University of BRISTOL

Massively Parallel Bayesian Inference

Importance weighting and more...

Sam Bowyer

Mini-Project Presentation

Supervisor: Laurence Aitchison

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Bayesian Inference

Bayesian inference relies on computing a posterior distribution,

$$P(z'|x) = \frac{P(x|z')P(z')}{\int_{\mathcal{Z}} P(x, z'')dz''} \tag{1}$$

given a prior $P(z')$ over latent variables $z' \in \mathcal{Z}$ and a likelihood $P(x|z')$ for data x.

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given a prior $P(z')$ over latent variables $z' \in \mathcal{Z}$ and a likelihood $P(x|z')$ for data x.

Problem: Computation of the normalising constant, (the marginal likelihood)

$$P(x) = \int_{\mathcal{Z}} P(x, z'')dz'', \tag{2}$$

is often intractable (especially if you have a large number of latent variables).

Bayesian Inference

Problem: Computing $P(x) = \int_{\mathcal{Z}} P(x, z'')dz''$.

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(One) solution: Importance Weighting—instead of trying to evaluate $P(x, z'')dz''$ for *every possible* latent setting $z'' \in \mathcal{Z}$, sample $K \in \mathbb{N}$ latent settings $z^1, ..., z^K \in \mathcal{Z}$ and attempt to reason about this collection.

Importance Weighting

In particular, draw K IID samples of your latents from the full joint space, $\mathcal{Z}$,

$$z = (z^1, ..., z^K) \in \mathcal{Z}^K, \tag{3}$$

$$z^k \in \mathcal{Z}, \ \ \forall k \in \mathcal{K} := \{1, \ldots, K\}, \tag{4}$$

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via some proposal distribution Q,

$$Q(z) = \prod_{k \in \mathcal{K}} Q(z^k). \tag{5}$$

(We can choose Q to be easy to sample from and have generally 'nice' qualities.)

Importance Weighting

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$$\mathcal{P}_{\text{global}}(z) = \tfrac{1}{K} \sum_{k \in \mathcal{K}} r_k(z). \tag{7}$$

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It is fairly easy to prove that this is unbiased:

$$\mathbb{E}_{Q(z)}[\mathcal{P}_{\text{global}}(z)] = P(x). \tag{8}$$

Importance Weighting: An Issue

Suppose each $z^k \in \mathcal{Z}$ is comprised of n individual latent variables:

$$z^k = (z_1^k, z_2^k, ..., z_n^k) \in \mathcal{Z} \tag{9}$$

(Note: z^k is a tuple, not a vector—each latent variable z_i^k might not be scalar-valued.)

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Massively Parallel Solution: Consider all possible K^n combinations of the latent samples within our collection $z = (z^1, ..., z^K) \in \mathcal{Z}^K$.

The Massively Parallel Framework

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Then we can write a combination of the samples with these indices as

$$z^{\mathbf{k}} = \left(z_1^{k_1}, z_2^{k_2}, \dots, z_n^{k_n}\right) \in \mathcal{Z}. \tag{10}$$

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Previously: we were essentially only using $\mathbf{k} \in \mathcal{K}^n$ where $k_1 = k_2 = \cdots = k_n$.
E.g. for the third sample drawn from Q,

$$z^3 = \left(z_1^3, z_2^3, \ldots, z_n^3\right) \in \mathcal{Z}.$$

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$$z^3 = \left(z_1^3, z_2^3, \dots, z_n^3\right) \in \mathcal{Z}.$$

The difference is that *now*, we don't require $k_1 = k_2 = \cdots = k_n$.

The Massively Parallel Framework

Before: We can index $|\mathcal{K}| = K$ samples.

$$k \in \mathcal{K}$$
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Now: We can index $|\mathcal{K}^n| = K^n$ samples.

$$\mathbf{k} = (k_1, ..., k_n) \in \mathcal{K}^n$$

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One choice is to have a graphical structure:

$$Q_{\text{MP}}(z) = \prod_{i=1}^{n} Q_{\text{MP}}\left(z_i | z_j \ \forall j \in \text{qa}(i)\right), \tag{11}$$

where $\text{qa}(i)$ is the set of indices of parents of z_i under the proposal's graphical model.

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where $\text{qa}(i)$ is the set of indices of parents of z_i under the proposal's graphical model. So the value of the ith latent variable depends only on the value of its parents.

(But *which* parents? We have K sets of parent samples to choose from...
Easy answer: for the kth child, only use the kth parents.)

