A weak convergence result for a Chebyshev-quantum walk on $\mathbb{Z}^2$

Laurent Miclo

Toulouse School of Economics
Institut de Mathématiques de Toulouse

Joint work with Simon Apers

Institut de Recherche en Informatique Fondamentale

Plan of the talk

1. Wave equations on graphs
2. Quantum walks on $\mathbb{Z}$
3. Quantum walks on lattices
4. Elements of proof

Plan

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The classical wave equation on $\mathbb{R}^d$ writes

$$\ddot{u} = \frac{1}{4d}\Delta u$$

or equivalently,

$$\dot{u} = v, \qquad \dot{v} = \frac{1}{4d}\Delta u \tag{1}$$

According to a blog of Tao mentioning Peres, the discrete analog for a Markov transition kernel P on a graph (V, E) is:

$$\forall\ t \in \mathbb{Z}, \qquad \begin{cases} u(t+1) = Pu(t) + v(t) \\ v(t+1) = Pv(t) - (I - P^2)u(t) \end{cases}$$

where $u(t)$ and $v(t)$ are functions defined on V and I is the identity operator.

Link between continuous and discrete settings

Consider the following scaling, with small $\epsilon > 0$: on the graph on $\epsilon\mathbb{Z}^d$ endowed with its usual random walk transition kernel P_ϵ

$$\forall\ t \in \epsilon\mathbb{Z}, \qquad \left\{ \begin{array}{lcl} u_\epsilon(t+\epsilon) & = & P_\epsilon u_\epsilon(t) + \epsilon v_\epsilon(t) \\ v_\epsilon(t+\epsilon) & = & P_\epsilon v_\epsilon(t) - \frac{1}{\epsilon}(I - P_\epsilon^2) u_\epsilon(t) \end{array} \right.$$

Consider a solution (u, v) to the continuous equation (1) starting from a continuous and compactly supported initial condition $(u(0), v(0))$. Take for $(u_\epsilon(0), v_\epsilon(0))$ the restriction of $(u(0), v(0))$ to $\epsilon\mathbb{Z}^d$. Then for any given $(t, x) \in \mathbb{R}_+ \times \mathbb{R}^d$, we have

$$\lim_{\epsilon \to 0_+} u_\epsilon(t_\epsilon, x_\epsilon) = u(t, x), \qquad \lim_{\epsilon \to 0_+} v_\epsilon(t_\epsilon, x_\epsilon) = v(t, x)$$

where for any $\epsilon > 0$, $t_\epsilon \in \epsilon\mathbb{Z}_+$ and $x_\epsilon \in \epsilon\mathbb{Z}^d$ are such that $\lim_{\epsilon \to 0_+} t_\epsilon = t$ and $\lim_{\epsilon \to 0_+} x_\epsilon = x$.

"Diffusions" on graphs

Consider the Markov semi-group dynamics on (V, E, P):

$$\forall\ t \in \mathbb{Z}_+, \qquad u(t+1) \;=\; Pu(t)$$

Renormalise it on $\sqrt{\epsilon}\mathbb{Z}^d$ through

$$\forall\ t \in \epsilon\mathbb{Z}_+, \qquad u_\epsilon(t+\epsilon) \;=\; P_{\sqrt{\epsilon}}[u_\epsilon(t)]$$

then we get the analog of the previous convergence

$$\lim_{\epsilon \to 0_+} u_\epsilon(t_\epsilon, x_\epsilon) \;=\; u(t, x)$$

where u is the solution to the heat equation

$$\dot{u} \;=\; \frac{1}{2d}\Delta u \tag{2}$$

Unitary dynamics

In the discrete wave framework, define

$$\forall\ t \in \mathbb{Z}_+, \qquad w(t) \ := \ \sqrt{I - P^2}\,u(t)$$

then the wave equation writes as

$$\forall\ t \in \mathbb{Z}, \qquad \begin{pmatrix} w(t+1) \\ v(t+1) \end{pmatrix} \ = \ U \begin{pmatrix} w(t) \\ v(t) \end{pmatrix}$$

with the unitary propagator

$$U \ := \ \begin{pmatrix} P & \sqrt{I - P^2} \\ -\sqrt{I - P^2} & P \end{pmatrix}$$

In particular, the following "energy" quantity

$$\|\sqrt{I - P^2}\,u(t)\|^2 + \|v(t)\|^2 \ = \ \|w(t)\|^2 + \|v(t)\|^2$$

is conserved through the evolution.

