Verification of ergodicity and mixing in anomalous diffusion systems

Marcin Magdziarz

Hugo Steinhaus Center
Wrocław University of Technology, Poland

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Outline

- Basic concepts in ergodic theory (ergodicity, mixing)
- Ergodic properties of Gaussian processes
  - Fractional Brownian motion
  - Langevin equation with fractional Gaussian noise
  - Fractional Langevin equation
- Ergodic properties of Lévy flights
  - Lévy autocorrelation function
  - Khinchin theorem for Lévy flights
  - Examples
- Ergodic properties of the generalized diffusion equation
- Verification of ergodicity and mixing in experimental data
  - Dynamical Functional
  - Main results with examples

Basic concepts in ergodic theory

$Y(t)$, $t \in \mathbb{R}$, **stationary** stochastic process

- system is in thermal equilibrium
- classical ergodic theorems apply

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Corresponding **dynamical system** (canonical representation of Y)

$$(\mathbb{R}^{\mathbb{R}}, \mathcal{B}, \mathbb{P}, S_t)$$

where

- $\mathbb{R}^{\mathbb{R}}$ – space of all functions $f : \mathbb{R} \to \mathbb{R}$
- $\mathcal{B}$ – Borel sets
- $\mathbb{P}$ – probability measure
- S_t – shift transformation, $S_t(f)(s) = f(t+s)$

Ergodicity

Definition

The stationary process $Y(t)$ is **ergodic** if for every invariant set A we have $\mathbb{P}(A) = 0$ or $\mathbb{P}(A^c) = 0$.

The set A is invariant if $S_t(A) = A$ for all t.

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Interpretation of ergodicity:

- the space cannot be divided into two regions such that a point starting in one region will always stay in that region
- the point will eventually visit all nontrivial regions of the space

Mixing

Definition

The stationary process $Y(t)$ is **mixing** if

$$\lim_{t \to \infty} \mathbb{P}(A \cap S_t(B)) = \mathbb{P}(A)\mathbb{P}(B)$$

for all $A, B \in \mathcal{B}$.

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Interpretation of mixing:

- it can be viewed as an asymptotic independence of the sets A and B under the transformation S_t
- the fraction of points starting in A that ended up in B after long time t, is equal to the product of probabilities of A and B

Remark. Mixing is stronger property than ergodicity

Birkhoff ergodic theorem (Boltzmann's hypothesis)

Theorem

If the stationary process $Y(t)$ *is ergodic, then*

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T g(Y(t))dt = \mathbb{E}(g(Y(0))),$$

provided that $\mathbb{E}(|g(Y(0))|) < \infty$.

Ergodic properties of Gaussian processes

- $Y(t)$ – stationary **Gaussian** process

G. Maruyama, Mem. Fac. Sci. Kyushu Univ. (1949)
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- $Y(t)$ – stationary **Gaussian** process
- **autocorrelation function** of $Y(t)$ is given by

$$r(t) = \frac{\mathbb{E}[(Y(0) - m)(Y(t) - m)]}{\mathbb{E}[Y^2(0)]},$$

where $m = E(Y(0))$.

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Corollary (Khinchin Theorem)

If the autocorrelation function of $Y(t)$ satisfies (1) then $Y(t)$ is ergodic.

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Examples – fractional Brownian motion

- **Fractional Brownian motion** (FBM) $B_H(t)$ is the mean-zero Gaussian process with autocovariance function

$$\mathbb{E}[B_H(s)B_H(t)] = \frac{1}{2}\left(s^{2H} + t^{2H} - |t-s|^{2H}\right), \qquad t, s \geq 0.$$

Here, $0 < H < 1$ is the Hurst index.

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- The autocorrelation function of $b_H(j)$ satisfies

$$r(j) \sim H(2H-1)j^{2H-2}$$

as $j \to \infty$. This implies

$$r(j) \to 0 \quad as \quad j \to \infty.$$

Thus, $b_H(j)$ is **ergodic and mixing**.

