Supplemental material

Identifying diffusive motions in single-particle trajectories on the plasma membrane via fractional time series models

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1. Introduction

In this Supplemental material we present details on ARFIMA models fitted to representative membrane protein trajectories corresponding to the free and confined motions. At the end we include videos illustrating the impact of the ARFIMA parameters on a simulated 2D trajectory.

2. Nav trajectories

For each trajectory we provide (i) a summary of the model, and for residuals (ii) results of the model validation tests (Ljung-Box and McLeod-Li) and (iii) results of the goodness of fit tests (Anderson and Darling) for different distributions. The p-values for Ljung-Box and McLeod-Li tests were calculated for the lag equal to 20.

2.1. Free state

Trajectory 1

\((1-B)^{-0.01} x(t) = Z(t) - 0.031 Z(t-1)\)

White noise variance = 0.110326E+05

Ljung-Box test, p-value = 0.86

McLeod-Li statistic test, p-value = 0.95

Anderson-Darling test for normality, p-value = 0.99

Trajectory 2

\((1-B)^{-0.22} x(t) = Z(t) - 0.37 Z(t-1)\)

White noise variance = 0.692959E+04

Ljung-Box test, p-value = 0.77

McLeod-Li test, p-value = 0.7
Anderson-Darling test for normality, p-value = 0.12

**Trajectory 3**

\[(1-B)^{-0.1}X(t) = Z(t) + 0.01 Z(t-1)\]

White noise variance = 0.636308E+04

Ljung-Box test, p-value = 0.71

McLeod-Li test, p-value = 0.51

Anderson-Darling test for normality, p-value = 0.57

**Trajectory 4**

\[(1-B)^{0.05}X(t) = Z(t) - 0.17 Z(t-1)\]

White noise variance = 0.624129E+04

Ljung-Box test, p-value = 0.92

McLeod-Li test, p-value = 0.78

Anderson-Darling test for normality, p-value = 0.94

**Trajectory 5**

\[(1-B)^{0.05}X(t) = Z(t) - 0.18 Z(t-1)\]

White noise variance = 0.119717E+05

Ljung-Box test, p-value = 0.75

McLeod-Li test, p-value = 0.96

Anderson-Darling test for normality, p-value = 0.15

### 2.2. Confined state

**Trajectory 1**

\[X(t) = 0.3 X(t-1) + Z(t)\]

White noise variance = .194799E+04

Ljung-Box test, p-value = .89

McLeod-Li test, p-value = .99

Anderson-Darling test for normality, p-value = 0.06

Anderson-Darling test for t location-scale, p-value = 0.08

Anderson-Darling test for NIG, p-value = 0.18

**Trajectory 2**

\[X(t) = 0.18 X(t-1) + Z(t)\]

White noise variance = 0.796564E+04

Ljung-Box test, p-value = 0.34

McLeod-Li test, p-value = 0.98

Anderson-Darling test for normality, p-value < 0.001

Anderson-Darling test for t location-scale, p-value < 0.001
Anderson-Darling test for NIG, p-value = 0.21

Trajectory 3
X(t) = 0.23 X(t-1) + Z(t)
White noise variance = 0.431889E+04
Ljung-Box test, p-value = 0.12
McLeod-Li test, p-value = 1
Anderson-Darling test for normality, p-value = 0.003
Anderson-Darling test for t location-scale, p-value = 0.18
Anderson-Darling test for NIG, p-value = 0.09

Trajectory 4
X(t) = 0.14 X(t-1) + Z(t)
White noise variance = 0.405302E+04
Ljung-Box test, p-value = 0.87
McLeod-Li test, p-value = 0.6
Anderson-Darling test for normality, p-value = 0.11
Anderson-Darling test for t location-scale, p-value = 0.73
Anderson-Darling test for NIG, p-value = 0 (convergence error)

Trajectory 5
X(t) = 0.11 X(t-1) + Z(t)
White noise variance = 0.610495E+04
Ljung-Box test, p-value = 0.92
McLeod-Li test, p-value = 0.44
Anderson-Darling test for normality, p-value = 0.003
Anderson-Darling test for t location-scale, p-value = 0.27
Anderson-Darling test for NIG, p-value = 0.89

3. Beta 2 trajectories

For each trajectory we provide (i) a summary of the model, and for residuals (ii) results of the model validation tests (Ljung-Box and McLeod-Li) and (iii) results of the goodness of fit tests (Anderson and Darling) for different distributions. The p-values for Ljung-Box and McLeod-Li tests were calculated for the lag equal to 20.

