ENFE 21

Brazilian Meeting on Statistical Physics

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The von Neumann entropy for the Pearson correlation matrix: A test of the entropic brain hypothesis for psychedelics

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Problem and motivation

2014: brain entropy increases for psychedelics;

frontiers in
HUMAN NEUROSCIENCE

The entropic brain: a theory of conscious states informed by neuroimaging research with psychedelic drugs

Robin L. Carhart-Harris[1]*, Robert Leech[2], Peter J. Hellyer[2], Murray Shanahan[3], Amanda Feilding[4], Enzo Tagliazucchi[5], Dante R. Chialvo[6] and David Nutt[1]

2017: validation via thresholding of Pearson matrices $\boldsymbol{R}$;

SCIENTIFIC REPORTS

Shannon entropy of brain functional complex networks under the influence of the psychedelic Ayahuasca

A. Viol[1,2,3], Fernanda Palhano-Fontes[4], Heloisa Onias[4], Draulio B. de Araujo[4] & G. M. Viswanathan[1,5]

Today: a threshold-free approach using the von Neumann entropy for $\boldsymbol{\rho} = \boldsymbol{R}/N$,

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

Psychedelics

Present in plants and animals; perennial human usage.

L. williamsii
(mescaline)

P. cubensis
(psilocybin)

C. purpurea
(ergolines $\to$ LSD)

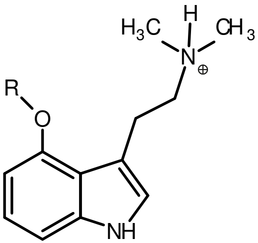
Ayahuasca

From the Quechua language, *aya* (dead) and *waska* (rope).

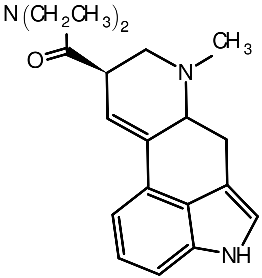
B. caapi
(β-carbolines)

P. viridis
(N,N-dimethyltryptamine)

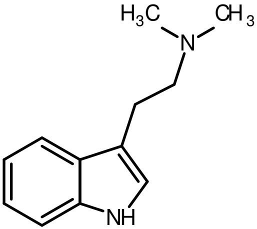
Chemical structure



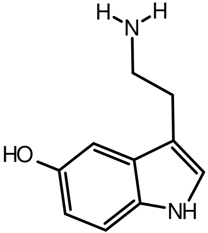
Psilocybin
($R = PO_3H^-$)



LSD

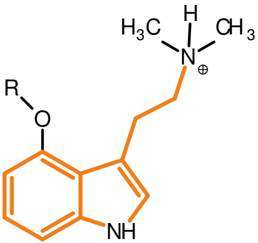


DMT



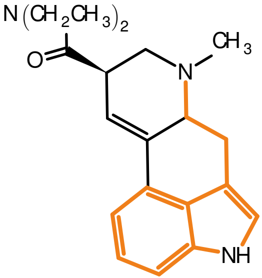
Serotonin

Chemical structure

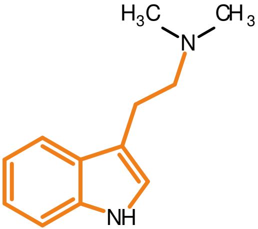


Psilocybin

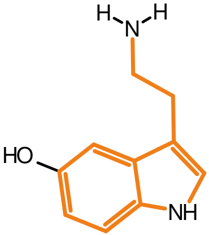
$(R = PO_3H^-)$



LSD

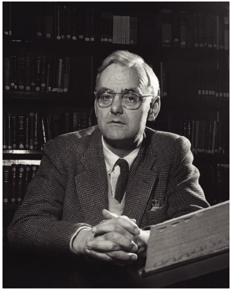


DMT

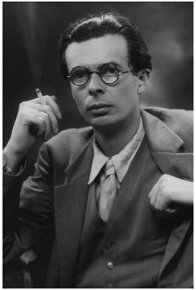


Serotonin

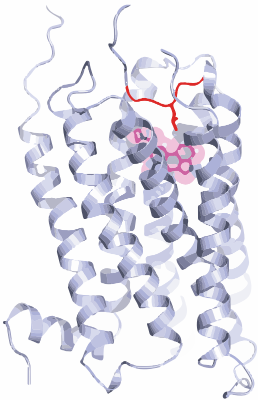
Definition



Humphry Osmond (1917–2004)



Aldous Huxley (1894–1963)



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

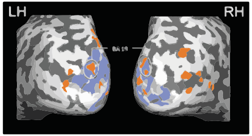
Psychedelic = *psychē* (ψυχή) + *dēloun* (δηλοῦν)
= "Mind-manifesting"

Serotonergic agonists
(5-HT_{2A}, 5-HT_{2B}, etc.)

