

Robust Optimisation Monte Carlo

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Robust Optimisation Monte Carlo
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Main messages

1. Optimisation Monte Carlo (OMC) is an existing method¹ 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.

¹Meeds and Welling, NIPS 2015.

Background: Optimisation Monte Carlo (OMC)

Contribution 1: An important failure mode of OMC

Contribution 2: Robust Optimisation Monte Carlo (ROMC)

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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
- ▶ Importance: such models and inference problems occur widely (evolutionary biology, neurosciences, health sciences, robotics, computer vision, machine learning, ...)

(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
 - ▶ \mathbf{x} : output data generated by the code
- ▶ 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.

- ▶ The deterministic function $g : (\boldsymbol{\theta}, \mathbf{u}) \mapsto \mathbf{x} = g(\boldsymbol{\theta}, \mathbf{u})$ and the distribution $p(\mathbf{u})$ define the conditional distribution $p(\mathbf{x}|\boldsymbol{\theta})$
- ▶ While well defined, evaluating $p(\mathbf{x}|\boldsymbol{\theta})$ is generally intractable
 - likelihood function $L(\boldsymbol{\theta}) = p(\mathbf{x}_o|\boldsymbol{\theta})$ is intractable
 - Bayesian inference is difficult
- ▶ Drawing samples $\mathbf{x}_i \sim p(\mathbf{x}|\boldsymbol{\theta})$ is possible for implicit models
 - 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)

- ▶ 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

- ▶ 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.
- ▶ Assumptions:
 - ▶ (approximate) derivative of $\Phi(\mathbf{x}) = \Phi(g(\boldsymbol{\theta}, \mathbf{u})) = \mathbf{f}(\boldsymbol{\theta}, \mathbf{u})$ wrt $\boldsymbol{\theta}$ is available
 - ▶ $\dim(\boldsymbol{\theta}) \leq \dim(\Phi(\mathbf{x}))$
- ▶ 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.)

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Application: Vision as inverse graphics

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

20 parameters:

Shape

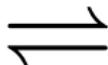
Rotation/Pose

Illumination

Colour

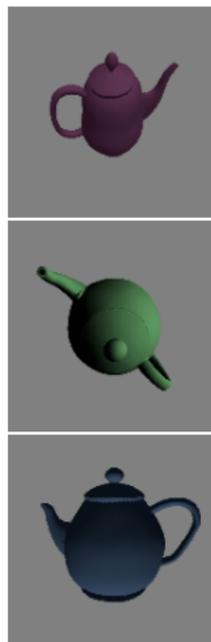
Renderer

(forward problem)



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.



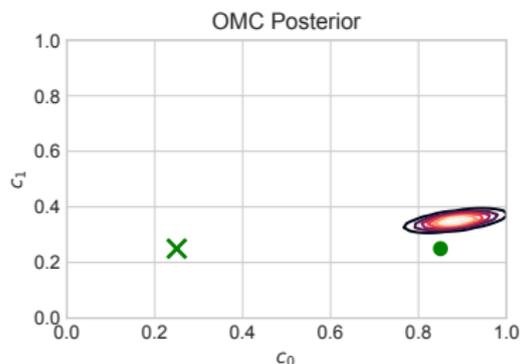
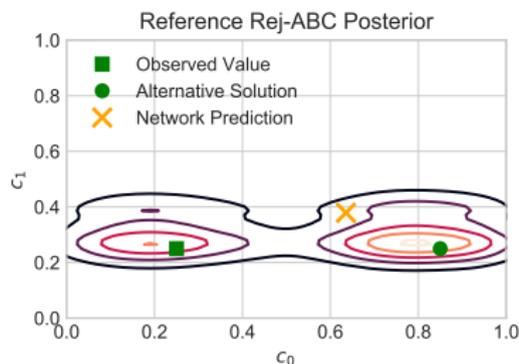
(a) Gray teapot under red light.



(b) Red teapot under white light.

