High-dimensional MCMC: Sampling from log-concave distrutions.

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July 8, 2016

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Smooth case Langevin diffusions and Euler discretization Sampling from strongly log-concave distribution Non-smooth potentials Numerical illustrations

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Introduction

- Sampling distribution over high-dimensional state-space has recently attracted a lot of research efforts in computational statistics and machine learning...
- Applications (non-exhaustive)
 - 1 Bayesian inference for high-dimensional models
 - 2 Bayesian non parametrics
 - 3 Aggregation of estimators and experts
- Most of the sampling techniques known so far do not scale to high-dimension... Challenges are numerous in this area...

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Logistic regression

• Likelihood: Binary regression set-up in which the binary observations (responses) (Y_1, \ldots, Y_n) are conditionally independent Bernoulli random variables with success probability $F(\boldsymbol{\beta}^T X_i)$, where

1 X_i is a d dimensional vector of known covariates,

2 β is a *d* dimensional vector of unknown regression coefficient

3 *F* is a distribution function.

■ logistic regression: *F* is the standard logistic distribution function,

 $F(t) = e^t / (1 + e^t)$

Problem: the number of predictor variables *d* can be large.

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Bayes 101

 Bayesian analysis requires a prior distribution for the unknown regression parameter

$$\pi(\boldsymbol{\beta}) \propto \exp\left(-\frac{1}{2}\boldsymbol{\beta}'\Sigma_{\boldsymbol{\beta}}^{-1}\boldsymbol{\beta}
ight) \quad \text{or} \quad \pi(\boldsymbol{\beta}) = \exp\left(-\sum_{i=1}^{d} \alpha_i |\beta_i|\right)$$

• The posterior of $\boldsymbol{\beta}$ is up to a proportionality constant given by

$$\pi(\boldsymbol{\beta}|(Y,X)) \propto \prod_{i=1}^{n} F^{Y_i}(\boldsymbol{\beta}'X_i)(1 - F(\boldsymbol{\beta}'X_i))^{1-Y_i}\pi(\boldsymbol{\beta})$$

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A daunting problem ?

The posterior density distribution of β is given by Bayes' rule, up to a proportionality constant by

 $\pi(\boldsymbol{\beta}|(Y,X)) \propto \exp(-U(\boldsymbol{\beta}))$.

where the potential $U(\boldsymbol{\beta})$ is given by

 $U(\boldsymbol{\beta}) = -\sum_{i=1}^{p} \{Y_i \log \frac{F(\boldsymbol{\beta}^T X_i)}{1 - F(\boldsymbol{\beta}^T X_i)} + \log(1 - F(\boldsymbol{\beta}^T X_i))\} + \|B\boldsymbol{\beta}\|^{1,2}$

 Classical composite objective function... The prior plays the role of regularization penalty.

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A daunting problem ?

- In the case of the ridge regression, the potential U is smooth strongly convex.
- In the case of the lasso regression, the potential U is non-smooth but still convex...
- A wealth of reasonably fast optimisation algorithms are available to solve this problem in high-dimension...

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Framework

Denote by π a target density w.r.t. the Lebesgue measure on \mathbb{R}^d , known up to a normalisation factor

$$x \mapsto \mathrm{e}^{-U(x)} / \int_{\mathbb{R}^d} \mathrm{e}^{-U(y)} \mathrm{d}y$$

Implicitly, $d \gg 1$.

Assumption: U is L-smooth : continuously differentiable and there exists a constant L such that for all $x, y \in \mathbb{R}^d$,

 $\left\|\nabla U(x) - \nabla U(y)\right\| \le L \|x - y\|.$

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Langevin diffusion

Langevin SDE:

 $\mathrm{d}Y_t = -\nabla U(Y_t)\mathrm{d}t + \sqrt{2}\mathrm{d}B_t \;,$

where $(B_t)_{t\geq 0}$ is a *d*-dimensional Brownian Motion.

Denote for all $x \in \mathbb{R}^d$, $\delta_x P_t$ the law Y_t started at x.

