Fast yet Simple Natural-Gradient Descent for Variational Inference

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The Goal of My Research

“To understand the fundamental principles of learning from data and use them to develop algorithms that can learn like living beings.”
Learning by exploring at the age of 6 months
Converged at the age of 12 months
Transfer Learning at 14 months
The Goal of My Research

“To understand the fundamental principles of learning from data and use them to develop algorithms that can learn like living beings.”
Bayesian Inference

• Compute the posterior distribution
  – Instead of just a point estimate (e.g. MLE).

• A natural representation of all the past information which can then be sequentially updated with new information
  – Useful for active learning, sequential experiment design, continual learning, RL.
  – But also for global optimization, causality, etc.
  – Eventually, for ML methods which can learn like humans (data efficient, robust, causal).
Uncertainty in Deep Learning

To estimate the confidence in the predictions of a deep-learning system
Example: Which is a Better Fit?

Frequency

Magnitude of Earthquake

Real data from Tohoku (Japan). Example taken from Nate Silver’s book “The signal and noise”
Example: Which is a Better Fit?

When the data is scarce and noisy, e.g., in medicine, and robotics.
Uncertainty for Image Segmentation

<table>
<thead>
<tr>
<th>Image</th>
<th>Truth</th>
<th>Prediction</th>
<th>Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) Input Image</td>
<td>(b) Ground Truth</td>
<td>(c) Semantic Segmentation</td>
<td>(d) Aleatoric Uncertainty</td>
</tr>
</tbody>
</table>

(taken from Kendall et al. 2017)
Variational Inference (VI)

• Approximate the posterior using optimization
  – Popular in reinforcement learning, unsupervised
    learning, online learning, active learning etc.

• We need accurate VI algorithms that are
  – general (apply to many models),
  – scalable (for large data and models),
  – fast (converge quickly),
  – simple (easy to implement).

• This talk: New algorithms with such features.
Gradient vs Natural-Gradient

- **Gradient Descent (GD)**
  - Rely on stochastic and automatic gradients.
  - Simple, general, and scalable, but can have suboptimal convergence.
  - Practical VI (2011), Black-box VI (2014), Bayes by backprop (2015), ADVI (2015), and many more.

- **Natural-Gradient Descent (NGD)**
  - Fast convergence, but computationally difficult, therefore not simple, general, and scalable
  - (Sato (2001), Riemannian CG (2010), Stochastic VI (2013), etc.

- **Fast and simple NGD** for complex models, such as those containing deep networks.
Talk Outline

• Variational Inference with gradient descent and natural-gradient descent.
• NGD with Conjugate-Computation VI
  – Generalization of forward-backward algorithms, SVI, Message Passing (*Alstats 2017*).
• Generalizations and Extensions,
  – Structured VAEs (*ICLR 2018*), Mixture of Exponential Family approximations, Evolution strategy (*ArXiv 2017*), etc.
Variational Inference

Gradient Descent (GD)
Vs
Natural-Gradient Descent (NGD)
A Naïve Method

\[ p(D|\theta) = \prod_{i=1}^{N} p(y_i | f_{\theta}(x_i)) \]

Data
Parameters
Neural network
Input
Output

Generate

\[ \theta \sim p(\theta) \]

Prior distribution
Bayesian Inference

Bayes’ rule: \[ p(\theta | D) = \frac{p(D | \theta) p(\theta)}{\int p(D | \theta) p(\theta) d\theta} \]

Posterior distribution

Intractable integral

![Graph showing narrow and wide posterior distributions](image-url)
Variational Inference

\[ p(\theta | \mathcal{D}) = \frac{p(\mathcal{D} | \theta)p(\theta)}{\int p(\mathcal{D} | \theta)p(\theta) d\theta} \]

Variational Approximation

\[ \approx q_\lambda(\theta) = \text{ExpFamily}(\lambda) \]

Maximize the Evidence Lower Bound (ELBO):

\[ \max_\lambda \mathcal{L}(\lambda) := \mathbb{E}_{q_\lambda} \left[ \log p(\mathcal{D}, \theta) - \log q_\lambda(\theta) \right] \]

