On the spectral analysis of second-order Markov chains

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Plan of the talk

Nonreversibility, why?

- Nonreversible Markov chains can avoid diffusive effects and go faster to equilibrium: [Diaconis, Holmes and Neal, 2000]

- The asymptotic variance of empirical estimators based on nonreversible Markov chains can be smaller: [Neal 2004]

- Typically nonreversible second order Markov chains enable better modelisations of physical dynamics: [Bacallado and Pande, 2009]

Second order Markov chains

V finite state space
Stochastic chain $(X_n)_{n\in\mathbb{N}}$ on V is second order iff

$$\mathcal{L}((X_m)_{m\geq n+1}|(X_m)_{m\in[\![0,n]\!]}) \quad = \quad \mathcal{L}((X_m)_{m\geq n+1}|X_n, X_{n-1})$$

Corresponding (time-homogeneous) kernel:

$$M(x, x'; x'') \quad := \quad \mathbb{P}[X_{n+1} = x''|X_n = x', X_{n-1} = x]$$

Initial law: $m = \mathcal{L}(X_0, X_1)$. It is said to be "trajectorially" reversible if

$$\mathcal{L}(X_0, X_1, \cdots, X_n) \quad = \quad \mathcal{L}(X_n, X_{n-1}, \cdots, X_0)$$

Trajectorial reversibility

Sufficient to check for $n = 1$ and $n = 2$. In particular, m is symmetrical and can be written

$$m(x, x') \quad = \quad \nu(x)L(x, x')$$

with L Markov kernel reversible with respect to ν.
Let $(\widetilde{X}_n)_{n\in\mathbb{N}}$ be a Markov chain associated to L. Usually, whatever the initial distributions,

$$\lim_{n\to\infty} \mathcal{L}(X_n, X_{n+1}) = m = \lim_{n\to\infty} \mathcal{L}(\widetilde{X}_n, \widetilde{X}_{n+1})$$

(by trajectorial reversibility, m is also invariant). Which convergence is faster?

Spectral gap

See M as an operator on $\mathcal{F}(V^2, \mathbb{C})$, via

$$M[F](x, x') \quad := \quad \sum_{x'' \in V} M(x, x'; x'') F(x', x'')$$

The subspace $\mathcal{F}_*(m, \mathbb{C}) := \{F \in \mathcal{F}(V^2, \mathbb{C}) \, : \, m[F] = 0\}$ is stable by M, let $\Theta_*(M) \subset \mathbb{C}$ be the spectrum of the restriction of M to $\mathcal{F}_*(m, \mathbb{C})$ and define

$$\lambda(M) \quad := \quad 1 - \max\{|\theta| \, : \, \theta \in \Theta_*(M)\} \quad \in \quad [0, 1]$$

It is the asymptotical rate of convergence: whatever the norm $\|\cdot\|$ on $\mathcal{M}(V^2)$,

$$\max_{m_0 \in \mathcal{P}(V^2)} \lim_{n \to \infty} \frac{1}{n} \ln \left(\| m_0 M^n - m \| \right) \quad = \quad \ln(1 - \lambda(M))$$

Questions

Assume that L is given (reversible wrt ν). Let $\lambda(L)$ be the usual spectral gap of L.

- Can we find M as above, with $\lambda(M) > \lambda(L)$?

- Are there some heuristic guidelines to construct such M?

- How much can $\lambda(M)$ be better than $\lambda(L)$?

Extension of L

L can be naturally extended into a "second order" Markov kernel $M^{(0)}$: take

$$\forall\ x, x', x'' \in V, \qquad M^{(0)}(x, x'; x'') \ := \ L(x', x'')$$

It may be that $M^{(0)}$ is not diagonalizable, but anyway $\mathrm{Spectrum}(M^{(0)}) = \mathrm{spectrum}(L) \cup \{0\}$, so

$$\lambda(L) \ = \ \lambda(M^{(0)})$$

To answer the previous questions, we will consider perturbations of $M^{(0)}$:

$$\forall\ a \in [0, 1], \qquad M^{(a)} \ := \ (1 - a)M^{(0)} + aM^{(1)}$$

where $M^{(1)}$ is trajectorially reversible wrt m and we will study $a \mapsto \lambda(M^{(a)})$.

