Parallel computations for Metropolis Markov chains with Picard maps

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Outline

- **Overview**
- **Picard Map** Φ for **Markov chain simulation**
- **Main theoretical results**
- **Simulations**
- (Technical Appendix, only if time allows) **Contraction of** Φ

S. Grazzi, G. Zanella, ***Parallel computations for Metropolis Markov chains with Picard maps.*** **arXiv:2506.09762**

Overview

Zeroth-order Parallel Sampling

- **Objective**: Sample from a distribution $\pi(\mathrm{d}x) = C\exp(-V(x))\mathrm{d}x$ on $\mathcal{X} = \mathbb{R}^d$, for some unknown constant C.
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Performance

(Parallel round) complexity: number of point-wise evaluations of V per parallel processor in order to obtain samples close to π (e.g. in total variation).

- **Important quantities**: dimension d, number of processors K.

Diagram Parallel sampling

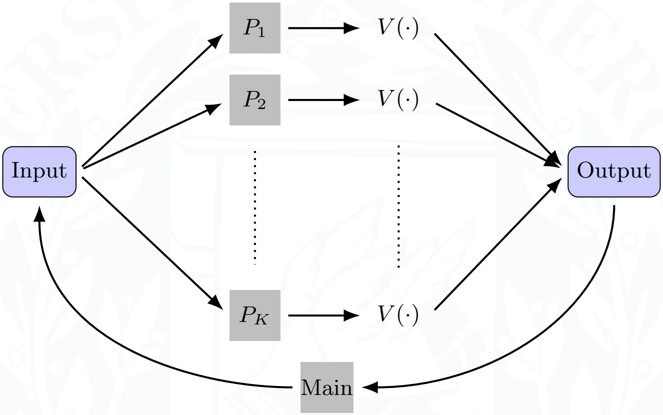

Figure 1: One parallel iteration of the algorithm

Markov chain Monte Carlo

- **Approach:** Markov chain Monte Carlo i.e. **simulate** a Markov chain

$$X_{i+1} = X_i + f(X_i, W_i)\,, \qquad\qquad i = 0, 1, \ldots \tag{1}$$

  whose limiting distribution coincides with π, for some i.i.d random variables $W_0, W_1, \ldots$

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How do we parallelize the recursion in (1)*, given its sequential nature?*

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- **Preview of our results:**

Algorithm	complexity	K	method
Sequential algorithm	$\mathcal{O}(d)$	1	exact
Online Picard	$\mathcal{O}(\sqrt{d})$	$\mathcal{O}(\sqrt{d})$	exact
Approx. Online Picard	$\mathcal{O}(1)$	$\mathcal{O}(d)$	approximate

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Picard map for Markov chain simulation

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- Compute X as the limit of the recursion $X^{(j)} = \Phi(X^{(j-1)}, W)$ for $j = 1, 2, \dots$

