Graph Cellular Automata and Beyond: Applications in Network Neuroscience

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Presentation Summary

Introduction

Introduction – From Lattices to Graphs

Classical cellular automata (CA) defined on lattices have long served as minimal models for emergent complexity (Wolfram, 1984). When the underlying lattice is replaced by an arbitrary graph, we obtain a graph cellular automaton (GCA).

Real-world networks are complex systems that can be modeled as graph cellular automata (GCA) (Marr & Hütt, 2005). In these GCA, the neighborhood of a cell is its graph neighborhood and the topology of the network thus becomes part of the dynamics. In particular, when the underlying graph is a digraph, the neighborhood splits into an *in*- and an *out*-neighborhood, so that a local rule can distinguish causal relationships.

Limitation. A GCA is still an intrinsically *pairwise* model, that is, each cell is a vertex, and all a cell can see is a set of adjacent vertices.

Introduction – Beyond GCA: Higher-Order Structures

It is commonly said that the cliques of a graph are its higher-order structures. In a digraph, its higher-order structures are its directed cliques. These are precisely the *directed simplices* of the directed flag complex (DFC) (Masulli & Villa, 2016; Reimann et al., 2017).

In neural data, directed cliques are natural candidates for representing groups of neurons acting in a coordinated and causally ordered manner. Their abundance and dimensionality have been related to structure and function in cortical microcircuits and in the human connectome (Reimann et al., 2017; Sizemore et al., 2018).

This motivated us to go beyond GCA and define the general concept of simplicial cellular automaton (SCA) and SCA associated with DFCs:

- its **cells** are simplices / directed simplices, eventually of different dimensions;
- its **neighborhoods** come from (directed) face sharing (Atkin, 1974; Riihimäki, 2022);
- its **rules** respect the dimensional stratification of the complex, and reduce to GCA rules in dimension 0.

Introduction – Scope of the Presentation

1. **GCA on digraphs.** Definitions of in-/out-neighborhood densities, families of density- and weight-based update rules, worked examples, and simulations on three random digraph models (Erdős–Rényi, Watts–Strogatz, Barabási–Albert).

2. **SCA on directed flag complexes.** Presentation of a formal framework for SCA. Definitions of state space, simplicial neighborhoods given by directed q-stars, and families of update rules built in analogy with the GCA ones. In this presentation, this framework is presented in a purely theoretical manner (no simulation or application to real data).

3. **Brain-inspired GCA.** A GCA whose underlying digraphs are **iPDC networks** estimated from scalp EEG of patients with left temporal lobe epilepsy (Siena Scalp EEG Database). The complexity of the emergent dynamics is quantified by complexity measures (e.g., average cell entropy and average mutual information), and compared across the pre-ictal, ictal, and post-ictal phases in different frequency bands.

Graph Cellular Automata

Graph Cellular Automata (GCA) – Definition

First proposed by (Marr et al. 2005).

Definition. Given a graph $G = (V, E)$, a graph cellular automaton (GCA) is a 4-tuple $(G, \mathcal{S}, \mathcal{N}, \tau)$, where $\mathcal{S}$ is the set of states, $\tau : \mathcal{S} \to \mathcal{S}$ is the transition function (local rule), and $\mathcal{N} : V \to \mathcal{P}(V)$, s.t. $\mathcal{N}(v) = \{w : (v, w) \in E\}$, is the neighborhood function.

Directed case. If G is a digraph, then we can have two neighborhood functions

$$\mathcal{N}_{in}(v) = \{w : (w, v) \in E\} \qquad \mathcal{N}_{out}(v) = \{w : (v, w) \in E\}.$$

and τ may read them separately (in-driven, out-driven, or mixed rules).

Remark. The states are associated with the vertices $v \in V$ of the (di)graph.

GCA – Active Neighbors and Neighborhood Densities

Definition: We define the number of active neighbors (undirected case), active in- and out-neighbors (directed case), at time t, respectively by

$$k^t(v) = \sum_{w \in \mathcal{N}(v)} s_t(w), \quad k^t_{in}(v) = \sum_{w \in \mathcal{N}_{in}(v)} s_t(w), \quad k^t_{out}(v) = \sum_{w \in \mathcal{N}_{out}(v)} s_t(w).$$

Definition: We define the neighborhood density (unidirected case), in- and out-neighborhood densities (directed case), at time t, respectively by

$$\Delta^t_{\mathcal{N}}(v) = k^t(v)/|\mathcal{N}^t(v)|, \quad \Delta_{\mathcal{N}^t_{in}}(v) = k^t_{in}(v)/|\mathcal{N}^t_{in}(v)|, \quad \Delta_{\mathcal{N}^t_{out}}(v) = k^t_{out}(v)/|\mathcal{N}^t_{out}(v)|.$$

Note that $\Delta_{\mathcal{N}^t}(v), \Delta_{\mathcal{N}^t_{in}}(v), \Delta_{\mathcal{N}^t_{out}}(v) \in [0, 1]$.