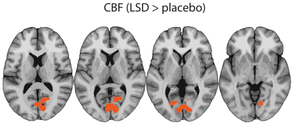
“Psychedelic Renaissance”

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

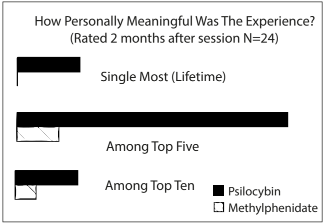
Vollenweider *et al.*, *Neuroreport* **9** (1998)



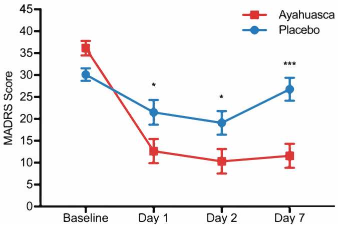
De Araujo *et al.*, *Hum. Brain Mapp.* **33** (2012)



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



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



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

Entropic brain hypothesis

"The entropy of [brain activity] indexes
the informational richness of conscious states."

Carhart-Harris, *Neuropharmacol.* **142** (2018)

Sedation,
depression,
addiction,
⋮

Low entropy
Rigid states

High entropy
Flexible states

Psychedelic state,
sensory deprivation,
early psychosis,
⋮

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

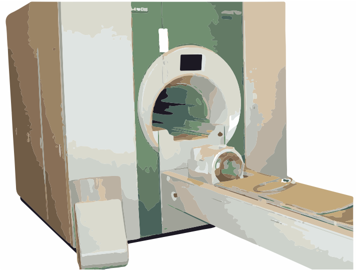
Tests: Tagliazucchi et al. (2014), Lebedev et al. (2016), Viol et al. (2017), ...

Data (Viol *et al.*, 2007)

9 healthy right-handed adults (5 women).

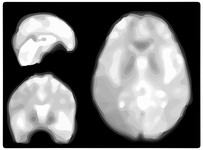
120–200 mL ayahuasca dosage: 0.8 mg/mL of DMT and 0.21 mg/mL of harmine.

Awake resting state in a functional magnetic resonance imaging (fMRI) session.



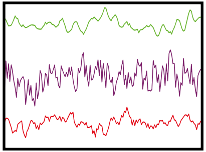
FMRI time series

Blood-oxygen-level-dependent (BOLD) signal.

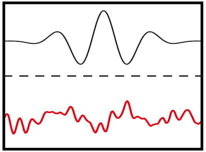


Onias *et al.*, *Epilepsy Behav.* **38** (2014)

parcellation

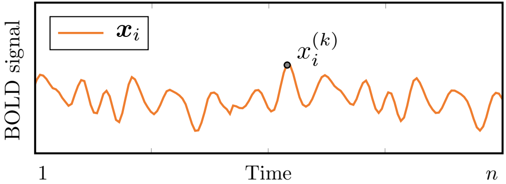


extraction



filtering

Time series vector $\boldsymbol{x}_i = (x_i^{(1)}, \ldots, x_i^{(n)}),\ i = 1, \ldots, N.$



Correlation

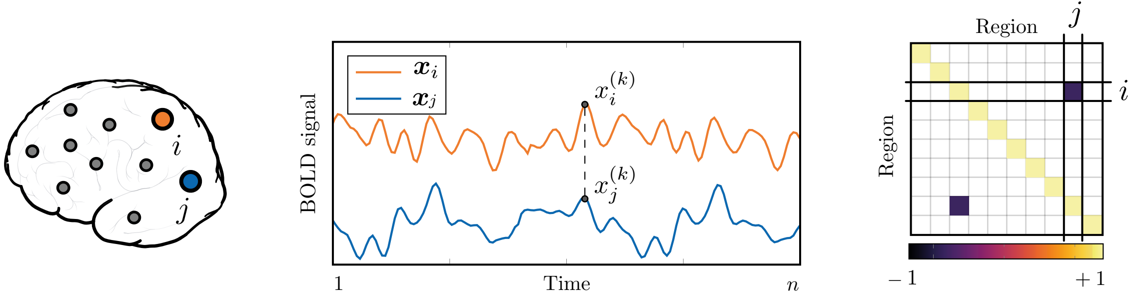
Pearson correlation coefficient: linear dependency of $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$,

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

Correlation

Pearson correlation coefficient: linear dependency of $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$,