- $\pi \propto e^{-U}$ is reversible \rightsquigarrow the unique invariant probability measure.
- The convergence to the stationary distribution takes place at geometrical rate.
- Precise estimates of the convergence rate (TV, relative entropy) can be obtained using:
 - Functional inequalities: Poincaré or Log-Sobolev inequalities
 - Coupling techniques: synchronous or reflection coupling, depending upon the assumptions (Eberle, 2015)

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Discretized Langevin diffusion

 Idea: Sample the diffusion paths, using for example the Euler-Maruyama (EM) scheme:

$$X_{k+1} = X_k - \gamma_{k+1} \nabla U(X_k) + \sqrt{2\gamma_{k+1}} Z_{k+1}$$

where

- $(Z_k)_{k\geq 1}$ is i.i.d. $\mathcal{N}(0, \mathbf{I}_d)$
- (γ_k)_{k≥1} is a sequence of stepsizes, which can either be held constant or be chosen to decrease to 0 at a certain rate.
- Euler discretization = gradient algorithm + noise.

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Discretized Langevin diffusion: constant stepzize

When $\gamma_k = \gamma$, then $(X_k)_{k \ge 1}$ is an homogeneous Markov chain with Markov kernel R_{γ} with density

$$r_{\gamma}(x,y) = (4\pi\gamma)^{-d/2} \exp\left(-(4\gamma)^{-1} \|y - x + \gamma \nabla U(x)\|^2\right)$$

- Under some appropriate conditions (a bit of positive curvature at infinity), this Markov chain is irreducible, positive recurrent \sim unique invariant distribution π_{γ} .
- Problem: $\pi_{\gamma} \neq \pi$.

The EM Markov chain

- When (γ_k)_{k≥1} is nonincreasing and non constant, (X_k)_{k≥1} is an inhomogeneous Markov chain associated with the sequence of Markov kernel (R_{γk})_{k≥1}.
- Denote by $\delta_x Q^p_{\gamma}$ the law of X_p stated at x.
- Reminder: the diffusion converges to the target distribution
- Question: since the EM disretization approximates the diffusion, can it be used to sample from π ?
 - Is $\delta_x Q^p_\gamma$ close to π for which p ?
 - Can we have some theoretical guarantees ? Particular attention to the dimension *d*, see also Dalalyan 2014.

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Metric on probability spaces

Definition

For μ,ν two probabilities measure on $\mathbb{R}^d,$ define

$$\|\mu - \nu\|_{\mathrm{TV}} = \sup_{|f| \le 1} |\mathbb{E}_{\mu}[f] - \mathbb{E}_{\nu}[f]|$$
.

$$W_2^2(\mu,\nu) = \inf_{\xi \in \mathcal{C}(\mu,\nu)} \int_{\mathbb{R}^{2d}} \|x - y\|^2 \,\xi(\mathrm{d} x,\mathrm{d} y) \; .$$

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Geometric convergence of the Langevin diffusion

If there exists a Lyapunov function for the generator of the diffusion then there exists $\kappa \in [0,1)$ such that for any initial distribution μ_0 and t > 0,

 $\|\mu_0 P_t - \pi\|_{\mathrm{TV}} \le C(\mu_0) \kappa^t ,$

for some explicit function of the initial probability $C(\mu_0)$.

- Explicit expressions of the constant (the way dimension impacts theses constants) critically depends on
 - the assumptions on the potential U
 - the technique of proofs (functional inequalities, coupling constructions, etc...)

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Foster-Lyapunov condition

• A function $V \in C^2(\mathbb{R}^d)$ is a Lyapunov function if $V \ge 1$ and if there exists $\theta > 0$, $b \ge 0$ such that,

 $\mathscr{A}V \leq -\theta V + b ,$

where $\mathscr{A}f = -\langle \nabla U, \nabla f \rangle + \Delta f$ is the generator of the diffusion **Example**: If there exist $\alpha > 1$, $\rho > 0$ and $M_{\rho} \ge 0$ such that for all $y \in \mathbb{R}^d$, $||y|| \ge M_{\rho}$:

 $\langle \nabla U(y), y \rangle \ge \rho \left\| y \right\|^{\alpha}$.

then $V(x) = \exp(U(x)/2)$ is a Lyapunov function.

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Geometric convergence of the Euler discretization

Let (γ_k)_{k≥1} be a sequence of positive and non-increasing step sizes
 Euler discretization:

 $X_{k+1} = X_k - \gamma_{k+1} \nabla U(X_k) + \sqrt{2\gamma_{k+1}} Z_{k+1} ,$

where $(Z_k)_{k\geq 1}$ is i.i.d. $\mathcal{N}(0, I_d)$, independent of X_0 .