Answer 1

Let $M^{(1)}$ be trajectorially reversible wrt m and satisfying

$$M^{(1)}(x, x'; x'') \quad > \quad L(x', x'')$$

if $x'' \neq x$, $L(x, x') > 0$ and $L(x', x'') > 0$. Namely, $M^{(1)}$ has less tendency to come back where it just came from than $M^{(0)}$.

Theorem

Assume that L is irreducible, that $L \neq \nu$ and that L is aperiodic. The mapping $[0, 1] \ni a \mapsto \lambda(M^{(a)})$ is differentiable at 0 and we have

$$\frac{d\lambda(M^{(a)})}{da}(0) \quad > \quad 0$$

Answer 2

In fact, initially the whole spectrum outside 0 is improving under the above perturbation: important to get quantitative bounds on the distance to equilibrium in chi-square distance.

It is sometimes (for instance if L is the random walk on a regular graph), to find the best perturbation to improve (initially) only the spectral gap. An heuristic (answer 2) is to keep going (symmetrically) in the direction indicated by the first eigenvector...

Homogeneous framework

V Abelian group, "speeds" given by $Y_n = X_{n+1} - X_n$. Change of variables:

$$(x, x') \leftrightarrow (x, y = x' - x) \qquad (\text{and } y' = x'' - x')$$

leads to

$$M(x, x'; x'') \leftrightarrow \delta_{x+y}(x') K_{x'}(y, y')$$

where $K_{x'}(y, y')$ is the change of speeds from y to y' above the (intermediate) position x'. Homogeneous setting: $K_x \equiv K$ does not depend on x and is a Markov kernel on S, generating set for V. Trajectorial reversibility leads to L being a random walk transition whose increments are distributed on S (according to a distribution μ which is symmetric).

A well-understood example

(V, S) given and take $\mu \equiv 1/|S|$ on S (symmetric). Then, $K^{(0)} = \mu$ and consider $K^{(1)}$ on S forbidding to reverse speed and transfering the weight to all the other directions:

$$\forall\ y, y' \in S, \qquad K^{(1)}(y, y') \ := \ \begin{cases} \frac{1}{|S|-1} & \text{, if } y' \neq -y \\ 0 & \text{, if } y' = -y \end{cases}$$

Define the interpolating kernel $K^{(a)}$, for $a \in [0, 1]$, as well as the corresponding second order kernels $M^{(a)}$. They are trajectorially reversible wrt

$$\forall\ x, x' \in V, \qquad m(x, x') \ := \ \begin{cases} \frac{1}{|V||S|} & \text{, if } x' - x \in S \\ 0 & \text{, otherwise} \end{cases}$$

Answer 3

Theorem

Let $\lambda := \lambda(L)$ *and define*

$$a_0 \quad := \quad (|S|-1)\frac{1-\sqrt{\lambda(2-\lambda)}}{1+\sqrt{\lambda(2-\lambda)}} \quad \geq \quad 0$$

Then $\lambda(M^{(a)})$ *is nondecreasing for* $a \in [0, a_0 \wedge 1]$ *and nonincreasing on* $[a_0 \wedge 1, 1]$. *Furthermore, with* $\Lambda := \max_{a\in[0,1]} \lambda(M^{(a)})$, *if* $a_0 \leq 1$,

$$\Lambda \quad = \quad \sqrt{\frac{1-\sqrt{\lambda(2-\lambda)}}{1+\sqrt{\lambda(2-\lambda)}}}$$

while if $a_0 > 1$,

$$\Lambda \quad = \quad 1 - \frac{|S|}{2(|S|-1)}\left(1-\lambda+\sqrt{\left(\frac{|S|-2}{|S|}\right)^2-\lambda(2-\lambda)}\right)$$