Results for colour inference task

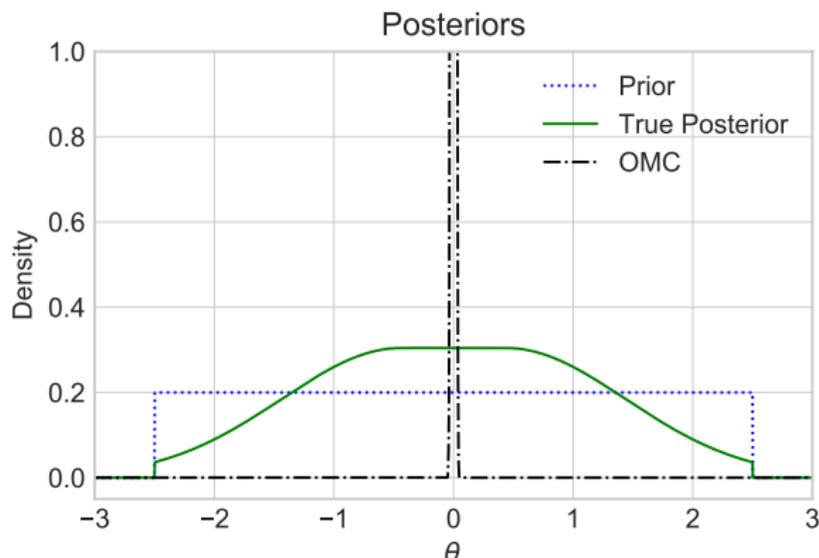
- ▶ We used OMC and the (simpler) rejection ABC algorithm.
- ▶ Rejection ABC uses trial and error instead of optimisation to determine the posterior samples. Slow but reliable.
- ▶ Same distance function $d(\mathbf{x}, \mathbf{x}_o) = \|\Phi(\mathbf{x}) - \Phi(\mathbf{x}_o)\|_2$.
- ▶ Summary statistics Φ : parameters $\hat{\theta}$ predicted by a neural network trained on images from the renderer with white light.
- ▶ Marginal joint posteriors for colours red (c_0) and green (c_1):



Why did OMC fail?

- ▶ The OMC weights $w_i = p(\theta_i^*) * (\det(\mathbf{J}_i^\top \mathbf{J}_i))^{-1/2}$ 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.

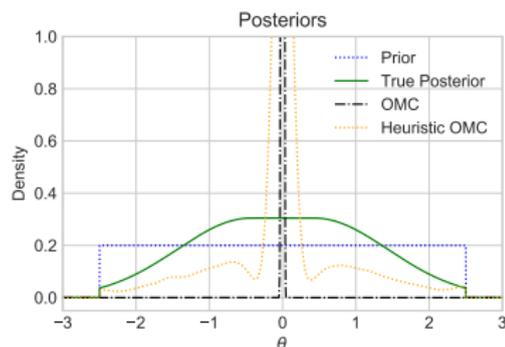
Note: stated OMC assumptions are not violated.



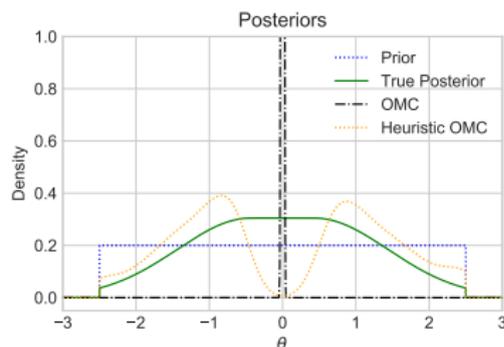
Stabilising the weights/matrices does not help

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



(a) Pseudo-inverse



(b) Pseudo-determinant

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Key properties of ROMC

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

1. **Fixes OMC's failure mode:** 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 $d(\mathbf{x}, \mathbf{x}_o)$:

$$\mathbf{u}_i \sim p(\mathbf{u}), \quad \theta_i^* = \arg \min_{\theta} d(g(\theta, \mathbf{u}_i), \mathbf{x}_o) \quad (i=1, \dots, n')$$

2. Use the minimal distances $d_i^* = d(g(\theta_i^*, \mathbf{u}_i))$ to choose an acceptance threshold ϵ / keep the n best θ_i^* .
3. For each i where $d_i^* \leq \epsilon$, define a proposal distribution q_i on the “acceptance region” $C_\epsilon^i = \{\theta : d(g(\theta, \mathbf{u}_i), \mathbf{x}_o) \leq \epsilon\}$.

