Multi-level Markov Chain Monte Carlo Methods for Bayesian Inverse Problems

Juan Pablo Madrigal Cianci

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ESI WS1: Multilevel and multifidelity sampling methods in UQ for PDEs

Chair of Scientific Computing and Uncertainty Quantification (CSQI), EPF Lausanne
Collaborators: Prof. Fabio Nobile, Prof. Raúl Tempone.

Introduction: Bayesian Inverse Problems

Given measured data $y \in Y$ modeled as

$$y = F(u) + e, \quad e \sim \mu_{\text{noise}}, \quad u \in X,$$

- u: Parameter $u \sim \mu_{\text{pr}}$.
- $F : X \to Y$.
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Goal: sample u **conditioned on** y from μ^y, with

$$\underbrace{\mu^y(u)}_{\text{Posterior}} := \mu(u|y) = \frac{1}{Z} \underbrace{\mu_{\text{noise}}(y - F(u))}_{\text{likelihood}} \underbrace{\mu_{\text{pr}}(u)}_{\text{prior}}$$

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Caveat: F usually gets evaluated numerically with discr. parameter L of high accuracy/cost. $\implies$ Induces F_{L}

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$$\frac{\mathrm{d}\mu_{\mathrm{L}}^{y}}{\mathrm{d}\mu_{\mathrm{pr}}}(u) = \frac{1}{Z_{\mathrm{L}}} e^{-\Phi_{\mathrm{L}}(u;y)}, \qquad \Phi_{\mathrm{L}}(u;y) = \|y - F_{\mathrm{L}}(u)\|_{\mathrm{Y}}^{2},$$

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with $\quad \mu_{\mathrm{L}}^{y} \to \mu^{y} \quad$ as $\mathrm{L} \to \infty$.

Introduction: MCMC- Metropolis Hastings

Constructs Markov chain $\{u^n_{\mathrm{L}}\}_{n=0}^N$ with invariant distribution μ^y_{L}

procedure MH(μ^y_{L}, Q,N,λ_0).

Sample $u^0 \sim \lambda_0$

for $n = 0, \dots, N-1$ **do**

Sample $z \sim Q(u^n, \cdot)$.

Set $u^{n+1} = z$ w/prob. α_{L}:

$$\alpha_{\mathrm{L}}(u^n, z) = \min\left[1, \frac{\mu^y_{\mathrm{L}}(z)Q(z, u^n)}{\mu^y_{\mathrm{L}}(u^n)Q(u^n, z)}\right],$$

set $u^{n+1} = u^n$ otherwise.

end for

Output $\{u^n\}_{n=0}^N$

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Accuracy is controlled by N and L.

Issue: Large N + Expensive F_L.

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Solution: ML-MCMC

ML-MCMC: motivation

Introduce $\{F_\ell\}_{\ell=0}^{L}$ of increasing accuracy/cost; $F_\ell \to F$ as $\ell \to \infty$.

(a) $\ell = 0$, F_0 (b) $\ell = 1$, F_1 (c) $\ell = 2$, F_2 (d) $\ell = 3$, F_3

Induces μ_ℓ^y, $\ell = 0, 1, \ldots, L$, with

$$\frac{d\mu_\ell^y}{d\mu_{pr}}(u) = \frac{1}{Z_\ell} \exp\left(-\|y - F_\ell(u)\|_Y^2\right)$$

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$$\mathbb{E}_{\mu^y}[\mathrm{QoI}] \simeq \mathbb{E}_{\mu^y_L}[\mathrm{QoI}_L] = \mathbb{E}_{\mu^y_0}[\mathrm{QoI}_0] + \sum_{\ell=1}^{L}\left(\mathbb{E}_{\mu^y_\ell}[\mathrm{QoI}_\ell] - \mathbb{E}_{\mu^y_{\ell-1}}[\mathrm{QoI}_{\ell-1}]\right)$$

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$u_{\star,\ell} \sim \mu^y_\ell$, $\quad u_{\star,\ell-1} \sim \mu^y_{\ell-1}$.

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Fact: Choosing $N_\ell < N_{\ell-1}$ very carefully gives a much cheaper estimator with same accuracy as SL.

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Theorem [DKST15] (Informal) : If $\exists\ \alpha_w, \beta, \gamma > 0$:

- T1. $|\mathbb{E}_{\mu_\ell^y}[\mathrm{QoI}_\ell] - \mathbb{E}_{\mu^y}[\mathrm{QoI}]| \leq C_w M^{-\alpha_w \ell}$,
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$$\mathrm{Cost}\left(e_{\mathrm{ML}}, \mathrm{tol}^2\right) \leq C_{\mathrm{ML}} \begin{cases} \mathrm{tol}^{-2}|\log \mathrm{tol}| & \text{if } \beta > \gamma, \\ \mathrm{tol}^{-2}|\log \mathrm{tol}|^3, & \text{if } \beta = \gamma, \\ \mathrm{tol}^{-2+(\gamma-\beta)/\alpha_w}|\log \mathrm{tol}|, & \text{if } \beta < \gamma. \end{cases}$$

$$\mathrm{Cost}\left(e_{\mathrm{SL}}, \mathrm{tol}^2\right) \leq C_{\mathrm{SL}} \mathrm{tol}^{-2-\gamma/\alpha_w}$$

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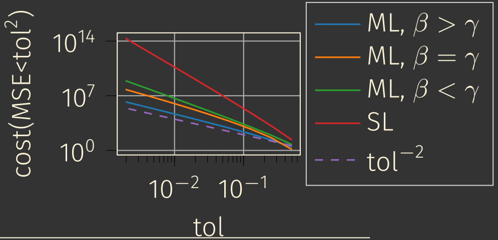

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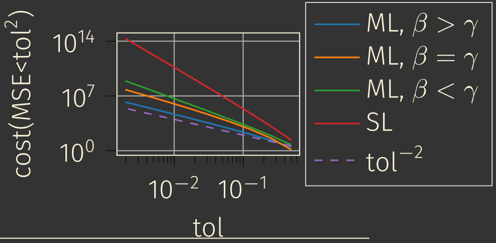

T2: $Y^m_\ell \xrightarrow{\ell\to\infty} 0 \implies \mathbb{V}_{\nu_\ell}[Y_\ell] \xrightarrow{\ell\to\infty} 0$

(Not trivial)

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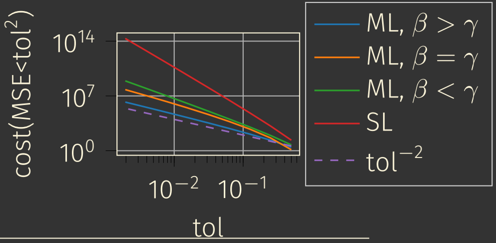

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Key: Construct coupled chains by coupling proposals.