Diagram Picard recursion

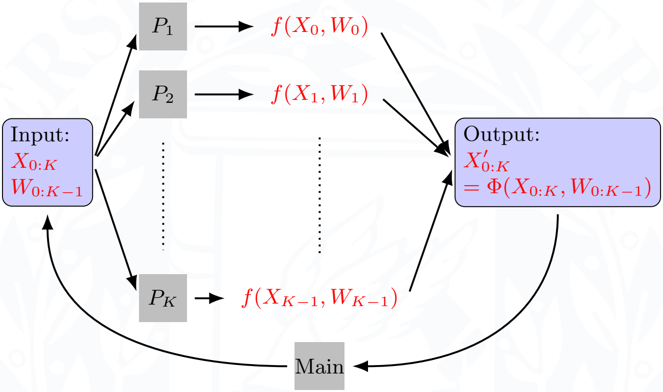

Figure 2: One parallel iteration of Picard recursion

Illustration Picard map

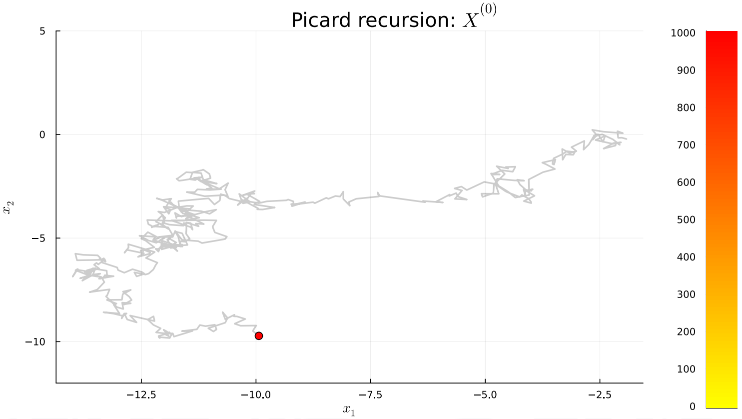

Figure 3: $X_1^{(i)}, X_2^{(i)}, \ldots$ of the Picard recursion for $K = 1000$ steps applied to a $d = 100$ dimensional RWM Markov chain. Gray line: Fixed point $X_1, \ldots, X_K$. The dashed line corresponds to the part of the trajectory that has converged to its fixed point.

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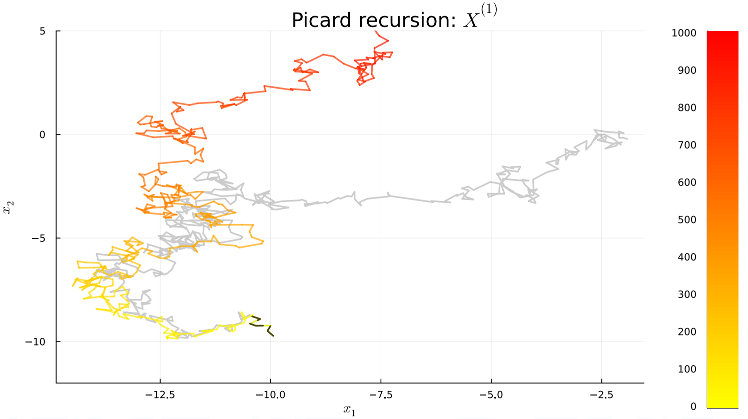

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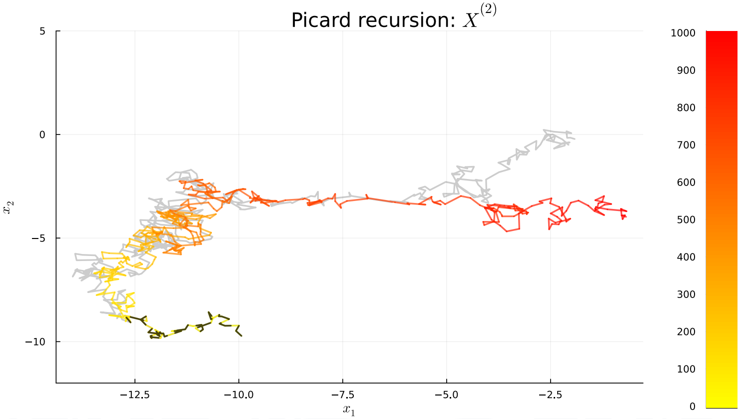

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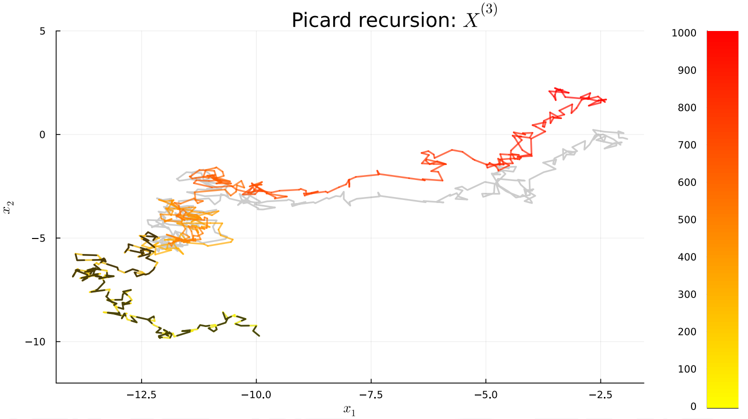

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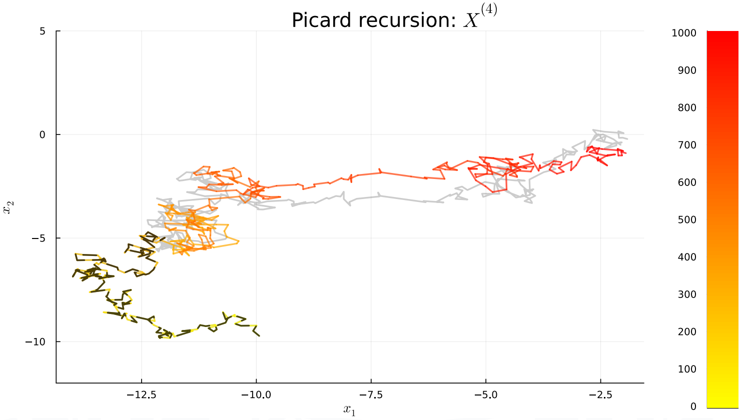

