# A new algorithm on constrained sampling : MAPLA.

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Paper : High-accuracy sampling from constrained spaces with the Metropolis-adjusted Preconditioned Langevin Algorithm, (SRINIVASAN; WIBISONO; WILSON, 2025)

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# Summary

# Unconstrained Sampling

**PROBLEM :** Sampling from a density with unconstrained support in the case of smooth log-concave density.

## Definition

Given an integer $p \geq 2$ and a measurable function $f : \mathbb{R}^p \longrightarrow \mathbb{R}$ such that the integral $\int_{\mathbb{R}^p} \exp\{-f(\theta)\}\, d\theta < \infty$. If $f$ is $m$-strongly convex with a $M$-Lipschitz continuous gradient then the density

$$\pi(\theta) \propto \exp\{-f(\theta)\}$$

is a smooth log-concave density.

with $f$ satisfies for all $\theta, \bar{\theta} \in \mathbb{R}^p$

$$\begin{aligned} f(\theta) - f(\bar{\theta}) - \nabla f(\bar{\theta})^\top (\theta - \bar{\theta}) &\geq \frac{m}{2} \|\theta - \bar{\theta}\|_2^2, \\ \|\nabla f(\theta) - \nabla f(\bar{\theta})\|_2 &\leq M \|\theta - \bar{\theta}\|_2. \end{aligned} \tag{1}$$

# Langevin Monte Carlo Algorithm (LMC)

- Given $\theta^{(0)} \in \mathbb{R}^p$ random or deterministic
- For $k \geq 0, \ \theta^{(k+1,h)} = \theta^{(k,h)} - h\nabla f(\theta^{(k,h)}) + \sqrt{2h}\xi^{k+1}$ with

Where $h > 0$ is the step-size and $\xi^{(k)} \underset{iid}{\sim} \mathcal{N}_p(0,\ I_p)$ independent of $(\theta_i)_{i=0\dots n}$

**Notice** that LMC is a gradient descent with an additional Gaussian random perturbation and also the Euler Discretization of the Langevin Dynamic (LD).

- the target distribution $P_\pi$ with density $\pi \propto \exp\{-f\}$
- the distribution of $\theta^{(K,h)}$ when $h$ is small and $K$ is large such that $T = Kh$ is large.

# An upper bound

## Theorem

*(DALALYAN, 2016) Let $\theta^\star \in \mathbb{R}^p$ be the global minimum of f and assume that for some $\alpha \geq 1$, we have $h \leq 1/(\alpha M)$ and $K \geq \alpha$. Then, for any time horizon $T = Kh$. The approximation $\nu P_\theta^K$ furnished by the LMC algorithm with the initial distribution $\nu = \mathcal{N}_p(\theta^*, M^{-1} I_p)$ satisfies*

$$\|\nu P_\theta^K - P_\pi\|_{TV} \leq \frac{1}{2} \exp\left(\frac{p}{4}\log\left(\frac{M}{m}\right) - \frac{Tm}{2}\right) + \left(\frac{pM^2 Th\alpha}{4(2\alpha - 1)}\right)^{1/2}.$$

**GOAL : Same result for constrained sampling**

# One approach for constrained sampling

**PROBLEM :** Sampling from a density with constrained support in the case of smooth log-concave density. (BUBECK; ELDAN; LEHEC, 2015)

- Let $\mathcal{K} \subset \mathbb{R}^n$ be a convex body such that $0 \in \mathcal{K}$, $B(0, r) \subset \mathcal{K} \subset B(0, R)$.
- Let $\text{Proj}_{\mathcal{K}}$ denote the Euclidean projection onto $K$.
- Let $f : \mathcal{K} \to \mathbb{R}$ be an $L$-Lipschitz and $\beta$-smooth convex function, i.e., $f$ is differentiable and satisfies the following conditions: for all $|\nabla f(x)| \leq L$, and $x, y \in K$, $|\nabla f(x) - \nabla f(y)| \leq \beta |x - y|$.

