Semiclassical Analysis of Metropolis Algorithm on Bounded Domain

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(joint work with P. Diaconis and G. Lebeau)

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The problem of hard spheres

Consider a fixed box in $\mathbb{R}^d$, $B = [-1,1]^d$. We consider the problem of placement of $N$ balls of radius $\epsilon > 0$ with centers in $B$ under the condition that the balls do not overlap. We denote $\mathcal{O}_{N,\epsilon} \subset B^N$ the set of all possible configurations. We endowe $\mathcal{O}_{N,\epsilon}$ with the normalized Lebesgue measure $dL/vol(\mathcal{O}_{N,\epsilon})$.

Problem:

Build a sample of points $X^1, \ldots, X^r \in \mathcal{O}_{N,\epsilon}$ distributed uniformly with respect to $dL$.

- This problem occurs in statistical physics in phase transition studies.
- It can be formulated in a more abstract setting.
Metropolis and al (50’s) proposed the following algorithm to solve this problem. Let $h > 0$ being fixed and $X^0 \in \mathcal{O}_{N,\epsilon}$.

- Starting from $X^0 = (x_1^0, \ldots, x_N^0)$, move one of the ball say $x_k^0$ uniformly at random in the ball $B(x_k^0, h)$, it results in a new position $x_k^1$. Denote $X^1 = (x_1^0, \ldots, x_k^1, \ldots, x_N^0)$ the new configuration. If $X^1 \in \mathcal{O}_{N,\epsilon}$, keep $X^1$.

- If $X^1 \notin \mathcal{O}_{N,\epsilon}$, throw away $X^1$ and restart the procedure from $X^0$.

- Once, $X^1$ is constructed, define $X^2$ by the same procedure starting from $X^1$, etc.

As $r$ goes to infinity, the point $X^r$ is chosen in $\mathcal{O}_{N,\epsilon}$ uniformly with respect to the uniform distribution.
Our framework is the following:

- \( \Omega \) denotes a bounded connected open subset of \( \mathbb{R}^d \) s.t. \( \partial \Omega \) has Lipschitz regularity.
- \( \rho \) is a measurable function on \( \overline{\Omega} \) such that
  * there exists \( m, M > 0 \), s.t. \( m \leq \rho(x) \leq M, \forall x \in \Omega \).
  * \( \int_{\Omega} \rho(x) dx = 1 \)
- \( B_1 \) denotes the unit ball in \( \mathbb{R}^d \) and \( |B_1| \) its volume.

We are willing to define a Markov kernel which permit to sample from \( \rho(x) dx \).
From the point of view of Markov chain, the algorithm is the following. We construct $x_{n+1} \in \Omega$ from $x_n \in \Omega$ according to the following procedure: choose $y \in \mathbb{R}^d$ uniformly at random in $B(x_n, h)$

- if $y \notin \Omega$ then $x_{n+1} := x_n$.
- if $y \in \Omega$, compute $A(x, y) = \rho(y)/\rho(x)$.
  - If $A(x, y) > 1$, let $x_{n+1} := y$
  - If $A(x, y) \leq 1$, let $x_{n+1} := x_n$ with probability $A(x, y)$ and $x_{n+1} := y$ with probability $1 - A(x, y)$. 

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The kernel associated to the preceding Markov chain is defined as follows. Introduce the following kernel on $\Omega$:

$$k_{h,\rho}(x, y) = \frac{1}{h^d|B_1|} 1_{|x-y|< h \min\left(\frac{\rho(y)}{\rho(x)}, 1\right)}$$

The Metropolis kernel on $\Omega$ is given by

$$t_{h,\rho}(x, dy) = m_{h,\rho}(x)\delta_x + k_{h,\rho}(x, y)dy.$$ 

with

$$m_{h,\rho}(x) = 1 - \int_{\Omega} k_{h,\rho}(x, y)dy$$

The Metropolis operator associated to this kernel is

$$T_{h,\rho}u(x) = m_{h,\rho}(x)u(x) + \int_{\Omega} u(y)k_{h,\rho}(x, y)dy$$
Basic properties

- The Metropolis kernel \( t_{h,\rho}(x, dy) \) is a Markov kernel \( (T_{h,\rho}(1) = 1) \).
- The operator \( T_{h,\rho} \) is self-adjoint on \( L^2(\Omega, \rho(x)dx) \) and \( \| T_{h,\rho} \|_{L^2 \rightarrow L^2} = 1 \).
- The probability measure \( \rho(x)dx \) is stationary for \( T_{h,\rho} \).
- \( \text{Spec}(T_{h,\rho}) \) is discrete near 1 (use this).

