Uncertainty Estimation with Noisy Optimizers

Master Seminar Beyond Deep Learning: Selected Topics on Novel Challenges

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Introduction: Bayesian Inference

Why Bayesian?

- Important tasks that have high risk or more interpretability require more than just "high accuracies".
- Autonomous driving, medical diagnosis, financial predictions for algorithmic trading...
- Bayesian Inference provides a framework where you can measure your confidence in your prediction.

Bayesian Inference

Given a dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i)_{i=1}^n\}$,

$$p(w|\mathcal{D}) = \frac{p(\mathcal{D}|w)p(w)}{p(\mathcal{D})} = \frac{p(\mathcal{D}|w)p(w)}{\int p(\mathcal{D}|w)p(w)} = \frac{p(\mathcal{D}|w)p(w)}{\sum_{i=1}^n p(\mathcal{D}|w)p(w)} \tag{1}$$

- **Frequentist** way: Directly maximizing the likelihood of the data given weights.
- In **Bayesian inference**, we put a prior distribution on weights and we try to find the posterior distribution
- **Likelihood**: $p(\mathcal{D}|w)$
- **Prior**: $p(w)$
- **Evidence**: $p(\mathcal{D}) = \int p(\mathcal{D}|w)p(w) \rightarrow$ Not tractable in complex models like deep neural networks!

Bayesian Inference

- Due to the **intractability of the evidence term**, we do not have an exact solution. But we can approximate to posterior!
- **Several methods** $\rightarrow$ variational inference(VI), Markov Chain Monte Carlo(MCMC), and ensemble methods like MC-Dropout...
- In the recent years, it has been shown that with slight modifications on well-known optimizers, they perform variational inference!
- This presentation's topic is on variational inference.

Variational Inference(VI)

Variational Inference: KL-Divergence

- Takes roots from relative entropy in information theory.
- A **non-negative, non-symmetric** measure between two probability distribution, defined as

$$\mathbb{KL}\left(q(x) \| p(x)\right) = \int q(x) \log \frac{q(x)}{p(x)} dx = \sum_{x \in X} p(x) \log \frac{p(x)}{q(x)}$$

- The integral version represents the continuous case and the summation version represents the discrete case

Variational Inference

- We try to approximate the true posterior distribution with a variational distribution $q_\theta(\mathbf{w})$, which is parametrized by θ - the parameters of the posterior distribution.
- **Example:** If we model our approximate posterior q to be a Gaussian distribution

$$q_\theta(\mathbf{w}) := \mathcal{N}(w|\mu, \, diag(\sigma^2)) \quad \text{or} \quad q_\theta(\mathbf{w}) := \mathcal{N}(w|\mu, \, \Sigma)$$

, the parameters would be

$$\theta = (\mu, \sigma) \quad \text{or} \quad \theta = (\mu, \Sigma)$$

, where μ, $\sigma \in \mathbb{R}^D$, and $\Sigma \in \mathbb{R}^{DxD}$.

Variational Inference

We try to maximize variational parameters θ:

$$\begin{aligned}\theta^\star &= \arg\min_\theta \mathbb{KL}[q_\theta(\mathrm{w}) \| p(w|\mathcal{D})] \\ &= \arg\min_\theta \underbrace{\mathbb{KL}[q_\theta(\mathrm{w} \mid \theta) \| p(\mathrm{w})] - \mathbb{E}_{q(\mathrm{w}|\theta)}[\log p(\mathcal{D} \mid \mathrm{w})]}_{\mathcal{F}(\mathcal{D},\theta) = -\mathcal{L}(\boldsymbol{\theta}, q) \to \text{negative ELBO}}\end{aligned} \tag{2}$$

It turns out that minimizing the KL-divergence is equal to maximizing the variational objective ELBO!

Reparametrization Trick:

In order to free our gradients of μ and Σ from the Gaussian distribution by using a parameter-free noise ϵ.

1. Draw samples from noise $\epsilon \sim \mathcal{N}(0, I)$
2. Set $\mathrm{w} = t(\epsilon, \theta = \{\mu, \Sigma\}) = \mu + \Sigma \circ \epsilon$

Natural Gradient

Natural Gradient

- Natural gradient method takes its roots from information geometry.
- In optimization of the deep learning cost functions, learning takes place in the space of parameters, which is actually a space of probability distributions.
- Aims to change the gradients direction from the steepest direction in the Euclidean space to the steepest direction the **natural parameter space**.
- **Good news:** This space can be a probability distribution space!

