UNIVERSIDADE FEDERAL DO RIO GRANDE DO NORTE
PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA

Matrizes de Pearson como operadores densidade: um teste da hipótese do cérebro entrópico usando a entropia de von Neumann

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Orientador: Prof. Dr. Gandhi Viswanathan
Co-orientadora: Dra. Aline Viol

Defesa de Mestrado, Natal, julho de 2021

Problema e motivação

Hipótese do cérebro entrópico (2014): aumento de entropia para estados psicodélicos.

Viol el at. (2017): validação via *thresholding* de matrizes de Pearson $\boldsymbol{R}$.

Hoje: testar a hipótese via operadores densidade $\boldsymbol{\rho} = \boldsymbol{R}/N$, utilizando a entropia de von Neumann

$$S(\boldsymbol{\rho}) = -\operatorname{tr}(\boldsymbol{\rho} \ln \boldsymbol{\rho}).$$

Psicodélicos

Presentes em plantas e animais; uso milenar.

L. williamsii
(mescalina)

P. cubensis
(psilocibina)

C. purpurea
(ergolinas)

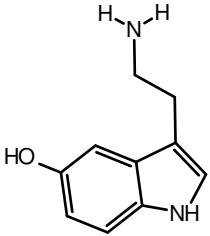
Ayahuasca

Do quíchua, *aya* (morto) e *waska* (cipó).

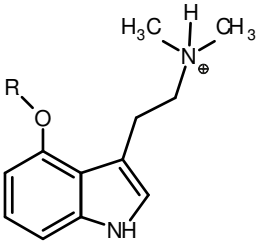
B. caapi
(β-carbolinas)

P. viridis
(N,N-dimetiltriptamina)

Estrutura molecular

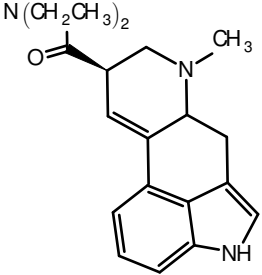


Serotonina (5-HT)

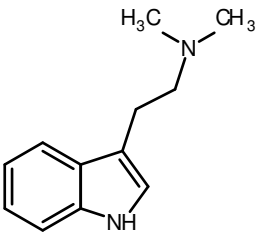


Psilocibina

($R = PO_3H^-$)

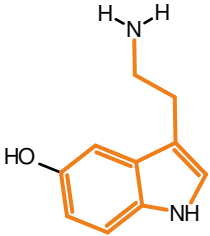


LSD



DMT

Estrutura molecular



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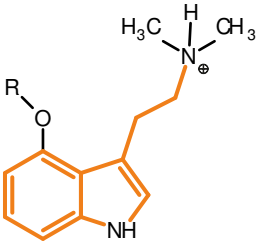

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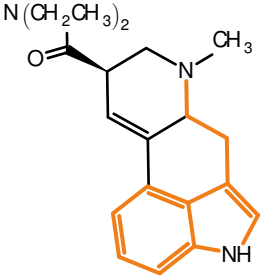

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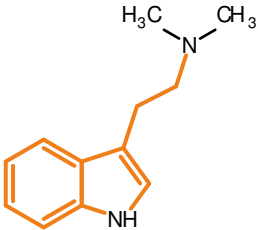
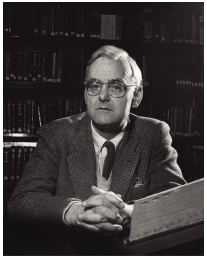


DMT

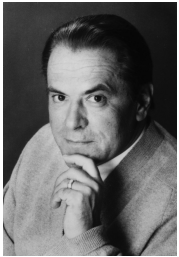
Definição



Humphry Osmond (1917–2004)

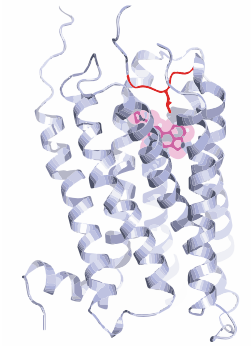
Aldous Huxley (1894–1963)