Definition

We define the spectral gap of the Metropolis operator \( T_{h,\rho} \) as 
\[
g(h, \rho) = \text{dist}(1, \text{spec}(T_h) \setminus \{1\}).
\]
This is the largest constant such that 
\[
\| u \|^2_{L^2(\rho)} - \langle u, 1 \rangle^2_{L^2(\rho)} \leq \frac{1}{g(h, \rho)} \langle u - T_{h,\rho}u, u \rangle_{L^2(\rho)}
\]
General densities

**Theorem 1**

Let $\Omega$ be an open, connected, bounded, Lipschitz subset of $\mathbb{R}^d$. There exists $h_0 > 0$, $\delta_0 \in ]0, 1/2[$ and constants $C_i > 0$ such that for $h \in ]0, h_0]$, the following holds true:

- $\text{Spec}(T_{h,\rho}) \subset [-1 + \delta_0, 1]$
- $1$ is a simple eigenvalue of $T_{h,\rho}$
- The spectral gap $g(h, \rho)$ satisfies
  $$C_1h^2 \leq g(h, \rho) \leq C_2h^2$$
- $\forall \lambda \in [0, \delta_0]$,
  $$\#(\text{Spec}(T_{h,\rho}) \cap [1 - \lambda, 1]) \leq C_3(1 + \lambda h^{-2})^{d/2}$$
If the density $\rho$ is smooth on $\Omega$ we can give a more precise description of the spectrum of $T_{h,\rho}$. For simplicity, we assume in this section that $\partial \Omega$ is smooth. Let us introduce the unbounded operator acting on $L^2(\Omega, \rho(x)dx)$, defined by

$$L_\rho(u) = \frac{-\alpha_d}{2}(\triangle u + \frac{\nabla \rho}{\rho} \cdot \nabla u)$$

$$D(L_\rho) = \{ u \in H^2(\Omega), \partial_n u|_{\partial \Omega} = 0 \}$$

where

$$\alpha_d = \frac{1}{vol(B_1)} \int_{B_1} z_1^2 dz = \frac{1}{d+2}$$
\( L_\rho \) is the self-adjoint realization of the Dirichlet form

\[
\frac{\alpha_d}{2} \int_\Omega |\nabla u(x)|^2 \rho(x) \, dx.
\]  

(1)

\( L_\rho \) has compact resolvant (thanks to Sobolev embeddings).

We denote

\[
\text{Spec}(L_\rho) = \{ \lambda_0 = 0 < \lambda_1 < \lambda_2 < \ldots \}
\]

and by \( m_j = \text{multiplicity}(\lambda_j) \). Observe that \( m_0 = 1 \) since \( \text{Ker}(L_\rho) \) is spanned by the constant function equal to 1.
Theorem 2

Let $\Omega$ be an open, connected, bounded and smooth subset of $\mathbb{R}^d$. Assume that the density $\rho$ is smooth on $\overline{\Omega}$, then for any $R > 0$ and $\varepsilon > 0$ such that $\lambda_{j+1} - \lambda_j > 2\varepsilon$ for $\lambda_{j+2} < R$, there exists $h_1 > 0$ such that one has for all $h \in ]0, h_1]$, 

$$ Spec \left( \frac{1 - T_{h,\rho}}{h^2} \right) \cap ]0, R] \subset \bigcup_{j \geq 1} [\lambda_j - \varepsilon, \lambda_j + \varepsilon], \quad (2) $$

and the number of eigenvalues of $\frac{1 - T_{h,\rho}}{h^2}$ in the interval $[\lambda_j - \varepsilon, \lambda_j + \varepsilon]$ is equal to $m_j$. 