The Massively Parallel Framework

Similarly, we work with a graphical structure on the generative distribution:

$$P(x, z^{\mathbf{k}}) = P\left(x | z_j^{k_j} \ \forall j \in \mathsf{pa}(x)\right) \prod_{i=1}^{n} P\left(z_i^{k_i} | z_j^{k_j} \ \forall j \in \mathsf{pa}(i)\right) \tag{12}$$

where $\mathsf{pa}(i)$ is the set of indices of parents of z_i under the generative graphical model (and $\mathsf{pa}(x)$ is the set of indices of parents for x)..

Massively Parallel Importance Weighting

Now we can define a new, *massively parallel* marginal likelihood estimator $\mathcal{P}_{\text{MP}}$,

$$\mathcal{P}_{\text{MP}}(z) = \tfrac{1}{K^n} \sum_{\mathbf{k} \in \mathcal{K}^n} r_{\mathbf{k}}(z) \tag{13}$$

$$r_{\mathbf{k}}(z) = \frac{P(x, z^{\mathbf{k}})}{\prod_{i=1}^{n} Q_{\text{MP}}(z_i^k | z_j^k \text{ for } j \in \text{qa}(i))}. \tag{14}$$

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This is also an unbiased marginal likelihood estimator [Heap and Aitchison, 2023]:

$$\mathbb{E}_{Q_{\text{MP}}}(z)[\mathcal{P}_{\text{MP}}(z)] = P(x). \tag{15}$$

What makes this 'massively parallel'?

Problem: We've got a sum over K^n terms. How do we compute this?

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Solution:

1. Write $r_{\mathbf{k}}(z)$ as a big tensor product [Aitchison, 2019, Heap and Aitchison, 2023]:

$$r_{\mathbf{k}}(z) = f^x_{\mathbf{k}_{\text{pa}(x)}}(z) \prod_i f^i_{k_i, \mathbf{k}_{\text{pa}(i)}}(z) \tag{17}$$

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2. Use efficient tensor-product implementations (e.g. opt-einsum [a. Smith and Gray, 2018]) which can be performed in parallel on GPUs.

Other Massively Parallel Applications

- Posterior moment estimation

$$m_{\mathsf{MP}}(z) = \tfrac{1}{K^n} \sum_{\mathbf{k} \in \mathcal{K}^n} \frac{r_{\mathbf{k}}(z)}{\mathcal{P}_{\mathsf{MP}}(z)} m(z^{\mathbf{k}}). \tag{18}$$

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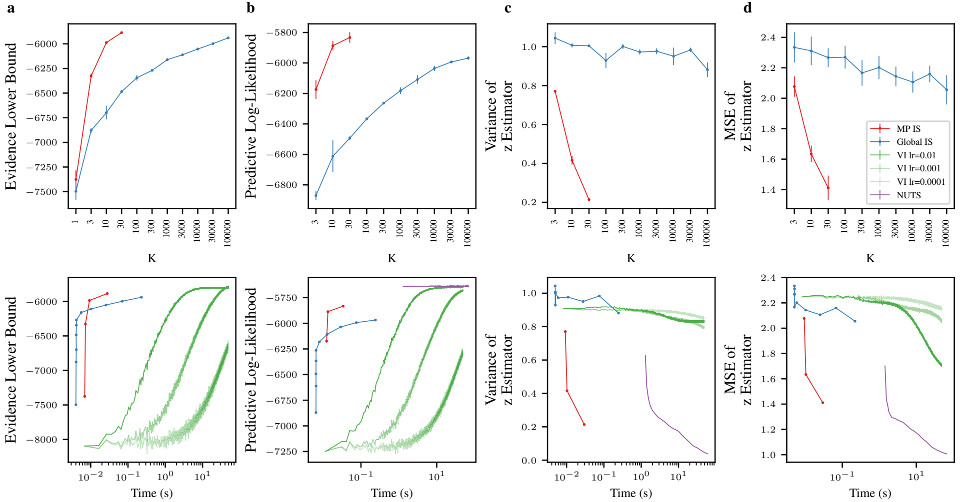
- Importance sampling

$$m_{\text{MP}}(z) = \sum_{\mathbf{k}\in\mathcal{K}} P(\mathbf{k}) m(z^{\mathbf{k}}) \qquad P(\mathbf{k}) = \frac{1}{K_n} \frac{1}{\mathcal{P}_{\text{MP}}(z)} r_{\mathbf{k}}(z). \tag{19}$$

Sampling $\mathbf{k}$ from $P(\mathbf{k})$ will give us $z^{\mathbf{k}}$ that are approximate samples from the true posterior $P(z|x)$.