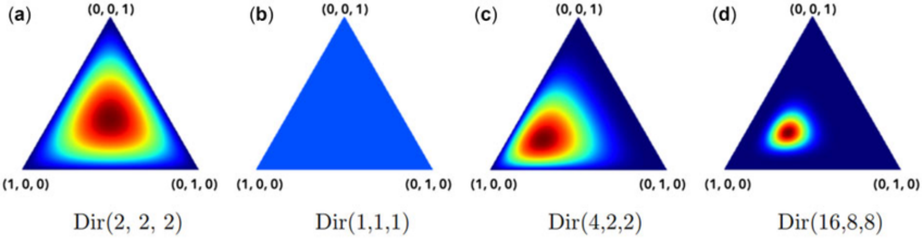
$$X_{k+1} = \text{Proj}_{\mathcal{K}} \left( X_k - \frac{\eta}{2} \nabla f(X_k) + \sqrt{\eta}\, \xi_k \right), \ \eta > 0$$

# Dirichlet distribution $\mathcal{D}(a)$

Let $\mathcal{K} := \Delta_{d+1} = \{x \in \mathbb{R}_+^d : \mathbf{1}^\top x \leq 1\}$ and

$$\pi(x) \propto \exp(-f(x)); \quad f(x) = -\sum_{i=1}^{d} a_i \log x_i - a_{d+1} \log\left(1 - \sum_{i=1}^{d} x_i\right) .$$

where $\mathbf{a} \in \mathbb{R}^{d+1}$ and $a_i > 0$,



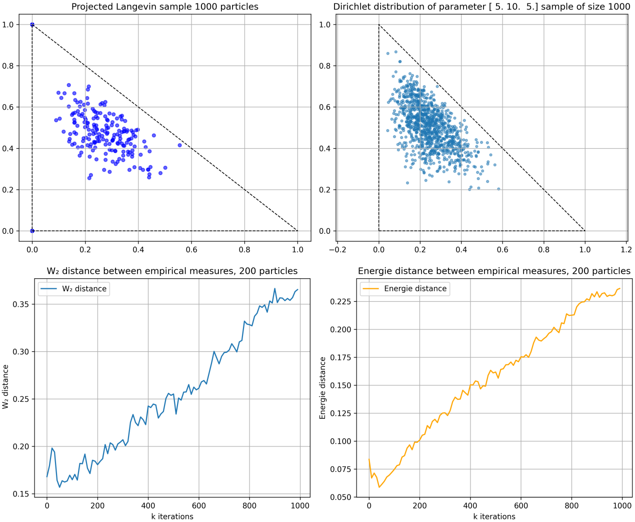
# Metrics

$$W_2^2(P,Q) = \inf\{\mathbb{E}[\|X - Y\|^2],\ X \sim P \text{ and } Y \sim Q\}$$

$$ED(\hat{P},\hat{Q}) = \frac{2}{N^2}\sum_{i,j=1}^{N}\|X_i - Y_j\| - \frac{1}{N^2}\sum_{i,j=1}^{N}\|X_i - X_j\| - \frac{1}{N^2}\sum_{i,j=1}^{N}\|Y_i - Y_j\|$$

where $\hat{P} = \frac{1}{N}\sum_{i=1}^{N}\delta_{X_i}$ and $\hat{Q} = \frac{1}{N}\sum_{i=1}^{N}\delta_{Y_i}$