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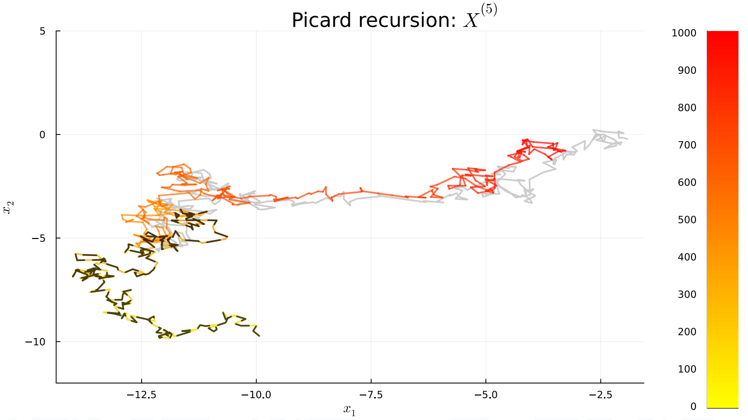

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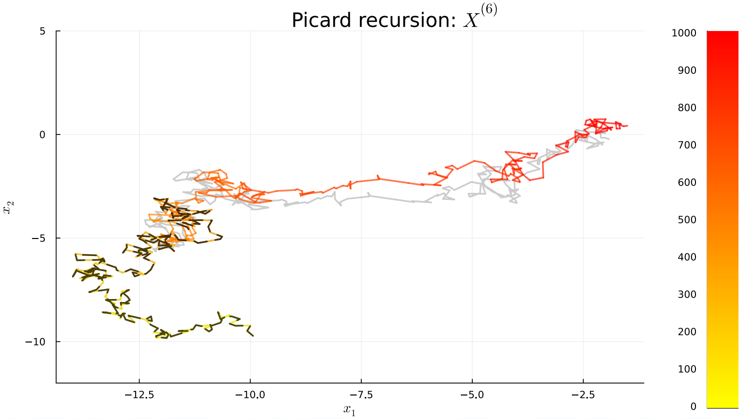

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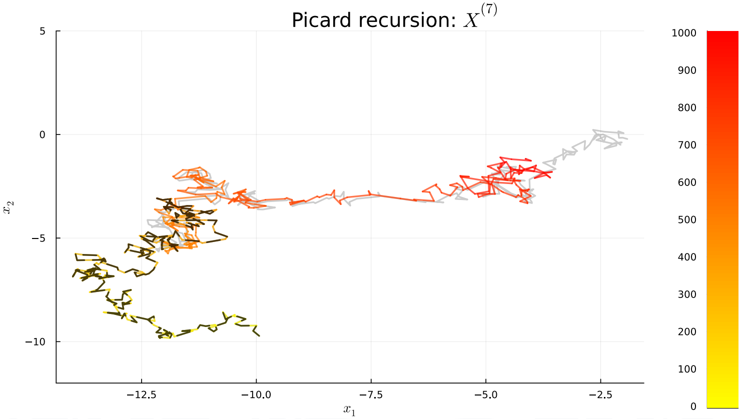

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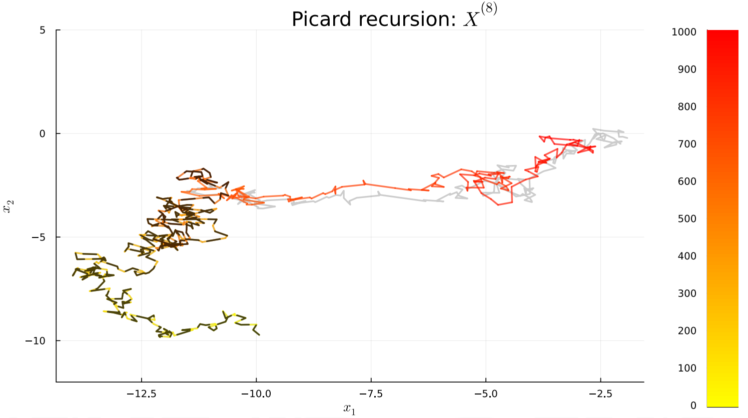

