Robust Optimisation Monte Carlo

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Reference

Borislav Ikonomov and Michael U. Gutmann
Robust Optimisation Monte Carlo
arXiv:1904.00670, 2019

Main messages

1. Optimisation Monte Carlo (OMC) is an existing method[1] that efficiently performs Bayesian inference with implicit models.
2. While efficient OMC under-estimates uncertainty by collapsing regions of near-constant likelihood into a single point.
3. A robust generalisation, robust OMC, explains and corrects this failure mode while maintaining OMC's benefits.

[1] Meeds and Welling, NIPS 2015.

Contents

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Overall topic of the talk

- Bayesian parameter inference for implicit models where
  1. the likelihood function is too costly to evaluate
  2. exact sampling – simulating data from the model – is possible

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  1. the likelihood function is too costly to evaluate
  2. exact sampling – simulating data from the model – is possible
- Importance: such models and inference problems occur widely (evolutionary biology, neurosciences, health sciences, robotics, computer vision, machine learning, ...)

Implicit models

(Diggle and Gratton, JRSS, 1982)

- Parametric statistical models specified by a data generating mechanism $g : (\boldsymbol{\theta}, \mathbf{u}) \mapsto \mathbf{x} = g(\boldsymbol{\theta}, \mathbf{u})$
  - $\boldsymbol{\theta}$: parameters of interest
  - $\mathbf{u}$: nuisance parameters with distribution $p(\mathbf{u})$
  - $\mathbf{x}$: generated data
- The (deterministic) function $g(\boldsymbol{\theta}, \mathbf{u})$ is generally not known in closed form but implemented as computer code
  - $\boldsymbol{\theta}$: input parameters
  - $\mathbf{u}$: random draws performed when running the code / seed of the random number generator used
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- Other names: Simulator-based models, stochastic simulation models, generative (latent-variable) models, ...

Bayesian inference for implicit models

- Task: Given
  - observed data $\mathbf{x}_o$,
  - an implicit model $g(\boldsymbol{\theta}, \mathbf{u})$, and
  - a prior distribution on $\boldsymbol{\theta}$,

  estimate the posterior $p(\boldsymbol{\theta}|\mathbf{x}_o)$ / obtain approximate samples from it.

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  $\rightarrow$ likelihood function $L(\boldsymbol{\theta}) = p(\mathbf{x}_o|\boldsymbol{\theta})$ is intractable
  $\rightarrow$ Bayesian inference is difficult

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- Drawing samples $\mathbf{x}_i \sim p(\mathbf{x}|\boldsymbol{\theta})$ is possible for implicit models
  $\rightarrow$ we can exploit this to perform Bayesian inference

Bayesian inference for implicit models

- Research fields: approximate Bayesian computation (ABC), likelihood-free inference, Bayesian indirect inference

  (overviews: Sisson et al 2018, Lintusaari et al 2017, Gutmann and Corander 2016, Drovandi 2015, Marin et al 2012)

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- ABC builds on the fact that samples from the posterior are given by samples from the prior for which simulated data $\mathbf{x}$ are close to the observed data $\mathbf{x}_o$.

- Two core ingredients of ABC algorithms:
  1. a distance function $d(\mathbf{x}, \mathbf{x}_o)$ between $\mathbf{x}$ and $\mathbf{x}_o$
  2. a search method to efficiently find such samples from the prior

Optimisation Monte Carlo (Meeds and Welling, NIPS 2015)

- Ingredients:
  - Distance $d(\mathbf{x}, \mathbf{x}_o) = ||\Phi(\mathbf{x}) - \Phi(\mathbf{x}_o)||_2$ with known Φ.
  - Search uses optimisation, which leads to increased efficiency.

