Spectra of Sample Auto-Covariance Matrices Derived from Time Series

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Outline

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Sample Auto-Covariance Matrices of Time Series

- Auto-covariance matrix of stationary stochastic process $(x_t)_{t\in\mathbb{Z}}$:

$$C_{ij} = \frac{1}{M}\sum_{t=1}^{M} x_{i+t}x_{j+t} = \frac{1}{M}(XX^T)_{ij} \ .$$

  Here $X = (x_{it})$ is $N \times M$ matrix with entries $x_{it} = x_{i+t}$.
  Expect finite sample fluctuation around mean

$$C_{ij} = \langle x_i x_j \rangle \pm O(1/\sqrt{M}) = \bar{C}(i-j) \pm O(1/\sqrt{M})$$

  $\Rightarrow$ C is randomly perturbed Toeplitz matrix.

- Spectrum of C as $N \to \infty$, $M \to \infty$ @ fixed $\alpha = N/M$?
  Known result as $\alpha \to 0$: Szegö's Theorem

$$\rho_0(\lambda) = \int_0^{2\pi} \frac{\mathrm{d}q}{2\pi}\,\delta(\lambda - \hat{C}(q))$$

Outline

Comparison with Wishart-Laguerre Ensemble

- Empirical covariances for N data, evaluated on the basis of M measurements for each variable. Express in terms of $N \times M$ matrices $X = (x_{it})$ as

$$C_{ij} = \frac{1}{M} \sum_{t=1}^{M} x_{it} x_{jt} = \frac{1}{M} (XX^T)_{ij} \ .$$

  Expect finite sample fluctuation around mean. For i.i.d. entries x_{it}

$$C_{ij} = \langle x_i x_j \rangle \pm O(1/\sqrt{M}) = \delta_{ij} \pm O(1/\sqrt{M})$$

- Spectrum of C as $N \to \infty$, $M \to \infty$ @ fixed $\alpha = N/M$?
  $\Rightarrow$ Marčenko Pastur-Law

$$\rho_\alpha(\lambda) = \left(1 - \frac{1}{\alpha}\right)_+ \delta(\lambda) + \frac{\sqrt{4\alpha - (\lambda - (1+\alpha))^2}}{2\pi\alpha\lambda} \, \mathbb{1}_{\lambda \in [\lambda_-, \lambda_+]}$$

Principal Differences

- Rows of X for the auto-covariance problem are sections of a single time series $(x_t)_{t\in\mathbb{Z}}$

$$X = \begin{pmatrix} x_1 & x_2 & x_3 & \dots & x_M \\ x_2 & x_3 & x_4 & \dots & x_{1+M} \\ \vdots & & & \ddots & \vdots \\ x_N & x_{N+1} & x_{N+2} & \dots & x_{N+M} \end{pmatrix}$$

- Number of random variables in the problem is $O(N)$, rather than $O(N^2)$ as in the Wishart Laguerre ensemble.
- Extensive body of knowledge about the Wishart-Laguerre ensemble and its variants (applications in multivariate statistics, signal-processing, finance, ...)

Principal Differences (contd.)

- Comparatively little is known about the auto-covariance problem
  - Existence of limiting spectral densityfor auto-covariance matrices of moving average processes with i.i.d. driving (Basak et. al 2011)
  - Universality of results: independence of statistics of i.i.d. driving (numerical, Sen 2010)
  - Existence of limiting spectral density for random Toeplitz matrices with i.i.d. entries (Bryc 2007)

Outline

Spectral Density and Resolvent

- Spectral density of sample covariance matrix from resolvent

$$\rho(\lambda) = \lim_{N\to\infty} \frac{1}{\pi N} \mathrm{Im}\ \mathrm{Tr} \left\langle \left[\lambda_\varepsilon \mathbf{1} - C\right]^{-1} \right\rangle , \qquad \lambda_\varepsilon = \lambda - \mathrm{i}\varepsilon$$

- Express as (S F Edwards & R C Jones, JPA, 1976)

$$\begin{aligned} \rho_\alpha(\lambda) &= \lim_{N\to\infty} \frac{1}{\pi N}\ \mathrm{Im}\ \frac{\partial}{\partial\lambda}\ \mathrm{Tr} \left\langle \ln \left[\lambda_\varepsilon \mathbf{1} - C\right] \right\rangle \\ &= \lim_{N\to\infty} -\frac{2}{\pi N}\ \mathrm{Im}\ \frac{\partial}{\partial\lambda} \left\langle \ln Z_N \right\rangle , \end{aligned}$$

where Z_N is a Gaussian integral:

$$Z_N = \int \prod_{k=1}^{N} \frac{\mathrm{d}u_k}{\sqrt{2\pi/\mathrm{i}}}\ \exp\left\{ -\frac{\mathrm{i}}{2} \sum_{k,\ell} u_k (\lambda_\varepsilon \delta_{k\ell} - C_{k\ell}) u_\ell \right\}$$