[DKST15]: Dodwell, et Al. (2015).

ML-MCMC: generating couplings

Γ is a **coupling** of $Q(u^n_{\ell,\ell},\cdot)$ and $R(u^n_{\ell,\ell-1},\cdot)$, if:

A. $(u'_{\ell,\ell-1}, u'_{\ell,\ell}) \sim \Gamma, \implies u'_{\ell,\ell-1} \sim R(u^n_{\ell,\ell-1},\cdot)$ and $u_{\ell,\ell} \sim Q(u^n_{\ell,\ell},\cdot)$.

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For any coupling:

B. $\mathbb{P}_\Gamma(u'_{\ell,\ell-1} \neq u'_{\ell,\ell}) \geq \left\| Q(u^n_{\ell,\ell}, \cdot) - R(u^n_{\ell,\ell-1}, \cdot) \right\|_{\mathrm{TV}}.$

We say it is a maximal coupling if B. holds with equality.

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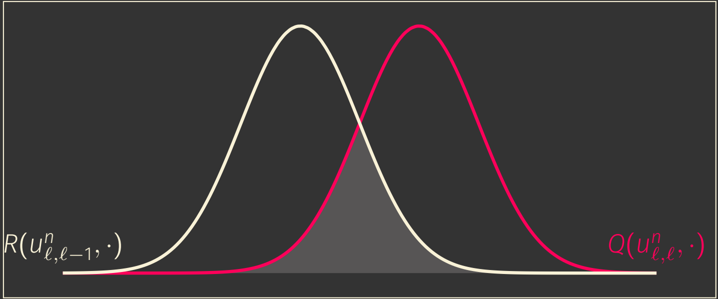

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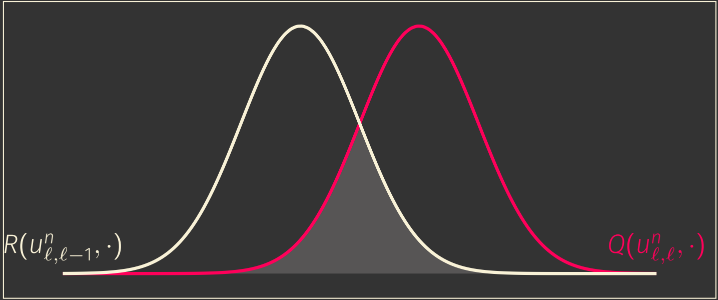

1. IMH $Q(u^n_{\ell,\ell},\cdot) = R(u^n_{\ell,\ell-1},\cdot) = Q(\cdot)$.
2. MxC: $Q(u^n_{\ell,\ell},\cdot)$, $R(u^n_{\ell,\ell-1},\cdot)$.

   (g)pCN, RWM, HMC,..

ML-MCMC: coupling via IMH

IMH: Couples chains by **always** proposing the same state (independently).

[DKST15]: Dodwell, et Al. (2015). [MCNT21]: MC, Nobile, Tempone. (2021.) [MC22]: MC. (2022.)

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procedure IMH($\{\mu^y_{\ell-1}, \mu^y_{\ell}\}, \{u^n_{\ell,\ell-1}, u^n_{\ell,\ell}\}, Q_\ell$)

Sample $z \sim Q_\ell$ and $w \sim \mathcal{U}(0,1)$.

for $j = \ell - 1, \ell$ **do**

Set $u^{n+1}_{\ell,j} = z$ if $w < \alpha_j(u^n_{\ell,j}, z)$, where

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Output $\{u^{n+1}_{\ell,\ell-1}, u^{n+1}_{\ell,\ell}\}$.

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- Induces joint kernel $\mathbf{p}_{\ell,IMH}$.
- Choosing Q_ℓ is critical
- [DKST15] proposes $Q_\ell(\cdot) = \frac{1}{N_{\ell-1}} \sum_{i=1}^{N_{\ell-1}} \delta_{u^i_{\ell-1,\ell-1}}(\cdot) \approx \mu^y_{\ell-1}$, however, **can give biased results**.
- [MCNT21,MC22] extend to a wider class of ind. proposals Q_ℓ w/ certain conditions (prior, KDE, Laplace approximation) . Difficult to find in some situations.

[DKST15]: Dodwell, et Al. (2015). [MCNT21]: MC, Nobile, Tempone. (2021.) [MC22]: MC. (2022.)

ML-MCMC: coupling via MxC

MxC: Γ^n of state-dependent proposals[MCN22][HJLT21] $Q^n = Q(u^n_{\ell,\ell}, \cdot)$, $R^n = R(u^n_{\ell,\ell-1}, \cdot)$

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procedure MxC($\mu^y_\ell, \mu^y_{\ell-1}, u^n_{\ell,\ell-1}, u^n_{\ell,\ell}, Q^n, R^n$)
    Sample $(u'_{\ell,\ell-1}, u'_{\ell,\ell}) \sim \Gamma^n$, $w \sim \mathcal{U}([0,1])$
    for $j = \ell-1, \ell$ **do**:
        if $w \leq \alpha_j(u^n_{\ell,j}, u'_{\ell,j})$ **then**
            Set $u^{n+1}_{\ell,j} = u'_{\ell,j}$.
        else
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- Induces joint kernel $\mathbf{p}_{\ell,MxC}$.
- ML-MCMC w/ state-dependent proposals.
- Proposes same state w.p. $1 - \left\| Q(u^n_{\ell,\ell}, \cdot) - R(u^n_{\ell,\ell-1}, \cdot) \right\|_{TV}$, small if $u^n_{\ell,\ell-1}, u^n_{\ell,\ell}$ are too far apart

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ML-MCMC: IMH convergence

Theorem 1: Convergence of joint IMH chain[MCNT21]**.**

A.1 $\exists\, c \in (0,1)$ independent of ℓ s.t. $\forall \ell \geq 1$:

$$\operatorname*{ess\,inf}_{z\in X} \left\{ \frac{Q_\ell(z)}{\mu_j^y(z)} \right\} \geq c > 0, j = \ell-1, \ell, \ \mu_{\text{pr}} - \text{a.s.} \tag{1}$$

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Then, $\forall \ell \geq 1\ \exists!$ a invariant ν_ℓ induced by $\mathbf{P}_{\ell,\mathrm{imh}}$. Furthermore,

$$\sup_{\|f\|_{L_\infty(X^2,\mu_{\mathrm{pr}}^2)}} \left| \int_{X^2} f(\mathbf{u}_\ell')\mathbf{p}_\ell^n(\mathbf{u}_\ell, \mathrm{d}\mathbf{u}_\ell') - \int_{X^2} f(\mathbf{u}_\ell)\nu_\ell(\mathrm{d}\mathbf{u}_\ell)\right| \leq 2(1-\rho_\ell)^n, \quad \forall \mathbf{u}_\ell \in X^2, n \in \mathbb{N},$$

$\rho_\ell := c \int_X \min\{\mu^y(z), \mu_{\ell-1}^y(z)\}\mu_{\mathrm{pr}}(\mathrm{d}z) = c[1 - d_{\mathrm{TV}}(\mu_\ell^y, \mu_{\ell-1}^y)]$.