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- Assumptions:
  - (approximate) derivative of $\Phi(\mathbf{x}) = \Phi(g(\boldsymbol{\theta}, \mathbf{u})) = \mathbf{f}(\boldsymbol{\theta}, \mathbf{u})$ wrt $\boldsymbol{\theta}$ is available
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  - $\dim(\boldsymbol{\theta}) \leq \dim(\Phi(\mathbf{x}))$
- Algorithm to generate n weighted samples $\boldsymbol{\theta}_i^*$:

1: **for** $i \leftarrow 1$ to n **do** ▷ Can be fully parallelised
2: $\mathbf{u}_i \sim p(\mathbf{u})$ ▷ Set seed
3: $\boldsymbol{\theta}_i^* = \arg\min_{\boldsymbol{\theta}} ||\mathbf{f}(\boldsymbol{\theta}, \mathbf{u}_i) - \Phi(\mathbf{x}_o)||$ ▷ Optimisation
4: Compute $\mathbf{J}_i$ with columns $\partial \mathbf{f}(\boldsymbol{\theta}_i^*, \mathbf{u}_i)/\partial\theta_k$
5: Compute $w_i = p(\boldsymbol{\theta}_i^*) * (\det(\mathbf{J}_i^\top \mathbf{J}_i))^{-1/2}$
6: Accept $\boldsymbol{\theta}_i^*$ as posterior sample with weight w_i

(Note that samples with too large final distances may be omitted.)

Contents

Application: Vision as inverse graphics

- Implicit model given by a graphics renderer
- We used Open Differential Renderer (Loper and Black, 2014)

20 parameters:
- Shape
- Rotation/Pose
- Illumination
- Colour

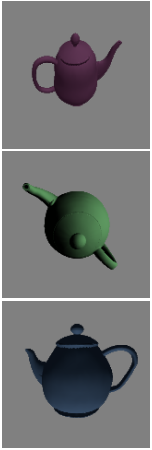
Renderer

(forward problem)

$\rightleftharpoons$

Inference

(inverse problem)



Why Bayesian inference and not point-estimation?

- In some cases, quantifying uncertainty is very important
- The inverse problem may have multiple solutions (posterior may be multi-modal)

  Example considered: Infer object colour when external lighting conditions are unknown.

(a) Gray teapot under red light.

(b) Red teapot under white light.

Results for colour inference task

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- Same distance function $d(\mathbf{x}, \mathbf{x}_o) = ||\Phi(\mathbf{x}) - \Phi(\mathbf{x}_o)||_2$.
- Summary statistics Φ: parameters $\hat{\theta}$ predicted by a neural network trained on images from the renderer with white light.

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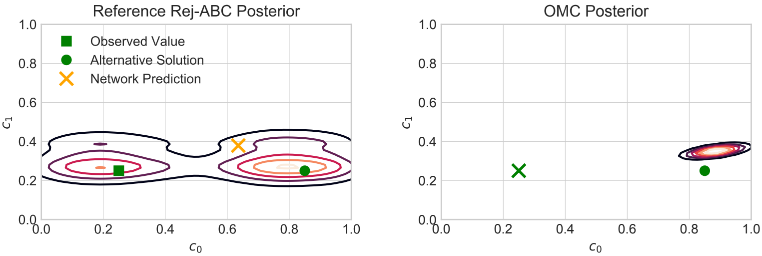
- Summary statistics Φ: parameters $\hat{\theta}$ predicted by a neural network trained on images from the renderer with white light.
- Marginal joint posteriors for colours red (c_0) and green (c_1):



Why did OMC fail?

- The OMC weights $w_i = p(\boldsymbol{\theta}_i^*) * (\det(\mathbf{J}_i^\top \mathbf{J}_i))^{-1/2}$ are unstable (ESS was 1.2!)
- $\det(\mathbf{J}_i^\top \mathbf{J}_i) \approx 0$ when the (approximate) likelihood function has nearly flat regions.