GCA – Families of Update Rules

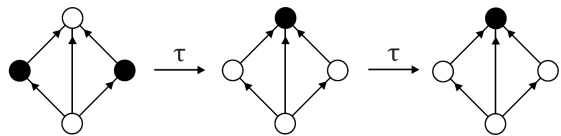
Rule	**Local map** $s_{t+1}(v)$
Density-based threshold	$\big(s_{t+1}(v) = 1$ if $\Delta_{\mathcal{N}^t}(v) > \delta; s_{t+1}(v) = 0$ otherwise$\big)$.
Node weight threshold	$\big(s_{t+1}(v) = 1$ if $\sum_{w \in \mathcal{N}^t(v)} \omega(v)\, s_t(w) > \delta; s_{t+1}(v) = 0$ otherwise$\big)$.
Edge/arc threshold	$\big(s_{t+1}(v) = 1$ if $\sum_{w \in \mathcal{N}^t(v)} \omega(w, v)\, s_t(w) > \delta; s_{t+1}(v) = 0$ otherwise$\big)$.

For the previous update rules, whenever appropriate, replace the neighborhood density by $\Delta_{\mathcal{N}^t_{in}}(v)$ or $\Delta_{\mathcal{N}^t_{out}}(v)$ to obtain the corresponding in and out versions.

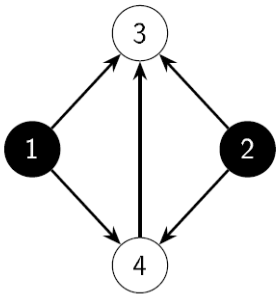
GCA – Example 1: Node Weight Threshold

Let $\mathcal{S} = \{0, 1\}$. For a chosen threshold $\delta > 0$, we can define the transition function depending on the node weights:

$$s_{t+1}(v) = \tau(s_t(v)) = \begin{cases} 1, & \text{if } \sum_{w \in \mathcal{N}_{in}^t(v)} \omega(v)\, s_t(w) > \delta, \\ 0, & \text{otherwise.} \end{cases}$$



GCA – Example 2: In-Density Threshold



$s_0 = (1, 1, 0, 0)$

$$s_{t+1}(v) = \begin{cases} 1, & \text{if } \Delta_{\mathcal{N}_{in}^t}(v) > \delta = 1/2, \\ 0, & \text{otherwise.} \end{cases}$$

- $0 \to 1$:

$$\Delta_{\mathcal{N}_{\text{in}}}(3) = \frac{s(1)+s(2)+s(4)}{3} = \frac{2}{3} > \frac{1}{2} \;\Rightarrow\; 1$$
$$\Delta_{\mathcal{N}_{\text{in}}}(4) = \frac{s(1)+s(2)}{2} = 1 > \frac{1}{2} \;\Rightarrow\; 1$$
$$v \in \{1, 2\} : \; \mathcal{N}_{\text{in}} = \varnothing \;\Rightarrow\; 0$$

$\Rightarrow s_1 = (0, 0, 1, 1)$.

- $1 \to 2$: $\Delta_{\mathcal{N}_{\text{in}}}(3) = \frac{0+0+1}{3} < \frac{1}{2}$, $\Delta_{\mathcal{N}_{\text{in}}}(4) = 0$

$$\Rightarrow \; s_2 = (0, 0, 0, 0).$$

Simplicial Cellular Automata

Simplicial Complexes

Definition. A (abstract) simplicial complex is a finite collection $\mathcal{X}$ of finite sets such that if $\sigma \in \mathcal{X}$, then for all $\tau \subseteq \sigma$ we have $\tau \in \mathcal{X}$ (closed under inclusion of subsets).

Each element $\sigma \in \mathcal{X}$ is an *abstract simplex*, or *n-simplex*, if $|\sigma| = n+1$. The *dimension* of σ is defined as $\dim \sigma = n$, and the dimension of $\mathcal{X}$ is $\dim \mathcal{X} = \max_{\sigma \in \mathcal{X}}(\dim \sigma)$

Example. A graph $G = (V, E)$ with the vertex set V is a 1-dimensional simplicial complex on V, where 0-simplices are vertices and 1-simplices are edges.

Directed Simplices and Directed Flag Complexes

Let $G = (V, E)$ be a finite digraph with $|V| = n$.

Definition. A directed k-simplex, $k < n$, is an ordered $(k+1)$-tuple of distinct vertices $\sigma = (v_0, v_1, \ldots, v_k)$ such that for every pair of indices $i < j$, the arc $(v_i, v_j) \in E$. The *dimension* of σ is $\dim(\sigma) = k$.

Equivalently, a directed k-simplex is a directed $(k+1)$-clique in G together with the total ordering of its vertices induced by the edge directions.

Definition. The directed flag complex (DFC) associated with G, $\mathrm{dFl}(G)$, is the set of all directed simplices of all dimensions:

$$\mathrm{dFl}(G) = \bigsqcup_{k=0}^{d} \mathrm{dFl}_k(G),$$

where $\mathrm{dFl}_k(G)$ denotes the set of all directed k-simplices of G and $d = d(G)$ is the dimension of the largest directed clique in G.