Outline

Performing the Average

- Standard Approach – Replica Method

$$\left\langle \ln Z_N \right\rangle = \lim_{n\to 0} \frac{1}{n} \ln \left\langle Z_N^n \right\rangle$$

- For integer n, Z_N^n is partition function of n identical copies of the system (n-th power of Gaussian integral)
- Experience: final result has structure of replica-symmetric high-temperature solution $\Leftrightarrow$ annealed calculation ($n = 1$). $\langle \ln Z_N \rangle \simeq \ln \langle Z_N \rangle \Rightarrow$ Do annealed calculation from the start

$$\langle Z_N \rangle = \left\langle \int \prod_k \frac{\mathrm{d}u_k}{\sqrt{2\pi/\mathrm{i}}} \exp\left\{ -\frac{\mathrm{i}}{2}\lambda_\varepsilon \sum_k u_k^2 + \frac{\mathrm{i}}{2} \sum_{k\ell} C_{k\ell} u_k u_\ell \right\} \right\rangle ,$$

Performing the Average (contd.)

- Insert definition of C

$$\langle Z_N \rangle = \left\langle \int \prod_k \frac{\mathrm{d}u_k}{\sqrt{2\pi/\mathrm{i}}} \exp\left\{ -\frac{\mathrm{i}}{2}\lambda_\varepsilon \sum_k u_k^2 + \frac{\mathrm{i}}{2}\alpha \sum_{i=1}^{M} z_i^2 \right\} \right\rangle$$

- with disorder dependence of Z_N only through the M variables

$$z_i = \frac{1}{\sqrt{N}} \sum_{k=1}^{N} x_{k+i} u_k \ , \quad 1 \le i \le M \ .$$

- By CLT (for weakly dependent rv's) normally distributed for large M with

$$\langle z_i \rangle = 0 \ , \qquad \langle z_i z_j \rangle = \frac{1}{N} \sum_{k\ell} \langle x_{k+i} x_{\ell+j} \rangle u_k u_\ell \equiv Q_{ij}$$

and Q given in terms of true process auto-covariance

$$Q_{ij} = \langle z_i z_j \rangle = \frac{1}{N} \sum_{k\ell} \bar{C}(i-j+k-\ell)\, u_k u_\ell$$

Exploiting Szegö's Theorem for Spectral Sums

- $\{z_i\}$ average is Gaussian

$$\langle Z_N \rangle = \int \prod_k \frac{\mathrm{d}u_{ka}}{\sqrt{2\pi/\mathrm{i}}} \exp\left\{ -\frac{\mathrm{i}}{2}\lambda_\varepsilon \sum_k u_k^2 - \frac{1}{2}\ln\det(\mathbb{1} - \mathrm{i}\alpha Q) \right\}$$

- Q is a Toeplitz matrix. $\Rightarrow$ evaluate $\ln\det(\mathbb{1} - \mathrm{i}\alpha Q)$ using
- **Szegö's theorem**: Given an $N \times N$ Toeplitz matrix A with elements $A_{ik} = a(i-k)$, where $a = (a(n)) \in \ell_1(\mathbb{Z})$. Then the spectral density has a weak limit

$$\rho_N(\lambda) = \frac{1}{N}\sum_{i=1}^{N} \delta(\lambda - \lambda_i) \xrightarrow{w} \int_{-\pi}^{\pi} \frac{\mathrm{d}q}{2\pi} \delta(\lambda - \hat{a}(q)) \ ,$$

as $N \to \infty$, where $\hat{a}(q)$ is called the 'symbol', and is nothing but the Fourier transform of a

$$\hat{a}(q) = \sum_{n=-\infty}^{\infty} a(n) \mathrm{e}^{\mathrm{i}qn} \ .$$

- Szegö (keeping track of finite-M finite-N expressions)

$$\ln\det(\mathbb{1} - \mathrm{i}\alpha Q) \sim \sum_{\mu=-(M-1)/2}^{(M-1)/2} \ln\Big(1 - \mathrm{i}\alpha Q_\mu\Big)$$

where

$$Q_\mu = \frac{1}{N}\sum_{k\ell} \hat{C}(q_\mu)\mathrm{e}^{-\mathrm{i}q_\mu(k-\ell)}\, u_k u_\ell = \hat{C}(q_\mu)|\hat{u}(q_\mu)|^2 \equiv Q(q_\mu)$$

with

$$\hat{u}(q_\mu) = \frac{1}{\sqrt{N}}\sum_{k=1}^{N} \mathrm{e}^{\mathrm{i}q_\mu k}\, u_k \ , \quad q_\mu = \frac{2\pi}{M}\mu$$

