Handling the Positive-Definite Constraint in the Bayesian Learning Rule

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Bayesian Learning Rule

Bayes vs Optimization

Unified via Bayesian Learning Rule

A Natural-gradient Variational Inference Algorithm

Challenges: How to deal with constraints
Contributions: Improved Bayesian Learning Rule
efficient updates for the positive-definite constraints
using Riemannian Gradient Descent

Two different worlds in ML

Bayesian:

Given: data **Infer:** posterior

latent variables

model: prior + likelihood

Unconstrained optimization:

Given: data **Min:** objective

decision variables

model: regularizer + loss

Distinct methods in each world:

Inference methods v.s. Optimizers

Scope

Challenges:
- unify methods in both worlds
- use inference techniques to design optimizers
- do optimization with uncertainty

The Bayesian learning rule (Khan & Rue 2019):
- **variational inference** approach unifies methods
- help to design new optimizers
- give an uncertainty estimation for decision variables

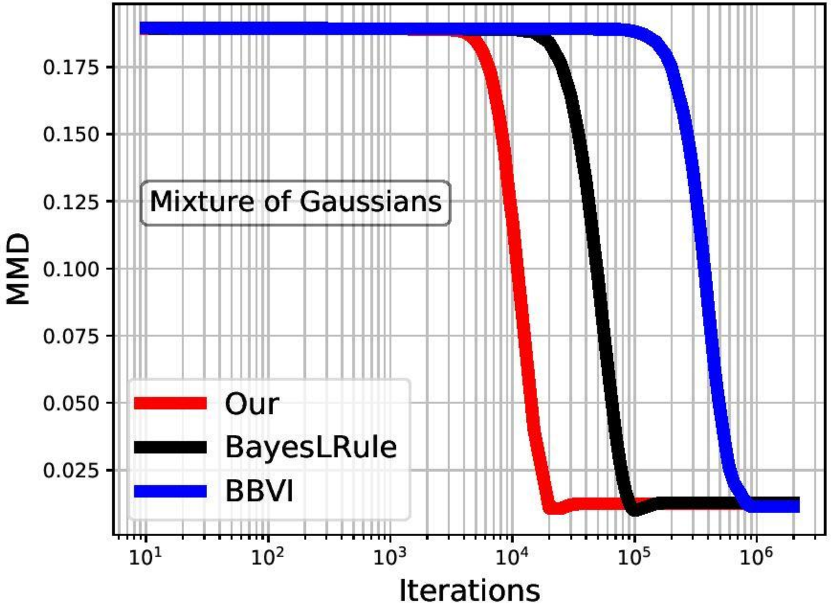
Issue of the rule: expensive to deal with constraints

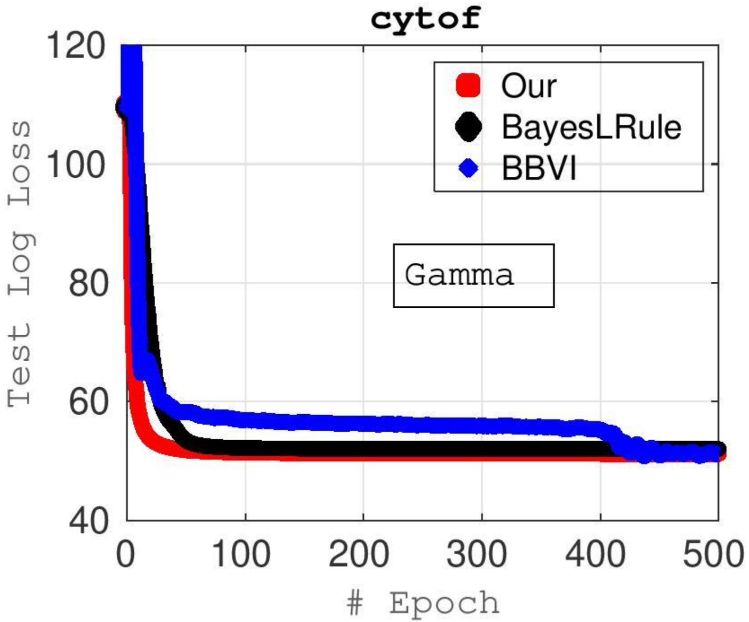
Example:

Gaussian posterior approximation (covariance matrix is **positive-definite**)

Our contributions

- new (constrained) parametrization
- closed-form correction term to address the constraint issue
- Gaussian, mixture of Gaussians, gamma, and more approximations