Simplicial Neighborhoods – q-Nearness and q-Stars

To define a cellular automaton on a simplicial complex, we first need a notion of "neighborhood of a simplex". The classical one comes from Q-analysis (Atkin, 1974; Johnson, 2013).

Definition. Let $\sigma, \tau \in \mathcal{X}$. They are q-near if they *share a q-face*, and we write $\sigma \sim_q \tau$. In particular, an n-simplex is n-near to itself.

Definition. The q-star of $\sigma \in \mathcal{X}$ is the set of all simplices q-near to it, and its cardinality is called q-degree:

$$\mathrm{st}_q(\sigma) = \{\tau \in \mathcal{X} : \sigma \sim_q \tau\}, \qquad \deg_q(\sigma) = |\,\mathrm{st}_q(\sigma)|.$$

The q-star is the simplicial analogue of the neighborhood $\mathcal{N}(v)$ of a vertex.

Simplicial Neighborhoods – Directed q-Nearness

Definition (Riihimäki, 2022). For $\sigma^{(n)} = [v_0, \ldots, v_n] \in \mathrm{dFl}(G)$, the i-th face map is

$$\hat{d}_i(\sigma^{(n)}) = \begin{cases} [v_0, \ldots, \widehat{v_i}, \ldots, v_n], & \text{if } i < n, \\ [v_0, \ldots, v_{n-1}, \widehat{v_n}], & \text{if } i \geq n, \end{cases}$$

where $\widehat{v_i}$ denotes deletion of the i-th vertex.

Definition. $\sigma^{(n)}$ is $(q, \hat{d}_i, \hat{d}_j)$-near to $\tau^{(m)}$, $0 \leq q \leq \min(n, m)$, if either $\sigma^{(n)} \subseteq \tau^{(m)}$, or

$$\hat{d}_i(\sigma^{(n)}) \;\supseteq\; \alpha^{(q)} \;\subseteq\; \hat{d}_j(\tau^{(m)}) \quad \text{for some } \alpha^{(q)} \in \mathrm{dFl}(G).$$

Definition. For $\sigma^{(n)}, \tau^{(m)} \in \mathrm{dFl}(G)$, we say that $\sigma^{(n)}$ is

- out-q-near to $\tau^{(m)}$, written $\sigma^{(n)} \sim_q^+ \tau^{(m)}$, if they are $(q, \hat{d}_i, \hat{d}_j)$-near with $i \leq j$;
- in-q-near to $\tau^{(m)}$, written $\sigma^{(n)} \sim_q^- \tau^{(m)}$, if they are $(q, \hat{d}_i, \hat{d}_j)$-near with $i \geq j$;
- bidirectionally q-near, written $\sigma^{(n)} \sim_q^\pm \tau^{(m)}$, if both hold.

Generic notation: $\sim_q^\bullet$, with $\bullet \in \{-, +, \pm\}$.

Simplicial Neighborhoods – Directed q-Stars

Definition. Given $\sigma \in \mathrm{dFl}(G)$ and $\bullet \in \{-, +, \pm\}$, the directed q-star of σ is

$$\mathsf{st}_q^\bullet(\sigma) = \{\tau \in \mathrm{dFl}(G) \ : \ \sigma \sim_q^\bullet \tau\}, \qquad \mathsf{deg}_q^\bullet(\sigma) = |\,\mathsf{st}_q^\bullet(\sigma|,$$

Definition. The collection $\mathrm{St} = \{\mathrm{St}_q^\bullet\}$ of simplicial neighborhood functions of an SCA is

$$\mathrm{St}_q^\bullet : \mathrm{dFl}(G) \longrightarrow \mathcal{P}(\mathrm{dFl}(G)), \qquad \sigma \longmapsto \mathsf{st}_q^\bullet(\sigma).$$

For the undirected case, simply replace $\mathrm{dFl}(G)$ with $\mathcal{X}$ and $\mathrm{St}_q^\bullet$ with St_q. Also, restricted to 0-simplices, the directed q-star reduces to the in-/out-neighborhood of a vertex of G.

Simplicial Configuration and State Space

Definition. A simplicial configuration at time t is a collection of binary functions, one for each dimension:

$$\mathbf{S}^t = \left(s_0^t,\ s_1^t,\ \ldots,\ s_d^t\right), \qquad s_k^t : \mathcal{X} \to \{0,1\}.$$

The full *state space* is $\mathcal{C} = \prod_{k=0}^{d} \{0,1\}^{|\mathcal{X}|}$. The state of a k-simplex σ at time t is thus $s_k^t(\sigma) \in \{0,1\}$.

For DFCs, we put $s_k^t : \mathrm{dFl}_k(G) \to \{0,1\}$ and $\mathcal{C} = \prod_{k=0}^{d} \{0,1\}^{|\mathrm{dFl}_k(G)|}$. Informally, $s_k^t(\sigma) = 1$ means that the directed $(k+1)$-clique σ is *active* at time t, and $s_k^t(\sigma) = 0$ means it is *non-active*.