- Enforce Q_μ definitions using δ-functions. $\Rightarrow$ Get Gaussian u_k-integrals.

$$\begin{aligned}\langle Z_N\rangle \quad = \quad & \int \prod_{\mu=0}^{(M-1)/2} \frac{\mathrm{d}\hat{Q}_\mu \mathrm{d}Q_\mu}{2\pi}\, \exp\Big\{ - \sum_{\mu=0}^{(M-1)/2} \mathrm{i}\hat{Q}_\mu Q_\mu \\ & - \sum_{\mu=0}^{(M-1)/2} \ln(1 - \mathrm{i}\alpha Q_\mu) - \frac{1}{2}\ln\det(\lambda_\varepsilon \mathbb{1} - R)\Big\}\end{aligned}$$

- Do Q_μ integrals using residues; gives R matrix elements

$$R_{k\ell} = \frac{2}{M} \sum_{\mu=0}^{(M-1)/2} \hat{Q}_\mu \hat{C}(q_\mu) \cos(q_\mu(k-\ell)) \ ,$$

with exponentially distributed $\hat{Q}_\mu$.

- R is Toeplitz matrix. Evaluate $\ln\det(\lambda_\varepsilon \mathbb{1} - R)$ using Szegö,

$$\ln\det(\lambda_\varepsilon \mathbb{1} - R) \sim \sum_{\nu=-(N-1)/2}^{(N-1)/2} \ln\left(\lambda_\varepsilon - R_\nu\right)$$

with

$$R_\nu = \sum_{\mu=0}^{(M-1)/2} \hat{Q}_\mu \hat{C}(q_\mu) S_{\nu\mu} \equiv R(p_\nu) \ , \qquad p_\nu = \frac{2\pi}{N}\nu$$

and

$$S_{\nu\mu} := \frac{1}{M} \sum_{\sigma=\pm 1} \frac{\sin(N(p_\nu - \sigma q_\mu)/2)}{\sin((p_\nu - \sigma q_\mu)/2)}$$

- Enforce R_ν definitions via δ-functions

$$\langle Z_N \rangle = \left\langle \int \prod_{\nu=0}^{(N-1)/2} \left\{ \frac{\mathrm{d}\hat{R}_\nu \mathrm{d}R_\nu}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}\hat{R}_\nu R_\nu}}{\lambda_\varepsilon - R_\nu} \, \mathrm{e}^{\mathrm{i}\hat{R}_\nu \sum_{\mu=0}^{(M-1)/2} \hat{Q}_\mu \hat{C}(q_\mu) S_{\nu\mu}} \right\} \right\rangle_{\{\hat{Q}_\mu\}}$$

- Do R_ν integrals using residues. Gives

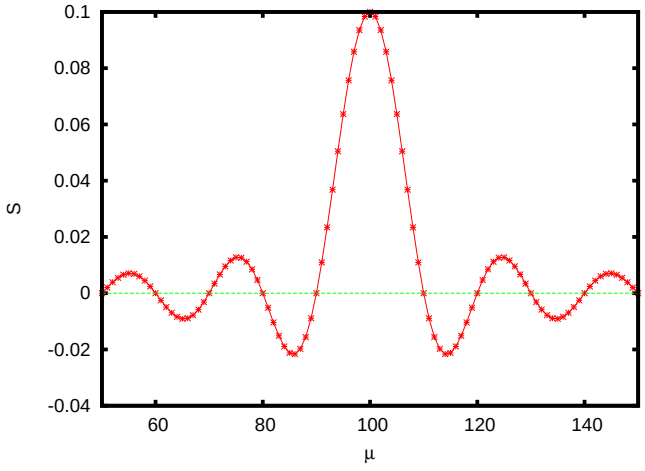
$$\langle Z_N \rangle = \left\langle \prod_{\nu=0}^{(N-1)/2} F_\nu \right\rangle_{\{Q_\mu\}}$$

with

$$F_\nu = \mathrm{i} \int_0^\infty \mathrm{d}\hat{R}_\nu \, \mathrm{e}^{-\mathrm{i}\hat{R}_\nu \left(\lambda_\varepsilon - \sum_\mu \hat{Q}_\mu \hat{C}(q_\mu) S_{\nu\mu} \right)}$$

Decoupling & Decorrelation Approximations

- S-kernel couples $\hat{Q}_\mu$ for $\mu \in I_\nu = \{\mu; |\mu - \nu/\alpha| \leq 1/\alpha\}$.