Performance (on MovieLens 100K Dataset)



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- Future work:

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- Future work:
  - Extend MCMC past $K = 2$.
  - Probabilistic programming language (e.g. Stan [Carpenter et al., 2017]).

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Thank you

Any questions?

Importance Weighting: Two Examples

1. Variational Autoencoders [Kingma and Welling, 2014]
   $\longrightarrow$ Importance Weighted Autoencoders [Burda et al., 2016].
   Update (θ, ϕ) by maximising $\mathcal{L}_{\text{global}}(\theta, \phi)$:

$$\log P_\theta(x) \geq \mathcal{L}_{\text{global}}(\theta, \phi) = \mathbb{E}_{Q(z|x)}[\log \mathcal{P}_{\text{global}}(z)] \tag{20}$$

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2. Wake-Sleep [Hinton et al., 1995]
   $\longrightarrow$ Reweighted Wake-Sleep [Bornschein and Bengio, 2015].
   Update (θ, ϕ) with:

$$\Delta\theta = \mathbb{E}_{Q(z|x)}[\nabla_\theta \log \mathcal{P}_{\text{global}}(z)], \tag{21}$$

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(Recent work [Heap and Aitchison, 2023] has ‘massively parallelised’ IWAE and RWS using the same framework introduced in this talk.)

Exploiting Conditional Independencies

$$\mathcal{P}_{\text{MP}}(z) = \frac{1}{K^n} \sum_{\mathbf{k} \in \mathcal{K}^n} r_{\mathbf{k}}(z) \qquad r_{\mathbf{k}}(z) = \frac{P(x, z^{\mathbf{k}})}{\prod_{i=1}^n Q_{\text{MP}}(z_i^k | z_j^k \text{ for } j \in \text{qa}(i))}. \tag{23}$$

Expressing $r_{\mathbf{k}}(z)$ as a product of many (low-rank) tensors,

$$r_{\mathbf{k}}(z) = f^x_{\mathbf{k}_{\text{pa}(x)}}(z) \prod_i f^i_{k_i, \mathbf{k}_{\text{pa}(i)}}(z) \tag{24}$$

$$f^x_{\mathbf{k}_{\text{pa}x}}(z) = P(x | z_j^{k_j} \text{ for all } j \in \text{pa}(x)), \tag{25}$$

$$f^i_{k_i, \mathbf{k}_{\text{pa}(i)}}(z) = \frac{P(z_i^{k_i} | z_j^{k_j} \text{ for all } j \in \text{pa}(i))}{Q_{\text{MP}}(z_i^{k_i} | z_j \text{ for all } j \in \text{qa}(i))}. \tag{26}$$

- $f^x_{\mathbf{k}_{\text{pa}(x)}}(z)$ is a tensor of rank $|\text{pa}(x)|$
- $f^i_{k_i, \mathbf{k}_{\text{pa}(i)}}(z)$ are tensors of rank $1 + |\text{pa}(i)|$

Modified Marginal Likelihood Estimator

We can calculate posterior moments nicely by differentiating through a modified version of our marginal liklihood estimator. Specifically, we introduce a 'source term' $e^{Jm(z^{\mathbf{k}})}$ for $J \in \mathbb{R}$:

$$\mathcal{P}_{\mathsf{MP}}^{\mathsf{exp}}(z, J) = \tfrac{1}{K^n} \sum_{\mathbf{k} \in \mathcal{K}^n} r_{\mathbf{k}}(z) e^{Jm(z^{\mathbf{k}})}. \tag{27}$$

Note that $\mathcal{P}_{\mathsf{MP}}^{\mathsf{exp}}(z, J = 0) = \mathcal{P}_{\mathsf{MP}}(z)$, and also that the source term, like the factors that make up $r_{\mathbf{k}}(z)$, can be thought of as a tensor indexed by some subset of $\mathbf{k}$ (depending on m), hence efficient computation of this sum is still possible.

$$\frac{\partial}{\partial J}\bigg|_{J=0} \log \mathcal{P}_{\mathsf{MP}}^{\mathsf{exp}}(z, J) = \frac{\frac{\partial}{\partial J}\big|_{J=0} \mathcal{P}_{\mathsf{MP}}^{\mathsf{exp}}(z, J)}{\mathcal{P}_{\mathsf{MP}}(z)} = \frac{\frac{1}{K^n} \sum_{\mathbf{k} \in \mathcal{K}^n} r_{\mathbf{k}}(z) m(z^{\mathbf{k}})}{\mathcal{P}_{\mathsf{MP}}(z)} = m_{\mathsf{MP}}(z). \tag{28}$$