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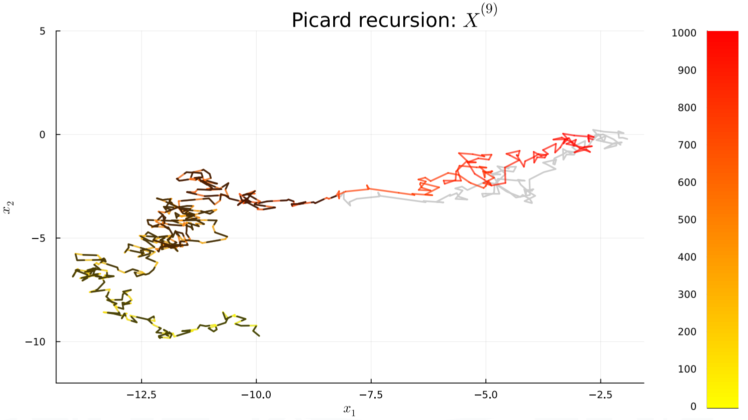

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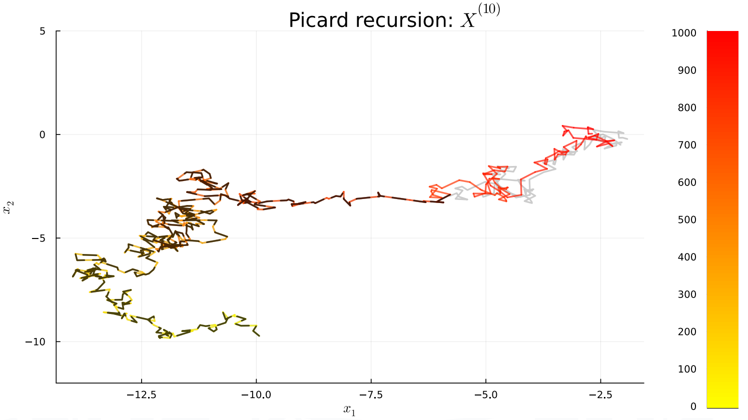

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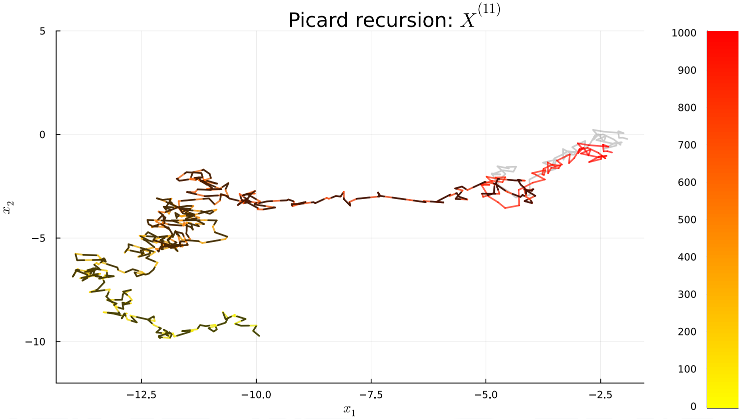

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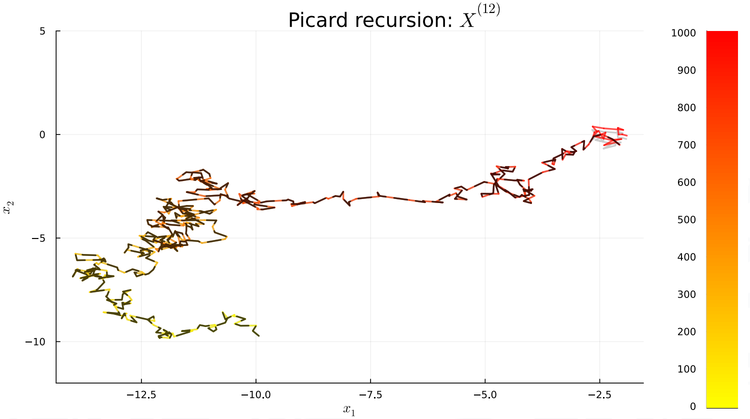