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Variational approach

Since, \( m \leq \rho(x) \leq M \) on \( \Omega \), we can easily suppose that \( \rho = 1 \) (and we denote \( T_h \) instead of \( T_{h,\rho} \)). The spectral gap is the largest constant such that

\[
\|u\|_{L^2}^2 - \langle u, 1 \rangle_{L^2}^2 \leq \frac{1}{g(h, \rho)} \langle u - T_h u, u \rangle_{L^2}
\]

A standard computation shows that

\[
\|u\|_{L^2}^2 - \langle u, 1 \rangle_{L^2}^2 = \frac{1}{2} \int_{\Omega \times \Omega} |u(x) - u(y)|^2 dxdy := \text{Var}(u)
\]

\[
\langle u - T_h u, u \rangle_{L^2} = \frac{h^{-d}}{2} \int_{\Omega \times \Omega} 1_{|x-y|<h} |u(x) - u(y)|^2 dxdy := \mathcal{E}_h(u).
\]
The following properties are easy to prove:

- 1 is a simple eigenvalue (use this)
- $g(h, \rho) \leq Ch^2$ (take $u \in C_0(\Omega)$ such that $\int_\Omega u(x)dx = 0$, $\|u\|_{L^2} = 1$, make a Taylor expansion and use again this)
Lower bound for the spectral gap

Let us show the lower bound on the spectral gap when $\Omega$ is convex. For any $u \in L^2(\Omega)$, we have

$$
\int_{\Omega \times \Omega} |u(x) - u(y)|^2 \, dx \, dy \leq 
C h^{-1} \sum_{k=0}^{K(h)-1} \int_{\Omega \times \Omega} |u(x + kh(y - x)) - u(x + (k + 1)h(y - x))|^2 \, dx \, dy,
$$

where $K(h)$ is the greatest integer $\leq h^{-1}$ and $K(h)h = 1$. 

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With the new variables $x' = x + kh(y - x)$, $y' = x + (k + 1)h(y - x)$, one has $dx' dy' = h^d dx dy$ and we get

$$\int_{\Omega \times \Omega} |u(x) - u(y)|^2 dx dy \leq Ch^{-d-1} K(h) \int_{\Omega \times \Omega} 1_{|x' - y'| < h\text{diam}(\Omega)} |u(x') - u(y')|^2 dx' dy',$$

This yields to

$$\text{Var}(u) \leq C'h^{-2} \mathcal{E}_h(u)$$

and proves the lower bound.
A simple quasimode calculus

Assume $\rho = 1$ and $\partial \Omega$ is smooth. Let $\lambda > 0$ and $u \in C^\infty(\overline{\Omega})$ satisfy

$\left(-\frac{\alpha_d}{2} \Delta - \lambda\right)u = 0$ in $\Omega$ and $\partial_n u|_{\partial \Omega} = 0$.

For $x \in \Omega$ s.t. $\text{dist}(x, \partial \Omega) > h$, Taylor expansion shows that

$T_h u(x) - u(x) = \frac{1}{|B_1|} \int_{|z| < 1, x + hz \in \Omega} (u(x + hz) - u(x))dz$

$= \frac{h}{|B_1|} \sum_{j=1}^{d} \partial_{x_j} u(x) \int_{|z| < 1} z_j dz + \frac{\alpha_d}{2} h^2 \Delta u(x) + O_{L^\infty}(h^4)$

$= \frac{\alpha_d}{2} h^2 \Delta u(x) + O_{L^\infty}(h^4)$

where the term of order $h$ and $h^3$ vanish for parity reason.
For $x \in \Omega$ s.t. $\text{dist}(x, \partial \Omega) < h$, we use local coordinates such that $\Omega = \{(x_1, x') \in \mathbb{R}^d, x_1 > 0\}$. Taylor expansion shows that

$$T_h u(x) - u(x) = \frac{1}{|B_1|} \int_{|z|<1, x_1+hz_1>0} (u(x + hz) - u(x)) dz$$

$$= \frac{h}{|B_1|} \sum_{j=1}^{d} \partial_{x_j} u(x) \int_{|z|<1, x_1+hz_1>0} z_j dz + O_{L\infty}(h^2)$$

- Parity argument $\implies$ term of index $j \geq 2$ vanish.
- $\partial_n u |_{\partial \Omega} = 0$ and $\text{dist}(x, \partial \Omega) < h$ $\implies$ term of index $j = 1$ is $O_{L\infty}(h^2)$.

