

Towards Markov Chain Monte Carlo Methods for Uncertainty Models Specified by Sets of Probability Distributions

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$\mathcal{M} := \{P_\theta : \theta \in \Theta\}$ \rightsquigarrow how to estimate $\underline{\mathbb{E}}_{\mathcal{M}} f$? $(= \inf_{P \in \mathcal{M}} \mathbb{E}_P f)$

Monte Carlo estimation:

$$X_1, \dots, X_n \stackrel{i.i.d.}{\sim} P_\theta \Rightarrow \mathbb{E}f \approx \hat{\mathbb{E}}f = \frac{1}{n} \sum f(x_i)$$

Draw samples via

- An ancillary RV $U \sim Q$
- Transformation function ϕ_P s.t.

$$X = \phi_P(U) \sim P_\theta$$

Set of samples $S_P(\bar{u}) := [\phi_P(u_i)]$

The estimator

$$\hat{\mathbb{E}}f = \frac{\sum f(S_P)}{|S_P|}$$

With \mathcal{M} :

• No clear notion of samples!

If $\exists \phi_P \forall P \in \mathcal{M}$

• sample common \bar{u}

• $\mathcal{Y}_{\mathcal{M}} := \{S_P(\bar{u}) : P \in \mathcal{M}\}$

$$\text{The estimator } \underline{\mathbb{E}}f = \inf_{S \in \mathcal{Y}_{\mathcal{M}}} \frac{\sum f(S)}{|S|}$$

We present a method for which $\mathcal{Y}_{\mathcal{M}}$ is finite.

(Avoids non-linear optimisation)

But how to keep track of the credal set splitting numerically?

Rejection Sampling:

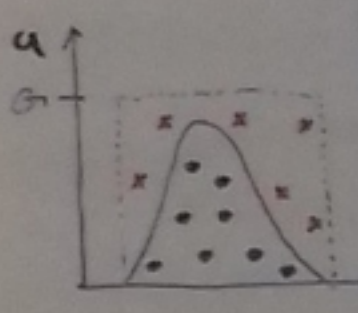
Initialize $S = []$

Repeat

sample $x, u \sim \text{Unif}$

$u < \frac{f(x)}{G} \Rightarrow S \leftarrow S + [x]$

$u > \frac{f(x)}{G} \Rightarrow S \leftarrow S$



With \mathcal{M} :

Initialize $\mathcal{Y}^* = \{(\mathcal{M}, S = [x])\}$

Repeat $\forall (\mathcal{M}, S) \in \mathcal{Y}^*$

$\mathcal{M}_1 := \{P \in \mathcal{M} : u < \frac{f(x)}{G}\}$

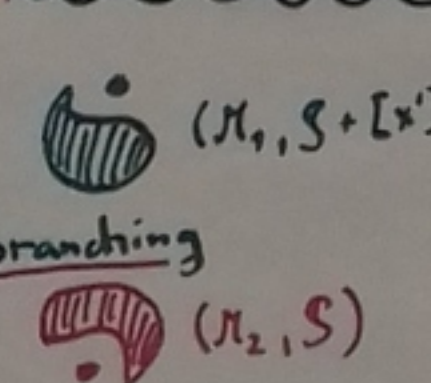
$\mathcal{M}_2 := \{P \in \mathcal{M} : u > \frac{f(x)}{G}\}$

$\mathcal{M}_1 = \emptyset \dots$ do nothing

$\mathcal{M}_2 = \emptyset \dots S \leftarrow S + [x]$

else $\mathcal{Y}^* \leftarrow \mathcal{Y}^* - (\mathcal{M}, S) \cup (\mathcal{M}_1, S + [x]) \cup (\mathcal{M}_2, S)$

$\mathcal{Y}^* \leftarrow \mathcal{Y}^* - (\mathcal{M}, S) \cup (\mathcal{M}_1, S + [x]) \cup (\mathcal{M}_2, S)$



Sometimes it is "easy"

Metropolis-Hastings algorithm:

(sample from q_θ)

Initialize $S = [x_0]$

Repeat

sample $u, v \sim \text{Unif}$

$X = \phi(x_{i-1}, u) \sim q(x'|x_{i-1})$

$A = \frac{p_\theta(x') q(x|x')}{p_\theta(x) q(x'|x)}$

$\{v < A \Rightarrow S \leftarrow S + [x']$

$\{v > A \Rightarrow S \leftarrow S + [x_{i-1}]$

Process

$S^* = S_M$ (burn-in phase)

$\hat{S} = S_K$ (subselection to remove correlations)

$\hat{\mathbb{E}}f = \frac{\sum f(\hat{S})}{|\hat{S}|}$ (estimation)

