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Estimation of drift and diffusion functions from unevenly sampled time-series data

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¹ Estimation of Drift and Diffusion Functions from Unevenly Sampled Time-Series Data

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Complex systems can often be modelled as stochastic processes. However, physical observations of such systems are often irregularly spaced in time, leading to difficulties in estimating appropriate models from data. Here we present extensions of two methods for estimating drift and diffusion functions from irregularly sampled time-series data. Our methods are flexible and applicable to a variety of stochastic systems, including non-Markov processes or systems contaminated with measurement noise. To demonstrate applicability, we use this approach to analyse an irregularly sampled paleoclimatological isotope record, giving insights into underlying physical processes.

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I. INTRODUCTION

The time-dependent behavior of complex systems con-6 7 sisting of a large number of subsystems can often be de-⁸ scribed by low-dimensional order parameter equations In many cases, a separation between slow ad-⁹ [1]. 10 justments and fast fluctuations allows for a description ¹¹ of continuous observables X of such systems with a ¹² Langevin-type equation

$$\frac{d}{dt}X(t) = f(X,t) + g(X,t)\Gamma(t)$$
(1)

¹³ where $\Gamma(t)$ denotes the stochastic force, with $\langle \Gamma(t) \rangle = 0$ ¹⁴ and $\langle \Gamma(t)\Gamma(t')\rangle = \delta(t-t')$ [2]. The same information is ¹⁵ expressed in the Fokker-Planck equation,

$$\frac{\partial}{\partial t}p(x,t|x',t') = \left[-\frac{\partial}{\partial x}D^{(1)}(x,t) + \frac{\partial^2}{\partial x^2}D^{(2)}(x,t)\right]p(x,t|x',t') \quad (2)$$

¹⁶ which contains the Kramers-Moyal (KM) coefficients

$$D^{(n)}(x,t) = \lim_{\tau \to 0} \frac{1}{n!\tau} \int_{-\infty}^{\infty} \left[x' - x \right]^n p(x',t+\tau|x,t) \, dx',$$
(3)

¹⁷ where x and x' denote values that can be taken by ¹⁸ X, and $p(\circ|\circ)$ is the transition probability. Here, the ¹⁹ first two coefficients are the drift and diffusion, respec-20 tively, connecting to (1) under the Itô interpretation, with $f(x,t) = D^{(1)}(x,t)$ and $g(x,t) = \sqrt{2D^{(2)}(x,t)}$. 21

It has been shown that it is possible to estimate the 6022 forms of such processes directly from regularly sampled time-series data using a technique called "direct estima-24 ²⁵ tion" [3, 4]. This approach has been applied to various $_{26}$ fields of science [5].

There are two main difficulties associated with apply-27 28 ing this approach to "real-world" time-series data. The ²⁹ first occurs when observations are contaminated by an-30 other undesirable signal, or measurement noise. In this 31 case, Böttcher et al. [6] introduced a method to para-32 metrically estimate drift and diffusion functions as well 33 as the amplitude of the measurement noise, an approach $_{34}$ has been expanded in subsequent studies [7–9].

The other difficulty involves the discrete sampling of ³⁶ the time-series data. For low sampling frequencies, is can $_{37}$ be difficult to perform or infer the limit $\tau \rightarrow 0$ required 38 for direct estimation. In this case, Honisch and Friedrich $_{39}$ [10] proposed a finite τ optimisation method that cor-⁴⁰ rectly recovers drift and diffusion functions even at large ⁴¹ sampling. However a related impediment is the presence ⁴² of irregular sampling. In this case, there is no obvious ⁴³ way to calculate averages in (3). This is commonly en-⁴⁴ countered in geoscientific measurements [e.g. 11, 12], but $_{45}$ also is encountered in turbulence measurements [13–15], ⁴⁶ astrophysical observations [16–19], and biological sys-47 tems [20]. Interpolation is sometimes used to side-step 48 these difficulties, however this can introduce a significant ⁴⁹ and hard-to-quantify bias [12, 21–23]. This motivates a 50 method for estimating drift and diffusion functions di-⁵¹ rectly from unaltered time-series data.