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Conversely, if (1) doesn't hold $\implies$ no geometric ergodicity.

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Importance: first result of its kind + guideline on implementation + $\nu_\ell = \nu_\ell(Q_\ell)$.

[MCNT21]: MC, Nobile, Tempone. (2021)

Theorem 2: Convergence of joint MxC chain[MCN22]

A.2.1 $\Phi_\ell(u;y) > 0, \ \forall u \in X, y \in Y.$

A.2.2 $\mu_{\text{pr}} = \mathcal{N}(0, \mathcal{C})$

A.2.3 $Q(u^n_{\ell,\ell}, \cdot) = \mathcal{N}(\sqrt{1-\rho^2}(u^n_{\ell,\ell}, \rho^2\mathcal{C}), \quad R(u^n_{\ell,\ell-1}, \cdot) = \mathcal{N}(\sqrt{1-\rho^2}u^n_{\ell,\ell-1}, \rho^2\mathcal{C})$

+ some technical conditions on the conv. of marginal pCN.

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ML-MCMC: MxC convergence

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+ some technical conditions on the conv. of marginal pCN.

Then, $\forall \ell \geq 1 \ \exists!$ invariant ν_ℓ induced by $\mathbf{P}_{\ell,\text{mc}}$. Furthermore, $\exists \varrho \in (0,1), M < +\infty$, $V_\ell : X^2 \to [1, \infty)$ s.t.

$$\sup_{\|f\|_{L_\infty(X^2, \mu^2_{\text{pr}})}} \left| \int_{X^2} f(\mathbf{u}'_\ell)\mathbf{p}^n_\ell(\mathbf{u}_\ell, d\mathbf{u}'_\ell) - \int_{X^2} f(\mathbf{u}_\ell)\nu_\ell(d\mathbf{u}_\ell) \right| \leq M V_\ell(\mathbf{u}_\ell)\varrho^n, \quad \forall \mathbf{u}_\ell \in X^2, n \in \mathbb{N}.$$

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ML-MCMC: MSE bound

Theorem 3: MSE Bound[MCNT21] (informal). $\mu p = \mu$, p **non-nec. reversible**, $\mu^0 \neq \mu$, and p mixes sufficiently fast. Then $\forall f \in L_2(\mathsf{X}, \mu)$:

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$$\mathrm{E}_{\mu^0, p}\left[\left|\frac{1}{N}\sum_{n=0}^{N} f(u^n) - \mathbb{E}_\mu[f]\right|^2\right] \leq C_{\gamma_{\mathrm{ps}}} \frac{\mathbb{V}_\mu[f]}{N}.$$

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Importance:

1. useful beyond ML-MCMC.
2. Needed for complexity result $(\mathrm{MSE}(\hat{Y}_{\ell, N_\ell}) \leq N_\ell^{-1} C_{\mathrm{mse}} \mathbb{V}_{\nu_\ell}[Y_\ell])$.
3. Similar results in literature[Rud12] **but** difficult to verify assumption if non-reversible (as ML-MCMC).

[MCNT21]: MC, Nobile, Tempone. (2021) , [Rud12]: Rudolf. (2012).

ML-MCMC: IMH complexity

Theorem 4: Complexity of ML-IMH algorithm [MCNT21] (informal) Suppose A.1 holds and:

A.3.1 $|\Phi_\ell(u;y) - \Phi(u;y)| \leq C_\Phi(u)s^{-\alpha\ell}, \ \forall u \in X.$

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T.3 $\mathrm{MSE}(\hat{Y}_{\ell,N_\ell}) \leq N_\ell^{-1} C_{\mathrm{mse}} \mathbb{V}_{\nu_\ell}[Y_\ell].$

Here, $\alpha_w = \min\{a_q, a\}, \ \beta = \min\{2\, a_q, \alpha(1 - 2/m)\}$

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Similar result for MxC if $\exists c_\ell \not\to 0$ s.t. $\int_{\Delta^c} \mathrm{p}_\ell(\mathbf{u}_\ell, \Delta)\nu_\ell(d\mathbf{u}_\ell) > c_\ell$ (strong)

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importance: Extends Dodwell's result beyond $Q_\ell = \mu_{\ell-1}^y$.

[MCNT21]: MC, Nobile, Tempone. (2021).

ML-MCMC: Some key points on the choice of method

Want marginals to stay close.

A1: $\operatorname*{ess\,inf}_{z \in X} \left\{ \frac{Q_\ell(z)}{\mu_j^y(z)} \right\} \geq c > 0.$

1. If $\mu_{\ell-1}^y$ available AND A1 $\implies$ use sub-sampling (IMH with $Q_\ell = \mu_{\ell-1}^y$). Indeed rate $1 - c[1 - d_{\mathrm{TV}}(\mu_\ell^y, \mu_{\ell-1}^y)] \overset{\ell \to \infty}{\to} 0$. (Tricky in practice since $\frac{1}{N_{\ell-1}} \sum_{i=1}^{N_{\ell-1}} \delta_{u^i_{\ell-1,\ell-1}}(\cdot) \approx \mu_{\ell-1}^y$).

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3. Otherwise, use MxC:
   - Easy to implement proposals (e.g., pCN) coupling algo.
   - Less efficient than a good IMH.