Metropolis-Hastings scheme uses rejection sampling \Rightarrow Branching

• each $P \in \mathcal{M}$ is specified by p_θ

\Rightarrow induces $A_\theta(x, x')$

• if all $P \in \mathcal{M}$ agree upon $\forall A \text{ or } \forall A > A$

proceed as in the precise case

else $\mathcal{M}_1 := \{P \in \mathcal{M} : v < A_P\}$

$\mathcal{M}_2 := \{P \in \mathcal{M} : v > A_P\}$

$\mathcal{Y}^* \leftarrow \mathcal{Y}^* - (\mathcal{M}, S) \cup (\mathcal{M}_1, S + [x]) \cup (\mathcal{M}_2, S + [x_{i-1}])$

For p_θ from the exponential family

$$p_\theta(x) = h(x) g(\theta) \exp(\eta(\theta) T(x))$$

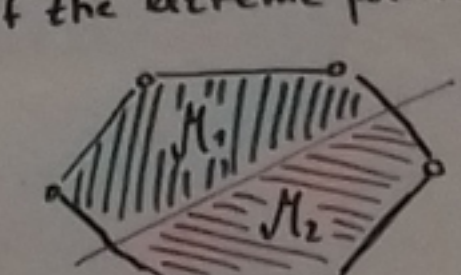
$$\Rightarrow A_\theta(x, x') = \frac{p_\theta(x') q(x|x')}{p_\theta(x) q(x'|x)}$$

$$= \frac{h(x') g(\theta') \exp(\eta(\theta') T(x')) q(x|x')}{h(x) g(\theta) \exp(\eta(\theta) T(x)) q(x'|x)}$$

$$\Rightarrow v < A \Leftrightarrow \ln(v) - \frac{h(x, x')}{g(\theta)} < \eta(\theta) [T(x') - T(x)]$$

The splitting boundary is a hyperplane

\Rightarrow we only need to keep track of the extreme points in $\eta(\theta)$



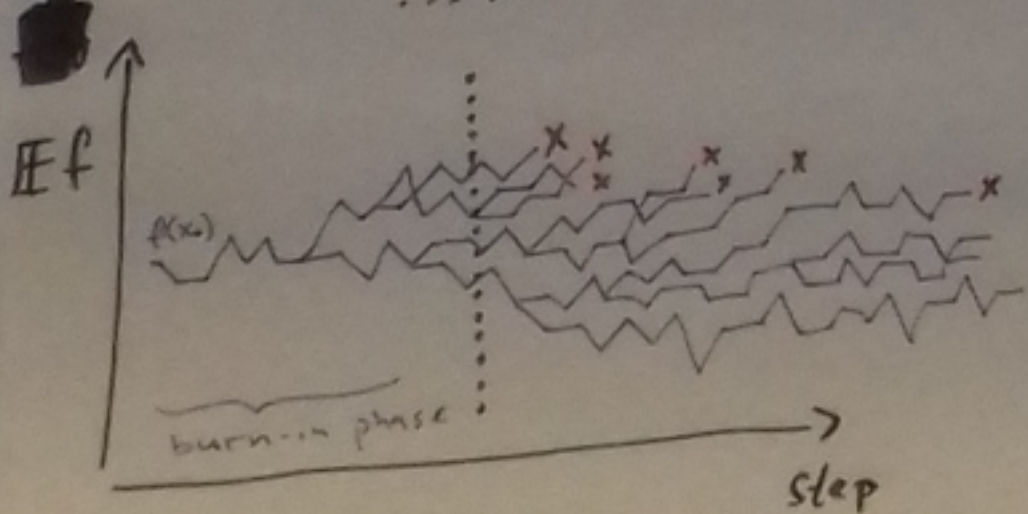
Taming the branches

Postponing branching:

for a transition kernel K
 $K_{\eta} = \tau \Rightarrow (\lambda K + (1-\lambda)I)\tau = \tau$

- if we randomly repeat the last sample we still target the same distribution.
- (Heuristic) we do this a couple of times when the chain would branch in order to decrease the number of branches.

"A cartoon of the evolution of a branching chain."



Terminating branches:

- we want to avoid wasting resources on unpromising branches.
- use a hypothesis test

$$H_0: \underline{\mathbb{E}}_{\mathcal{M}_1} f = \underline{\mathbb{E}}_{\mathcal{M}_{\min}} f$$

$$H_A: \underline{\mathbb{E}}_{\mathcal{M}_1} f > \underline{\mathbb{E}}_{\mathcal{M}_{\min}} f$$

UTOPIAE

Funded by the EU's H2020 programme through the UTOPIAE Marie Curie Innovative Training Network, H2020-MSCA-ITN-2016 Grant Agreement no. 722734

Conclusions:

- We optimise only over a finite set to obtain the final $\underline{\mathbb{E}}f$.
- Naïvely parallelizable.
- $P(\text{"This will eventually work well"}) > 0.5$

Future work:

- Theoretical justification for the heuristic patches.
- Resources allocation via sequential D-M.