• Markov kernel R_{γ} and $x \in \mathbb{R}^d$ by

 $R_{\gamma}(x,A) = \int_{A} \frac{1}{(4\pi\gamma)^{d/2}} \exp\left(-(4\gamma)^{-1} \|y - x + \gamma \nabla U(x)\|^{2}\right) \mathrm{d}y \;.$

• The sequence $(X_n)_{n\geq 0}$ is a (possibly) time-nonhomogeneous Markov chain whose distribution is specified by the Markov kernels $(R_{\gamma_n})_{n\geq 1}$.

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Level-0 results

- The Markov kernel R_{γ} is strongly Feller, irreducible, and hence all the compact sets are therefore small.
- Typically, the R_{γ} satisfies a Foster-Lyapunov drift condition of a particular form, *i.e.* there exists $\kappa \in [0, 1)$, b > 0 such that for all $\gamma > 0$

 $R_{\gamma}V \leq \kappa^{\gamma}V + \gamma b$.

• R_{γ} admits a unique stationary distribution π_{γ} and is *V*-uniformly geometrically ergodic, in the sense that, for some constant $C < \infty$ and $\kappa \in [0, 1)$, such that for all $x \in \mathbb{R}^d$,

$$\left\| R_{\gamma}^{k}(x,\cdot) - \pi_{\gamma} \right\|_{V} \le C(\gamma) \kappa^{\gamma k} V(x)$$

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Example: A drift condition for R_{γ}

Theorem

Assume U is L-smooth and there exist $\rho>0,\,\alpha>1$ and $M_{\rho}\geq 0$ such that :

$$\left\langle
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angle \geq
ho \left\|y
ight\|^lpha \ , \quad ext{for all } y\in \mathbb{R}^d, \ \|y\|\geq M_
ho$$

Then for all $\bar{\gamma} \in (0, L^{-1})$, there exists $b \ge 0$ and s > 0 such that

 $R_{\gamma}V(x) \leq \kappa^{\gamma}V(x) + \gamma b$, for all $\gamma \in (0, \bar{\gamma}]$ and $x \in \mathbb{R}^d$,

where

$$V(x) = \exp(U(x)/2).$$

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Control of moments

By a straightforward induction, we get for all $n \ge 0$ and $x \in \mathbb{R}^d$,

$$Q_{\gamma}^{n}V \leq \kappa^{\Gamma_{1,n}}V + b\sum_{i=1}^{n}\gamma_{i}\kappa^{\Gamma_{i+1,n}} ,$$

where
$$\Gamma_{n,p} = \sum_{k=n}^{p} \gamma_k$$
.

Note that we have

$$\sup_{n\geq 1}\sum_{i=1}^n \gamma_i \kappa^{\Gamma_{i+1,n}} < \infty \; .$$

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Wasserstein distance convergence

• We assume in this part that U is strongly convex: there exist and m > 0, such that for all $x, y \in \mathbb{R}^d$,

 $\langle \nabla U(x) - \nabla U(y), x - y \rangle \ge m \|x - y\|^2$.

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Wasserstein distance convergence

Theorem

Assume that U is strongly convex. Then,

(i) For all probability measures $x, y \in \mathbb{R}^d$ and $t \ge 0$,

 $W_2(\delta_x P_t, \delta_y P_t) \le e^{-mt} \|x - y\|$

(ii) In addition, for any $x \in \mathbb{R}^d$,

 $W_2(\delta_x P_t, \pi) \le C(d) \mathrm{e}^{-mt}$.

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Elements of proof

$$\begin{cases} \mathrm{d}Y_t &= -\nabla U(Y_t)\mathrm{d}t + \sqrt{2}\mathrm{d}B_t \ ,\\ \mathrm{d}\tilde{Y}_t &= -\nabla U(\tilde{Y}_t)\mathrm{d}t + \sqrt{2}\mathrm{d}B_t \ , \end{cases}$$

where $(Y_0, \tilde{Y}_0) = (x, y)$. This SDE has a unique strong solution $(Y_t, \tilde{Y}_t)_{t \ge 0}$ associated to $(B_t)_{t \ge 0}$. Moreover