$S_{\nu\mu}$ at $\nu = 10$ as a function of μ,for $\alpha = 0.1$

- Approximations (using smoothness of $\hat{C}(q_\mu)$ on q_μ scale)

$$\textbf{(i)} \qquad \sum_\mu \hat{Q}_\mu \hat{C}(q_\mu) S_{\nu\mu} \simeq \frac{\alpha}{2} \hat{C}(p_\nu) \sum_{\mu \in I_\nu} Q_\mu$$

$$\textbf{(ii)} \qquad \left\langle \prod_{\nu=0}^{(N-1)/2} F_\nu \right\rangle_{\{\hat{Q}_\mu\}} \simeq \prod_{\nu=0}^{(N-1)/2} \left\langle F_\nu \right\rangle_{\{\hat{Q}_\mu\}}$$

Closed Form Approximation & Scaling

- Allow closed form expression of $\langle Z_N \rangle$, and hence $\rho_\alpha(\lambda)$

$$\langle Z_N \rangle = \prod_{\nu=0}^{(N-1)/2} \left\{ \frac{2\,\mathrm{i}}{\alpha \hat{C}(p_\nu)} \int_0^\infty \mathrm{d}y \, \frac{\mathrm{e}^{-\mathrm{i}y\lambda_\varepsilon 2/(\alpha \hat{C}(p_\nu))}}{\left(1-\mathrm{i}y\right)^{2/\alpha}} \right\}$$

- Gives

$$\rho_\alpha(\lambda) = \int_0^\pi \frac{\mathrm{d}q}{\pi} \, \frac{1}{\hat{C}(q)} \, \rho_\alpha^{(0)} \left(\frac{\lambda}{\hat{C}(q)} \right)$$

- As $\hat{C}(q) \equiv 1$ for uncorrelated data, we have to identify $\rho_\alpha^{(0)}$ with the spectral density for auto-covariance matrices of i.i.d. (uncorrelated) data.
- Our approximations give

$$\rho_\alpha^{(0)}(\lambda) = -\lim_{\varepsilon \to 0} \frac{1}{\pi} \mathrm{Im} \frac{\partial}{\partial \lambda} \ln I_\alpha \left(\frac{2}{\alpha} \lambda_\varepsilon \right)$$

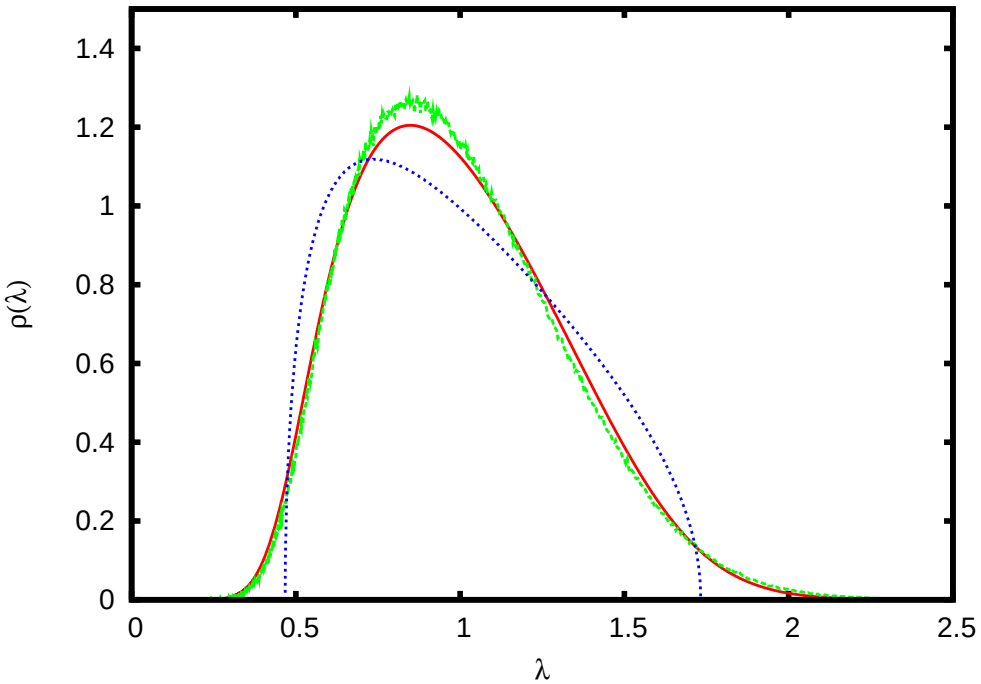
with

$$I_\alpha(x) = \mathrm{i}\,(-x)^{-1+2/\alpha} \mathrm{e}^{-x} \Gamma(1-2/\alpha, -x) \,, \quad \mathrm{Im}\, x < 0 \,.$$

