

PAC-Bayes & Variational Inference

Badr-Eddine Chérif-Abdellatif

badr-eddine.cherief-abdellatif@cnr.fr



**SORBONNE
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Overview of the course

The course will be divided in 5 lectures :

- Lecture 1 : Introduction & Motivation
- Lecture 2 : Basics of PAC-Bayes Theory
- Lecture 3 : Advances in PAC-Bayes Theory
- Lecture 4 : Basics of Variational Inference
- Lecture 5 : Advances in Variational Inference

Lecture 4 : Basics of Variational Inference

Outline

- Variational inference (VI) : compute an approximate posterior distribution by maximizing the ELBO

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- Some difficulties : compute the gradients of the ELBO
- Design faster and simpler methods by incorporating natural gradients

Introduction to Variational Inference

A short story of variational inference

- 1760's & 1770's : Bayes' and Laplace's early works on the concept of 'inverse probability'.
- 1950's & 1960's : Bayesian inference is impossible.
- 1970's & 1980's : Early work on approximate Bayesian inference (Metropolis-Hastings, importance sampling).
- 1990's : Gibbs sampling & better computation. Early work on variational inference.
- 2000's : VI in practice. Bayesian models can be fit faster.
- 2010's : VI is scalable and general. Large classes of models & large datasets can be studied.
- 2020's : ?

Notations

Assume that we observe $\mathcal{S}_1, \dots, \mathcal{S}_n$ i.i.d from P^* . We denote the collection of r.v. $\mathcal{S} = (\mathcal{S}_1, \dots, \mathcal{S}_n)$. We consider a model $\{P_\theta, \theta \in \Theta\}$, a prior π on Θ .

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The posterior

$$\pi_n(d\theta) \propto p_\theta(\mathcal{S})\pi(d\theta)$$

Remark : the prior is sometimes simply written as $p(\theta)$ and the posterior $p(\theta|\mathcal{S})$.

Frequentist Inference

A typical example of frequentist estimator :

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Maximum Likelihood Estimation

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Maximum Likelihood Estimation

$$\hat{\theta} = \arg \max_{\theta \in \Theta} \log p_{\theta}(\mathcal{S})$$

which can be computed using

Stochastic Gradient Descent

$$\theta_{t+1} = \theta_t + \eta_t \hat{\nabla}_{\theta} \log p_{\theta_t}(\mathcal{S})$$

where t is the iteration number, η_t is the step size, and $\hat{\nabla}_{\theta} \log p_{\theta_t}(\mathcal{S})$ is a stochastic estimate of the gradient of $\theta \mapsto \log p_{\theta}(\mathcal{S})$ at $\theta = \theta_t$.

Major Difficulty

The exact posterior $\pi_n(d\theta) \propto \prod_{i=1}^n p_{\theta}(\mathcal{S}_i)\pi(d\theta)$ is often difficult to compute in complex models.

Bayesian Inference

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Example : Bayesian Neural Networks

Data \mathcal{S}_i contains input $X_i \in \mathbb{R}^d$ and a scalar output $y_i \in \mathbb{R}$. θ is the vector of network weights. The likelihood $p_\theta(\mathcal{S}_i)$ is a Gaussian distribution $p(y_i | f_\theta(X_i))$ whose parameter $f_\theta(\cdot)$ is a neural network parameterized by θ . The prior is usually taken as $\pi = \mathcal{N}(0, I)$.

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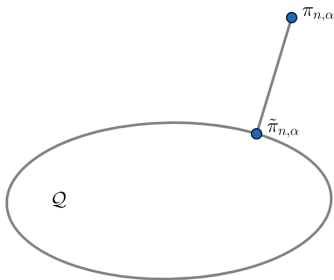
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How can we compute this posterior ?