Psicodélico = *psychē* (ψυχή) + *dēloun* (δηλοῦν)
= "Tornar manifesto a mente"



Stan Grof (1931–)

"Amplificadores não específicos do inconsciente"



Wacker et al., *Cell* **168** (2017)

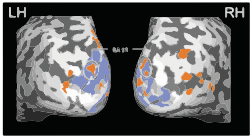
Agonistas serotoninérgicos
(5-HT_{2A}, 5-HT_{2B}, etc.)

Renascença psicodélica

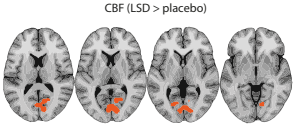
Farmacologia e neurociência.

Psilocybin induces schizophrenia-like psychosis in humans via a serotonin-2 agonist action

Vollenweider et al., *Neuroreport* **9** (1998)

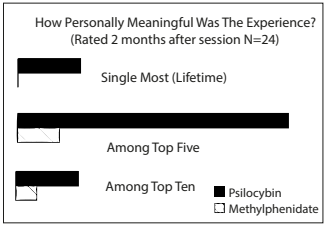


De Araujo et al., *Hum. Brain Mapp.* **33** (2012)

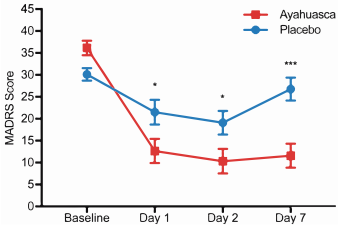


Carhart-Harris et al., *PNAS* **11** (2016)

Psiquiatria; potencial terapêutico.



Griffiths et al., *Psychopharmacol.* **187** (2006)



Palhano-Fontes et al., *Psychol. Med.* **49** (2019)

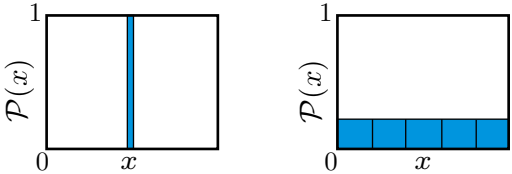
Hipótese do cérebro entrópico

"A entropia da atividade cerebral indexa a riqueza informacional de estados de consciência"

Carhart-Harris et al., *Front. Hum. Neurosci.* **8** (2014)

Entropia (teoria da informação): incerteza de um sistema;

$$S(X) = -\sum_{x \in \mathcal{X}} \mathcal{P}(x) \log \mathcal{P}(x). \qquad \text{(Shannon)}$$



$S = 0$ $\qquad$ $S = \log|\mathcal{X}|$

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$S\Big($ $\Big) \; < \; S\Big($ $\Big)$

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Carhart-Harris et al., *Front. Hum. Neurosci.* **8** (2014)

Estado de coma, depressão, adicção, ⋮

Estado psicodélico, privação sensorial, psicose, ⋮

Entropia reduzida
Rigidez de estados

Entropia elevada
Flexibilidade de estados

$$S(X) = -\sum_{x \in \mathcal{X}} \mathcal{P}(x) \log \mathcal{P}(x)$$

Testes: Tagliazucchi et al. (2014), Lebedev et al. (2016), Viol et al. (2017), ...

Dados (Viol et al., 2017)

9 adultos saudáveis, destros.

Dose de 120–200 mL de ayahuasca (0,8 mg/mL de DMT; 0,21 mg/mL harmina).

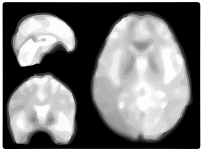
Estado de repouso desperto.

Sessão de *functional magnetic resonance imaging* (fMRI) antes e 40 minutos depois da ingestão.

Séries temporais de fMRI

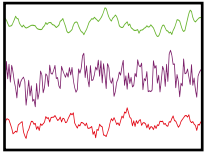
Sinal BOLD (*blood-oxygen-level-dependent*).