Outline

The Scaling Function — Spectrum for i.i.d. Data

- Spectral density for $x_n \sim \mathcal{N}(0,1)$ i.i.d. @ $\alpha = 0.1$

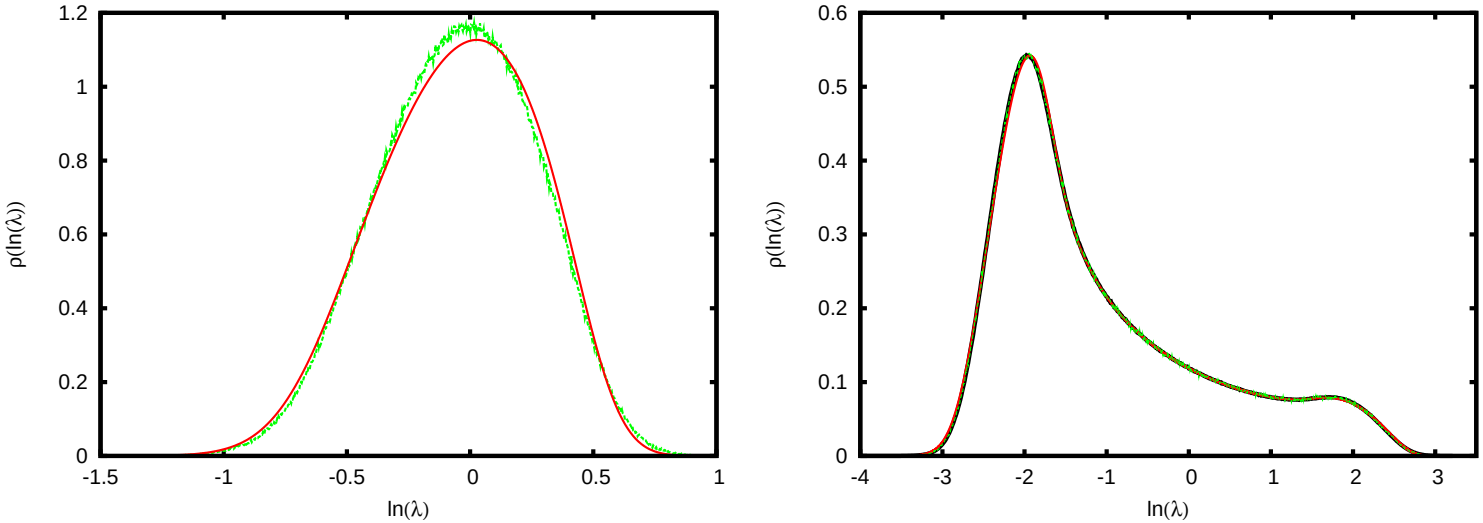


Simulation results (green); analytic approximation for $\rho_\alpha^{(0)}(\lambda)$ (red), Marčenko-Pastur law (blue-dashed).

AR-1 Process @ $\alpha = 0.1$

- (Logarithmic) Spectral density for AR-1 process @ $\alpha = 0.1$

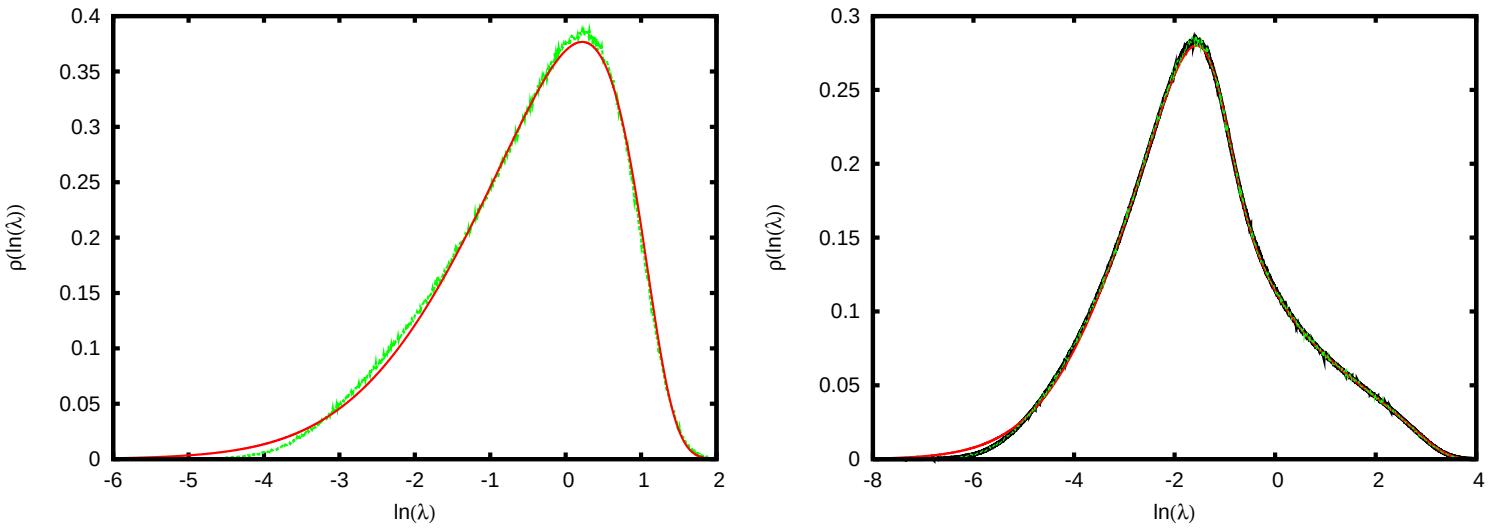
$$x_n = a_1 x_{n-1} + \sqrt{1 - a_1^2}\,\xi_n$$