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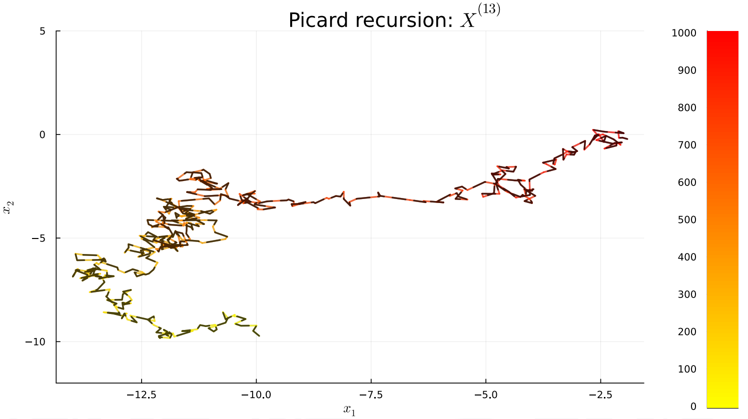

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- Piecewise constant $x \mapsto f(x, w)$:
  - The contraction of the Picard map for RWM is **non-standard**.
  - $X \mapsto \Phi(X, W)$ for RWM is **constant in a neighborhood of its fixed point**.
  - The fixed point of Φ can be reached exactly.

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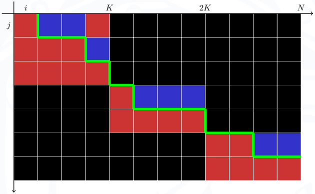

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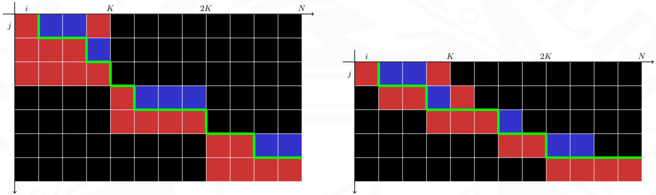

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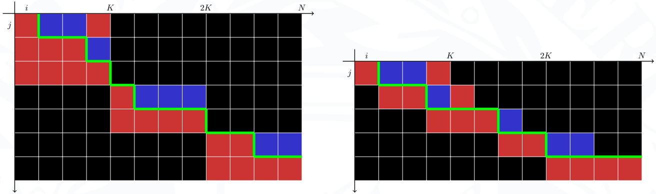

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- **Key challenges for analyzing the convergence:**
  - For each (j, i) square: probability of (error) vs (correct guess).

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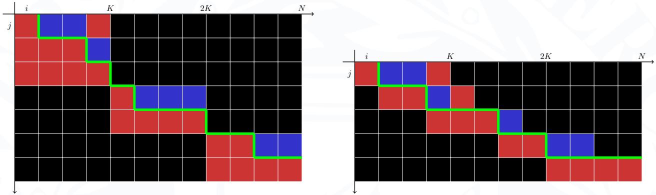

Figure 4: The color of the (j, i) entry represents the state of the ith step: ■ for $f(X_i^{(j)}, W_i) = f(X_i^{(j-1)}, W_i)$ (correct guess), ■ for $f(X_i^{(j)}, W_i) \neq f(X_i^{(j-1)}, W_i)$ (error). ■ where no processor has been allocated. ▬: number of steps simulated according to RWM.

- **Key challenges for analyzing the convergence:**
  - For each (j, i) square: probability of ■ (error) vs ■ (correct guess).
  - For each row j: probability of a strike of $n > 1$ consecutive ■ (or equivalently the probability of the first ■).

Theoretical results

Probability of an error (■)

- Technical assumption: V is L-smooth and Hessian-Lipschitz.

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After $j \geq \log(d)$ steps we have

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- $T_{K,N}$: number of iterations of OPA for simulating N steps with K processors

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Corollary 1 (Complexity OPA)

For log-concave distributions, the Online Picard algorithm with $K = \mathcal{O}(\sqrt{d})$ outputs a random variable X, with $\|\mathcal{L}(X) - \pi\|_{\mathrm{TV}} \leq \epsilon$ after

$$J = \mathcal{O}\left(\frac{L}{m}\sqrt{d}\,\mathrm{polylog}(\epsilon^{-1})\right) \quad \text{parallel iterations.}$$

- Corollary 1 was obtained by combining Theorem 2 with known mixing time bounds of RWM (Andrieu et al. 2024)

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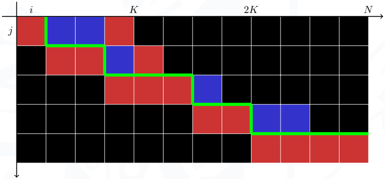

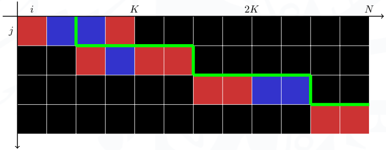

Figure 5: Illustration of OPA (left) vs AOPA with $r = 50\%$ (right). The color of the (j, i) entry represents the state of the ith step: ■ for $f(X_i^{(j)}, W_i) = f(X_i^{(j-1)}, W_i)$ (correct guess), ■ for $f(X_i^{(j)}, W_i) \neq f(X_i^{(j-1)}, W_i)$ (error). ■ where no processor has been allocated.

