Statistical mechanics of time series

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Natural and social multivariate systems are commonly studied through sets of simultaneous and time-spaced measurements of the observables that drive their dynamics, i.e., through sets of time series. Typically, this is done via hypothesis testing: the statistical properties of the empirical time series are tested against those expected under a suitable null hypothesis. This is a very challenging task in complex interacting systems, where statistical stability is often poor due to lack of stationarity and ergodicity. Here, we describe an unsupervised, data-driven framework to perform hypothesis testing in such situations. This consists of a statistical mechanical theory - derived from the Maximum Entropy principle - for ensembles of time series designed to preserve, on average, some of the statistical properties observed on an empirical set of time series. We showcase its possible applications on a set of stock market returns from the NYSE.

I. INTRODUCTION

Hypothesis testing lies at the very core of the scientific method. In its general formulation, it hinges upon contrasting the observed statistical properties of a system with those expected under a null hypothesis. In particular, hypothesis testing allows to discard potential models of a system when empirical measurement that would be exceedingly unlikely under them are made.

However, there is often no theory to guide the investigation of a system’s dynamics. What is worse, in many practical situations one may be given a single - and possibly unreproducible - set of experimental data. This is indeed the case when dealing with most complex systems, whose collective dynamics often are neither stationary nor ergodic, ranging from climate \textsuperscript{[1,2]} to brain activity \textsuperscript{[3]} and financial markets \textsuperscript{[4-6]}. This, in turn, makes hypothesis testing in complex systems a very challenging task, that potentially prevents from assessing which properties observed in a given data sample are “untypical”, i.e, unlikely to be observed again in a sample collected at a different point in time.

This issue is usually tackled by constructing ensembles of artificial time series sharing some characteristics with those generated by the dynamics of the system under study. This can be done either via modelling or in a purely data-driven way. In the latter case, the technique most frequently used by both researchers and practitioners is bootstrapping \textsuperscript{[7,8]}, which amounts to generating partially randomised versions of the available data via resampling, that can then be used as a null benchmark to perform hypothesis testing. Depending on its specificities, bootstrapping can account for autocorrelations and cross-correlations in time series sampled from multivariate systems. However, it relies on assumptions, such as sample independence and some form of stationarity \textsuperscript{[9]}, which limit its power when dealing with complex systems.

As far as model-driven approaches are concerned, the literature is extremely vast \textsuperscript{[10]}. Broadly speaking, modelling approaches rely on a priori structural assumptions for the system’s dynamics, and on identifying the parameter values that best explain the available set of observations within a certain class of models (e.g., via Maximum Likelihood \textsuperscript{[10]}). A widely used class for multivariate time series is that of autoregressive models, such as VAR \textsuperscript{[11]}, ARMA \textsuperscript{[12]}, and GARCH \textsuperscript{[13]}, which indeed were originally introduced, among other reasons, to perform hypothesis testing \textsuperscript{[12]}. In such models, the future values of each time series are given by a linear combination of past values of one or more time series, each characterised by their own idiosyncratic noise to capture the fluctuations of individual variables. Such a structure is most often dictated by its simplicity rather than by first principles. As a consequence, once calibrated, autoregressive models produce rather constrained ensembles of time series that do not allow to explore scenarios that differ substantially from those observed empirically.

Here we propose a novel formalism to perform hypothesis testing on sets of time series based on the ensemble theory of statistical mechanics. Starting from the Maximum Entropy principle, we will introduce a (gran)canonical ensemble of correlated time series subject to constraints based on the properties of an empirically observed set of measurements. This, in turn, will result in a multivariate probability distribution which allows to unbiasedly sample values centred on such measurements, which represents the main contribution of this paper. The theory we propose in the following shares some similarities with the canonical ensemble of complex networks \textsuperscript{[14-17]}, and, as we will show, inherits its powerful calibration method based on Likelihood maximization \textsuperscript{[18]}.

The paper is organized as follows. In Section \textsuperscript{[1]} we outline the general formalism of our approach. As a formative example, in Section \textsuperscript{[2]} we show how the methodology introduced can be used to reconstruct an unknown probability density function from repeated measurements over time. In Section \textsuperscript{[3]} we proceed to study the most general case of multivariate time series, showing how our

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approach recovers collective statistical properties of interacting systems without directly accounting for such interactions in the set of constraints imposed on the ensemble. In Section VI we briefly mention an interesting analogy between our approach and Jaynes’ Maximum Caliber principle [19]. In Section VI we conclude with a final discussion.