Pré-processamento.

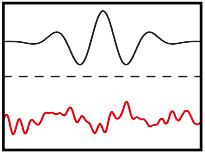


Onias et al., *Epilepsy Behav.* **38** (2014)

parcelamento

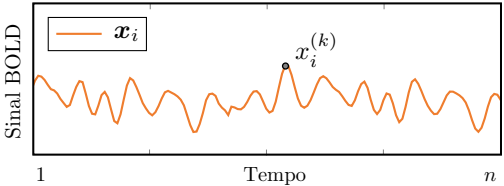


extração



filtro

Vetor série temporal $\boldsymbol{x}_i = (x_i^{(1)}, \ldots, x_i^{(n)})\,;\; i = 1, \ldots, N.$



Correlação das séries temporais

Coeficiente de correlação de Pearson R_{ij}: influência linear do par $\boldsymbol{x}_i, \boldsymbol{x}_j$;

$$R_{ij} = \frac{1}{n}\sum_{k=1}^{n}\left[\frac{x_i^{(k)} - \langle \boldsymbol{x}_i \rangle}{\sigma_i}\right]\left[\frac{x_j^{(k)} - \langle \boldsymbol{x}_j \rangle}{\sigma_j}\right] \equiv \frac{\langle \boldsymbol{X}_i \boldsymbol{X}_j \rangle}{\sigma_i \sigma_j},$$

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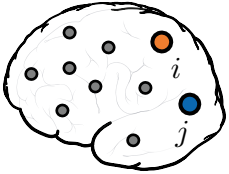

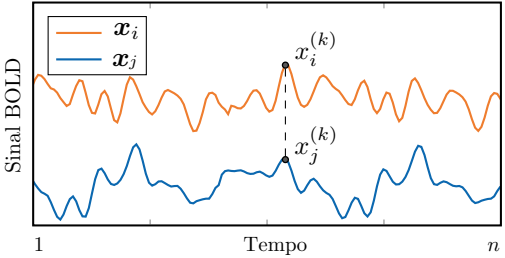

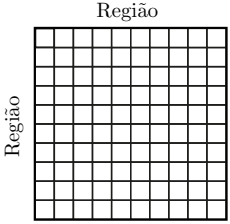

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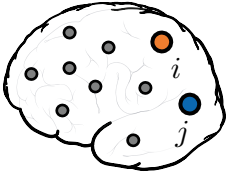

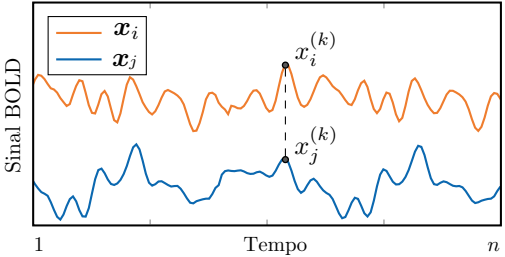

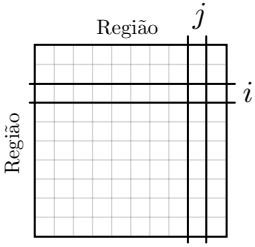

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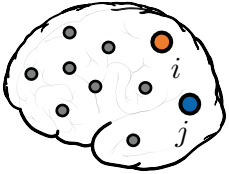

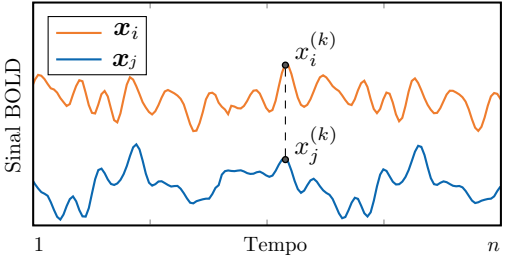

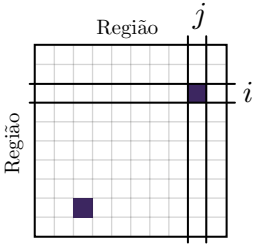

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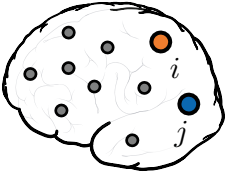