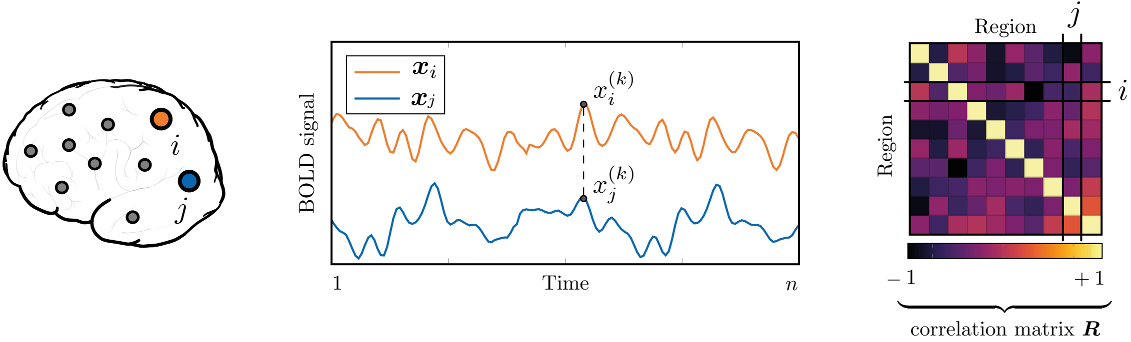
$$R_{ij} = \frac{1}{n} \sum_{k=1}^{n} \left[\frac{x_i^{(k)} - \langle \boldsymbol{x}_i \rangle}{\sigma_i} \right] \left[\frac{x_j^{(k)} - \langle \boldsymbol{x}_j \rangle}{\sigma_j} \right] .$$



Correlation

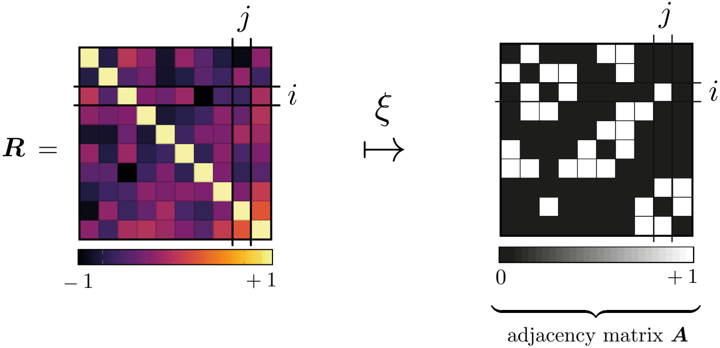
Pearson correlation coefficient: linear dependency of $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$,

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

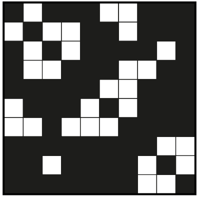


Thresholding

Let $|\xi| < 1$. Define $\boldsymbol{A}$ such that $A_{ij} = 1$ if $|R_{ij}| \geq \xi$. Otherwise, $A_{ij} = 0$.

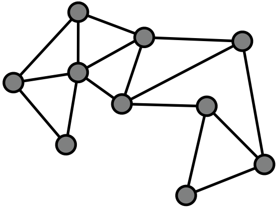


Graph theory and brain networks

$\boldsymbol{A} =$ 

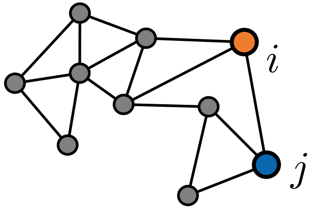
Graph theory and brain networks

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



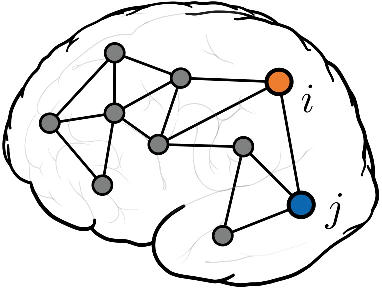
Graph theory and brain networks

$$\boldsymbol{A} = \begin{array}{cc} \begin{matrix} & & & & & & & & j & \end{matrix} & \\ \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix} & \begin{matrix} \\ \\ i \\ \\ \\ \\ \\ \\ \\ \\ \end{matrix} \end{array} \Longrightarrow$$