II. GENERAL FRAMEWORK DESCRIPTION

Let $\mathcal{W}$ be the set of all real-valued sets of $N$ time series of length $T$ (i.e., the set of real-valued matrices of size $N \times T$), and let $\mathcal{W} \in \mathcal{W}$ be the empirical set of data we want to perform hypothesis testing on (i.e., $\mathcal{W}_{it}$ stores the value of the $i$-th variable in the system sampled at time $t$, so that $\mathcal{W}_{it}$ for $t = 1, \ldots, T$ represents the sampled time series of variable $i$). Our aim is to define a probability density function $P(W)$ on $\mathcal{W}$ such that the expectation values $\langle O_i(W) \rangle$ of a set of observables ($\ell = 1, \ldots, L$) coincide with the value $O_\ell$ of the corresponding quantity as empirically measured from $\mathcal{W}$.

Following Boltzmann and Gibbs, we can achieve the above by invoking the Maximum Entropy principle, i.e., by identifying $P(W)$ as the distribution that maximises the entropy functional $S(W) = -\sum_{W \in \mathcal{W}} P(W) \ln P(W)$, while satisfying the $L$ constraints $\langle O_i(W) \rangle = \sum_{W \in \mathcal{W}} O_i(W) P(W) = \overline{O}_i$ and the normalisation condition $\sum_{W} P(W) = 1$. As is well known [20] [21], this reads

$$P(W) = \frac{e^{-H(W)}}{Z}, \quad (1)$$

where $H(W) = \sum_{\ell} \beta_\ell O_\ell(W)$ is the Hamiltonian of the system, $\beta_\ell (\ell = 1, \ldots, L)$ are Lagrange multipliers introduced to enforce the constraints, and $Z = \sum_{W} e^{-H(W)}$ is the partition function of the ensemble, which verifies $\langle O_i(W) \rangle = \partial \ln Z / \partial \beta_i$, $\forall \ell$.

Figure I provides a sketch representation of the ensemble theory just introduced. The rationale of enforcing the aforementioned constraints is that of finding a distribution $P(W)$ that assigns low probability to regions of the phase space $W$ where the observables associated to the Lagrange multipliers $\beta_\ell$ take values that are exceedingly different from those measured in the empirical set $\mathcal{W}$, and high probability to regions where some degree of similarity with $\mathcal{W}$ is retained [22]. This, in turn, allows to test whether other properties (not encoded in any of the constraints) of $\mathcal{W}$ are statistically significant by measuring how often they appear in instances drawn from the ensemble. The existence and uniqueness of the Lagrange multipliers ensuring the ensemble’s ability to preserve the constraints $O_\ell$ is a well known result, and they are equivalent to those that would be obtained from the maximization of the Likelihood of drawing the empirical matrix $\mathcal{W}$ from the ensemble [22].

III. SINGLE TIME SERIES

As a warm up example to showcase our approach, we are first going to apply it to univariate stationary systems. In particular, we shall reconstruct an unknown probability density function from univariate time series data.

Let us then consider an $1 \times T$ empirical data matrix $\mathcal{W}$ coming from $T$ repeated sampling of an observable of the system under consideration. If the processes is stationary and time-independent, this is equivalent to sampling $T$ times a random variable from its given, unknown, distribution and therefore the task of the model can be translated into reconstructing the unknown distribution given the data. Let us consider a vector $\alpha \in [0,1]^d$ and the associated empirical $\alpha$-quantiles $\overline{q}_\alpha$, calculated on $\mathcal{W}$. In order to fully capture the information present in the data $\mathcal{W}$, we are going to constrain our ensemble to preserve, as averages, one or more quantities derived from $\overline{q}_\alpha$. Possible choices may be:

- The number of data points falling within each pair of empirically observed adjacent quantiles:
  $$\overline{N}_{\alpha_i} = \sum_t \Theta(\mathcal{W}_t - \overline{q}_{\alpha_{i-1}}) \Theta(\mathcal{W}_t + \overline{q}_{\alpha_i})$$
- The cumulative values of the data points falling within each pair of adjacent quantiles:
  $$\overline{M}_{\alpha_i} = \sum_t \mathcal{W}_t \Theta(\mathcal{W}_t - \overline{q}_{\alpha_{i-1}}) \Theta(\mathcal{W}_t + \overline{q}_{\alpha_i})$$
- The cumulative squared values of the data points falling within each pair of adjacent quantiles:
  $$\overline{M}^2_{\alpha_i} = \sum_t \mathcal{W}_t^2 \Theta(\mathcal{W}_t - \overline{q}_{\alpha_{i-1}}) \Theta(\mathcal{W}_t + \overline{q}_{\alpha_i})$$

In each of the above constraints we assumed $i = 2, \ldots, d$, and we have used $\Theta(\cdot)$ to indicate Heaviside’s step function (i.e., $\Theta(x) = 1$ for $x > 0$, and $\Theta(x) = 0$ otherwise). In general we are not required to use the same $\alpha$ for all constraints, for example we can freely choose to impose on the ensemble the ability to preserve $\overline{N}_{\alpha_i}, \forall i \in [1,d]$ together with the total cumulative values $\overline{M} = \sum_i \overline{M}_{\alpha_i}$, and total cumulative squared values $\overline{M}^2 = \sum_i \overline{M}^2_{\alpha_i}$, as well as each $\overline{M}_{\alpha_i}$ and $\overline{M}^2_{\alpha_i}$ separately.

A defined set of constraints will lead to a different Hamiltonian, to a different number of Lagrange multipliers and therefore to a different statistical model. If we choose, for example, to adopt all the constraints specified above, the Hamiltonian $H$ of the ensemble will depend on a total of $3(d - 1)$ parameters:

$$H(W) = \sum_{i=1}^d \sum_{t=1}^T \left[ a_i + W_t \alpha_i + W_t^2 \beta_i \right] \times$$
$$\times \Theta(\mathcal{W}_t - \overline{q}_{\alpha_{i-1}}) \Theta(\mathcal{W}_t + \overline{q}_{\alpha_i}). \quad (2)$$

The freedom to choose the amount of constraints of course comes with a cost. First of all, it must be noted that the Likelihood of the data matrix $\mathcal{W}$ will be in general a non linear function of the Lagrange multipliers and therefore of the constraints. These latter can vary both...
Starting from an empirical set of time series $W$, we construct its unbiased randomization by finding the probability measure $P(W)$ on the phase space $W$ which maximises Gibbs’ entropy while preserving the constraints $\{O_l(W)\}_{l=1}^L$. The probability distribution $P(W)$ depends on $L$ parameters that can be found by maximising the likelihood of drawing $W$ from the ensemble. In the Figure, orange, turquoise and black are used to indicate positive, negative or empty values of the entries $W_{it}$, respectively, while brighter shades of each color are used to display higher absolute values. As it can be seen, the distribution $P(W)$ assigns higher probabilities to those sets of time series that are more consistent with the constraints and therefore more similar to $W$. See [16] for a similar chart in the case of the canonical ensemble of complex networks.

In magnitude (by choosing different values for the entries of $\alpha$) and in size (by choosing a different $d$). In general, tackling the issue of finding the optimal positions for the constraints, given their number $d$, can become highly not trivial and goes out of the scope of the present work. However, loosely speaking, the Likelihood of finding $W$ after a random draw from the defined ensemble is an increasing function of the number constraints, coherently with the idea that a larger number of parameter leads to better statistics on the data used to train the model. As a result, in order to avoid overfitting, given a set of constraints, we can compare different values of $d$ by using standard model selection techniques such as the Bayesian [24] or Akaike information criteria [21].

In the following we are going to show how to apply the methodology just outlined to a synthetic dataset. For this example, let us assume that the data generating process follows a balanced mixture of a truncated standard Normal distribution and a truncated Student’s $t$-distribution with $\nu = 5$ degree of freedom. The two models we are going to use to build the respective ensembles are specified by the following Hamiltonians:

$$H_1 = \sum_i [\alpha_i N_{\alpha_i} + \beta_i M_{\alpha_i}]$$

$$H_2 = \sum_i [\alpha_i N_{\alpha_i} + \beta M_{\alpha_i} + \gamma M_{\alpha_i}^2]$$