Variational Inference

Idea of VI : choose a family \mathcal{Q} of probability distributions on Θ and approximate π_n by a distribution in \mathcal{Q} :

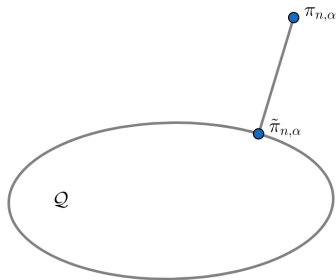
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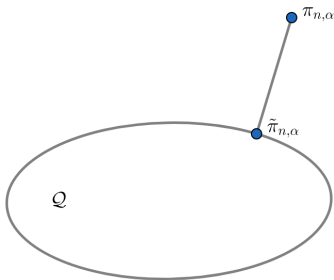
- parametric ($\Theta \subset \mathbb{R}^d$) :

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- mean-field ($\Theta = \Theta_1 \times \Theta_2$) :

$$q(d\theta) = q_1(d\theta_1) \times q_2(d\theta_2).$$

Shape of the variational approximation ?

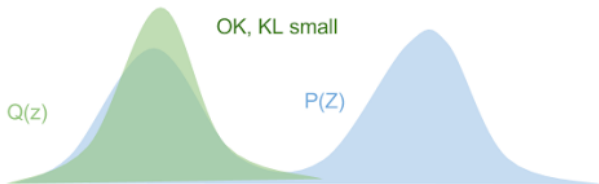
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Evidence lower bound (ELBO)

Define the joint likelihood with $\mathcal{S} = (\mathcal{S}_1, \dots, \mathcal{S}_n)$:

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Then we have :

$$\log p(\mathcal{S}) = \text{KL}(q \parallel \pi_n) + \underbrace{\mathbb{E}_{\theta \sim q} \left[\log \left(\frac{p(\mathcal{S}, \theta)}{q(\theta)} \right) \right]}_{\text{ELBO}(q)}$$

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We always have $\text{ELBO}(q) \leq \log p(\mathcal{S})$ (hence the name).

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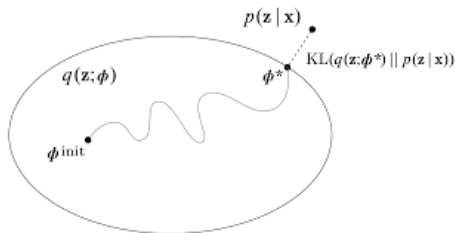
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This is a very simple and powerful approach that applies to many models and scales to large data, but... how about the derivation of the gradients?

Let us recall the expression of the ELBO :

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- Black-Box Variational Inference.
- The Reparameterization Trick.

Black-Box Variational Inference

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- First rewrite the gradient of that objective as the expectation of an easy-to-implement function of θ and \mathcal{S} , where the expectation is taken with respect to q_λ .

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- Then optimize that objective by sampling from q_λ , evaluate the function, and form the corresponding Monte Carlo estimate of the gradient.
- Finally use these stochastic gradients in a stochastic optimization algorithm to update λ .

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$$\begin{aligned}\nabla_\lambda \text{ELBO}(q_\lambda) &= \nabla_\lambda \int g_{\mathcal{S}}(\lambda, \theta) q_\lambda(\theta) d\theta \\ &= \int \{ \nabla_\lambda g_{\mathcal{S}}(\lambda, \theta) q_\lambda(\theta) + g_{\mathcal{S}}(\lambda, \theta) \nabla_\lambda q_\lambda(\theta) \} d\theta \\ &= \int \{ \nabla_\lambda g_{\mathcal{S}}(\lambda, \theta) q_\lambda(\theta) + g_{\mathcal{S}}(\lambda, \theta) \nabla_\lambda \log q_\lambda(\theta) q_\lambda(\theta) \} d\theta \\ &= \mathbb{E}_{\theta \sim q_\lambda} [\nabla_\lambda g_{\mathcal{S}}(\lambda, \theta) + g_{\mathcal{S}}(\lambda, \theta) \nabla_\lambda \log q_\lambda(\theta)].\end{aligned}$$

REINFORCE Gradients (cont.)

$$g_{\mathcal{S}}(\lambda, \theta) = \log p(\mathcal{S}, \theta) - \log q_{\lambda}(\theta).$$

$$\nabla_{\lambda} \text{ELBO}(q_{\lambda}) = \mathbb{E}_{\theta \sim q_{\lambda}} [\nabla_{\lambda} g_{\mathcal{S}}(\lambda, \theta) + g_{\mathcal{S}}(\lambda, \theta) \nabla_{\lambda} \log q_{\lambda}(\theta)].$$

REINFORCE Gradients (cont.)