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ML-MCMC Example: Subsurface flow

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$$\begin{cases} -\nabla_x \cdot (e^{u(x)} \nabla_x h(x,u)) = 1, \quad x \in D, \; u \in \mathrm{X}, \\ +\text{Suitable BCs} \end{cases}, \tag{2}$$

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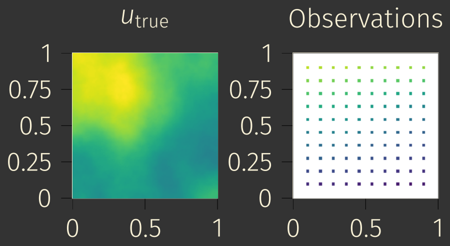
- Introduce a FE mesh of $K^* = (16 \times 2^4 + 1)^2$ elements.
- Data y generated by sampling $u_{\mathrm{true}} \sim \mu_{\mathrm{pr}}$, solving (2), obs. at 100 points in $[0, 0.9]^2$ and polluting with 1% Gaussian noise.
- $u \sim \mathcal{N}(0, \mathcal{A}^{-2}) =: \mu_{\mathrm{pr}}$, $\mathcal{A} : \Delta + \frac{1}{2} I$



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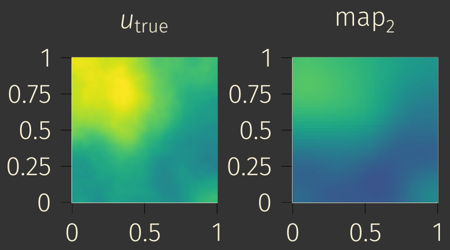

ML-MCMC Example: Subsurface flow –concentration

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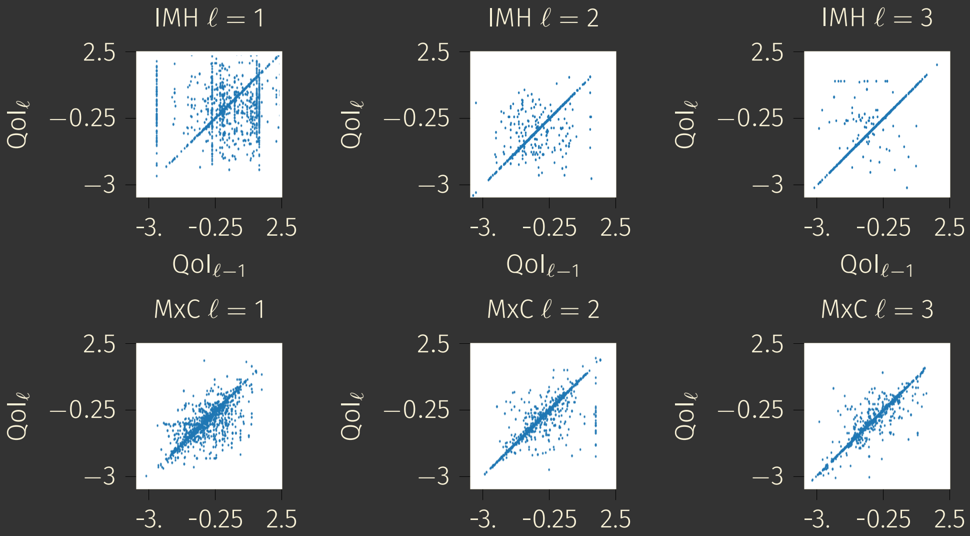

ML-MCMC Example: Subsurface flow –rates

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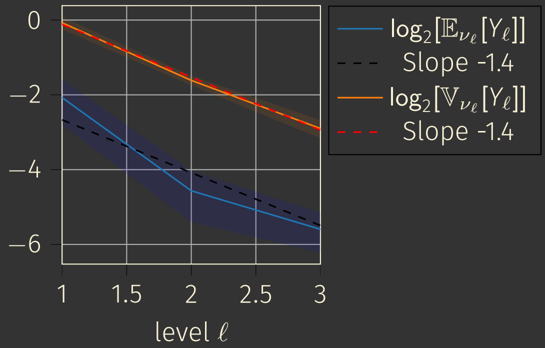
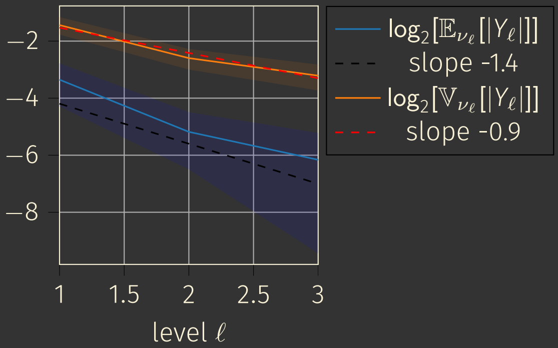


MxC



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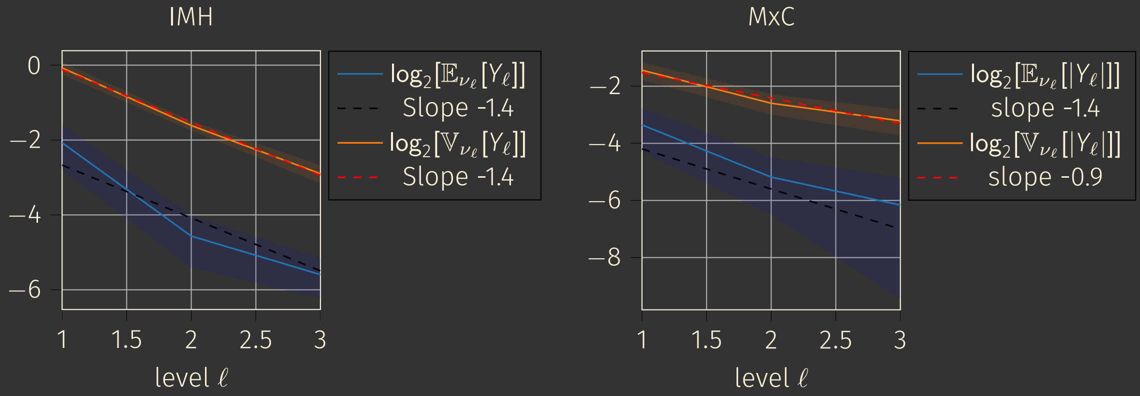

pay a price for applicability of MxC

ML-MCMC Example: Subsurface flow –costs

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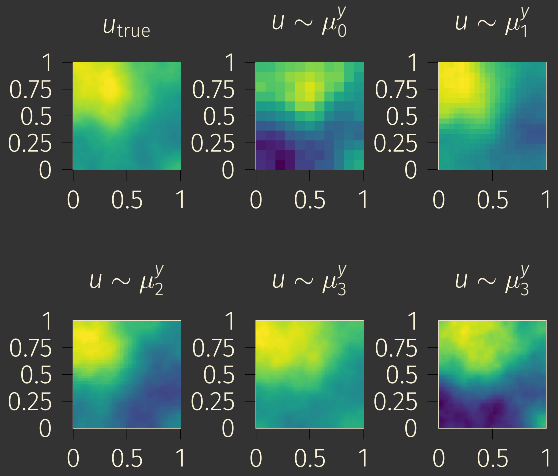