The model resulting from $H_1$ will have a total of $2(d-1)$ parameter and will preserve the average number of data point contained within each pair of adjacent quantiles together with their cumulative values, while the model coming from $H_2$ will be characterised by $d+1$ parameters and will preserve the average number of data point contained within each pair of adjacent quantiles together with the overall mean and variance calculated across all data points. In order to find the Lagrange multipliers able to preserve the chosen constraints, we first need to find the partitions functions of the two ensembles $Z_{1,2} = \sum_W e^{-H_{1,2}(W)}$. In order to do that, we first need to specify the sum over the phase space:

$$\sum_{W \in W} \equiv \prod_{t=1}^T \int_{Q_{\alpha_t}} dw_t .$$
The above expression leads to the following partition functions (in Appendix A we present a detailed derivation of the partition function shown in Section IV; the following result can be obtained with similar steps):

\[
Z_1 = \prod_{t=1}^{T} \sum_{i=1}^{d-1} e^{-\alpha_i} e^{-\beta_i \gamma_{a_i}} - e^{-\beta_i \gamma_{a_{i+1}}}
\]

\[
Z_2 = \prod_{t=1}^{T} \sum_{i=1}^{d-1} \sqrt{\frac{\pi}{4\gamma}} e^{\frac{\beta_i^2}{2\gamma} - \alpha_i} \left( -\text{erf} \left( \frac{\beta_i + 2\gamma \gamma_{a_i}}{2\gamma} \right) + \text{erf} \left( \frac{\beta_i + 2\gamma \gamma_{a_{i+1}}}{2\gamma} \right) \right)
\]

where with erf we indicate the Gaussian error function $\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$.

In Figure 2 we show how the models resulting from the partition functions $Z_1$ and $Z_2$ are able to reconstruct the underlying true distribution starting from different amount of information (i.e. different sample sizes) and quantiles vector set to $\bar{\theta} = [-\infty, 0.025; 0.05; 0.5; 0.75; \infty]$ (the steps to obtain the ensemble’s probability density function from its partition function are outlined in Appendix A for the case discussed in Section IV). First of all we note that, as expected, estimating the unknown distribution from more data gives estimates that are closer to the real underlying distribution. Moreover, looking at Figure 2 we can qualitatively see that the model described by $Z_1$ does a better job than $Z_2$ at inferring the underlying pdf. We can verify both statements more quantitatively by calculating the Kullback-Leibler divergence of the probability density function. We can verify both statements more quantitatively by calculating the Kullback-Leibler divergence of the probability density function.

\[
AIC = T \cdot \ln \left( \frac{1}{T} \sum_{i=1}^{T} L_{\text{empirical}} \right) + 2k
\]

where with $L_{\text{empirical}}$ we indicate the likelihood function for the empirical data vector set $\bar{\theta}$.

\[
KL \left( \tilde{P}, P \right) = \int_{-\infty}^{\infty} \tilde{P}(W) \log \frac{\tilde{P}(W)}{P(W)} dW
\]

\[
W_{it} > 0 \quad (W_{it} < 0) \quad \text{indicates that the time } t \text{ value of the } i^{\text{th}} \text{ variable is higher (lower) than its empirical mean. Also, without loss of generality, let us assume that } W_{it} \in \mathbb{R}_{\neq 0}, \text{ and that } W_{it} = 0 \text{ indicates missing data. For later convenience, let us define } A^\pm = \Theta(\pm W) \text{ and } w^\pm = \pm W \Theta(\pm W) \text{ (we shall denote the corresponding quantities measured on the empirical set as } \bar{A}^\pm \text{ and } \bar{w}^\pm \text{), and let us constrain the ensemble to preserve the values of the following observables:}
\]

- The number of positive (above-average) and negative (below-average) values $N^+ = \sum_i A^+_i$, and the number of missing values $N^- = T - N^+ - N^-$ recorded for each time series ($i = 1, \ldots, N$).

- The cumulative positive and negative values recorded for each time series: $\bar{A}^+_i = \sum_t A^+_it$ ($i = 1, \ldots, N$).

- The number of positive, negative, and missing values recorded at each sampling time: $\bar{M}^+_t = \sum_i A^+_it$, $\bar{M}^-_t = N - \bar{M}^+_t - \bar{M}^-_t$ ($t = 1, \ldots, T$).

- The cumulative positive and negative value recorded at each sampling time: $\bar{W}^+_t = \sum_i \overline{W}^+_it$ ($t = 1, \ldots, T$).