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Let's compute the first term of the gradient :

$$\begin{aligned}\mathbb{E}_{\theta \sim q_\lambda} [\nabla_\lambda g_S(\lambda, \theta)] &= -\mathbb{E}_{\theta \sim q_\lambda} [\nabla_\lambda \log q_\lambda(\theta)] \\ &= -\int \nabla_\lambda \log q_\lambda(\theta) q_\lambda(\theta) d\theta \\ &= -\int \nabla_\lambda q_\lambda(\theta) d\theta \\ &= -\nabla_\lambda \int q_\lambda(\theta) d\theta = -\nabla_\lambda 1 = 0.\end{aligned}$$

Final value of the gradient $\nabla_{\lambda} \text{ELBO}(q_{\lambda})$:

$$\mathbb{E}_{\theta \sim q_{\lambda}}[\{\log p(\mathcal{S}, \theta) - \log q_{\lambda}(\theta)\} \nabla_{\lambda} \log q_{\lambda}(\theta)]$$

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To compute the noisy gradient of the ELBO we need :

- Sampling from q_{λ} .
- Evaluating $\nabla_{\lambda} \log q_{\lambda}$.
- Evaluating $\log q_{\lambda}$ and $\log p(\mathcal{S}, \theta)$.

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To compute the noisy gradient of the ELBO we need :

- Sampling from q_{λ} .
- Evaluating $\nabla_{\lambda} \log q_{\lambda}$.
- Evaluating $\log q_{\lambda}$ and $\log p(\mathcal{S}, \theta)$.

The method is not model-specific : black-box criteria are satisfied.

Algorithm 1 Black Box Variational Inference

Input: data x , joint distribution p , mean field variational family q .

Initialize $\lambda_{1:n}$ randomly, $t = 1$.

repeat

 // Draw S samples from q

for $s = 1$ **to** S **do**

$z[s] \sim q$

end for

$\rho = t$ th value of a Robbins Monro sequence (Eq. 2)

$\lambda = \lambda + \rho \frac{1}{S} \sum_{s=1}^S \nabla_{\lambda} \log q(z[s]|\lambda) (\log p(x, z[s]) - \log q(z[s]|\lambda))$

$t = t + 1$

until change of λ is less than 0.01.

Problem : BBVI has a large variance...

Can be fixed using Rao-Blackwellization and/or Control Variates.

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Algorithm 2 Black Box Variational Inference (II)

Input: data x , joint distribution p , mean field variational family q .

Initialize $\lambda_{1:m}$ randomly, $t = 1$.

repeat

 // Draw S samples from the variational approximation

for $s = 1$ to S **do**

$z[s] \sim q$

end for

for $i = 1$ to n **do**

for $s = 1$ to S **do**

$f_i[s] = \nabla_{\lambda_i} \log q_i(z[s]|\lambda_i)(\log p_i(x, z[s]) - \log q_i(z[s]|\lambda_i))$

$h_i[s] = \nabla_{\lambda_i} \log q_i(z[s]|\lambda_i)$

end for

$\hat{a}_i^* = \frac{\sum_{d=1}^{n_i} \text{Cov}(f_i^d, h_i^d)}{\sum_{d=1}^{n_i} \text{Var}(h_i^d)}$

$\hat{\nabla}_{\lambda_i} \mathcal{L} \triangleq \frac{1}{S} \sum_{s=1}^S f_i[s] - \hat{a}_i^* h_i[s]$

end for

$\rho = t$ th value of a Robbins Monro sequence

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Example :

$$\varepsilon \sim \mathcal{N}(0, 1),$$

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$$\theta \sim \mathcal{N}(\mu, \sigma).$$

The idea of the reparameterization trick is to write the expectation with respect to ν (which does not depend on λ) and then pull the gradient inside the expectation.