# First case : Corner issue, case of $\mathcal{D}([5, 10, 5])$



# Solution : Removing the points on the boundary of the polytope

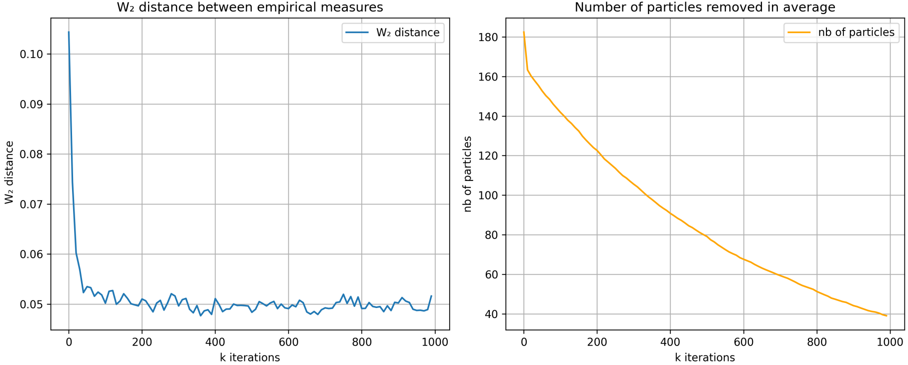
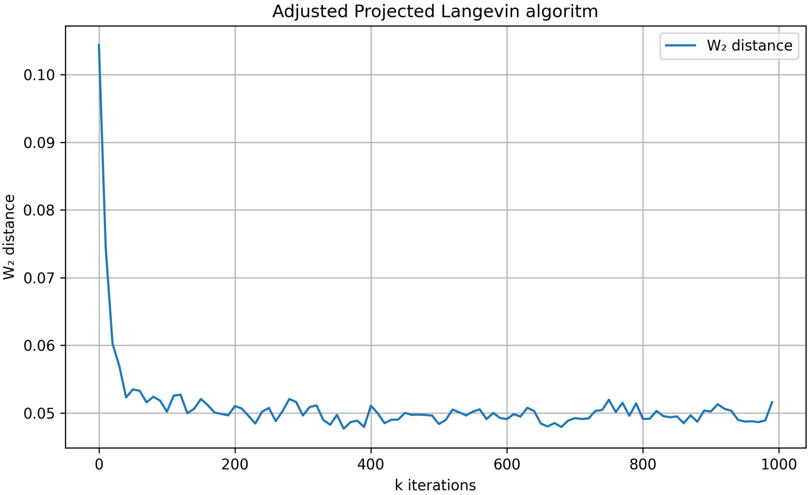
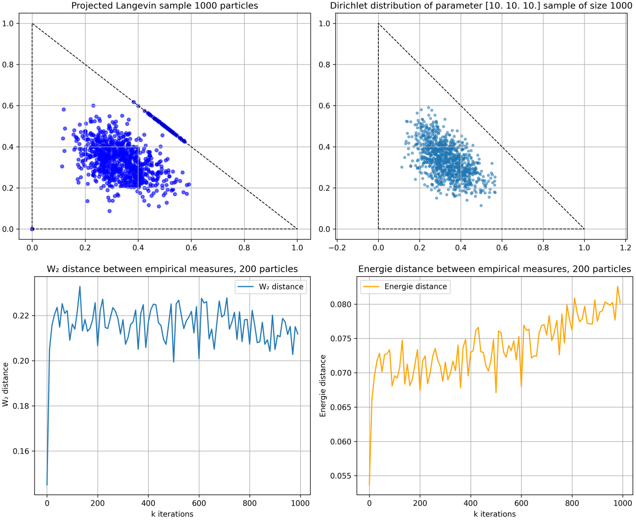



Figure: $W_2$ distance between the empirical measures (Left) and number of particle removed (Right)

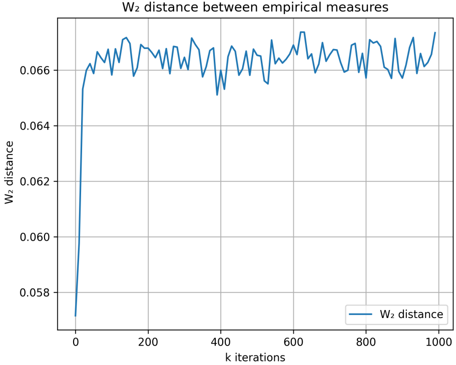
# Solution : Metropolis-Hastings Adjustment



# Second case : Diagonal issue, case of $\mathcal{D}([10, 10, 10])$



# Solution : Removing the points on the boundary of the polytope



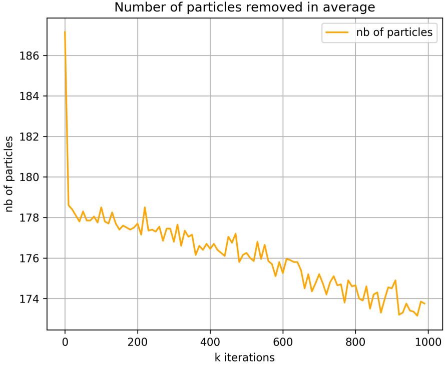
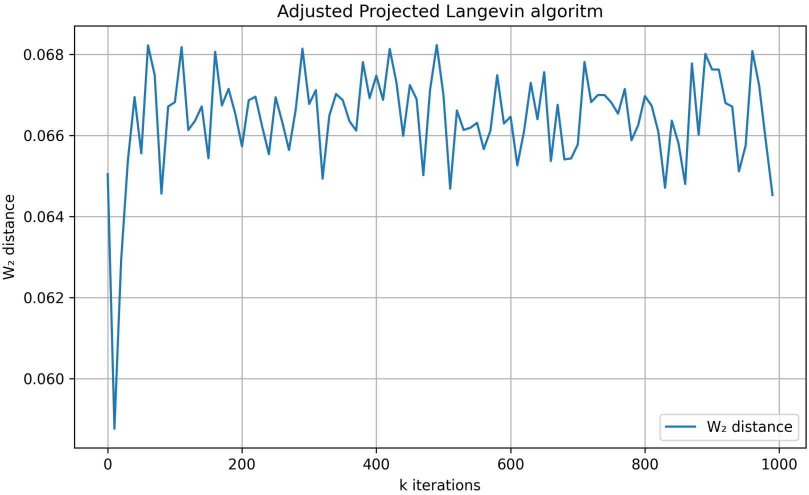