52 In the next section we review current estimation tech-⁵³ niques, and propose two extensions for irregular sam-⁵⁴ pling. Section III shows numerical examples where we 55 demonstrate the functionality of our new methods. In 56 Section IV we apply this framework to an empirical data-57 set, namely a paleoclimatological isotope record [24]. ⁵⁸ Summaries are given in Section V, where further appli-⁵⁹ cations are proposed.

II. ESTIMATION OF CONDITIONAL MOMENTS

62 We consider a stationary scalar process X(t) that $_{63}$ is observed at a set of N increasing points in time, $_{64}$ { t_1, t_2, \ldots, t_N }, with no guarantee of a regular sam-⁶⁵ pling. Observations at these points are denoted as $_{66}$ { $X(t_1), X(t_2), \ldots, X(t_N)$ }. The finite-time KM coeffi-⁶⁷ cients of X(t) are defined as [10]

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 $D_{\tau}^{(n)}(x) = \frac{1}{n!\tau} M^{(n)}(x,\tau),$ 75 (4)

⁶⁸ which are calculated using the finite-time conditional mo-69 ments

$$M^{(n)}(x,\tau) = \int_{-\infty}^{\infty} [x' - x]^n p(x', t + \tau | x, t) \, dx'.$$
 (5)

⁷² as finite-time KM coefficients in an appropriate method ⁸³ written as, [e.g. 26],

73 in order to estimate drift and diffusion functions of the 74 underlying process.

Conditional moment estimates are denoted as $\hat{M}^{(n)}(x_i, au_j)$, and are evaluated at a set of evalua- τ_{τ} tion points in $x_i \in \{x_1, x_2, \ldots, x_{\max}\}$, and $\tau_j \in$ 78 $\{\tau_1, \tau_2, \ldots, \tau_{\max}\}.$

Histogram Based Regression А.

The simplest way of estimating conditional moments 80 ⁷⁰ The task is to make an estimate of these moments from ⁸¹ is by means of regressogram, [e.g. 25], also known as his- τ_1 data X(t). These moments will subsequently be used τ_2 togram based regression (HBR). This estimator can be

$$\hat{M}^{(n)}(x_i,\tau_j) = \frac{\sum_{k=1}^{N} I(X(t_k) \in B^{(x)}(x_i)) [X(t_k + \tau_j) - X(t_k)]^n}{\sum_{k=1}^{T} I(X(t_k) \in B^{(x)}(x_i))},$$
(6)

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⁸⁴ where $I(\circ)$ is the indicator function, and binning is in- $_{90}$ times, and also bin data by time-step. We shall refer to $B^{(x)}(x_i) := [x_i - B^{(x)}(x_i)] = [x_i - B^{(x)}(x_i)]$ $\frac{1}{2}b_x, x_i + \frac{1}{2}b_x)$, where b_x is the width of the bin.

 $_{92}$ The estimator for conditional moments can be written as

В. Histogram-Time Based Regression 87

One simple way to extend HBR to account for uneven time-sampling is to average over all pairs of increasing 89

$$\hat{M}^{(n)}(x_i,\tau_j) = \frac{\sum_{k=1}^{N-1} \sum_{l=k+1}^{N} \widetilde{I(X(t_k) \in B^{(x)}(x_i))} \widetilde{I(\Delta t_{l,k} \in B^{(\tau)}(\tau_j))} [X(t_l) - X(t_k)]^n}{\sum_{k=1}^{T-1} \sum_{l=k+1}^{T} I(X(t_k) \in B^{(x)}(x_i)) I(\Delta t_{l,k} \in B^{(\tau)}(\tau_j))}$$
(7)