Gradient descent (GD):

\[ \lambda \leftarrow \lambda + \rho \nabla_\lambda \mathcal{L} \]
VI with Natural-Gradient Descent


\[ \lambda \leftarrow \lambda + \rho F(\lambda)^{-1} \nabla_\lambda \mathcal{L} \]

Fisher Information Matrix (FIM)

\[ F(\lambda) := \mathbb{E}_{q_\lambda} \left[ \nabla \log q_\lambda(\theta) \nabla \log q_\lambda(\theta)^\top \right] \]

• Fast convergence due to optimization in Riemannian manifold (not Euclidean space).
• But requires additional computations.
• Can we simplify/reduce this computation?
Can we simplify NGD computation? Yes, by using algorithms such as message passing/ backprop.

Conjugate-Computation VI
Khan and Lin, AI-STATS 2017
The key idea: Expectation Parameters

Expectation/moment/mean parameters

\[ \mu := \mathbb{E}_{q_\lambda} [\phi(\theta)] \]

Sufficient statistics

For Gaussians, it’s mean and correlation matrix

\[ \mathbb{E}_{q_\lambda} [\theta] = m \quad \mathbb{E}_{q_\lambda} [\theta\theta^\top] = mm^\top + V \]

A key relationship:

\[ F(\lambda)^{-1} \nabla_\lambda \mathcal{L} = \nabla_\mu \mathcal{L} \]

Natural Gradient wrt natural parameter

Gradient wrt expectation parameter

NGD: \[ \lambda \leftarrow \lambda + \rho \nabla_\mu \mathcal{L} \]
Conjugate-Computation VI (CVI)

\[ \lambda \leftarrow \lambda + \rho \nabla_{\mu} \mathcal{L} \]

• In a “conjugate” model, this is equivalent to simply adding the natural parameters of the factors of a model.

• This is a type of conjugate computation, and enables “simple” updates for complex models.
CVI on Bayesian Linear Regression

\[ q_\lambda(\theta) := \mathcal{N}(m, V) \]

\[
\mathbb{E}_q \left( (y - X\theta)^\top (y - X\theta) + \gamma \theta^\top \theta \right) - \log q_\lambda(\theta)
\]

\[-\mathbb{E}_{q_\lambda} [\theta]^\top X^\top y + \text{trace} \left[ X^\top X \mathbb{E}_{q_\lambda} [\theta \theta^\top] \right] \]

\[
\nabla \mathbb{E}_{q_\lambda} [\theta] = \begin{pmatrix} -X^\top y & + & 0 & - & V^{-1}m \end{pmatrix}
\]

\[
\nabla \mathbb{E}_{q_\lambda} [\theta \theta^\top] = \begin{pmatrix} X^\top X & + & \gamma I & - & V^{-1} \end{pmatrix}
\]
NGD $\equiv$ Newton’s Method

$$m \leftarrow (1 - \rho)m - \rho \left[ X^\top X + \gamma I \right]^{-1} X^\top y$$

*Least-square solution*

For $\rho=1$, converges in 1 step (Newton’s method).

Gradient descent is suboptimal:

$$m \leftarrow m - \alpha \left[ (X^\top X + \gamma I) m - X^\top y \right]$$

This property generalizes to all “conjugate” models, where forward-backward algorithm returns the natural-gradients of ELBO.
Conditionally-Conjugate Models

VMP: Sequential update with $\rho = 1$

SVI: Update local variable with $\rho = 1$ and global variable with $\rho$ in $(0,1)$

For CVI, $\rho$ can follow any schedule, and updates can be sequential or parallel.