Natural Gradient

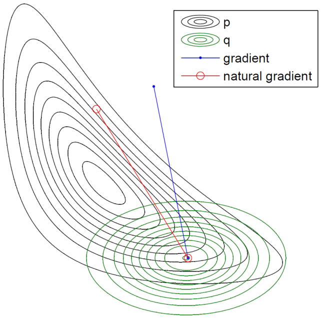


Figure 1: Gradient and vs natural gradient directions for mean of variational distribution q. VI with a diagonal covariance is applied to the posterior $p(x, y) \propto \exp\left[-9(xy-1)^2 - x^2 - y^2\right]$.[1]

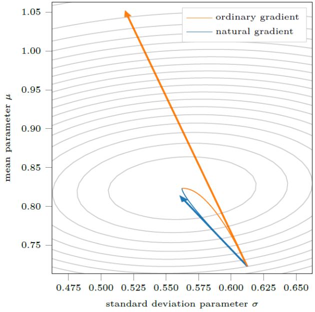


Figure 2: Arrows correspond the gradients and the curves correspond the path of gradients.[2]

[1] A gradient-based algorithm competitive with variational bayesian em for mixture of gaussians, 2009 Kuusela et al. [2009]

[2] Natural gradients inpractice: Non-conjugate variational inference in gaussian process models Salimbeni et al.

Natural Gradient: Fisher Information Matrix

- Natural gradient method scales the gradient with a inverse of **Fisher Information Matrix(FIM)** of a **score function**.
- In **probabilistic setting**, this score function is a **probability distribution**.
- The likelihood function can be a proper choice in this task, but in a Bayesian setting that we are trying to approximate the true posterior, our variational posterior $q_\theta(\mathrm{w})$ would be the right choice for score function
- FIM is given by:

$$\mathrm{F} = \mathop{\mathbb{E}}_{q_\theta(\mathrm{w})}\left[\nabla_\theta q_\theta(\mathrm{w}) \nabla_\theta q_\theta(\mathrm{w})^{\mathrm{T}}\right] \tag{3}$$

Natural Gradient

- Let $\tilde{\nabla}_\theta$ be the term for natural gradient. Then, the mathematical equation for the natural gradient of our variational objective is defined as

$$
\begin{aligned}
\tilde{\nabla}_\theta \mathcal{L}(\boldsymbol{\theta}, q) &\stackrel{\text{def}}{=} \nabla_\theta \mathcal{L}(\theta) \mathbb{E}_{\mathbf{z}} \left[(\nabla \log p_\theta(\mathbf{z}))^T (\nabla \log p_\theta(\mathbf{z})) \right]^{-1} \\
&\stackrel{\text{def}}{=} \nabla_\theta \mathcal{L}(\boldsymbol{\theta}, q) \mathbf{F}^{-1}
\end{aligned}
\tag{4}
$$

Natural Gradient

2 major variants of natural gradient that are frequently in use. The first one in named **natural gradient for point estimation(NGPE)** and the second one is **natural gradient for variational inference(NGVI)**:

1. **NGPE:** NGPE tries to estimate just the likelihood $p(\mathcal{D}|w)$ by optimizing over a loss function. For this task, the FIM is constructed by calculating the $\mathrm{F} = \mathrm{Cov}_{\mathcal{D}\sim p(\mathcal{D})}[\nabla_{\mathrm{w}} \log p(\mathcal{D}|w)]$.

2. **NGVI:** We try to fit the parameters of a variational posterior $q_\theta(\mathrm{w})$ to maximize our variational objective ELBO. We need to compute the FIM of our variational posterior q instead of the predictive distribution, which is $\mathrm{F} = \mathrm{Cov}_{\mathrm{w}\sim q_\theta(\mathrm{w})}[\nabla_{\mathrm{w}} \log q_\theta(\mathrm{w})]$.

Variational Inference using Noisy Natural Gradients[a]

[a] Noisy Natural Gradient as Variational Inference (Zhang et al. [2018])

Variational Inference Using Noisy Gradient

The following updates for μ and Λ:

$$\begin{aligned} \mu &\leftarrow \mu + \alpha\Lambda^{-1}\left[\nabla_{\mathbf{w}}\log p(\mathcal{D}|w) - \tfrac{\eta}{N}\mathbf{w}\right] \\ \Lambda &\leftarrow \left(1 - \tfrac{\beta}{N}\right)\Lambda - \beta\left[\nabla^2_{\mathbf{w}}\log p(\mathcal{D}|w), \mathbf{w}) - \tfrac{\eta}{N}\mathbf{I}\right] \end{aligned} \tag{5}$$

where $q_\theta(\mathbf{w}) = \mathcal{N}(w|\mu, \Sigma)$, the precision matrix $\Lambda = \Sigma^{-1}$, a spherical Gaussian prior $p(\mathbf{w}) = \mathcal{N}(\mathbf{0}, \mathbf{I}/\eta)$, and then $\nabla^2_{\mathbf{w}}\log p(\mathbf{w}) = \eta\mathbf{I}$.