Simplicial Cellular Automata (SCA) – Definition

Similarly to the GCA, for simplicial complexes and DFCs, we can build a "higher-order graph cellular automaton", in the sense of associating binary states to the simplices.

Definition. A simplicial cellular automaton (SCA) is a 4-tuple $(\mathcal{X}, \mathcal{C}, \mathrm{St}, \Phi)$, where $\mathcal{X}$ is simplicial complex, $\mathcal{C}$ is a state space, St is a collection of simplicial neighborhood functions, and Φ is the **global update rule**

$$\mathbf{S}^{t+1} = \Phi(\mathbf{S}^t), \qquad \Phi : \mathcal{C} \to \mathcal{C},$$

defined by a collection of local rules.

For DFCs associated with digraphs, the definition of SCA is analogous. Also, notice that a **GCA is the dimension-0 restriction of a SCA**.

SCA – Active Neighbors and Simplicial Neighborhood Densities

Definition. Let $s_t(\sigma) := s^t_{\dim \sigma}(\sigma)$ be the state of the cell σ at time t. We define the number of active q-neighbors of $\sigma \in \mathrm{dFl}(G)$ at time t, for $\bullet \in \{-, +, \pm\}$, by

$$k_q^{t,\bullet}(\sigma) = \sum_{\tau \in \mathrm{st}_q^\bullet(\sigma)} s_t(\tau),$$

Definition: We define the simplicial q-neighborhood densities at time t by

$$\Delta_q^{\bullet,t}(\sigma) \;=\; \frac{k_q^{t,\bullet}(\sigma)}{|\,\mathrm{st}_q^\bullet(\sigma)|} \;=\; \frac{k_q^{t,\bullet}(\sigma)}{\deg_q^\bullet(\sigma)}, \qquad \bullet \in \{-, +, \pm\},$$

with the convention $0/0 = 0$ for simplices isolated at level q. We write $\Delta_q^{in} := \Delta_q^-$ and $\Delta_q^{out} := \Delta_q^+$. Note that $\Delta_q^{-,t}(\sigma), \Delta_q^{+,t}(\sigma), \Delta_q^{\pm,t}(\sigma) \in [0, 1]$.

SCA – Families of Update Rules

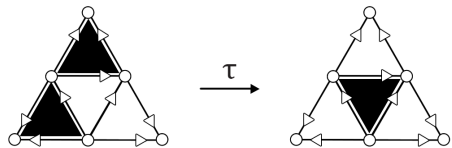
Rule	**Local map** $s_{t+1}(\sigma)$
q-Density-based threshold	($s_{t+1}(\sigma) = 1$ if $\Delta_q^{\pm,t}(\sigma) > \delta$; $s_{t+1}(\sigma) = 0$ otherwise).
Simplex weight threshold	($s_{t+1}(\sigma) = 1$ if $\sum_{\tau \in \mathsf{st}_q^{\pm}(\sigma)} \widetilde{\omega}(\sigma)\, s_t(\tau) > \delta$; $s_{t+1}(\sigma) = 0$ otherwise).
q-Arc weight threshold	($s_{t+1}(\sigma) = 1$ if $\sum_{\tau \in \mathsf{st}_q^{\pm}(\sigma)} \omega(\tau, \sigma)\, s_t(\tau) > \delta$; $s_{t+1}(\sigma) = 0$ otherwise).

Here $\widetilde{\omega}(\sigma) = \prod_i \widetilde{\omega}(v_i)$ is the product-weight of the directed simplex σ. Also, for the previous update rules, whenever appropriate, replace $\mathsf{st}_q^{\pm}$ and $\Delta_q^{\pm,t}$ by $\mathsf{st}_q^{-}, \Delta_q^{-,t}$ or $\mathsf{st}_q^{+}, \Delta_q^{+,t}$ to obtain the corresponding **in** and **out** versions. For $q = 0$ and cells restricted to 0-simplices, these three families collapse exactly onto the density-, node-weight-, and arc-weight-based GCA rules.

SCA — Example 1: Simplicial Out-Neighborhood Density

Let $\mathrm{dFl}_k(G)$ be the DFC associated with a digraph G and let $\mathcal{C} = \prod_{k=0}^{d} \{0,1\}^{|\mathrm{dFl}_k(G)|}$ be the state space. For a chosen threshold $\delta > 0$, we can define the transition function depending on the simplicial out-q-neighborhood density

$$s_{t+1}(\sigma) = \tau(s_t(\sigma)) = \begin{cases} 1, & \text{if } \Delta_q^{+,t}(\sigma) > \delta, \\ 0, & \text{otherwise.} \end{cases}$$



Simulation Studies

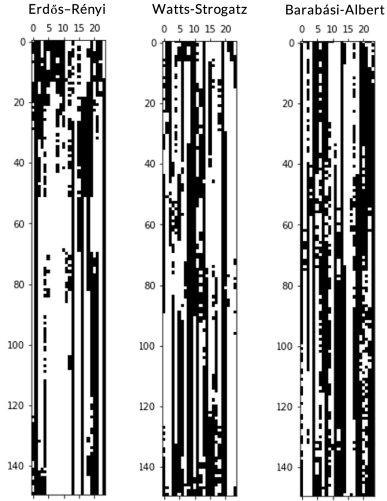
Simulations: Random Digraph Models

We performed simulations on three different random digraph models:

- **Erdős–Rényi Random Digraphs**: $G(n, p)$
- **Watts-Strogatz Random Digraphs**: $WS(n, N, p)$
- **Barabási-Albert Random Digraphs**: $BA(n, \alpha, \beta, \gamma)$

We used digraphs with $n = 26$ vertices. The models were implemented in Python using the NetworkX library.