Images taken from Hoffman et al. (2013) and https://www.zybuluo.com/nanmeng/note/369145
Convergence Rates for CVI

\[ \mathbb{E} \left[ \| (\lambda_k - \lambda_{k+1})/\rho \|^2 \right] \leq \left[ \frac{2LC_0}{\alpha_*^2 t} + \frac{c\sigma^2}{M\alpha_*} \right] \]

Lipschitz constant of (nonconvex) ELBO
Gradient noise variance
Strong convexity of the Fisher Information Matrix
Mini-batch size

See Khan et al. UAI 2016. The proof is based on Ghadimi, Lan, and Zhang (2014)
NGD for Deep Learning

Using CVI on Bayesian deep learning with Gaussian approximation. Reduces to a Newton step.
CVI for Bayesian Neural Network

\[
\mathbb{E}_q \left( \sum_{i=1}^{N} \log p(y_i | f_\theta(x_i)) + \gamma \theta^\top \theta - \log q_\lambda(\theta) \right)
\]

neural network

\[
m \leftarrow m - \beta (S + \gamma I)^{-1} \left[ g_i(\theta) + \gamma m \right]
\]

\[
S \leftarrow (1 - \beta) S + \beta H_i(\theta)
\]

Back-propagated gradient & Hessian

\[
\theta \sim q_\lambda(\theta), \quad g_i(\theta) := -\nabla_\theta \log p(y_i | f_\theta(x_i)),
\]

\[
V^{-1} \leftarrow S + \gamma I, \quad H_i(\theta) := -\nabla^2_\theta \log p(y_i | f_\theta(x_i))
\]
CVI for Bayesian Neural Network

\[
(X^\top X + \gamma I)^{-1} X^\top y
\]

\[
m \leftarrow m - \beta (S + \gamma I)^{-1} [g_i(\theta) + \gamma m]
\]

\[
S \leftarrow (1 - \beta) S + \beta H_i(\theta)
\]

\[
\theta \sim q_\lambda(\theta), \quad g_i(\theta) := -\nabla_\theta \log p(y_i | f_\theta(x_i)),
\]

\[
V^{-1} \leftarrow S + \gamma I, \quad H_i(\theta) := -\nabla^2_\theta \log p(y_i | f_\theta(x_i))
\]

Back-propagated gradient & Hessian
MLE vs NGD-VI

RMSprop for MLE

\[ \theta \leftarrow \mu \]
\[ g \leftarrow \frac{1}{M} \sum_{i} \nabla_{\theta} \log p(D_i | \theta) \]
\[ s \leftarrow (1 - \beta)s + \beta g^2 \]
\[ \mu \leftarrow \mu + \alpha \frac{g}{\sqrt{s + \delta}} \]

NGD for mean-field VI

\[ \theta \leftarrow \mu + \epsilon, \text{ where } \epsilon \sim \mathcal{N}(0, Ns + \lambda) \]
\[ g \leftarrow \frac{1}{M} \sum_{i} \nabla_{\theta} \log p(D_i | \theta) \]
\[ s \leftarrow (1 - \beta)s + \beta \frac{g^2}{M} \sum_{i} \left[ \nabla_{\theta}^2 \log p(D_i | \theta) \right]^2 \]
\[ \mu \leftarrow \mu + \alpha \frac{g^2 + \lambda \mu / \sqrt{N}}{\sqrt{s + \lambda / \sqrt{N}}} \]

Variational Online-Newton (VON)

Variational Online Gauss-Newton (VOGN)

Variational RMSprop (Vprop)
Variational Adam (Vadam)

### Adam for MLE

\[
\begin{align*}
\theta & \leftarrow \mu \\
g & \leftarrow \frac{1}{M} \sum_i \nabla_{\theta} \log p(D_i | \theta) \\
s & \leftarrow (1 - \beta)s + \beta g^2 \\
m & \leftarrow (1 - \gamma)m + \gamma g \\
\hat{m} & \leftarrow m / (1 - (1 - \gamma)^t) \\
\hat{s} & \leftarrow s / (1 - (1 - \beta)^t) \\
\mu & \leftarrow \mu + \alpha \frac{\hat{m}}{\sqrt{\hat{s}} + \delta}
\end{align*}
\]

### Variational Adam

\[
\begin{align*}
\theta & \leftarrow \mu + \epsilon, \text{ where } \mathcal{N}(0, Ns + \lambda) \\
g & \leftarrow \frac{1}{M} \sum_i \nabla_{\theta} \log p(D_i | \theta) \\
s & \leftarrow (1 - \beta)s + \beta g^2 \\
m & \leftarrow (1 - \gamma)m + \gamma (g + \lambda \mu / N) \\
\hat{m} & \leftarrow m / (1 - (1 - \gamma)^t) \\
\hat{s} & \leftarrow s / (1 - (1 - \beta)^t) \\
\mu & \leftarrow \mu + \alpha \frac{\hat{m}}{\sqrt{\hat{s}} + \lambda / N}
\end{align*}
\]
Adam vs Vadam (on Logistic-Reg)

