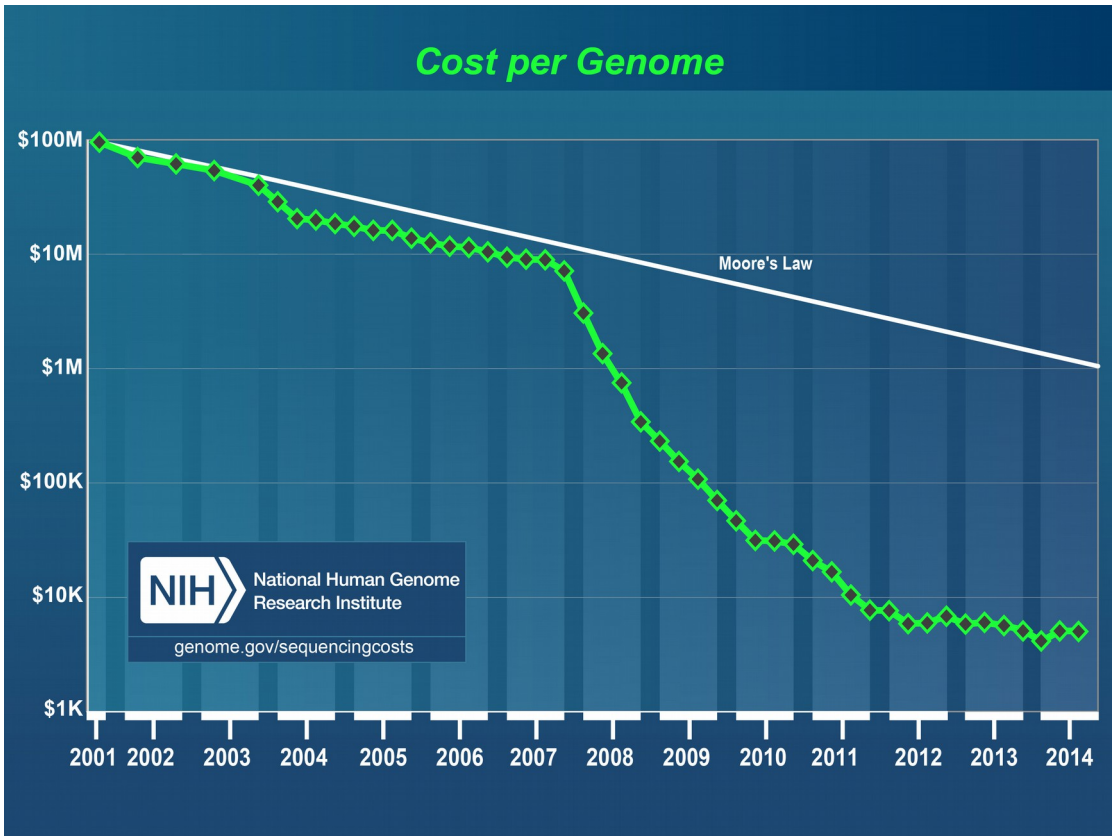
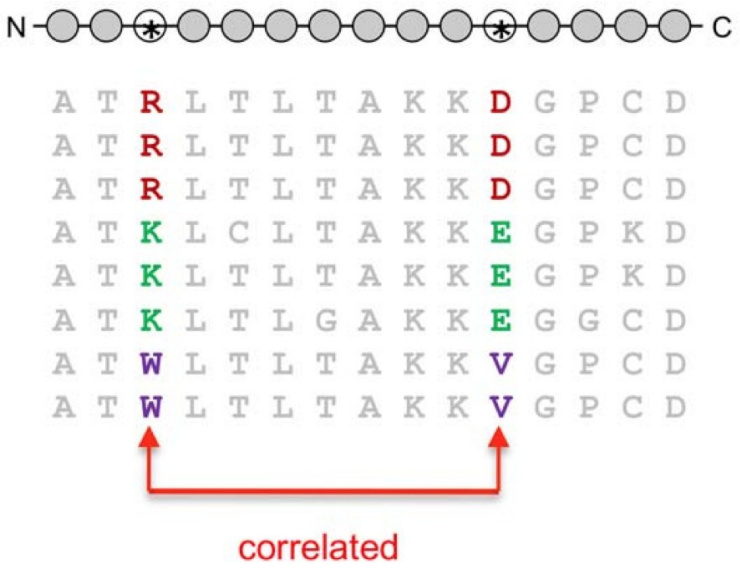
Dario Villamaina

École normale supérieure & Institut Philippe Meyer

Random matrices and correlation data analysis



Motivation: Analysis of sequences



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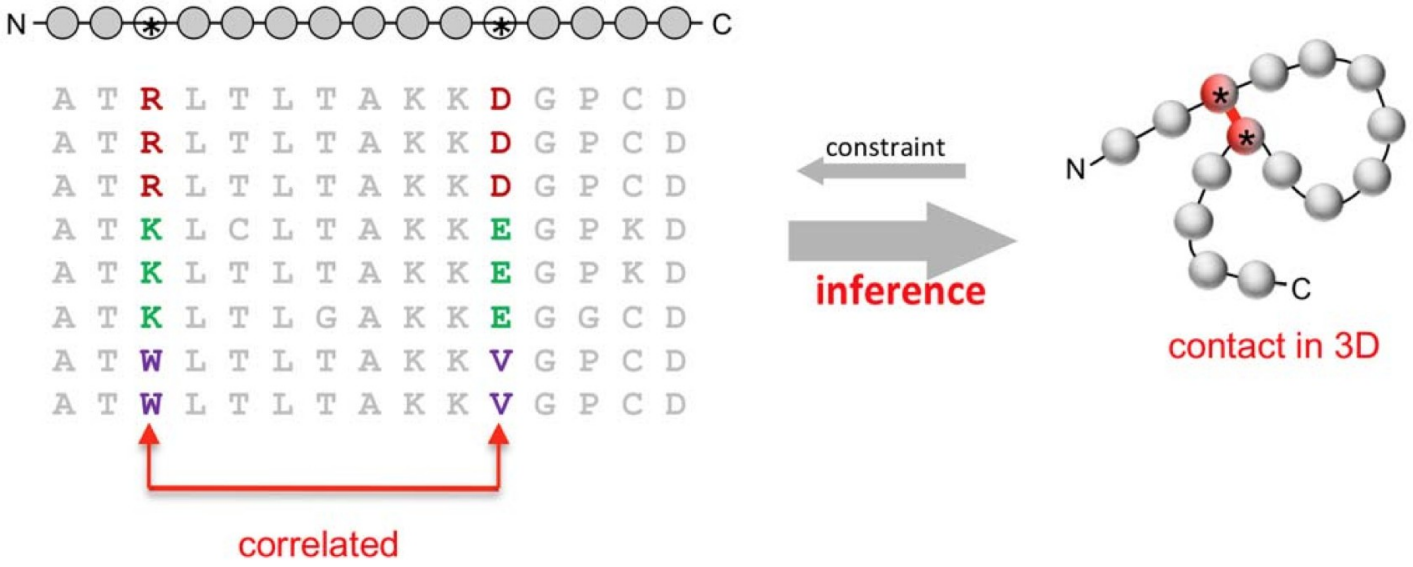

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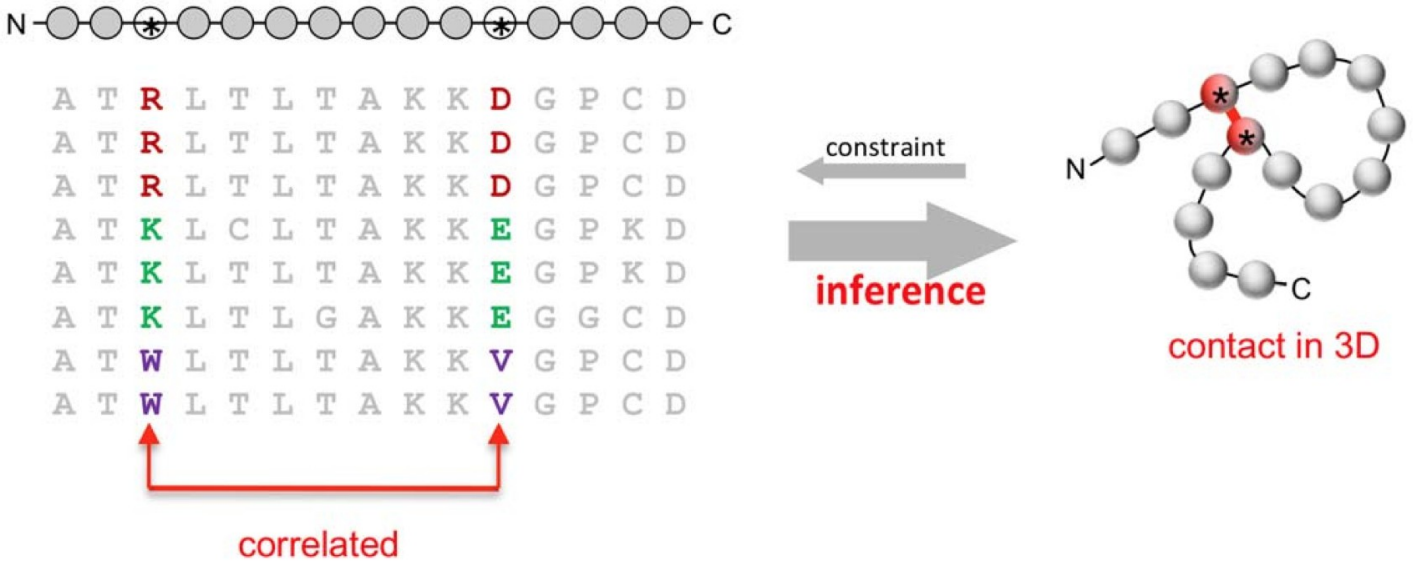


