Markov Chains and Unitary Dynamics

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Plato's Allegory of the Cave by Jan Saenredam, according to Cornelis van Haarlem, 1604

Our objectives here

- To provide a rough sketch of a **very unusual strategy** to study Markov Chains.
- The strategy exploits **beautiful** mathematical tools which are not well known among Probabilists, but in the cluttered Mathematical Physics *bag of tricks*.
- The sketch only considers **Simple Markov Chains**, just to argue that the strategy can deal with *well known stuff*, though from a **rather spooky point-of-view**.
- We also indicate a **weird open question** that it poses, even for simple Markov Chains.

Halmos Idea

Paul Halmos' dilation theory: *Represent operator-theoretic structures in terms of conceptually simpler ones acting on larger spaces, in such a way that the first is a* **projection** *of the later.*

Inspired by this idea, we

- Construct a *dilation* for stochastic semigroup, acting on the probability simplex $\Delta_N \in \mathbb{R}^N$ as **Unitary** operators on the Complex Hilbert space $\mathbb{C}^N$.
- Next, using standard mathematical tools from **quantum mechanics** and **quantum computing**, we rewrite the problem as a Dynamical System of **Rotations** *in a* **Euclidian Sphere**.

Unusual perspective:

the classical Semigroup trajectory is the orthogonal projection, **a shadow**, of **Rotations** on a Euclidean Sphere into a Probability Simplex **inscribed** in that sphere.

Markov Chains Setup

Finite state space: $\Sigma = \{1, \ldots, N\}$.

Dynamics defined by a $N \times N$ Rate Matrix $\mathbf{Q}$, where $q_{ij} \equiv \mathbf{Q}_{ij}$ denotes the rate with which the chain jumps from state i to state j. The total rate of jumping out of state i is $-q_i \equiv \sum_{j \neq i} q_{ij}$

Stochastic Semigroup: $S_t = e^{tQ}$.

Acting on l_1 space of probability measures on Σ:

$$\textbf{Simplex :}\ \Delta_N = \{\pi \in \mathbb{R}^N : \pi_l \geq 0, \sum_l^N \pi_l = 1\}.$$

So, if $\pi^0 = (\pi_i)_{i \in S} \in \Delta_N$ is a probability vector in $\mathbb{R}^N$ describing the distribution at time 0 of the chain then

$$\pi^t = \pi^0 S_t$$

is the probability vector at time t.

We focus on the dynamics of $\{\pi_t\}_{t \geq 0}$.

Probabilities to Probability Amplitudes

Notation: write $v = (v_l)_{l=i}^N$ for a column vector in $\mathbb{R}^N$ or $\mathbb{C}^N$.

We say that $|\psi\rangle \equiv (\psi_l)_{l=i}^N \in \mathbb{C}^N$ is a Probability Amplitude vector if

$$\sum_{l=1}^{N} |\psi_l|^2 = 1,$$

where, if $z \in \mathbb{C}$, $|z|^2 = z\overline{z}$.

Given a probability vector $\pi = (\pi_l)_{l=1}^N$ we define its **Representation**

$$|\psi\rangle = |\psi(\pi)\rangle = (\psi_l)_{l=1}^N \in \mathbb{C}^N$$

such that

$$\pi_l = |\psi_l|^2, \; 1 \leq l \leq N$$

Remark: the precise definition of $|\psi\rangle$ is *not essential* in our setting, as long as

$$\pi_I = |\psi_I|^2, 1 \leq I \leq N$$

.

For the **Standard Representation** we set, for $1 \leq I \leq N$

$$\psi_I = \sqrt{\pi_I}$$

In a more *whimsical mood*, inspired by the *Plato Cave Allegory* we can also take the **Plato Representation** and set

$$\psi_I = \pi_I + i\sqrt{\pi_I(1-\pi_I)}, 1 \leq I \leq N.$$

so that $\pi_I = |\psi_I|^2 = \mathbf{Re}(\psi_{\mathbf{I}})$ (*real part*), $1 \leq I \leq N$.

With this Plato Representation choice:
The real *shadow of each Probability Amplitude is the actual Probability*.

Now with *Angle Parameters*

Let $\theta = (\theta_l)_{l=1}^{N}$ be such that $\pi_l = cos^2(\theta_l/2),\ 1 \leq l \leq N$.