Conjecture

This result is interesting if $|S| = 2$, but not so good if $|S| > 2$. $K^{(1)}$ defined above is not the appropriate perturbation and a more relevant one would be $K^{(1)} = \mathrm{Id}$ (which forces to keep going always with the same speed). What we believe for the associated second order Markov chains (trajectorially reversible wrt the same m as before): There exists $a_0 \in [0, 1]$ such that $\lambda(M^{(a)})$ is nondecreasing for $a \in [0, a_0]$ and nonincreasing on $[a_0, 1]$. Furthermore there exists two values $0 < c_1 < c_2$ (maybe depending on $|S|$), such that

$$c_1 \sqrt{\lambda(L)} \;\leq\; \lambda(M^{(a_0)}) \;\leq\; c_2 \sqrt{\lambda(L)}$$

(true if $|S| = 2$, as a consequence of Theorem 2).

The first task is to get the spectral decomposition of $M^{(0)}$:

Proposition

The spectrum of the transition operator $M^{(0)}$ is equal to the spectrum of L with the same multiplicities, except for the eigenvalue 0, whose multiplicity is $|V|^2 - |V|$. In particular $M^{(0)}$ is diagonalizable if and only if 0 is not an eigenvalue of L. When 0 is an eigenvalue of L, let d be the dimension of the corresponding eigenspace. Then the canonical form of $M^{(0)}$ contains d 2×2-Jordan blocks $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$.

Idea: consider the functions $F(x, x') := f(x')$ (f eigenvector of L), $F(x, x') := \delta_{x_0}(x) f(x')$ (with $L[f](x_0) = 0$) and $F(x, x') := f(x)$ (with $L[f] = 0$).

Perturbations, according to Kato

Opening The Book at the right pages:

Lemma

There exists $a_0 \in (0,1)$ such that the number s of distinct eigenvalues of $M^{(a)}$ does not depend on $a \in (0, a_0)$. It is possible to parameterize these eigenvalues by $(\theta_l(a))_{l \in [\![s]\!]}$ in such a way that for any $l \in [\![s]\!]$, the mapping $(0, a_0) \ni a \mapsto \theta_l(a)$ is analytical. Furthermore these mappings admit continuous extension to $[0, a_0)$ and the set $\{\theta_l(0) : l \in [\![s]\!]\}$ coincides with the spectrum of $M^{(0)}$ (note nevertheless that the cardinal of this spectrum can be stricly less than s, when occurs a splitting phenomenon of some eigenvalues at 0). Moreover for any $l \in [\![s]\!]$, we can find a continuous mapping $[0, a_0) \ni a \mapsto F_l(a) \in \mathcal{F}(V^2, \mathbb{C}) \setminus \{0\}$ such that for any $a \in [0, a_0)$, F_l is an eigenfunction associated to the eigenvalue $\theta_l(a)$ of $M^{(a)}$, and such that the mapping $(0, a_0) \ni a \mapsto F_l(a) \in \mathcal{F}(V^2, \mathbb{C}) \setminus \{0\}$ is analytical.

The main ingredient

Proposition

Let $l \in [\![s]\!]$ be such that $\theta_l(0) \neq 0$. Then the limit $\lim_{a \to 0_+} \theta_l'(a)$ exists and belongs to $\mathbb{R}$. Furthermore if $|\theta_l(0)| \neq 1$, then the sign of $\theta_l'(0)$ is the opposite sign of $\theta_l(0)$.