Data Sequences

Empirical Correlation matrix

$\hat{C}$

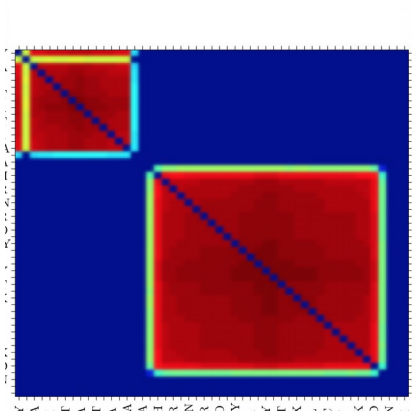
3D Contacts prediction

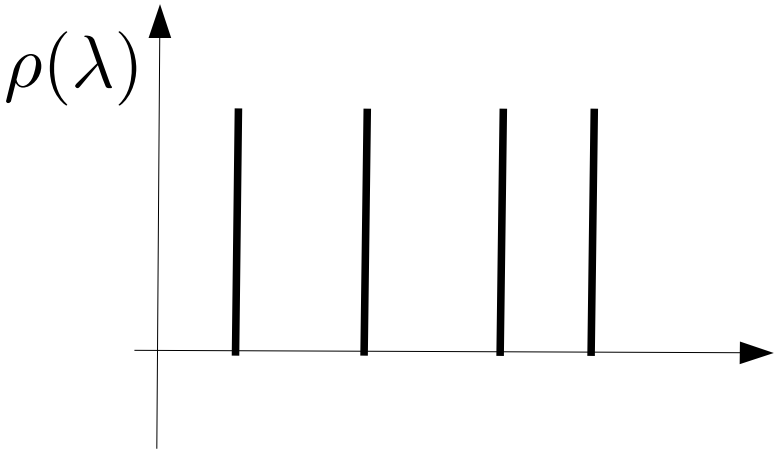
Sites in contact are associated with high localized eigenvectors of the correlation matrix

Population Covariance

Infinite statistics

C (One matrix)

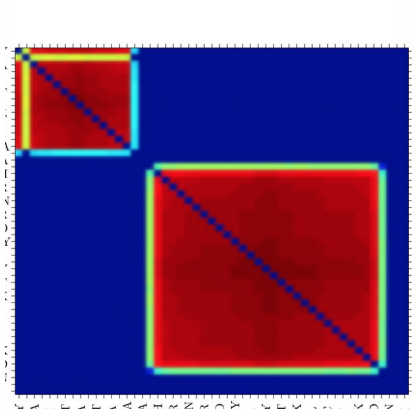




Population Covariance *vs* Empirical Covariance

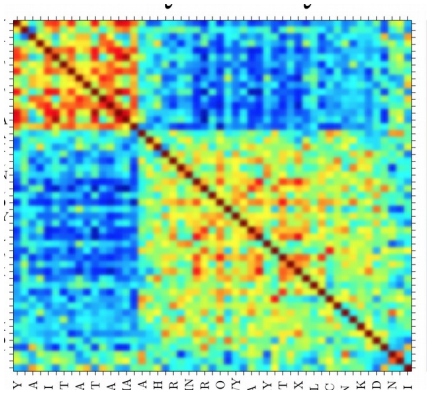
Infinite statistics

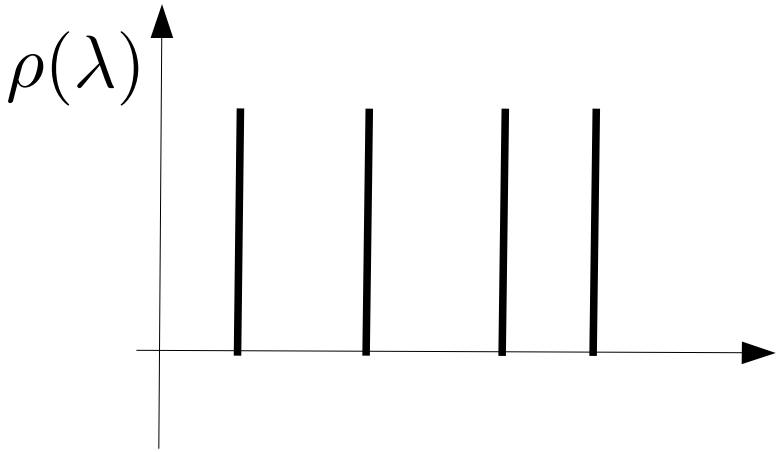
C (One matrix)

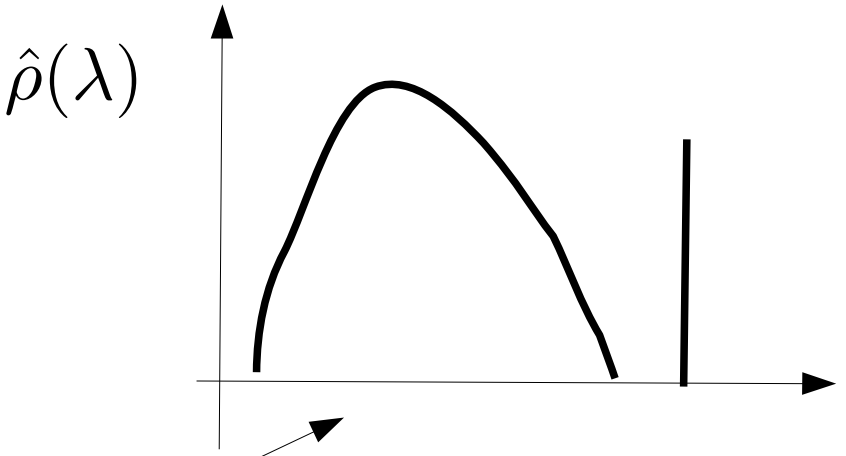


Finite statistics

$\hat{C}$ (Ensembles of matrices)







Part of the signal is hidden
by finite sampling effects!

Random Matrix Model

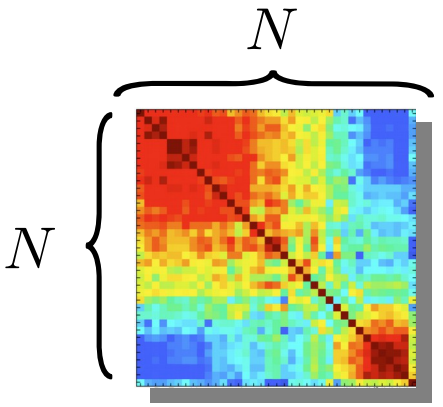
Number of measures (M)

$$\hat{X} = \overbrace{\begin{pmatrix} -0.2526 & -0.8387 & 0.9620 & -0.2771 & 0.2107 \\ 0.8294 & -0.2004 & -1.0053 & 0.3873 & -0.4419 \\ 0.5982 & 1.0760 & 0.5182 & 0.2671 & 0.4277 \\ -0.0285 & -1.0486 & -0.7054 & 1.1440 & -1.0764 \\ -1.1416 & -0.5782 & -0.1396 & -0.9523 & 0.2344 \end{pmatrix}}^{\text{Number of variables } (N)}$$

Gaussian sample with correlation matrix C

$$\hat{C} \propto \hat{X} \times \hat{X}^T$$

$$\hat{C}_{ij} = \frac{1}{M} \sum_t x_{i,t} x_{j,t}$$



Efficiency parameter $r = \frac{N}{M}$

Perfect sampling limit $\hat{C} \underset{r \to 0}{\to} C$

Toy model : Finite rank correlation matrix

$$C \propto \begin{pmatrix} \gamma & & 0 \\ & 1 & \\ 0 & & \ddots \\ & & & 1 \end{pmatrix} \qquad \boldsymbol{\xi}_1 \propto \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

continuous limit $\Longrightarrow$ $\rho_C(\lambda) = (1-\alpha)\delta(\lambda - 1) + \alpha\delta(\lambda - \gamma)$

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continuous limit $\Rightarrow$ $\rho_C(\lambda) = (1-\alpha)\delta(\lambda - 1) + \alpha\delta(\lambda - \gamma)$