⁹³ where $\Delta t_{l,k} := t_l - t_k (> 0)$, and binning in τ is facil-¹⁰⁶ ⁹⁴ itated with a bounded half closed interval $B^{(\tau)}(\tau_i) :=$ $[\max(0, \tau_i - \frac{1}{2}b_{\tau}), \tau_i + \frac{1}{2}b_{\tau}).$ 95

Both HBR and HTBR provide simple methods of es-96 timating moments, however the histogram based nature 97 of both methods results in undesirable properties. 98

1. Histograms assign the same weight to every point 99 inside each bin, resulting in sharp cut-offs between 100

data across the edge of a bin. 101

102 103 104 of bins. 105

C. Kernel Based Regression

To address the deficiencies of the histogram based ap-¹⁰⁸ proach, Lamouroux and Lehnertz [26] introduced kernel 2. The width of the bins sets the resolution length-¹⁰⁹ based regression (KBR) method. For this, each estimate scale. This length-scale dependence is not explicit, 100 at x is assigned an estimate by averaging over all obserit is indirectly determined by the number and range $_{111}$ vations weighted by the distance of the observation X(t) $_{112}$ to x. Moments are then estimated with

$$\hat{M}^{(n)}(x_i, \tau_j) = \frac{\sum_{k=1}^{N} K_h(x_i - X(t_k)) [X(t_k + \tau_j) - X(t_k)]^n}{\sum_{k=1}^{T} K_h(x_i - X(t_k))}$$
(8)

¹¹³ where $K_h(\circ) = K(\circ/h)/h$ is a scaled kernel, h is the ¹¹⁴ bandwidth, and $K(\circ)$ is the kernel function. Here we use ¹¹⁵ the Epanechnikov kernel [27]

$$K(x) = \begin{cases} \frac{3}{4}(1-x^2) & \text{if } x^2 < 1, \\ 0 & \text{otherwise.} \end{cases}$$
(9)

¹¹⁶ for its computationally desirable properties [28].

Kernel-based methods have a number of advantages 130 kernel density estimation is employed 117

¹¹⁸ over histogram based approached, including a higher con-¹¹⁹ vergence rate in the limit of a large number of data points [28, 29]. The introduction of a bandwidth gives an ex-120 121 plicit indication of the length scale of averaging, although 122 there is no optimal bandwidth. However, as points are 123 indexed at set time-shifts τ_i in the future, this method is ¹²⁴ unsuitable for unevenly spaced data.

D. Kernel-Time Based Regression

To extend KBR to unevenly spaced data, kernel den-127 sity estimation is applied to the τ component as well as $_{128}$ the *x* component. We shall refer to this method as kernel-129 time based regression (KTBR). To enable this, bivariate

$$\hat{M}^{(n)}(x_i,\tau_j) = \frac{\sum_{k=1}^{T-1} \sum_{l=k+1}^{T} K_h^{(2)}(x_i - X(t_k),\tau_j - \Delta t_{l,k}) \left[X(t_l) - X(t_k) \right]^n}{\sum_{k=1}^{T-1} \sum_{l=k+1}^{T} K_h^{(2)}(x_i - X(t_k),\tau_j - \Delta t_{l,k})}$$
(10)

125

¹³¹ where $K_h^{(2)}(\circ, \circ)$ is a bandwidth scaled, Euclidian dis-¹³³ where h_x and h_{τ} and the bandwidths in x and τ , re-132 tance 2D kernel

 $K_{h}^{(2)}(x,\tau) = \frac{C}{h_{x}h_{\tau}}K\left(\left(\left(x/h_{x}\right)^{2} + \left(\tau/h_{\tau}\right)^{2}\right)^{\frac{1}{2}}\right)$

¹³⁴ spectively [30]. The prefactor C is defined such that the ¹³⁵ kernel integrates to unity. We use the Epanechnikov ker-136 nel (9), therefore $C = 8/3\pi$.