Begin by differentiating $M^{(a)} F_l(a) = \theta_l(a) F_l(a)$ to get

$$(M^{(1)} - M^{(0)}) F_l(a) + M^{(a)} F_l'(a) \quad = \quad \theta_l'(a) F_l(a) + \theta_l(a) F_l'(a)$$

To eliminate $F_l'(a)$, multiply by $\widetilde{F}_l(a)$, an eigenvector of $(M^{(a)})^*$ (the dual operator of $M^{(a)}$ in $\mathbb{L}^2(m)$) associated to the eigenvalue $\theta_l(a)$ and integrate with respect to m:

$$m[\widetilde{F}_l(a)(M^{(1)} - M^{(0)}) F_l(a)] \quad = \quad \theta_l'(a) m[\widetilde{F}_l(a) F_l(a)]$$

Duality

M trajectorially reversible wrt to m and M^* its dual. Define the tilde operation on $\mathcal{F}(V^2)$ as the exchange of coordinates:

$$\forall\ F \in \mathcal{F}(V^2), \forall\ x, x' \in V, \qquad \widetilde{F}(x, x') \ := \ F(x', x)$$

Then we have

$$\forall\ F \in \mathcal{F}(V^2), \qquad M^*[F] \ = \ \widetilde{M[\widetilde{F}]}$$

(in general not a second order Markov kernel).
Thus if F is an eigenvector associated to θ, wrt M, then $\widetilde{F}$ is an eigenvector associated to θ, wrt M^*. As a consequence, we know how to compute $\widetilde{F}_I(a)$ in the previous equation, especially when $a = 0$ ...

Singular values

There are completely useless here:
Let M and M^* be as above. The spectrum of the Markovian operator M^*M in $\mathbb{L}^2(m)$ is the union, with multiplicities, of the spectra of the $M^2_{x'}$, for $x' \in V$, where $M_{x'}$ is the transition kernel on $V_{x'} = \{x \in V : L(x', x) > 0\}$ defined by

$$\forall\, x, x'' \in V_{x'}, \qquad M_{x'}(x, x'') \;:=\; M(x, x'; x'')$$

Unfortunately, the information contained in the $M_{x'}$, for $x' \in V$, is of a local nature (it just describes how the "speed" evolves above the point $x' \in V$) and is not sufficient to deduce the global rate of convergence to equilibrium.

Links with the works of Neal?

Let $(X_n)_{n\in\mathbb{N}}$ be a second order trajectory reversible Markov chain whose transition kernel is M and let $f \in \mathcal{F}(V)$ be a function satisfying $\nu[f] = 0$. For $n \in \mathbb{N}$ large, the variance of the random variable $(f(X_1) + \cdots + f(X_n))/\sqrt{n}$ admits a limit $\sigma(M, f)$. Under the assumption

$$\forall\, x'' \neq x \in V, \qquad M(x, x'; x'') \;\geq\; L(x', x'')$$

Neal has proven that

$$\sigma(M, f) \;\leq\; \sigma(M^{(0)}, f) \quad (= \sigma(L, f))$$

His proof is based on a clever decomposition of trajectories and also gives a probabilistic proof of Peskun's theorem. But the link with our results is not clear!

Best improvement of spectral gap

We are looking for the perturbation signed kernel $D^\dagger$ leading to the best gap improvement:

$$\frac{d}{d\epsilon}\lambda(M^{(0)}+\epsilon D^\dagger)\Big|_{\epsilon=0} \quad = \quad \sup_{D\in\mathcal{D}} \frac{d}{d\epsilon}\lambda(M^{(0)}+\epsilon D)\Big|_{\epsilon=0}$$

where $\mathcal{D}$ imposes normalization and trajrev conditions.
Assume that L is the transition kernel of a rw on a n-regular graph and that, up to a factor, there is only one eigenfunction f associated to $\pm(1-\lambda(L))$. For $x' \in V$, let $\{x_1, x_2, ..., x_n\} := \{x : L(x', x) > 0\}$ ordered such that $f(x_1) \leq f(x_2) \leq \cdots \leq f(x_n)$. Then a maximizer $D^\dagger$ is given by

$$D^\dagger(x_i, x'; x_j) \quad = \quad J(i,j) - I(i,j)$$

where I and J are the identity and reverse diagonal matrices.