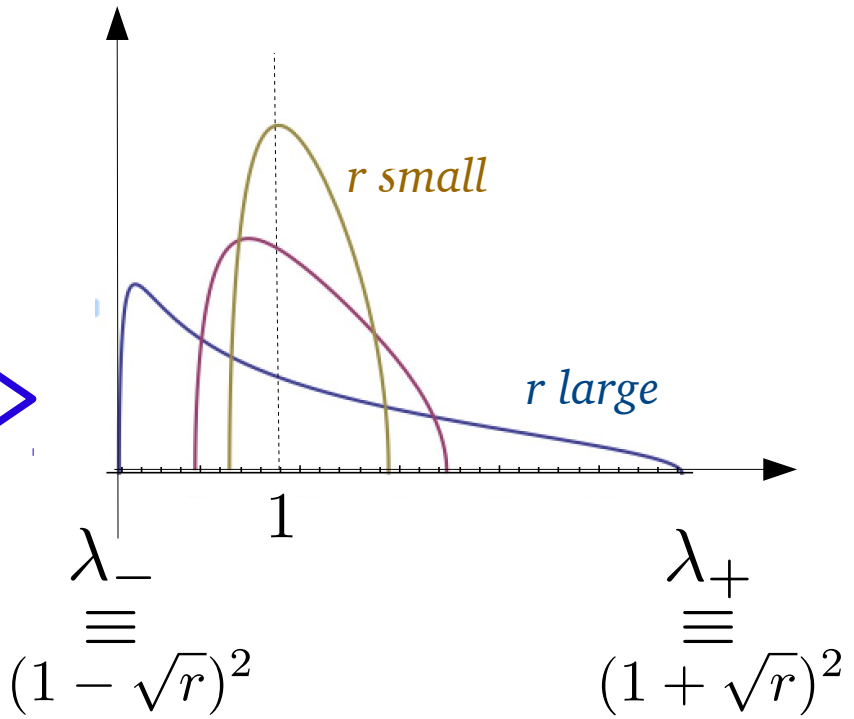
Case $\gamma = 1 \quad \alpha = 0$ (Null model)

$$\hat{C} \equiv XX^t$$

Wishart ensemble

$$\rho_{\hat{C}}(\lambda) = \frac{\sqrt{(\lambda - \lambda_-)(\lambda_+ - \lambda)}}{2\lambda\pi r}$$

Marcenko-Pastur distribution

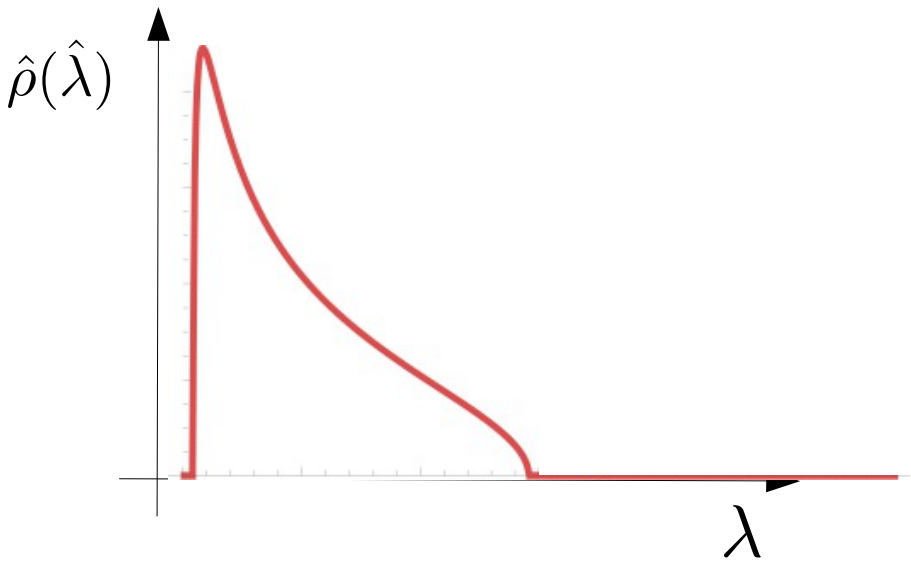


The transition in the eigenvalue spectrum

Case of γ finite and $\alpha \to 0$

Weak signal $\gamma < \gamma_c \equiv 1 + \sqrt{r}$

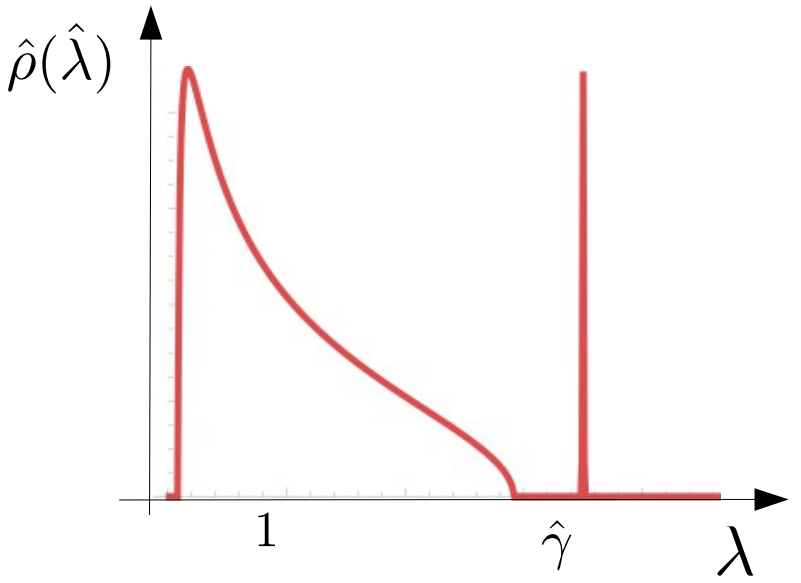
$$\hat{\rho}(\hat{\lambda}) \simeq \hat{\rho}_{bulk}(\hat{\lambda})$$



Strong signal $\gamma > \gamma_c$

$$\hat{\rho}(\hat{\lambda}) \simeq (1-\alpha)\hat{\rho}_{bulk}(\hat{\lambda}) + \alpha\,\delta(\hat{\lambda} - \hat{\gamma})$$

delta peak



Noise undressing of empirical correlation matrices

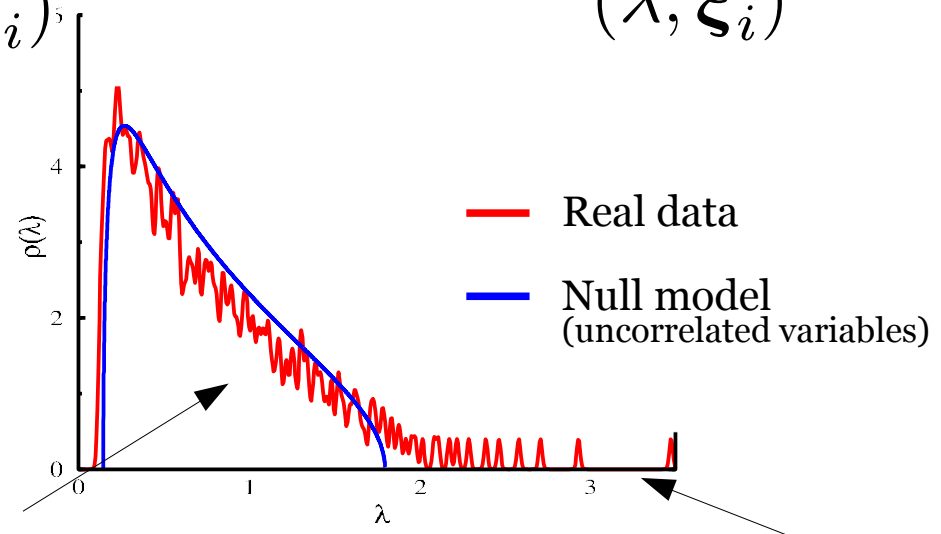
L Laloux, P Cizeau, JP Bouchaud, M Potters - Physical Review Letters, (1999)

(Measured)

$$\hat{C} \quad (\hat{\lambda}, \hat{\boldsymbol{\xi}}_i)$$

(True)

$$C \quad (\lambda, \boldsymbol{\xi}_i)$$



(Only noise ?)
Bulk eigenvalues

Signal

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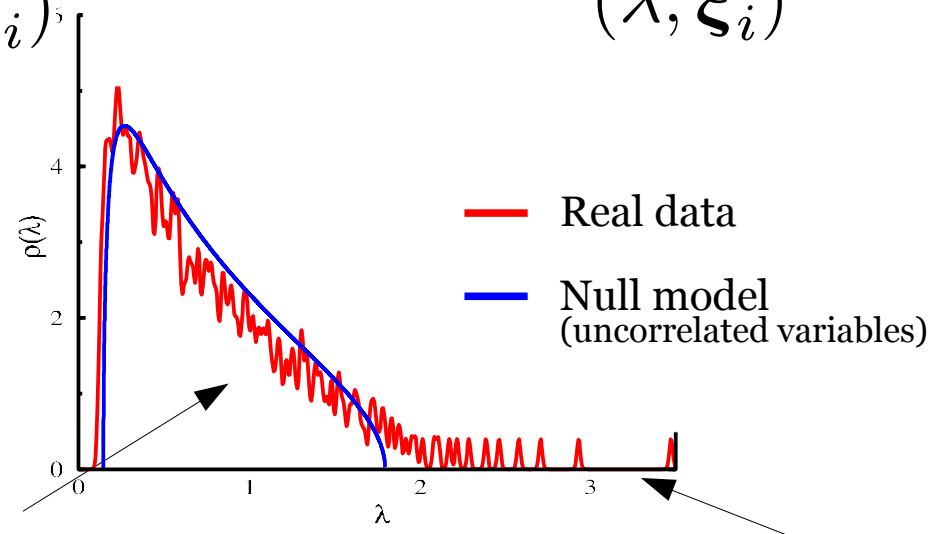
(Measured) $\hat{C}$ $(\hat{\lambda}, \hat{\boldsymbol{\xi}}_i)$ → (True) C $(\lambda, \boldsymbol{\xi}_i)$



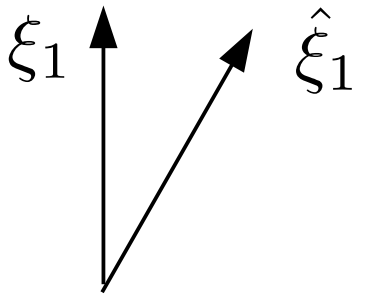
(Only noise ?)
Bulk eigenvalues

Signal

What about eigenvectors ?