Simulation – Neighborhood Density Threshold



Brain-Inspired GCA and the Complexity of Brain Networks

Three Notions of Brain Connectivity

- **Structural (anatomical) connectivity**: Refers to a set of anatomical connections that link neural elements.
- **Functional connectivity**: Refers to the temporal interdependence of activation patterns of anatomically separate brain areas (estimators: correlation, coherence – undirected and symmetric).
- **Effective connectivity**: Reflects the causal relationships between activated brain regions by characterizing the influence that one brain structure has on another (estimators: PDC, DTF – directed and asymmetric.).

Why Partial Directed Coherence?

The Partial Directed Coherence (PDC), proposed by (Baccalá & Sameshima, 2001), was designed to satisfy:

- **Directionality**: For time series $\mathbf{x}_i$ and $\mathbf{x}_j$, distinguish $\mathbf{x}_j \to \mathbf{x}_i$ from $\mathbf{x}_i \to \mathbf{x}_j$.
- **Frequency domain**: Representation of Granger causality in the frequency domain (neural interactions are rhythm-specific).
- **Direct vs. indirect**: Separate $\mathbf{x}_1 \to \mathbf{x}_3$ (direct) from $\mathbf{x}_1 \to \mathbf{x}_2 \to \mathbf{x}_3$ (indirect).
- **Multivariate**: Condition on all other recorded series.

Significance tests and confidence intervals for PDC was introduced latter with the asymptotic theory (Baccalá et al., 2013).

Granger Causality

For two time series $\mathbf{x}(n)$ and $\mathbf{y}(n)$, the series $\mathbf{x}(n)$ Granger-causes $\mathbf{y}(n)$ if the past values of $\mathbf{x}(n)$ contain information that helps to predict $\mathbf{y}(n)$. In other words, let $\mathcal{U}_n$ be all information up to time n and $\mathcal{U}_n \setminus \mathbf{x}(n)$ the same information with the past of $\mathbf{x}(n)$ removed, then:

$$\mathbf{x}(n) \text{ Granger-causes } \mathbf{y}(n) \iff \operatorname{var}\big[\,\mathbf{y}(n) \,|\, \mathcal{U}_{n-1}\,\big] \;<\; \operatorname{var}\big[\,\mathbf{y}(n) \,|\, \mathcal{U}_{n-1} \setminus \mathbf{x}(n)\,\big].$$

Granger causality is not reciprocal, i.e. $\mathbf{x}(n)$ Granger-causes $\mathbf{y}(n)$ does not imply that $\mathbf{y}(n)$ Granger-causes $\mathbf{x}(n)$.

The Multivariate Autoregressive (MVAR) Model

Let $\mathbf{x}(n) = [x_1(n), \ldots, x_N(n)]^{\mathsf{T}}$ be N jointly stationary, zero-mean time series. The MVAR(p) model is

$$\mathbf{x}(n) \;=\; \sum_{r=1}^{p} \mathbf{A}_r\, \mathbf{x}(n-r) \;+\; \mathbf{w}(n), \qquad \mathbf{w}(n) \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_{\mathbf{w}}),$$

with

- $\mathbf{A}_r = [a_{ij}(r)]$ the $N \times N$ coefficient matrix at lag r and $\mathbf{w}(n)$ serially uncorrelated innovations.
- $a_{ij}(r)$ = influence of $x_j(n-r)$ on $x_i(n)$ (row = target, column = source).
- Granger causality $j \not\to i \iff a_{ij}(r) = 0$ for all $r = 1, \ldots, p$.
- $\boldsymbol{\Sigma}_{\mathbf{w}}$ is generally **not diagonal**: instantaneous (zero-lag) correlation is absorbed here.
- Coefficient estimation methods: Yule-Walker (Levinson-Wiggins-Robinson); Nuttall-Strand / Vieira-Morf; ARfit.

Partial Directed Coherence (PDC) - Going to the Frequency Domain

Define the matrix:

$$\bar{\mathbf{A}}(f) \;=\; \mathbf{I} - \mathbf{A}(f) \;=\; \mathbf{I} - \sum_{r=1}^{p} \mathbf{A}_r \, e^{-i2\pi fr}.$$

Its inverse is the transfer function:

$$\mathbf{H}(f) = \bar{\mathbf{A}}^{-1}(f), \qquad \mathbf{S}(f) = \mathbf{H}(f)\, \boldsymbol{\Sigma}_{\mathbf{w}}\, \mathbf{H}^{\mathsf{H}}(f)$$

where $\mathbf{S}(f)$ is the power spectral density matrix.