Iteration 1

M = 5,
Rho = 0.01,
Gamma = 0.01
Adam vs Vadam (on Neural Nets)

Epoch 0

- Adam
- Vadam (mean)
- Vadam (samples)

(By Runa E.)
LeNet-5 on CIFAR10

Figure 2: Evaluation metrics on Train and Test sets for both optimizers. Adam overfits while VOGN does a good job of keeping test and train errors close. VOGN outperforms Adam on CIFAR10 but underperforms on MNIST for test accuracy. For test log loss, VOGN is better than Adam in both cases. Model architectures given in Table 1.

(By Anirudh Jain)
Stochastic, Low-Rank, Approximate, Natural-Gradient (SLANG)

NeurIPS 2018

- Low-rank + diagonal covariance matrix.
- SLANG is linear in D!

\[
\mathbf{m} \leftarrow \mathbf{m} - \rho \left[ \mathbf{U}\mathbf{U}^\top + \mathbf{D} \right]^{-1} [g_i + \gamma \mathbf{m}]
\]

\[
(1 - \beta) \mathbf{S} + \beta \mathbf{H}_i(\theta)
\]

\[
D \times L \quad L \times D \\
\quad + \quad \text{gradient} \\
D \times M \quad M \times D \\
\quad = \quad \text{gradient} \quad \text{fast_eig} \\
D \times L \quad L \times D
\]

\( \beta \approx 1 \)
SLANG is Faster than GD

Classification on USPS with BNNs

<table>
<thead>
<tr>
<th>Method</th>
<th>Mean-Field</th>
<th>SLANG(1)</th>
<th>SLANG(2)</th>
<th>SLANG(3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neg. ELBO</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Neg. Test LogLik</td>
<td></td>
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Figure 4: This figure compares the convergence behavior on two datasets: USPS 3vs5 (top) and MNIST (bottom). The left plot shows the negative ELBO, and the right plot shows the negative test log-likelihood. SLANG converges faster than the mean-field method, and SLANG with just one rank outperforms BBB on 7 out of 10 datasets.
Generalization and Extensions
Deep Nets + Graphical Models

Neural Nets +
Linear Dynamical System

Neural Nets + GMM

Published as a conference paper at ICLR 2018

To reproduce our results is available at
Amortized Inference on VAE + Probabilistic Graphical Models (PGM)

Graphical model + Deep Model

Structured Inference Network

Backprop on DNN, and forward-backward on PGM.

ICLR 2018
Going Beyond Exponential Family

• Fast and Simple NGD for approximations outside exponential family,
  – Scale mixture of Gaussians, e.g., T-distribution,
  – Finite mixture of Gaussian,
  – Matrix Variate Gaussian,
  – Skew-Gaussians.

• The updates can be implemented using message passing and back-propagation.
Summary of the Talk

• Fast yet simple NGD for VI using Conjugate-Computation VI (AI-STATS 2017),
  – Generalization of forward-backward algorithm, Stochastic VI, Variational Message Passing etc.
  – Beyond conjugacy: Extends fast and simple NGD to deep nets (ICML 2018, NeurIPS 2018).