Chebyshev polynomials

For any $t \in \mathbb{Z}_+$, the t-step propagator U^t writes as

$$U^t = \begin{pmatrix} T_t(P) & \sqrt{I - P^2}\, U_{t-1}(P) \\ -\sqrt{I - P^2}\, U_{t-1}(P) & T_t(P) \end{pmatrix}$$

where $(T_t)_{t \in \mathbb{Z}_+}$ and $(U_t)_{t \in \mathbb{Z}_+}$ are respectively the families of Chebyshev polynomials of the first and second kind: for any $t \in \mathbb{Z}_+$ and $\theta \in \mathbb{R}/(2\pi\mathbb{Z})$,

$$\begin{aligned} T_t(\cos(\theta)) &= \cos(t\theta) \\ U_t(\cos(\theta)) &= \frac{\sin((t+1)\theta)}{\sin(\theta)} \end{aligned}$$

The fact that for any $t \in \mathbb{Z}_+$, U^t is a unitary extension of $T_t(P)$, also known as "block encoding", is important in the quantum computing literature, starting with the seminal work of Szegedy, who constructed a different unitary extension of a Markov transition kernel.

Plan

Quantum dynamics

The preceding considerations suggest to define a quantum dynamics via

$$\forall\ n \in \mathbb{Z}_+, \qquad \varphi_n \quad := \quad U^n[\varphi_0]$$

where φ_0 is a given element of $\mathbb{L}^2(V) \oplus \mathbb{L}^2(V)$. More precisely, we are interested in the case where $\varphi_0 := \begin{pmatrix} e_{x_0} \\ 0 \end{pmatrix}$ where e_{x_0} is the indicator function of an initial vertex x_0 from V. Then we have

$$U^n \begin{pmatrix} e_{x_0} \\ 0 \end{pmatrix} \quad = \quad \begin{pmatrix} T_n(P)\, e_{x_0} \\ -\sqrt{I - P^2}\, U_{n-1}(P)\, e_{x_0} \end{pmatrix}$$

We focus our attention on the evolution of u-coordinate, i.e. $(T_n(P)\, e_{x_0})_{n \in \mathbb{Z}_+}$, and more particularly on the associated measures $(\nu_n)_{n \in \mathbb{Z}_+}$ on V given by

$$\forall\ n \in \mathbb{Z}_+, \forall\ x \in V, \qquad \nu_n(x) \quad := \quad (T_n(P)(x_0, x))^2$$

On $\mathbb{Z}$ (1)

Take for P the usual random walk transition kernel on $\mathbb{Z}$.
Consider Q_1 the shift operator on $\mathbb{Z}$: we have

$$\forall\, x \in \mathbb{Z}, \qquad Q_1[e_x] \;=\; e_{x+1}$$

where e_x is the indicator function of x. We have

$$P \;=\; \frac{Q_1 + Q_1^{-1}}{2}$$

and for any $n \in \mathbb{Z}_+$, P^n corresponds to the (shifted and scaled) binomial distribution centred at 0 of variance n.

Taking into account the formula

$$\forall\ z \in \mathbb{C}\backslash\{0\}, \qquad T_n\left(\frac{z+z^{-1}}{2}\right) = \frac{z^n+z^{-n}}{2}$$

we get

$$T_n(P) = T_n\left(\frac{Q_1+Q_1^{-1}}{2}\right) = \frac{Q_1^n+Q_1^{-n}}{2}$$

namely

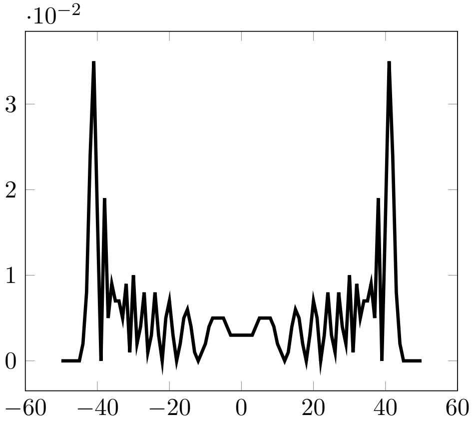
$$T_n(P)(0,x) = \frac{e_n(x)+e_{-n}(x)}{2}$$