Definition. The PDC is defined by (Baccalá & Sameshima, 2001):

$$\pi_{ij}(f) \;=\; \frac{\bar{A}_{ij}(f)}{\sqrt{\bar{\mathbf{a}}_j^{\mathsf{H}}(f)\, \bar{\mathbf{a}}_j(f)}} \;=\; \frac{\bar{A}_{ij}(f)}{\sqrt{\sum_{k=1}^{N} \left|\bar{A}_{kj}(f)\right|^2}}$$

where $\bar{\mathbf{a}}_j(f)$ is the j-th column of $\bar{\mathbf{A}}(f)$.

Properties of PDC

1. **Asymmetric**: $|\pi_{ij}| \neq |\pi_{ji}|$ in general.
2. **Frequency domain**: π_{ij} measures the influence from j to i at frequency f.
3. **Direct**: Indirect paths are excluded by construction.
4. **Normalisation**: $\sum_{i=1}^{N} |\pi_{ij}(f)|^2 = 1$ for every j and every f, and $0 \leq |\pi_{ij}(f)|^2 \leq 1$.
5. **Exact null equivalence**: $\pi_{ij}(f) = 0 \ \forall f \iff a_{ij}(r) = 0 \ \forall r \iff \mathbf{x}_j$ does not Granger-cause $\mathbf{x}_i$ given all other channels.
6. **Multivariate**: Automatically conditioned on the other $N - 2$ series.

Information PDC (iPDC)

The information PDC (iPDC), introduced by (Takahashi et al., 2010a, 2010b), is a modification of the PDC expression that formalizes the relationship between PDC and information flow:

$$\left|\iota\pi_{ij}(f)\right|^2 \;=\; \frac{\left|\bar{A}_{ij}(f)\right|^2 / \sigma_{ii}}{\bar{\mathbf{a}}_j^{\mathsf{H}}(f)\,\boldsymbol{\Sigma}_{\mathbf{w}}^{-1}\,\bar{\mathbf{a}}_j(f)}.$$

The denominator is a quadratic form in the full inverse innovation covariance $\boldsymbol{\Sigma}_{\mathbf{w}}^{-1}$(off-diagonal terms included).

We can verify that $\iota\pi_{ij}(f)$ is still bounded, $0 \leq |\iota\pi_{ij}(f)|^2 \leq 1$, and still zero exactly when $\mathbf{x}_j \not\to \mathbf{x}_i$.

Also, it reduces to PDC when $\boldsymbol{\Sigma}_{\mathbf{w}} = \sigma^2\mathbf{I}$.

EEG Data (Siena Scalp EEG Database)

The EEG data were obtained from the Siena Scalp EEG Database (Detti et al., 2020). We chose eight patients with left temporal lobe epilepsy (TLE) based on the quality of the signal.

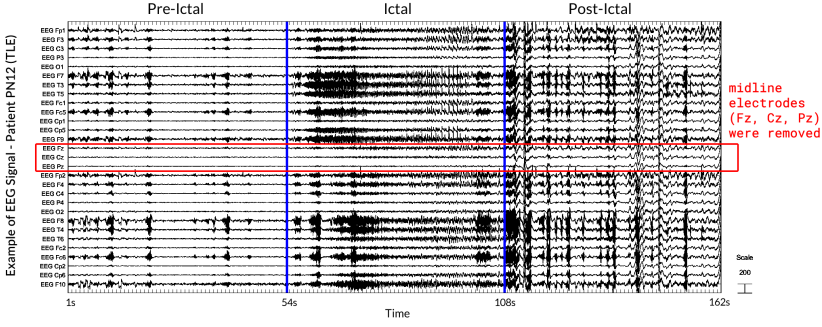
Public available at `https://physionet.org/content/siena-scalp-eeg/1.0.0`.

Table: Patient information.

Pat. id	Age	Gender	Localization	Lateralization	Time (min)
PN01	46	Male	Temporal Lobe	Left	809
PN06	36	Male	Temporal Lobe	Left	722
PN07	20	Female	Temporal Lobe	Left	523
PN09	27	Female	Temporal Lobe	Left	410
PN12	71	Male	Temporal Lobe	Left	246
PN13	34	Female	Temporal Lobe	Left	519
PN14	49	Male	Temporal Lobe	Left	1408
PN16	41	Female	Temporal Lobe	Left	303

Data Preprocessing

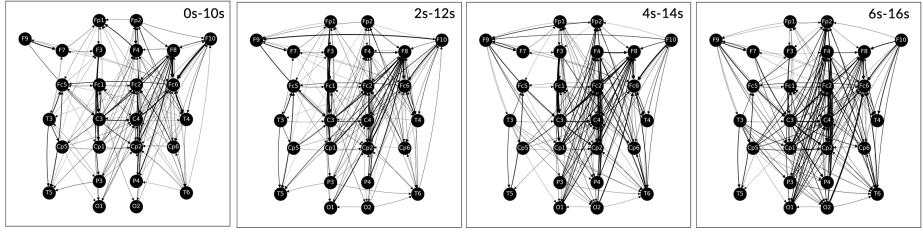
- **1)** Downsampling: from 512 Hz to 256 Hz. **2)** 1 Hz high-pass filter; notch filter at 50 Hz. **3)** The midline electrodes (Fz, Cz, and Pz) were removed (final number of channels: 26). **4)** An ICA was performed to remove artifactual components.
- Next, we identified the **pre-ictal, ictal, and post-ictal phases**, and then divided the signals from each phase into 30s epochs: 30s immediately before the seizures, 30s starting on the seizures onset, and 30s immediately after the seizures.