Problems:

1. Hessian is hard to compute and not differentiable in every point(Ex: ReLU).
2. Hessian might have negative eigen-values if the negative log-likelihood is not convex, which means that our update for Λ might not be positive semi-definite.

Variational Inference Using Noisy Gradient

Idea: Approximate Hessian with NGPE FIM $\mathrm{F} = \mathrm{Cov}_{\mathcal{D}\sim p(\mathcal{D})}[\nabla_{\mathrm{w}} \log p(\mathcal{D}|w)]$, which prevents both of the problems stated:

$$\Lambda \leftarrow \left(1 - \frac{\beta}{N}\right)\Lambda + \beta\left[\underbrace{\nabla_{\mathrm{w}} \log p(\mathcal{D}|w)\nabla_{\mathrm{w}} \log p(\mathcal{D}|w)^{\mathrm{T}}}_{\mathrm{F}} + \frac{\eta}{N}\mathbf{I}\right] \tag{6}$$

Observation: With a fixed prior variance η, Λ will become a damped version of the moving average of the FIM

Rewriting the equations with the FIM approximation of Hessian:

$$
\begin{aligned}
\Lambda &= N\bar{\mathbf{F}} + \eta \mathbf{I} \\
\bar{\mathbf{F}} &\leftarrow (1-\tilde{\beta})\bar{\mathbf{F}} + \tilde{\beta}[\nabla_{\mathbf{w}} \log p(\mathcal{D}|w) \nabla_{\mathbf{w}} \log p(\mathcal{D}|w)^{\mathrm{T}}] \\
\mu &\leftarrow \mu + \tilde{\alpha}\left(\bar{\mathbf{F}} + \tfrac{\eta}{N}\mathbf{I}\right)^{-1}\left[\nabla_{\mathbf{w}} \log p(\mathcal{D}|w) - \tfrac{\eta}{N}\mathbf{w}\right]
\end{aligned}
\tag{7}
$$

Noisy Adam

- Estimating Λ^{-1} as a full covariance Gaussian is unrealistic since the number of parameters needed for a full covariance matrix is $(\mathbf{dim(w)})^2$.
- Zhang et al. (2018) proposed a solution by approximating the FIM with a **diagonal matrix f**. For their noisy natural gradient version of Adam, the updates for μ and **f** are:

$$\begin{aligned} \mu &\leftarrow \mu + \tilde{\alpha}\left[\nabla_{\mathrm{w}} \log p(\mathcal{D}|w) - \tfrac{\eta}{N}\mathbf{w}\right] / \left(\bar{\mathbf{f}} + \tfrac{\eta}{N}\right) \\ \bar{\mathbf{f}} &\leftarrow (1-\tilde{\beta})\bar{\mathbf{f}} + \tilde{\beta}(\nabla_{\mathrm{w}} \log p(\mathcal{D}|w))^2 \end{aligned} \tag{8}$$

Noisy K-FAC

They use a Kronecker-factored approximation[1] to the FIM to perform efficient approximate natural gradient updates, given by

$$
\begin{aligned}
\mathrm{F}_l = \mathbb{E}\left[\mathrm{vec}\{\mathcal{D}\mathrm{W}_l\}\,\mathrm{vec}\{\mathcal{D}\mathrm{W}_l\}^\top\right] = \mathbb{E}\left[\mathbf{g}_l\mathbf{g}_l^\top \otimes \mathbf{a}_l\mathbf{a}_l^\top\right] \\
\approx \mathbb{E}\left[\mathbf{g}_l\mathbf{g}_l^\top\right] \otimes \mathbb{E}\left[\mathbf{a}_l\mathbf{a}_l^\top\right] = \mathrm{S}_l \otimes \mathrm{A}_l = \tilde{\mathrm{F}}_l
\end{aligned}
\tag{9}
$$

where, $\mathbf{a}_l$ and $\mathbf{s}_l$ correspond to input activations and outputs at layer l, $\mathcal{D}v = \nabla_v \log p(\mathcal{D}|w)$, $\mathbf{g}_l = \mathcal{D}\mathbf{s}_l$ and the gradient of weights at layer l is $\mathcal{D}\mathrm{W}_l = \mathbf{a}_l\mathbf{g}_l^T$.