Left: i.i.d. data, simulation (green) and analytic result (red).
Right: $a_1 = 0.8$. Comparing scaling based on the empirical scaling function (black) with that based on the analytic result (red) and simulations (green).

AR-1 Process @ $\alpha = 0.8$

- (Logarithmic) Spectral density for AR-1 process @ $\alpha = 0.8$



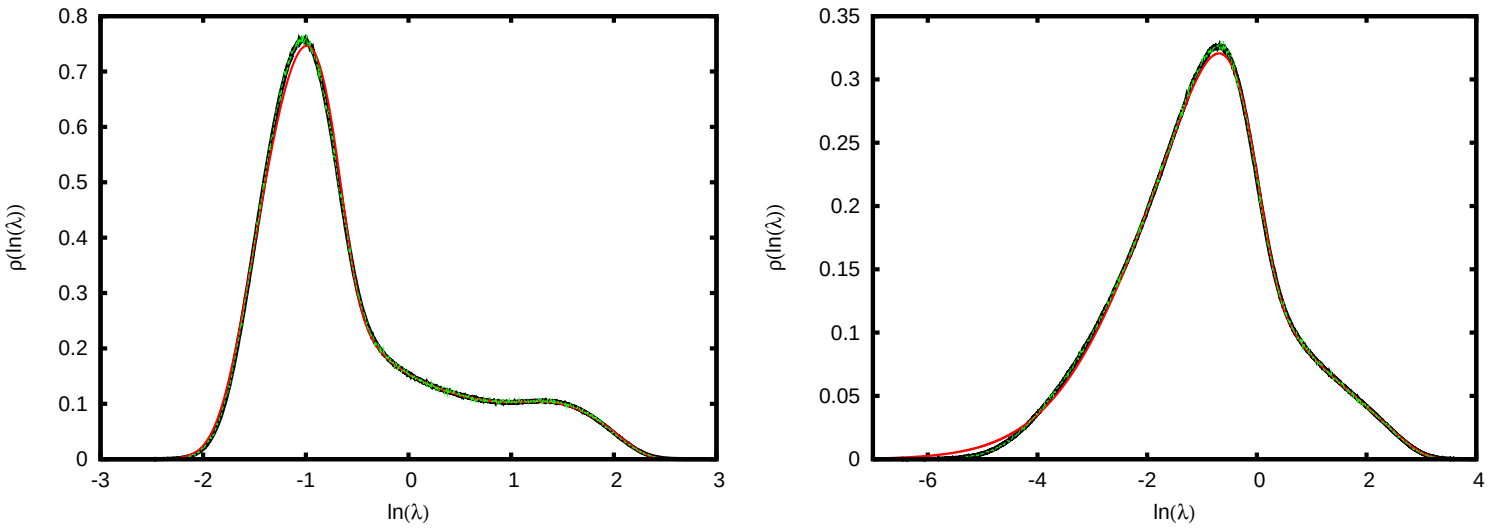
Left: i.i.d. data, simulation (green) and analytic result (red).
Right $a_1 = 0.8$. Comparing scaling based on the empirical scaling function (black) with that based on the analytic result (red) and simulations (green).

AR-2 Process (Two Real Eigenvalues)

- (Logarithmic) Spectral density for AR-2 process

$$x_n + a_1 x_{n-1} + a_2 x_{n-2} = \sigma \xi_n$$

$$a_1 = 0.5,\ a_2 = -3/16\ , \qquad \sigma \text{ such that } \bar{C}(0) = 1\ .$$



Comparing scaling based on the empirical scaling function (black) with that based on the analytic result (red) and simulations (green).

