#### Particle-MALA and Particle-mGRAD

Gradient-based MCMC methods for high-dimensional state-space models<sup>1</sup>

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<sup>&</sup>lt;sup>1</sup>https://arxiv.org/pdf/2401.14868

## Talk outline

#### $1. \ State-space \ models/Feynman-Kac \ representation$

- 2. Existing methods
- 3. Particle extensions of MALA and aMALA
- 4. Particle extensions of mGRAD and aGRAD
- 5. Numerical illustration
- 6. Summary

 $\mathbf{x}_1 \longrightarrow \mathbf{x}_2 \longrightarrow \mathbf{x}_3 \longrightarrow \cdots$ 









- Examples:
  - econometrics/finance,
  - ecology,
  - engineering,
  - epidemiology,
  - weather forcasting,
  - ...



• T observations:  $\mathbf{y}_1, \ldots, \mathbf{y}_T$ .

$$\begin{array}{cccc} \mathbf{y}_1 & \mathbf{y}_2 & \mathbf{y}_T \\ \uparrow g_1 & \uparrow g_2 & & \uparrow g_T \\ \mathbf{x}_1 & \overbrace{f_2} & \mathbf{x}_2 & \overbrace{f_3} & \cdots & \overbrace{f_T} & \mathbf{x}_T \end{array}$$

$$ig \in \mathcal{X} \coloneqq \mathbb{R}^D$$
,

 $\begin{array}{cccc} \mathbf{y}_1 & \mathbf{y}_2 & \mathbf{y}_T \\ \uparrow g_1 & \uparrow g_2 & & \uparrow g_T \\ \mathbf{x}_1 & \xrightarrow{f_2} & \mathbf{x}_2 & \xrightarrow{f_3} & \cdots & \xrightarrow{f_T} & \mathbf{x}_T \end{array}$ • T observations:  $\mathbf{y}_1, \dots, \mathbf{y}_T$ . • D-dimensional latent states:  $\mathbf{x}_t = \begin{bmatrix} x_{t,1} \\ \vdots \\ x_{t,D} \end{bmatrix} \in \mathcal{X} \coloneqq \mathbb{R}^D$ , • Joint smoothing distribution:  $\pi_T(\mathbf{x}_{1:T}) = p(\mathbf{x}_{1:T}|\mathbf{y}_{1:T}) \propto \prod f_t(\mathbf{x}_t|\mathbf{x}_{t-1})g_t(\mathbf{y}_t|\mathbf{x}_t).$ 

 $\begin{array}{cccc} \mathbf{y}_1 & \mathbf{y}_2 & \mathbf{y}_T \\ \uparrow g_1 & \uparrow g_2 & \uparrow g_T \\ \mathbf{x}_1 & \xrightarrow{f_2} \mathbf{x}_2 & \xrightarrow{f_3} \cdots & \xrightarrow{f_T} \mathbf{x}_T \end{array}$  $\begin{array}{l} T \text{ observations: } \mathbf{y}_1, \dots, \mathbf{y}_T. \\ D \text{-dimensional latent states: } \mathbf{x}_t = \begin{bmatrix} x_{t,1} \\ \vdots \\ x_{t,D} \end{bmatrix} \in \mathcal{X} \coloneqq \mathbb{R}^D, \\ \end{array}$  $\pi_T(\mathbf{x}_{1:T}) = p(\mathbf{x}_{1:T}|\mathbf{y}_{1:T}) \propto \prod f_t(\mathbf{x}_t|\mathbf{x}_{t-1})g_t(\mathbf{y}_t|\mathbf{x}_t).$ 

Assumption: densities ft and gt are differentiable (in the states); densities/gradients can be evaluated pointwise.

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- Assumption: densities  $f_t$  and  $g_t$  are differentiable (in the states); densities/gradients can be evaluated pointwise.
- Goal: find efficient MCMC algorithms targetting  $\pi_T(\mathbf{x}_{1:T})$ .

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- Assumption: densities ft and gt are differentiable (in the states); densities/gradients can be evaluated pointwise.
- Goal: find efficient MCMC algorithms targetting  $\pi_T(\mathbf{x}_{1:T})$ .
- **Problem:**  $\pi_T(\mathbf{x}_{1:T})$  may be high dimensional (*T* or *D* large).

• More generally: we are interested in a distribution  $\pi_T(\mathbf{x}_{1:T}) \propto \prod_{t=1}^T M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) G_t(\mathbf{x}_{t-1:t}) = \prod_{t=1}^T Q_t(\mathbf{x}_{t-1:t}),$ on  $\mathcal{X}^T$  (with  $\mathcal{X} \coloneqq \mathbb{R}^D$ ), where

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-  $M_t(\cdot | \mathbf{x}_{t-1})$  is a density of a mutation kernel;  
-  $G_t(\mathbf{x}_{t-1:t}) > 0$  is called *potential function*.

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$$\begin{aligned} \pi_T(\mathbf{x}_{1:T}) \propto \prod_{t=1}^T M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) G_t(\mathbf{x}_{t-1:t}) &= \prod_{t=1}^T Q_t(\mathbf{x}_{t-1:t}), \\ \text{on } \mathcal{X}^T \text{ (with } \mathcal{X} \coloneqq \mathbb{R}^D \text{), where} \\ &- M_t(\cdot | \mathbf{x}_{t-1}) \text{ is a density of a mutation kernel;} \\ &- G_t(\mathbf{x}_{t-1:t}) > 0 \text{ is called potential function.} \end{aligned}$$

• Assumption:  $M_t$  and  $G_t$  are differentiable; both functions and their gradients can be evaluated point-wise.

$$\pi_T(\mathbf{x}_{1:T}) \propto \prod_{t=1}^T M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) G_t(\mathbf{x}_{t-1:t}) = \prod_{t=1}^T Q_t(\mathbf{x}_{t-1:t}),$$
  
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Then,  $Q_t(\mathbf{x}_{t-1:t}) = p(\mathbf{x}_t, \mathbf{y}_t | \mathbf{x}_{t-1})$  and  $\pi_t(\mathbf{x}_{1:t}) = p(\mathbf{x}_{1:t} | \mathbf{y}_{1:t})$ .