Then we have the inverse FIM as

$$
\begin{aligned}
\tilde{\mathrm{F}}_l^{-1}\,\mathrm{vec}\{\nabla_{\mathrm{W}_l} h\} = \mathrm{S}_l^{-1} \otimes \mathrm{A}_l^{-1}\,\mathrm{vec}\{\nabla_{\mathrm{W}_l} h\} \\
= \mathrm{vec}\left[\mathrm{A}_l^{-1}\nabla_{\mathrm{W}_l} h \mathrm{S}_l^{-1}\right]
\end{aligned}
\tag{10}
$$

[1] Optimizing Neural Networks with Kronecker-factored Approximate Curvature

Noisy K-FAC

- By plugging in this inverse FIM approximation to eqn. (7), we will have the MVG posterior. The update rule for $\bar{\mathsf{A}}_l$ and $\bar{\mathsf{S}}_l$ is as follows:

$$\begin{aligned} \bar{\mathsf{A}}_l &\leftarrow (1-\tilde{\beta})\bar{\mathsf{A}}_l + \tilde{\beta}\mathbf{a}_l\mathbf{a}_l^\top \\ \bar{\mathsf{S}}_l &\leftarrow (1-\tilde{\beta})\bar{\mathsf{S}}_l + \tilde{\beta}\mathcal{D}\mathbf{s}_l\mathcal{D}\mathbf{s}_l^\top \end{aligned} \tag{11}$$

- And the Σ_l can be decomposed as the Kronecker product of two terms:

$$\begin{aligned} \Sigma_l &= \frac{1}{N}\left[\mathsf{S}_l^\gamma\right]^{-1} \otimes \left[\mathsf{A}_l^\gamma\right]^{-1} \\ &\triangleq \frac{1}{N}\left(\bar{\mathsf{S}}_l + \frac{1}{\pi_l}\sqrt{\frac{\eta}{N}}\mathbf{I}\right)^{-1} \otimes \left(\bar{\mathsf{A}}_l + \pi_l\sqrt{\frac{\eta}{N}}\mathbf{I}\right)^{-1} \end{aligned} \tag{12}$$

Noisy K-FAC

Algorithm 1: Noisy K-FAC. Subscript l denotes layers, . We assume zero momentum for simplicity. Differences from standard K-FAC are shown in red.

input : α: Stepsize
input : β: Exponential moving average parameter
input : $\lambda, \eta, \gamma_{\text{ex}},$: KL weighting, prior variance, extrinsic damping term
input : Stats and inverse update intervals T_{stats} and T_{inv}

$k \leftarrow 0$ and initialize $\{\boldsymbol{\mu}_l\}_{l=1}^{L}, \{S_l\}_{l=1}^{L}, \{A_l\}_{l=1}^{L}$ Calculate the intrinsic damping term $\gamma_{\text{in}} = \frac{\eta}{N}$, total damping term $\gamma = \gamma_{\text{in}} + \gamma_{\text{ex}}$.
while *not converged* **do**
  $k \leftarrow k + 1$
  $W_l \sim \mathcal{MN}\left(M_l, \frac{1}{N}\left[A_l^{\gamma_{\text{in}}}\right]^{-1}, \left[S_l^{\gamma_{\text{in}}}\right]^{-1}\right)$
  if $k \equiv 0 \pmod{T_{stats}}$ **then**
    Update the factors $\{S_l\}_{l=1}^{L}, \{A_l\}_{l=0}^{L-1}$ using eq.(11)
  if $k \equiv 0 \pmod{T_{inv}}$ **then**
    Calculate the inverses $\left\{\left[S_l^{\gamma}\right]^{-1}\right\}_{l=1}^{L}, \left\{\left[A_l^{\gamma}\right]^{-1}\right\}_{l=0}^{L-1}$ using eq. (13).
  $V_l = \nabla_{W_l} \log p(\mathcal{D}|w) - \gamma_{\text{in}} \cdot W_l$
  $M_l \leftarrow M_l + \alpha \left[A_l^{\gamma}\right]^{-1} V_l \left[S_l^{\gamma}\right]^{-1}$

Variational Online Gauss-Newton(VOGN)[a]

[a] Fast and Scalable Bayesian Deep Learning by Weight-Perturbation in Adam(Khan et al. [2018])

Variational Online Gauss-Newton (VOGN)

Shown[1] that we can express the NGVI update in terms of the MLE objective.