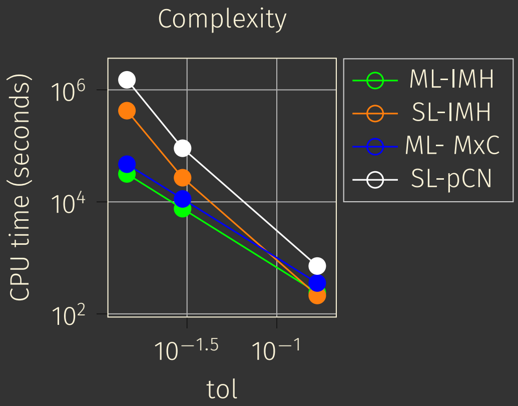

ML-MCMC

1. Proposed methods can be understood as generalizations of current ML-MCMC techniques.
   1.1 IMH: First extension of SS approach to allow wider class of proposals.
   1.2 MxC: ML-MCMC allowing state-dependent proposals.
2. Theoretical analysis for convergence and cost of both proposed methods, MxC can be refined.
3. Identification of cases on when should each method be used.
4. MxC easy to implement but lower perfomance than SS or good IMH (when applicable).

Perspectives/open problems

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- combine ML-MCMC with tempering for multi-modal problems.

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Thanks!

Sanity check: Gaussians

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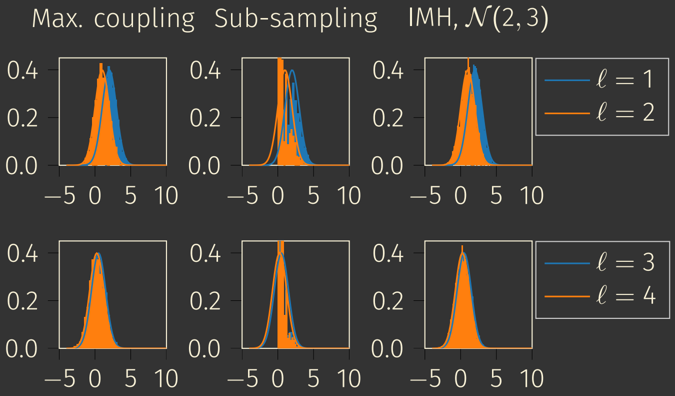
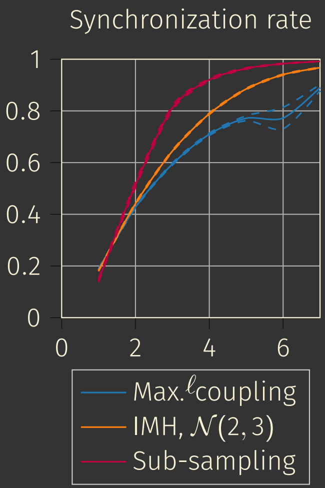


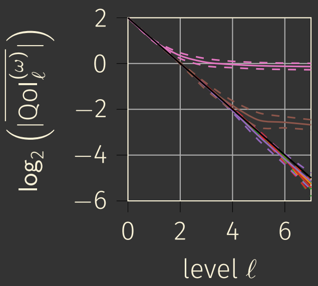


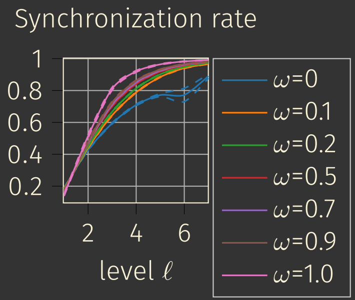
Sanity check: Gaussians

$\mathrm{QoI}_\ell = u_\ell \implies \mathbb{E}_{\mu^y_\ell}[\mathrm{QoI}_\ell] = 2^{-\ell+2}$

$\mathbf{p}_{c,\ell} = (1-\omega)\mathbf{p}_{\ell,MxC} + \omega\mathbf{p}_{\ell,IMH}$, $\omega \in (0,1)$

Using the mixed kernel with the SS of [1], we obtain for different values of $\omega \in (0,1)$





1: Dodwell, et Al. 2015.

Examples: Subsurface flow

Let $\bar{D} = [0,1]^2$, $\partial D = \Gamma_N \cup \Gamma_D$, $\mathring{\Gamma}_N \cap \mathring{\Gamma}_D = \emptyset$, $\Gamma_D := \{(x_1, x_2) \in \partial D,\ \text{s.t. } x_1 = \{0,1\}\}$.

$$\begin{cases} -\nabla_x \cdot (\kappa(x,u)\nabla_x u(x,u)) = 1, & x \in D,\ u \in X, \\ u(x,u) = 0 & x \in \Gamma_D,\ u \in X,\ , \\ \partial_n u(x,u) = 0 & x \in \Gamma_N,\ u \in X, \end{cases} \tag{3}$$

$$\log(\kappa(x,u)) = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} \sqrt{\lambda_{m,n}}\phi_{m,n}(x)u_{m,n}, \quad u_{n,m} \sim \mathcal{N}(0,1)$$

$\lambda_{m,n} = \frac{1}{\pi m^2}\frac{1}{\pi n^2}$,
$\phi_{m,n}(x) = \sin(m\pi x_1)\sin(n\pi x_2),\ m,n \in \mathbb{N}$.

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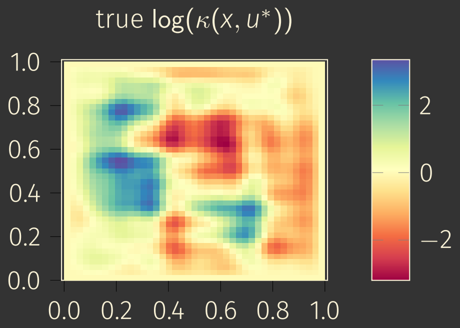

Goal: Estimate $\mathbb{E}_{\mu^y}[\mathrm{QoI}]$.