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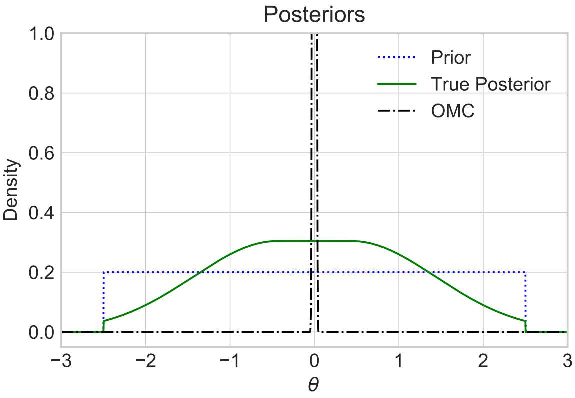

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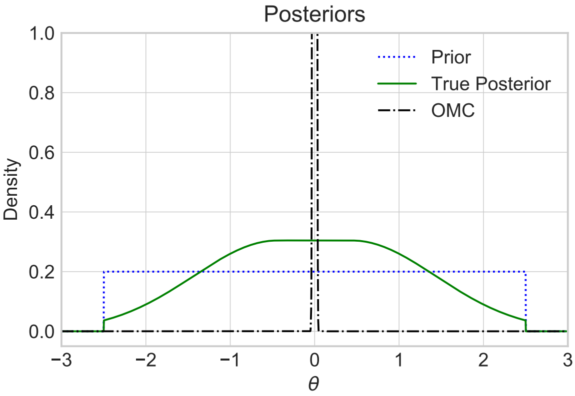
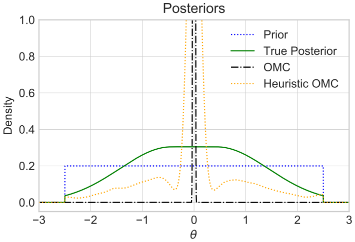
  Note: stated OMC assumptions are not violated.

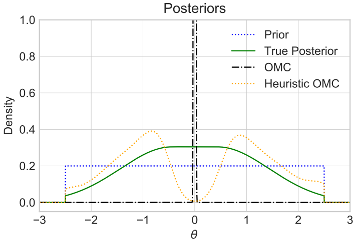


Stabilising the weights/matrices does not help

- Taking the pseudo-inverse or pseudo-determinant of $\mathbf{J}_i^\top \mathbf{J}_i$ does not help.



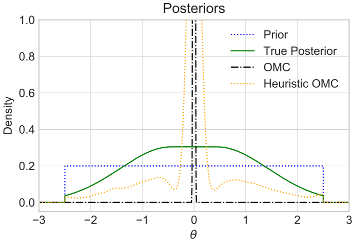
(a) Pseudo-inverse



(b) Pseudo-determinant

Stabilising the weights/matrices does not help

- Taking the pseudo-inverse or pseudo-determinant of $\mathbf{J}_i^\top \mathbf{J}_i$ does not help.
- The weights are not the real issue. The problem is more fundamental:
  OMC uses a single point to represent an entire region where the likelihood is (nearly) constant.



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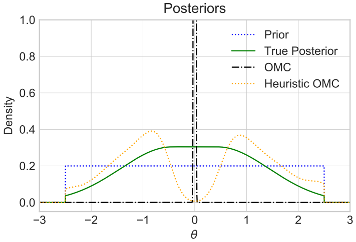

(b) Pseudo-determinant

Contents

Key properties of ROMC

(Ikonomov and Gutmann, *arXiv:1904.00670*, 2019)

1. Fixes OMC's failure case: It handles likelihood functions that are (nearly) flat on significant regions in parameter space.
2. Works for general distance functions $d(g(\boldsymbol{\theta}, \mathbf{u}), \mathbf{x}_o)$ and not only Euclidean distances between summary statistics.
   (condition $\dim(\boldsymbol{\theta}) \leq \dim(\Phi(\mathbf{x}))$ disappears)
3. Does not require (approximate) derivatives, while OMC does.
4. Can be run as post-processing to OMC or from scratch.