As the domain in τ only has positive support, kernel 138 estimations at $\tau < h_{\tau}$ can be biased. To account for this, ¹³⁹ we use a boundary correction method [31] that replaces (11) $_{140}$ the application of kernel (11) inside (10), with

$$K_h^{(2)}(x_i - X(t_k), \tau_j - \Delta t_{l,k}) \to \left[K_h^{(2)}(x_i - X(t_k), \tau_j - \Delta t_{l,k}) + K_h^{(2)}(x_i - X(t_k), \tau_j + \Delta t_{l,k}) \right].$$
(12)

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NUMERICAL EXAMPLES III.

To validate the presented methods, we test them on a 142 143 set of three synthetic data-sets.

Α. **Ornstein-Uhlenbeck** process

First we examine an Ornstein-Uhlenbeck process given 145 146 by the drift and diffusion functions

$$D^{(1)}(x) = -x, (13a)$$

$$D^{(2)}(x) = 1. (13b)$$

¹⁴⁷ We consider a discrete time-series sampling of X(t) con-¹⁴⁸ sisting of 10⁷ points with irregular time sampling, $\Delta t \sim$ ¹⁴⁹ $\mathcal{N}(5 \times 10^{-3}, 3.2 \times 10^{-7})$. The solution is integrated [32] 150 with an internal time-step of $\delta t \leq 10^{-4}$, to ensure nu-¹⁵¹ merical accuracy.

To estimate the conditional moments of this data, we 152 ¹⁵³ use three separate methods. First, the moments are es-154 timated using HTBR (6). Sampling in x is performed 155 by 11 evenly spaced bins in the range [-2, 2]. Sampling ¹⁵⁶ in τ is performed by a single bin, [0,0.01]. Here τ is ¹⁵⁷ small enough that the drift and diffusion functions can 158 be directly estimated from the moments

$$\hat{D}^{(n)}(x) \approx \frac{1}{n!\tau} \hat{M}^{(n)}(x,\tau).$$
 (14)



FIG. 1. Results for an Ornstein-Uhlenbeck process. Estimated functions $D^{(1)}(x)$ and $D^{(2)}(x)$ are shown in the top

¹⁵⁹ Second, the moments are estimated using KTBR (10). 160 Evaluation points in x are 30 evenly spaced points in -2, 2], with a bandwidth of $h_x = 0.3$. Sampling in τ is 161 performed with a single evaluation point at $\tau = 5 \times 10^{-3}$. 162 with a bandwidth of $h_{\tau} = 2.5 \times 10^{-3}$. As with HTBR, the 163 direct estimation method (14) is utilized. Finally, to com-164 pare with the two previous methods, naive resampling is 165 performed on the time-series data. The data X(t) is lin-166 ¹⁶⁷ early interpolated to a regular sampling of $\Delta t = 5 \times 10^{-3}$. and then direct estimation is applied with the same bin 169 sampling as the HTBR estimate. The drift and diffu-¹⁷⁰ sion functions are shown in Fig. 1. In this example and all the following examples—KBR performed simi-171 larly to HBR except with finer resolution, and hence will 172 not shown for conciseness. 173

174 175 176 $_{177}$ cally underestimated when using HBR with interpolated $_{206}$ Finally, the data Y(t) is also linearly interpolated to a 178 time-sampling.

Multiplicative process with measurement noise В. 179

Next we examine a multiplicative process with mea-180 ¹⁸¹ surement noise. The drift and diffusion functions are set 182 as

$$D^{(1)}(x) = -x, (15a)$$

$$D^{(2)}(x) = 1 + x^2.$$
(15b)