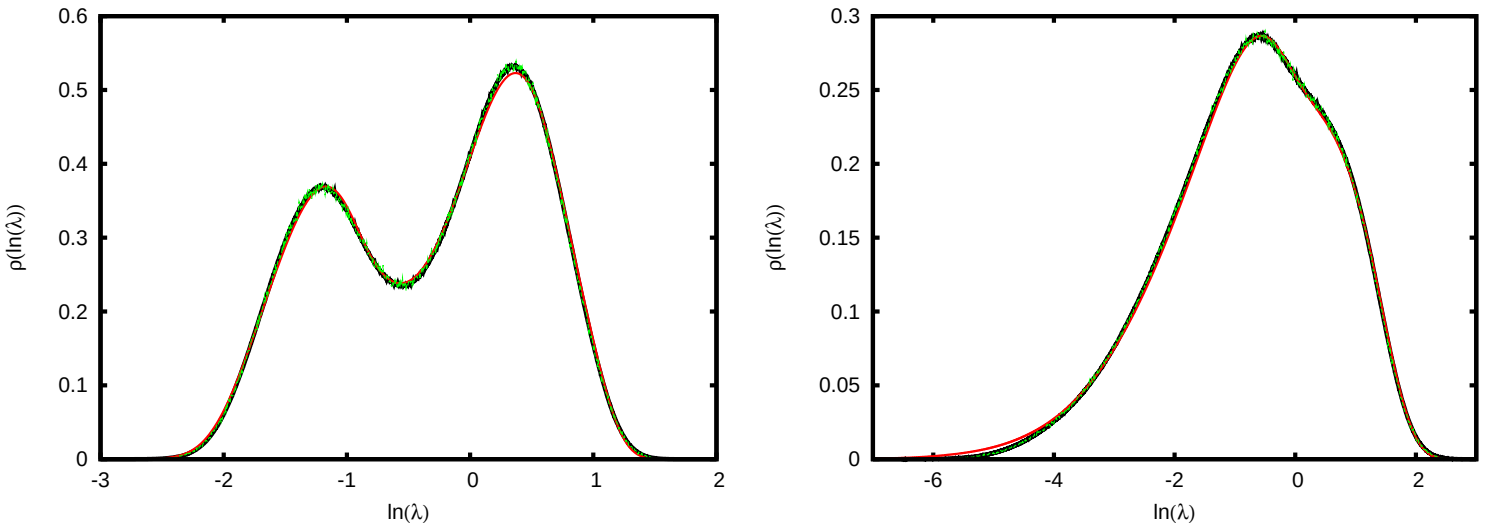
Left: $\alpha = 0.1$, **Right**: $\alpha = 0.8$.

AR-2 Process (Complex Conjugate Eigenvalues)

- (Logarithmic) Spectral density for AR-2 process

$$x_n + a_1 x_{n-1} + a_2 x_{n-2} = \sigma \xi_n$$

$$a_1 = 0.5,\ a_2 = 5/16\ , \qquad \sigma \text{ such that } \bar{C}(0) = 1\ .$$



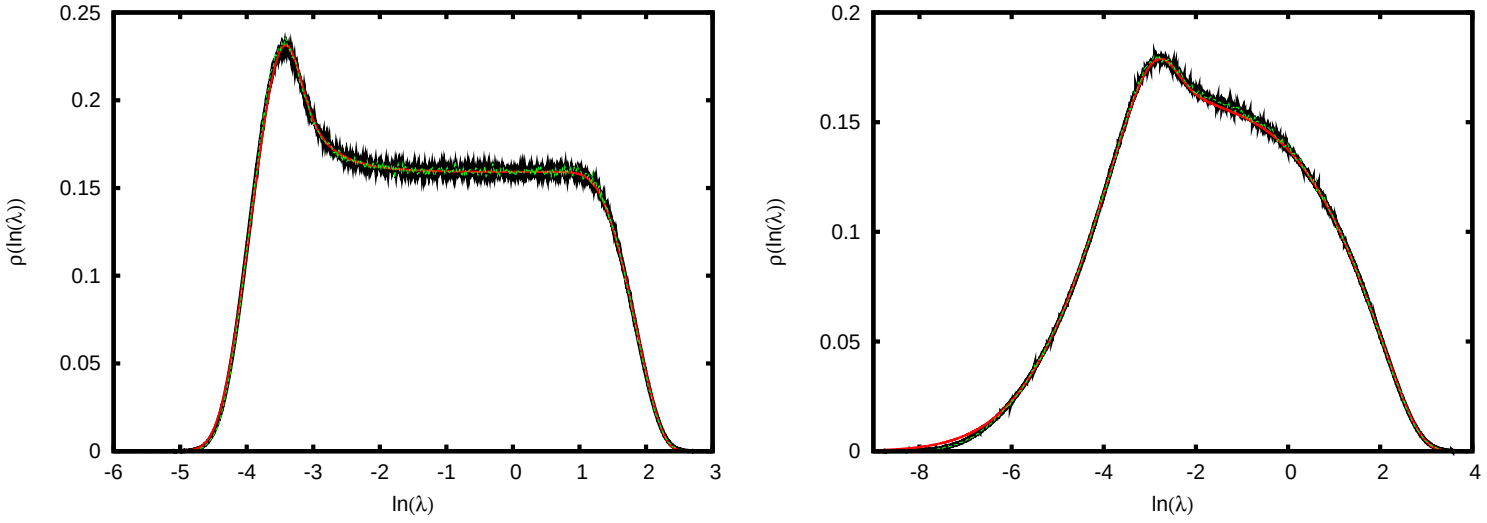
Comparing scaling based on the empirical scaling function (black) with that based on the analytic result (red) and simulations (green).