Approximate posterior is represented by weighted samples θ_{ij} :

$$\theta_{ij} \sim q_i(\theta), \quad w_{ij} = \mathbb{1}_{C_\epsilon^i}(\theta_{ij}) \frac{p(\theta_{ij})}{q_i(\theta_{ij})} \quad (i=1, \dots, n; \quad j=1, \dots, m)$$

Construction of the proposal distribution

(General idea, see paper for details)

- ▶ Using θ_i^* and the optimisation trajectory, we build a model of the acceptance regions $C_\epsilon^i = \{\theta : d(g(\theta, \mathbf{u}_i), \mathbf{x}_o) \leq \epsilon\}$
- ▶ Simple but effective: model C_ϵ^i as a hypercube or ellipse and define q_i to be the uniform distribution on it.
- ▶ Note: When computing the weight,

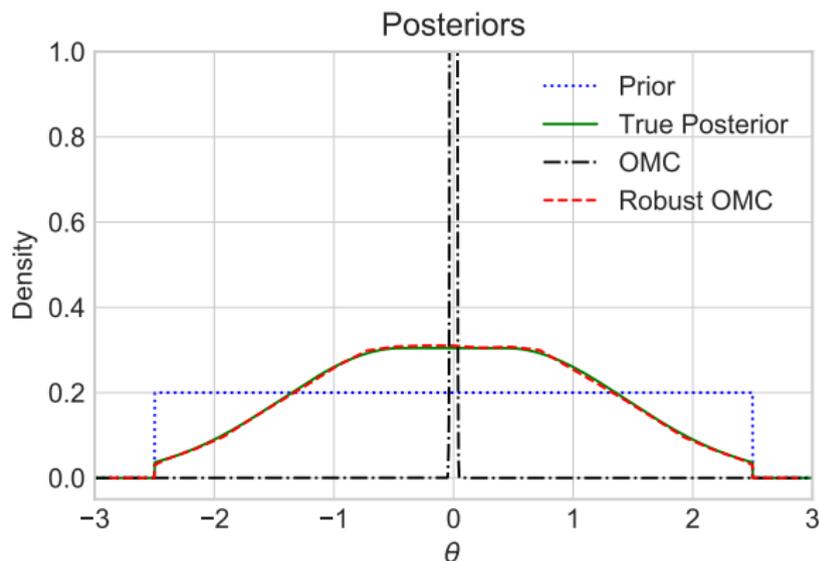
$$w_{ij} = \mathbb{1}_{C_\epsilon^i}(\theta_{ij}) \frac{p(\theta_{ij})}{q_i(\theta_{ij})}$$

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

- ▶ Check requires evaluating the distance $d(g(\theta, \mathbf{u}_i), \mathbf{x}_o)$ and can be omitted/approximated to accelerate the inference.

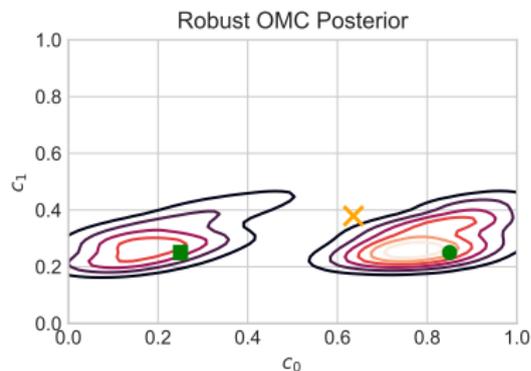
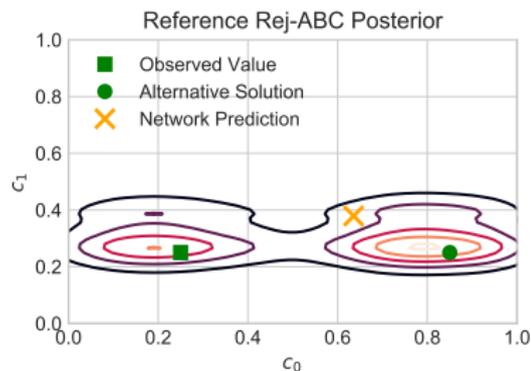
Results on the toy example

- ▶ 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.



Results on the colour inference task

- ▶ 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 $\epsilon \rightarrow 0$.

Assumption 1. The distance $d(g(\boldsymbol{\theta}, \mathbf{u}), \mathbf{x}_o)$ is given by the Euclidean distance between summary statistics $\|\mathbf{f}(\boldsymbol{\theta}, \mathbf{u}) - \Phi(\mathbf{x}_o)\|_2$.

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

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

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_ϵ^i .

Explanation of OMC's failure mode

Identified failure mode is due to violation of Assumptions 3 and 4 when the likelihood is nearly flat in a region of the parameter space:

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

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

For non-uniform priors, Assumption 5 may also not hold:

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

Paper available at: *arXiv:1904.00670*

- ▶ Talk was on Bayesian inference for implicit models.
 - ▶ Implicit models: statistical models that are defined by a data generating process.
 - ▶ 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.