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#### 2. Existing methods

#### 2.1 'Classical' MCMC

- 2.2 Conditional sequential Monte Carlo (CSMC)
- 2.3 Particle-RWM: An existing combination of MCMC and CSMC

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• Note:  $\mathbf{x}$  is thus (TD)-dimensional.

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 $=:h(\mathbf{u})$ 

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- Two interpretations of the auxiliary sampler:
  - 1. Standard MH conditional on  $\mathbf{u}$ , i.e. targetting  $\pi(\mathbf{x};\mathbf{u}) = \pi(\mathbf{x})q(\mathbf{u}|\mathbf{x})$ .
  - 2. MH with randomised acceptance ratio<sup>3</sup> (since  $\mathbb{E}[h(\mathbf{u})|\mathbf{x}, \tilde{\mathbf{x}}] = 1$ ).

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  - 2. MH with randomised acceptance ratio<sup>3</sup> (since  $\mathbb{E}[h(\mathbf{u})|\mathbf{x}, \tilde{\mathbf{x}}] = 1$ ).
- Efficiency of auxiliary sampler  $\leq$  efficiency of marginal sampler.<sup>4</sup>

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<sup>&</sup>lt;sup>3</sup>Ceperley and Dewing (1999)

# A simple MCMC algorithm

Independent Metropolis–Hastings (IMH)<sup>5</sup>:

$$q(\tilde{\mathbf{x}}|\mathbf{x}) = M(\tilde{\mathbf{x}}).$$



- must grow **linearly** in *D* ~→ horizontal line;
- can grow sublinearly in D → increasing line;
- must grow superlinearly in  $D \rightsquigarrow$  decreasing line.

• [Marginal sampler] Random-walk Metropolis (RWM)<sup>6</sup>:

 $q(\tilde{\mathbf{x}}|\mathbf{x}) = \mathcal{N}(\tilde{\mathbf{x}}; \mathbf{x}, \delta \mathbf{I}).$ 

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- Can sample from  $q(\tilde{\mathbf{x}}|\mathbf{x})$  by sampling
  - 1.  $\mathbf{u} \sim N(\mathbf{x}, \frac{\delta}{2}\mathbf{I});$

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- [Auxiliary sampler] Not integrating out u in the acceptance ratio is statistically equivalent to the marginal sampler.

<sup>&</sup>lt;sup>6</sup>Metropolis et al. (1953)



 $(\text{Average ESJD}) = \frac{1}{TD} \sum_{t=1}^{T} \sum_{d=1}^{D} (x_{t,d}^{\text{new}} - x_{t,d}^{\text{old}})^2 \implies \text{Informally, to stably approximate marginals, the number of iterations}$ 

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 [Marginal sampler] Metropolis-adjusted Langevin algorithm (MALA)<sup>7</sup>:

$$q(\tilde{\mathbf{x}}|\mathbf{x}) = N(\tilde{\mathbf{x}}; \mathbf{x} + \frac{\delta}{2}\nabla \log \pi(\mathbf{x}), \delta \mathbf{I}).$$

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 1. u ~ N(x + δ/2∇ log π(x), δ/2I);
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# Scaling with D $M_t(\mathbf{x}_t|\mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{x}_{t-1}, \mathbf{I}), G_t(\mathbf{x}_{t-1:t}) = N(\mathbf{y}_t; \mathbf{x}_t, \mathbf{I}); T = 25, N = 31$



 $(\text{Average ESJD}) = \frac{1}{TD} \sum_{t=1}^{T} \sum_{d=1}^{D} (x_{t,d}^{\text{new}} - x_{t,d}^{\text{old}})^2 \implies \text{Informally, to stably approximate marginals, the number of iterations}$ 

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[Marginal sampler] Preconditioned
 Crank–Nicolson–Langevin (PCNL)<sup>9</sup> algorithm:

 $q(\tilde{\mathbf{x}}|\mathbf{x}) = N(\tilde{\mathbf{x}}; (1-\beta)\mathbf{m} + \beta[\mathbf{x} + \frac{\delta}{2}\mathbf{C}\nabla\log G(\mathbf{x})], (1-\beta^2)\mathbf{C}),$ 

where  $\beta \coloneqq 2/(2+\delta)$ .

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• [Marginal sampler] Marginal gradient (mGRAD)<sup>10</sup> algorithm:

$$q(\tilde{\mathbf{x}}|\mathbf{x}) = N(\tilde{\mathbf{x}}; (\mathbf{I} - \mathbf{A})\mathbf{m} + \mathbf{A}[\mathbf{x} + \frac{\delta}{2}\nabla \log G(\mathbf{x})], \mathbf{B}),$$

where  $\mathbf{B}\coloneqq \frac{\delta}{2}\mathbf{A}^2+\mathbf{A}$  and  $\mathbf{A}=(\mathbf{C}+\frac{\delta}{2}\mathbf{I})^{-1}\mathbf{C}.$ 

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• **Problem:** 'Classical' MCMC methods do not exploit the 'decorrelation-over-time' property the state-space model.
Summary of 'classical' MCMC methods

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 Problem: 'Classical' MCMC methods do not exploit the 'decorrelation-over-time' property the state-space model.
→ suboptimal scaling with T (for fixed D).



approximate marginals, the number of iterations

- can be **constant** in  $T \rightsquigarrow$  horizontal line: •
- must increase in T → decreasing line.