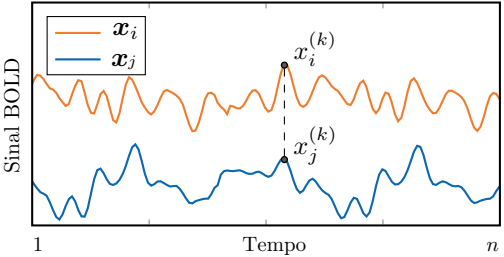

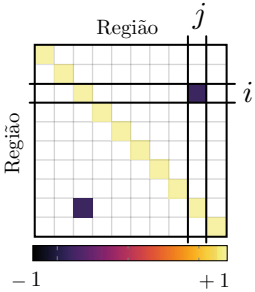

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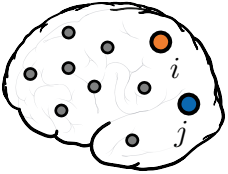
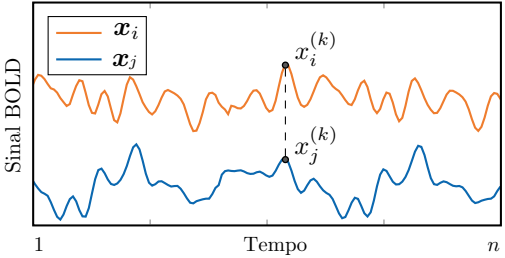
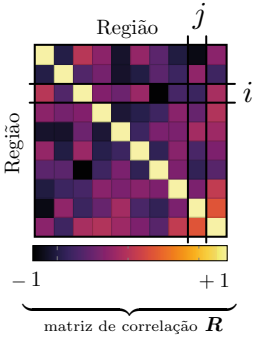
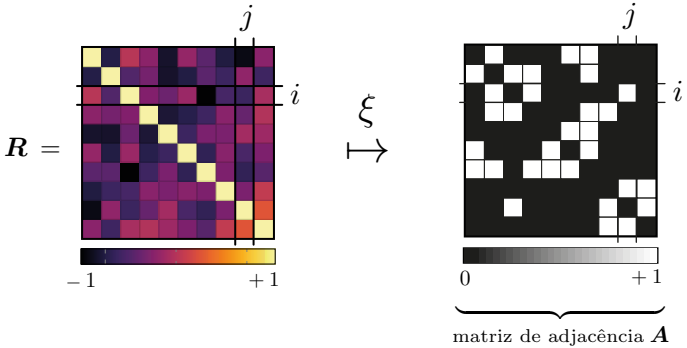






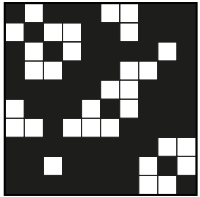
Limiarização (*thresholding*)

Seja $|\xi| < 1$. Defina $\boldsymbol{A}$ tal que $A_{ij} = 1$ se $|R_{ij}| \geq \xi$. Do contrário, $A_{ij} = 0$.



Teoria de grafos

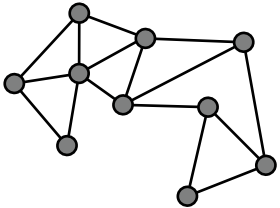
A matriz $\boldsymbol{A}$ assume a representação de grafo.

$\boldsymbol{A} =$ 

Teoria de grafos

A matriz $\boldsymbol{A}$ assume a representação de grafo.