The two representations of $\pi = (\pi_l)_{l=1}^{N}$ as $|\psi\rangle = (\psi_l)_{l=1}^{N}$

Plato representation: For $1 \leq l \leq N$

$$
\begin{aligned}
\psi_l &= \cos^2(\tfrac{\theta_l}{2}) + i\sin(\tfrac{\theta_l}{2})\cos(\tfrac{\theta_l}{2}) \\
&= \frac{\mathbf{1+e^{i\theta_l}}}{\mathbf{2}}
\end{aligned}
$$

Standard representation: For $1 \leq l \leq N$

$$
\psi_l = \sqrt{\pi_l} = \cos\left(\frac{\theta_l}{2}\right)
$$

There are $(N-1)$ real-valued free parameters, as $\sum_{l=1}^{N} \cos^2(\theta_l/2) = 1$ or

$$
\sum_{l=1}^{N} \cos\left(\frac{\phi_N + \theta_l}{2}\right)\cos\left(\frac{\phi_N - \theta_l}{2}\right) = 0, \text{ with } \cos(\phi_N) = \frac{2}{N} - 1
$$

.

Unitary Dynamics of Probability Amplitude Vectors

Given the stochastic dynamics $\{\pi^t\}_{t\geq 1}$ we now identify the corresponding Unitary Dynamics $\{|\psi_t\rangle\}_{t\in\mathbb{R}}$.

To start, we define the associated *Density Matrix*

$$\rho = |\psi\rangle \langle\psi| \,,$$

where $\langle\psi|$ indicates the conjugate transpose of the column vector $|\psi\rangle = (\psi_l)_{l=1}^N$ and

$$|\psi_l|^2 = \pi_l = \cos^2(\theta_l/2), \;\; 1 \leq l \leq N$$

with

$$\sum_{l=1}^{N} \cos^2(\theta_l/2) = 1$$

This linear operator ρ, acting on the Hilbert space $\mathcal{H}_N$, is the natural analog of the probability distribution $\pi \in \Delta_N$.

The density matrix is Hermitian, has trace one and is a projector in $\mathcal{H}_N$ (that is $\rho^2 = \rho$).

The stochastic dynamics

$$\pi^t = \pi^0 S_t$$

Will now be represented by equivalent unitary dynamics

$$|\psi_t\rangle = U_t |\psi_0\rangle \Longleftrightarrow \rho_t = U_t \rho_0 U_t^*$$

To identify $\{U_t\}_{t \geq 0}$ corresponding to a given Markov Chain we need a bit of **Lie Algebra theory**.

$su(N)$ Lie Algebra Generators

Write $\{(|l\rangle)_{l=1}^{N}\}$ for the standard basis of the Hilbert Space $\mathcal{H}_N \subset \mathbf{C}^N$

The generators of the Lie algebra $su(N)$ can be divided into three groups:

First, $(N-1)$ **diagonal** matrices (Cartan sub-algebra of $su(N)$)

$$\Lambda_j = \sqrt{\frac{2}{j(j+1)}}\Big(|1\rangle\langle 1| + |2\rangle\langle 2| + \ldots + |j\rangle\langle j| - j.\, |j{+}1\rangle\langle j{+}1| \Big)$$

for $1 \leq j \leq N-1$.

And two other groups, one with **symmetric**

$$\Lambda_{lk}^{S} = |k\rangle\langle l| + |l\rangle\langle k|$$

and the other with **antisymmetric** matrices

$$\Lambda_{lk}^{A} = i(|k\rangle\langle l| - |l\rangle\langle k|)$$

for $1 \leq l < k \leq N$.

Generators are Hermitian, traceless and orthogonal.

Now we can write the $N \times N$ density matrix $\rho_t = \big| |\psi_t\rangle \langle\psi_t| \big|$ as

$$\rho_t = \frac{1}{N}\mathbf{1} + \sqrt{\frac{N-1}{2N}}\mathbf{r_t}.\boldsymbol{\Lambda}$$

where $\mathbf{r}.\boldsymbol{\Lambda} = \sum_{l=1}^{N^2-1} r_l.\Lambda_l$, is the inner product of $\mathbf{r} \in \Omega_N \subset \mathbf{R}^{N^2-1}$ and the *vector of generators* $\boldsymbol{\Lambda} = (\Lambda_l)_{l=1}^{N^2-1}$.

Probability Simplex: components of $\mathbf{r}_t$ corresponding to the $(N-1)$ Diagonal Generators.

Dynamics is defined with the Antisymmetric Generators.