Figure: $W_2$ distance between the empirical measures (Left) and number of particle removed (Right)

# Solution : Metropolis Hasting Adjustment



# Metropolis-Adjusted Preconditioned Langevin Algorithm (MAPLA)

**Idea :** The procedure is adjusting the Markov chain of the discrete version (Euler) of the following SDE with Metropolis-Hastings filter.
Given a function $\mathscr{G} : \mathrm{int}(\mathcal{K}) \to \mathbb{S}_+^d$ called a metric,

$$\mathrm{d}X_t = \mathfrak{m}(X_t)\mathrm{d}t + \sqrt{2} \cdot \mathscr{G}(X_t)^{-1/2}\,\mathrm{d}B_t \tag{2}$$

$$\mathfrak{m}(X_t) = -\mathscr{G}(X_t)^{-1}\nabla f(X_t) \tag{3}$$

The discretization gives MAPLA

$$X_{k+1} - X_k = -h \cdot \mathscr{G}(X_k)^{-1}\nabla f(X_k) + \sqrt{2h} \cdot \mathscr{G}(X_k)^{-1/2}\,\xi_k \;; \quad \xi_k \sim \mathcal{N}\left(0,\ \mathrm{I}_{d\times d}\right)$$

$(X_k)_{k\geq 0}$ is an homogeneous Markov chain defined by a collection of transition probability $\mathbf{P} = \{\mathcal{P}_x,\ x \in \mathcal{K}\}$, for any $x \in \mathcal{K}$

$$\mathcal{P}_x = \mathcal{N}\left(x - h \cdot \mathscr{G}(x)^{-1}\nabla f(x),\ 2h \cdot \mathscr{G}(x)^{-1}\right)$$

**Take this kernel as a proposal in the Metropolis-Hastings filter**

# Related Algorithms

Other proposal distributions $P_X \sim \mathcal{N}(\mathfrak{m}(X), 2h \cdot \mathscr{G}(X)^{-1})$

| Algorithm | Mean $\mathfrak{m}(X)$ |
|---|---|
| MAPLA | $X - h \cdot \mathscr{G}(X)^{-1} \nabla f(X)$ |
| ManifoldMALA (*GIROLAMI*;*CALDERHEAD*,2011) | $X + h \cdot \{(\nabla \cdot \mathscr{G}^{-1})(X) - \mathscr{G}(X)^{-1} \nabla f(X)\}$ |
| Dikin (*KOOK*;*VEMPALA*,2024) | $X$ |

# Algorithm

Generate $X_0 \sim \Pi_0$ (initialization)

1. Generate a proposal $Z$ from $\mathcal{P}_X$ where $X$ is current the iterate
2. If $Z \notin \mathcal{K}$, reject $Z$ and set $X$ to be $X'$ (next iterate).
3. If $Z \in \mathcal{K}$, compute the Metropolis-Hastings acceptance probability $p_{X \to Z}$.
4. With probability $p_{X \to Z}$, set $X' = Z$ (accept); otherwise set $X' = X$ (reject).