- Let's denote the MLE objective $f_i(\boldsymbol{\theta}) := -\log p\left(\mathcal{D}_i \mid \boldsymbol{\theta}\right)$ and and minibatch stochastic-gradient estimates as

$$f(\boldsymbol{\theta}) := \frac{1}{N} \sum_{i=1}^{N} f_i(\boldsymbol{\theta}), \quad \hat{\mathrm{g}}(\boldsymbol{\theta}) := \frac{1}{M} \sum_{i \in \mathcal{M}} \nabla_\theta f_i(\boldsymbol{\theta}), \tag{13}$$

- show the the NGVI update can be written in terms of stochastically approximated Hessian of f as

$$\boldsymbol{\mu}_{t+1} = \boldsymbol{\mu}_t - \beta_t \left(\hat{\mathrm{g}}\left(\boldsymbol{\theta}_t\right) + \tilde{\eta}\boldsymbol{\mu}_t\right) / \left(\mathrm{s}_{t+1} + \tilde{\eta}\right), \quad \mathrm{s}_{t+1} = \left(1 - \beta_t\right) \mathrm{s}_t + \beta_t \operatorname{diag}\left[\widehat{\nabla}^2_{\theta\theta} f\left(\boldsymbol{\theta}_t\right)\right] \tag{14}$$

where $\boldsymbol{\theta}_t \sim \mathcal{N}\left(\boldsymbol{\theta} \mid \boldsymbol{\mu}_t, \boldsymbol{\sigma}_t^2\right)$ with $\boldsymbol{\sigma}_t^2 := 1/\left[N\left(\mathrm{s}_t + \tilde{\eta}\right)\right]$ and $\tilde{\eta} := \eta/N$.

[1] Fast and Scalable Bayesian Deep Learning by Weight-Perturbation in Adam(Khan et al. [2018]

Variational Online Gauss-Newton (VOGN)

Resembles the online-Newton method, since s_t contains an online estimate of the diagonal of the Hessian.
Problem: Hessian can be negative again!

Solution

Approximate Hessian with

$$\nabla^2_{\theta_j \theta_j} f(\boldsymbol{\theta}) \approx \frac{1}{M} \sum_{i \in \mathcal{M}} \left[\nabla_{\theta_j} f_i(\theta) \right]^2 := \hat{h}_j(\boldsymbol{\theta}) \tag{15}$$

which is guaranteed to be positive if initial σ^2 is positive!

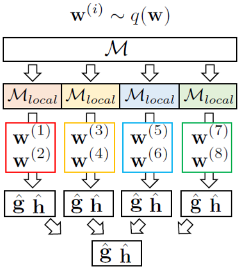
As a result, the new update rule for s_t becomes

$$\mathbf{s}_{t+1} = (1 - \beta_t)\, \mathbf{s}_t + \beta_t \hat{h}_j(\boldsymbol{\theta}) \tag{16}$$

Variational Online Gauss-Newton (VOGN)

Algorithm 1: Variational Online Gauss Newton (VOGN)

Initialise $\boldsymbol{\mu}_0$, $\mathbf{s}_0$, $\mathbf{m}_0$.
$N \leftarrow \rho N$, $\tilde{\delta} \leftarrow \tau\delta/N$.
repeat
  Sample a minibatch $\mathcal{M}$ of size M.
  Split $\mathcal{M}$ into each GPU (local minibatch $\mathcal{M}_{local}$).
  for each GPU in parallel **do**
    for $k = 1, 2, \ldots, K$ **do**
      Sample $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$.
      $\mathbf{w}^{(k)} \leftarrow \boldsymbol{\mu} + \epsilon\boldsymbol{\sigma}$ with $\boldsymbol{\sigma} \leftarrow (1/(N(\mathbf{s} + \tilde{\delta} + \gamma)))^{1/2}$.
      Compute $\mathbf{g}_i^{(k)} \leftarrow \nabla_w \ell(\mathbf{y}_i, \mathbf{f}_{w^{(k)}}(\mathbf{x}_i)), \forall i \in \mathcal{M}_{local}$ using the method described in Appendix B.
      $\hat{\mathbf{g}}_k \leftarrow \frac{1}{M}\sum_{i\in\mathcal{M}_{local}} \mathbf{g}_i^{(k)}$.
      $\hat{\mathbf{h}}_k \leftarrow \frac{1}{M}\sum_{i\in\mathcal{M}_{local}} (\mathbf{g}_i^{(k)})^2$.
    end for
    $\hat{\mathbf{g}} \leftarrow \frac{1}{K}\sum_{k=1}^{K} \hat{\mathbf{g}}_k$ and $\hat{\mathbf{h}} \leftarrow \frac{1}{K}\sum_{k=1}^{K} \hat{\mathbf{h}}_k$.
  end for
  AllReduce $\hat{\mathbf{g}}$, $\hat{\mathbf{h}}$.
  $\mathbf{m} \leftarrow \beta_1\mathbf{m} + (\hat{\mathbf{g}} + \tilde{\delta}\boldsymbol{\mu})$.
  $\mathbf{s} \leftarrow (1 - \tau\beta_2)\mathbf{s} + \beta_2\hat{\mathbf{h}}$.
  $\boldsymbol{\mu} \leftarrow \boldsymbol{\mu} - \alpha\mathbf{m}/(\mathbf{s} + \tilde{\delta} + \gamma)$.
until stopping criterion is met