showing that

$$\nu_n = \frac{1}{4}(\delta_n+\delta_{-n})$$

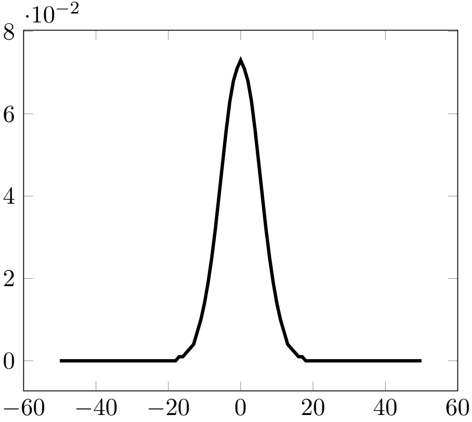
Lazy on $\mathbb{Z}$ (1)

Rather consider the lazy transition kernel $P_L = (I + P)/2$ on $\mathbb{Z}$, the expansion of $T_n(P_L)$ is no longer so simple. Instead, we retrieve the fickle (but still ballistic) behaviour usually associated to the quantum walk on the line. Here is picture for ν_{50}:



Lazy on $\mathbb{Z}$ (2)

To be compared with the picture for $P_L^{50}(0,\cdot)$ illustrating the diffusive behaviour of the usual random walk:



Plan

On $\mathbb{Z}^2$ (1)

On the 2-dimensional lattice consider the commuting operators Q_1 and Q_2 described by $Q_1 e_{(x,y)} = e_{(x+1,y)}$ and $Q_2 e_{(x,y)} = e_{(x,y+1)}$ for any $(x,y) \in \mathbb{Z}^2$. Set $P_1 = (Q_1 + Q_1^{-1})/2$ and $P_2 = (Q_2 + Q_2^{-1})/2$, we are interested in the usual random walk transition kernel

$$P \quad := \quad \frac{P_1 + P_2}{2}$$

Introduce the expansion in two commuting variables X, Y:

$$T_n\left(\frac{X+Y}{2}\right) \quad =: \quad \sum_{(p,q)\in[\![0,n]\!]} a_{n,p,q} T_p(X) T_q(Y)$$

for a set of real coefficients $(a_{n,p,q})_{p,q\in[\![0,n]\!]}$.

On $\mathbb{Z}^2$ (2)

Since P_1 and P_2 are commuting, we deduce:

$$T_n\left(\frac{P_1+P_2}{2}\right) = \sum_{(p,q)\in[\![0,n]\!]} a_{n,p,q}\, T_p(P_1)\, T_q(P_2)$$

$$= \sum_{(p,q)\in[\![0,n]\!]} a_{n,p,q} \left(\frac{Q_1^p + Q_1^{-p}}{2}\right)\left(\frac{Q_2^q + Q_2^{-q}}{2}\right)$$

and we get:

$$\forall\ (p,q)\in\mathbb{Z}^2, \qquad (T_n(P)((0,0),(p,q)))^2 = a^2_{n,|p|,|q|}/2^{2k(|p|,|q|)}$$

where $k(|p|,|q|)\in\{0,1,2\}$ denotes the number of nonzero entries among $|p|,|q|$. We will see that the points of the form $(0,q)$ and (p,q) do not play an important role.