Outline

- Bayesian learning rule
- Key idea from a geometric viewpoint
- Example of our new rule
- Experimental results

Variational inference

Variational Inference (VI): data $\mathcal{D}$, latent variables $\mathbf{w}$, approx: $p(\mathbf{w}|\mathcal{D})$

$$\min_{\lambda} \mathcal{L}(\lambda) = \mathbb{E}_{q(w|\lambda)}[\ell(\mathcal{D}, \mathbf{w})] + \mathbb{D}_{\mathrm{KL}}[q(\mathbf{w}|\lambda) || \exp(-R(\mathbf{w}))]$$

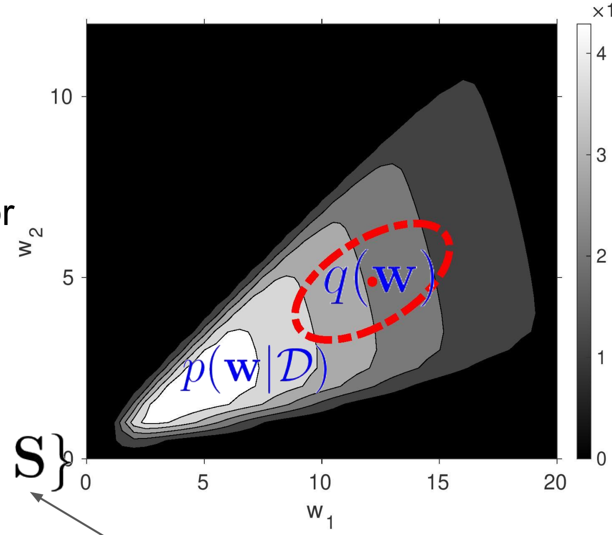
negative ELBO

loss/negative log-likelihood

$$\ell(\mathcal{D}, \mathbf{w}) = -\log p(\mathcal{D}|\mathbf{w})$$

regularizer/negative log-prior

$$R(\mathbf{w}) = -\log p(\mathbf{w})$$



Example:

$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mu, \mathbf{S})$, Gaussian approximation $\lambda = \{\mu, \mathbf{S}\}$

the mean

the precision matrix

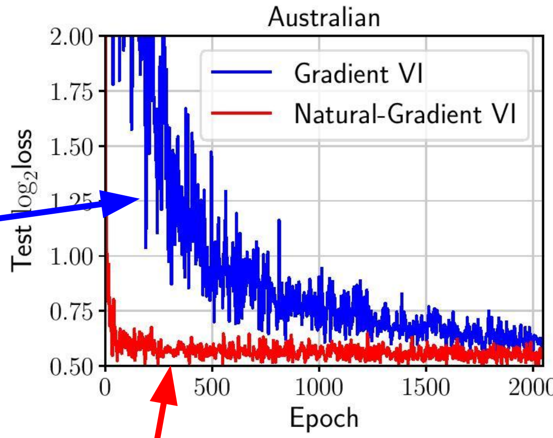
Issue: positive-definite constraint

The VI framework bridges the gap between the Bayesian world and the optimization world.

Handling the constraint

λ' is a unconstrained transformation

BBVI is **slow**



Black-box gradient VI (BBVI): $\lambda' = \lambda' - t\nabla_{\lambda'}\mathcal{L}(\lambda')$

Why NGVI instead of BBVI ?

- **fast** iteration progress

Natural-gradient VI (NGVI): $\lambda' = \lambda' - t\mathbf{F}(\lambda')^{-1}\nabla_{\lambda'}\mathcal{L}(\lambda')$

Fisher matrix of $q(\mathbf{w}|\lambda')$

Issue: **high** iteration cost in NGVI

Notation: ∇ denotes the ordinary/standard derivative in this talk

Bayesian learning rule

Bayesian learning rule is NGVI with low iteration cost

Under a right (**constrained**) parametrization λ

low iteration cost if easy to compute

$\nabla_m \mathcal{L}(\lambda) = \mathbf{F}(\lambda)^{-1} \mathcal{L}(\lambda)$, $\mathbf{m}$ is an auxiliary parameter.