# Mixing Time and Warm start

## Definition

We introduce the important indicator of convergence

$$\tau_{\mathrm{mix}}(\delta; \mathbf{P}, \mathcal{C}) \stackrel{\mathrm{def}}{=} \sup_{\pi_0 \in \mathcal{C}} \inf\{k \geq 0 : \mathrm{d}_{\mathrm{TV}}(\mathbb{T}_{\mathbf{P}}^{k} \pi_0, \nu) \leq \delta\}$$

with the operator $\mathbb{T}_{\mathbf{P}}$, $(\mathbb{T}_{\mathbf{P}} \mu)(S) = \int_{\mathcal{K}} \mathcal{P}_y(S) \cdot \mathrm{d}\mu(y)$

How to choose $\pi_0$? we choose it be *warm* relative to the target $\pi$

- $\mathrm{Warm}(L_\infty, M, \pi) = \{\pi_0 \in \mathcal{P}(\mathcal{K}), \sup_{A \in \mathcal{F}(\mathcal{K})} \frac{\pi_0(A)}{\pi(A)} \leq M\}$
- $\mathrm{Warm}(L_1, M, \pi) = \{\pi_0 \in \mathcal{P}(\mathcal{K}), \left\| \frac{\mu_0}{\nu} \right\|_{L^1(\mu_0)} = M\}$

**Now one can wonder what kind of assumption to do on $\mathcal{K}$,$\mathscr{G}$ and $f$ to derive a bound**

# Assumptions on $\mathscr{G}$ : *Self-concordance*

- Properties introduced by Nestrerov in optimization.

The metric $\mathscr{G} : \mathrm{int}(\mathcal{K}) \to \mathbb{S}_+^d$ is ***self-concordant*** if

$$\forall\, x \in \mathrm{int}(\mathcal{K}),\ v \in \mathbb{R}^d, \quad \|\mathscr{G}(x)^{-1/2}\mathrm{D}\mathscr{G}(x)[v]\mathscr{G}(x)^{-1/2}\|_{op} \leq 2 \cdot \|v\|_{\mathscr{G}(x)} \,.$$

The metric is ***strongly self-concordant*** if for all $x \in \mathrm{int}(\mathcal{K})$ and $v \in \mathbb{R}^d$,

$$\|\mathscr{G}(x)^{-1/2}\mathrm{D}\mathscr{G}(x)[v]\mathscr{G}(x)^{-1/2}\|_{\mathrm{F}} \leq 2 \cdot \|v\|_{\mathscr{G}(x)} \,.$$

# Assumptions on $f$ : Curvature and Lipschitzness

The potential $f : \mathrm{int}(\mathcal{K}) \to \mathbb{R}$ satisfies a **$(\mu, \mathscr{G})$*-curvature lower bound*** where $\mu \geq 0$ if for any $x \in \mathrm{int}(\mathcal{K})$,

$$\nabla^2 f(x) \succeq \mu \cdot \mathscr{G}(x)$$

The potential $f$ satisfies a **$(\lambda, \mathscr{G})$*-curvature upper bound*** where $\lambda \geq 0$ if for any $x \in \mathrm{int}(\mathcal{K})$,

$$\nabla^2 f(x) \preceq \lambda \cdot \mathscr{G}(x) \ .$$

the potential $f$ satisfies a **$(\beta, \mathscr{G})$*-gradient upper bound*** where $\beta \geq 0$ if for any $x \in \mathrm{int}(\mathcal{K})$,

$$\|\nabla f(x)\|_{\mathscr{G}(x)^{-1}} \leq \beta \ .$$

# Assumption on $K$ : symmetry

The metric $\mathscr{G}$ is said to be ***symmetric*** with parameter $\nu \geq 1$ if for any $x \in \mathrm{int}(\mathcal{K})$,

$$\mathcal{E}_x^{\mathscr{G}}(1) \subseteq \mathcal{K} \cap (2x - \mathcal{K}) \subseteq \mathcal{E}_x^{\mathscr{G}}(\sqrt{\nu})$$

With $\mathcal{E}_x^{\mathscr{G}}(r)$ the Dikin ellipsoid of radius $r$ defined as

$$\mathcal{E}_x^{\mathscr{G}}(r) = \{y : \|y - x\|_{\mathscr{G}(x)} < r\}$$

# First case Theorem : Self-concordant version

Define the quantity $b_{\mathrm{SC}}(d, \lambda, \beta)$

$$b_{\mathrm{SC}}(d, \lambda, \beta) \stackrel{\text{def}}{=} c_1 \cdot \min\left\{\frac{1}{d^3}, \frac{1}{d \cdot \lambda}, \frac{1}{\beta^2}, \frac{1}{\beta^{2/3}}, \frac{1}{(\beta \cdot \lambda)^{2/3}}\right\}$$

