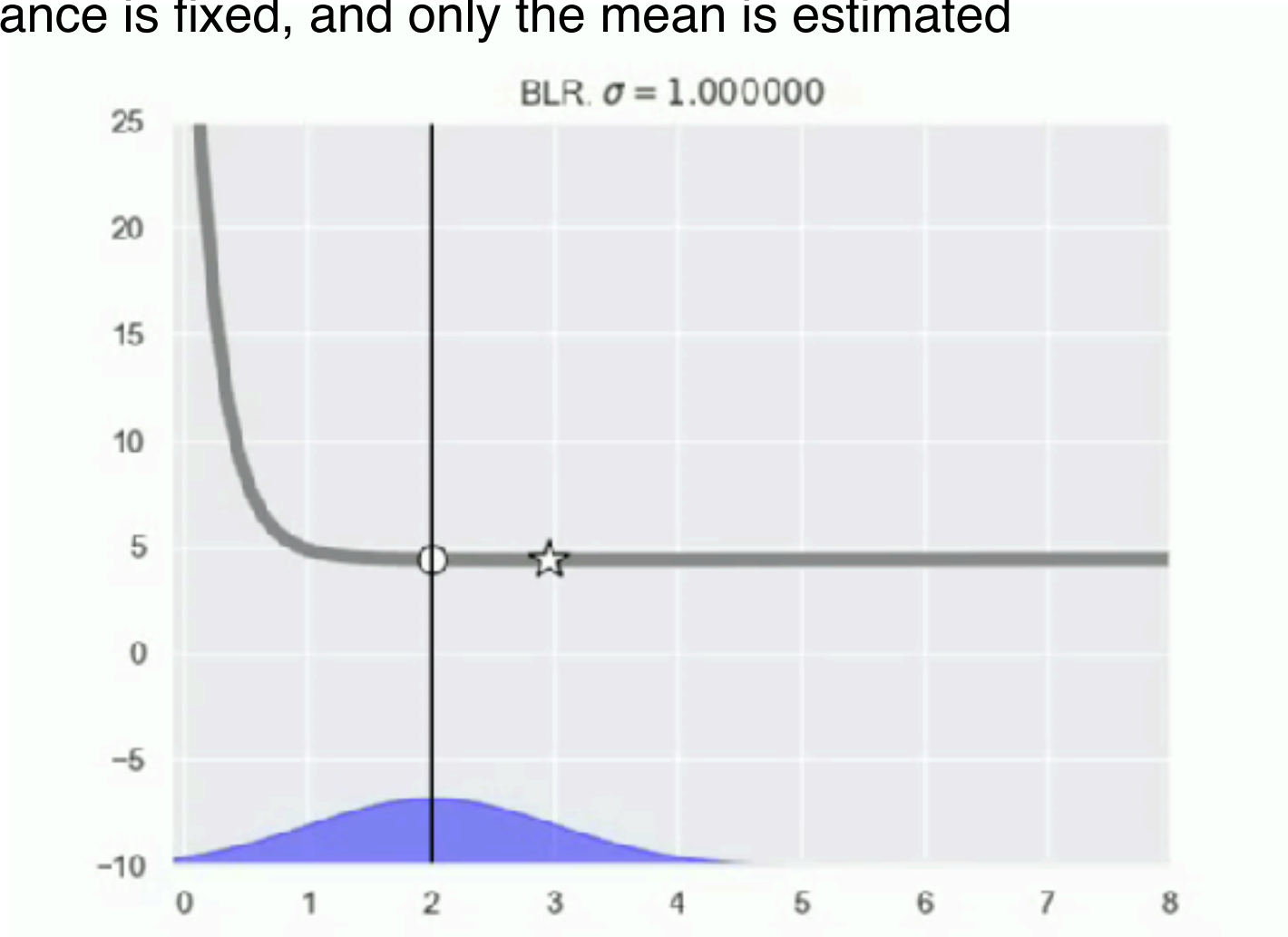


SGD: Implicit Regularization

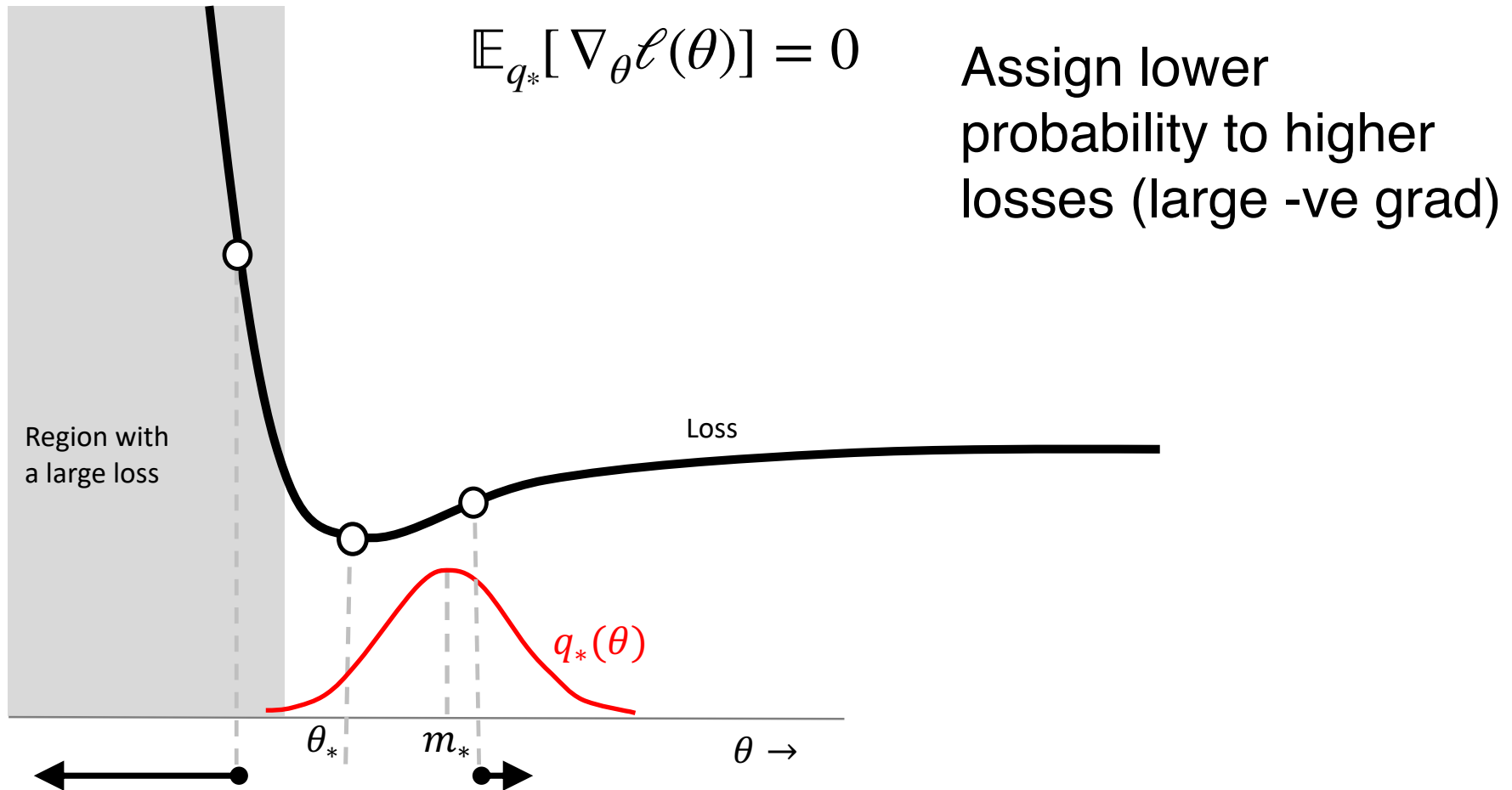


Bayes: Implicit Regularization

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

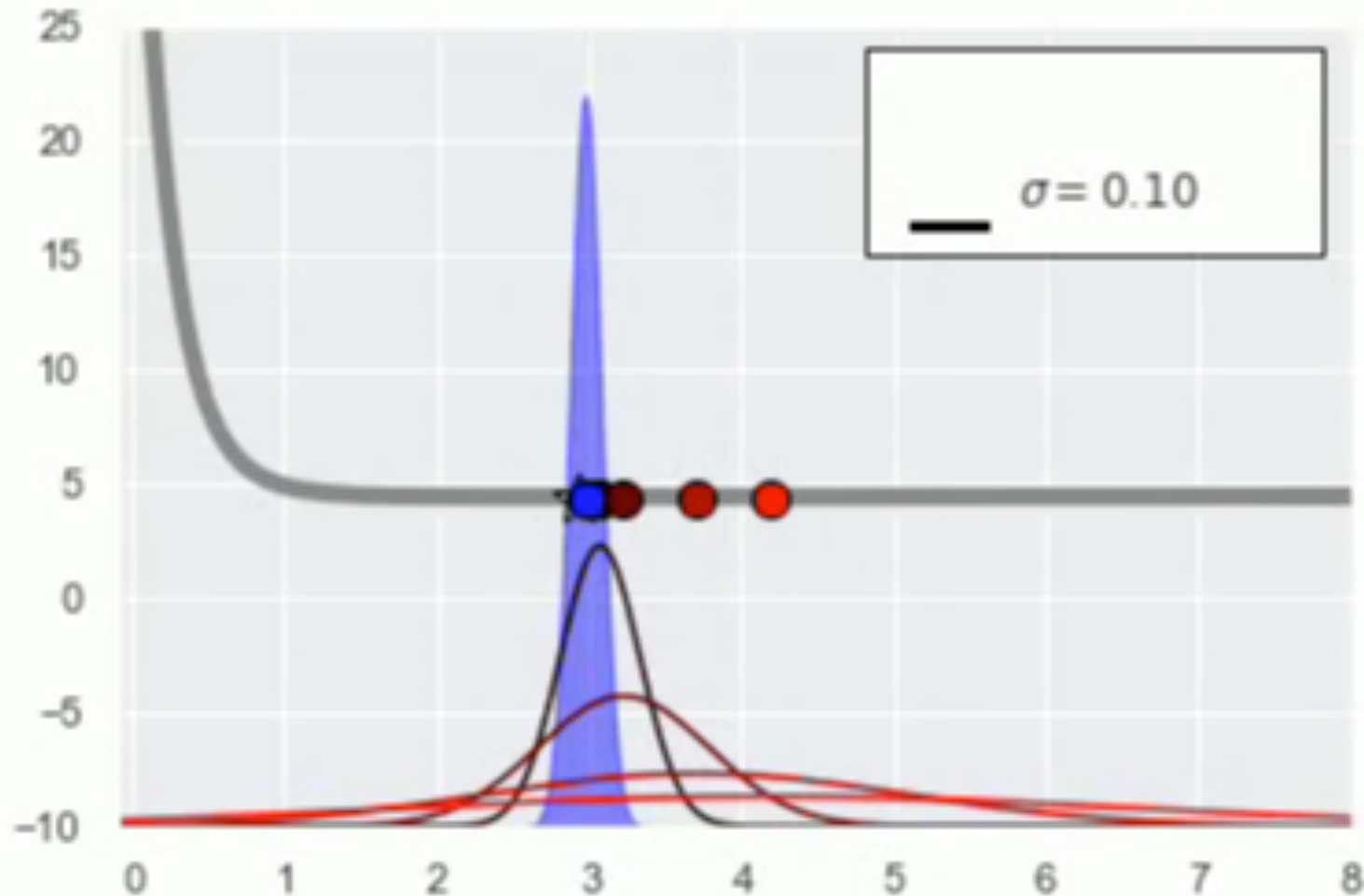


Bayes: Implicit Regularization



Bayes: Implicit Regularization

Bayes solutions (blue) compared to SGD solutions (red lines)



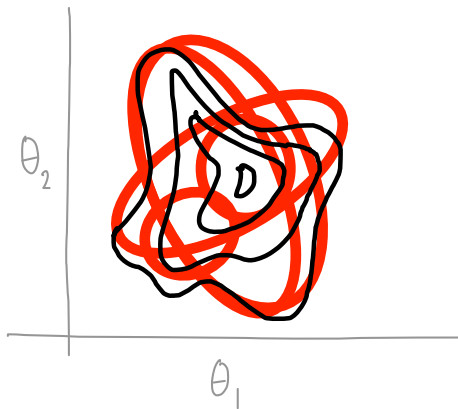
Deriving Learning-Algorithms from the Bayesian Learning Rule

Posterior Approximation \longleftrightarrow Learning-Algorithm

Complex



Simple



Bayes' rule

Mixture
of Newton

Newton

Gradient
Descent

Newton's Method from Bayes

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

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

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

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

Derived by choosing a **multivariate Gaussian**

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

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

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:

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

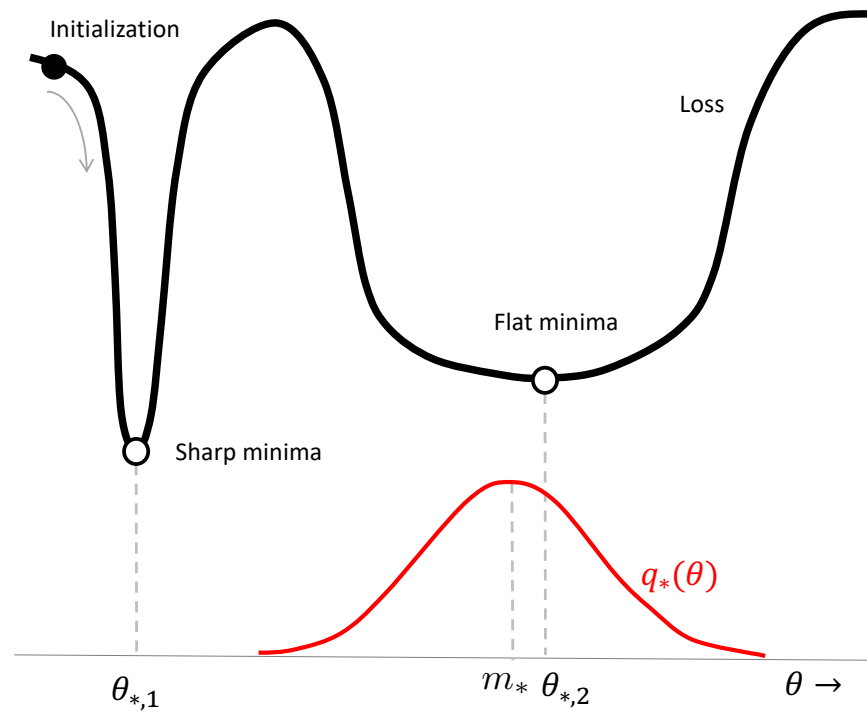
$$\nabla_{\mathbb{E}_q(\theta\theta^{\top})} \mathbb{E}_q[\ell(\theta)] = \mathbb{E}_q[H_{\theta}]$$

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

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

Bayes leads to robust solutions

Avoiding sharp minima



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

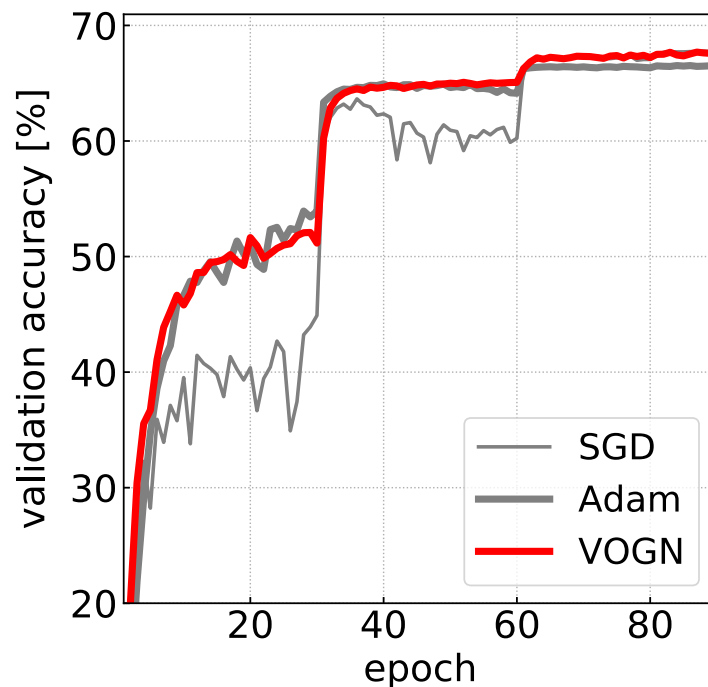
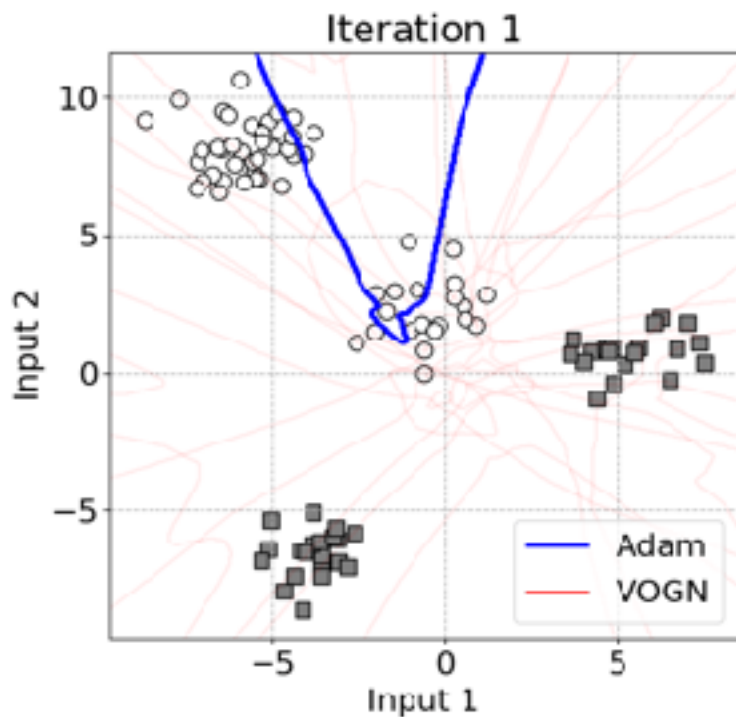
We can compute uncertainty using a variant of Adam.