The reparameterization trick (cont.)

$$g_{\mathcal{S}}(\lambda, \theta) = \log p(\mathcal{S}, \theta) - \log q_{\lambda}(\theta).$$

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$$\begin{aligned}\nabla_{\lambda} \text{ELBO}(q_{\lambda}) &= \nabla_{\lambda} \mathbb{E}_{\theta \sim q_{\lambda}}[g_{\mathcal{S}}(\lambda, \theta)] \\ &= \nabla_{\lambda} \mathbb{E}_{\varepsilon \sim \nu}[g_{\mathcal{S}}(\lambda, t_{\lambda}(\varepsilon))] \\ &= \mathbb{E}_{\varepsilon \sim \nu}[\nabla_{\lambda} \{g_{\mathcal{S}}(\lambda, t_{\lambda}(\varepsilon))\}] \\ &= \mathbb{E}_{\varepsilon \sim \nu}[\nabla_{\lambda} t_{\lambda}(\varepsilon)^T \nabla_{\theta} g_{\mathcal{S}}(\lambda, t_{\lambda}(\varepsilon)) + \nabla_{\lambda} g_{\mathcal{S}}(\lambda, t_{\lambda}(\varepsilon))] \\ &= \mathbb{E}_{\varepsilon \sim \nu}[\nabla_{\lambda} t_{\lambda}(\varepsilon)^T \nabla_{\theta} \{\log p(\mathcal{S}, t_{\lambda}(\varepsilon)) - \log q_{\lambda}(t_{\lambda}(\varepsilon))\} \\ &\quad - \underbrace{\nabla_{\lambda} \log q_{\lambda}(t_{\lambda}(\varepsilon))}_{\nu(\varepsilon)}] \end{aligned}$$

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and the gradient $\nabla_{\lambda} \text{ELBO}(q_{\lambda})$ is :

$$\mathbb{E}_{\varepsilon \sim \nu}[\nabla_{\lambda} t_{\lambda}(\varepsilon)^T \nabla_{\theta} \{\log p(\mathcal{S}, t_{\lambda}(\varepsilon)) - \log q_{\lambda}(t_{\lambda}(\varepsilon))\}].$$

REINFORCE vs Reparameterization Trick

$$\mathbb{E}_{\theta \sim q_\lambda} [\{\log p(\mathcal{S}, \theta) - \log q_\lambda(\theta)\} \nabla_\lambda \log q_\lambda(\theta)]$$

- Differentiates the density $q_\lambda(\theta)$.
- Works for both discrete and continuous models.
- Works for a large class of variational families.
- But the variance can be a big problem.

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- Works for both discrete and continuous models.
- Works for a large class of variational families.
- But the variance can be a big problem.

$$\mathbb{E}_{\varepsilon \sim \nu} [\nabla_\lambda t_\lambda(\varepsilon)^T \nabla_\theta \{\log p(\mathcal{S}, t_\lambda(\varepsilon)) - \log q_\lambda(t_\lambda(\varepsilon))\}]$$

- Differentiates the densities $p(\mathcal{S}, \theta)$, $q_\lambda(\theta)$.
- Works for differentiable models only.
- Works for reparameterized variational families only.
- But the variance behaves much better.

Natural Gradient Variational Inference

SGD and Information Geometry

The standard SGD algorithm

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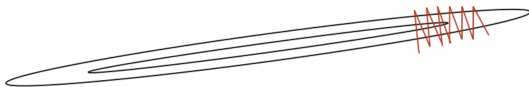
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- Is there a 'good' **parameterization** ?
- Is there a 'good' **distance** ?

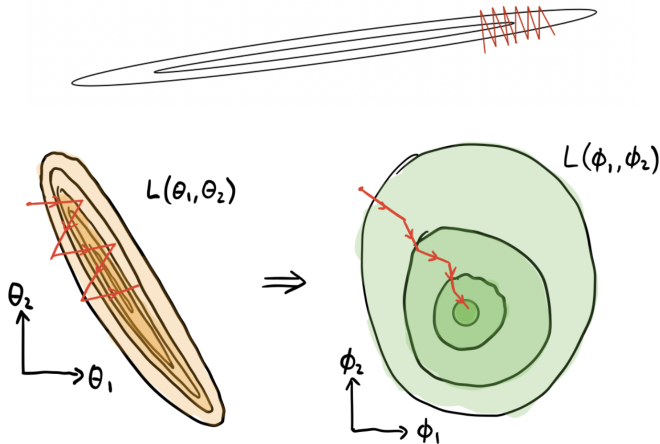
Which choice of the parameterization in SGD?

SGD bounces around in high curvature directions and makes slow progress in low curvature directions.