Since $\text{meas}(\{\text{dist}(x, \partial \Omega) < h\}) = O(h)$, it follows that

$$1_{\text{dist}(x, \partial \Omega) < h} (T_h u - u) = O_{L^2}(h^{5/2}).$$

Combining the two estimates, we get

$$T_h u - (1 - h^2 \lambda) u = O(h^{5/2}).$$
Using the min-max principle, this shows that for any eigenvalue $\lambda_k$ of $-\Delta$ with Neumann condition and with multiplicity $m_k$, we have

$$\# \text{Spec}(\frac{1 - T_h}{h^2}) \cap [\lambda - Ch^{\frac{1}{2}}, \lambda + Ch^{\frac{1}{2}}] \geq m_k.$$  

To show the converse inequality, we consider (for a fixed $R > 0$) a family $(\lambda_h, u_h) \in [0, R] \times L^2(\Omega)$ such that $\|u_h\|_{L^2} = 1$ and

$$T_h u_h = (1 - h^2 \lambda_h) u_h$$

We want to show that $\lambda_h$ converges to an eigenvalue of $-\Delta$ with Neuman condition when $h \to 0$. For this purpose, we need some compactness on $(u_h)_{h \in [0, h_0]}$. 

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Comparaison with the random walk on the torus

Since $\Omega$ is bounded, it is contained in a large box $]-A, A[^d$. We denote $\Pi = (\mathbb{R}/2A \mathbb{Z})^d$. Since $\Omega$ is Lipschitz, using local coordinates, we can define an extension map

$$ P : L^2(\Omega) \to L^2(\Pi) $$

which is also bounded from $H^1(\Omega)$ into $H^1(\Pi)$. Any function $v \in L^2(\Pi)$ can be extended in Fourier series $v(x) = \sum_{k \in \mathbb{Z}^d} c_k(v)e^{2ik\pi x/A}$. The $L^2$ and $H^1$ norm on $\Pi$ can be expressed as follows

- $\|v\|_{L^2(\Pi)}^2 = (2A)^d \sum_k |c_k|^2$.
- $\|v\|_{H^1(\Pi)}^2 = (2A)^d \sum_k (1 + \frac{4\pi^2 k^2}{A^2})|c_k|^2$.
Recall that for $u \in L^2(\Omega)$,

$$\mathcal{E}_h(u) = \langle u - T_h u, u \rangle_{L^2(\Omega)} = \frac{h^{-d}}{2} \int_{\Omega \times \Omega} 1_{|x-y|<h} |u(x) - u(y)|^2 \, dx \, dy.$$ 

For $v \in L^2(\Pi)$, we define

$$\tilde{\mathcal{E}}_h(v) = \langle v - \tilde{T}_h v, v \rangle_{L^2(\Pi)} = \frac{h^{-d}}{2} \int_{\Pi \times \Pi} 1_{|x-y|<h} |v(x) - v(y)|^2 \, dx \, dy.$$ 

where $\tilde{T}_h$ is the metropolis operator on the torus.

Remark

A simple calculus using the Fourier expansion, shows that $\tilde{T}_h = \Gamma(-h^2 \Delta)$ where $\Gamma$ is a smooth function decreasing to 0 at infinity.
Lemma 1

There exist $C_0, C_1, h_0 > 0$ such that the following holds true for any $h \in ]0, h_0]$ and any $u \in L^2(\Omega)$.

$$\frac{\mathcal{E}_h(u)}{C_0} \leq \tilde{\mathcal{E}}_h(P(u)) \leq C_0 \left( \mathcal{E}_h(u) + h^2 \|u\|_{L^2}^2 \right). \quad (3)$$

As a by-product, any $u \in L^2(\Omega)$ such that

$$\|u\|_{L^2(\rho)}^2 + h^{-2} \langle (1 - T_h)u, u \rangle_{L^2(\rho)} \leq 1$$

admits a decomposition $u = u_L + u_H$ with $u_L \in H^1(\Omega)$, $\|u_L\|_{H^1} \leq C_1$, and $\|u_H\|_{L^2} \leq C_1 h$. 
Proof.