¹⁸³ Irregularly sampled data X(t) is produced similarly to ¹⁸⁴ example III A, however we also add δ -correlated mea-185 surement noise

$$Y(t) = X(t) + \sigma\zeta(t), \tag{16}$$

 $_{^{186}}$ where σ denotes the amplitude of the measurement noise, 187 and $\zeta \sim \mathcal{N}(0,1)$. We seek to estimate coefficients of 188 parameterised drift and diffusion functions

$$\hat{D}^{(1)}(x) = p_1 + p_2 x, \tag{17a}$$

$$\hat{D}^{(2)}(x) = p_3 + p_4 x + p_5 x^2,$$
 (17b)

using the method of Lind *et al.* [7]. The time-series Y(t)¹⁹⁰ is used to estimate noisy moments, $\hat{M}^{(n)}(y,\tau)$. These ¹⁹¹ moments are separated with linear regression

$$\hat{M}^{(1)}(y_i, \tau_i) \approx \hat{m}_1(y_i)\tau_i + \hat{\gamma}_1(y_i),$$
 (18a)

$$\hat{M}^{(2)}(y_i, \tau_j) \approx \hat{m}_2(y_i)\tau_j + \hat{\gamma}_2(y_i) + \sigma^2,$$
 (18b)

and bottom plots, respectively. Estimates from HBR are from $_{192}$ along with uncertainties $\sigma^2_{\hat{m}_1}(y_i), \sigma^2_{\hat{\gamma}_1}(y_i)$, etc... These interpolated data. ¹⁹⁴ $m_1(y), \gamma_1, m_2(y)$, and γ_2 , which depend solely on param-¹⁹⁵ eters p_1, \ldots, p_5 , and σ , see Lind *et al.* [7] for more details. ¹⁹⁶ The parameters vary the fit function

$$F = \sum_{i=1}^{8} \left\{ \frac{[\hat{m}_{1}(y_{i}) - m_{1}(y_{i})]^{2}}{\sigma_{\hat{m}_{1}}^{2}(y_{i})} + \frac{[\hat{\gamma}_{1}(y_{i}) - \gamma_{1}(y_{i})]^{2}}{\sigma_{\hat{\gamma}_{1}}^{2}(y_{i})} + \frac{[\hat{m}_{2}(y_{i}) - m_{2}(y_{i})]^{2}}{\sigma_{\hat{m}_{2}}^{2}(y_{i})} + \frac{[\hat{\gamma}_{2}(y_{i}) - \gamma_{2}(y_{i}) - \sigma^{2}]^{2}}{\sigma_{\hat{\gamma}_{2}}^{2}(y_{i})} \right\}, \quad (19)$$

¹⁹⁷ which is minimised using simulated annealing [33].

For HTBR, sampling in y is performed with 50 equally 198 ¹⁹⁹ spaced bins in the range [-6, 6]. Sampling in τ is per-200 formed by 8 equally spaced bins with centers from $\tau_1 =$ $_{201} 5 \times 10^{-3}$ to $\tau_8 = 4 \times 10^{-2}$, with bin-widths $b_{\tau} = 5 \times 10^{-3}$. $_{202}$ For KTBR, evaluation points in x are 50 equally spaced We find that the estimates of drift and diffusion func- 203 points in the range [-6, 6], with $h_x = 0.18$. Sampling tions are in good accordance with the true values for 204 in time is performed with 8 equally spaced points from both HTBR and KTBR. These functions are systemati- $_{205} \tau_1 = 5 \times 10^{-3}$ to $\tau_8 = 4 \times 10^{-2}$, with $h_{\tau} = 2.5 \times 10^{-3}$. 207 regular sampling of $\Delta t = 5 \times 10^{-3}$ and then processed ²⁰⁸ in the same way as the HTBR example. The optimised ²⁰⁹ parameters are shown in Table I.

The parameters of the drift and diffusion functions are very close to the true values for both HTBR and KTBR. For HBR with interpolated time-sampling, while some estimated well, the absolute gradient of the drift, the constant diffusion term, and the quadratic term are all overestimated. Finally the measurement noise amplitude σ is underestimated.