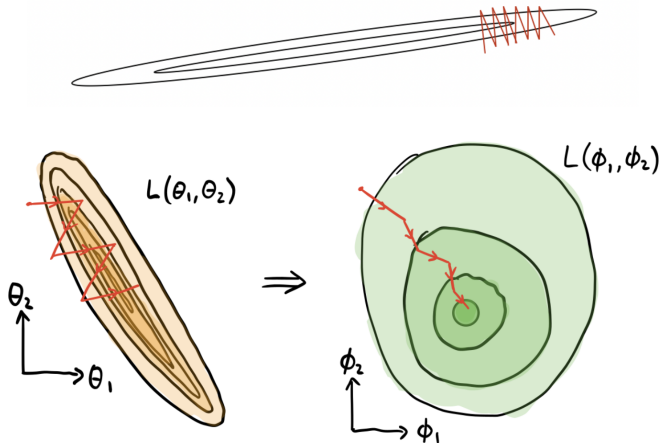
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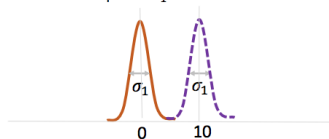
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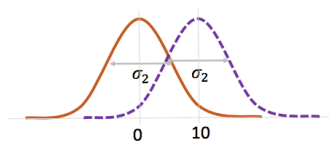
Toward a 'parameterization-invariant' parameterization in SGD?

Is the Euclidean distance a good one?

Two Gaussians with mean 1 and 10 respectively
and variances equal to σ_1 have Euclidean distance = 10



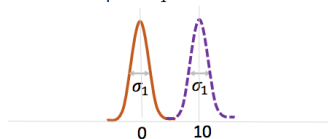
Same as the top row but with the variance $\sigma_2 > \sigma_1$
but still Euclidean distance = 10



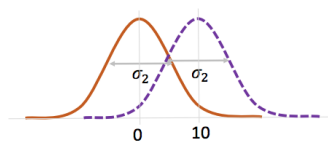
(a) Gradient-based methods use the Euclidean distance which is a poor metric to measure distance between distributions. The bottom two distributions are almost identical while the top ones barely overlap, yet Euclidean distance is the same.

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Toward a 'distance' between probability distributions?

Probability distributions & Information Geometry

'Shortest path' between two probability distributions?



Mapping a manifold to a flat coordinate system distorts distances !

Exponential families

We define the exponential family of sufficient statistic T , natural parameter λ , carrier measure h and log-partition function A :

$$q_{\lambda}(\theta) = h(\theta) \exp \left(\lambda^T T(\theta) - A(\lambda) \right).$$

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Example of Gaussian distributions :

$$T(\theta) = [\theta, \theta^2]^T$$

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Why exponential families ? Because the 'natural parameterization' addresses both questions by defining a manifold !

The exponential family & Information Geometry

The exponential family induces a Riemannian manifold with a metric defined by the Fisher Information Matrix :

$$\|\lambda - \lambda_t\|_{F(\lambda_t)}^2 = (\lambda - \lambda_t)^T F(\lambda_t) (\lambda - \lambda_t)$$

where $F(\lambda) = \mathbb{E}_{\theta \sim q_\lambda} [\nabla_\lambda \log q_\lambda(\theta) \nabla_\lambda \log q_\lambda(\theta)^T]$.



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The Fisher metric approximates the KL divergence :

$$\text{KL}(q_\lambda \| q_{\lambda_t}) = (\lambda - \lambda_t)^T F(\lambda_t) (\lambda - \lambda_t) + \mathcal{O}((\lambda - \lambda_t)^3).$$

Natural parameters & Information Geometry

We use the natural parameterization and replace the Euclidean distance by the Riemannian metric :

$$\lambda_{t+1} = \arg \max_{\lambda} \left\{ \lambda^T \hat{\nabla}_{\lambda} \text{ELBO}(q_{\lambda_t}) - \frac{\|\lambda - \lambda_t\|_{\hat{F}(\lambda_t)}^2}{2\eta} \right\},$$

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$$\lambda_{t+1} = \lambda_t + \eta \underbrace{F(\lambda_t)^{-1} \hat{\nabla}_{\lambda} \text{ELBO}(q_{\lambda_t})}_{\tilde{\nabla}_{\lambda} \text{ELBO}(q_{\lambda_t})}.$$

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Therefore, steepest descent in the Fisher metric (which approximates KL divergence) is invariant to parameterization, to the first order (hence the name "natural gradient").