Dynamic iPDC Networks Estimated from the EEG Data

- iPDC $\rightarrow$ **delta** [1 - 4 Hz), **theta** [4 - 8 Hz), and **alpha** [8 - 13 Hz);
- iPDC $\rightarrow$ **Sliding window technique** for each epoch, sliding the window in 10s cuts; overlap of 8s (11 digraphs on each seizure phase).
- VAR autoregression coefficients: estimated through the **Nuttall-Strand's method**. Order for the VAR models: **fixed order $p = 12$**.
- Only the statistically significant connections were considered (estimated asymptotically with a **significance level of 0.1%**). Arc weights were removed.

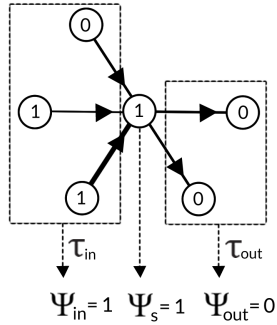
iPDC networks - Patient PN01 - Delta band [1 Hz, 4Hz) (seizure onset)



Brain-Inspired Graph Cellular Automata

Inspired by the model introduced in (Joyce et al., 2012), here we propose a similar model called brain-inspired graph cellular automata (BGCA). This elementary cellular automaton is based on epilepsy EEG data (see next section) and it's created by associating a binary 3-bit neighborhood to every node, $\Psi(v) = (\psi_{in}(v), \psi_s(v), \psi_{out}(v))$:

$$\begin{cases} \psi_{in}(v) = 1, \text{ if } \Delta_{\mathcal{N}_{in}}(v) > \tau_{in}, \\ \psi_{in}(v) = 0, \text{ otherwise }, \\ \psi_s(v) = s_i, \\ \psi_{out}(v) = 1, \text{ if } \Delta_{\mathcal{N}_{out}}(v) > \tau_{out}, \\ \psi_{out}(v) = 0, \text{ otherwise }. \end{cases}$$



Rule 110

Neighborhood $(\Psi_{in}^t, \Psi_s^t, \Psi_{out}^t)$	New State Ψ_s^{t+1}
111	0
110	1
101	1
100	0
011	1
010	1
001	1
000	0

Complexity Measures

In our brain-inspired GCA, the underlying digraph is derived from physiological data (iPDC networks representing the effective connectivity of epileptic brain regions); thus, the GCA becomes a biologically grounded computational model whose emergent behavior can be investigated through information-theoretic complexity measures. Three such measures were chosen:

- **Average Cell Entropy** (ACE): Quantifies the marginal unpredictability of individual network nodes.
- **Average Mutual Information** (AMI): Measures directed information flow along network edges.
- **Average Normalized Hamming Distance** (AHD): Captures the rate at which the system changes over time.

The measures ACE and AMI are implemented in the Python library `CellPyLib` through the functions `average_cell_entropy()` and `average_mutual_information()`, respectively.

Complexity Measures – Average Cell Entropy (ACE)

Shannon entropy, in the context of cellular automata, measures the unpredictability of the state sequence generated by each cell over time. For a single cell i, the cell entropy H_i is computed as:

$$H_i = -\sum_{s \in \mathcal{S}} p_i(s) \log_2 p_i(s),$$

where $p_i(s)$ is the empirical probability of cell i occupying state s over the trajectory of the automaton, with the convention $0 \log_2 0 = 0$. The Average Cell Entropy (ACE) is then the arithmetic mean of H_i across all N cells:

$$\overline{H} = \frac{1}{N} \sum_{i=1}^{N} H_i.$$

Complexity Measures – Average Mutual Information (AMI)

For a temporal lag τ (equal to 1 by default), define the random variables $X = x_i(t)$ and $Y = x_i(t+\tau)$. The mutual information of cell i is

$$I_i(X;Y) = \sum_{x,y} p_i(x,y) \log_2 \left(\frac{p_i(x,y)}{p_i(x) p_i(y)} \right),$$

where

- $p_i(x)$ is the marginal probability of state x,
- $p_i(y)$ is the marginal probability of state y,
- $p_i(x,y)$ is the joint probability of observing state x followed by state y after a temporal distance τ.