A general observation

Let S and V be finite sets with cardinals s and v. Let K be a $S \times S$ matrix and for any $y \in S$, let Q_y be a $V \times V$ matrix. consider P the $(V \times S) \times (V \times S)$ matrix defined by

$$\forall\ (x,y),(x',y') \in V \times S,\ P((x,y),(x',y')) \quad = \quad K(y,y')Q_y(x,x')$$

Assume there is a basis $(\varphi_l)_{l \in [\![v]\!]}$ of $\mathcal{F}(V,\mathbb{C})$ consisting of eigenfunctions for Q_y, independent of $y \in S$. The corresponding eigenvalues are allowed to depend on $y \in S$ and are denoted by $(\sigma_l(y))_{l \in [\![v]\!]}$. For fixed $l \in [\![v]\!]$, consider K_l the $S \times S$ matrix defined by

$$\forall\ y,y' \in S, \qquad K_l(y,y') \quad := \quad \sigma_l(y)K(y,y')$$

Assume that it is diagonalizable (in $\mathbb{C}$) and denote by $(\theta_{l,k})_{k \in [\![s]\!]}$ and $(\psi_{l,k})_{k \in [\![s]\!]}$ its eigenvalues and corresponding eigenvectors. Then P is diagonalizable, its eigenvalues are the $\theta_{l,k}$ for $(l,k) \in [\![v]\!] \times [\![s]\!]$ and a corresponding family of eigenvectors is $(\varphi_l \otimes \psi_{l,k})_{(l,k) \in [\![v]\!] \times [\![s]\!]}$.

Abelian groups

Homogeneous setting: $Q_y(x, x') := \delta_{x+y}(x')$
Joint diagonalizability equivalent to the commutation relations

$$\forall\ y, y' \in S, \qquad Q_y Q_{y'} \quad = \quad Q_{y'} Q_y$$

and this leads to the Abelianness of V. It is isomorphe to a group product $\prod_{l \in [\![1,r]\!]} \mathbb{Z}_{N_l}$ and consider V^* the set of mappings $\rho : V \to \mathbb{T}$ of the form,

$$\forall\ x = (x_l)_{l \in [\![1,r]\!]} \in V, \qquad \rho(x) \quad = \quad \exp\left(2\pi i \sum_{l \in [\![1,r]\!]} k_l x_l / N_l\right)$$

For such representations, $Q_y[\rho] = \rho(y)\rho$ and thus we are led to introduce $A_\rho := \triangle(\rho)K$, where $\triangle(\rho)$ is the $(\rho(y))_{y \in S}$ diagonal matrix: if all these matrices are diagonalizable, then M is diagonalizable and its spectrum is the union of the spectra of the A_ρ, with $\rho \in V^*$ (with multiplicities).

Centro-Hermitian matrices

The trajectorial reversibility is equivalent to the reversibility of $\widehat{K}$ defined by $\widehat{K}(y, y') := K(y^{-1}, y')$ (say wrt μ). Then μ is invariant for K and if in addition we assume that K is reversible wrt μ (as in our examples), it is interesting to consider

$$B_\rho \quad := \quad \triangle(\sqrt{\mu}\rho^{-1/2})A_\rho\triangle(\rho^{1/2}/\sqrt{\mu})$$

This matrix is centro-Hermitian

$$\forall\ y, y' \in S, \qquad B_\rho(y, y') \quad = \quad \overline{B_\rho(-y, -y')}$$

and furthermore symmetric if μ is uniform.

A simple example

$V = \mathbb{Z}_N$ and $S = \{-1, +1\}$ ($N \geq 2$). The natural state space: set of nearest neighbors. Consider for $a \in [0, 1]$,

$$M^{(a)}(x, x'; x'') := \begin{cases} (1+a)/2 & \text{, if } x' = x+1 \text{ and } x'' = x'+1 \\ (1+a)/2 & \text{, if } x' = x-1 \text{ and } x'' = x'-1 \\ (1-a)/2 & \text{, if } x' = x+1 \text{ and } x'' = x'-1 \\ (1-a)/2 & \text{, if } x' = x-1 \text{ and } x'' = x'+1 \\ 0 & \text{, otherwise} \end{cases}$$