- The first inequality is trivial. The second one is obtained by working in local coordinates for which the boundary is an half-space.

- We observe that (thanks to Parseval identity)

\[ \tilde{\mathcal{E}}(v) = \frac{(2A)^d}{2} \sum_k |c_k|^2 \theta(hk/A), \]

\[ \theta(\xi) = \int_{|z| \leq 1} |e^{2i\pi \xi z} - 1|^2 dz. \]

The by-product is obtained by projecting the extension \( v = P(u) \) on low frequencies \( h|k| \leq \delta \) and high frequencies \( h|k| > \delta \) for some fixed \( \delta > 0 \). Hence, it suffices to use the fact that the function \( \theta \) is quadratic near 0 and has a positive lower bound for \( |\xi| \geq \delta \). \qed
Total variation estimate

The **total variation distance** between two probability measures $\mu, \nu$ is defined by

$$\|\mu - \nu\|_{TV} = \sup_{A \text{ measurable}} |\mu(A) - \nu(A)| = \frac{1}{2} \sup_{f \in L^\infty, |f| \leq 1} |\int f d\mu - \int f d\nu|$$

**Theorem 3**

Under the same assumption as above, the following estimate holds true for all $n \in \mathbb{N}$:

$$C_4 e^{-ng(h, \rho)} \leq \sup_{x \in \Omega} \|t^n_{h, \rho}(x, dy) - \rho(y)dy\|_{TV} \leq C_5 e^{-ng(h, \rho)}.$$
Proof of total variation estimates

Let \( \Pi_0 \) be the orthogonal projector in \( L^2(\Omega) \) on the space of constant functions

\[
\Pi_0(u)(x) = 1_\Omega(x) \int_{\Omega} u(y) \rho(y) \, dy.
\]  

(4)

Then, by definition

\[
2 \sup_{x_0 \in \Omega} \left\| t^n_h(x_0, dy) - \rho(y) \, dy \right\|_{TV} = \left\| T^n_h - \Pi_0 \right\|_{L^\infty \rightarrow L^\infty}.
\]  

(5)

Thus, we have to prove that for \( h > 0 \) small and any \( n \), one has

\[
\left\| T^n_h - \Pi_0 \right\|_{L^\infty \rightarrow L^\infty} \leq C_0 e^{-ng(h, \rho)}.
\]  

(6)

Since \( g(h, \rho) = O(h^2) \), we can suppose that \( nh^2 \gg 1 \).
Denote \( \lambda_{j,h} \) the eigenvalues of \( T_h \) and \( \Pi_j \) the associated spectral projector. We fix \( \alpha > 0 \) small and use the spectral decomposition
\[ T_h - \Pi_0 = T_{h,1} + T_{h,2} \]
with
\[ T_{h,1} = \sum_{1 - h^2 - \alpha < \lambda_{j,h} < 1} \lambda_{j,h} \Pi_j \]
and \( T_{h,2} \) spectrally localized in \([-1 + \delta_0, 1 - h^2 - \alpha] \).

It is easy to see that
\[ \| T^n_h - \Pi_0 \|_{L^2 \rightarrow L^2} \leq Ce^{-ng(h,\rho)}. \]

Since, we deal with \( L^\infty \rightarrow L^\infty \) norm, we need:

- to control \( \| \Pi_j \|_{L^2 \rightarrow L^\infty} \)
- a bound on the number of eigenvalues in any interval \([\alpha_h, 1]\) with \( 1 - \delta_0 < \alpha_h < 1 - Ch^2 \).
Control of small eigenvalues

For this purpose, we use Lemma 1 and show that there exists $\delta_0 > 0$ s.t.

- for any $0 \leq \lambda \leq \delta_0/h^2$,
  \[ \#(\text{Spec}(T_h) \cap [1 - h^2\lambda, 1]) \leq C(1 + \lambda)^{d/2} \]

- any eigenfunction $T_h(u) = \lambda u$ with $\lambda \in [1 - \delta_0, 1]$ satisfies the bound
  \[ \|u\|_{L^\infty} \leq C_2 h^{-d/2} \|u\|_{L^2}. \]

Using these estimates we get easily:

\[ \|T_{2,h}^n\|_{L^\infty \to L^\infty} \leq Ch^{-3d/2} e^{-nh^2-\alpha} << e^{-ng(h,\rho)} \]

since $g(h, \rho) \sim h^2$. 