The average mutual information over all cells is

$$\bar{I} = \frac{1}{N} \sum_{i=1}^{N} I_i(X;Y).$$

Complexity Measures – Average Normalized Hamming Distance (AHD)

The Hamming distance is a measure of the dissimilarity between two cellular automaton configurations. Given two configurations $\mathbf{x}(t)$ and $\mathbf{y}(t)$ of length N, the Hamming distance is defined as the number of cells whose states differ.
The normalized Hamming distance is given by

$$d_H(\mathbf{x}(t), \mathbf{y}(t)) = \frac{\#\{i : x_i(t) \neq y_i(t)\}}{N},$$

where $\#\{\cdot\}$ denotes the cardinality of the set, i.e., the number of cells with different states, and N is the total number of cells. Consequently,

$$0 \leq d_H \leq 1,$$

where $d_H = 0$ indicates identical configurations and $d_H = 1$ indicates that all cells differ.

Complexity Measures – Average Normalized Hamming Distance

To characterize the overall dynamical behavior of a cellular automaton, the Hamming distance can be averaged over multiple consecutive time steps. Let $\mathbf{x}(t)$ and $\mathbf{x}(t+1)$ denote the automaton configurations at times t and $t+1$, respectively. The average Hamming distance over $T-1$ transitions is defined as

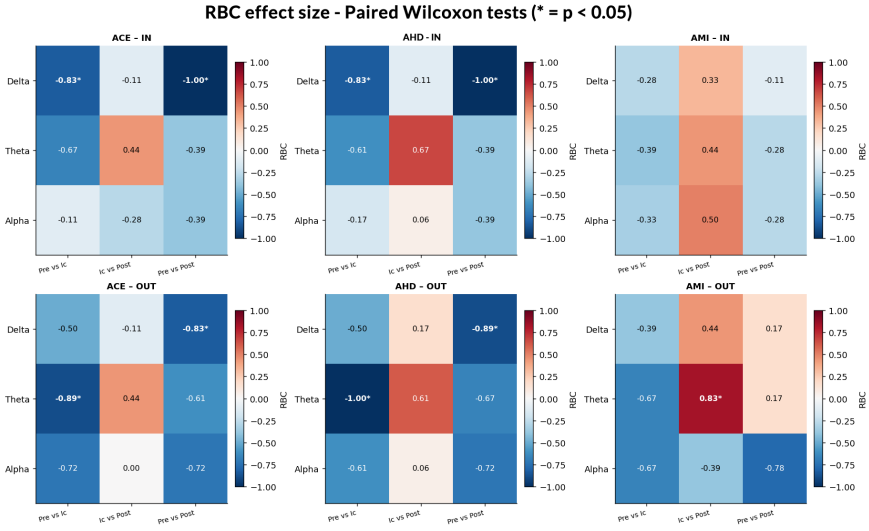
$$\overline{d}_H = \frac{1}{T-1} \sum_{t=1}^{T-1} d_H(\mathbf{x}(t), \mathbf{x}(t+1)) \,.$$

Substituting the definition of the normalized Hamming distance yields

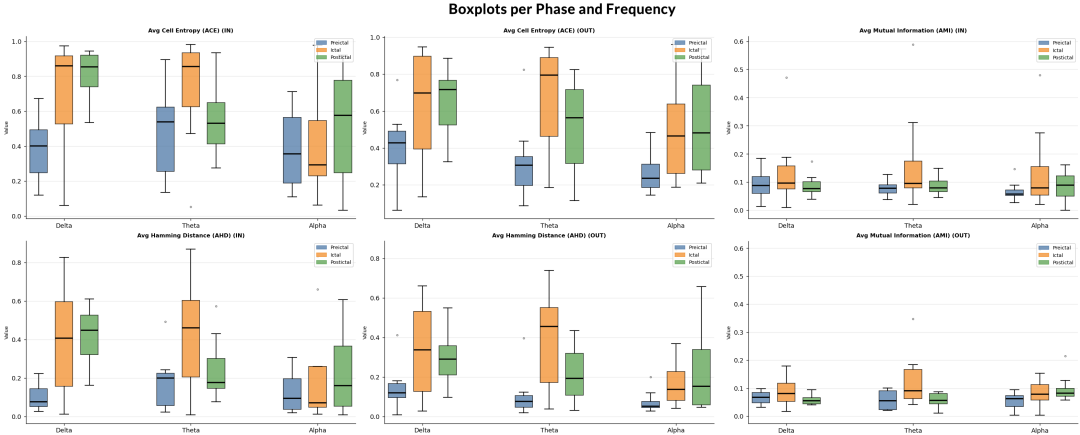
$$\overline{d}_H = \frac{1}{T-1} \sum_{t=1}^{T-1} \frac{\#\left\{i : x_i(t) \neq x_i(t+1)\right\}}{N}.$$

The average Hamming distance quantifies the mean fraction of cells that change state between successive iterations of the cellular automaton. Low values indicate relatively stable dynamics, whereas high values indicate greater temporal variability and more rapidly evolving configurations.

RBC Effect Size – Complexity Measures (ACE, AMI, AHD)



Boxplots – Complexity Measures (ACE, AMI, AHD)



Thank you!

hbaldo@usp.br

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