π_t (Probability Vector) $\Longleftrightarrow |\psi_t\rangle \Longleftrightarrow \rho_t \Longleftrightarrow \mathbf{r_t}$ (Vector in a Sphere)

We now define U_t

Stochastic Semigroup $e^{tQ} \Longleftrightarrow U_t$ Unitary dynamics

Expression of U_t

Suppose the Markov chain starts at state $l \in \{1, \ldots, N\}$

Let $\{\phi_{lk}(t)\}_{1 \leq l,k \leq N}$ be given from Kolmogorov's equation

$$\cos^2(\phi_{lk}(t)/2) = P_t(X_t = k | X_0 = l) = (e^{tQ})_{lk}$$

and $\alpha_{lk}(t)$ be the **Conditional Probability Amplitude** given by

$$\alpha_{lk}(t) = \frac{\cos(\phi_{lk}(t)/2)}{\sin(\phi_{ll}(t)/2)}$$

.

Then

$$U_t = e^{i \frac{\phi_{ll}}{2}(t) \left(\sum_{k \neq l} \alpha_{lk}(t) \Lambda_{lk}^A \right)}$$

describes the unitary dynamics corresponding to $\{\pi_t\}_{t \geq 0}$.

Equivalent Euclidean formulation

Since

$$\rho_t = \frac{1}{N}\mathbf{1} + \sqrt{\frac{N-1}{2N}}\mathbf{r_t}.\mathbf{\Lambda}$$

The orthogonal rotation dynamics of unit-norm $\mathbf{r_t} \in \mathbb{R}^{N^2-1}$, with $\mathbf{r_0} = (\delta_{lk})_{k=1}^{N^2-1}$ (initial state is l) given by

$$\mathbf{r_t} = \mathbf{R}_t \mathbf{r_0}$$

is an equivalent Euclidean Rotation view of the unitary dynamics of $|\psi_t\rangle$.

Plato's Cave Shadow:

$(N-1)$ of the components of $\mathbf{r_t}$ follow
exactly
the classical trajectory of π_t on the probability simplex.

Example: Two state Markov Chain: **qubits**

For $N = 2$, we have $su(2)$: Lie algebra associated to Unitary transformations in $\mathbb{C}^2$. Generators here are the **Pauli Matrices**

$$\Lambda_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \Lambda_{12}^S = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \Lambda_{12}^A = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

and we have

$$\rho_t = \frac{1}{2}(\mathbf{1} + \mathbf{r_t}.\sigma)$$

where $\mathbf{r_t} \in \mathcal{S}^2 \in \mathbb{R}^3$ and $\mathbf{r}.\sigma \equiv \sum_{l=1}^{3} r_l \sigma_l$

For probability vector $\pi = [p, 1-p]$, set $\cos^2(\theta/2) = p$ and get, (Plato Representation)

$$\mathbf{r} = \begin{bmatrix} \sin^2\theta \\ \sin\theta\cos\theta \\ \cos\theta \end{bmatrix} \in S^2 \in \mathbb{R}^3$$

Two state Markov Chain: Bloch Sphere

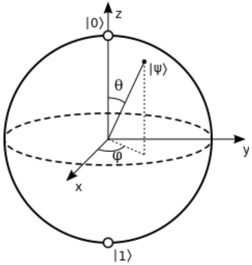


Figure: $|0\rangle$ and $|1\rangle$ indicates the two Markov Chain states

Trajectories $\mathbf{r}_t \in \mathbb{R}^3$ (spherical coordinates):

$$\phi_t = \pi/2 - \theta_t, \text{ and } \cos(\theta_t) = 2\pi_t - 1,$$

with $\pi_t = \pi_0 e^{tQ}$, solution of associated Kolmogorov's equation

In *Quantum Computing* this describes the smallest amount of Quantum information:
the *quantum bit* or **qubit**.

Weird stuff

Quantum Mechanics exhibits several, **experimentally verified**, *strange phenomena*.

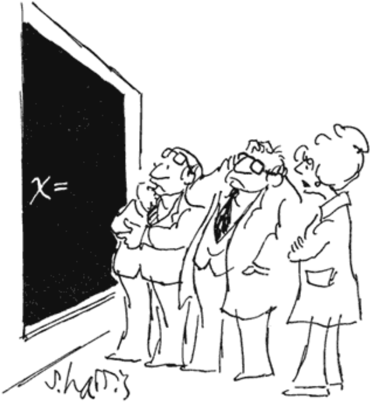
A important *weird* ingredient in **Quantum Computing** is **Entanglement** between two or more qubits.

Already in 1932 E. Majorana introduced a method (there are others) that allow representing pure states of Quantum Spin system, with $S > 1/2$, in terms of groups of qubits ($S = 1/2$).

The approach we just presented tells us that a Markov chain shadows the dynamics of Quantum Spins which *could* be entangled.

Question: Are these crazy Quantum Weirdness stuff relevant from our Markov Chain Shadow?...

Thanks!



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