217 C. Bistable system with correlated noise

Finally we examine a bistable process X(t) driven by 219 correlated noise $\eta(t)$ [34]. This system is defined as

$$\frac{d}{dt}X = D^{(1)}(X) + \sqrt{2D^{(2)}(X)}\eta(t), \qquad (20a)$$

$$\frac{d}{dt}\eta = -\frac{1}{\theta}\eta + \frac{1}{\theta}\xi(t), \qquad (20b)$$

 $_{220}$ where θ is the correlation time of the noise. The drift $_{221}$ and diffusion functions are set as

$$D^{(1)}(x) = x - \frac{1}{2}x^3,$$
 (21a)

$$D^{(2)}(x) = 1 + \frac{1}{20} \ln \cosh 2x,$$
 (21b)

²²² and the correlation time is $\theta = 0.01$. An unevenly spaced ²²³ time-series is produced in the same way as example III A, ²²⁴ however only X(t) is observed.

We estimate the drift and diffusion functions using the 226 non-parametric method of [34]. This involves compar-227 ing estimates of moments, $\hat{M}^{(n)}(x,\tau)$, with theoretical 228 estimates

$$M^{(n)}(x,\tau) \approx \sum_{i=1}^{3} \lambda_i^{(n)}(x) r_i(\tau,\theta), \qquad (22)$$

TABLE I. True and optimised parameter values for a multiplicative process with measurement noise. Parameters are rounded to either 2 significant figures or at least 2 decimal places. The HBR column represents results from interpolated Y(t) data. We note that entering the true parameter values into function (19) with estimates gathered from interpolated HBR result in a value of F two orders of magnitude higher than the optimised minimum.

Parameter	True	HTBR	KTBR	HBR
p_1	0	-0.0050	-0.0040	-0.014
p_2	-1	-0.99	-1.00	-1.48
p_3	1	0.99	1.00	1.62
p_4	0	0.0062	0.013	0.0020
p_5	1	0.97	0.98	1.11
σ	1	1.00	1.00	0.76



FIG. 2. Results for a bistable system with correlated noise. As Fig. 1.

²²⁹ where functions r_i are prescribed basis functions and ²³⁰ $\lambda_i^{(n)}(x)$ are the corresponding coefficients. Coefficients ²³¹ are found through least squares, and then $\lambda_1^{(n)}(x)$ are ²³² directly related to estimates of the drift and diffusion ²³³ functions at points in x. For a detailed description of the ²³⁴ method, see Lehle and Peinke [34].

For HTBR, sampling in x is performed by 16 equally spaced bins in the range [-2, 2]. Sampling in τ is performed by 30 spaced bins with from $\tau_1 = 5 \times 10^{-3}$ to $\tau_{30} = 1.5 \times 10^{-1}$, with bin-widths $b_{\tau} = 5 \times 10^{-3}$. For KTBR, evaluation points in x are 50 equally spaced points in the range [-2, 2], with $h_x = 0.24$. Sampling $\tau_1 = 5 \times 10^{-3}$ to $\tau_{30} = 1.5 \times 10^{-1}$, with $h_{\tau} = 2.5 \times 10^{-3}$. Finally, the data X(t) is also linearly interpolated to a regular sampling of $\Delta t = 5 \times 10^{-3}$ and then processed in solute error between estimated moments $\hat{M}^{(n)}(x,\tau)$ and fitted moments (22) is on the order of 10^{-5} . The drift solute fituation for the same shown in Fig. 2. 251 252 253 254 estimated. 255

IV. APPLICATION TO 256 PALEOCLIMATOLOGICAL DATA 257

258 259 260 foraminifera [24, 35]. Of particular interest are large and ₃₁₀ suggestive. 261 rapid negative excursions in carbon isotope ratios, δ^{13} C, 311 262 263 264 265 266 267 climate response to hyperthermal events, and provide $_{317}$ plays characteristic excursions to low δ^{13} C values. 268 an analogue to modern anthropogenic forcing [44–47]. ³¹⁸ Beyond reproducing observations, the form of the esti-269 270 Recently Arnscheidt and Rothman [48] suggested that 319 mated drift and diffusion functions can give insight into 271 the time-variability of these records can be modelled as 320 physical processes. The drift term indicates an average $_{272}$ stochastic processes, invoking a single-variable correlated $_{321}$ relaxation timescale of $\tau_{\text{eff}} = 47$ kyr, possibly reflecting ²⁷³ additive-multiplicative (CAM) process

$$\frac{d}{dt}X = -\frac{1}{\tau_{\text{eff}}}X + v\left(X - c\right)\Gamma(t), \qquad (23)$$