Examples: Subsurface flow: discretization and setup

1. Reorder $\log(\kappa(x,u))$ in terms of a single index j s.t $\lambda_{m,n} =: \lambda_j > \lambda_{j+1}$, and truncate at K:

$$\log(\kappa(x,u)) \approx \sum_{j=1}^{K} \sqrt{\lambda_j}\phi_j(x)u_j, \quad u_j \sim N(0,1),\ j = 1,\dots,K. \tag{4}$$

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4. Set $K = 50$, $\ell \in \{0,1,2,3,4\}$, $\mathrm{L} = 4$, $u \mapsto F_\ell(u)$: sol PDE at level ℓ, using a log-permeability field modeled by (4), and observed at a grid of 4×4 points inside D $\Phi_\ell(u,y) = \frac{1}{2\sigma^2_{\text{noise}}} \|y - F_\ell(u)\|^2$, 1% noise.

Examples: Subsurface flow: discretization and setup

1. Reorder $\log(\kappa(x,u))$ in terms of a single index j s.t $\lambda_{m,n} =: \lambda_j > \lambda_{j+1}$, and truncate at K:

$$\log(\kappa(x,u)) \approx \sum_{j=1}^{K} \sqrt{\lambda_j}\phi_j(x)u_j, \quad u_j \sim N(0,1),\ j = 1,\dots,K. \tag{4}$$

2. We introduce $\ell = \{0,1,2,3,4\}$, For each ℓ, the solution to Equation (3) is numerically approximated using FE on a mesh of $2^\ell \cdot 22 \times 2^\ell \cdot 22$ piece-wise linear elements.
3. Data y is obtained by solving PDE using a discretization level $\mathrm{L}^* = 6$, with $u_k \sim \mathcal{N}(0,1)$, $k = 1,2,\dots,K^* = 150$. $\eta \sim \mathcal{N}(0, \sigma^2_{\mathrm{noise}} I_{16\times 16})$
4. Set $K = 50$, $\ell \in \{0,1,2,3,4\}$, $\mathrm{L} = 4$, $u \mapsto F_\ell(u)$: sol PDE at level ℓ, using a log-permeability field modeled by (4), and observed at a grid of 4×4 points inside D $\Phi_\ell(u,y) = \frac{1}{2\sigma^2_{\mathrm{noise}}} \|y - F_\ell(u)\|^2$, 1% noise.
5. $\mu_{\mathrm{pr}} = \bigotimes_{i=1}^{K} \mathcal{N}(0,1)$,

Examples: subsurface

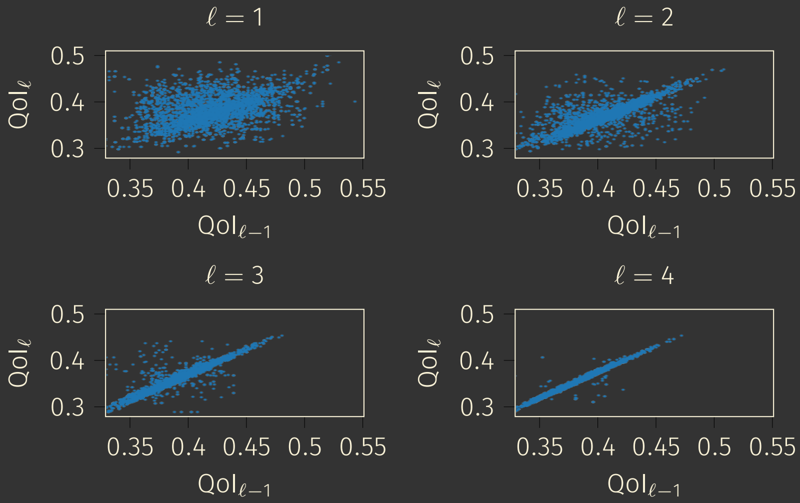
We implement our Maximal Coupling method with ω_ℓ given by $\omega_1 = 0.1$, and $\omega_2 = \omega_3 = \omega_4 = 0.5$.

As a verification of our method, we run our ML-MCMC algorithm 50 independent times, with $N_\ell = [5000, 5000, 5000, 2000, 1000]$ samples per level, per run, for $\ell = 0, 1, \ldots, 4$.

We want to (i) check that chains stay correlated, (ii) verify assumptions form complexity Theorem.

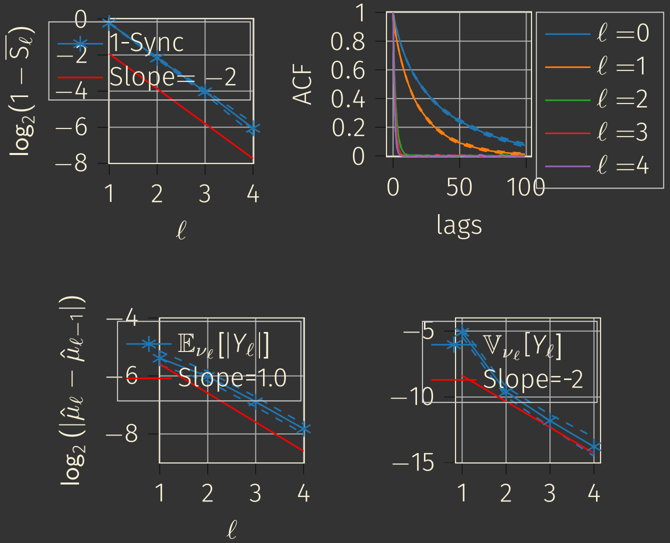
Examples: subsurface: results

Verification that chains stay increasingly more sync'd $\rightarrow$ concentrate around a diagonal



Verification of rates in cost Theorem:

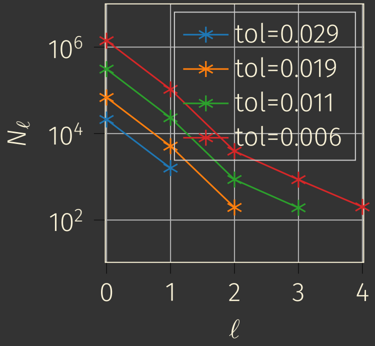
$$|\mathbb{E}_{\mu^y_\ell}[\mathrm{QoI}_\ell] - \mathbb{E}_{\mu^y}[\mathrm{QoI}]| \le C_w M^{-\alpha_w \ell}, \quad \mathbb{V}_{\nu_\ell}[Y_\ell] \le C_v M^{-\beta\ell}.$$

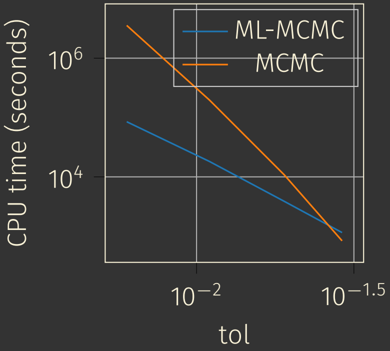


Examples: subsurface: results

$N_\ell = \left\lceil 2\text{tol}^{-2}\sqrt{V_\ell/C_\ell}\left(\sum_{k=0}^{L}\sqrt{V_k C_k}\right)\right\rceil$, Here: $V_\ell = \mathbb{V}_{\nu_\ell}(Y_\ell)$, C_ℓ cost of 1 sample at ℓ.