Examples – Langevin equation with fractional Gaussian noise

- **Langevin equation with fractional Gaussian noise** has the form

$$dW_H(t) = -\lambda W_H(t)dt + \sigma dB_H(t), \quad \lambda, \sigma > 0. \tag{2}$$

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$$W_H(t) = \sigma \int_{-\infty}^{t} e^{-\lambda(t-s)} dB_H(s).$$

- The autocorrelation function of $W_H(t)$ satisfies

$$r(t) \propto t^{2H-2}$$

as $t \to \infty$. This implies that $W_H(t)$ is **ergodic and mixing**.

- Fractional Langevin equation for a single particle of mass m in the absence of external force has the form

$$m\frac{dV}{dt} = -\gamma \int_0^t \frac{1}{(t-u)^{\beta}} V(u)du + \sigma \frac{dB_H(t)}{dt}, \tag{3}$$

where $\gamma > 0$ is the friction constant, $\beta = 2 - 2H$, $H > 1/2$.

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where $\gamma > 0$ is the friction constant, $\beta = 2 - 2H$, $H > 1/2$.

- Solution to (3) is a stationary Gaussian process, whose autocovariance function $c(t)$ in the Laplace space yields

$$\widetilde{c}(\omega) = \frac{1}{\omega + c\omega^{\beta-1}}.$$

From Tauberian theorem, $c(t) \to 0$ as $t \to \infty$. Thus, the process $V(t)$ is **ergodic and mixing**.

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- **Main difficulty**: the second moment is infinite – autocorrelation function is not defined
- **Examples of Lévy flight dynamics:** animal foraging patterns, transport of light in special optical materials, bulk mediated surface diffusion, transport in micelle systems or heterogeneous rocks, single molecule spectroscopy, wait-and-switch relaxation, etc.

Lévy autocorrelation function

- $Y(t)$ – **stationary α-stable process** (Lévy flight) of the form

$$Y(t) = \int_{-\infty}^{\infty} K(t,x) dL_\alpha(x), \qquad t \in \mathbb{R}. \tag{4}$$

Here, $K(t,x)$ is the kernel function and $L_\alpha(x)$ is the α-stable Lévy motion with the Fourier transform $\mathbb{E} e^{izL_\alpha(x)} = e^{-x|z|^\alpha}$, $0 < \alpha < 2$.

I. Eliazar, J. Klafter, Physica A (2007); J. Phys. A: Math. Theor. (2007)

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Definition (Lévy autocorrelation function)

Lévy autocorrelation function corresponding to $Y(t)$ is defined as

$$R(t) = \int_{-\infty}^{\infty} \min\{|K(0,x)|, |K(t,x)|\}^\alpha dx \tag{5}$$

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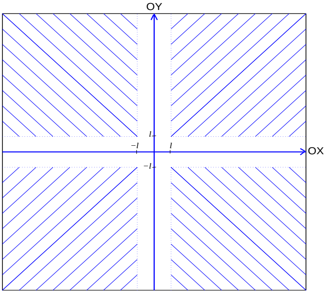
Lévy autocorrelation function

Interpretation: For every $l > 0$ we have

$$R(t) = l^{\alpha} \cdot \nu_{0t}\{(x, y) : \min\{|x|, |y|\} > l\},$$

where ν_{0t} is the Lévy measure of the vector $(Y(0), Y(t))$.



Remark: $Y(0)$ and $Y(t)$ are independent if and only if ν_{0t} is concentrated on the axes OX and OY.

Maruyama's mixing theorem and its refinement

Theorem (Maruyama, 1970)

An i.d. stationary process Y_t is mixing if and only if

(i) *correlation function $r(t)$ of Gaussian part converges to 0 as $t \to \infty$,*

(ii) $\lim_{t\to\infty} \nu_{0t}(|xy| > \delta) = 0$ *for every* $\delta > 0$,

(iii) $\lim_{t\to\infty} \int_{0<x^2+y^2\le 1} xy\nu_{0t}(dx, dy) = 0$,

where ν_{0t} is the Lévy measure of (Y_0, Y_t).