Weak convergence

Introduce the probability measure μ_n on $[-1,1]^2$ given by

$$\mu_n \quad := \quad \frac{\sum_{p,q} a^2_{n,|p|,|q|} \delta_{(p/n,q/n)}}{\sum_{p,q} a^2_{n,|p|,|q|}}$$

where $\delta_{(p/n,q/n)}$ is the Dirac mass at $(p/n, q/n) \in [0,1]^2$.
Our main result is:

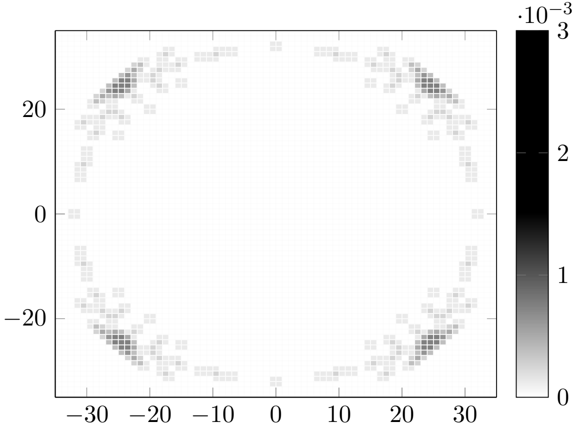
Theorem 1

There exists a continuous probability measure μ on $[-1,1]^2$ such that $\mu_n \to_{n\to\infty} \mu$.

The measure μ will be described through its moments.

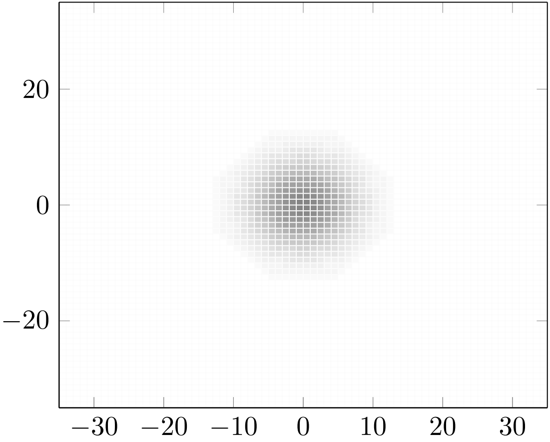
Ballistic picture

The ballistic feature of the above theorem is illustrated by the following picture of ν_{50}:



Diffusive picture

To be compared with the picture for $P^{50}(0,\cdot)$ illustrating the diffusive behaviour of the usual random walk:



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Moments

Remove the normalisation and consider

$$\gamma_n \quad := \quad \sum_{p,q \in [\![0,n]\!]} a_{n,p,q}^2 \delta_{(p/n,q/n)}$$

so that $\mu_n = \frac{\gamma_n}{\gamma_n([0,1]^2)}$.
We will find a continuous probability measure γ on $[0,1]^2$ such that

$$\forall\ K, L \in \mathbb{Z}_+, \qquad \lim_{n\to\infty} \gamma_n[\varphi_{K,L}] \quad = \quad \gamma[\varphi_{K,L}]$$

where

$$\varphi_{K,L}\ :\ [0,1]^2 \ni (x,y) \quad \mapsto \quad x^{2K} y^{2L}$$

The Stone-Weierstrass theorem implies the weak convergence of γ_n toward γ and by consequence Theorem 1 with $\mu = \gamma$.

Moments as an integral

Introduce the function h given for any $x, y \in [0, 2\pi]$ by

$$h(x,y) := T_n\left(\frac{\cos(x)+\cos(y)}{2}\right) = \sum_{p,q\in[\![0,n]\!]} a_{n,p,q}\cos(px)\cos(qy)$$

We have the following approximation

Proposition 1

$$\lim_{n\to\infty}\left|\gamma_n[\varphi_{K,L}] - \frac{1}{\pi^2 n^{2(K+L)}}\int_{[0,2\pi]^2}\left(\partial_x^K \partial_y^L h(x,y)\right)^2 dxdy\right| = 0$$

Arguments for Proposition 1 (1)

In one hand, compute the partial derivative in the integral:

$$\partial_x^K \partial_y^L h(x,y) = \sum_{p,q\in[\![0,n]\!]} a_{n,p,q} p^K q^L \xi_K(px)\xi_L(qy)$$

where $\xi_r(z)$ denotes the r-th derivative $\cos^{(r)}(z)$, and on the other hand, use the orthogonality relations: for any $p, p' \in \mathbb{Z}_+$,

$$\frac{1}{2\pi}\int_0^{2\pi} \xi_r(px)\xi_r(p'x)\,dx = \begin{cases} 1 & \text{, if } p = p' = 0 \text{ and } r \equiv 0[2] \\ 1/2 & \text{, if } p = p' \geqslant 1 \\ 0 & \text{, otherwise} \end{cases}$$