## Theorem

*For precision $\delta \in (0, 1/2)$ and warmness parameter $M \geq 1$, if the step size $h$ is bounded as $0 < h \leq b_{SC}(d, \lambda, \beta)$, $\mathcal{C} \in \{\mathrm{Warm}(L_\infty, M, \pi), \mathrm{Warm}(L_1, M, \pi)\}$ that*

$$\tau_{\mathrm{mix}}(\delta; \mathbf{T}, \mathcal{C}) = \frac{c_2}{h} \cdot \max\left\{1, \min\left\{\frac{1}{\widetilde{\mu}^2}, \nu\right\}\right\} \cdot \log\left(\frac{\mathfrak{m}_{\mathcal{C}}}{\delta}\right) ,$$

$$\mathfrak{m}_{\mathcal{C}} = \begin{cases} M^{1/2}, & \mathcal{C} = \mathrm{Warm}(L_\infty, M, \pi) \\ M^{1/3}, & \mathcal{C} = \mathrm{Warm}(L_1, M, \pi) \end{cases} , \quad \widetilde{\mu} = \frac{\mu}{8 + 4\sqrt{\mu}}$$

where $c_1, c_2$ are universal positive constants.

# Assumptions on $\mathscr{G}$ : *Self-concordance*$_{++}$

The metric is said to be ***lower trace self-concordant*** with parameter $\alpha \geq 0$ if for all $x \in \mathrm{int}(\mathcal{K})$ and $v \in \mathbb{R}^d$,

$$\mathrm{tr}(\mathscr{G}(x)^{-1}\mathrm{D}^2\mathscr{G}(x)[v,v]) \geq -\alpha \cdot \|v\|^2_{\mathscr{G}(x)} \, .$$

The metric is said to be ***average self-concordant*** if for any $x \in \mathrm{int}(\mathcal{K})$ and $\varepsilon > 0$, there exists $r_\varepsilon > 0$ such that for any $h \in (0, \frac{r_\varepsilon^2}{2d}]$,

$$\mathbb{P}_{\xi \sim \mathcal{N}(x, 2h \cdot \mathscr{G}(x)^{-1})}\left(\|\xi - x\|^2_{\mathscr{G}(\xi)} - \|\xi - x\|^2_{\mathscr{G}(x)} \leq 4h \cdot \varepsilon\right) \geq 1 - \varepsilon$$

$\boxed{\text{\textit{self-concordant}}_{++} = \textbf{\textit{strong, lower-trace and average}}\ \text{\textit{self-concordance}}}$

# Summary and main results

| Conditions | | Mixing time scaling |
|---|---|---|
| $f$ is $\begin{cases} (\mu,\mathscr{G})\text{-curv. lower-bdd.} \\ (\lambda,\mathscr{G})\text{-curv. upper-bdd.} \\ (\beta,\mathscr{G})\text{-grad. upper-bdd.} \end{cases}$ & | $\mathscr{G}$ is $\begin{cases} \text{self-concordant} \\ \nu\text{-symmetric} \end{cases}$ | $\min\left\{\nu, \frac{1}{\mu}\right\} \cdot \max\{d^3, d\lambda, \beta^2\}$ (Theorem 4.1) |
| | $\mathscr{G}$ is $\begin{cases} \text{self-concordant}_{++} \\ \nu\text{-symmetric} \end{cases}$ | $\min\left\{\nu, \frac{1}{\mu}\right\} \cdot \max\{d\beta, d\lambda, \beta^2\}$ (Theorem 4.2) |
| $f$ is linear | & $\mathscr{G}$ is $\begin{cases} \text{self-concordant}_{++} \\ \nu\text{-symmetric} \end{cases}$ | $\nu \cdot d^2$ (Theorem 4.3) |

# Elements of proof : One-step overlap technique, Lovász (1999)

Let $s \in (0, 1/2)$. The $s$-conductance of $\mathbf{T} = \{\mathcal{P}_x : x \in \mathcal{K}\}$ (MAPLA) with stationary distribution $\pi$ (thanks to MF) supported on $\mathcal{K}$ is defined as

$$\Phi_{\mathbf{T}}^{s} = \inf_{\substack{A \in \mathcal{F}(\mathcal{K}) \\ \nu(A) \in (s, 1-s)}} \frac{1}{\min\{\nu(A) - s,\ 1 - \nu(A) - s\}} \cdot \int_A \mathcal{P}_x(\mathcal{K} \setminus A) \cdot \mathrm{d}\nu(x) .$$

The (ordinary) conductance $\Phi_{\mathbf{P}}$ of $\mathbf{P}$ is the limit of $\Phi_{\mathbf{P}}^{s}$ as $s \to 0$.