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Newton's method	Gaussian	—"—"	1.3
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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).

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).

RMSprop/Adam from Bayes

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])

Variational Online Newton Methods

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

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

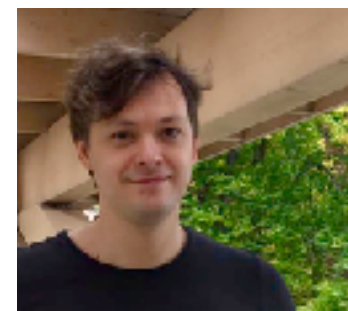
$$s \leftarrow (1 - \rho)s + \rho(\sum_i g_i^2)$$

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

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

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

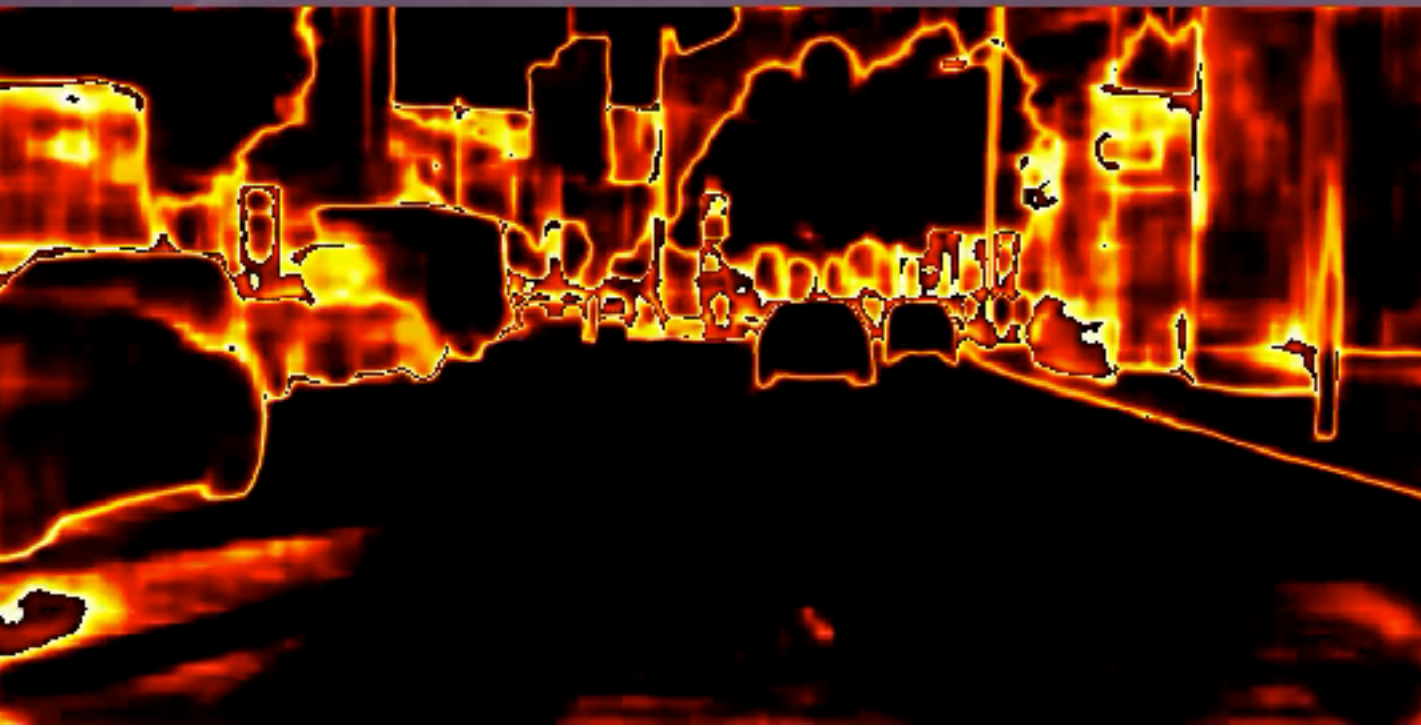
The BLR variant from [3] led to the **winning solution** for the NeurIPS 2021 challenge for “approximate inference in deep learning”. Watch **Thomas Moellenhoff’s** talk at <https://www.youtube.com/watch?v=LQInIN5EU7E>.