The above list amounts to $8(N + T)$ constraints, and the Hamiltonian $H$ depends on the very same number of parameters:

\[
H(W) = \frac{1}{2} \sum_{i=1}^{N} \sum_{t=1}^{T} \left[ (\alpha_i^N + \alpha_i^T) A^+_it + (\beta_i^N + \beta_i^T) A^-_it \right. \nonumber \\
+ \left. (\gamma_i^N + \gamma_i^T) w^+_it + (\sigma_i^N + \sigma_i^T) w^-_it \right]
\]

where we have introduced the Lagrange multipliers associated to all constraints. This choice for the Hamiltonian naturally generalizes the framework introduced in [23].

In order to calculate the partition function $Z = \sum W e^{-H(W)}$, we first need to properly specify the sum over the phase space. Given the matrix representation we have chosen for the system, and the fact that $w^+_it = w^-_it A^+_it$, this reads:

\[
\sum_{W \in W} = \prod_{i=1}^{N} \prod_{t=1}^{T} \int_{-\infty}^{+\infty} dw^-_it = \nonumber \\
= \prod_{i=1}^{N} \prod_{t=1}^{T} \sum_{(A^+_it, A^-_it) = (1,0) (0,0)} \int_{0}^{+\infty} dw^-_it \int_{0}^{+\infty} dw^+_it
\]

where the sum specifies whether the entry $A^-_it$ stores a positive, negative or missing value, respectively. This signifies that negative and positive events (this in general holds for any discretization of the
First of all, the partition function factorises into the product of independent factors (see Appendix A). The above distribution allows comparisons between empirical PDFs (shown as histograms) and PDFs reconstructed with our ensemble approach from the Hamiltonians in Eq. (9), shown in red and orange respectively. In both panels the true empirical PDF is shown as a black dashed line. a) Results obtained by calibrating the models on 40 data points. b) Results obtained by calibrating the models on 4000 data points. See the main text for additional information about the quality of the models.

The above expression leads to the following partition function (see Appendix A):

$$Z = \sum_{W \in W} e^{-H(W)} = \prod_{i=1}^{N} \prod_{t=1}^{T} Z_{it}$$

$$= \prod_{i=1}^{N} \prod_{t=1}^{T} \left[ 1 + \frac{e^{-(\alpha_i^N + \alpha_i^T)}}{\alpha_i^N + \alpha_i^T} + \frac{e^{-(\beta_i^N + \beta_i^T)}}{\beta_i^N + \beta_i^T} \right]$$

(9)

$$= \prod_{i=1}^{N} \prod_{t=1}^{T} \left( 1 + e^{\frac{\alpha_i^N - \alpha_i^T}{\beta_i^N - \beta_i^T}} + e^{\frac{\beta_i^N - \beta_i^T}{\alpha_i^N - \alpha_i^T}} \right),$$

where the quantities $\mu_i^{1,2}$, $\epsilon_i$, and $T_i$ are functions of the Lagrange multipliers (see Appendix A).

Some considerations about Eq. (9) are now in order. First of all, the partition function factorises into the product of independent factors $Z_{it}$, and therefore into a collection of $N \times T$ statistically independent sub-systems. However, it is crucial to notice that their parameters (i.e., the Lagrange multipliers) are coupled through the system of equations specifying the constraints ($\partial \ln Z / \partial \beta_{it}$, $\forall t$). As we shall demonstrate later, this ensures that part of the original system’s correlation structure is retained within the ensemble. Moreover, with the above positions, the aforementioned physical analogy becomes clear: the system described by Eq. (9) can be interpreted as a system of $N \times T$ orbitals with energies $\epsilon_{it}$ and local temperatures $T_{it}$ that can be populated by fermions belonging to two different species characterised by local chemical potentials $\mu_{it}^1$ and $\mu_{it}^2$, respectively.

From the partition function in Eq. (9) we can finally calculate the probability distribution $P(W)$:

$$P(W) = \prod_{i=1}^{N} \prod_{t=1}^{T} [P_{it}^+ A_{it}^+ \left[ P_{it}^- - P_{it}^+ \right]]^{-A_{it}^- A_{it}^+}$$

$$\times \left[ Q_{it}^{-}(w_{it}^+) \right]^A_{it}$$

(10)

where $P_{it}^\pm$ and $Q_{it}^{-}(w_{it}^+)$ are functions of the Lagrange multipliers (see Appendix A) and correspond, respectively, to the probability of drawing a positive (negative) value for the $i$-th variable at time $t$ and to its probability distribution.