• Generalizations and Extensions,
  – VAEs (ICLR 2018), Mixture of Exponential Family, Evolution strategy (ArXiv 2017), etc.
Related Works

Sorry, if I miss some important work! Please email me.
EM, Forward-Backward, and VI

- Sato (2001), *Online Model Selection Based on the Variational Bayes*.
- Jordan et al. (1999), *An Introduction to Variational Methods for Graphical Models*.
- Winn and Bishop (2005), *Variational Message Passing*.
NGD: Author Name Starting with an H

- Honkela et al. (2007), *Natural Conjugate Gradient in Variational Inference*.
- Honkela et al. (2010), *Approximate Riemannian Conjugate Gradient Learning for Fixed-Form Variational Bayes*.
- Hensman et al. (2012), *Fast Variational Inference in the Conjugate Exponential Family*.
- Hoffman et al. (2013), *Stochastic Variational Inference*.
NGD: Author Name Starting with an S

• Salimans and Knowles (2013), *Fixed-Form Variational Posterior Approximation through Stochastic Linear Regression.*
  – Approximate Natural-Gradient steps.
• Seth and Khardon (2016), *Monte Carlo Structured SVI for Two-Level Non-Conjugate Models.*
  – Applies to models with two level of hierarchy.
• Salimbani et al. (2018), *Natural Gradients in Practice: Non-Conjugate Variational Inference in Gaussian Process Models.*
  – Fast convergence on GP models
NGD for Bayesian Deep Learning

• Zhang et al. (2018), *Noisy Natural Gradient as Variational Inference*
  
  – For Bayesian deep learning (similar to Variational Adam).
Issues and Open Problems

• Automatic natural-gradient computation.
• Good implementation of message passing.
  – Gradient with respect to covariance matrices.
• Structured approximation for covariance.
• Comparisons on really large problems.
• Applications.
• Flexible posterior approximations.
References

Available at https://emtiyaz.github.io/publications.html

Conjugate-Computation Variational Inference: Converting Variational Inference in Non-Conjugate Models to Inferences in Conjugate Models,
(AISTATS 2017) M.E. Khan and W. Lin [Paper] [Code]

Faster Stochastic Variational Inference using Proximal-Gradient Methods with General Divergence Functions,
References

Available at https://emtiyaz.github.io/publications.html

Variational Message Passing with Structured Inference Networks,

Fast and Scalable Bayesian Deep Learning by Weight-Perturbation in Adam,
(ICML 2018) M.E. Khan, D. Nielsen, V. Tangkaratt, W. Lin, Y. Gal, and A. Srivastava,[ ArXiv Version ] [ Code ] [ Slides ]

Fast yet Simple Natural-Gradient Descent for Variational Inference in Complex Models,
Invited paper at (ISITA 2018) M.E. Khan and D. Nielsen, [ Pre-print ]

SLANG: Fast Structured Covariance Approximations for Bayesian Deep Learning with Natural Gradient,

Fast and Simple Natural-Gradient Variatioional Inference with Mixture of Exponential Family,
Fast yet Simple Natural-Gradient Descent for Variational Inference in Complex Models

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Abstract—Bayesian inference plays an important role in advancing machine learning, but faces computational challenges when applied to complex models such as deep neural networks. Variational inference circumvents these challenges by formulating Bayesian inference as an optimization problem and solving it using gradient-based optimization. In this paper, we argue in favor of natural-gradient approaches which, unlike their gradient-based counterparts, can improve convergence by exploiting the information geometry of the solutions. We show how to derive fast yet simple natural-gradient updates by using a duality associated with exponential-family distributions. An attractive feature of these methods is that, by using natural-gradients, they are able to extract accurate local approximations for individual model components. We summarize recent results for Bayesian deep learning showing the superiority of natural-gradient approaches over their gradient counterparts.

Index Terms—Bayesian inference, variational inference, natural gradients, stochastic gradients, information geometry, exponential-family distributions, nonconjugate models.

prove the rate of convergence [7]–[9]. Unfortunately, these approaches only apply to a restricted class of models known as conditionally-conjugate models, and do not work for non-conjugate models such as Bayesian neural networks.

This paper discusses some recent methods that generalize the use of natural gradients to such large and complex non-conjugate models. We show that, for exponential-family approximations, a duality between their natural and expectation parameter-spaces enables a simple natural-gradient update. The resulting updates are equivalent to a recently proposed method called Conjugate-computation Variational Inference (CVI) [10]. An attractive feature of the method is that it naturally obtains local exponential-family approximations for individual model components. We discuss the application of the CVI method to Bayesian neural networks and show some recent results from a recent work [11] demonstrating
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Slides, papers, and code available at
https://emtiyaz.github.io