### Talk outline

- 2. Existing methods
- 2.1 'Classical' MCMC
- 2.2 Conditional sequential Monte Carlo (CSMC)
- 2.3 Particle-RWM: An existing combination of MCMC and CSMC

• For the moment: *D* small.

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  - Induces  $\pi_T$ -invariant MCMC kernel.
- Sequentially builds proposal in the 'time'-direction:
  - using N + 1 interacting samples ('particles'),
  - avoids curse of dimensionality in T (for fixed D).

#### Algorithm 1 (CSMC). Given $\mathbf{x}_{1:T} \in \mathcal{X}^T$ :

- 1. for t = 1, ..., T,
  - 1.1 set  $\mathbf{x}_t^0 \coloneqq \mathbf{x}_t$ ,
  - 1.2 [resampling] if t > 1, set  $a_{t-1}^0 := 0$ ; sample  $a_{t-1}^n = i$  w.p.  $W_{t-1}^i$ , for  $n \in [N]$ ,
  - 1.3 [sampling] isample  $\mathbf{x}_t^n \sim M_t(\cdot | \mathbf{x}_{t-1}^{a_{t-1}^n})$  for  $n \in [N]$ ,
  - 1.4 [weighting] for  $n \in [N]_0$ , set  $w_t^n \propto G_t(\mathbf{x}_{t-1}^{a_{t-1}^n}, \mathbf{x}_t^n)$ .
  - 1.5 for  $n \in [N]_0$ , set  $W^n_t \coloneqq w^n_t / \sum_{m=0}^N w^m_t$ ;
- 2. sample  $l_T = i \in [N]_0$  w.p.  $W_T^i$ .
- 3. [ancestral tracing] for  $t = T 1, \ldots, 1$ , set  $l_t \coloneqq a_t^{l_{t+1}}$ .
- 4. return  $\mathbf{x}'_{1:T} \coloneqq (\mathbf{x}_1^{l_1}, \dots, \mathbf{x}_t^{l_T}).$





- Set  $\mathbf{x}_1^0 \coloneqq \mathbf{x}_1$ . Sample  $\mathbf{x}_1^{1:N} \sim \prod_{n=1}^N M_1(\mathbf{x}_1^n)$ .



$$\begin{array}{ll} \bullet & {\rm Set} \; {\bf x}_t^0 \coloneqq {\bf x}_t, \, a_{t-1}^0 \coloneqq 0. \\ \bullet & {\rm Sample} \; ({\bf x}_t^{1:N}, a_{t-1}^{1:N}) \sim \prod_{n=1}^N W_{t-1}^{a_{t-1}^n} M_t({\bf x}_t^n | {\bf x}_{t-1}^{a_{t-1}^n}), \\ & - \; {\rm where} \; W_t^n \propto G_t({\bf x}_{t-1}^{a_{t-1}^n}, {\bf x}_t^n). \end{array}$$



time

$$\begin{array}{l} \text{ Set } \mathbf{x}_{t}^{0} \coloneqq \mathbf{x}_{t}, \, a_{t-1}^{0} \coloneqq 0. \\ \text{ Sample } (\mathbf{x}_{t}^{1:N}, a_{t-1}^{1:N}) \sim \prod_{n=1}^{N} W_{t-1}^{a_{t-1}^{n}} M_{t}(\mathbf{x}_{t}^{n} | \mathbf{x}_{t-1}^{a_{t-1}^{n}}), \\ \text{ - where } W_{t}^{n} \propto G_{t}(\mathbf{x}_{t-1}^{a_{t-1}^{n}}, \mathbf{x}_{t}^{n}). \end{array}$$



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Given reference path  $\mathbf{x}_{1:T}$  (current state of MCMC chain):

 $\begin{array}{ll} \bullet & {\rm Set} \; \mathbf{x}_{t}^{0} \coloneqq \mathbf{x}_{t}, \, a_{t-1}^{0} \coloneqq 0. \\ \bullet & {\rm Sample} \; (\mathbf{x}_{t}^{1:N}, a_{t-1}^{1:N}) \sim \prod_{n=1}^{N} W_{t-1}^{a_{t-1}^{n}} M_{t}(\mathbf{x}_{t}^{n} | \mathbf{x}_{t-1}^{a_{t-1}^{n}}), \\ & - \; {\rm where} \; W_{t}^{n} \propto G_{t}(\mathbf{x}_{t-1}^{a_{t-1}^{n}}, \mathbf{x}_{t}^{n}). \end{array}$ 



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time



time



time



time



time

1. Sample  $l_T \sim W_T^{l_T}$ . 2. Set  $l_t \coloneqq a_t^{l_{t+1}}$ , for  $t = T - 1, \dots, 1$ . 3. Return  $\mathbf{x}'_{1:T} \coloneqq (\mathbf{x}_1^{l_1}, \dots, \mathbf{x}_T^{l_T})$  (new state of MCMC chain). • induces  $\pi_T$ -invariant MCMC kernel  $P_{\mathsf{CSMC}}(\mathbf{x}'_{1:T}|\mathbf{x}_{1:T})$ .

- induces  $\pi_T$ -invariant MCMC kernel  $P_{\mathsf{CSMC}}(\mathbf{x}'_{1:T}|\mathbf{x}_{1:T})$ .
- T "accept-reject decisions".