G. Maruyama, Theory Probab. Appl. (1970)
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Ergodic properties of Lévy flights

Theorem

The stationary Lévy flight process $Y(t)$ is ergodic if and only if its Lévy autocorrelation function satisfies

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T R(t)dt = 0.$$

M. Magdziarz, Stoch. Proc. Appl. (2009)
M. Magdziarz, A. Weron, Ann. Phys. (2011)

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Corollary (Khinchin Theorem for Lévy flights)

If the autocorrelation function of Lévy flight $Y(t)$ satisfies

$$\lim_{t\to\infty} R(t) = 0.$$

then $Y(t)$ is ergodic.
Moreover, the temporal and ensemble averages coincide

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T g(Y(t))dt = \mathbb{E}[g(Y(0))],$$

provided that $\mathbb{E}[|g(Y(0))|] < \infty$.

A. Weron, M. Magdziarz, Phys. Rev. Lett. (2010)

- α-**stable Ornstein-Uhlenbeck** process is defined as

$$Y_1(t) = \sigma \int_{-\infty}^{t} e^{-\lambda(t-x)} dL_\alpha(x), \quad \lambda, \sigma > 0.$$

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- The Lévy autocorrelation function corresponding to $Y_1(t)$ satisfies

$$R(t) \propto e^{-\alpha\lambda t}$$

as $t \to \infty$. Thus, $Y_1(t)$ is **ergodic and mixing**.

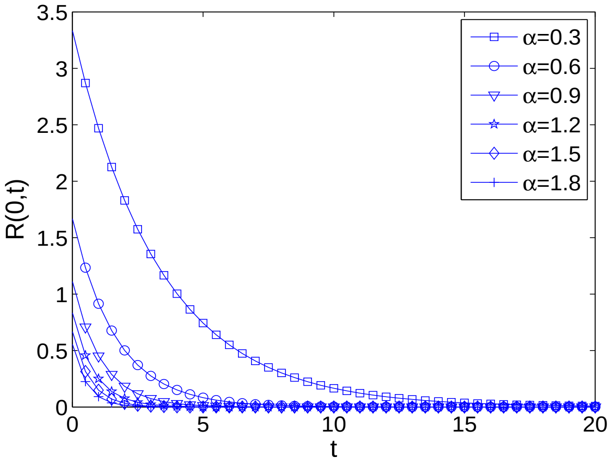

Figure: Lévy autocorrelation function corresponding to the α-stable Ornstein-Uhlenbeck process $Y_1(t)$.

Examples - α-stable Ornstein-Uhlenbeck process

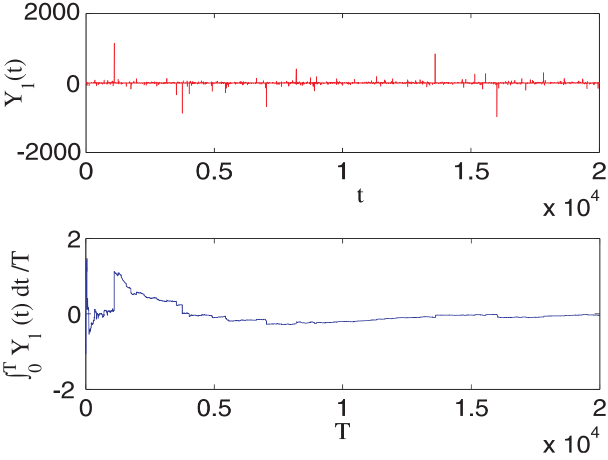

Figure: Top panel: simulated trajectory of the 1.2-stable Ornstein-Uhlenbeck process $Y_1(t)$. Bottom panel: the temporal average corresponding to $Y_1(t)$. Clearly $\lim_{T\to\infty} \frac{1}{T}\int_0^T Y_1(t)dt = 0 = \mathbb{E}(Y_1(0))$.

- α-**stable Lévy noise** is defined as

$$l_\alpha(t) = L_\alpha(t+1) - L_\alpha(t).$$

It is a stationary sequence of independent and identically distributed α-stable random variables.

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- α-**stable Lévy noise** is defined as

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  It is a stationary sequence of independent and identically distributed α-stable random variables.