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Nash inequality

Let \( E_\alpha = \text{span}(e_j,h, 1 - h^{2-\alpha} < \lambda_{j,h} < 1) \).

Lemma 2 (Nash inequality)

There exists \( C, D, \alpha > 0 \), s.t. any function \( u \in E_\alpha \) satisfies:

\[
\|u\|_{L^2}^{2+1/D} \leq C h^{-2}(\|u\|_{L^2}^2 - \|T_h u\|_{L^2}^2 + h^2 \|u\|_{L^2}^2) \|u\|_{L^1}^{1/D}.
\]

Proof.

- Use Lemma 1 to show that there exists \( p > 2, \alpha > 0 \) such that any function \( u \in E_\alpha \) satisfies

\[
\|u\|_{L^p}^2 \leq C h^{-2}(\mathcal{E}_h(u) + h^2 \|u\|_{L^2}^2)
\]

- Use the bound \( \mathcal{E}_h(u) \leq \langle (1 - T_h)u, u \rangle \) on \( E_\alpha \) and interpolate between \( L^p \) and \( L^1 \) to get the \( L^2 \) estimate.

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Control of $T_{h,1}$

We want to control the norm $\| T_{h,1}^n \|_{L^2 \to L^\infty} = \| T_{h,1}^n \|_{L^1 \to L^2}$.

- Take $g \in L^2$ s.t. $\|g\|_{L^1} = 1$ and denote $c_n = \| T_{h,1}^n g \|_{L^2}^2$.

Thanks to the preceding Lemma:

$$c_n^{1+2D} \leq Ch^{-2}(c_n - c_{n+1} + h^2 c_n)$$

Hence, for $0 \leq n \leq h^{-2}$, $c_n \leq (h^{-2}/(1+n))^{2D}$.

- This permit to show that for some large $n \sim h^{-2}$,

$$\| T_{h,1}^n \|_{L^2 \to L^\infty} = \| T_{h,1}^n \|_{L^1 \to L^2} = O(1)$$

Combined with $\| T_h^p \|_{L^2 \to L^2} \leq Ce^{-pg(h,\rho)}$, this completes the proof.
The problem of hard spheres

Consider a fixed box in \( \mathbb{R}^d \), \( B = [-1, 1]^d \). We consider the problem of placement of \( N \) balls of radius \( \epsilon > 0 \) with centers in \( B \) under the condition that the balls do not overlap. We denote \( \mathcal{O}_{N, \epsilon} \subset B^N \) the set of all possible configurations:

\[
\mathcal{O}_{N, \epsilon} = \left\{ X = (x_1, \ldots, x_N) \in B^N, \forall 1 \leq i < j \leq N, |x_i - x_j| > \epsilon \right\}.
\]

We endow \( \mathcal{O}_{N, \epsilon} \) with the normalized Lebesgue measure \( \mu = dL/vol(\mathcal{O}_{N, \epsilon}) \).

**Problem:**

Build a sample of points \( X^1, \ldots, X^r \in \mathcal{O}_{N, \epsilon} \) distributed uniformly with respect to \( \mu \).

This problem occurs in statistical physics in phase transition studies.

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Metropolis and al (50’s) proposed the following algorithm to solve this problem. Let $h > 0$ being fixed and $X^0 \in \mathcal{O}_N, \epsilon$.

- Starting from $X^0 = (x^0_1, \ldots, x^0_N)$, move one of the ball say $x^0_k$ uniformly at random in the ball $B(x^0_k, h)$, it results in a new position $x^1_k$. Denote $X^1 = (x^0_1, \ldots, x^1_k, \ldots, x^0_N)$ the new configuration. If $X^1 \in \mathcal{O}_N, \epsilon$, keep $X^1$.

- If $X^1 \notin \mathcal{O}_N, \epsilon$, throw away $X^1$ and restart the procedure from $X^0$.

- Once, $X^1$ is constructed, define $X^2$ by the same procedure starting from $X^1$, etc.