Problem:  $\mathbf{x}'_{1:T} = (\mathbf{x}_1^{l_1}, \dots, \mathbf{x}_T^{l_T}) \& \mathbf{x}_{1:T} = (\mathbf{x}_1^0, \dots, \mathbf{x}_T^0)$  coalesce
# Mixing



Problem:  $\mathbf{x}'_{1:T} = (\mathbf{x}_1^{l_1}, \dots, \mathbf{x}_T^{l_T}) \& \mathbf{x}_{1:T} = (\mathbf{x}_1^0, \dots, \mathbf{x}_T^0)$  coalesce

- controlling the 'acceptance rates' requires  $N \sim T$  (Andrieu et al., 2018; Koskela et al., 2020)

#### Algorithm 2 (CSMC). Given $\mathbf{x}_{1:T} \in \mathcal{X}^T$ :

- 1. for t = 1, ..., T,
  - 1.1 set  $\mathbf{x}_t^0 \coloneqq \mathbf{x}_t$ ,
  - 1.2 [resampling] if t > 1, set  $a_{t-1}^0 := 0$ ; sample  $a_{t-1}^n = i$  w.p.  $W_{t-1}^i$ , for  $n \in [N]$ ,
  - 1.3 [sampling] sample  $\mathbf{x}_t^n \sim M_t(\cdot | \mathbf{x}_{t-1}^{a_{t-1}^n})$  for  $n \in [N]$ ,
  - 1.4 [weighting] for  $n \in [N]_0$ , set  $w_t^n \propto G_t(\mathbf{x}_{t-1}^{a_{t-1}^n}, \mathbf{x}_t^n)$ .
  - 1.5 for  $n \in [N]_0$ , set  $W^n_t \coloneqq w^n_t / \sum_{m=0}^N w^m_t$ ;
- 2. sample  $l_T = i \in [N]_0$  w.p.  $W_T^i$ .
- 3. [ancestral tracing] for  $t = T 1, \ldots, 1$ , set  $l_t \coloneqq a_t^{l_{t+1}}$ .
- 4. return  $\mathbf{x}'_{1:T} \coloneqq (\mathbf{x}_1^{l_1}, \dots, \mathbf{x}_t^{l_T}).$

Algorithm 2 (CSMC). Given  $\mathbf{x}_{1:T} \in \mathcal{X}^T$ :

- 1. for t = 1, ..., T,
  - 1.1 set  $\mathbf{x}_t^0 \coloneqq \mathbf{x}_t$ ,
  - 1.2 [resampling] if t > 1, set  $a_{t-1}^0 \coloneqq 0$ ; sample  $a_{t-1}^n = i$  w.p.  $W_{t-1}^i$ , for  $n \in [N]$ ,
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- 2. sample  $i \in [N]$  w.p.  $\frac{W_T^i}{1 W_T^0}$ ; set  $l_T \coloneqq i$  w.p.  $1 \wedge \frac{1 W_T^0}{1 W_T^i}$ ; otherwise, set  $l_T \coloneqq 0$ ;
- 3. [ancestral tracing] for  $t = T 1, \ldots, 1$ , set  $l_t \coloneqq a_t^{l_{t+1}}$ .
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- 3. [backward sampling] for t = T 1, ..., 1, sample  $l_t = i \in [N]_0$  w.p.  $\frac{W_t^i Q_{t+1}(\mathbf{x}_t^i, \mathbf{x}_{t+1}^{l_{t+1}})}{\sum_{n=0}^N W_t^n Q_{t+1}(\mathbf{x}_t^n, \mathbf{x}_{t+1}^{l_{t+1}})};$
- 4. return  $\mathbf{x}'_{1:T} \coloneqq (\mathbf{x}_1^{l_1}, \dots, \mathbf{x}_t^{l_T}).$



time



time



time



time



time



time



- Forms new lineage  $\mathbf{x}'_{1:T} = (\mathbf{x}_1^{l_1}, \dots, \mathbf{x}_T^{l_T}).$
- Frees us from having to grow N with T (Lee et al., 2020).



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• all acceptance rates  $\rightarrow 0$  (Finke and Thiery, 2023);



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- even with backward sampling.

# Scaling with D $M_t(\mathbf{x}_t|\mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{x}_{t-1}, \mathbf{I}), G_t(\mathbf{x}_{t-1:t}) = N(\mathbf{y}_t; \mathbf{x}_t, \mathbf{I}); T = 25, N = 31$



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# Summary of the CSMC algorithm

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- Problem: The CSMC algorithm cannot use 'local' moves.
   → curse of dimension in D (for fixed T).

#### Talk outline

#### 2. Existing methods

- 2.1 'Classical' MCMC
- 2.2 Conditional sequential Monte Carlo (CSMC)
- 2.3 Particle-RWM: An existing combination of MCMC and CSMC

Algorithm 3 (Particle-RWM). Modify CSMC as follows:

- 1c. [sampling] sample  $\mathbf{u}_t \sim N(\mathbf{x}_t, \frac{\delta_t}{2}\mathbf{I})$ , and  $\mathbf{x}_t^n \sim N(\mathbf{u}_t, \frac{\delta_t}{2}\mathbf{I})$ , for  $n \in [N]$ ,
- 1d. [weighting] for  $n \in [N]_0$ , set  $w_t^n \propto Q_t(\mathbf{x}_{t-1}^{a_{t-1}^n}, \mathbf{x}_t^n)$ .