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).

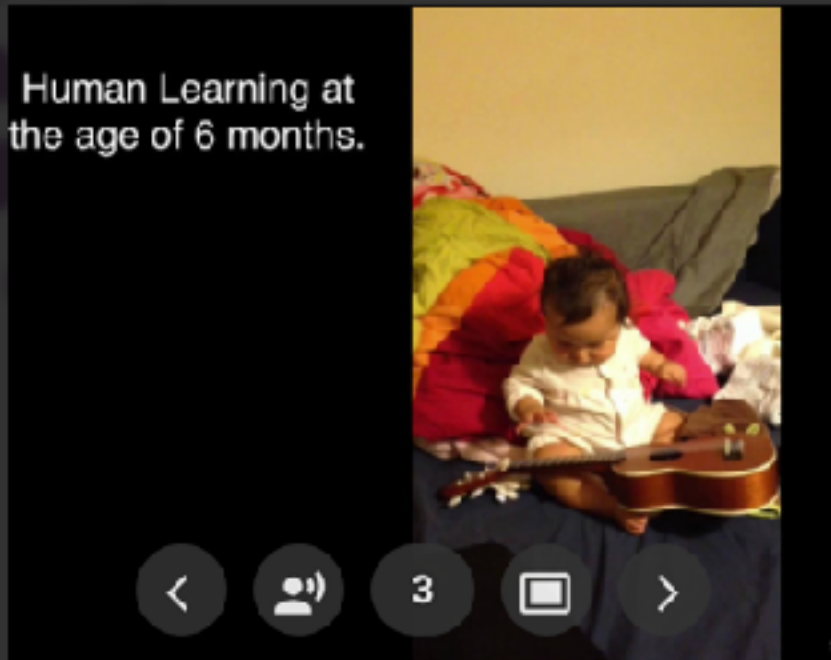
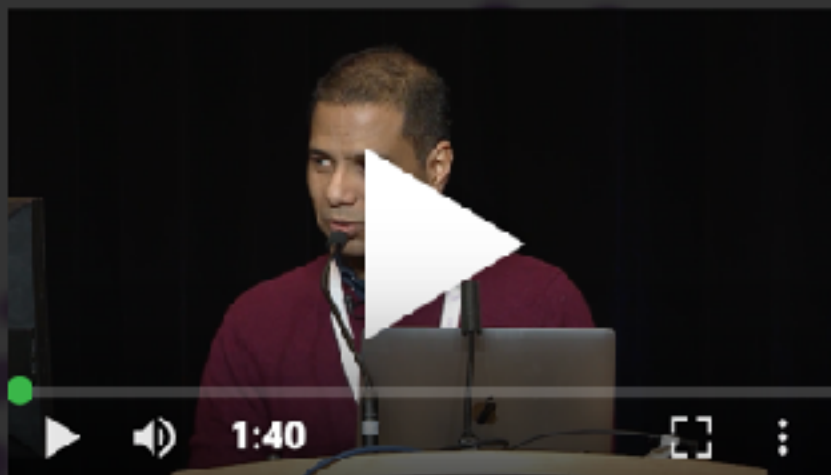