This is a homogeneous situation with

$$K^{(a)} = \begin{pmatrix} \frac{1+a}{2} & \frac{1-a}{2} \\ \frac{1-a}{2} & \frac{1+a}{2} \end{pmatrix}$$

We have $V^* \leftrightarrow \{\exp(2\pi ikx/N) : k \in [\![0, N-1]\!]\}$ and we must study for $\rho \in V^*$,

$$B_\rho^{(a)} := \begin{pmatrix} \frac{1+a}{2}\rho & \frac{1-a}{2} \\ \frac{1-a}{2} & \frac{1+a}{2}\bar{\rho} \end{pmatrix}$$

Eigenvalues of $B_\rho^{(a)}$

Writing $\rho =: C + iS$, we get with $a_0(\rho) := \frac{1-|S|}{1+|S|} \in [0,1]$,

• If $a \in [0, a_0(\rho))$, the matrix $B_\rho^{(a)}$ is diagonalizable in $\mathbb{R}$ and its eigenvalues are

$$\theta_{\rho,\pm}^{(a)} = \frac{1+a}{2} C \pm \frac{\sqrt{(1-a)^2 - S^2(1+a)^2}}{2}$$

• If $a \in (a_0(\rho), 1]$, the matrix $B_\rho^{(a)}$ is diagonalizable in $\mathbb{C}$ and its eigenvalues are

$$\theta_{\rho,\pm}^{(a)} = \frac{1+a}{2} C \pm i \frac{\sqrt{S^2(1+a)^2 - (1-a)^2}}{2}$$

Define

$$\theta_{\rho,*}^{(a)} := \max\left\{ \left|\theta_{\rho,-}^{(a)}\right|, \left|\theta_{\rho,+}^{(a)}\right| \right\}$$

We have

$$\lambda(M^{(a)}) = 1 - \max(\{\theta_{\rho,*}^{(a)} : \rho \in V^* \setminus \{1\}\} \cup \{a\})$$

Basic computations

• Let $\rho \in \mathbb{T} \setminus \mathbb{R}$ be given. On $[0, a_0(\rho)]$ the mapping $a \mapsto \theta^{(a)}_{\rho,*}$ is strictly concave and decreasing. For $a \in [a_0(\rho), 1]$, we have $\theta^{(a)}_{\rho,*} = \sqrt{a}$. In particular, we get $\theta^{(a)}_{\rho,*} \geq \sqrt{a} \geq a$, so

$$\lambda(M^{(a)}) \quad = \quad 1 - \max\{\theta^{(a)}_{\rho,*} \, : \, \rho \in V^* \setminus \{1\}\}$$

• Let $\rho, \rho' \in \mathbb{T}$ be such that their respective real parts satisfy $C > C' \geq 0$. Then for any $a \in [0, 1]$ we have,

$$\theta^{(a)}_{\rho,*} \quad \geq \quad \theta^{(a)}_{\rho',*}$$

Symmetry implies

$$\lambda(M^{(a)}) \quad = \quad 1 - \theta^{(a)}_{\rho_0,*}$$

with $\rho_0 = \exp(2\pi i \lfloor N/2 \rfloor / N)$

Behavior of the spectral gap

- N even: $\rho_0 = -1$ and $\lambda(L) = 0$, as well as $\lambda(M^{(a)}) = 0$, for any $a \in [0,1]$ (by periodicity).
- N odd: let $C_N := \cos(\pi/N)$ and $a_N = \frac{1-\sqrt{1-C_N^2}}{1+\sqrt{1-C_N^2}}$. The evolution

of the spectral gap of $\lambda(M^{(a)})$ is given by

$$\lambda(M^{(a)}) \quad = \quad \begin{cases} 1 - \frac{1+a}{2} C_N - \frac{\sqrt{(1+a)^2 C_N^2 - 4a}}{2} & , \text{ if } a \in [0, a_N] \\ 1 - \sqrt{a} & , \text{ if } a \in [a_N, 1] \end{cases}$$

The largest spectral gap of $M^{(a)}$ correspond to the choice $a = a_N$ and we get

$$\lambda(M^{(a_N)}) \quad \sim \quad \frac{\pi}{N}$$

(to be compared with $\lambda(L) \sim \frac{\pi^2}{2N^2}$).