<sup>&</sup>lt;sup>12</sup>Finke and Thiery (2023); see also Malory (2021)

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  - Step 1c marginally proposes (for  $n \neq 0$ ):

 $\mathbf{x}_t^n \sim \mathrm{N}(\mathbf{x}_t, \delta_t \mathbf{I}).$ 

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- Reduces to RWM if N = T = 1.
- Dimensionally stable if  $\delta_t = O(D^{-1})$ .<sup>12</sup>

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- Set  $\mathbf{x}_1^0 \coloneqq \mathbf{x}_1$ .
- Sample  $(\mathbf{u}_1, \mathbf{x}_1^{1:N}) \sim \mathrm{N}(\mathbf{u}_1; \mathbf{x}_1^0, \frac{\delta_1}{2}\mathbf{I}) \prod_{n=1}^N \mathrm{N}(\mathbf{x}_1^n; \mathbf{u}_1, \frac{\delta_1}{2}\mathbf{I}).$



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# Particle-RWM $(D \to \infty)$



- Set  $\mathbf{x}_1^0 \coloneqq \mathbf{x}_1$ .
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time

- Set  $\mathbf{x}_t^0 \coloneqq \mathbf{x}_t$ ,  $a_{t-1}^0 \coloneqq 0$ . Sample  $(\mathbf{u}_t, \mathbf{x}_t^{1:N}, a_{t-1}^{1:N}) \sim \mathcal{N}(\mathbf{u}_t; \mathbf{x}_t^0, \frac{\delta_t}{2}\mathbf{I}) \prod_{n=1}^N W_{t-1}^{a_{t-1}^n} \mathcal{N}(\mathbf{x}_t^n; \mathbf{u}_t, \frac{\delta_t}{2}\mathbf{I})$ , - where  $W_t^n \propto Q_t(\mathbf{x}_{t-1}^{a_{t-1}^n}, \mathbf{x}_t^n)$ .



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 $\overline{(\text{Average ESJD}) = \frac{1}{TD} \sum_{t=1}^{T} \sum_{d=1}^{D} (x_{t,d}^{\text{new}} - x_{t,d}^{\text{old}})^2} \implies \text{Informally, to stably approximate marginals, the number of iterations}$ 

- can be constant in T → horizontal line;
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- must grow **linearly** in  $D \rightsquigarrow$  horizontal line;
- can grow sublinearly in *D* ~→ increasing line;
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Extended target distribution (admits  $\pi_T(\mathbf{x}_{1:T})$  as a marginal!):

$$\pi'_{T}(\mathbf{x}_{1:T}, \mathbf{u}_{1:T}) \coloneqq \pi_{T}(\mathbf{x}_{1:T}) \prod_{t=1}^{T} N(\mathbf{u}_{t}; \mathbf{x}_{t}, \frac{\delta_{t}}{2}\mathbf{I})$$

$$\propto \prod_{t=1}^{T} \underbrace{N(\mathbf{x}_{t}; \mathbf{u}_{t}, \frac{\delta_{t}}{2}\mathbf{I})}_{=:M'_{t}(\mathbf{x}_{t}|\mathbf{x}_{t-1}; \mathbf{u}_{t})} \underbrace{M_{t}(\mathbf{x}_{t}|\mathbf{x}_{t-1})G_{t}(\mathbf{x}_{t-1:t})}_{=:G'_{t}(\mathbf{x}_{t-1:t})},$$

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Equivalent formulation of Particle-RWM:

1. sample  $\mathbf{u}_t \sim N(\mathbf{x}_t, \frac{\delta_t}{2}\mathbf{I})$ , for  $t = 1, \dots, T$ ;

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  - $M_t(\mathbf{x}_t|\mathbf{x}_{t-1})$  by  $M_t'(\mathbf{x}_t|\mathbf{x}_{t-1};\mathbf{u}_t)$ ;

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$$\pi'_{T}(\mathbf{x}_{1:T}, \mathbf{u}_{1:T}) \coloneqq \pi_{T}(\mathbf{x}_{1:T}) \prod_{t=1}^{T} N(\mathbf{u}_{t}; \mathbf{x}_{t}, \frac{\delta_{t}}{2}\mathbf{I})$$

$$\propto \prod_{t=1}^{T} \underbrace{N(\mathbf{x}_{t}; \mathbf{u}_{t}, \frac{\delta_{t}}{2}\mathbf{I})}_{=:M'_{t}(\mathbf{x}_{t}|\mathbf{x}_{t-1}; \mathbf{u}_{t})} \underbrace{M_{t}(\mathbf{x}_{t}|\mathbf{x}_{t-1})G_{t}(\mathbf{x}_{t-1:t})}_{=:G'_{t}(\mathbf{x}_{t-1:t})},$$

- 1. sample  $\mathbf{u}_t \sim N(\mathbf{x}_t, \frac{\delta_t}{2}\mathbf{I})$ , for  $t = 1, \dots, T$ ;
- 2. run standard CSMC algorithm but replace

$$\begin{array}{l} - \ M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) \ \text{by} \ M_t'(\mathbf{x}_t | \mathbf{x}_{t-1}; \mathbf{u}_t); \\ - \ G_t(\mathbf{x}_{t-1:t}) \ \text{by} \ G_t'(\mathbf{x}_{t-1:t}). \end{array}$$

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- 1. State-space models/Feynman–Kac representation
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- 3. Particle extensions of MALA and aMALA
- 4. Particle extensions of mGRAD and aGRAD
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- 3. Particle extensions of MALA and aMALA
- 3.1 Exploiting filter gradients (gradients w.r.t.  $\log \pi_t$ )
- 3.2 Exploiting smoothing gradients (gradients w.r.t.  $\log \pi_T$ )

Algorithm 4 (Particle-MALA). Modify CSMC as follows:

- 1c. [sampling] sample  $\mathbf{u}_t \sim N(\mathbf{x}_t + \frac{\delta_t}{2} \nabla_{\mathbf{x}_t} \log \pi_t(\mathbf{x}_{1:t}), \frac{\delta_t}{2} \mathbf{I})$ , and  $\mathbf{x}_t^n \sim N(\mathbf{u}_t, \frac{\delta_t}{2} \mathbf{I})$ , for  $n \in [N]$ ,
- 1d. [weighting] set  $\bar{\mathbf{x}}_t \coloneqq \frac{1}{N+1} \sum_{n=0}^N \mathbf{x}_t^n$  and, for  $n \in [N]_0$ ,

$$w_t^n \propto Q_t(\mathbf{x}_{t-1}^{a_{t-1}^n}, \mathbf{x}_t^n) F_t(\mathbf{x}_{t-1}^{a_{t-1}^n}, \mathbf{x}_t^n, \bar{\mathbf{x}}_t).$$