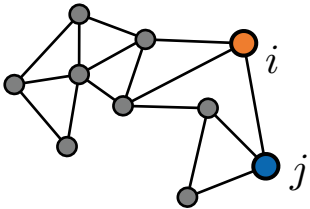
$$\boldsymbol{A} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix} \implies$$



Teoria de grafos

A matriz $\boldsymbol{A}$ assume a representação de grafo.

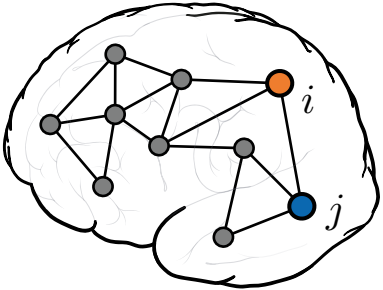
$$
\boldsymbol{A} = \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array}
\begin{array}{c}
\begin{array}{cccccccc} & & & & & & j & \end{array} \\
\left(\begin{array}{cccccccc|c}
0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\
\hline
\mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} \\
\hline
0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1
\end{array}\right)
\end{array}
\begin{array}{c} \\ \\ \\ i \\ \\ \\ \\ \\ \\ \end{array}
\Longrightarrow
$$



Teoria de grafos

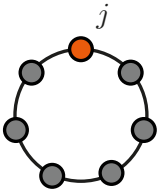
A matriz $\boldsymbol{A}$ assume a representação de grafo.

$$
\boldsymbol{A} = \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array}
\begin{array}{c}
\begin{array}{cccccccccc} & & & & & & & & j & \end{array} \\
\left(\begin{array}{cccccccc|c|c}
0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\
1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
\hline
\mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} \\
\hline
0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\
1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0
\end{array}\right)
\end{array}
\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ i \\ \end{array}
\Longrightarrow
$$

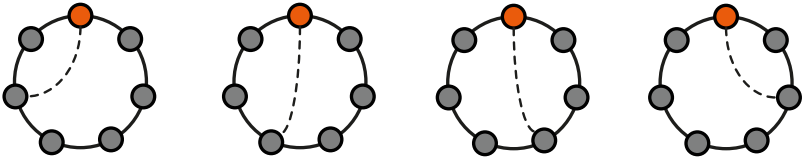


Distribuição de grau

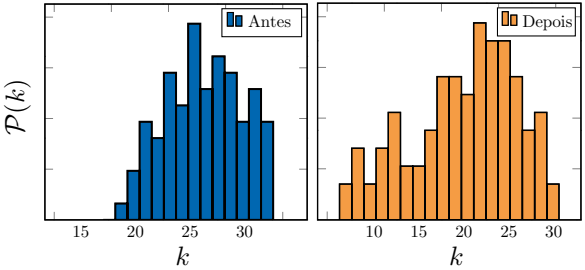
O grau k_j é a soma de conexões do j-ésimo nó. Se $k = 2$ para todos os nós,



A distribuição de grau $\mathcal{P}(k)$ nos informa sobre os padrões da rede. Se $k_j = 3$,



Entropia de Shannon da distribuição de grau



Dado $\mathcal{P}(k)$ das redes de antes e depois da ayahuasca, calcula-se

$$S[\mathcal{P}(k)] = -\sum_k \mathcal{P}(k) \ln \mathcal{P}(k).$$

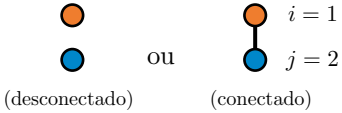
Viol et al. (2017): $\Delta S = S_{\text{depois}} - S_{\text{antes}} > 0.$

***Thresholding*: prós e contras**

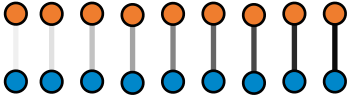
Pró: elimina ruído; p-valor $< \alpha$.

Contra: elimina sinal; $N = 2$,

$$\boldsymbol{A} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \text{ ou } \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$



$$\boldsymbol{R} = \begin{pmatrix} 1 & R_{12} \\ R_{12} & 1 \end{pmatrix}, R_{12} \in [-1, +1]$$



Pró: preserva topologia; Viol et al., *Physica A* **561** (2021).