As an example application of the ensemble defined above, let us consider the daily returns of the most capitalized NYSE stocks over $T = 560$ trading days (spanning October 2016 - November 2018). In this example, the aforementioned constraints force the ensemble to preserve, on average, the number of positive and negative returns and the overall positive and negative return for each time series and for each trading day, leading to $6(N \times T)$ constraints. When these constraints are enforced, an explicit expression for the marginal distributions can be obtained (see Appendix A):

$$P(W_{it} = x) = (1 - P_{it}^+) \lambda_{it}^+ e^{\lambda_{it}^- x} \Theta(-x) +$$

$$+ P_{it}^+ \lambda_{it}^- e^{-\lambda_{it}^+ x} \Theta(x),$$

(11)

where $\lambda_{it}^\pm$ are also functions of the Lagrange multipliers (see Appendix A). The above distribution allows
both to efficiently sample the ensemble numerically and to obtain analytical results for several observables.

Figure 3 and Tables I and II illustrate how the above first-moment constraints translate into explanatory power of higher-order statistical properties. Indeed, in the large majority of cases, the empirical return distributions of individual stocks and trading days and their higher-order moments (variance, skewness, and kurtosis) are statistically compatible with the corresponding ensemble distributions, i.e., with the distributions of such quantities computed over large numbers (10^6 in all cases shown) of time series independently generated from the ensemble. Notably, this is the case without constraints explicitly aimed at enforcing such level of agreement. This, in turn, further confirms that the ensemble can indeed be exploited to perform reliable hypothesis testing by sampling random scenarios that are however closely based on the empirically available data.

In that spirit, in Figure 4 we show an example of ex-post anomaly detection, where the original time series of a stock is plotted against the 95% confidence intervals obtained from the ensemble for each data point $W_{it}$. As it can be seen, the results are non-trivial, since the returns flagged as anomalous are not necessarily the largest ones in absolute value. This is because the constraints imposed on the ensemble reflect the collective nature of

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FIG. 3: Comparisons between empirical statistical properties and ensemble averages. In these plots we demonstrate the model’s ability to partially reproduce non-trivial statistical properties of the original set of time series that are not explicitly encoded as ensemble constraints. a) Empirical vs ensemble average values of the variances of the returns calculated for each stock (red dots) and each day (blue dots). b) Same plot for the skewness of the returns. c) Comparison between the ensemble and empirical cumulative distributions (and associated survival functions) for the returns of two randomly selected stocks (Microsoft and Pepsi Company). Dots correspond to the cumulative distribution and survival functions obtained from the empirical data. Dashed lines correspond to the equivalent functions obtained by pooling together 10^6 time series independently generated from the ensemble. Different colours refer to different stocks as reported in the legend. Remarkably, a Kolmogorov-Smirnov test (0.01 significance) shows that 92% of the stocks returns empirical distributions are compatible with their ensemble counterparts. d) Same plot for the returns of all stocks on two randomly chosen days. In this case, 82% of daily returns empirical distributions are compatible with their ensemble counterparts (K-S test at 0.01 significance).
FIG. 4: Applications of the ensemble theory we propose to a system of stocks. a) Anomaly detection performed on each single trading day of a randomly selected stock (Google). A return measured on a specific day for a specific stock is marked as anomalous if it exceeds the associated 95% confidence interval on that specific return. b) Comparison between the empirical spectrum of the estimated correlation matrix (black dashed line), its ensemble counterpart (orange line) and the one prescribed by the Marchenko-Pastur law (blue line). The inset shows the empirical largest eigenvalue (dashed line) against the ensemble distribution for it.