Estimation of true eigenvectors from the empirical ones

Scalar product between the largest true and empirical eigenvectors



Estimation of true eigenvectors from the empirical ones

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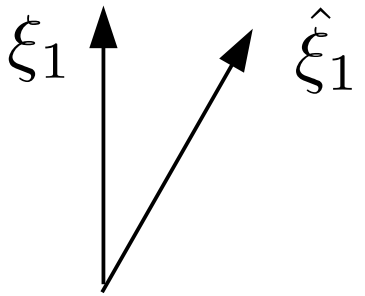
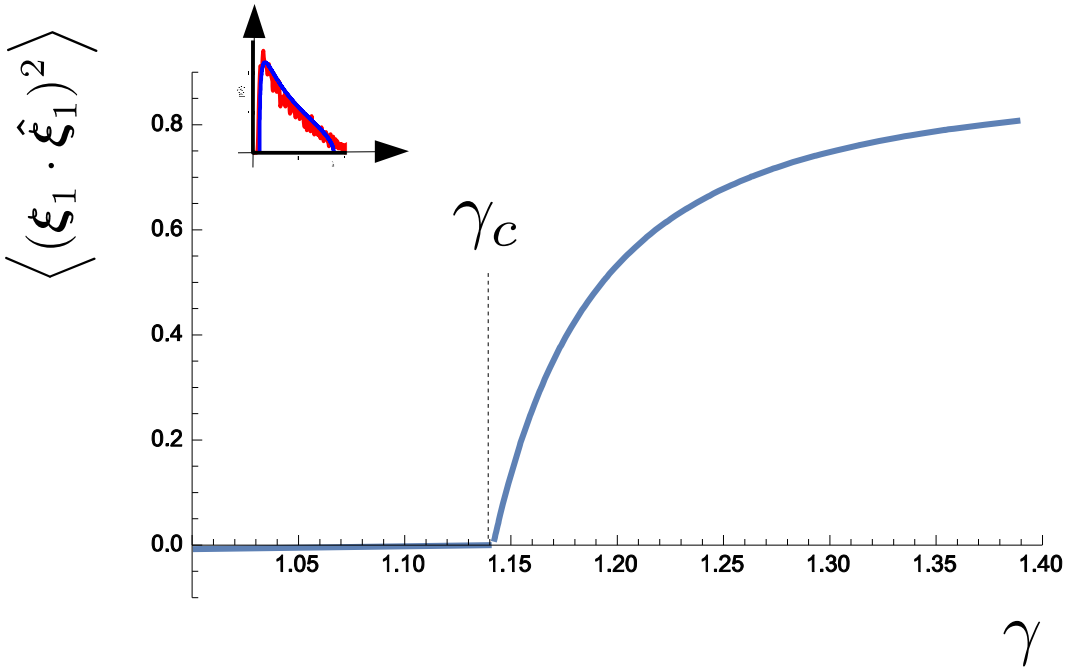
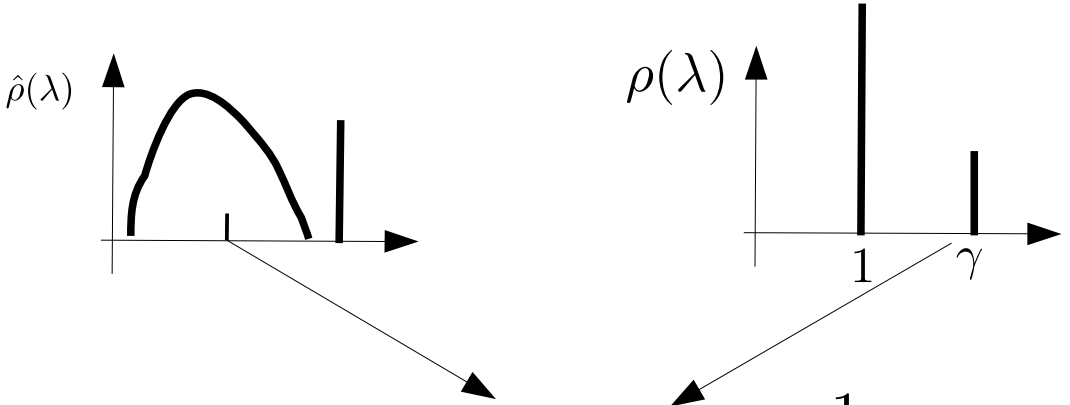




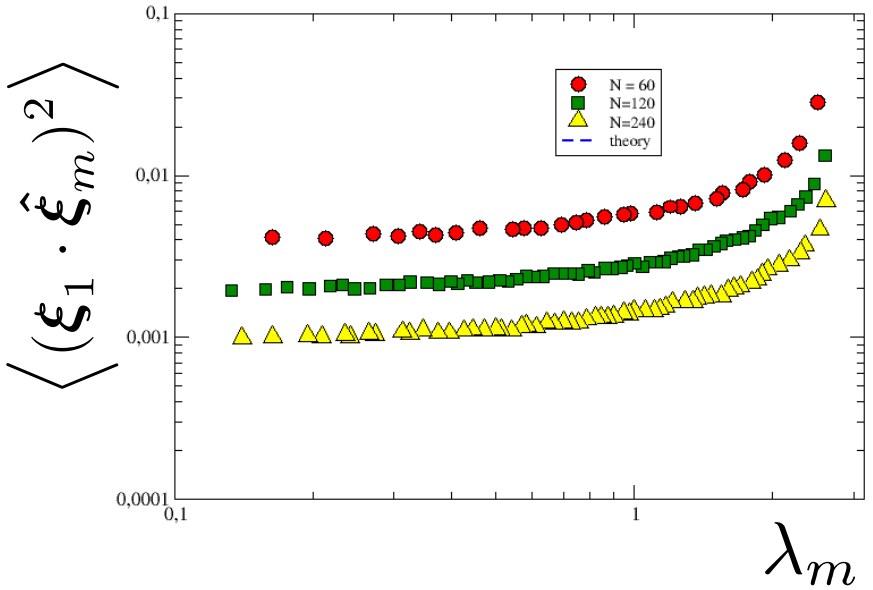
$$\left\langle (\boldsymbol{\xi}_1 \cdot \hat{\boldsymbol{\xi}}_1)^2 \right\rangle \equiv w_1^2 = \begin{cases} 0 & \gamma < 1 + \sqrt{r} \\ \dfrac{(\gamma - 1)^2 - r}{(\gamma - 1)(\gamma + r - 1)} & \gamma > 1 + \sqrt{r} \end{cases}$$

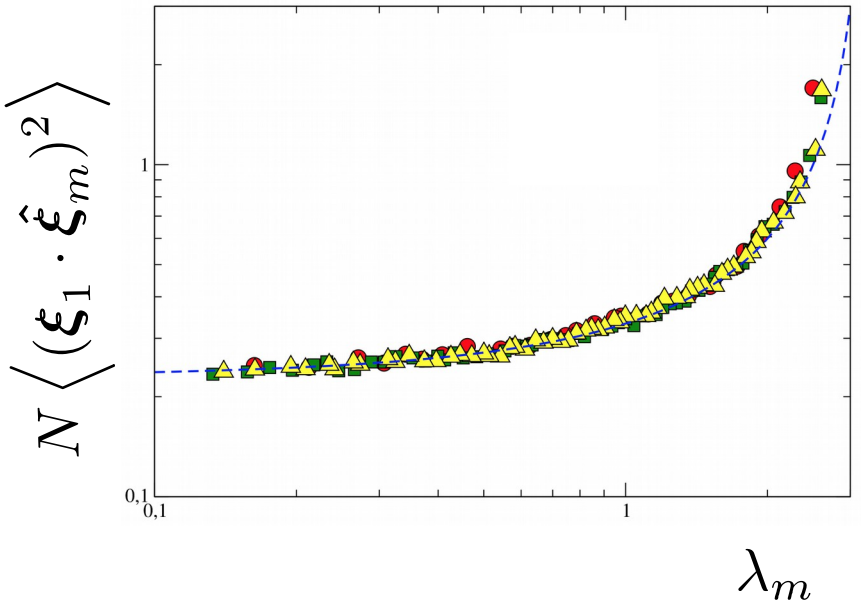
Estimation of true eigenvectors from the empirical ones