Image
Segmentation



Uncertainty
(entropy of
class probs)

NeurIPS 2019 Tutorial



Deep Learning with Bayesian Principles

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

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Past and New Work

- Natural Gradient Variational Inference

1. Khan and Lin. "Conjugate-computation variational inference: Converting variational inference in non-conjugate models to inferences in conjugate models." *Alstats* (2017).
2. Khan and Nielsen. "Fast yet simple natural-gradient descent for variational inference in complex models." (2018) *ISITA*.

- Mixture of Exponential family

3. Lin et al. "Fast and Simple Natural-Gradient Variational Inference with Mixture of Exponential-family Approximations," *ICML* (2019).

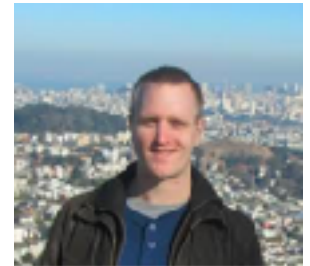
- Generalization of natural gradients

4. Lin et al. "Handling the Positive-Definite Constraint in the Bayesian Learning Rule", *ICML* (2020)
5. Lin et al. "Tractable structured natural gradient descent using local parameterizations", *ICML*, (2021)

- Gaussian approx \longleftrightarrow Newton-variants



Wu Lin (UBC)



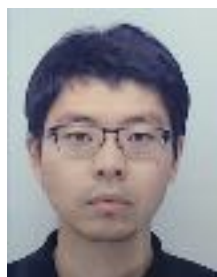
Mark Schmidt (UBC)



Frank Nielsen (Sony)

Gaussian Approximation and DL

1. Khan, et al. "Fast and scalable Bayesian deep learning by weight-perturbation in Adam." *ICML* (2018).
2. Mishkin et al. "SLANG: Fast Structured Covariance Approximations for Bayesian Deep Learning with Natural Gradient" *NeurIPS* (2018).
3. Osawa et al. "Practical Deep Learning with Bayesian Principles." *NeurIPS* (2019).



Voot Tangkaratt
(Postdoc, RIKEN-AIP)



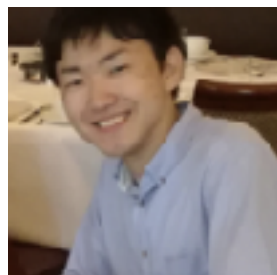
Aaron Mishkin
(Intern From UBC)
Frederik Kunstner
(Intern From EPFL)
Didrik Nielsen
(Past: RA)



Yarin Gal
(UOxford)



Akash Srivastava
(UEdinburgh)



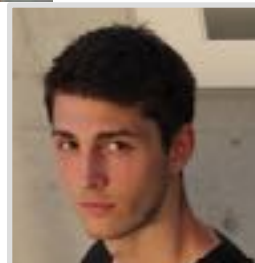
Kazuki Osawa
(Tokyo Tech)



Rio Yokota
(Tokyo Tech)



Anirudh Jain
(Intern from
IIT-ISM, India)



Runa Eschenhagen
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Extensions

- Binary Neural Networks (Bernoulli approx)
 1. Meng, et al. "Training Binary Neural Networks using the Bayesian Learning Rule." *ICML* (2020).
- Gaussian Process
 2. Chang et al. "Fast Variational Learning in State-Space GP Models", *MLSP* (2020)
 - For sparse GPs, BLR is a generalization of [1]



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How to design AI that learn like us?

- Three questions
 - Q1: What do we know? (model)
 - Q2: What do we not know? (uncertainty)
 - Q3: **What do we need to know? (action & exploration)**
- Posterior approximation is the key
 - (Q1) Models == representation of the world
 - (Q2) Posterior approximations == representation of the model
 - (Q3) **Use posterior approximations for knowledge representation, transfer, and collection.**

Approximate Bayesian Inference Team

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

We have many open positions!
Come, join us.



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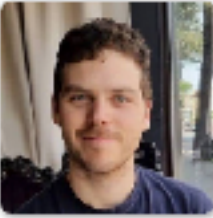
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