$$\left\|Y_t - \tilde{Y}_t\right\|^2 = \left\|Y_0 - \tilde{Y}_0\right\|^2 - 2\int_0^t \left\langle (\nabla U(Y_s) - \nabla U(\tilde{Y}_s)), Y_s - \tilde{Y}_s \right\rangle \mathrm{d}s \;,$$

which implies using Grönwall's inequality that

$$\left\|Y_t - \tilde{Y}_t\right\|^2 \le \left\|Y_0 - \tilde{Y}_0\right\|^2 - 2m \int_0^t \left\|Y_s - \tilde{Y}_s\right\|^2 \mathrm{d}s \le \left\|Y_0 - \tilde{Y}_0\right\|^2 \mathrm{e}^{-2mt}$$

The proof follows since for all $t \ge 0$, the law of (Y_t, \tilde{Y}_t) is a coupling between $\delta_x P_t$ and $\delta_y P_t$.

Coupling between the Langevin and the EM discretization

Consider the synchronuous coupling between $(Y_t)_{t\geq 0}$ and $(X_k)_{k\geq 0}$ defined by

$$\begin{cases} dY_t = -\nabla U(Y_t)dt + \sqrt{2}dB_t\\ X_{k+1} = X_k - \gamma_{k+1}\nabla U(X_k) + \sqrt{2\gamma_{k+1}}(B_{\Gamma_{k+1}} - B_{\Gamma_k}) \end{cases}$$

started at $(y, x) \in \mathbb{R}^d \times \mathbb{R}^d$.

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Bound in Wasserstein distance of order $\ensuremath{2}$

• We make an additional regularity assumption on U: The potential U is three times continuously differentiable and there exists \tilde{L} such that for all $x, y \in \mathbb{R}^d$:

$$\left\|\nabla^2 U(x) - \nabla^2 U(y)\right\| \leq \tilde{L} \left\|x - y\right\| \ .$$

• Then for all $x \in \mathbb{R}^d$ and $n \ge 1$,

$$W_2^2(\delta_x Q_{\gamma}^n, \pi) \le u_n^{(1)}(\gamma) \int_{\mathbb{R}^d} \|y - x\|^2 \, \pi(\mathrm{d} y) + u_n^{(2)}(\gamma) \;,$$

where $u_n^{(1)}(\gamma)$ and $u_n^{(2)}(\gamma)$ are explicit.

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Decreasing step sizes

If
$$\lim_{k\to+\infty} \gamma_k = 0$$
 and $\lim_{k\to+\infty} \Gamma_k = +\infty$, then

$$\lim_{p \to +\infty} W_2^2(\delta_x Q_\gamma^p, \pi) = 0 ,$$

with explicit convergence.

• Order of convergence of $W_2^2(\delta_x Q_{\gamma}^n, \pi)$ for $\gamma_k = \gamma_1 k^{-\alpha}$: $\mathcal{O}(n^{-2\alpha})$.

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Fixed step sizes

When $(\gamma_k)_{k\geq 1}$ is held constant:

• We optimize γ and p to get $W_1(\delta_x Q^p_{\gamma}, \pi) \leq \epsilon$. In particular, we find:

$$p = \mathcal{O}(\sqrt{d}\epsilon^{-1})$$
.

• At fixed number of iteration p, we can choose γ such that $W_1(\delta_x Q^p_{\gamma}, \pi) \leq Cn^{-1}$.

• Letting $p \to +\infty$, we get:

$$W_2(\pi_\gamma,\pi) \le C\gamma$$

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Convergence of the Euler discretization in total variation

• If
$$\lim_{\gamma_k \to +\infty} \gamma_k = 0$$
, and $\sum_k \gamma_k = +\infty$ then
$$\lim_{p \to +\infty} \|\delta_x Q_{\gamma}^p - \pi\|_{\mathrm{TV}} = 0 .$$

If the step sizes are constant $\gamma_k = \gamma$ for all $k \in \mathbb{N}$, we can optimize γ and p to get

$$\|\delta_x Q^p_\gamma - \pi\|_{\rm TV} \le \epsilon \; ,$$

for a target precision $\epsilon > 0$.