²⁷⁴ where τ_{eff} , v, and c are constants and $\Gamma(t)$ is white noise [49–53]. A non-parametric verification of this CAM hy-275 276 pothesis has been unreachable with previous estimation methods, as the δ^{13} C record is unevenly sampled in time. 277 In this section, we apply KTBR to a section of this un- 330 278 279 evenly sampled paleoclimate record.

We choose a stationary section of the record, from 53 280 Ma to 46 Ma, containing a series of representative ex-281 282 Thermal Maximum [48, 54]. The sampling in this time-283 284 285 $_{287}$ range [-0.8, 0.5], with $h_x = 0.4$. Sampling in time is per- $_{338}$ ment noise or non-Markovian processes, both HTBR and 288 ²⁸⁹ to $\tau_{30} = 116$ kyr, with $h_{\tau} = 5$ kyr. The higher or-³⁴⁰ rate estimates of the original drift and diffusion functions. ²⁹⁰ der moments in $M^{(4)}(x,\tau) \simeq 3 \left(M^{(2)}(x,\tau)\right)^2$ are eval-³⁴¹ Additionally, KTBR is applied to a series of irregularly ²⁹¹ uated using (10) and are comparable, showing a small ³⁴² spaced paleoclimatological measurements. The inferred $_{292}$ error of $\sim 5 \times 10^{-3}$, validating the continuity of the $_{343}$ model is able to produce similar time-dependent behavior ²⁹³ record [55, 56]. To estimate the drift and diffusion func- ³⁴⁴ and statistics, revealing underlying dynamics. ²⁹⁴ tions from these moments, we use the approach of Lehle ³⁴⁵ ²⁹⁵ and Peinke [34], while the correlation time is estimated ³⁴⁶ While example III A shows that interpolation results in 296 through a grid search, $\theta \approx 0.4$ kyr. The moments are fit 347 an absolute underestimate in the magnitude of estimated 297 well, with an absolute error between estimated moments 348 drift and diffusion functions, example III B shows the op- $\hat{M}^{(n)}(x,\tau)$ and fitted moments (22) on the order of 10^{-4} . 349 posite bias (with an underestimated measurement noise 299 The estimated drift and diffusion functions are shown in 350 amplitude). Interpolation in example IIIC has little ef-300 Fig. 4.

The estimates of the drift and diffusion functions com- 301 The drift function has a strongly linear form, and is pare well with the true values for both HTBR and KTBR. $_{302}$ well approximated by the CAM model (23) with τ_{eff} = For the interpolated HBR the drift function is reproduced $_{303}$ 47 kyr ($R^2 = 0.98$). For the diffusion function, while a well, whilst the diffusion function is systematically under- $_{304}$ CAM model (23) with the coefficients v = -3.2 and c = $_{305}$ -1.2 falls within the confidence intervals ($R^2 = 0.67$), we 306 cannot reject a likely piecewise diffusion of

$$D^{(2)}(x) = \begin{cases} p_1 + p_2(x - p_3) & \text{if } x \le p_3, \\ p_1 & \text{otherwise,} \end{cases}$$
(24)

Paleoclimate proxies preserve a record of Earth's cli- $_{307}$ with best fitting coefficients of $p_1 = 3.30, p_2 = -11.50,$ mate variability. This variability is commonly studied $_{308}$ and $p_3 = -0.36$ ($R^2 = 0.99$), although we note that this through carbon and oxygen isotopes records from benthic 309 parameterization is not unique, and only meant to be