Scalar product between the largest true and bulk eigenvectors

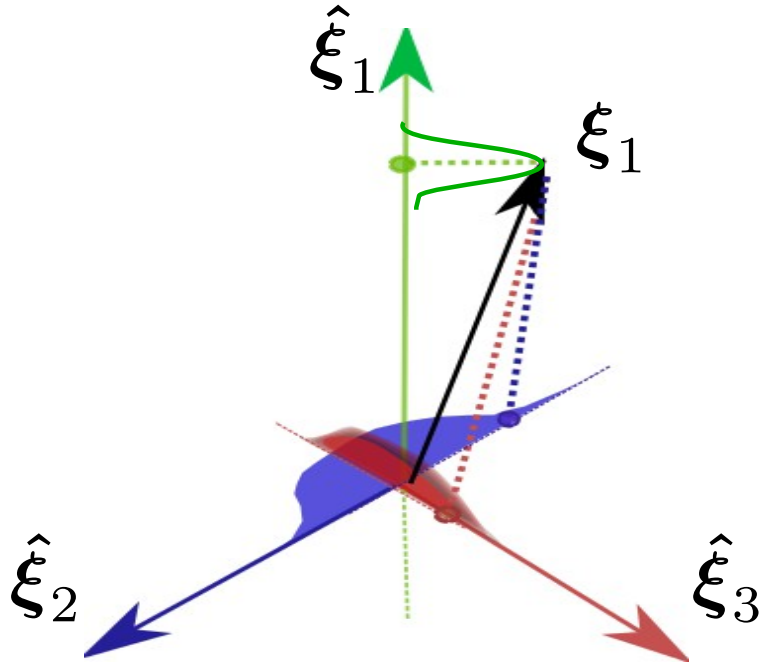


$$(\hat{\boldsymbol{\xi}}_m \cdot \boldsymbol{\xi}_1) \sim \frac{1}{\sqrt{N}}$$





Summary on empirical eigenvectors



$$\left\langle |\boldsymbol{\xi}_1 \cdot \hat{\boldsymbol{\xi}}_1|^2 \right\rangle = \mathcal{O}(1) \qquad \left\langle |\boldsymbol{\xi}_1 \cdot \hat{\boldsymbol{\xi}}_{m>1}|^2 \right\rangle = \mathcal{O}(N^{-1})$$

Two questions:

Is it possible to calculate analytically the scalar products ?

Is there information stored in bulk empirical eigenvectors ?

Part 1: How to calculate the scalar products?

$$g(\lambda,\hat{\lambda}) = \lim_{N\to\infty} \frac{1}{N}\mathrm{Tr}\left[\left(\lambda - C\right)^{-1} \cdot \left\langle\left(\hat{\lambda} - \hat{C}\right)^{-1}\right\rangle\right]$$

Projection on the eigenvectors

$$\begin{cases} \left(\lambda - C\right)^{-1}_{ij} = \sum_m (\lambda - \lambda_m)^{-1} \xi_{m,i}\, \xi_{m,j} \\ \left(\hat{\lambda} - \hat{C}\right)^{-1}_{ij} = \sum_m (\hat{\lambda} - \hat{\lambda}_m)^{-1} \hat{\xi}_{m,i}\, \hat{\xi}_{m,j} \end{cases}$$

Continuous limit of the spectrum

$$\hat{\rho}(\hat{\mu}) = \frac{1}{N}\sum_m \left\langle \delta(\hat{\mu} - \hat{\lambda}_m)\right\rangle$$

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Continuous limit of the spectrum

$$\hat{\rho}(\hat{\mu}) = \frac{1}{N}\sum_m \left\langle \delta(\hat{\mu}-\hat{\lambda}_m)\right\rangle$$

$$g(\lambda,\hat{\lambda}) = \int d\mu\, d\hat{\mu}\, \frac{\rho(\mu)}{\lambda-\mu}\,\frac{\hat{\rho}(\hat{\mu})}{\hat{\lambda}-\hat{\mu}}\, W^2(\mu,\hat{\mu})$$

$$N\left\langle (\hat{\xi}_{\hat{\mu}}\cdot\xi_\mu)^2\right\rangle$$

$$\mathrm{Im}\frac{1}{\lambda-\mu-i\epsilon} = \pi\delta(\lambda-\mu)$$

$$W^2(\lambda,\hat{\lambda}) = \frac{g(\lambda+i\epsilon,\hat{\lambda}+i\epsilon) - g(\lambda+i\epsilon,\hat{\lambda}-i\epsilon)}{2\pi\,\rho(\lambda)\,\hat{\rho}(\hat{\lambda})}$$

An extension of the Edwards-Jones technique

SF Edwards and RC Jones Journal of Physics A: Mathematical and General, 9(10), 1595 (1976)

$$\left\langle \mathrm{Tr}((\lambda - C)^{-1}(\hat{\lambda} - \hat{C})^{-1}) \right\rangle = \left\langle \int \mathcal{D}Y\mathcal{D}Z(Y \cdot Z)^2 \exp(-\frac{1}{2}(Y(\lambda - C)Y^{\dagger} + Z(\hat{\lambda} - \hat{C})Z^{\dagger}) \right\rangle$$

$$\langle ... \rangle \propto \int \prod_{i,t} dx_{i,t} \exp\left(-\frac{1}{2} x_{i,t} C_{ij}^{-1} x_{j,t}\right) \qquad \hat{C}_{ij} = \frac{1}{M} \sum_{t} x_{i,t} x_{j,t}$$

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Gaussian integrals

Replica-based calculation

Saddle point equation

$$N \to \infty \quad M \to \infty \quad r = \frac{N}{M}$$

$$g(\lambda, \hat{\lambda}) = \frac{2}{N} \int d\phi \; d\hat{\phi} \frac{\partial}{\partial \eta}\bigg|_{\eta=0} e^{-N S_{\eta}(\phi, \hat{\phi})}$$

$$S_{\eta}(\phi, \hat{\phi}) = \frac{1}{2}\left(\int d\mu \rho(\mu) \ln((\lambda - \mu)(\hat{\lambda} - \mu\,\hat{\phi}) - \eta) + \frac{1}{r} \ln(1 - r\phi) + \phi\,\hat{\phi} \right)$$

Equations for the densities

O. Ledoit and S. Péché, Probability Theory and Related Fields 151.1-2 (2011).
JW Silverstein Journal of Multivariate Analysis, 55(2), (1995)

$$g(\lambda, \hat{\lambda}) = \int d\mu \frac{\rho(\mu)}{(\lambda - \mu)(\hat{\lambda} - \mu\,\hat{\phi}^*)}$$

Saddle point equation

$$\frac{\hat{\phi}^* - 1}{r\hat{\phi}^*} = \int d\mu \frac{\rho(\mu)}{(\hat{\lambda} - \hat{\mu}\hat{\phi}^*)}$$

$$\lambda \gg 1 \quad \Longrightarrow \quad \hat{\rho}(\hat{\lambda}) = \frac{1}{\pi}\mathrm{Im} \int d\mu \frac{\rho(\mu)}{(\hat{\lambda} - \mu\,\hat{\phi}^*)}$$

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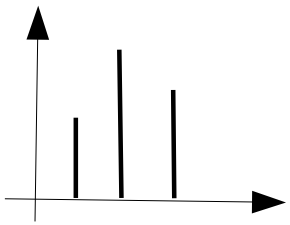
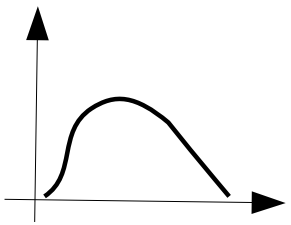
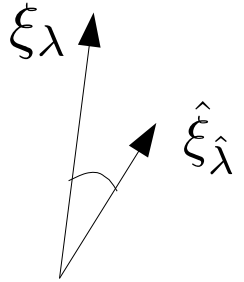
Input $\rho(\lambda)$ ⟹ **Noise dressing** $\hat{\rho}(\hat{\lambda})$ ⟹ **Scalar products** $W^2(\lambda,\hat{\lambda})$





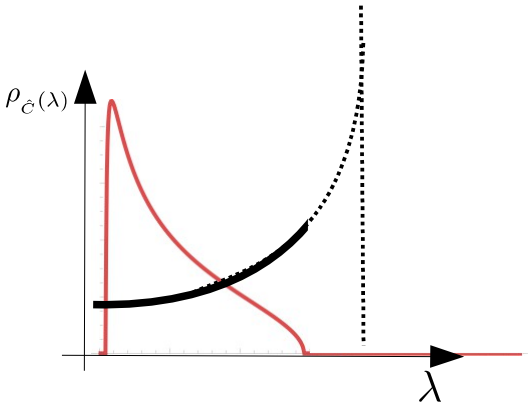


The transition from eigenvectors point of view

$$\rho(\lambda) = (1-\alpha)\delta(\lambda-1) + \alpha\delta(\lambda-\gamma)$$

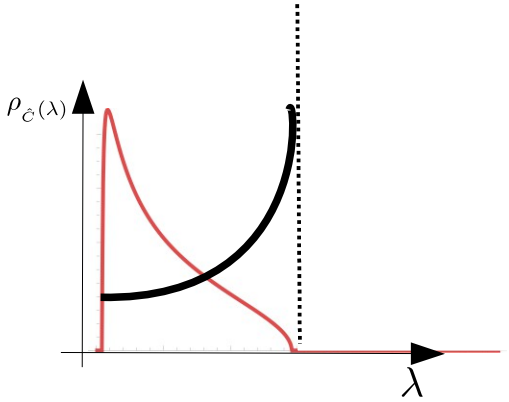
$$W^2(\gamma,\hat{\lambda}) = \frac{\gamma r}{\hat{\lambda} + \gamma(\gamma - \hat{\lambda} + r - 1)} \qquad \text{(with a divergence in } \hat{\lambda} = \gamma + \frac{r\gamma}{\gamma - 1}\text{)}$$