We get the equality

$$\frac{1}{\pi^2 n^{2(K+L)}}\int \left(\partial_x^K \partial_y^L h(x,y)\right)^2 dxdy = \gamma_n[\varphi_{K,L} w_K(n\,\cdot) \otimes w_L(n\,\cdot)]$$

Arguments for Proposition 1 (2)

where

$$\forall\ k \in \mathbb{Z}_+,\ \forall\ r \in \mathbb{Z}_+, \qquad w_k(r) \quad := \quad \begin{cases} 2 & \text{, if } k \text{ is even and } r = 0 \\ 0 & \text{, if } k \text{ is odd and } r = 0 \\ 1 & \text{, otherwise} \end{cases}$$

So to prove Proposition 1 it is sufficient to show that

$$\lim_{n \to \infty} \sum_{p \in \mathbb{Z}_+} a_{n,p,0}^2 \quad = \quad 0$$

This convergence also shows that the behaviours of μ_n and ν_n are the same for large n.

Arguments for Proposition 1 (3)

The access to the previous quantity is provided by expansion of

$$\frac{4}{\pi}\int\left(\frac{1}{2\pi}\int_{[0,2\pi]} T_n\left(\frac{\cos(x)+\cos(y)}{2}\right)\,dy\right)^2 dx$$
$$= \quad a_{n,0,0}^2 + \sum_{p\in[\![0,n]\!]} a_{n,p,0}^2$$

The integral inside the square for fixed x can be transformed by the change of variable $\cos(z) = (\cos(x)+\cos(y))/2$. Next an application of the Riemann-Lebesgue theorem implies that this integral converges to zero for large n. The desired result follows by dominated convergence theorem.

Removing the boundary region

For $\epsilon \in (0,1)$, consider

$$A_\epsilon := \left\{(x,y) \in [0,2\pi]^2 \; : \; \left|\frac{\cos(x)+\cos(y)}{2}\right| \leqslant 1-\epsilon\right\}$$

$$B_\epsilon := [0,2\pi]^2 \backslash A_\epsilon$$

We have

Lemma 2

$$\lim_{\epsilon\to 0_+} \lim_{n\to\infty} \left|\gamma_n[\varphi_{K,L}] - \frac{1}{\pi^2 n^{2(K+L)}} \int_{A_\epsilon} \left(\partial_x^K \partial_y^L h(x,y)\right)^2 dxdy\right| = 0$$

It amounts to show that

$$\lim_{\epsilon\to 0_+} \sup_{n\geqslant 1} \frac{1}{n^{2(K+L)}} \int_{B_\epsilon} \left(\sum_{p,q\in[\![0,n]\!]} a_{n,p,q} p^K q^L \xi_K(px)\xi_L(qy)\right)^2 dxdy = 0$$

Arguments for Lemma 2

The proof is based on an approximative orthogonality relations:

$$\int_{-\eta}^{\eta} \xi_K(px)\xi_K(p'x)\,dx \quad = \quad \frac{\sin((p+p')\eta)}{p+p'} - \frac{\sin((p-p')\eta)}{p-p'}$$

where $\eta \in (0,\pi)$ corresponds to the boundary of B_ϵ and is given by $\cos(\eta) = 1 - 2\epsilon$. Cauchy-Schwartz inequality implies that the integral at the end of the previous slide is bounded above by

$$\sum_{p,q} a_{n,p,q}^2 \left(\eta^2 + 2\sum_{r\in\mathbb{N}} \left(\frac{\sin(r\eta)}{r}\right)^2\right)^2$$

The desired convergence is a consequence of $\sum_{p,q} a_{n,p,q}^2 \leqslant 4$ (consequence of Proposition 1 with $K = L = 0$) and

$$\lim_{\eta\to 0_+} \sum_{r\in\mathbb{N}} \left(\frac{\sin(r\eta)}{r}\right)^2 \quad = \quad 0$$