The ROMC framework

ROMC is a framework for inference. It has three key steps:

1. Same as OMC but with general distances $d(\mathbf{x}, \mathbf{x}_o)$:

$$\mathbf{u}_i \sim p(\mathbf{u}), \qquad \boldsymbol{\theta}_i^* = \arg\min_{\boldsymbol{\theta}} d(g(\boldsymbol{\theta}, \mathbf{u}_i), \mathbf{x}_o) \qquad \text{(i=1, \ldots n')}$$

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3. For each i where $d_i^* \leq \epsilon$, define a proposal distribution q_i on the "acceptance region" $C_\epsilon^i = \{\boldsymbol{\theta} : d(g(\boldsymbol{\theta}, \mathbf{u}_i), \mathbf{x}_o) \leq \epsilon\}$.

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Approximate posterior is represented by weighted samples $\boldsymbol{\theta}_{ij}$:

$$\boldsymbol{\theta}_{ij} \sim q_i(\boldsymbol{\theta}), \qquad w_{ij} = \mathbb{1}_{C_\epsilon^i}(\boldsymbol{\theta}_{ij}) \frac{p(\boldsymbol{\theta}_{ij})}{q_i(\boldsymbol{\theta}_{ij})} \qquad \text{(i=1, ... n; j=1, ..., m)}$$

Construction of the proposal distribution

(General idea, see paper for details)

- Using $\boldsymbol{\theta}_i^*$ and the optimisation trajectory, we build a model of the acceptance regions $C_\epsilon^i = \{\boldsymbol{\theta} : d(g(\boldsymbol{\theta}, \mathbf{u}_i), \mathbf{x}_o) \leq \epsilon\}$

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- Note: When computing the weight,

$$w_{ij} = \mathbb{1}_{C_\epsilon^i}(\boldsymbol{\theta}_{ij}) \frac{p(\boldsymbol{\theta}_{ij})}{q_i(\boldsymbol{\theta}_{ij})}$$

the indicator function checks whether $\boldsymbol{\theta}_{ij}$ is in the true acceptance region C_ϵ^i. $\Rightarrow$ Some robustness to modelling errors.

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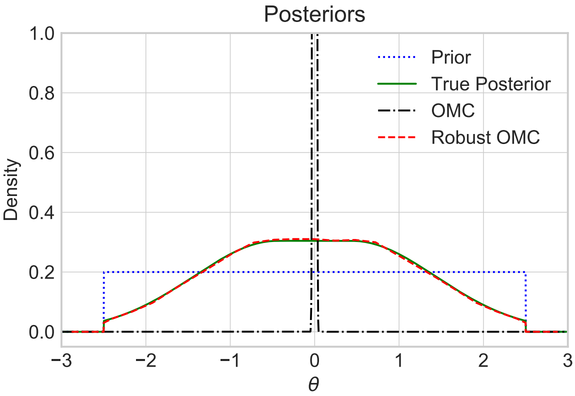
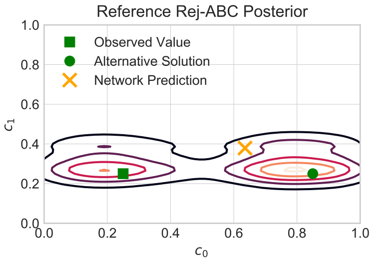
  the indicator function checks whether $\boldsymbol{\theta}_{ij}$ is in the true acceptance region C_ϵ^i. $\Rightarrow$ Some robustness to modelling errors.
- Check requires evaluating the distance $d(g(\boldsymbol{\theta}, \mathbf{u}_i), \mathbf{x}_o)$ and can be omitted/approximated to accelerate the inference.

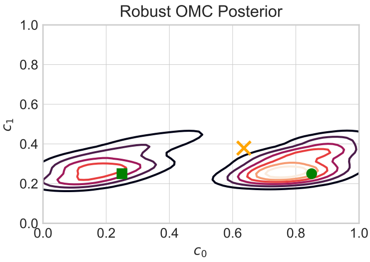
Results on the toy example

- Acceptance regions C_ϵ^i given by intervals on the line.
- ROMC handles the (nearly) flat likelihood function correctly.
- ROMC accurately represents uncertainty while OMC does not.