$\gamma < \gamma_c$

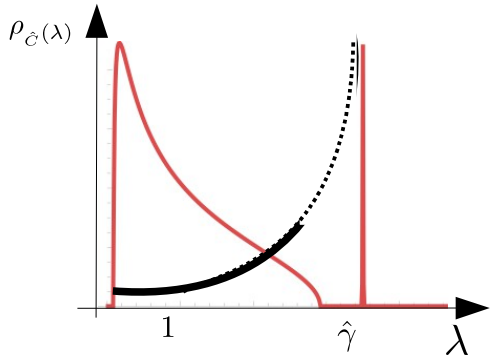


$$\int_{\lambda_-}^{\lambda_+} W^2(\gamma,\hat{\lambda})\rho(\hat{\lambda})d\hat{\lambda} = 1$$

$\gamma \equiv \gamma_c$



$\gamma > \gamma_c$



$$\int_{\lambda_-}^{\lambda_+} W^2(\gamma,\hat{\lambda})\rho(\hat{\lambda})d\hat{\lambda} = 1 - W_1^2$$

Estimation of the principal component

Inverse problem : How to estimate $\boldsymbol{\xi}_1$?

$$\boldsymbol{\xi}_1^{(est)} = w_1 \hat{\boldsymbol{\xi}}_1 + \sum_m^N w_m \hat{\boldsymbol{\xi}}_m$$

Estimation of the principal component

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The *ws* are Gaussian variables (fairly verified for large *N*)

$$P\left(\boldsymbol{\xi}_1^{(est)} | \{\hat{\xi}\}\right)$$

"standard approach"

$$\left\langle \boldsymbol{\xi}_1^{(est)} \right\rangle = \langle w_1 \rangle \, \hat{\boldsymbol{\xi}}_1$$

Main limitation: reconstruction impossible for weak signals

$$\gamma < \gamma_c \longrightarrow \langle w_1 \rangle = 0$$

One question left:

Is it possible to calculate analytically the scalar products ?

YES !!

Is there information stored in bulk empirical eigenvectors ?

The mutual information

$$I(x;y) = \left\langle \log\left(\frac{P(x,y)}{P(x)P(y)}\right)\right\rangle$$

It measures how much knowing X reduces uncertainty about Y

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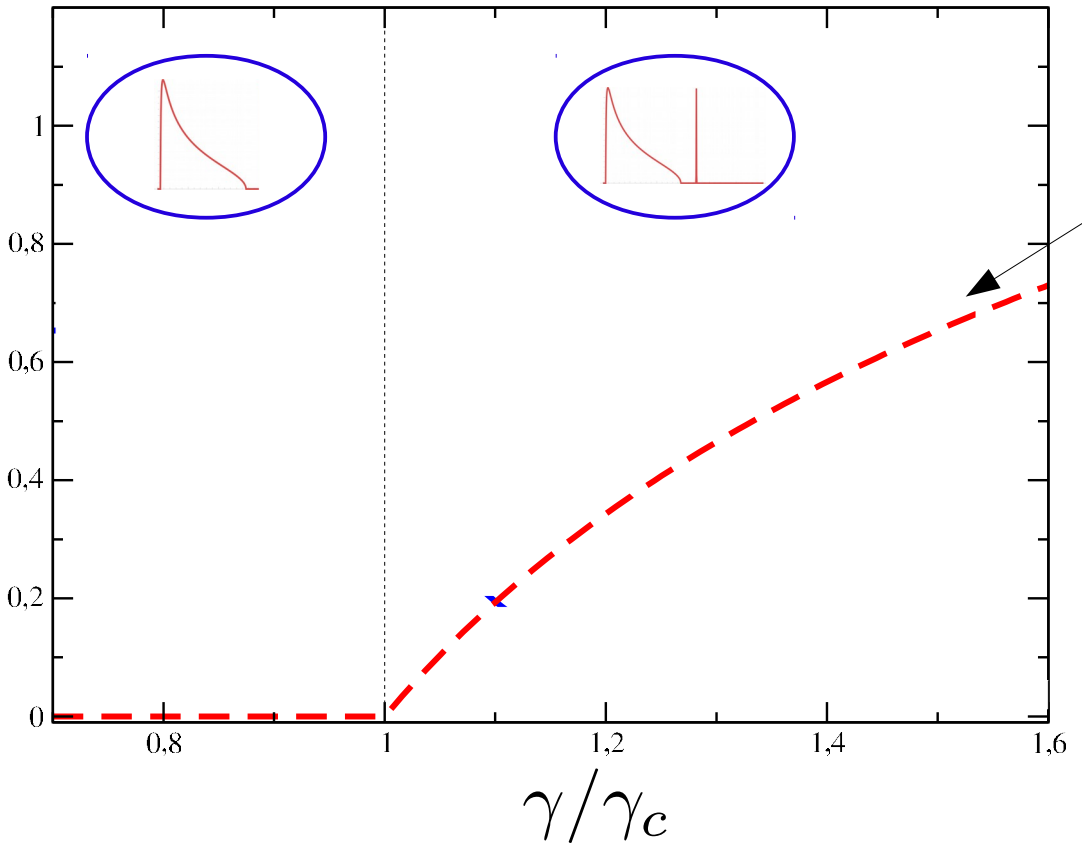

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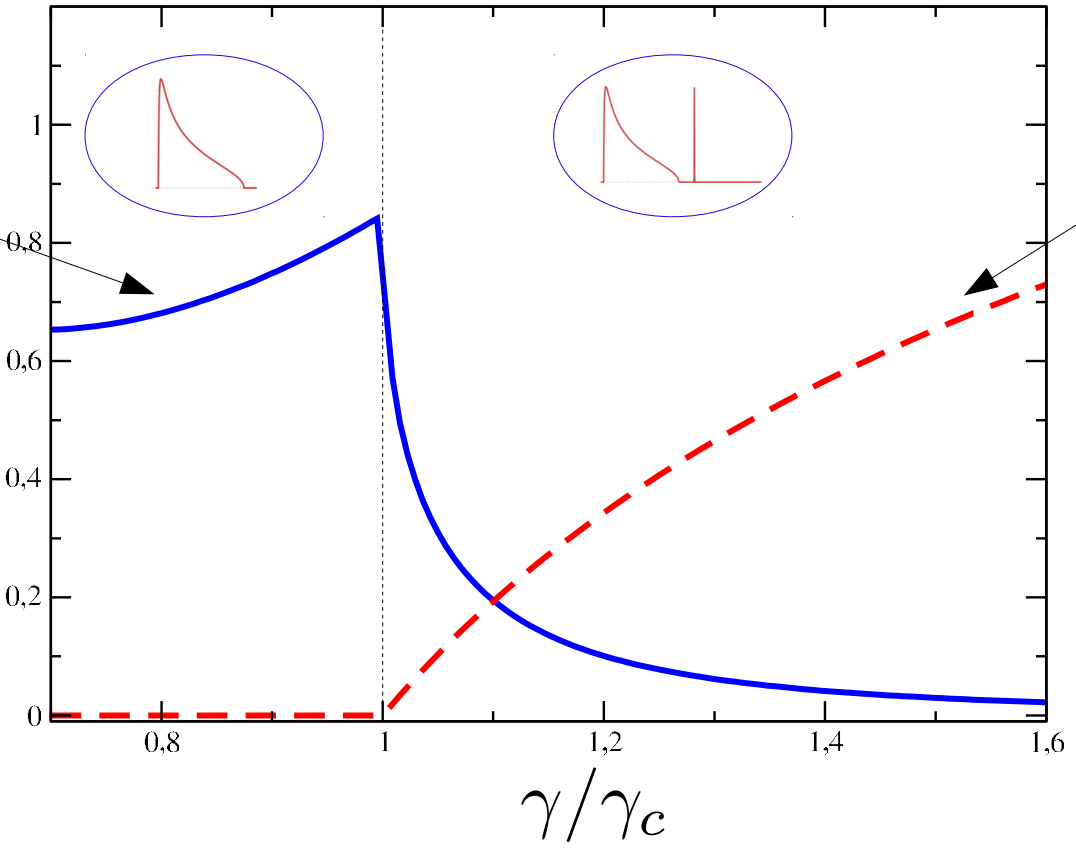
It measures how much knowing X reduces uncertainty about Y

$I\left(\boldsymbol{\xi}_1;\{\hat{\boldsymbol{\xi}}_{m\neq 1}\}\right)$

Information related to bulk eigenvectors



$I\left(\boldsymbol{\xi}_1;\hat{\boldsymbol{\xi}}_1\right)$

Information related to the first eigenvector

Three questions:

Is it possible to calculate analytically the scalar products ?

YES !!

Is there information stored in bulk empirical eigenvectors ?

YES !!

Is it possible to exploit this information
to improve the noise undressing procedure ?