But the computation of the natural gradient $\tilde{\nabla}_{\lambda} \text{ELBO}(q_{\lambda_t})$ can be really cumbersome due to $F(\lambda_t)^{-1} \dots$

Use the Mean Parameterization !

There is a one-to-one mapping between the natural parameterization and the mean parameterization :

$$\mu(\lambda) = \mathbb{E}_{\theta \sim q_\lambda} [T(\theta)].$$

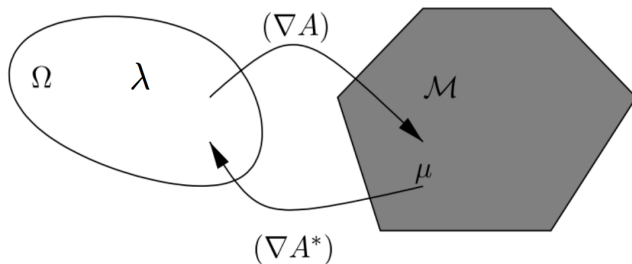
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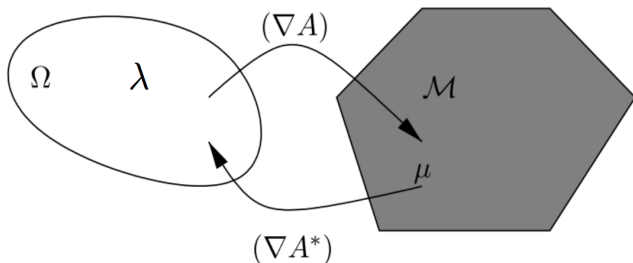


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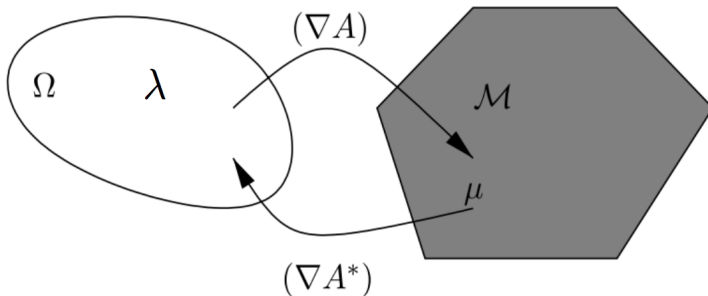
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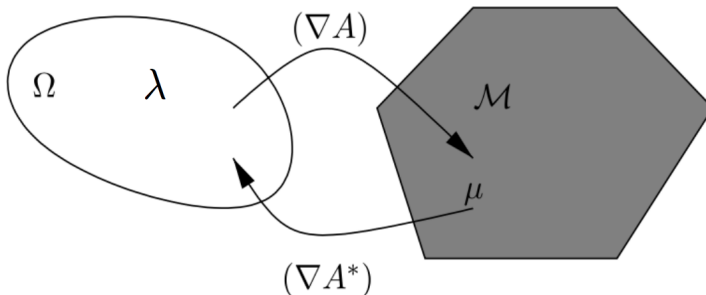
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Final learning rule

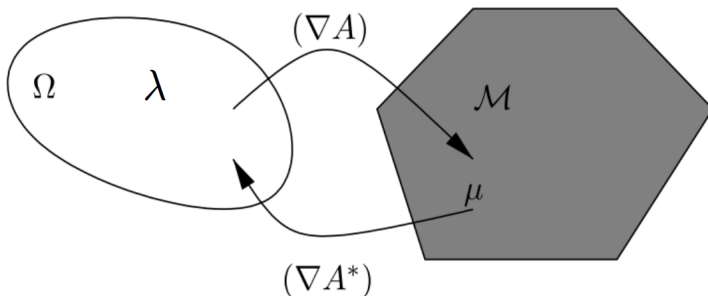


Final learning rule



Learning algorithm :