We can assume that $C_\ell \lessapprox 2^{\gamma\ell}$, $\gamma = 2$

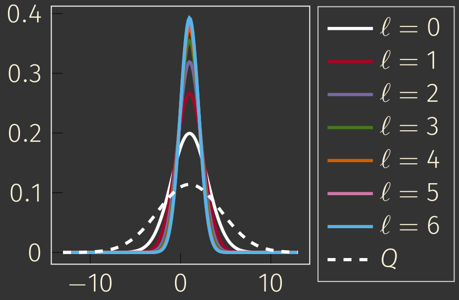




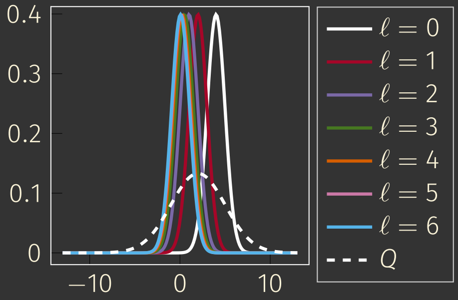
In words: In a single-level we would need $O(10^6)$ PDE solves at the finest level. **With the ML-MCMC approach we need just** $O(10^2)$

Coupling via independent sampler: illustrative example.

Dodwell et. Al. 2015, proposes to sub-sample from the previous chain targeting $\mu^y_{\ell-1} \to \{u^n_{\ell,\ell}\}_{n=0}^{N_\ell} \subset \{u_{0,0}\}_{n=0}^{N_0}$. however this can only work if $\mathrm{supp}(\mu^y_\ell) \subset \mathrm{supp}(\mu^y_{\ell-1})$.



(a) ✓



(b) ✗

Coupling via independent sampler: illustrative example.

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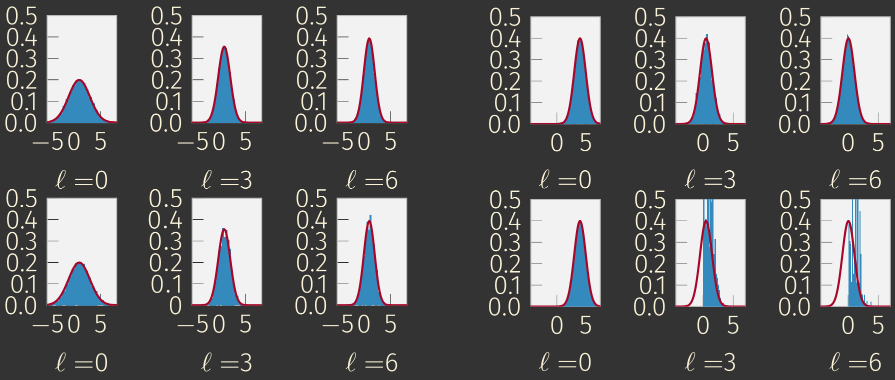
Top: ours. **Bottom:** Dodwell et Al. 2015

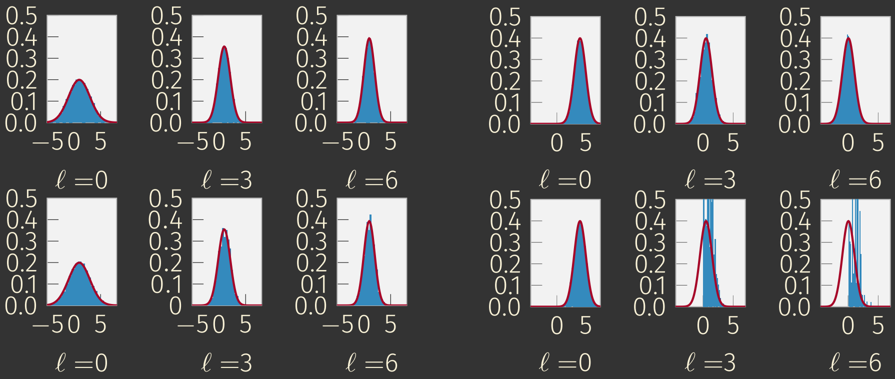


(a) ✓ Both methods work (b) ✗ Only our method works

Coupling via independent sampler: illustrative example.

Dodwell et. Al. 2015, proposes to sub-sample from the previous chain targeting $\mu^y_{\ell-1} \rightarrow \{u^n_{\ell,\ell}\}_{n=0}^{N_\ell} \subset \{u_{0,0}\}_{n=0}^{N_0}$. however this can only work if $\mathrm{supp}(\mu^y_\ell) \subset \mathrm{supp}(\mu^y_{\ell-1})$.

Difficulty finding Q (IMH) suitable for realistic problems $\rightarrow$ Try localized proposals



(a) ✓ Both methods work

(b) ✗Only our method works

Maximal coupling: An example

Sample $u'_{\ell,\ell-1} \sim R(u^n_{\ell,\ell-1}, \cdot)$, and $u'_{\ell,\ell} \sim Q(u^n_{\ell,\ell}, \cdot)$ s.t. $\mathbb{P}(u'_{\ell,\ell-1} \neq u'_{\ell,\ell}) = \|Q - R\|_{\mathrm{TV}}$

4: Jacob et Al. 2019.

Maximal coupling: An example

Sample $u'_{\ell,\ell-1} \sim R(u^n_{\ell,\ell-1}, \cdot)$, and $u'_{\ell,\ell} \sim Q(u^n_{\ell,\ell}, \cdot)$ s.t. $\mathbb{P}(u'_{\ell,\ell-1} \neq u'_{\ell,\ell}) = \|Q - R\|_{\mathrm{TV}}$

Mixture approach [4]:

1. Case 1: With probability $a = \int \min\{Q, R\} dz$ sample

$$u'_{\ell,\ell} \sim \frac{\min\{Q, R\}}{a}, \quad u'_{\ell,\ell} = u'_{\ell,\ell-1}.$$

2. Case 2: Otherwise

$$u'_{\ell,\ell} \sim \frac{Q - \min\{Q, R\}}{1 - a}, \quad u'_{\ell,\ell-1} \sim \frac{R - \min\{Q, R\}}{1 - a} \text{ independently.}$$

4: Jacob et Al. 2019.