Learning rate	α
Momentum rate	β_1
Exp. moving average rate	β_2
Prior precision	δ
External damping factor	γ
Tempering parameter	τ
# MC samples for training	K
Data augmentation factor	ρ

Figure 3: Table is prepared from the experimental results of [Khan et al., 2018, Zhang et al., 2018]

Variational Adam(Vadam)

- Assuming that variational posterior q is from an exponential-family distribution with natural parameter η, Khan et al. (2018) proposed the following natural-momentum method:

$$\eta_{t+1} = \eta_t + \bar{\alpha}_t \tilde{\nabla}_\eta \mathcal{L}_t + \bar{\gamma}_t \left(\eta_t - \eta_{t-1}\right) \tag{17}$$

where $\tilde{\nabla}$ it the natural-gradients with respect to natural parameter space and the gradient scaled by the Fisher information matrix of $q(\theta)$.

Variational Adam(Vadam)

- They show that the eqn.(17) can be expressed as VON update with momentum:

$$\begin{aligned}\mu_{t+1} &= \mu_t - \bar{\alpha}_t \left[\frac{1}{\mathrm{s}_{t+1} + \tilde{\eta}}\right] \circ \left(\nabla_\theta f(\boldsymbol{\theta}_t) + \tilde{\eta}\boldsymbol{\mu}_t\right) + \bar{\gamma}_t \left[\frac{\mathrm{s}_t + \tilde{\eta}}{\mathrm{s}_{t+1} + \tilde{\eta}}\right] \circ \left(\boldsymbol{\mu}_t - \boldsymbol{\mu}_{t-1}\right) \\ \mathrm{s}_{t+1} &= (1 - \bar{\alpha}_t)\,\mathrm{s}_t + \bar{\alpha}_t \nabla^2_{\theta\theta} f(\boldsymbol{\theta}_t)\end{aligned} \tag{18}$$

where $\mathbf{w}_t \sim \mathcal{N}\left(\theta \mid \mu_t, \sigma_t^2\right)$ with $\sigma_t^2 := 1/[N(\mathrm{s}_t + \tilde{\lambda})]$.

Noisy Adam vs Vadam

Algorithm 2: Noisy Adam. Differences from standard Adam are shown in red.

input : α: Stepsize
input : β_1, β_2: Exponential decay rates for updating μ and **f**
input : $, \eta, \gamma_{\text{ex}},$: prior variance, extrinsic damping term

$\mathrm{m} \leftarrow 0$;
Calculate the intrinsic damping term $\gamma_{\text{in}} = \frac{\eta}{N}$, total damping term $\gamma = \gamma_{\text{in}} + \gamma_{\text{ex}}$.
while *not converged* **do**
$\quad \mathrm{w} \sim \mathcal{N}\left(\boldsymbol{\mu}, \frac{1}{N} \operatorname{diag}\left(\mathrm{f} + \gamma_{\text{in}}\right)^{-1}\right)$
$\quad \mathrm{g} \leftarrow \nabla_{\mathrm{w}} \log p(\mathcal{D}|w)$
$\quad \mathrm{m} \leftarrow \beta_1 \cdot \mathrm{m} + (1 - \beta_1) \cdot (\mathrm{g} + \gamma_{\text{in}} \cdot \mathrm{w})$
$\quad \mathrm{f} \leftarrow \beta_2 \cdot \mathrm{f} + (1 - \beta_2) \cdot (\mathrm{g} \circ \mathrm{g})$. (Update momentum)
$\quad \tilde{\mathrm{m}} \leftarrow \mathrm{m} / \left(1 - \beta_1^k\right)$
$\quad \hat{\mathrm{m}} \leftarrow \tilde{\mathrm{m}} / (\mathrm{f} + \gamma)$
$\quad \mu \leftarrow \mu + \alpha \cdot \hat{\mathrm{m}}$ (Update parameters)