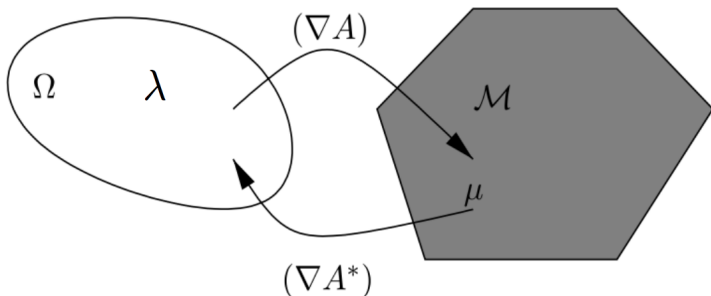
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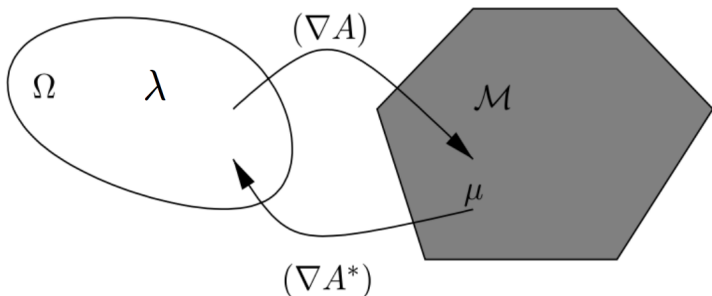
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The Gaussian example

For a Gaussian approximation $\mathcal{N}(m, \text{diag}(\sigma^2))$,

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Question : how about the derivation of the gradients ?

$$\text{ELBO}(q_\lambda) = \mathbb{E}_{\theta \sim q_\lambda}[g_S(\lambda, \theta)]$$

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Bonnet's and Price's formula :

$$\nabla_m \mathbb{E}_{\theta \sim q_\lambda}[g_S(\lambda, \theta)] = \mathbb{E}_{\theta \sim q_\lambda}[\nabla_\theta g_S(\lambda, \theta)],$$

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Or using the reparameterization trick :

$$\begin{aligned}\nabla_{\sigma^2} \mathbb{E}_{\theta \sim q_\lambda}[g_S(\lambda, \theta)] &= \nabla_{\sigma^2} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, I)}[g_S(\lambda, m + \sigma \varepsilon)] \\ &= \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, I)}[\nabla_{\sigma^2} g_S(\lambda, m + \sigma \varepsilon)] \\ &= \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, I)}[\nabla_\theta g_S(\lambda, m + \sigma \varepsilon) \varepsilon / 2\sigma].\end{aligned}$$

Adam-like algorithm

Adam

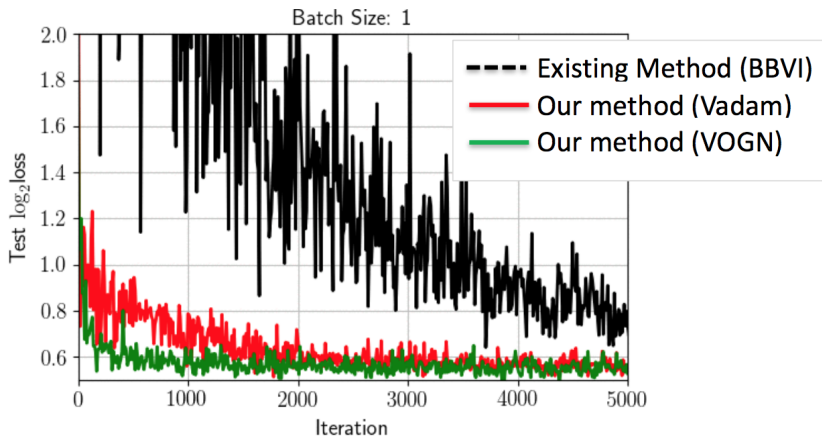
```
1: while not converged do
2:    $\theta \leftarrow \mu$ 
3:   Randomly sample a data example  $\mathcal{D}_i$ 
4:    $\mathbf{g} \leftarrow -\nabla \log p(\mathcal{D}_i | \theta)$ 
5:    $\mathbf{m} \leftarrow \gamma_1 \mathbf{m} + (1 - \gamma_1) \mathbf{g}$ 
6:    $\mathbf{s} \leftarrow \gamma_2 \mathbf{s} + (1 - \gamma_2) (\mathbf{g} \circ \mathbf{g})$ 
7:    $\hat{\mathbf{m}} \leftarrow \mathbf{m} / (1 - \gamma_1^t)$ ,  $\hat{\mathbf{s}} \leftarrow \mathbf{s} / (1 - \gamma_2^t)$ 
8:    $\mu \leftarrow \mu - \alpha \hat{\mathbf{m}} / (\sqrt{\hat{\mathbf{s}}} + \delta)$ 
9:    $t \leftarrow t + 1$ 
10: end while
```