An application: reconstruction of localized eigenvectors

discrete approximation : $w_m \to \sqrt{\langle w_m^2 \rangle}\, \sigma_m \equiv \overline{w}_m \sigma_m$

(± 1)

$$\boldsymbol{\xi}_1^{(est)}(\boldsymbol{\sigma}) = \overline{w}_1 \hat{\boldsymbol{\xi}}_1 + \sum_m^N \overline{w}_m \hat{\boldsymbol{\xi}}_m \sigma_m$$

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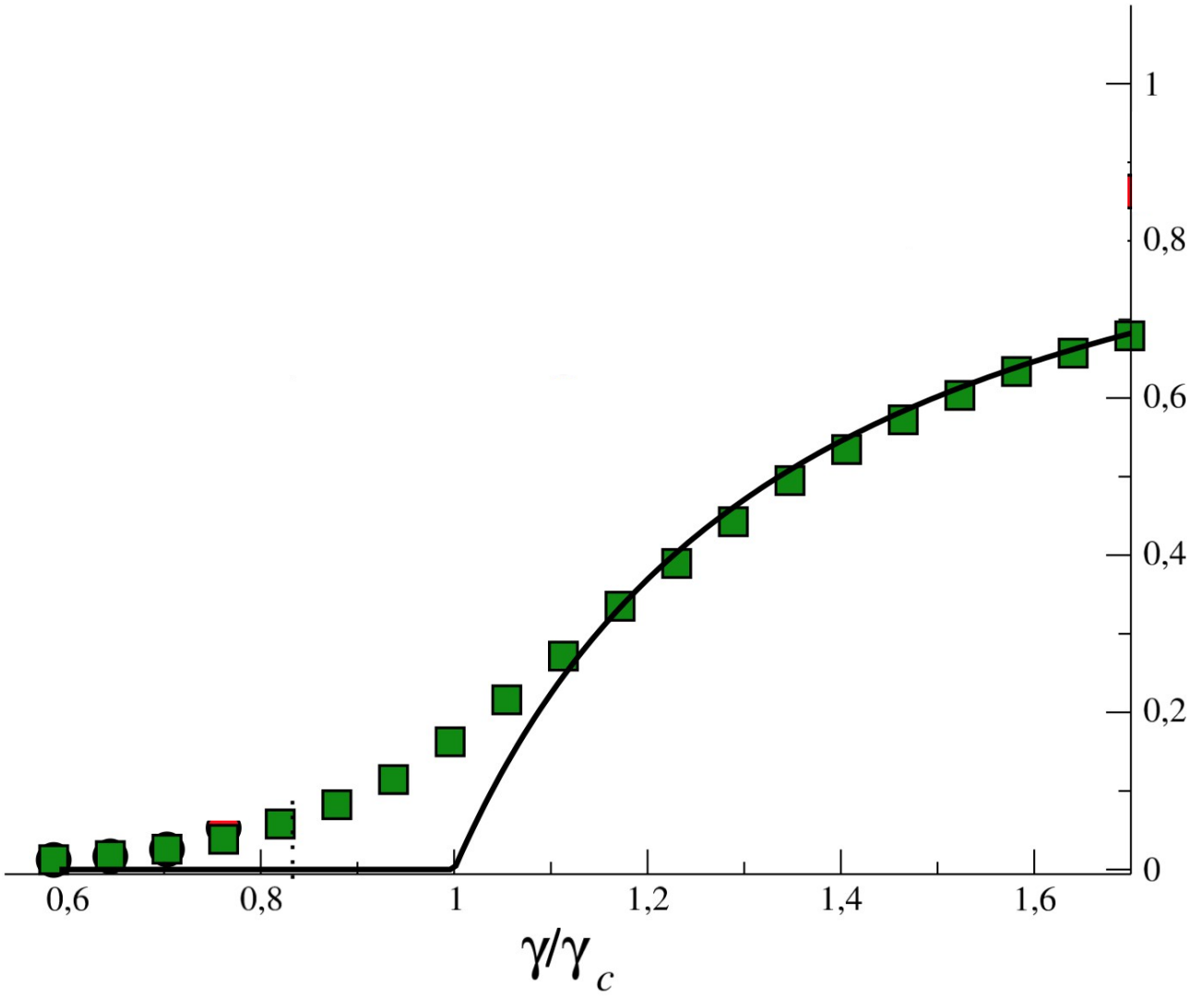
The estimation problem is mapped onto an Ising model

$$E(\boldsymbol{\sigma}) = -\sum_i \left(\xi_{1,i}^{(est)}(\boldsymbol{\sigma}) \right)^4$$

Estimate: finding $\overline{\boldsymbol{\sigma}}$ for which $E(\overline{\boldsymbol{\sigma}})$ attains its minimal value

An application: reconstruction of localized eigenvectors

Montecarlo results (simulated annealing)



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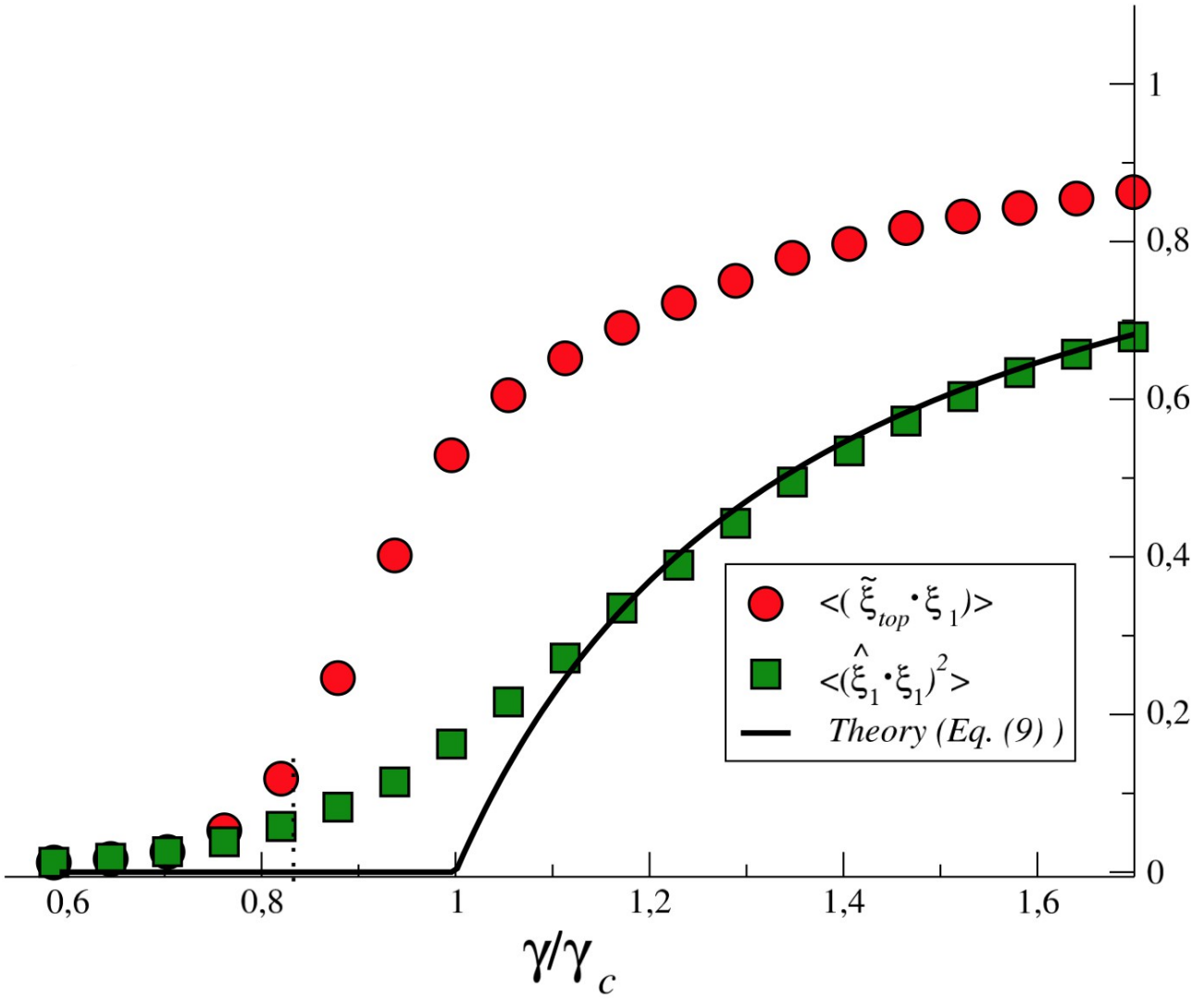