Contra: fabrica complexidade; Cantwell et al., *Phys. Rev. E* **101** (2020).

Pró: $\boldsymbol{A}$ é computacionalmente inócuo.

Contra: $\{\boldsymbol{A}_1, \ldots, \boldsymbol{A}_m\}$ é intimidador ($m \gg 1$).

Alternativa: matrizes de Pearson como operadores densidade

Seja $\boldsymbol{\rho}$ o operador densidade do ensemble de M vetores de estado $|\psi_j\rangle$,

$$\boldsymbol{\rho} = \sum_{j=1}^{M} p_j |\psi_j\rangle\langle\psi_j|.$$

$\boldsymbol{\rho}$ é (i) hermitiano, (ii) tem traço normalizado, e (iii) é positivo semidefinido.

A entropia de $\boldsymbol{\rho}$ é dada pela entropia de von Neumann

$$S(\boldsymbol{\rho}) = -\operatorname{tr}(\boldsymbol{\rho}\ln\boldsymbol{\rho}) = -\sum_{i=1}^{N} \lambda_i \ln\lambda_i.$$

Proposição: a matriz $\boldsymbol{\rho} = \boldsymbol{R}/N$ satisfaz as condições (i)–(iii) de operadores densidade.

Prova : (i) hermiticidade; por inspeção,

$$R_{ij} = \frac{\langle \boldsymbol{X}_i \boldsymbol{X}_j \rangle}{\sigma_i \sigma_j} = R_{ji} \in \mathbb{R}.$$

(ii) traço normalizado; a diagonal é dada por

$$R_{ii} = \frac{\langle \boldsymbol{X}_i^2 \rangle}{\sigma_i^2} = 1,$$

logo, $\operatorname{tr} \boldsymbol{R}/N = 1$.

(iii) positividade semidefinida (autovalores não negativos); basta mostrar $\boldsymbol{R}$ positivo semidefinido, isto é, $\boldsymbol{v} \cdot \boldsymbol{R}\, \boldsymbol{v} \geq 0$ para todo $\boldsymbol{v} \in \mathbb{R}^N$.

$$\begin{aligned}\sum_{ij}^{N} v_i \left(\sum_{k}^{n} X_i^{(k)} X_j^{(k)} \right) v_j &= \sum_{k}^{n} \sum_{ij}^{N} \left(v_i X_i^{(k)} v_j X_j^{(k)} \right) \\ &= \sum_{k}^{n} \left| \sum_{i}^{N} v_i X_i^{(k)} \right|^2 \geq 0.\end{aligned}$$

$\blacksquare$

Observação: $S(\boldsymbol{\rho}) \in [0, \ln N]$.

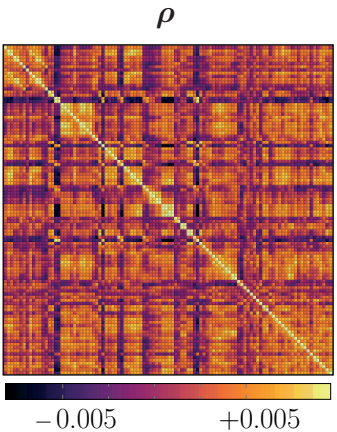
Com efeito, $\boldsymbol{x}_i$ e $\boldsymbol{x}_j$ independentes implica não correlação: $\langle \boldsymbol{X}_i \boldsymbol{X}_j \rangle = \langle \boldsymbol{X}_i^2 \rangle \delta_{ij}$,

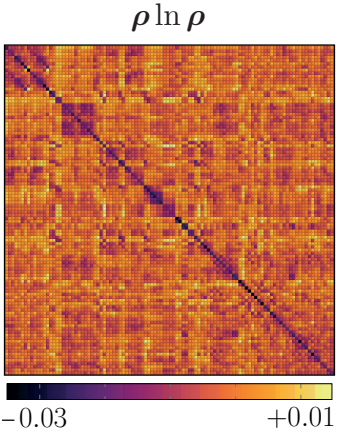
$$R_{ij} = \delta_{ij} \quad \Longrightarrow \quad \underset{\text{(estado misto)}}{\boldsymbol{\rho} = \boldsymbol{I}/N} \quad \Longrightarrow \quad S = \ln N.$$

Pares totalmente correlacionados: $R_{ij} = 1$ para todo i, j, tal que $\boldsymbol{R}^2 = N\boldsymbol{R}$.