3.1. Free state

Trajectory 1
(1-B)^0.2 X(t) = Z(t) + 0.31 Z(t-1)
White noise variance = 1.05  
Ljung-Box test, p-value = .83  
McLeod-Li test, p-value = .34  
Anderson-Darling test for normality, p-value = 0.001  

**Trajectory 2**

$(1-B)^{0.13}X(t) = Z(t) + 0.11 Z(t-1)$  
White noise variance = 1.56  
Ljung-Box test, p-value = 0.93  
McLeod-Li test, p-value = 0.76  
Anderson-Darling test for normality, p-value = 0.53  

**Trajectory 3**

$(1-B)^{0.2}X(t) = Z(t) + 0.21 Z(t-1)$  
White noise variance = 1.80  
Ljung-Box test, p-value = 0.32  
McLeod-Li test, p-value = 0.11  
Anderson-Darling test for normality, p-value = 0.86  

**Trajectory 4**

$(1-B)^{0.04}X(t) = Z(t) + 0.02 Z(t-1)$  
White noise variance = 1.35  
Ljung-Box test, p-value = 0.36  
McLeod-Li test, p-value = 0.66  
Anderson-Darling test for normality, p-value = 0.34  

**Trajectory 5**

$(1-B)^{-0.04}X(t) = Z(t) + 0.09 Z(t-1)$  
White noise variance = 1.165842  
Ljung-Box test, p-value = 0.63  
McLeod-Li test, p-value = 0.28  
Anderson-Darling test for normality, p-value = 0.52  

3.2. Confined state  

**Trajectory 1**

$X(t) = 0.02 X(t-1) + Z(t)$  
White noise variance = 0.033  
Ljung-Box test, p-value = 0.74  
McLeod-Li test, p-value = 0.63
Anderson-Darling test for normality, p-value < 0.001
Anderson-Darling test for t location-scale, p-value < 0.001
Anderson-Darling test for NIG, p-value = 0.04

**Trajectory 2**

X(t) = -0.05 X(t-1) + Z(t)
White noise variance = 0.079
Ljung-Box test, p-value = 0.12
McLeod-Li test, p-value = 0.4
Anderson-Darling test for normality, p-value < 0.001
Anderson-Darling test for t location-scale, p-value < 0.001
Anderson-Darling test for NIG, p-value < 0.001

**Trajectory 3**

X(t) = 0.07 X(t-1) + Z(t)
White noise variance = 0.088
Ljung-Box test, p-value = 0.93
McLeod-Li test, p-value = 0.79
Anderson-Darling test for normality, p-value < 0.001
Anderson-Darling test for t location-scale, p-value = 0.08
Anderson-Darling test for NIG, p-value = 0.11

**Trajectory 4**

X(t) = 0.09 X(t-1) + Z(t)
White noise variance = 0.1
Ljung-Box test, p-value = 0.5
McLeod-Li test, p-value = 0.95
Anderson-Darling test for normality, p-value < 0.001
Anderson-Darling test for t location-scale, p-value < 0.001
Anderson-Darling test for NIG, p-value = 0.01

**Trajectory 5**

X(t) = 0.33 X(t-1) + Z(t)
White noise variance = 0.015
Ljung-Box test, p-value = 0.25
McLeod-Li test, p-value = 0.42
Anderson-Darling test for normality, p-value = 0.03
Anderson-Darling test for t location-scale, p-value = 0.64
Anderson-Darling test for NIG, p-value = 0.35
4. Empirical vs model simulated MSD values

We present here a comparison of MSD exponents calculated for the representative trajectories and MSD values obtained for the simulated trajectories of the fitted models.

4.1. Free state

![Figure S1. 95% confidence intervals of estimated MSD exponents for 1000 simulated trajectories of the fitted FIMA processes for the X-coordinate of free state Nav1.6 and beta 2 receptor five representative trajectories. The dashed horizontal line stands for the MSD exponent obtained for the analyzed empirical trajectory.](image1)

4.2. Confined state

![Figure S2. 95% confidence intervals of estimated MSD exponents for 1000 simulated trajectories of the fitted AR processes for the X-coordinate of confined state Nav1.6 and beta 2 receptor five representative trajectories. The dashed horizontal line stands for the MSD exponent obtained for the analyzed empirical trajectory.](image2)
5. Illustration of the impact of ARFIMA parameters on a 2D simulated trajectory

5.1. Impact of the AR parameter $\varphi$ on ARFIMA(1,d,1) with $d = 0.25$ and $\psi = 0.3$

![ARimpact.avi](attachment:ARimpact.avi)

5.2. Impact of the FI parameter $d$ on ARFIMA(1,d,1) with $\varphi = 0.3$ and $\psi = 0.3$

![FIimpact.avi](attachment:FIimpact.avi)

5.3. Impact of the MA parameter $\psi$ on ARFIMA(1,d,1) with $d = 0.25$ and $\varphi = 0.3$

![MAimpact.avi](attachment:MAimpact.avi)