As $r$ goes to infinity, the point $X^r$ is chosen in $\mathcal{O}_N, \epsilon$ uniformly with respect to the uniform distribution $\mu$.

**Question**

What is the speed of convergence?
Let $\varphi = 1_{B_{\mathbb{R}^d}(0,1)}$ and introduce the following kernels for $j = 1, \ldots, N$:

$$k_{j,h}(x, dy) = \delta_{x_1} \otimes \cdots \otimes \delta_{x_{j-1}} \otimes h^{-d} \varphi \left( \frac{x_j - y_j}{h} \right) dy_j \otimes \delta_{x_{j+1}} \otimes \cdots \otimes \delta_{x_N}$$

Let $m_{j,h}(x) = \int_{\mathbb{R}^d \setminus \mathcal{O}_{N,\varepsilon}} k_{j,h}(x, dy)$ and let

$$t_{j,h}(x, dy) = m_{j,h}(x) \delta_x + k_{j,h}(x, dy).$$

Define the partial operators $T_{j,h}$ with kernel $t_{j,h}(x, dy)$, then the Metropolis operator on $L^2(\mathcal{O}_{N,\varepsilon})$ is

$$T_h = N^{-1} \sum_{j=1}^{N} T_{j,h}$$

Denote $t_h(x, dy) = \sum_j t_{j,h}(x, dy)$ the kernel of $T_h$. Then, $T_h$ admits $\mu$ as stationary measure and $t_h^n(x, dy)$ converges to $\mu$ as $n \to \infty$. 

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Proposition

There exists $\alpha > 0$ such that for $N\epsilon \leq \alpha$, the set $\Omega_{N,\epsilon}$ is connected and Lipschitz.

Proof. To prove the “Lipschitz boundary“ use the following observations:

- A domain $\Omega \subset \mathbb{R}^p$ has Lipschitz boundary iff it satisfies the following cone property:

$$\forall a \in \partial \Omega, \exists \delta > 0, \exists \nu_a \in S^{p-1}, \forall b \in B(a, \delta) \cap \partial \Omega \text{ we have}$$

$$b + \Gamma_+(\nu_a, \delta) \subset \Omega \text{ and } b + \Gamma_-(\nu_a, \delta) \subset \mathbb{R}^p \setminus \overline{\Omega}.$$  

where for $\nu \in S^p$,

$$\Gamma_+(\nu_a, \delta) = \{ \xi \in \mathbb{R}^p, \pm \langle \xi, \nu \rangle > (1 - \delta)|\xi|, |\langle \xi, \nu \rangle| < \delta \}$$
For $x \in \overline{O}_{N,\epsilon}$ we set

$$R(x) = \{ i \in \mathbb{N}_N, x_i \in \partial \Omega \}$$

$$S(x) = \{ \tau = (\tau_1, \tau_2) \in \mathbb{N}_N, \tau_1 < \tau_2 \text{ and } |x_{\tau_1} - x_{\tau_2}| = \epsilon \}$$

$$r(x) = \#R(x), \quad s(x) = \#S(x)$$

Any $x \in \overline{O}_{N,\epsilon}$ belongs to $\partial O_{N,\epsilon}$ iff $r(x) + s(x) \geq 1$. 

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Semiclassical Analysis of Metropolis Algorithm on Bounded Domain
Thanks to the preceding proposition, we can consider the Neumann Laplacian $|\Delta|_N$ on $\mathcal{O}_{N,\epsilon}$ defined by

$$|\Delta|_N = -\frac{\alpha_d}{2N} \Delta,$$

$$D(|\Delta|_N) = \{ u \in H^1(\mathcal{O}_{N,\epsilon}), -\Delta u \in L^2(\mathcal{O}_{N,\epsilon}), \partial_n u|_{\partial \mathcal{O}_{N,\epsilon}} = 0 \}.$$

We still denote $0 = \nu_0 < \nu_1 < \nu_2 < \ldots$ the spectrum of $|\Delta|_N$ and $m_j$ the multiplicity of $\nu_j$. 
Theorem (part 1)