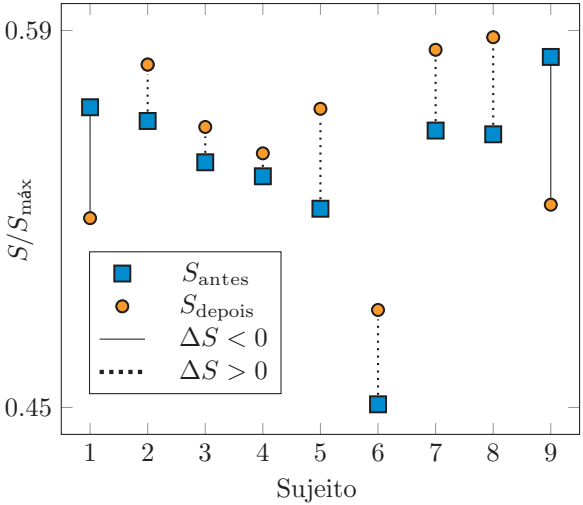
$$\underset{\text{(estado puro)}}{\boldsymbol{\rho}^2 = \boldsymbol{\rho}} \quad \Longrightarrow \quad \operatorname{tr}(\boldsymbol{\rho} \ln \boldsymbol{\rho}) \;=\; \operatorname{tr}(\boldsymbol{\rho} \ln \boldsymbol{\rho}^2) \;=\; 2 \operatorname{tr}(\boldsymbol{\rho} \ln \boldsymbol{\rho}) = 0.$$

Resultados

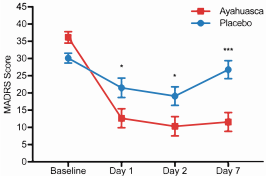

$\boldsymbol{\rho}$
-0.005
$+0.005$


$\boldsymbol{\rho} \ln \boldsymbol{\rho}$
-0.03
$+0.01$

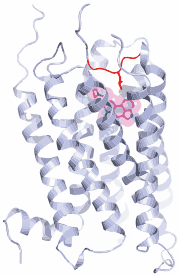
Resultados


0.59
0.45
$S/S_{\text{máx}}$
1
2
3
4
5
6
7
8
9
Sujeito
S_{antes}
S_{depois}
$\Delta S < 0$
$\Delta S > 0$

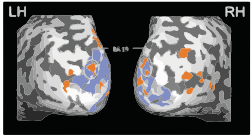
“Big picture”



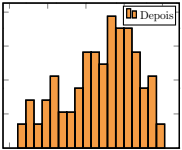
Palhano-Fontes et al., *Psychol. Med.* **49** (2019)

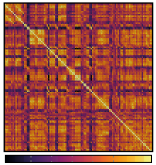


Wacker et al., *Cell* **168** (2017)



De Araujo et al., *Hum. Brain Mapp.* **33** (2012)





Conclusão

- Método matematicamente robusto e independente de *threshold*; reduz-se arbitrariedade.
- Parcimonioso: uma única matriz $\boldsymbol{\rho}$ para cada amostra.
- Consistente com a hipótese do cérebro entrópico (grosso modo).
- Genérico e prontamente implementável: preço de ativos, sistemas complexos em geral.

"To study the abnormal is the best way of understanding the normal"– William James

CAPES

PPGF Programa de Pós-Graduação Física Universidade Federal do Rio Grande

LaTeX