	d	ε	L	m
γ	$\mathcal{O}(d^{-1})$	$\mathcal{O}(\varepsilon^2/\log(\varepsilon^{-1}))$	$\mathcal{O}(L^{-2})$	$\mathcal{O}(m)$
p	$\mathcal{O}(d\log(d))$	$\mathcal{O}(\varepsilon^{-2}\log^2(\varepsilon^{-1}))$	$\mathcal{O}(L^2)$	$\mathcal{O}(m^{-2})$

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Non-smooth potentials

The target distribution has a density π with respect to the Lebesgue measure on \mathbb{R}^d of the form $x \mapsto \mathrm{e}^{-U(x)} / \int_{\mathbb{R}^d} \mathrm{e}^{-U(y)} \mathrm{d}y$ where U = f + g, with $f : \mathbb{R}^d \to \mathbb{R}$ and $g : \mathbb{R}^d \to (-\infty, +\infty]$ are two lower bounded, convex functions satisfying:

1 f is continuously differentiable and gradient Lipschitz with Lipschitz constant L_f , *i.e.* for all $x, y \in \mathbb{R}^d$

 $\left\|\nabla f(x) - \nabla f(y)\right\| \le L_f \left\|x - y\right\| .$

2 g is lower semi-continuous and $\int_{\mathbb{R}^d} e^{-g(y)} dy \in (0, +\infty)$.

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Moreau-Yosida regularization

Let h: R^d → (-∞, +∞] be a l.s.c convex function and λ > 0. The λ-Moreau-Yosida envelope h^λ : R^d → R and the proximal operator prox_h^λ : R^d → R^d associated with h are defined for all x ∈ R^d by

$$\mathbf{h}^{\lambda}(x) = \inf_{y \in \mathbb{R}^d} \left\{ \mathbf{h}(y) + (2\lambda)^{-1} \left\| x - y \right\|^2 \right\} \le \mathbf{h}(x) \; .$$

For every $x \in \mathbb{R}^d$, the minimum is achieved at a unique point, $\operatorname{prox}_{\mathrm{h}}^{\lambda}(x)$, which is characterized by the inclusion

 $x - \operatorname{prox}_{\mathrm{h}}^{\lambda}(x) \in \gamma \partial \mathrm{h}(\operatorname{prox}_{\mathrm{h}}^{\lambda}(x))$.

■ The Moreau-Yosida envelope is a regularized version of *g*, which approximates *g* from below.

Properties of proximal operators

• As $\lambda \downarrow 0$, converges h^{λ} converges pointwise h, *i.e.* for all $x \in \mathbb{R}^d$, $h^{\lambda}(x) \uparrow h(x)$, as $\lambda \downarrow 0$.

• The function \mathbf{h}^{λ} is convex and continuously differentiable

 $\nabla \mathbf{h}^{\lambda}(x) = \lambda^{-1}(x - \mathrm{prox}^{\lambda}_{\mathbf{h}}(x))$.

■ The Moreau-Yosida envelope is *L*-smooth: $\|\nabla h^{\lambda}(x) - \nabla h^{\lambda}(y)\| \le \lambda^{-1} \|x - y\|$, for all $x, y \in \mathbb{R}^d$.

MY regularized potential

- If g is not differentiable, but the proximal operator associated with g is available, its λ-Moreau Yosida envelope g^λ can be considered.
- This leads to the approximation of the potential $U^{\lambda}: \mathbb{R}^d \to \mathbb{R}$ defined for all $x \in \mathbb{R}^d$ by

$$U^{\lambda}(x) = f(x) + g^{\lambda}(x) .$$

Theorem

Under (H), for all
$$\lambda > 0$$
, $0 < \int_{\mathbb{R}^d} e^{-U^{\lambda}(y)} dy < +\infty$.

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Some approximation results

Theorem

Assume (H).

- **1** Then, $\lim_{\lambda \to 0} \|\pi^{\lambda} \pi\|_{\mathrm{TV}} = 0.$
- **2** Assume in addition that g is Lipschitz. Then for all $\lambda > 0$,

$$\|\pi^{\lambda} - \pi\|_{\mathrm{TV}} \le \lambda \|g\|_{\mathrm{Lip}}^2$$

If g = ι_K where K is a convex body of R^d. Then for all λ > 0 we have

$$\|\pi^{\lambda} - \pi\|_{\mathrm{TV}} \le 2 \left(1 + \mathsf{D}(\mathcal{K}, \lambda)\right)^{-1}$$

where $D(\mathcal{K}, \lambda)$ is explicit in the proof, and is of order $\mathcal{O}(\lambda^{-1})$ as λ goes to 0.