Let \( N \geq 2 \) and \( \epsilon > 0 \) small be fixed. Let \( R > 0 \) be given and \( \beta > 0 \) small. Then, there exists \( h_0 > 0, \delta_0 \in ]0, 1/2[ \) and constants \( C_i > 0 \) such that for any \( h \in ]0, h_0] \), the following hold true:

i) The spectrum of \( T_h \) is a subset of \([-1 + \delta_0, 1]\), 1 is a simple eigenvalue of \( T_h \), and \( \text{Spec}(T_h) \cap [1 - \delta_0, 1] \) is discrete. Moreover,

\[
\text{Spec} \left( \frac{1 - T_h}{h^2} \right) \cap ]0, R] \subset \bigcup_{j \geq 1} [\nu_j - \beta, \nu_j + \beta]; \\
\# \text{Spec} \left( \frac{1 - T_h}{h^2} \right) \cap [\nu_j - \beta, \nu_j + \beta] = m_j \quad \forall \nu_j \leq R;
\]

and for any \( 0 \leq \lambda \leq \delta_0 h^{-2} \), the number of eigenvalues of \( T_h \) in \([1 - h^2 \lambda, 1]\) (with multiplicity) is bounded by \( C_1(1 + \lambda)^{dN/2} \).
Theorem (part 2)

ii) The spectral gap $g(h)$ satisfies

$$\lim_{h \to 0^+} h^{-2} g(h) = \nu_1$$

and the following estimate holds true for all $n \in \mathbb{N}$:

$$\sup_{x \in O_N, \epsilon} \left\| t_h^n(x, dy) - \frac{dy}{vol(O_N, \epsilon)} \right\|_{TV} \leq C_4 e^{-ng(h)}.$$
Simple observations

- For any smooth function $u$, we still have
  \[(1 - T_h)u = h^2 |\Delta|_N u + O_{L^2}(h^{5/2})\]

- The kernel of $T_h$ inside the domain is not a smooth function anymore.

- To get regularity of eigenfunction, we still need to compare the operator with the usual random walk on the torus.

- Eigenfunctions of $T_h$ are also eigenfunctions for $T_h^M$ for any $M \in \mathbb{N}$.
Lemma

Let $\epsilon$ be small. There exists $h_0 > 0$, $c_0, c_1 > 0$ and $M \in \mathbb{N}^*$ such that for all $h \in ]0, h_0]$, one has

$$T_h^M(x, dy) = \mu_h(x, dy) + c_0 h^{-Nd} \varphi_N d(\frac{x - y}{c_1 h}) dy$$

where for all $x \in O_{N,\epsilon}$, $\mu_h(x, dy)$ is a positive Borel measure.

Proof. We have to show that there exists $M \in \mathbb{N}$, s.t. for any $u$ non negative

$$T_h^M u(x) \geq c_0 h^{-Nd} \int_{O_{N,\epsilon}} u(y) \varphi_N d \left( \frac{x - y}{c_1 h} \right) dy.$$

To simplify, replace $O_{N,\epsilon}$ by $\mathbb{R}^{Nd}$, then $M = N$ works since

$$T_h^N u(x) \geq T_{1,h} \cdots T_{N,h} u(x) \geq C h^{-Nd} \int_{x - y \in [-h, h]^{Nd}} u(y) dy.$$
Denote $\tilde{\mathcal{E}}(\nu)$ the Dirichlet form on the torus $\Pi^{Nd}$. As a consequence of the preceding lemma we get

**Lemma**

There exist $C_0, h_0 > 0$ such that the following holds true for any $h \in ]0, h_0]$ and any $u \in L^2(\mathcal{O}_N, \epsilon)$

$$\tilde{\mathcal{E}}_h(E(u)) \leq C_0(\langle (1 - T^M_h)u, u \rangle_{L^2(\mathcal{O}_N, \epsilon)} + h^2 \|u\|_{L^2}^2)$$

From this Lemma, we can prove the following:

**Lemma**

For any $0 \leq \lambda \leq \delta_0/h^2$, the number of eigenvalues of $T_h$ in $[1 - h^2 \lambda, 1]$ is bounded by $C_1(1 + \lambda)^{Nd/2}$. Moreover, any eigenfunction $T_h(u) = \lambda u$ with $\lambda \in ]1 - \delta_0, 1]$ satisfies the bound

$$\|u\|_{L^\infty} \leq C_2 h^{-Nd/2} \|u\|_{L^2}$$