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- can be **constant** in  $T \rightsquigarrow$  horizontal line;
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- 4. Particle extensions of mGRAD and aGRAD
- 4.1 Exploiting conditionally Gaussian prior dynamics
- 4.2 Exploiting unconditionally Gaussian prior dynamics
- 4.3 Interpolation between CSMC and Particle-MALA/aMALA

# Conditionally Gaussian prior dynamics

• For the moment, assume that

$$M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \mathbf{m}_t(\mathbf{x}_{t-1}), \mathbf{C}_t).$$

Assuming  $M_t(\mathbf{x}_t|\mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{m}_t(\mathbf{x}_{t-1}), \mathbf{C}_t)$ 

#### Algorithm 6 (Particle-mGRAD). Modify CSMC as follows:

- 1c. [sampling] sample  $\mathbf{u}_t \sim N(\mathbf{x}_t + \frac{\delta_t}{2} \nabla_{\mathbf{x}_t} \log G_t(\mathbf{x}_{t-1:t}), \frac{\delta_t}{2} \mathbf{I})$ and  $\mathbf{x}_t^n \sim M_t'(\cdot | \mathbf{x}_{t-1}^{a_{t-1}^n}; \mathbf{u}_t)$ , for  $n \in [N]$ ,
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  - Here,

 $M'_t(\mathbf{x}_t|\mathbf{x}_{t-1};\mathbf{u}_t) \propto \mathrm{N}(\mathbf{x}_t;\mathbf{m}_t(\mathbf{x}_{t-1}),\mathbf{C}_t) \,\mathrm{N}(\mathbf{u}_t;\mathbf{x}_t,\frac{\delta_t}{2}\mathbf{I}),$ 

is the 'fully-adapted auxiliary-particle filter' proposal for the pseudo observation  $\mathbf{u}_t$ :

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• Step 1c marginally proposes (for  $n \neq 0$ ):

$$\mathbf{x}_{t}^{n} \sim \mathrm{N}((\mathbf{I} - \mathbf{A}_{t})\mathbf{m}_{t}(\mathbf{x}_{t-1}^{a_{t-1}^{n}}) + \mathbf{A}_{t}[\mathbf{x}_{t} + \frac{\delta_{t}}{2}\nabla_{\mathbf{x}_{t}}\log G_{t}(\mathbf{x}_{t-1:t})], \mathbf{B}_{t}),$$

where  $\mathbf{B}_t \coloneqq \frac{\delta_t}{2} \mathbf{A}_t^2 + \mathbf{A}_t$  and  $\mathbf{A}_t = (\mathbf{C}_t + \frac{\delta_t}{2} \mathbf{I})^{-1} \mathbf{C}_t$ .

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• Reduces to mGRAD if N = T = 1.

Assuming  $M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{m}_t(\mathbf{x}_{t-1}), \mathbf{C}_t(\mathbf{x}_{t-1}))$ 

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- 4.3 Interpolation between CSMC and Particle-MALA/aMALA
### Gaussian prior dynamics

• Now assume  $\mathbf{m}_t(\mathbf{x}_{t-1}) = \mathbf{F}_t \mathbf{x}_{t-1} + \mathbf{b}_t$ , i.e.:

$$M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \mathbf{F}_t \mathbf{x}_{t-1} + \mathbf{b}_t, \mathbf{C}_t).$$

### Twisted Particle-aGRAD

Assuming  $M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{F}_t \mathbf{x}_{t-1} + \mathbf{b}_t, \mathbf{C}_t)$ 

Algorithm 7 (Twisted Particle-aGRAD). For  $t \in [T]$ , sample  $\mathbf{u}_t \sim N(\mathbf{x}_t + \frac{\delta_t}{2} \nabla_{\mathbf{x}_t} \log G_t(\mathbf{x}_{t-1:t}), \frac{\delta_t}{2} \mathbf{I})$ . Then, run the CSMC algorithm with the following modifications.

- 1c. [sampling]  $\mathbf{x}_t^n \sim M_t'(\cdot | \mathbf{x}_{t-1}^{a_{t-1}^n}; \mathbf{u}_{t:T})$ , for  $n \in [N]$ ,
- 1d. [weighting] (\*omitted\*)
  - 3. [backward sampling] (\*omitted\*)

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  - Here,

 $M_t'(\mathbf{x}_t|\mathbf{x}_{t-1};\mathbf{u}_{t:T})$ 

$$\propto \int_{\mathcal{X}^{T-t}} \left[ \prod_{s=t}^T \mathrm{N}(\mathbf{x}_s; \mathbf{F}_s \mathbf{x}_{s-1} + \mathbf{b}_s, \mathbf{C}_s) \, \mathrm{N}(\mathbf{u}_s; \mathbf{x}_s, \frac{\delta_s}{2} \mathbf{I}) \right] \mathrm{d}\mathbf{x}_{t+1:T},$$

is the **'fully-twisted particle filter'** proposal for the pseudo observations  $\mathbf{u}_{t:T}$ :

### Twisted Particle-aGRAD

Assuming  $M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{F}_t \mathbf{x}_{t-1} + \mathbf{b}_t, \mathbf{C}_t)$ 

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is the **'fully-twisted particle filter'** proposal for the pseudo observations  $\mathbf{u}_{t:T}$ :

• Reduces to aGRAD if N = T = 1.