- The Lévy autocorrelation function of $l_\alpha(t)$ satisfies

$$R(t) = 0$$

  This corresponds to the well known property that independent random variables are uncorrelated. Thus, $l_\alpha(t)$ is **ergodic and mixing**.

- **Fractional α-stable Lévy motion** is defined as

$$L_{\alpha,H}(t) = \int_{-\infty}^{\infty} \left[(t-x)_+^{H-1/\alpha} - (-x)_+^{H-1/\alpha}\right] dL_\alpha(x).$$

Here $x_+ = \max\{x, 0\}$.

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- The Lévy autocorrelation function of $l_{\alpha,H}(t)$ yields

$$\lim_{t\to\infty} R(t) = 0.$$

  Therefore, the fractional α-stable Lévy noise is **ergodic and mixing**.

Summary for Lévy autocorrelation function

- Lévy autocorrelation function seems to be a perfect tool for verification of ergodic properties of Lévy flights
- it works also for the whole family of infinitely divisible processes (α-stable, tempered α-stable, Pareto, exponential, gamma, Poisson, Linnik, Mittag-Leffler, etc.)

Generalized diffusion equation (GDE)

Definition (I.M. Sokolov, J. Klafter, Phys. Rev. Lett. (2006))

$$\frac{\partial w(x,t)}{\partial t} = \Phi_t \frac{\partial^2}{\partial x^2} w(x,t)$$

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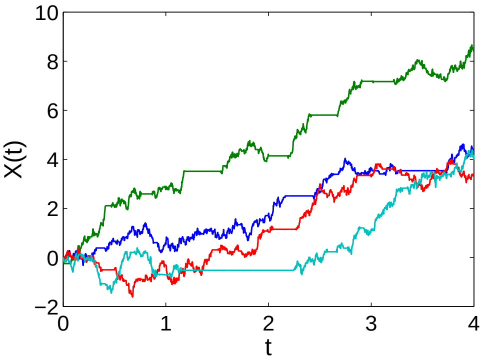

Figure: Typical trajectories of the process corresponding to GDE

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- $\Psi(u)$ is the Laplace exponent of the underlying waiting time $T > 0$, i.e. $\mathbb{E}\left(e^{-uT}\right) = e^{-\Psi(u)}$
- T – any infinitely divisible distribution
- for $\Psi(u) = u^\alpha$ we have $\Phi_t = {}_0D_t^{1-\alpha}$ and we recover the celebrated fractional diffusion equation

Theorem (M. Magdziarz (2010))

The PDF of the process $X(t) = B(S_\Psi(t))$ is the solution of GDE. Here, B is the Brownian motion and S_Ψ is the inverse subordinator corresponding to T.

GDE – ergodicity and mixing

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Let $\mathbb{E}(T) < \infty$. Then the increments of the process $X(t) = B(S_\Psi(t))$ corresponding to GDE are ***ergodic*** *and* ***mixing****.*

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- **Consequences:**
  Recently, in J-H. Jeon et al., Phys. Rev. Lett (2010), GDE with tempered stable waiting times was used to model the dynamics of lipid granules in fission yeast cells. The above theorem implies that this dynamics is ergodic and mixing.

Testing ergodicity and mixing in experimental data

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- $Y(1)$, $Y(2)$, $Y(3)$, ..., $Y(N)$ – experimentally measured one realization of some random process $Y(n)$
- we assume that $Y(n)$ is stationary and infinitely divisible (Gaussian, α-stable, tempered α-stable, Pareto, exponential, gamma, Poisson, Linnik, Mittag-Leffler, etc.)

Dynamical Functional

Definition (A. Weron et al. (1994))

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Remark 1: $D(n)$ is just the Fourier transform of $Y(n) - Y(0)$ evaluated for the Fourier-space variable $k = 1$.

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Definition (A. Weron et al. (1994))

The **dynamical functional** $D(n)$ corresponding to the process $Y(n)$ is defined as

$$D(n) = \mathbb{E}(\exp\{i[Y(n) - Y(0)]\})$$

Remark 1: $D(n)$ is just the Fourier transform of $Y(n) - Y(0)$ evaluated for the Fourier-space variable $k = 1$.