- Setup:
  - Optimisation via a gradient-free method (Bayesian optimisation with GP surrogate modelling)
  - Acceptance regions were modelled as ellipses (derived from the GP surrogate model)
- ROMC posterior matches reference posterior well.
- Effective sample size: 97% (vs. approx. 0.5% for OMC)





ROMC generalises OMC (see paper for the proof)

Theorem: Under the below assumptions, ROMC becomes equivalent to standard OMC as $\epsilon \to 0$.

Assumption 1. The distance $d(g(\boldsymbol{\theta}, \mathbf{u}), \mathbf{x}_o)$ is given by the Euclidean distance between summary statistics $||\mathbf{f}(\boldsymbol{\theta}, \mathbf{u}) - \Phi(\mathbf{x}_o)||$.

Assumption 2. The proposal distribution $q_i(\boldsymbol{\theta})$ is the uniform distribution on C^i_ϵ.

Assumption 3. The acceptance regions C^i_ϵ are approximated by the ellipsoid $C^i_\epsilon = \{\boldsymbol{\theta} : (\boldsymbol{\theta} - \boldsymbol{\theta}^*_i)^\top \mathbf{J}_i{}^\top \mathbf{J}_i(\boldsymbol{\theta} - \boldsymbol{\theta}^*_i) \leq \epsilon\}$ where $\mathbf{J}_i$ is the Jacobian matrix with columns $\partial \mathbf{f}(\boldsymbol{\theta}^*_i, \mathbf{u}_i)/\partial\theta_k$.

Assumption 4. The matrix square root $\mathbf{A}_i$ of $\mathbf{J}_i{}^\top \mathbf{J}_i$ is full rank, i.e. $\text{rank}(\mathbf{A}_i) = \dim(\boldsymbol{\theta})$.

Assumption 5. The prior $p(\boldsymbol{\theta})$ is constant on the acceptance regions C^i_ϵ.

Explanation of the failure case

Identified failure case is due to violation of Assumptions 3 and 4:

Assumption 3. The acceptance regions C^i_ϵ are approximated by the ellipsoid $C^i_\epsilon = \{\boldsymbol{\theta} : (\boldsymbol{\theta} - \boldsymbol{\theta}^*_i)^\top \mathbf{J}_i{}^\top \mathbf{J}_i (\boldsymbol{\theta} - \boldsymbol{\theta}^*_i) \leq \epsilon\}$ where $\mathbf{J}_i$ is the Jacobian matrix with columns $\partial \mathbf{f}(\boldsymbol{\theta}^*_i, \mathbf{u}_i)/\partial \theta_k$.

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Explanation of the failure case

Identified failure case is due to violation of Assumptions 3 and 4:

Assumption 3. The acceptance regions C_ϵ^i are approximated by the ellipsoid $C_\epsilon^i = \{\boldsymbol{\theta} : (\boldsymbol{\theta} - \boldsymbol{\theta}_i^*)^\top \mathbf{J}_i{}^\top \mathbf{J}_i (\boldsymbol{\theta} - \boldsymbol{\theta}_i^*) \leq \epsilon\}$ where $\mathbf{J}_i$ is the Jacobian matrix with columns $\partial \mathbf{f}(\boldsymbol{\theta}_i^*, \mathbf{u}_i)/\partial \theta_k$.

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For non-uniform priors, OMC then also risks violating Assumption 5:
Assumption 5. The prior $p(\boldsymbol{\theta})$ is constant on the acceptance regions C_ϵ^i.

Conclusions

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  - Optimisation Monte Carlo (OMC): Bayesian inference method that uses optimisation to increase computational efficiency.
- We showed that OMC under-estimates posterior uncertainty by collapsing regions of near-constant likelihood into a point.
- We proposed a robust generalisation of OMC, robust OMC, that explains and corrects this failure mode while maintaining OMC's benefits due to optimisation.