Left: $\alpha = 0.1$, **Right**: $\alpha = 0.8$.

A Process with Long Range Auto-Correlation

- A process with power-law decay of auto-correlation

$$\bar{C}(n) = \frac{1}{1+(n/2)^2} \ ,$$

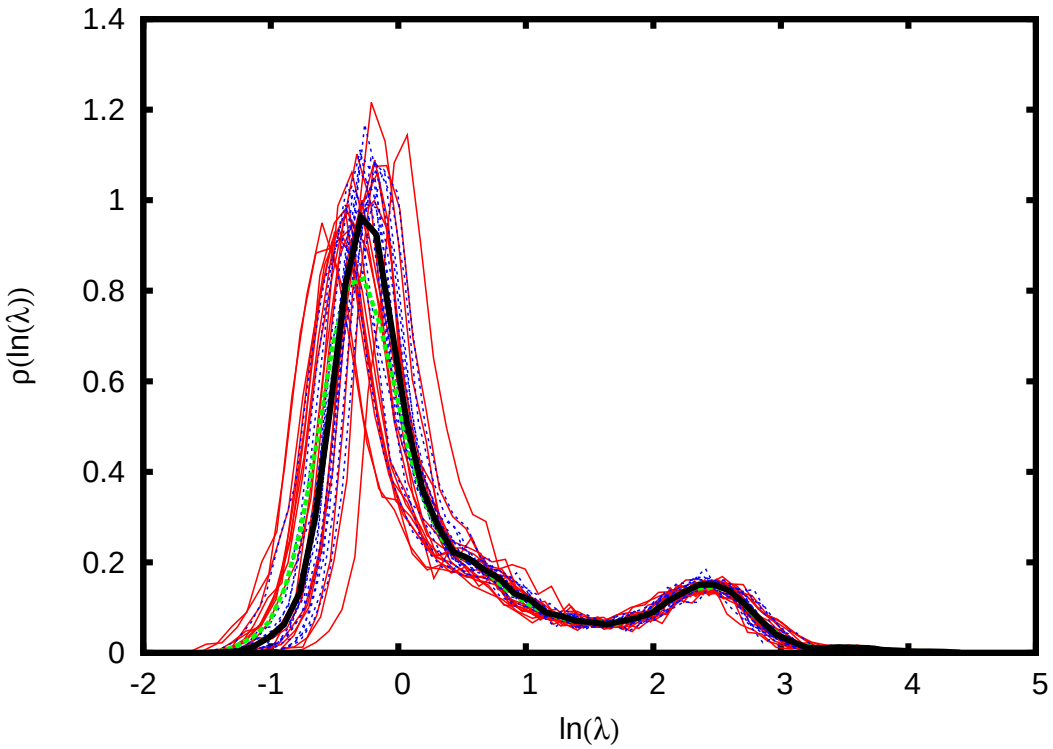


Comparing scaling based on the empirical scaling function (black) with that based on the analytic result (red) and simulations (green).

Left: $\alpha = 0.1$, **Right**: $\alpha = 0.8$.

An application (Work in Progress)

- DNA-Methylation Levels for different cancers



Spectral density of auto-covariance matrices of DNA mathylation levels with $N = 100$ at $\alpha = N/M = 0.025$. Thin red lines are for individual patients from the P class, dashed blue are for individual patients from the N class. The thicker green and black lines correspond to average spectra of the P and N classes, respectively.

Outline

Summary

- Computed DOS of sample auto-covariance matrices using annealed calculation.
- Key ingredient: Szegö's theorem for Toeplitz matrices
- Rectangular window and decorrelation approximation $\Rightarrow$ Closed form approximation.
- Use of Szegös theorem suggests a scaling form for DOS.
  - results suggest that scaling is exact
  - ideas for independent proof
- Applications: time-series analysis, signal processing, information theory, finance ...
- **Thanks!** K. Anand, L. Dall'Asta, P. Vivo