Maximal coupling: An example

Sample $u'_{\ell,\ell-1} \sim R(u^n_{\ell,\ell-1}, \cdot)$, and $u'_{\ell,\ell} \sim Q(u^n_{\ell,\ell}, \cdot)$ s.t. $\mathbb{P}(u'_{\ell,\ell-1} \neq u'_{\ell,\ell}) = \|Q - R\|_{\mathrm{TV}}$

Mixture approach [4]:

1. Case 1: With probability $a = \int \min\{Q, R\} \mathrm{d}z$ sample
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$$u'_{\ell,\ell} \sim \frac{Q - \min\{Q, R\}}{1-a}, \quad u'_{\ell,\ell-1} \sim \frac{R - \min\{Q, R\}}{1-a} \text{ independently.}$$

$u_{\ell,\ell} \sim Q$

$$\begin{aligned}\mathbb{P}(u_{\ell,\ell} \in A) &= a \int_A \frac{\min\{Q, R\}}{a} + (1-a) \int_A \frac{Q - \min\{Q, R\}}{1-a} \\ &= \int_A Q \mathrm{d}z\end{aligned}$$

4: Jacob et Al. 2019.

Maximal coupling: An example

Sample $u'_{\ell,\ell-1} \sim R(u^n_{\ell,\ell-1}, \cdot)$, and $u'_{\ell,\ell} \sim Q(u^n_{\ell,\ell}, \cdot)$ s.t. $\mathbb{P}(u'_{\ell,\ell-1} \neq u'_{\ell,\ell}) = \|Q - R\|_{\mathrm{TV}}$

Mixture approach [4]:

1. Case 1: With probability $a = \int \min\{Q, R\}\mathrm{d}z$ sample
$$u'_{\ell,\ell} \sim \frac{\min\{Q, R\}}{a}, \quad u'_{\ell,\ell} = u'_{\ell,\ell-1}.$$
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$$u'_{\ell,\ell} \sim \frac{Q - \min\{Q, R\}}{1 - a}, \quad u'_{\ell,\ell-1} \sim \frac{R - \min\{Q, R\}}{1 - a} \text{ independently.}$$

$u_{\ell,\ell-1} \sim R$

$$\begin{aligned}\mathbb{P}(u_{\ell,\ell-1} \in A) &= a \int_A \frac{\min\{Q, R\}}{a} + (1 - a) \int_A \frac{R - \min\{Q, R\}}{1 - a} \\ &= \int_A R\mathrm{d}z\end{aligned}$$

4: Jacob et Al. 2019.

Maximal coupling: An example

Sample $u'_{\ell,\ell-1} \sim R(u^n_{\ell,\ell-1}, \cdot)$, and $u'_{\ell,\ell} \sim Q(u^n_{\ell,\ell}, \cdot)$ s.t. $\mathbb{P}(u'_{\ell,\ell-1} \neq u'_{\ell,\ell}) = \|Q - R\|_{\mathrm{TV}}$

Mixture approach [4]:

1. Case 1: With probability $a = \int \min\{Q, R\}\mathrm{d}z$ sample
$$u'_{\ell,\ell} \sim \frac{\min\{Q, R\}}{a}, \quad u'_{\ell,\ell} = u'_{\ell,\ell-1}.$$
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$$u'_{\ell,\ell} \sim \frac{Q - \min\{Q, R\}}{1-a}, \quad u'_{\ell,\ell-1} \sim \frac{R - \min\{Q, R\}}{1-a} \text{ independently.}$$

$\mathbb{P}(u_{\ell,\ell-1} = u_{\ell,\ell}) = 1 - \|Q - R\|_{\mathrm{TV}}$

$$\begin{aligned}\mathbb{P}(u_{\ell,\ell-1} = u_{\ell,\ell}) &= \int \min\{Q, R\}\mathrm{d}z = \frac{1}{2}\int Q\mathrm{d}z + \frac{1}{2}\int R\mathrm{d}z - \int \frac{1}{2}|Q - R|\mathrm{d}z \\ &= 1 - \frac{1}{2}\int |Q - R|\mathrm{d}z = 1 - \|Q - R\|_{\mathrm{TV}}.\end{aligned}$$

4: Jacob et Al. 2019.

Maximal coupling: An example

Sample $u'_{\ell,\ell-1} \sim R(u^n_{\ell,\ell-1}, \cdot)$, and $u'_{\ell,\ell} \sim Q(u^n_{\ell,\ell}, \cdot)$ s.t. $\mathbb{P}(u'_{\ell,\ell-1} \neq u'_{\ell,\ell}) = \|Q - R\|_{\mathrm{TV}}$

Mixture approach [4]:

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Basis for more complicated algorithms. Again: Max coupling is not unique.

4: Jacob et Al. 2019.

Reflection Maximal coupling

Create coupling from $\mathcal{N}(m(u^n_{\ell,\ell}),\tilde{\mathcal{C}})$ and $\mathcal{N}(m(u^n_{\ell,\ell-1}),\tilde{\mathcal{C}})$. $\varphi_0 = \mathcal{N}(0,I)$

procedure REFLECTION-COUPLING$(m(u^n_{\ell,\ell}), m(u^n_{\ell,\ell}))$

Set $z^n = m(u^n_{\ell,\ell}) - m(u^n_{\ell,\ell-1})$ and set $e^n = z^n / \|z^n\|_X$.

Sample $\xi \sim \varphi_0$, and $w \sim \mathcal{U}([0,1])$.

if $w \leq \min\left\{1, \frac{\varphi_0(\xi+z^n)}{\varphi_0(\xi)}\right\}$ **then**

Set $\zeta = \xi + z^n$. ▷ case I

else

Set $\zeta = \xi - 2\langle e^n, \xi\rangle_X e^n$. ▷ case II

end if

Set $u'_{\ell,\ell} = m(u^n_{\ell,\ell}) + \tilde{\mathcal{C}}^{1/2}\xi$ and $u'_{\ell,\ell-1} = m(u^n_{\ell,\ell-1}) + \tilde{\mathcal{C}}^{1/2}\zeta$

Output $(u'_{\ell,\ell-1}, u'_{\ell,\ell})$.

end procedure