 $\overline{(\text{Average ESJD}) = \frac{1}{TD} \sum_{t=1}^{T} \sum_{d=1}^{D} (x_{t,d}^{\text{new}} - x_{t,d}^{\text{old}})^2} \implies \text{Informally, to stably}}$  approximate marginals, the number of iterations

- can be **constant** in  $T \rightsquigarrow$  horizontal line;
- must increase in  $T \rightsquigarrow$  decreasing line.



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- must grow **linearly** in *D* ~→ horizontal line;
- can grow sublinearly in *D* ~→ increasing line;
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 $\overline{(\text{Average ESJD}) = \frac{1}{TD} \sum_{t=1}^{T} \sum_{d=1}^{D} (x_{t,d}^{\text{new}} - x_{t,d}^{\text{old}})^2 } \Longrightarrow \text{Informally, to stably approximate marginals, the number of iterations}$ 

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### Talk outline

#### 4. Particle extensions of mGRAD and aGRAD

- 4.1 Exploiting conditionally Gaussian prior dynamics
- 4.2 Exploiting unconditionally Gaussian prior dynamics
- 4.3 Interpolation between CSMC and Particle-MALA/aMALA

• Assume  $M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{m}_t, \mathbf{C}_t).$ 

- Assume  $M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{m}_t, \mathbf{C}_t).$
- Recall: Particle-mGRAD/Particle-aGRAD marginally propose:

 $\mathbf{x}_t^n \sim \mathrm{N}(\mathbf{a}_t, \mathbf{B}_t), \quad \text{for } n \neq 0,$ 

where (with  $\mathbf{A}_t = (\mathbf{C}_t + rac{\delta_t}{2}\mathbf{I})^{-1}\mathbf{C}_t$ ),

$$\mathbf{a}_t \coloneqq (\mathbf{I} - \mathbf{A}_t)\mathbf{m}_t + \mathbf{A}_t[\mathbf{x}_t + \frac{\delta_t}{2}\nabla_{\mathbf{x}_t}\log G_t(\mathbf{x}_{t-1:t})],$$
$$\mathbf{B}_t \coloneqq \frac{\delta_t}{2}\mathbf{A}_t^2 + \mathbf{A}_t,$$

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- If prior is highly informative (all eigenvalues of  $\mathbf{C}_t$  small) then  $\mathbf{A}_t \approx \mathbf{0}$  and

- Assume  $M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{m}_t, \mathbf{C}_t).$
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 $N(\mathbf{a}_t, \mathbf{B}_t) \approx \widetilde{N(\mathbf{m}_t, \mathbf{C}_t)}.$ 

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$$\mathbf{a}_t \coloneqq (\mathbf{I} - \mathbf{A}_t)\mathbf{m}_t + \mathbf{A}_t[\mathbf{x}_t + \frac{\delta_t}{2}\nabla_{\mathbf{x}_t}\log G_t(\mathbf{x}_{t-1:t})],\\ \mathbf{B}_t \coloneqq \frac{\delta_t}{2}\mathbf{A}_t^2 + \mathbf{A}_t,$$

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$$N(\mathbf{a}_t, \mathbf{B}_t) \approx N(\mathbf{x}_t + \frac{\delta_t}{2} \nabla_{\mathbf{x}_t} \log \pi_t(\mathbf{x}_{1:t}), \delta_t \mathbf{I}).$$

(marginal) Particle-MALA/Particle-aMALA proposal 51 / 61

# Scaling with prior informativeness $M_t(\mathbf{x}_t|\mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{x}_{t-1}, \lambda \mathbf{I}), G_t(\mathbf{x}_{t-1:t}) = N(\mathbf{y}_t; \mathbf{x}_t, \mathbf{I}); T = D = 10, N = 31$



(Average ESJD) =  $\frac{1}{TD} \sum_{t=1}^{T} \sum_{d=1}^{D} (x_{t,d}^{\text{new}} - x_{t,d}^{\text{old}})^2$ .

Convergence to CSMC for highly informative priors

**A1**  $M_t(\cdot | \mathbf{x}_{t-1}) = N(\mathbf{m}_t, \mathbf{C}_t)$ , with  $G_t$  bounded and  $\mathbf{C}_t$  invertible. **A2**  $\exists C_0, C_1 \ge 0$  such that  $\|\nabla \log G_t(\mathbf{x}_t)\|_2 \le C_0 + C_1 \|\mathbf{x}_t\|_2$ .

**Proposition 1.** For some  $D, T, N \ge 1$ , assume A1–A2, and assume that there exists a sequence  $(\lambda_k)_{k\ge 1}$  in  $(0,\infty)$  with  $\max_{t\in[T]} \max \operatorname{eigenval}(\mathbf{C}_{t,k}) \le \lambda_k \to 0$  as  $k \to \infty$ . Then for any  $\varepsilon > 0$ , there exists a sequence  $(F_{T,k})_{k\ge 1}$  of subsets of  $\mathcal{X}^T$  with  $\lim_{k\to\infty} \pi_{T,k}(F_{T,k}) = 1$  such that

$$\begin{split} \sup_{\mathbf{x}_{1:T} \in F_{T,k}} & \|P_{\mathsf{Particle-mGRAD},k}(\cdot | \mathbf{x}_{1:T}) \\ & \mathbf{x}_{1:T} \in F_{T,k} & -P_{\mathsf{CSMC},k}(\cdot | \mathbf{x}_{1:T}) \|_{\mathrm{TV}} \in \mathrm{O}(\lambda_{k}^{(1-\varepsilon)/4}); \\ & \sup_{\mathbf{x}_{1:T} \in F_{T,k}} & \|P_{\mathsf{Particle-aGRAD},k}(\cdot | \mathbf{x}_{1:T}) \\ & \mathbf{x}_{1:T} \in F_{T,k} & -P_{\mathsf{CSMC},k}(\cdot | \mathbf{x}_{1:T}) \|_{\mathrm{TV}} \in \mathrm{O}(\lambda_{k}^{(1-\varepsilon)/4}). \end{split}$$

Convergence to Particle-MALA for uninformative priors

A3  $\max_{d \in [D]} \int_{\mathcal{X}} x_{t,d}^2 G_t(\mathbf{x}_t) \, \mathrm{d}\mathbf{x}_t < \infty$ , where  $x_{t,d}$  is the dth component of  $\mathbf{x}_t$ .