Behavior of the whole spectrum

For N odd. For any $a \in [0,1]$, the spectrum of $M^{(a)}$ is included into $[-1,1] \cup \mathcal{C}(\sqrt{a})$. The eigenvalues go by pairs. At $a = 0$, one starts from zero and the other one from an eigenvalue of L and they go in the direction of each other (except for the pair containing 1). When they meet, they begin to leave the real line and go on the circle $\mathcal{C}(\sqrt{a}) \subset \mathbb{C}$. They will keep on moving on the circle, in a conjugate way. Putting aside the exceptional pair, the last pair to leave the real line is the one containing the eigenvalue corresponding to the spectral gap. Once this pair has left the interval $[-1,1]$, all the eigenvalues (except the two exceptional ones) have the same modulus and so all of them correspond to the spectral gap. At $a = 1$, all eigenvalues are regularly distributed on the unit circle $\mathcal{C}(1)$ and are all of multipicity 2 ($M^{(1)}$ has two irreducible classes).

Spectral problem of Theorem 2

$V = \prod_{l \in [\![1,r]\!]} \mathbb{Z}_{N_l}$ is a finite Abelian group generated by the symmetric subset S. For $a \in [0,1]$, consider the homogeneous speed transition kernel

$$K^{(a)}(y,y') := \begin{cases} \left(1 + \frac{a}{s-1}\right)\frac{1}{|S|} & \text{, if } y' \neq -y \\ (1-a)/|S| & \text{, if } y' = -y \end{cases}$$

For $\rho \in V^*$, we want to find the spectral decomposition of the centro-Hermitian matrix $A_\rho^{(a)} := \triangle(\rho)K^{(a)}$.
Note that $\rho \in V^*$ can be identified with the vector $(\rho(y))_{y \in S} \in \mathbb{T}^S$.

A first reduction

Proposition

Let $a \in [0,1]$ and $\rho \in V^*$ be fixed and assume that ρ as a vector is not proportional to $\mathbb{1}$. Denote $b^{(a)} := a/(|S|-1)$, $c_\rho^{(a)} := (1+b^{(a)})|S|^{-1}\sum_{y\in S}\rho(y)$ and consider the matrix

$$C_\rho^{(a)} := \begin{pmatrix} 0 & -b^{(a)} \\ 1 & c_\rho^{(a)} \end{pmatrix}$$

The matrix $A_\rho^{(a)}$ is in the same conjugacy class as a block diagonal matrix whose diagonal blocks are the 2×2 block $C_\rho^{(a)}$, with multiplicity one, complemented with some 1×1 block(s) $(b^{(a)})$ and/or $(-b^{(a)})$.

Idea: $\mathrm{Vect}(\mathbb{1},\rho)$ and $\{f \in \mathcal{F}(S,\mathbb{C}) : \mu[f]=0 \text{ and } \mu[\bar{\rho}f]=0\}$ are stable by $A_\rho^{(a)}$.

A second reduction

Lemma

Let $a' = b^{(a)} \in [0,1]$ and $\rho' \in \mathbb{T}$ be such that its real part is given by $s^{-1} \sum_{y \in S} \rho(y)$. Then $C_\rho^{(a)}$ is in the same conjugacy class as

$$\widehat{B}_{\rho'}^{(a')} := \begin{pmatrix} \frac{1+a'}{2}\rho' & \frac{1-a'}{2} \\ \frac{1-a'}{2} & \frac{1+a'}{2}\overline{\rho'} \end{pmatrix}$$

This comes from applying the above reduction to the previous $\mathbb{Z}_N$ example. Theorem 2 follows, essentially because the largest modulus of the eigenvalues of $A_\rho^{(a)}$ is just $\theta_{\rho',*}^{(a')}$, at least if $\mathbb{1}$ are ρ are not proportional.