Remark 2: If $Y(n)$ is Gaussian, then the dynamical functional is equal to

$$D(n) = \exp\{\sigma^2[r(n) - 1]\},$$

where $r(n)$ is the autocorrelation function of $Y(n)$ and σ^2 is the variance of $Y(0)$.

Dynamical Functional – main results

Theorem

*$Y(n)$ is **mixing** if and only if*

$$\lim_{n\to\infty} D(n) = |\mathbb{E}(\exp\{iY(0)\})|^2.$$

Equivalently,

$$\lim_{n\to\infty} E(n) = 0,$$

where $E(n) = D(n) - |\mathbb{E}(\exp\{iY(0)\})|^2$.

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Theorem

*$Y(n)$ is **ergodic** if and only if*

$$\lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} E(k) = 0.$$

Applications: the case of many realizations of $Y(n)$

- Suppose that the number of experimental realizations of $Y(n)$ is **large enough to calculate ensemble averages**

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ALGORITHM of testing mixing and ergodicity:

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4. If the convergence
$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} E(k) = 0$$
holds for large n, then $Y(n)$ is **ergodic**, otherwise we have **ergodicity breaking**

Example: ergodicity of Ornstein-Uhlenbeck process

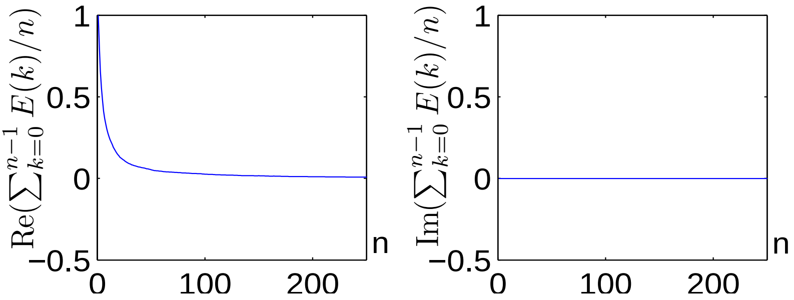

Figure: Verification of ergodicity for the Ornstein-Uhlenbeck process given by the Langevin equation $dY(n) = -Y(n)dt + dB(n)$.

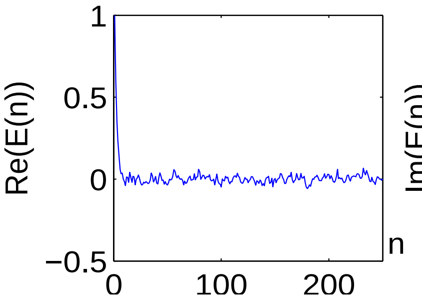

Figure: Verification of mixing property for the Ornstein-Uhlenbeck process given by the Langevin equation $dY(n) = -Y(n)dt + dB(n)$.

Example: Mixing breaking and ergodicity breaking of a Gaussian process

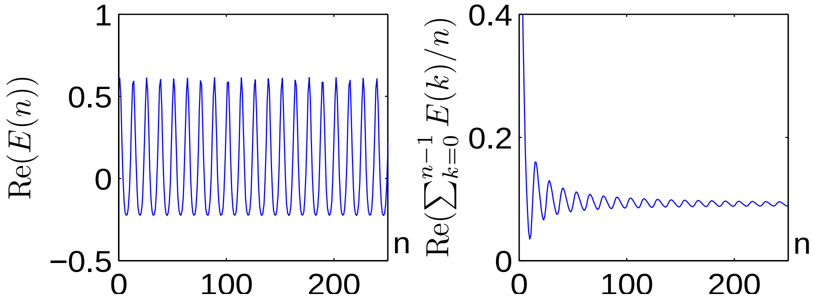

Figure: Verification of mixing breaking and ergodicity breaking for the Gaussian stationary process of the form $Y(n) = \sqrt{T}\cos(0.5n + \theta)$. Here, T is exponentially distributed random variable.