TABLE I: Fraction of empirical moments compatible with their corresponding ensemble distribution at different significance levels specified in terms of quantiles (e.g., 0.01-0.99 denotes that the 1st and 99th percentiles of the ensemble distribution are used as bounds to determine whether the null hypothesis of an empirical moment being compatible with the ensemble distribution can be rejected or not). Moments are calculated both for each stock and each trading day. In the last column, we also report, for each moment, the median relative error between the empirical value and its ensemble average.

| Stat | Sample | Significance null hypothesis | median rel. err. |
|------|--------|------------------------------|-----------------|
|      |        | 0.01-0.99 | 0.05-0.95 | 0.1-0.9 |         |
| Var  | stock  | 0.95       | 0.76      | 0.59    | 0.2    |
|      | day    | 0.88       | 0.78      | 0.69    | 0.14   |
| Skew | stock  | 1          | 0.98      | 0.95    | 0.13   |
|      | day    | 0.78       | 0.58      | 0.49    | 0.46   |
| Kurt | stock  | 0.78       | 0.61      | 0.51    | 0.60   |
|      | day    | 0.85       | 0.68      | 0.55    | 0.1    |

TABLE II: Fraction of empirical return distributions (both for stocks and trading days) that are compatible with their ensemble counterparts based on Kolmogorov-Smirnov tests at different significance levels.

| Aggregation level | K-S test significance |
|-------------------|-----------------------|
|                   | 0.01 | 0.05 |
| stocks            | 0.92 | 0.68 |
| days              | 0.82 | 0.75 |

financial market movements, thus resulting in the statistical validation of events that are anomalous with respect to the overall heterogeneity present in the market.

Following the above line of reasoning, in Figure 4 we show a comparison between the eigenvalue spectrum of the empirical correlation matrix of the data, and the average eigenvalue spectrum of the ensemble. As is well known, the correlation matrix spectrum of most complex interacting systems normally features a large bulk of small eigenvalues which is often approximated by the Marchenko-Pastur (MP) distribution \[26\] of Random Matrix Theory (i.e., the average eigenvalue spectrum of the correlation matrix of a large system of uncorrelated variables with finite second moments) \[27-29\], plus a few large and isolated eigenvalues that contain information about the relevant correlation structure of the system (e.g., they can be associated to clusters of strongly correlated variables \[30\]). As it can be seen in the Figure, the ensemble’s average eigenvalue spectrum captures the spectral bulk much better than the MP distribution, and the ensemble distribution for the largest eigenvalue is very close to the one empirically observed, demonstrating that the main source of correlation in the market is well captured by the ensemble. Conversely, the average distance between the empirically observed largest eigenvalue and its ensemble distribution can be interpreted as the portion of the market’s collective movement which cannot be explained by the constraints imposed on the ensemble.

In Appendix B, we also apply the above ensemble approach to a dataset of weekly and hourly temperature time series recorded in North-American cities, which we use to showcase the approach’s ability to capture inherent time periodicities in empirical data.
V. RELATIONSHIP WITH MAXIMUM CALIBER PRINCIPLE

Before concluding, let us point out an interesting connection between our approach and Jaynes’ Maximum Caliber principle [19]. It has recently been shown [31] that the time-dependent probability distribution that maximizes the caliber of a two-state system evolving in discrete time can be calculated by mapping the time domain of the system as a spatial dimension of an Ising-like model. This is exactly equivalent to our mapping of a time-dependent system onto a data matrix, where the system’s time dimension is mapped onto a discrete spatial dimension of the lattice representing the matrix.

From this perspective, our ensemble approach represents a novel way to calculate and maximize the caliber of systems sampled in discrete time with a continuous number of states. This also allows to interpret some recently published results on correlation matrices in a different light. Indeed, in [17] the authors obtain a probability distribution on the data matrix of sampled multivariate systems starting from a Maximum Entropy ensemble on their corresponding correlation matrices. Following the steps outlined in our paper, the same results could be achieved via the Maximum Caliber principle by first mapping the time dimension of the system onto a spatial dimension of a corresponding lattice, and by then imposing the proper constraints on it.

VI. DISCUSSION

In this paper we have put forward a novel formalism - grounded in the ensemble theory of statistical mechanics - to perform hypothesis testing on time series data. Whereas in physics and in the natural sciences, hypothesis testing is carried out through repeated controlled experiments, this is rarely the case in complex interacting systems, where the lack of statistical stability and controllability often hamper the reproducibility of experimental results. This, in turn, prevents from assessing whether the observations made are consistent with a given hypothesis on the dynamics of the system under study.