Algorithm 3: Vadam. Differences from standard Adam are shown in red

input : α: Stepsize
input : β_1, β_2: Exponential decay rates for updating μ and **f**
input : η:prior variance

$\mathrm{m} \leftarrow 0$;
while *not converged* **do**
$\quad w \leftarrow \boldsymbol{\mu} + \boldsymbol{\sigma} \circ \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathrm{I}), \boldsymbol{\sigma} \leftarrow 1/\sqrt{N\mathrm{s} + \lambda}$
$\quad \mathrm{g} \leftarrow -\nabla \log p\left(\mathcal{D}_i \mid \boldsymbol{\theta}\right)$
$\quad \mathrm{m} \leftarrow \beta_1 \mathrm{m} + (1 - \beta_1)\left(\mathrm{g} + \mu \frac{\eta}{N}\right)$
$\quad \mathrm{s} \leftarrow \beta_2 \mathrm{s} + (1 - \beta_2)(\mathrm{g} \circ \mathrm{g})$
$\quad \hat{\mathrm{m}} \leftarrow \mathrm{m} / \left(1 - \beta_1^t\right), \quad \hat{\mathrm{s}} \leftarrow \mathrm{s} / \left(1 - \beta_2^t\right)$
$\quad \mu \leftarrow \mu - \alpha \hat{\mathrm{m}} / \left(\sqrt{\hat{\mathrm{s}}} + \frac{\eta}{N}\right)$

Vadam and VOGN Convergence

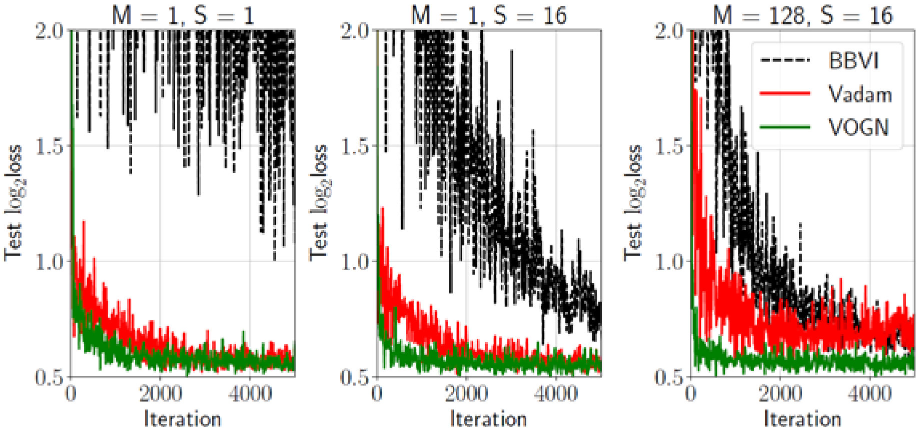


Figure 4: Results on the Australian-Scale dataset using a neural network with a hidden layer of 64 units for different minibatch sizes M and number of MC samples S. Figure taken from Khan et al. [2018]

Comparison

Comparison of Optimizers

	Noisy Adam	Vadam	Noisy K-FAC	VOGN
Prior	Spherical Gaussian	Spherical Gaussian	Spherical Gaussian	Spherical Gaussian
Posterior	Gaussian with diag. cov.	Gaussian with diag. cov.	Matrix-Variate Gaussian	Gaussian with diag. cov.
FIM Approximation	GM	GM	GM	GGN
Gradient Estimators of Gaussian	Opper Estimator	Reparametrization Trick	Opper Estimator	Reparametrization Trick

Table 1: Difference and similarities between the noisy optimizers. GM corresponds to Gradient Magnitude, and GGN corresponds to Generalized Gauss-Newton approximation.

- **Noisy Adam and Vadam** $\leftarrow$ algorithmically very similar and both easy to implement.
- Derivation of **Vadam** uses **natural-momentum** term from **Polyak's heavy ball method**, which noisy Adam doesn't provide.
- **Noisy K-FAC** $\rightarrow$ more complex weight distribution due to covariances.