Bayesian learning rule (BayesLRule): $\lambda = \lambda - t \nabla_m \mathcal{L}(\lambda)$

line search for the step-size (expensive)

The rule:

- simple way to implement NGVI but gives rise to **constrained** optimization

Example of the rule

Gaussian posterior approximation:

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mu, \mathbf{S})$$

the mean **the precision matrix**

Issue: **S** must be **positive-definite**

We define: $\bar{\ell}(\mathbf{w}) := R(\mathbf{w}) + \ell(\mathcal{D}, \mathbf{w})$

regularizer loss

Recall: minimize the negative ELBO $\mathcal{L}(\lambda)$

This work: we address this constraint issue by using Riemannian gradient descent

$\mathcal{L}(\lambda)$ can be re-written as $\mathcal{L}(\lambda) = \mathbb{E}_{q(w|\lambda)}[\bar{\ell}(\mathbf{w})] + \mathbb{E}_{q(w|\lambda)}[\log q(\mathbf{w}|\lambda)]$

Bayesian learning rule for $\min_{\lambda} \mathcal{L}(\lambda)$

$$\mathbf{S} = (1-t)\mathbf{S} + t\mathbb{E}_q[\nabla_w^2 \bar{\ell}(\mathbf{w})]$$
$$\mu = \mu - t\mathbf{S}^{-1}\mathbb{E}_q[\nabla_w \bar{\ell}(\mathbf{w})]$$

Recall: Newton's update for $\min_{w} \bar{\ell}(\mathbf{w})$

$$\mathbf{w} = \mathbf{w} - t[\nabla_w^2 \bar{\ell}(\mathbf{w})]^{-1} \nabla_w \bar{\ell}(\mathbf{w})$$

require line search for step-size t

The Bayesian learning rule
- bring the two worlds closer
- recover many optimizers (Khan & Rue 2019)

Key idea of this work

a **(shortest curve) line** as t varies

(Euclidean) gradient descent/BBVI: $L(t) = \lambda - t\nabla_\lambda \mathcal{L}(\lambda)$

starting point   Euclidean direction

$\mathcal{M}$ is a manifold induced by $q(\mathbf{w}|\mathbf{x})$, x is constrained, $\mathbf{F}(\mathbf{x})$ is the Fisher matrix

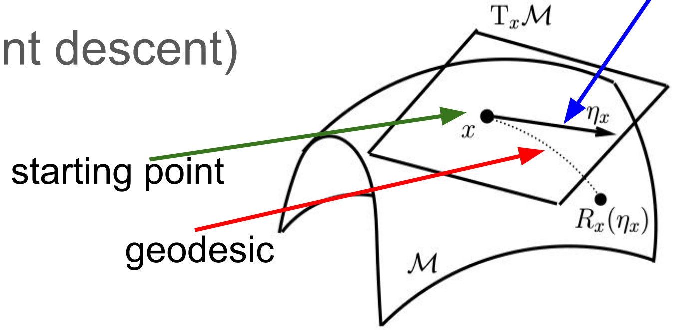
geodesic: generalization of the “shortest” curve in the manifold

natural-gradient descent/BLR

$N(t) = x - t\mathbf{F}(\mathbf{x})^{-1}\nabla_x \mathcal{L}(\mathbf{x})$

manifold direction: $-\mathbf{F}(\mathbf{x})^{-1}\nabla_x \mathcal{L}(\mathbf{x})$, let $\eta_x := -t\mathbf{F}(\mathbf{x})^{-1}\nabla_x \mathcal{L}(\mathbf{x})$

geodesic: $R(t) = R_x(\eta_x)$ (Riemannian gradient descent)



Key idea of this work

Natural-gradient descent/Bayesian learning rule(BLR):

- like a “2nd-order” method in a Euclidean case
- 1st-order method in a (Riemannian) manifold
- 1st-order approximation of the geodesic at the starting point

Challenges:

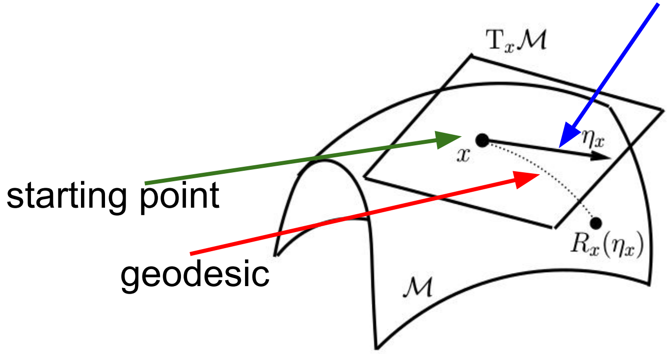
- hard to exactly compute a geodesic (manifold exponential map)
- NGD ignores the **curvature** of a geodesic

natural-gradient descent/BLR

$$N(t) = x - t\mathbf{F}(\mathbf{x})^{-1}\nabla_x \mathcal{L}(\mathbf{x})$$

This work:

- approximate a geodesic
- efficiently capture the curvature of a geodesic



Contributions of this work

capture the curvature of a geodesic

Under a **new** (constrained) parametrization, our rule:

- efficiently approximate a geodesic as: $\lambda = \lambda - t\nabla_m \mathcal{L}(\lambda) + \text{correction}$
  - efficiently approximate **Christoffel symbols/Levi-Civita coefficients**
- efficiently compute natural-gradients $\nabla_m \mathcal{L}(\lambda) = \mathbf{F}(\lambda)^{-1}\mathcal{L}(\lambda)$

Example: Gaussian approximation $q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mu, \mathbf{S})$

the mean

the precision matrix
(positive-definite constraint)

Bayesian learning rule (BayesLRule):

$$\mathbf{S} = (1-t)\mathbf{S} + t\mathbb{E}_q[\nabla_w^2 \bar{\ell}(\mathbf{w})]$$
$$\mu = \mu - t\mathbf{S}^{-1}\mathbb{E}_q[\nabla_w \bar{\ell}(\mathbf{w})]$$

require line search for step-size t

Our rule (iBayesLRule):

$$\mu = \mu - t\mathbf{S}^{-1}\mathbb{E}_q[\nabla_w \bar{\ell}(\mathbf{w})] + \mathbf{0}$$
$$\mathbf{S} = (1-t)\mathbf{S} + t\mathbb{E}_q[\nabla_w^2 \bar{\ell}(\mathbf{w})] + \frac{t^2}{2}\mathbf{G}\mathbf{S}^{-1}\mathbf{G}$$

no need to do line search

$$\mathbf{G} := \mathbf{S} - \mathbb{E}_q[\nabla_w^2 \bar{\ell}(\mathbf{w})]$$

same time complexity in terms of big O notation

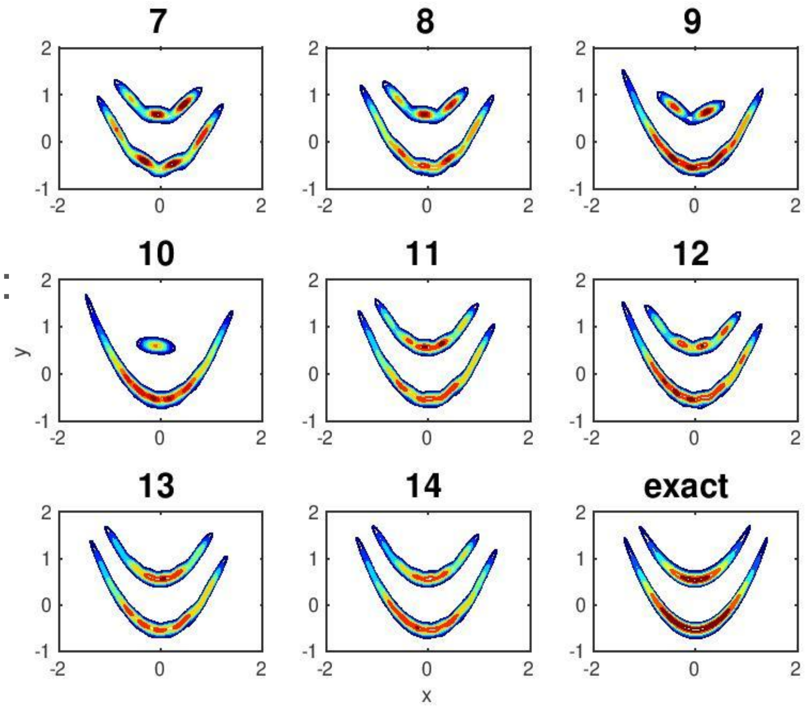
More examples

Our approach can work on useful approximations:

- gamma
- inverse Gaussian
- Wishard

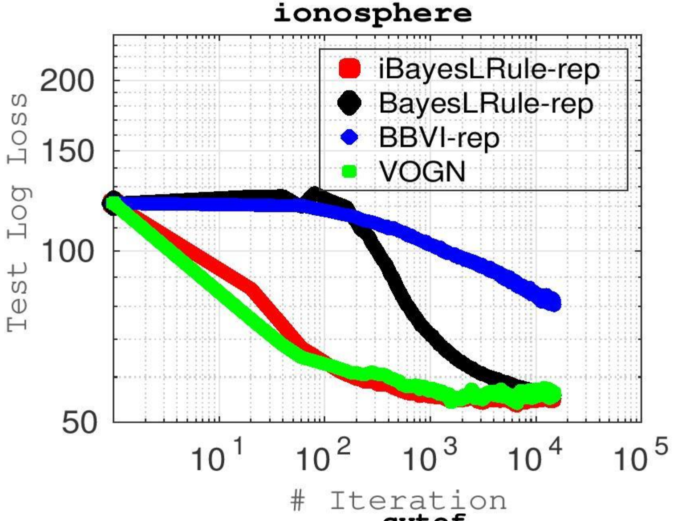
Mixture extensions:

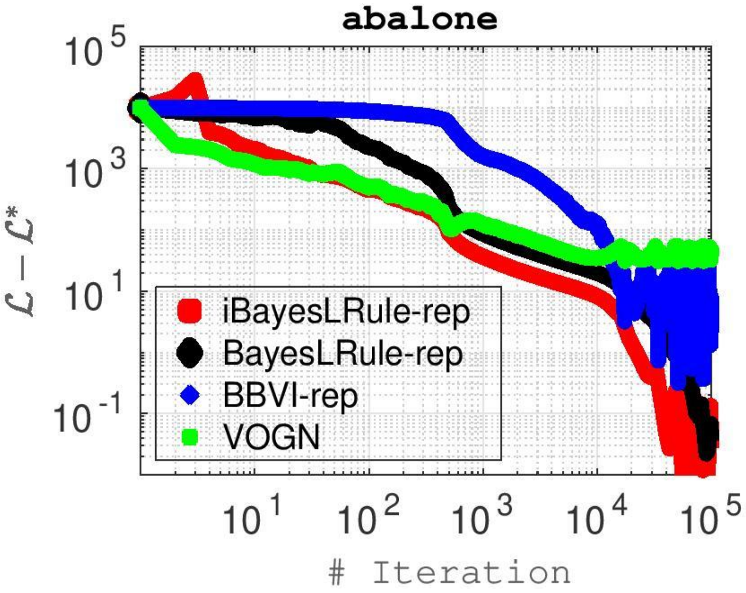
- finite mixture models (e.g., mixture of Gaussians)
- skew Gaussian (continuous Gaussian mixture)
- Student's T (Gaussian scale mixtures)



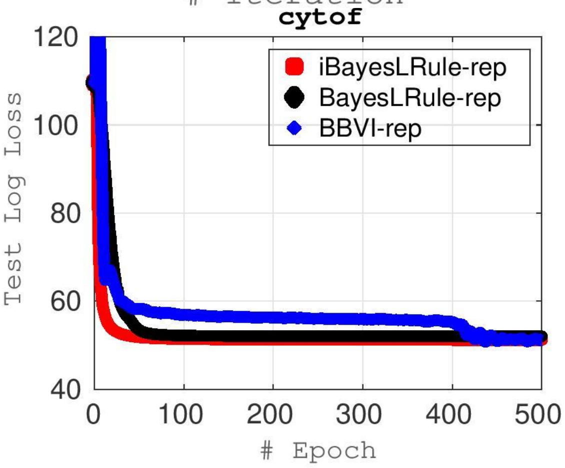
Experimental results

Full Gaussian:





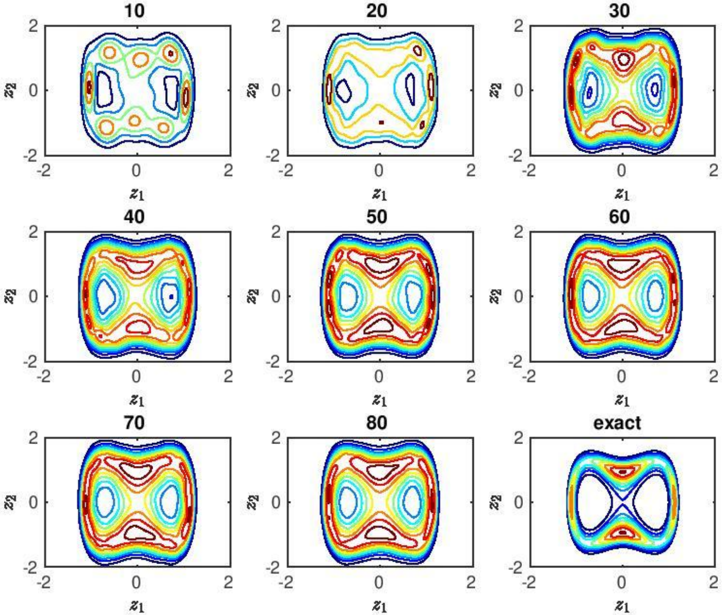
Gamma:

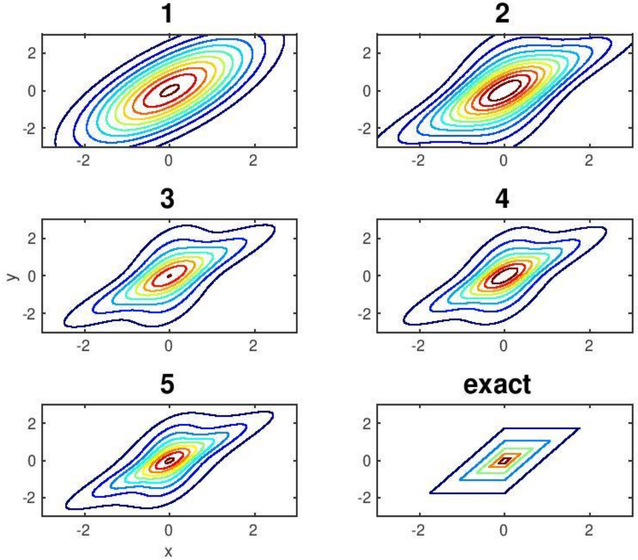


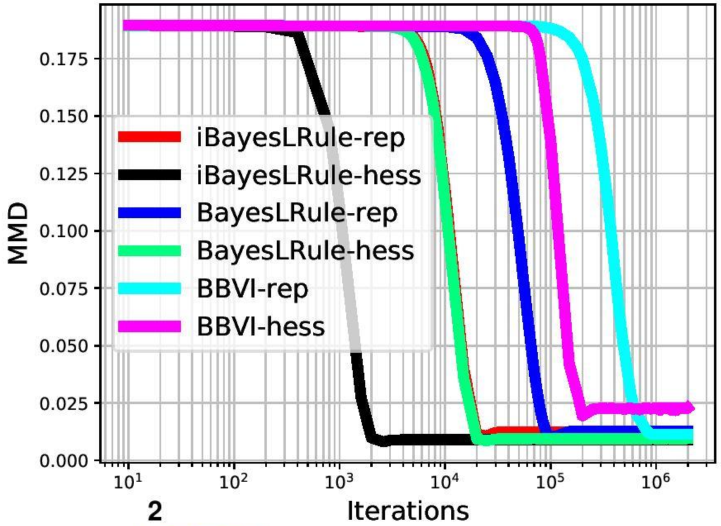
More experimental results

Mixture of full Gaussians: 2-dim , 20-dim, 300-dim

# of mixing components







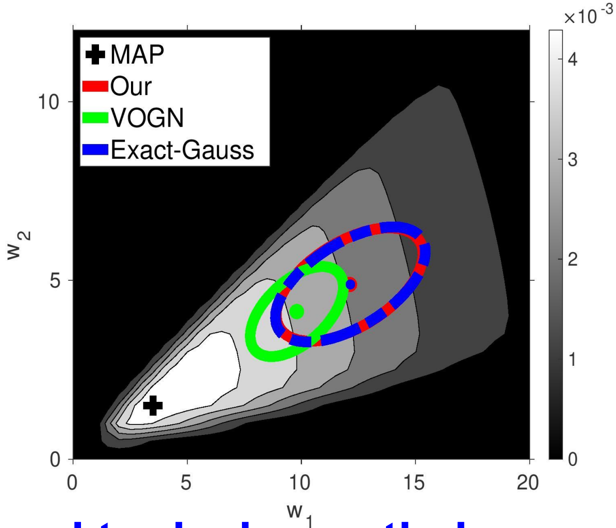
Conclusion

Improved Bayesian learning rule (under a new constrained parametrization):

- handle positive-definite constraints
- use natural-gradients with low iteration cost
- no line search for many useful approximations
- as accurate as the original Bayesian learning rule
- easy to design new optimizers (e.g., ADAM-like optimizer)

Thank You

Approaches to handle constraints



Example: Gaussian posterior approximation

Issue: parameter constraint (eg, covariance matrix)

Existing approaches to handle the constraint:

- block-box gradient VI: unconstrained, slow, accurate, **hard to design optimizers**
- Bayes learning rule: constrained, fast, accurate, **line search (expensive)**
- Gauss-Newton (VOGN): constrained, fast, specific approximation, **inaccurate**

This work:

constrained, fast, no line search, accurate, easy to design new optimizers