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  - All convergence results also apply to Metropolis within Gibbs.
  - For Metropolis within Gibbs, we have instantaneous convergence for isotropic Gaussian targets, suggesting better performance for well-conditioned targets.

Simulations

Logistic Regression

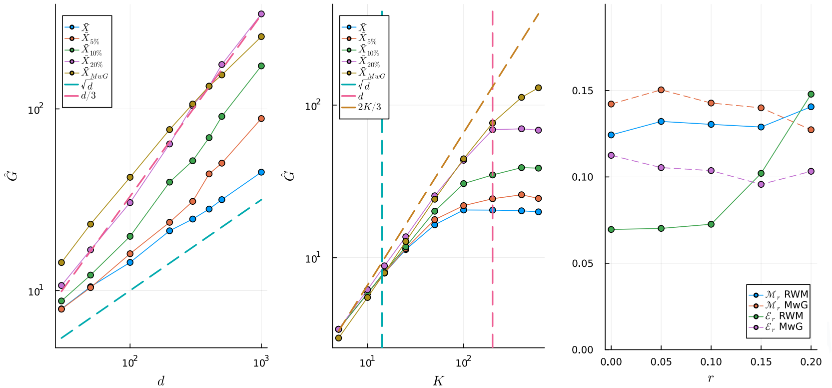

Figure 6: Performance of OPA ($\bar{X}$) and its AOPA ($\bar{X}_r,\ r = 0\%, \ldots, 20\%$) applied to RWM and MwG ($\bar{X}_{MwG}$). Average speedup $\hat{G} = N/T_{K,N}$, $K = d$, $d = 10^2, \ldots, 10^3$ (Left panel) and $d = 200$, $K = 2, 3, \ldots, 10^3$. Right panel: Average error on 1st $(\mathcal{M}_r)$ and 2nd $(\mathcal{E}_r)$ moment estimation for the AOPA with $r = 0\%, \ldots, 20\%$

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Conclusion

- **Recap**:

Algorithm	complexity	K	method
Sequential algorithm	$\mathcal{O}(d)$	1	exact
Online Picard	$\mathcal{O}(\sqrt{d})$	$\mathcal{O}(\sqrt{d})$	exact
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  - Develop more advanced algorithms combining **"cheap" predictions** with **Picard maps** (e.g. Parareal framework)

- Andrieu, Christophe et al. (2024). “Explicit convergence bounds for Metropolis Markov chains: isoperimetry, spectral gaps and profiles”. In: *The Annals of Applied Probability* 34.4, pp. 4022–4071.
- Grazzi, Sebastiano and Giacomo Zanella (2025). *Parallel computations for Metropolis Markov chains with Picard maps*. arXiv: 2506.09762 [stat.CO]. URL: https://arxiv.org/abs/2506.09762.
- Pozza, Francesco and Giacomo Zanella (2024). “On the fundamental limitations of multiproposal Markov chain Monte Carlo algorithms”. In: *arXiv preprint arXiv:2410.23174*.

Contraction of the Picard map

Lemma 1

Under Assumptions 3, for every $x, y \in \mathcal{X}$,

$$\mathbb{P}(f(x, W) \neq f(y, W)) \leq \frac{hL^{1/2}}{d^{1/2}} \left(\sqrt{\frac{2}{\pi}} + \frac{h\gamma}{2} \right) \|x - y\|, \qquad W \sim \nu.$$

Lemma 2

Under Assumption 2 and for all $x, y \in \mathcal{X}^{K+1}$ with $x_0 = y_0, w_0 \in \mathcal{W}$ and $1 < i \leq d$,

$$\mathbb{E}[\|\Phi_i(x, W) - \Phi_i(y, W)\|^2] \leq \frac{15h^2}{L} \sum_{\ell=1}^{i-1} \left(\mathbb{P}(f(x_\ell, W_\ell) \neq f(y_\ell, W_\ell)) + \delta(d)\right).$$

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Lemma 3 and 4 implies Theorem 1, i.e.

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