Example: Ergodicity breaking of a α-stable process

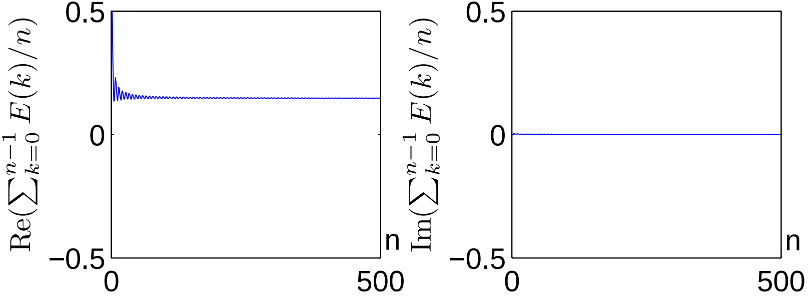

Figure: Verification of ergodicity breaking for the α-stable stationary process of the form $Y(n) = A^{1/2}(G_1 \cos(n) + G_2 \sin(n))$. Here, $A > 0$ is the one-sided α-stable random variable, G_1 and G_2 are standard normal random variables.

Applications: the case of one realization of $Y(n)$

- Suppose that we have only one realization of $Y(n)$. Then, **only necessary conditions** for ergodicity and mixing can be checked

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3. Check if
$$\widehat{E}(n) \approx 0$$
for large n. Here $\widehat{E}(n) = \widehat{D}(n) - \widehat{a}$. The above condition is **necessary for mixing**. Therefore, its violation implies that $Y(n)$ does not have the mixing property. This condition is **not sufficient for mixing**.

4. Check if

$$\frac{1}{n}\sum_{k=0}^{n-1}\widehat{E}(k) \approx 0.$$

for large n. The above condition is **necessary for ergodicity**. Therefore, its violation implies ergodicity breaking of $Y(n)$. This condition is **not sufficient for ergodicity**.

Example: Mixing breaking of a α-stable process – one trajectory case

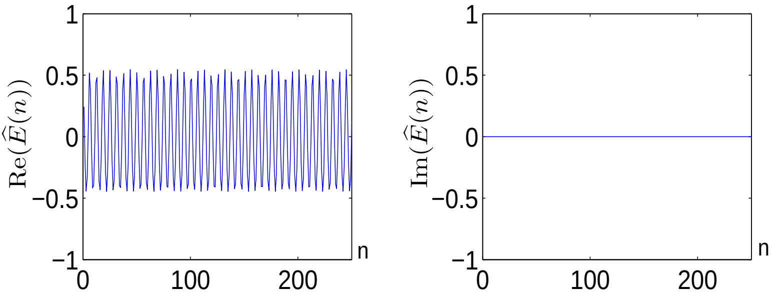


Figure: Verification of mixing breaking from one trajectory of the α-stable stationary process of the form $Y(n) = A^{1/2}(G_1 \cos(n) + G_2 \sin(n))$. Here, $A > 0$ is the one-sided α-stable random variable, G_1 and G_2 are standard normal random variables.

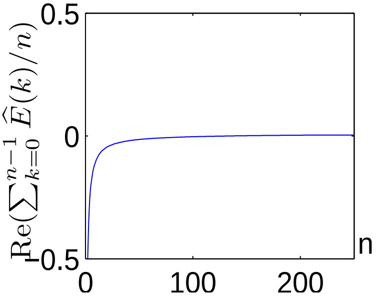
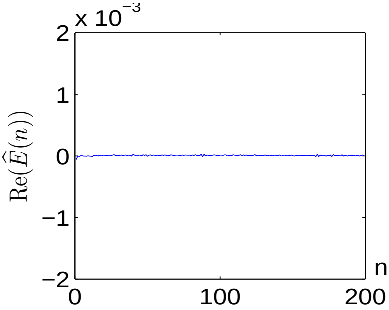


Figure: The real and imaginary parts of the function $\sum_{k=0}^{n-1}\widehat{E}(k)/n$ corresponding to the longest trajectory of the Golding-Cox data (X coordinate). The necessary condition for ergodicity is clearly satisfied.

Golding-Cox experimental data – mixing



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