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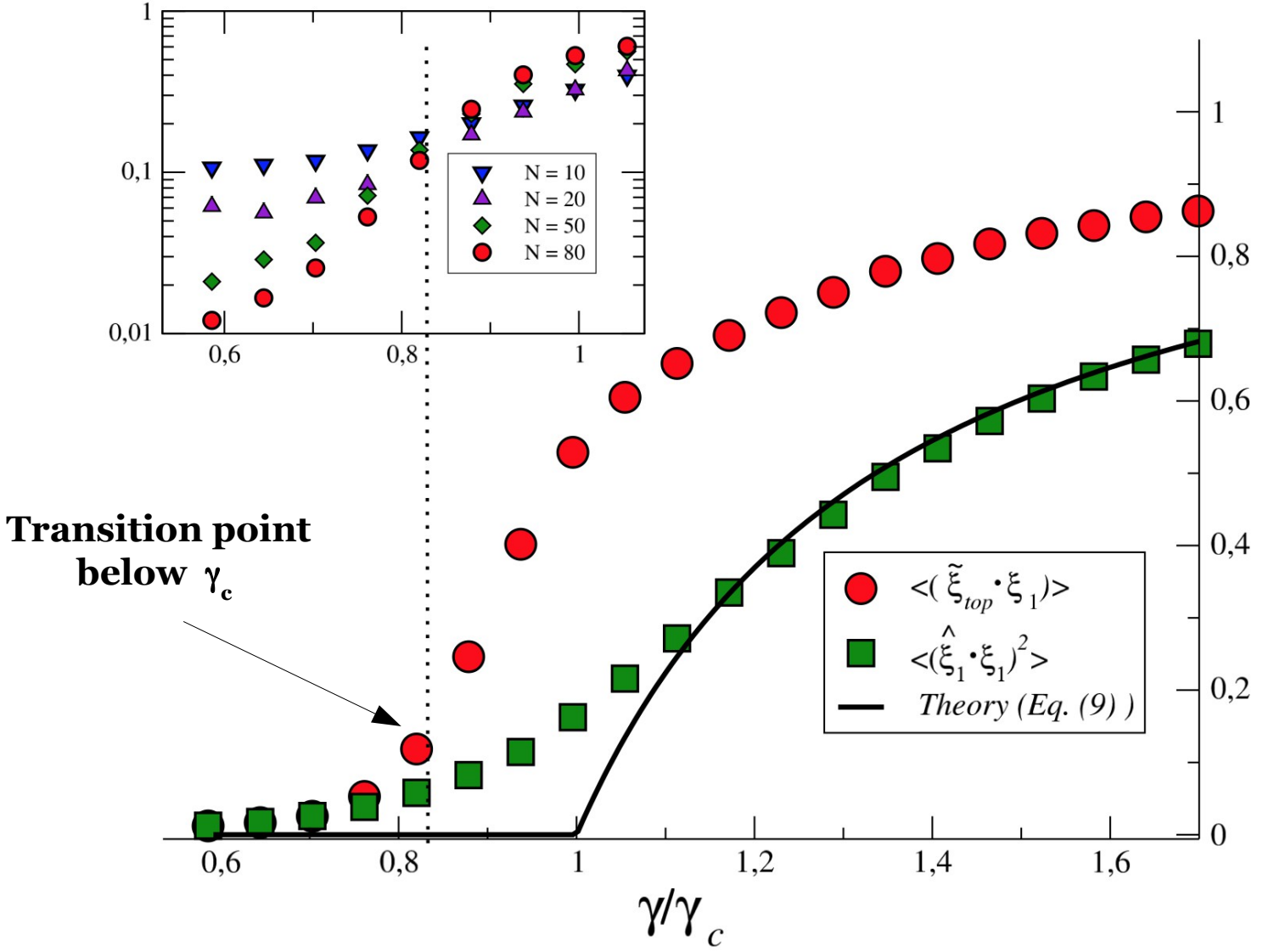


Conclusions and Perspectives

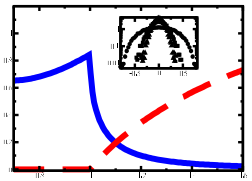
R. Monasson and D. Villamaina (arXiv:1503.00287)

General formalism for the calculation of the scalar products between the empirical eigenvectors and the true ones of a correlation matrix

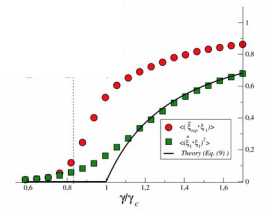
$$\mathrm{Tr}\left[(\lambda - C)^{-1} \cdot \langle(\hat{\lambda} - \hat{C})^{-1}\rangle\right]$$

Large deviations ?

Importance of minor components for the reconstruction of eigenvectors



Analogy between spin models and estimations of localized eigenvectors



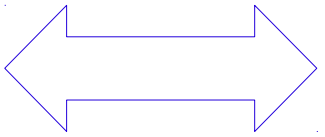
Smarter algorithms ?

Perspectives: analogy with the Hopfield model

Hopfield

$$m^\mu = \sum_j \xi_j^\mu \sigma_j$$

$$H_{opf}(\boldsymbol{\sigma}) = -\frac{1}{2}\sum_\mu (m^\mu)^2$$



Eigenvector estimation

$$m^i = \sum_m \overline{w}_m \hat{\xi}_{m,i} \sigma_m$$

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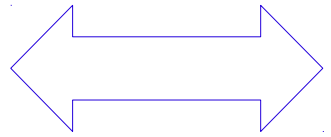

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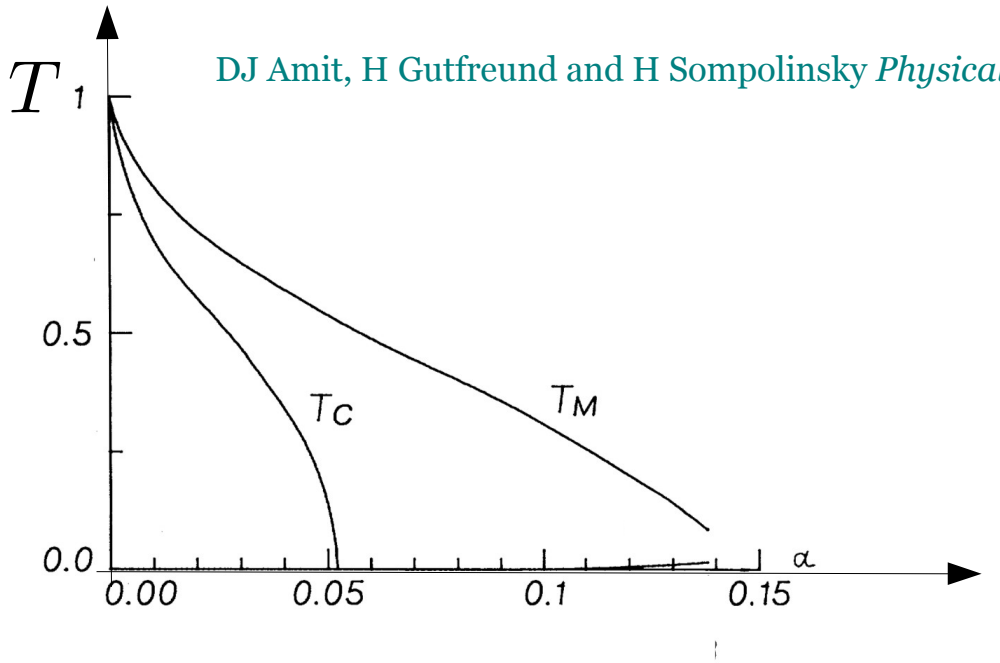

DJ Amit, H Gutfreund and H Sompolinsky *Physical Review Letters* 55, 1530 (1985)

$$\alpha = \frac{\text{\# of patterns}}{\text{\# of spins}}$$

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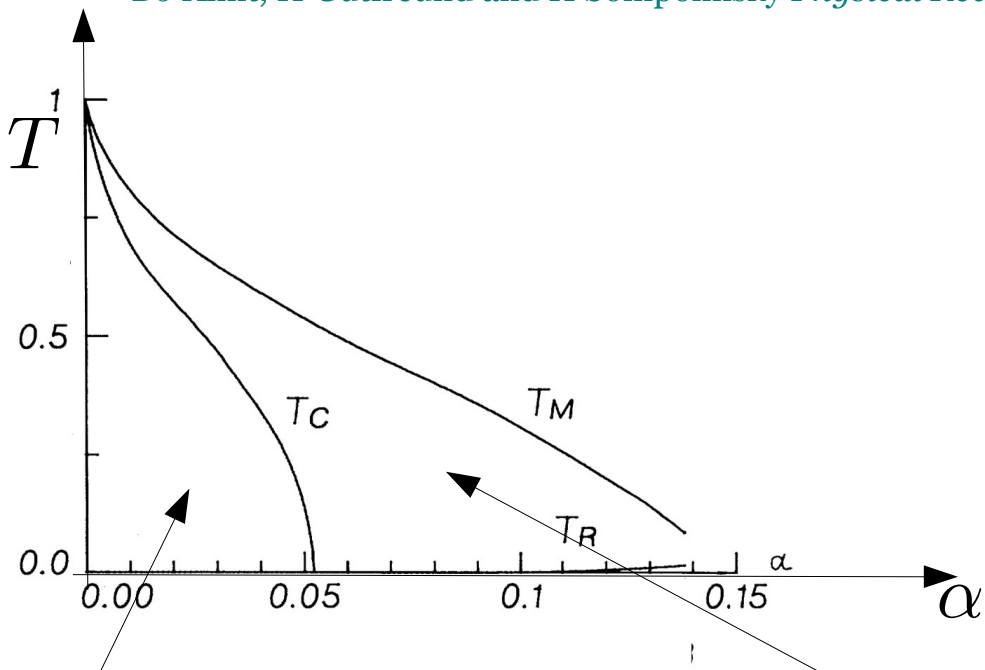

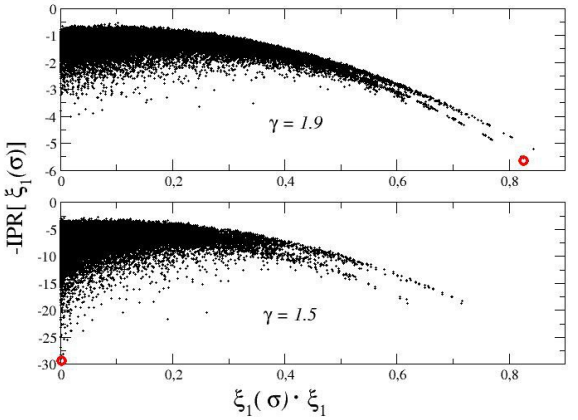

$$\alpha = \frac{\text{\# of patterns}}{\text{\# of spins}}$$

High γ

(small quenched disorder)

Small γ

(high quenched disorder)

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