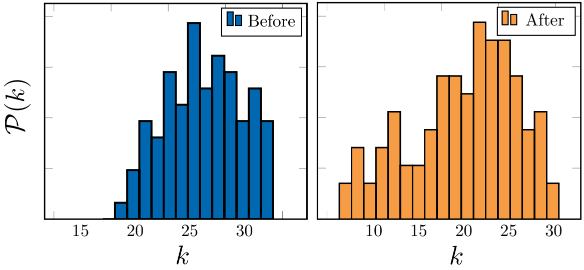


Graph theory and brain networks

$$\boldsymbol{A} = \begin{array}{c} \\ \\ \end{array}\begin{array}{cc} \begin{array}{cccccccccc} & & & & & & & & j & \end{array} & \\ \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix} & \begin{array}{c} \\ \\ i \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \end{array} \quad \Longrightarrow$$



Entropy of the degree distribution of functional brain networks



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

Viol *et al.* (2017):

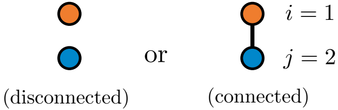
$$\Delta S = S_{\mathrm{after}} - S_{\mathrm{before}} > 0 \ .$$

Pros and cons of thresholding

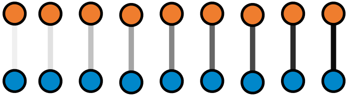
Pros: noise reduction, ...

Cons: complexity from randomness, ...

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



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



Alternative: Pearson matrices as density operators

The density operator

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

is (i) Hermitian, (ii) has unit trace, and (iii) is positive semidefinite.

The entropy is given by the von Neumann entropy

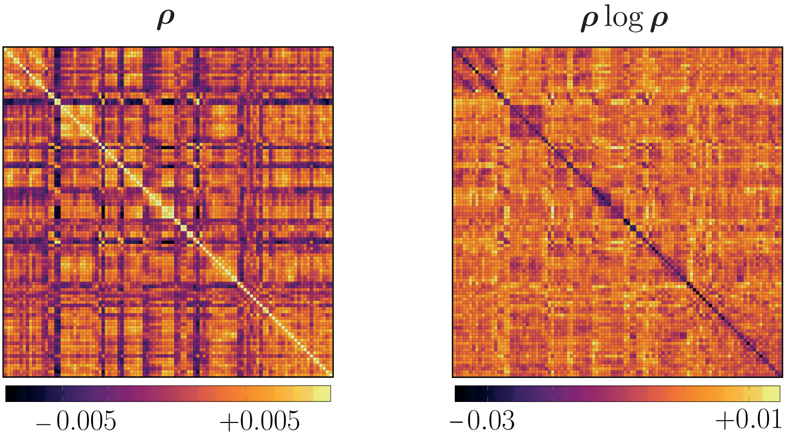
$$S(\boldsymbol{\rho}) = -\operatorname{tr}(\boldsymbol{\rho}\log\boldsymbol{\rho}) = -\sum_{i=1}^{N} \lambda_i \log \lambda_i \; .$$

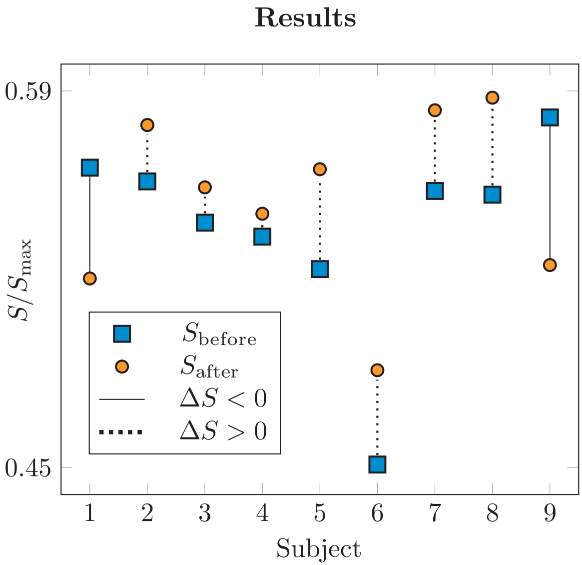
Proposition: the matrix $\boldsymbol{\rho} \equiv \boldsymbol{R}/N$ satisfies (i)–(iii).

Proof: Left to the reader :-).

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

Results


$\boldsymbol{\rho}$
$\boldsymbol{\rho} \log \boldsymbol{\rho}$
-0.005
$+0.005$
-0.03
$+0.01$


Results
0.59
0.45
$S/S_{\max}$
1
2
3
4
5
6
7
8
9
Subject
S_{before}
S_{after}
$\Delta S < 0$
$\Delta S > 0$

Concluding remarks

- Threshold-free and mathematically robust method.
- Consistent with the entropic brain hypothesis (roughly speaking).
- Readily available to complex systems in general.

Preprint available at arXiv:2106.05379

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