(see Vempala 2005) If $\pi_0 \in \mathrm{Warm}(L_\infty, M, \pi)$, then

$$\mathrm{d}_{\mathrm{TV}}(\mathbb{T}_{\mathbf{T}}^{k}\pi_0, \pi) \leq \sqrt{M} \cdot \left(1 - \frac{{\Phi_{\mathbf{T}}}^2}{2}\right)^k \leq \sqrt{M} \cdot \exp\left(-\frac{k \cdot {\Phi_{\mathbf{T}}}^2}{2}\right)$$

By setting the right hand side to be less than $\delta$ for $\delta \in (0, 1/2)$

$$\tau_{\mathrm{mix}}(\delta; \mathbf{T}, \mathcal{C}) = \frac{2}{{\Phi_{\mathbf{T}}}^2} \cdot \log\left(\frac{\sqrt{M}}{\delta}\right) \leq \frac{C'}{h} \cdot \max\left\{1, \min\left\{\frac{1}{\widetilde{\mu}^2}, \nu\right\}\right\} \cdot \log\left(\frac{\sqrt{M}}{\delta}\right)$$

The most important part shows that

$$\Phi_{\mathbf{T}} \geq C \cdot \sqrt{h} \cdot \min\left\{1, \max\left\{\widetilde{\mu}, \frac{1}{\sqrt{\nu}}\right\}\right\} .$$

# Sampling from a Dirichlet distribution

Let $\mathcal{K} := \Delta_{d+1} = \{x \in \mathbb{R}_+^d : \mathbf{1}^\top x \leq 1\}$ and

$$\pi(x) \propto \exp(-f(x)); \quad f(x) = -\sum_{i=1}^{d} a_i \log x_i - a_{d+1} \log\left(1 - \sum_{i=1}^{d} x_i\right) .$$

where $\mathbf{a} \in \mathbb{R}^{d+1}$ and $a_i > -1$, $f$ is satisfies $(a_{\min}, \mathscr{G})$-curvature lower bound, $(a_{\max}, \mathscr{G})$-curvature upper bound, and $(\|a\|, \mathscr{G})$-gradient upper bound.

Which metrics $\mathscr{G}$ ? $\mathscr{G}$ is the norm induced by the Hessian of the log-barrier of the polytope $\Delta_{d+1}$ $K = \left\{x \in \mathbb{R}^d : Ax \leq b\right\}$, $\varphi(x) = -\sum_{i=1}^m \log\left(b_i - a_i^\top x\right)$

and $\nabla^2\varphi(x) = \sum_{i=1}^m \frac{a_i a_i^\top}{(b_i - a_i^\top x)^2}$

# DikinWalk vs MAPLA : Mixing Time

DikinWalk Algorithm (KOOK; VEMPALA, 2024) is the discretization of the process with the drift equal to $0_d$

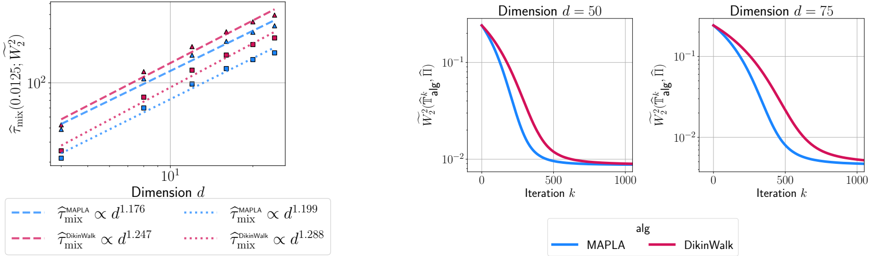



Figure: The dashed and dotted lines correspond to $C_h = 0.1$ and $0.2$ respectively. The markers indicate the average over 20 simulations.

