STU FCHPT



Nested Sampling Approach to Set-membership Estimation

R. Paulen*, L. Gomoescu**, B. Chachuat**

*Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Slovakia

** Centre for Process Systems Engineering, Department of Chemical Engineering Imperial College London, United Kingdom

Nested Sampling Approach to Set-membership Estimation

Motivation

- Set-membership estimation is an alternative to statistical estimation
- It drops the need of knowing statistical distributions but requires set-based tools





Motivation



• Sampling techniques well-developed for Bayesian statistics



E. Corsaro and J. De Ridder (2014)

• This talk: A novel algorithm based on <u>nested sampling</u> that leverages efficient strategies from Bayesian estimation







 $\mathcal{P}_{\mathbf{e}} := \{ \boldsymbol{p} \in \mathcal{P}_0 \mid -\overline{\boldsymbol{e}} \leq \boldsymbol{y}(t_i) - \boldsymbol{F}(\boldsymbol{p}, t_i) \leq \overline{\boldsymbol{e}}, \forall i \in \{1, \dots, N\} \} := \{ \boldsymbol{p} \in \mathcal{P}_0 | \boldsymbol{h}(\dot{\boldsymbol{x}}, \boldsymbol{x}, \boldsymbol{p}) \leq 0 \}$



Nested sampling (NS) (Skilling, 2006)

- \mathbb{E} (Posterior) $\propto \mathbb{E}$ (Likelihood × Prior) = $\int_{\boldsymbol{p}} \mathcal{L}(\boldsymbol{p}) \pi(\boldsymbol{p}) d\boldsymbol{p}$ is hard to calculate.
- It is easier to get the probability mass contained within the level sets of $\mathcal{L}(oldsymbol{p})$

$$X(\lambda) = \int_{\mathcal{L}(\boldsymbol{p}) \ge \lambda} \pi(\boldsymbol{p}) \mathrm{d}\boldsymbol{p}$$

• ...and calculate the evidence in 1D.

$$\mathcal{Z} = \int_0^1 \mathcal{L}(\boldsymbol{p}) \mathrm{d}X$$

• The posterior is a free by-product.



Feroz et al. (2013)

Nested sampling (NS) (Skilling, 2006)



- Initialization: Draw N_{live} samples (live points) from the prior in a list L
- Iterations:
 - 1. Find the lowest value of $\mathcal{L}(p)$ within the list *L* and remove the point from the list
 - 2. Draw N_{prop} samples (proposals) from the prior within a region enclosing $\mathcal{L}(p)$
 - 3. Include them in the list *L* if their likelihood value is higher than the current lowest one









Nested sampling (NS) (Skilling, 2006)

- Effective sampling from the prior is necessary for multimodal distributions (disconnected sets)
- E.g. X-means clustering algorithm (Pelleg and Moore, 2000)



Feroz et al. (2009)

Stopping criterion:

- The algorithm estimates contribution of the enclosed probability mass
- Stop once the contribution to the mass from the live points is below threshold





Nested sampling (NS) – Features

- NS samples more sparsely from the prior in regions where the likelihood is low and more densely where the likelihood is high.
- The algorithm can be applied to multi-modal likelihood functions.
- The likelihood function evaluations can be easily parallelized.
- The procedure runs with an evolving collection of N_{live} points, where N_{live} can be chosen small for speed or large for accuracy.



E. Corsaro and J. De Ridder (2014)

NS for Set-membership estimation (SME)



How to transform SME into Bayesian-like setup to apply NS?

Naïve way:

$$\pi(\boldsymbol{p}) := \begin{cases} 1, & \text{if } \boldsymbol{p} \in \mathcal{P}_0 \\ 0, & \text{otherwise} \end{cases} \qquad \mathcal{L}(\boldsymbol{p}) := \begin{cases} 1, & \text{if } \boldsymbol{p} \in \mathcal{P}_e \\ 0, & \text{otherwise} \end{cases}$$

Proposed way:

$$\mathcal{P}_{e} := \{ \boldsymbol{p} \in \mathcal{P}_{0} \mid -\overline{\boldsymbol{e}} \leq \boldsymbol{y}(t_{i}) - \boldsymbol{F}(\boldsymbol{p}, t_{i}) \leq \overline{\boldsymbol{e}}, \forall i \in \{1, \dots, N\} \}$$
$$\mathcal{L}(\boldsymbol{p}) := \begin{cases} 1 & \text{if } \boldsymbol{p} \in \mathcal{P}_{e} \\ \prod_{i=1}^{N} e^{-\frac{1}{2}(\boldsymbol{y}(t_{i}) - \boldsymbol{F}(\boldsymbol{p}, t_{i}))^{T} \boldsymbol{Q}(\boldsymbol{y}(t_{i}) - \boldsymbol{F}(\boldsymbol{p}, t_{i}))} & \text{otherwise} \end{cases}$$
$$Q := \operatorname{diag}^{-2}\left(\frac{1}{3}\overline{\boldsymbol{e}}\right)$$



DEUS 1.0.0 available

- \bullet DEsign under Uncertainty using Sampling methods
- A Python package that implements Nested sampling algorithm
 - Bayesian estimation
 - Set-membership estimation
 - Design space characterization
- Available at: https://github.com/omega-icl/DEUS
- Input files for all the presented case studies can be retrieved







Sampling of an n-dimensional box



 $\mathcal{P}_{e} := \{ p \in [-10^{m}, 10^{m}]^{n} | 0 \le p_{i} \le 2, \forall i \in \{0, \dots, n\} \} \qquad n \in \{2, \dots, 10\}, m \in \{1, \dots, 5\}$ For n = 2, m = 1: Solution in less than 1s (naïve way of sampling takes 63s). For n = 10: • m = 1: 106s • m = 5: 1100s • m = 5: 1100s

The computational burden scales <u>quadratically</u> with the size of the search space n and <u>linearly</u> with the volume of initial search domain \mathcal{P}_0 .

 p_2

(a) $N_{\text{live}} := 150$



Simple nonlinear static problem



Solution in 3 seconds (no parallelization) after 7,200 function evaluations.

Jaulin, L. and Walter, E. (1993). Set inversion via interval analysis for nonlinear bounded-error estimation. Automatica, 29(4).

Paulen, Gomoescu, Chachuat

Nested Sampling Approach to Set-membership Estimation



Three-parameter dynamic estimation



Kieffer, M. and Walter, E. (2011). International Journal of Adaptive Control & Signal Processing.



State/parameter dynamic estimation

- Anaerobic digester model with 6 states and 3 measured outputs
- 5 kinetic parameters and 6 initial conditions to estimate



- Inner approximation obtained in 1 hour of algorithm run
- Obtaining an outer-approximation is infeasible with state of the art tools

Paulen, Gomoescu, Chachuat



Paulen, Gomoescu, Chachuat

Nested Sampling Approach to Set-membership Estimation

ITMS 26240220084, APVV (Grant no. 15-0007)

Acknowledgements: MSCA IF (Grant no. 790017), ITN (Grant no. 675585),

- A novel technique based on Bayesian nested sampling for inner-approximation of the solution set of set-membership estimation.
- Favourable computational performance obtained.
- Inner-approximation cannot replace a validated outer-approximation but it is helpful in certain specific tasks:
 - scenario-based optimization
 - identifiability analysis

Conclusions

• a priori analysis of a set-membership problems

Questions: radoslav.paulen@stuba.sk

IFAC World Congress 2020 15 / 15