To demonstrate that this linear drift and piecewise difthroughout the Cenozoic [36-40]. These excursions have $_{312}$ fusion cannot be rejected by the data, we numerically been interpreted as "hyperthermal" warming events, and 313 integrate a sample path with these functions. The timeare speculated to be linked to the release of isotopically 314 series and distributions of the original data and SDE depleted organic carbon from permafrost or methane 315 simulation are shown in Fig. 3. The SDE matches the clathrates [41-43]. Such records offer insights to Earth's $_{316}$ skewed distribution of the original record, and also dis-

> 322 the stabilizing feedback of weathering of carbonate and ³²³ silicate rocks [e.g. 58]. The piecewise nature of the dif-324 fusion suggests a "tipping-point" beyond which fluctu-325 ations are amplified, indicating an imbalance in typical ³²⁶ weathering feedback mechanisms [59–61]. Further work 327 should investigate whether this behavior is reflected in ³²⁸ related oxygen isotope records, as well as other epochs in 329 the Cenozoic.

DISCUSSION AND CONCLUSION v.

331 We present two methods to estimate conditional mo-332 ments from irregularly spaced time-series. These mocursions but excluding the anomalous Paleocene–Eocene 333 ments are used alongside parametric and non-parametric ³³⁴ methods to facilitate the accurate estimation of drift and span is approximately log-normally distributed, with 335 diffusion functions of stochastic differential equations. $\log_{10} \Delta t \sim \mathcal{N}(-2.7, 0.2)$. To calculate moments, eval- 336 We demonstrate this for three numerical examples, in uation points in x are 50 equally spaced points in the $_{337}$ a number of settings. Even in the presence of measureformed with 30 equally spaced points from $\tau_1 = 3.5$ kyr $_{339}$ KTBR are able to produce moments that result in accu-

> This study also illustrates the dangers of interpolation. ³⁵¹ fect on the estimated drift function, but not the diffusion



FIG. 3. Climate variations in the Early Eocene, recorded in benthic foraminiferal δ^{13} C data [24]. A running mean of 1-Ma has been subtracted to remove longer-scale climate effects. Time-series data and a simulated trajectory are shown in the top and bottom plots, respectively. Histograms are shown in the right plot. By convention, axes for $\delta^{13}C$ are reflected.

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352 function, as is the case with weak measurement noise [62]. 353 Overall, the bias may be small because longer time-scale 354 information is included in the inversion, or the interpo-355 lation bias may be masked by the non-Markovian nature 356 of the process. 357

In addition to being applicable to a wide class of 358 stochastic systems, these methods could allow for the 359 handling of other non-ideal sampling conditions. Data 360 with inconvenient gaps, for example, can be approached 361 by this outlook when framed as irregularly sampled pro-362 cesses. This method is also capable of estimating higher-363 order moments (n > 2 in (7) and (10)), which are useful 364 for analysis of jump-diffusion processes [63]. On the effect 365 of number of data points on the robustness of the esti-366 mated drift and noise functions, as HTBR and KTBR are 384 367 368 inherently frequency based calculations we expect them 385 two anonymous reviewers for their helpful comments and ³⁷⁰ The methods here are demonstrated in one dimension, ³⁸⁷ ence Foundation (EAR-1644644).

function. These smaller errors average out for the drift $_{371}$ however extensions to higher dimensions is straightfor-372 ward.

> 373 In the broader picture for stochastic process estima-³⁷⁴ tion, the methods presented here extend time-shift condi-³⁷⁵ tioning from index-based to histogram and kernel based methods. This reflects similar work regarding sample autocorrelation function estimators [12, 18, 66]. We note 378 that it is not strictly required to match similar conditioning on x and τ . In theory hybrid methods could be used, 379 $_{380}$ for example, kernel conditioning in x combined with his- $_{381}$ togram conditioning in τ , however it is not clear if such an approach would have significant advantages. 382 383

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FIG. 4. Results for early Eocene δ^{13} C record. Estimated drift and diffusion functions $D^{(1)}(x)$ and $D^{(2)}(x)$ are shown in the top and bottom plots, respectively. Best estimates are plotted as black lines, and bootstrapped 95% confidence intervals are shown as grey regions [57].

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