**Proposition 2.** For some  $D, T, N \ge 1$ , assume A1–A3, and assume that there exists a sequence  $(\lambda_k)_{k\ge 1}$  in  $(0,\infty)$  with  $\min_{t\in[T]} \min \operatorname{eigenval}(\mathbf{C}_{t,k}) \ge \lambda_k \to \infty$  as  $k \to \infty$ . Then for any  $\varepsilon > 0$ , there exists a sequence  $(F_{T,k})_{k\ge 1}$  of subsets of  $\mathcal{X}^T$  with  $\lim_{k\to\infty} \pi_{T,k}(F_{T,k}) = 1$  such that

$$\begin{split} \sup_{\mathbf{x}_{1:T}\in F_{T,k}} & \|P_{\mathsf{Particle-m}\mathsf{GRAD},k}(\cdot|\mathbf{x}_{1:T}) \\ & -P_{\mathsf{Particle-MALA},k}(\cdot|\mathbf{x}_{1:T})\|_{\mathsf{TV}} \in \mathcal{O}(\lambda_{k}^{-(1-\varepsilon)/4}); \\ \sup_{\mathbf{x}_{1:T}\in F_{T,k}} & \|P_{\mathsf{Particle-a}\mathsf{GRAD},k}(\cdot|\mathbf{x}_{1:T}) \\ & -P_{\mathsf{Particle-a}\mathsf{MALA},k}(\cdot|\mathbf{x}_{1:T})\|_{\mathsf{TV}} \in \mathcal{O}(\lambda_{k}^{-(1-\varepsilon)/4}). \end{split}$$

### Talk outline

- $1. \ State-space \ models/Feynman-Kac \ representation$
- 2. Existing methods
- 3. Particle extensions of MALA and aMALA
- 4. Particle extensions of mGRAD and aGRAD
- 5. Numerical illustration
- 6. Summary

### Multivariate stochastic volatility model

• Potential function/observation density:

$$G_t(\mathbf{x}_{t-1:t}) = g_t(\mathbf{y}_t | \mathbf{x}_t) = \mathcal{N}(\mathbf{y}_t; \mathbf{0}, \operatorname{diag}(\exp \mathbf{x}_t)).$$

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• Mutation kernel/transition density:

$$M_t(\mathbf{x}_t|\mathbf{x}_{t-1}) = f_t(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; 0.9\mathbf{x}_{t-1}, \tau \mathbf{H}),$$

where, with  $\rho=0.25$  ,

$$\mathbf{H} = \begin{bmatrix} 1 & \rho & \cdots & \rho \\ \rho & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \rho \\ \rho & \cdots & \rho & 1 \end{bmatrix}$$

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- The prior variance  $\tau>0$  controls 'prior informativeness'.

## Multivariate stochastic volatility model, continued T = 128, D = 30, N = 31; $\delta_t$ tuned to achieve 75 % acceptance rate



Proposed methods which do not require (conditionally or unconditionally) Gaussian dynamics compared with Particle-RWM as a baseline.

### Multivariate stochastic volatility model, continued T = 128, D = 30, N = 31; $\delta_t$ tuned to achieve 75 % acceptance rate



Proposed methods which require only *conditionally* Gaussian dynamics, i.e.,  $M_t(\mathbf{x}_t | \mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{m}_t(\mathbf{x}_{t-1}), \mathbf{C}_t(\mathbf{x}_{t-1}))$  (Particle-mGRAD algorithm also needs  $\mathbf{C}_t(\mathbf{x}_{t-1}) = \mathbf{C}_t$ ). ' $(\kappa = 0$ ' indicates no gradient usage. <sup>57 / 61</sup>

## Multivariate stochastic volatility model, continued $T = 128, D = 30, N = 31; \delta_t$ tuned to achieve 75% acceptance rate



Proposed methods which require *unconditionally* Gaussian dynamics i.e.,  $M_t(\mathbf{x}_t|\mathbf{x}_{t-1}) = N(\mathbf{x}_t; \mathbf{F}_t \mathbf{x}_{t-1} + \mathbf{b}_t, \mathbf{C}_t)$ , compared with aGRAD (which also makes this assumption) as baseline. '( $\kappa = 0$ )' indicates no gradient usage.<sup>58 / 61</sup>

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- All our methods are exact (they leave  $\pi_T(\mathbf{x}_{1:T})$  invariant).

### Summary, continued

The methods mentioned in this work (new methods are in *italic*).

Method	Special case if $N = T = 1$
CSMC <sup>†</sup>	IMH
Particle-RWM	RWM
Particle-aMALA	aMALA
Particle-MALA	MALA
Particle-aMALA+	aMALA
Particle-aGRAD	aGRAD
Particle-mGRAD	mGRAD
Particle-aGRAD+	aGRAD
Twisted Particle-aGRAD(+)	aGRAD
Particle-PCNL & more <sup>‡</sup>	PCNL

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- More details: https://arxiv.org/pdf/2401.14868
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