# DikinWalk vs MAPLA : Acceptance rate

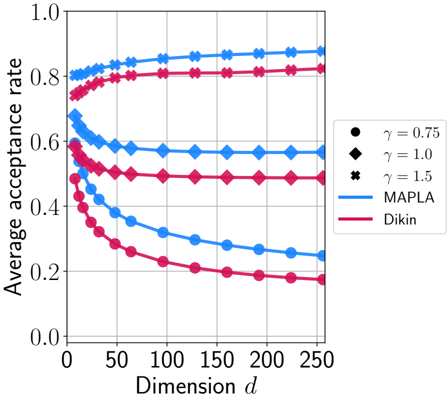



Figure: Variation of $\widehat{R}_{\text{accept}}$ with dimension $d$ when stepsize $h \propto d^{-\gamma}$.

# END !

# PLMC bound

Assume that $r = 1$ and let $\epsilon > 0$. Then one has

$$d_{\mathrm{TV}}(X_N, \mu) \leq \epsilon$$

provided that $\eta = \widetilde{\mathcal{O}}\left(\frac{R^2}{N}\right)$ and that $N$ satisfies the following: if $\mu$ is uniform, then

$$N = \widetilde{\Omega}\left(\frac{R^6 n^7}{\epsilon^8}\right),$$

and otherwise

$$N = \widetilde{\Omega}\left(\frac{R^6 \max(n, RL, R\beta)^{12}}{\epsilon^{12}}\right).$$

# MAPLA Algorithm

**Algorithm 1:** Metropolis-adjusted Preconditioned Langevin Algorithm (MAPLA)

**Input** : Potential $f$ of $\Pi$, convex support $\mathcal{K} \subset \mathbb{R}^d$, metric $\mathscr{G} : \mathrm{int}(\mathcal{K}) \to \mathbb{S}_+^d$, step size $h > 0$, iterations $K$, initial distribution $\Pi_0$

Sample $x_0 \sim \Pi_0$.
**for** $k \leftarrow 0$ **to** $K - 1$ **do**
    Sample a random vector $\xi_k \sim \mathcal{N}(\mathbf{0}, \mathrm{I}_{d \times d})$.
    Generate proposal $z = x_k - h \cdot \mathscr{G}(x_k)^{-1} \nabla f(x_k) + \sqrt{2h} \cdot \mathscr{G}(x_k)^{-1/2}\, \xi_k$.
    **if** $z \notin \mathcal{K}$ **then**
        Set $x_{k+1} = x_k$.
    **else**
        Compute acceptance ratio $p_{\text{accept}}(z; x_k)$ defined in Eq. (1), where $p_y$ is the density of $\mathcal{N}\left(y - h \cdot \mathscr{G}(y)^{-1} \nabla f(y),\ 2h \cdot \mathscr{G}(y)^{-1}\right)$.
        Obtain $U \sim \mathrm{Unif}([0, 1])$.
        **if** $U \leq p_{\text{accept}}(z; x_k)$ **then**
            Set $x_{k+1} = z$.
        **else**
            Set $x_{k+1} = x_k$.
        **end**
    **end**
**end**
**Output:** $x_K$

# Références

BUBECK, S.; ELDAN, R.; LEHEC, J. *Sampling from a log-concave distribution with Projected Langevin Monte Carlo*. 2015.

DALALYAN, A. S. *Theoretical guarantees for approximate sampling from smooth and log-concave densities*. 2016. Disponível em: ⟨https://arxiv.org/abs/1412.7392⟩.

GIROLAMI, M.; CALDERHEAD, B. Riemann manifold Langevin and Hamiltonian Monte Carlo methods. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, Wiley Online Library, v. 73, n. 2, p. 123–214, 2011.

KOOK, Y.; VEMPALA, S. S. Gaussian Cooling and Dikin Walks: The Interior-Point Method for Logconcave Sampling. In: AGRAWAL, S.; ROTH, A. (Ed.). *Proceedings of Thirty Seventh Conference on Learning Theory*. [S.l.]: PMLR, 2024. (Proceedings of Machine Learning Research, v. 247), p. 3137–3240.

SRINIVASAN, V.; WIBISONO, A.; WILSON, A. *High-accuracy sampling from constrained spaces with the Metropolis-adjusted Preconditioned Langevin Algorithm*. 2025.