Evaluation

Evaluation

	Test log-likelihood				
Dataset	**MC-Dropout**	**BBVI**	**Vadam**	**Noisy Adam**	**Noisy K-FAC**
Boston	-2.46 +/- 0.06	-2.73 +/- 0.05	-2.85 +/- 0.07	-2.558 +/- 0.032	**-2.417 +/- 0.029**
Concrete	-3.04 +/- 0.02	-3.24 +/- 0.02	-3.39 +/- 0.02	-3.145 +/- 0.023	**-3.039 +/- 0.025**
Energy	-1.99 +/- 0.02	-2.47 +/- 0.02	-2.15 +/- 0.07	-1.629 +/- 0.020	**-1.421 +/- 0.005**
Kin8nmm	0.95 +/- 0.01	0.95 +/- 0.01	0.76 +/- 0.00	1.112 +/- 0.008	**1.148 +/- 0.007**
Naval	3.80 +/- 0.01	4.46 +/- 0.03	4.72 +/- 0.22	6.231 +/- 0.041	**7.079 +/- 0.034**
Power	-2.80 +/- 0.01	-2.88 +/- 0.01	-2.88 +/- 0.01	-2.803 +/- 0.010	**-2.776 +/- 0.011**
Wine	**-0.93 +/- 0.01**	1.00 +/- 0.001	-1.00 +/- 0.01	-0.976 +/- 0.016	-0.969 +/- 0.014
Yacht	**-1.55 +/- 0.03**	-2.41 +/- 0.02	-1.70 +/- 0.03	-2.412 +/- 0.006	-2.316 +/- 0.006

Table 2: Comparison of Noisy Adam, Noisy K-FAC and Vadam with other popular methods. Table is prepared from the experimental results of [Khan et al., 2018, Zhang et al., 2018]

Evaluation

Dataset/ Architecture	Optimiser	Train/Validation Accuracy (%)	Validation NLL	Epochs	Time/ epoch (s)	ECE	AUROC
CIFAR-10/ LeNet-5 (no DA)	Adam	71.98 / **67.67**	**0.937**	210	6.96	**0.021**	0.794
	BBB	66.84 / 64.61	1.018	800	11.43†	0.045	0.784
	MC-dropout	68.41 / **67.65**	0.99	210	6.95	0.087	**0.797**
	VOGN	70.79 / **67.32**	**0.938**	210	18.33	0.046	**0.8**
CIFAR-10/ AlexNet (no DA)	Adam	100.0 / 67.94	2.83	161	3.12	0.262	0.793
	MC-dropout	97.56 / **72.20**	1.077	160	3.25	0.140	**0.818**
	VOGN	79.07 / 69.03	**0.93**	160	9.98	**0.024**	0.796
CIFAR-10/ AlexNet	Adam	97.92 / 73.59	1.480	161	3.08	0.262	0.793
	MC-dropout	80.65 / **77.04**	**0.667**	160	3.20	0.114	0.828
	VOGN	81.15 / 75.48	0.703	160	10.02	**0.016**	**0.832**
CIFAR-10/ ResNet-18	Adam	97.74 / **86.00**	0.55	160	11.97	0.082	**0.877**
	MC-dropout	88.23 / 82.85	0.51	161	12.51	0.166	0.768
	VOGN	91.62 / 84.27	**0.477**	161	53.14	**0.040**	**0.876**
ImageNet/ ResNet-18	SGD	82.63 / **67.79**	**1.38**	90	44.13	0.067	0.856
	Adam	80.96 / 66.39	1.44	90	44.40	0.064	0.855
	MC-dropout	72.96 / 65.64	1.43	90	45.86	**0.012**	0.856
	OGN	85.33 / 65.76	1.60	90	63.13	0.128	0.854
	VOGN	73.87 / **67.38**	**1.37**	90	76.04	0.029	0.854
	K-FAC	83.73 / 66.58	1.493	60	133.69	0.158	0.842
	Noisy K-FAC	72.28 / 66.44	1.44	60	179.27	0.080	0.852

Figure 5: Performance comparisons on different dataset/architecture combinations. Figure taken from Osawa et al. [2019]

- The distributed version of momentum employed VOGN method proposed by Osawa et al. (2019) has very promising results as well.
- VOGN and Noisy K-FAC has a comparable performance with standart Adam and MC-Dropout if data augmentation(DA) is applied.

Questions?

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