Simplifying the integral (1)

Applying twice Fa di Bruno's formula we can rewrite $\partial_x^K \partial_y^L h(x,y)$ as

$$\sum_{\substack{m_1+2m_2+\cdots+Km_K=K \\ n_1+2n_2+\cdots+Ln_L=L}} \frac{K!}{m_1!m_2!\cdots m_K!}\frac{L!}{n_1!n_2!\cdots n_L!}$$

$$T_n^{(\sum m_\ell + \sum n_\ell)}\left(\frac{\cos(x)+\cos(y)}{2}\right)\prod_{k\in[\![K]\!]}\left(\frac{\xi_k(x)}{2k!}\right)^{m_k}\prod_{l\in[\![L]\!]}\left(\frac{\xi_l(y)}{2l!}\right)^{n_l}$$

For $(x,y)\in A_\epsilon$ with fixed $\epsilon\in(0,1)$, it appears the dominant term in the above sum corresponds to $m_1 = K$ and $n_1 = L$. So introducing

$$I_{K,L}(\epsilon,n) \quad := \quad \frac{1}{\pi^2 n^{2(K+L)}}\int_{A_\epsilon}\left(T_n^{(K+L)}\left(\frac{\cos(x)+\cos(y)}{2}\right)\right.$$
$$\left.\left(\frac{-\sin(x)}{2}\right)^K\left(\frac{-\sin(y)}{2}\right)^L\right)^2 dxdy$$

Simplifying the integral (2)

we get

$$\lim_{n\to\infty} \frac{1}{\pi^2 n^{2(K+L)}} \int_{A_\epsilon} \left(\partial_x^K \partial_y^L h(x,y)\right)^2 \, dxdy - I_{K,L}(\epsilon, n) \quad = \quad 0$$

Introduce $\theta(x,y)$ the unique solution in $[0,\pi]$ of

$$\cos(\theta(x,y)) \quad = \quad \frac{\cos(x)+\cos(y)}{2}$$

and define

$$J_{K,L}(\epsilon,n) \quad := \quad \frac{1}{\pi^2 2^{2(K+L)}} \int_{A_\epsilon} \xi_{K+L}^2(n\theta(x,y)) \left(\frac{\sin(x)}{\sin(\theta(x,y))}\right)^{2K} \left(\frac{\sin(y)}{\sin(\theta(x,y))}\right)^{2L} \, dxdy$$

Simplifying the integral (3)

Applying Fa di Bruno's formula to the derivative $\partial_\theta^{K+L} T_n(\cos(\theta))$ and keeping the dominant term, we get

$$\lim_{\epsilon\to 0_+} \limsup_{n\to\infty} |I_{K,L}(\epsilon,n) - J_{K,L}(\epsilon,n)| = 0$$

so that

$$\lim_{\epsilon\to 0_+} \lim_{n\to\infty} |\gamma_n[\varphi_{K,L}] - J_{K,L}(\epsilon,n)| = 0$$

Finally using symmetry, the change of variables $[0,\pi]^2 \ni (x,y) \mapsto (x,\theta(x,y))$ and the Riemann-Lebesgue theorem give us:

$$\lim_{\epsilon\to 0_+} \limsup_{n\to\infty} J_{K,L}(\epsilon,n)$$
$$= \frac{1}{\pi^2}\int_{[0,\pi]^2} \left(\frac{\sin(x)}{\sin(\theta(x,y))}\right)^{2K} \left(\frac{\sin(y)}{\sin(\theta(x,y))}\right)^{2L} dxdy$$

The limiting probability measure

From the last limit, we deduce the weak convergence for large n of the γ_n toward the probability measure γ which is the image of the measure $\frac{1}{\pi^2}dxdy$ on $[0,\pi]^2$ by the mapping

$$\Psi \ : \ [0,\pi]^2 \ni (x,y) \quad \mapsto \quad \left(\frac{\sin(x)}{\sin(\theta(x,y))}, \frac{\sin(y)}{\sin(\theta(x,y))} \right) \qquad (3)$$

In particular it appears that γ is a probability measure, so that $\mu = \gamma$, as announced previously.

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