The evolution of the spectrum of $M^{(a)}$ can also be described in a similar fashion as before.

Bad news!

Theorem 2 does not provide great improvements of the spectral gap, except if $|S| = 2$. Consider a family of examples parametrized by N belonging to a set $\mathcal{N}$, endowed with a filter so that the notion $N \to \infty$ has a meaning. Put N to all the notations introduced.

Proposition

Assume that there exists $s \in \mathbb{N} \setminus \{0, 1, 2\}$ *such that for any* $N \in \mathcal{N}$, $|S_N| = s$. *Under the assumption that* $\lim_{N\to\infty} \lambda_N = 0$, *we have as* $N \to \infty$,

$$\begin{aligned} \Lambda_N &= \lambda(M^{(1)}) \\ &\sim \frac{s}{2(s-1)} \left(1 + \left(\frac{s}{s-2}\right)^2\right) \lambda_N \end{aligned}$$

Example 1

We add 0 to the generating set S of the previous cyclic example: Let $\mathcal{N} = \mathbb{N} \setminus \{0, 1, 2\}$ and for $N \in \mathcal{N}$, we take $V_N = \mathbb{Z}_N$ and $S_N = \{-1, 0, 1\}$, so that $s := |S_N| = 3$.
For $N \in \mathcal{N}$ large,

$$\lambda_N \sim \frac{4\pi^2}{3N^2}$$

and Proposition 8 gives us

$$\begin{aligned} \Lambda_N &\sim \frac{15}{2}\lambda_N \\ &\sim \frac{10\pi^2}{N^2} \end{aligned}$$

Example 2

This family of examples corresponds to the nearest neighbor multidimensional torus models. Let $r \in \mathbb{N} \setminus \{0,1\}$ be fixed. We denote $\mathcal{N} = (\mathbb{N} \setminus \{0,1,2\})^r$ and for $N = (N_1, ..., N_r) \in \mathcal{N}$, consider the group $V_N = \prod_{l \in [\![1,r]\!]} \mathbb{Z}_{N_l}$ and the generating set $S_N := \{\pm e_l \, : \, l \in [\![1,r]\!]\}$ where $e_l = (\delta_l(k))_{k \in [\![1,r]\!]}$. Let us say that $N \to \infty$ if all its coordinates N_1, ..., N_r go to infinity. Then as $N \to \infty$, we have

$$\lambda_N \sim \frac{\pi^2}{2r} \sum_{l \in I_N} \frac{1}{N_l^2}$$

where $I_N := \{l \in [\![1,r]\!] \, : \, N_l \text{ is odd}\}$. In particular $\lim_{N\to\infty} \lambda_N = 0$ and Proposition 8 implies that as $N \to \infty$,

$$\Lambda_N \sim \frac{r}{2r-1} \left(1 + \left(\frac{r}{r-1}\right)^2\right) \lambda_N$$

Example 3

The third family of examples comes back to the cyclic group, but with a different set of generators, of cardinal 4. We take

$$\mathcal{N} \quad := \quad \{n^2 \,:\, n \in \mathbb{N} \setminus \{0,1\} \text{ and } n \text{ odd}\}$$

so that $\sqrt{N}$ is an odd integer for $N \in \mathbb{N}$. The notion $N \to \infty$ is the usual one.
For $N \in \mathbb{N}$, we consider $V_N := \mathbb{Z}_N$ and $S_N := \{\pm 1, \pm\sqrt{N}\}$. It appears that

$$\lambda_N \quad \sim \quad \frac{\pi^2}{4N}$$

for N large. Again Proposition 8 shows only a modest improvement for the spectral gap of $M^{(1)}$: for N large,

$$\Lambda_N \;\sim\; \frac{10}{3}\lambda_N \;\sim\; \frac{5\pi^2}{6N}$$

Hope...

The conjecture would lead to more serious improvements of the spectral gap.
Theoretically, Examples 1 and 3 (or Example 2 with r=2) could be used to check this hope, since third and fourth algebraic equations admit explicit solutions ...