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The MYULA algorithm-I

Given a regularization parameter $\lambda > 0$ and a sequence of stepsizes $\{\gamma_k, k \in \mathbb{N}^*\}$, the algorithm produces the Markov chain $\{X_k^{\mathrm{M}}, k \in \mathbb{N}\}$: for all $k \ge 0$,

$X_{k+1}^{\rm M} = X_k^{\rm M} - \gamma_{k+1} \left\{ \nabla f(X_k^{\rm M}) + \lambda^{-1} (X_k^{\rm M} - \operatorname{prox}_g^{\lambda}(X_k^{\rm M})) \right\} + \sqrt{2\gamma_{k+1}} Z_{k+1} ,$

where $\{Z_k, k \in \mathbb{N}^*\}$ is a sequence of i.i.d. *d*-dimensional standard Gaussian random variables.

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The MYULA algorithm-II

- The ULA target the smoothed distribution π^{λ} .
- To compute the expectation of a function $h : \mathbb{R}^d \to \mathbb{R}$ under π from $\{X_k^M ; 0 \le k \le n\}$, an importance sampling step is used to correct the regularization.
- This step amounts to approximate $\int_{\mathbb{R}^d} h(x) \pi(x) \mathrm{d}x$ by the weighted sum

$$\mathbf{S}_n^h = \sum_{k=0}^n \omega_{k,n} h(X_k) \ , \ \text{with} \ \omega_{k,n} = \left\{ \sum_{k=0}^n \gamma_k \mathrm{e}^{\bar{g}^{\lambda}(X_k^{\mathrm{M}})} \right\}^{-1} \gamma_k \mathrm{e}^{\bar{g}^{\lambda}(X_k^{\mathrm{M}})} \ ,$$

where for all $x \in \mathbb{R}^d$

$$\bar{g}^{\lambda}(x) = g^{\lambda}(x) - g(x) = g(\operatorname{prox}_{g}^{\lambda}(x)) - g(x) + (2\lambda)^{-1} \left\| x - \operatorname{prox}_{g}^{\lambda}(x) \right\|^{2}$$

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Image deconvolution

- Objective recover an original image $x \in \mathbb{R}^n$ from a blurred and noisy observed image $y \in \mathbb{R}^n$ related to x by the linear observation model y = Hx + w, where H is a linear operator representing the blur point spread function and w is a Gaussian vector with zero-mean and covariance matrix $\sigma^2 I_n$.
- This inverse problem is usually ill-posed or ill-conditioned: exploits prior knowledge about x.
- Consider the ℓ_1 norm prior, $\pi({m x}) \propto \exp{(-lpha \|{m x}\|_1)}$, then

 $\pi(\boldsymbol{x}|\boldsymbol{y}) \propto \exp\left[-\|\boldsymbol{y} - H\boldsymbol{x}\|^2/2\sigma^2 - \alpha\|\boldsymbol{x}\|_1\right].$

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Microscopy dataset



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HPD credible region

- We want to test if the molecules are indeed present in true image (as opposed to being noise artefacts for example),
- Uncertainty about their position.
- For this, it can be relevent to compute the HPD credible region

$$C^*_{\alpha} = \{x : U(x) \le \eta_{\alpha}\}$$

with $\eta_{\alpha} \in \mathbb{R}$ chosen such that $\mathbb{P}(\boldsymbol{x} \in C_{\alpha}^* | \boldsymbol{y}) = 1 - \alpha$ holds. Here we use $\alpha = 0.01$ related to the 99% confidence level.

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Convergence of MYULA



Figure : Convergence of MYULA and PMALA after 5×10^6 iterations

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Comparison with PMALA



Figure : Microscopy experiment: (a) HDP region thresholds η_{α} for MYULA $(2 \times 10^6 \text{ iterations } \lambda = 1, \gamma = 0.6)$ and PMALA $(2 \times 10^7 \text{ iterations})$, (b) relative approximation error of MYULA.

Application of MYULA

- We check that a group of three molecules are in the image by a test.
- MYULA $(2 \times 10^6$ iterations $\lambda = 1, \gamma = 0.6$) and PMALA $(2 \times 10^7$ iterations) give the same answer.

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Thank you for your attention.

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