Vadam

```
1: while not converged do
2:    $\theta \leftarrow \mu + \sigma \circ \epsilon$ , where  $\epsilon \sim \mathcal{N}(0, \mathbf{I})$ ,  $\sigma \leftarrow 1 / \sqrt{N\mathbf{s} + \lambda}$ 
3:   Randomly sample a data example  $\mathcal{D}_i$ 
4:    $\mathbf{g} \leftarrow -\nabla \log p(\mathcal{D}_i | \theta)$ 
5:    $\mathbf{m} \leftarrow \gamma_1 \mathbf{m} + (1 - \gamma_1) (\mathbf{g} + \lambda \mu / N)$ 
6:    $\mathbf{s} \leftarrow \gamma_2 \mathbf{s} + (1 - \gamma_2) (\mathbf{g} \circ \mathbf{g})$ 
7:    $\hat{\mathbf{m}} \leftarrow \mathbf{m} / (1 - \gamma_1^t)$ ,  $\hat{\mathbf{s}} \leftarrow \mathbf{s} / (1 - \gamma_2^t)$ 
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```

Figure 1. Comparison of Adam (left) and one of our proposed method Vadam (right). Adam performs maximum-likelihood estimation while Vadam performs variational inference, yet the two pseudocodes differ only slightly (differences highlighted in red). A major difference is in line 2 where, in Vadam, weights are perturbed during the gradient evaluations.

Fast Convergence



Performance

Table 1. Performance comparisons for BNN regression. The better method out of BBVI and Vadam is shown in boldface according to a paired t-test with p -value > 0.01 . Both methods perform comparably but MC-Dropout outperforms them.

Dataset	N	D	Test RMSE			Test log-likelihood		
			MC-Dropout	BBVI	Vadam	MC-Dropout	BBVI	Vadam
Boston	506	13	2.97 ± 0.19	3.58 ± 0.21	3.93 ± 0.26	-2.46 ± 0.06	-2.73 ± 0.05	-2.85 ± 0.07
Concrete	1030	8	5.23 ± 0.12	6.14 ± 0.13	6.85 ± 0.09	-3.04 ± 0.02	-3.24 ± 0.02	-3.39 ± 0.02
Energy	768	8	1.66 ± 0.04	2.79 ± 0.06	1.55 ± 0.08	-1.99 ± 0.02	-2.47 ± 0.02	-2.15 ± 0.07
Kin8nm	8192	8	0.10 ± 0.00	0.09 ± 0.00	0.10 ± 0.00	0.95 ± 0.01	0.95 ± 0.01	0.76 ± 0.00
Naval	11934	16	0.01 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	3.80 ± 0.01	4.46 ± 0.03	4.72 ± 0.22
Power	9568	4	4.02 ± 0.04	4.31 ± 0.03	4.28 ± 0.03	-2.80 ± 0.01	-2.88 ± 0.01	-2.88 ± 0.01
Wine	1599	11	0.62 ± 0.01	0.65 ± 0.01	0.66 ± 0.01	-0.93 ± 0.01	-1.00 ± 0.01	-1.01 ± 0.01
Yacht	308	6	1.11 ± 0.09	2.05 ± 0.06	1.32 ± 0.10	-1.55 ± 0.03	-2.41 ± 0.02	-1.70 ± 0.03

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- It is possible to use SGD to perform (approximate) Bayesian inference.
- The major difficulty is to compute the gradients.
- There exists many ways to deal with this derivation (e.g. REINFORCE & reparameterization trick).
- Convergence can be accelerated using the natural gradient.

Next lecture

We'll focus on 3 different topics :

- Learning Latent Variable Models.
- Theory of Variational Inference.
- Bayesian Model Averaging in Deep Learning.