The framework introduced here overcomes the above issues by means of a data-driven and assumptions-free paradigm, which entails the generation of ensembles of randomized counterparts of a given data sample. The only guiding principle underpinning such a paradigm is that of entropy maximization, which allows to interpret the ensemble’s partition function in terms of a precise physical analogy. Indeed, as we have shown, in our framework events in a data sample correspond to fermionic particles in a physical system with multiple energy levels. Notably, even though the Hamiltonians used throughout the paper correspond to non-interacting systems, and therefore the correlations in the original data are not captured in terms of interactions between particles (as is instead the case in Ising-like models), the ensemble introduced here is still capable of partially capturing properties typical of interacting systems through the ‘environment’ the particles are embedded in, i.e., a system of coupled local temperatures and chemical potentials.

All in all, our framework is rather flexible, and can be easily adapted to the data at hand by removing or adding constraints from the ensemble’s Hamiltonian. For example, the constraints in the applications showcased here (i.e., on the sums of above and below average values) result in two fermionic species of particles. More stringent constraints (e.g., on the data belonging to certain percentiles of the empirical distribution) would result in other species being added to the ensemble.

As we have shown, our framework is capable of capturing several non-trivial statistical properties of empirical data that are not necessarily associated with the constraints imposed on the ensemble. As such, it can provide valuable insight on a variety of complex systems by both allowing to test theoretical models for their structure and by allowing to uncover new information in the statistical properties that are not fully captured by the ensemble.

Appendix A: Explicit calculation of the partition function

We want to find a probability density function $P(W)$ on $W$ such that the expectation values of a set of observables coincide with their empirical value, i.e $\langle O_\ell(W) \rangle = \overline{O}_\ell$ ($\ell = 1, \ldots, L$), where $W \in W$ is the empirical set of measurements. At first, this problem may appear almost impossible to solve, given that $P(W)$ may be determined by a number of degrees of freedom way larger than the number of constraints we are imposing. However, as introduced in the main text, this can be done by using the Maximum Entropy principle, or, in other words, by adding another (functional) constraint on the probability distribution, which requires that $P(W)$ should also maximise the Gibbs entropy:

$$S(W) = - \sum_{W \in W} P(W) \ln P(W) , \quad (A1)$$

while preserving the constraints:

$$\langle O_\ell(W) \rangle = \sum_{W \in W} O_\ell(W) P(W) = O_\ell(W) = \overline{O}_\ell , \quad (A2)$$

and the normalization:

$$\sum_{W \in W} P(W) = 1 . \quad (A3)$$

Eqs. (A1)-(A3) define a constrained optimization problem, whose solution is found by solving the following...
where, as usual in such scenarios, each constraint has been coupled with a Lagrange multiplier $\alpha, \beta_t \ (t = 1, \ldots, L)$. Defining $H(W) = \sum_t \beta_t O_t(W)$ as the Hamiltonian of the ensemble and $Z = e^{\alpha+1} = \sum_W e^{-H(W)}$ is its partition function, the solution of Eq. (A4) reads:

$$P(W) = \frac{e^{-H(W)}}{Z}.$$  \hspace{1cm} (A6)

This is the general probability density function ruling the ensemble theory we are proposing. Of course, the sum $\sum_W$ on the phase space of the system used in the above equations still needs to be properly specified.

We are going to do so while considering the Hamiltonian specified in the main paper. As pointed out above, in order to find the partition function $Z$ of the system, we just need to sum $e^{-H(W)}$ over all possible configurations, i.e., over the set of all the $N \times T$ real valued matrices $W$. Recalling the notations introduced in the main text $A^k = \Theta(\pm W)$ and $\omega^\pm = \pm W \Theta(\pm W)$, we can write the sum over the phase space as follows:

$$Z = \sum_{W \in \mathcal{W}} \prod_{i=1}^{N} \prod_{t=1}^{T} \sum_{\{(A^k, A^\gamma) = (1,0)\}}^{(0,1)} \int_0^{+\infty} dw^+_{it} \int_0^{+\infty} dw^-_{it}.$$  \hspace{1cm} (A7)

We can now calculate the partition function $Z$ of the ensemble:

$$Z = \sum_{W \in \mathcal{W}} e^{-H(W)} = \prod_{i=1}^{N} \prod_{t=1}^{T} \sum_{\{(A^k, A^\gamma) = (1,0)\}}^{(0,1)} \int_0^{+\infty} dw^+_{it} \int_0^{+\infty} dw^-_{it} \times$$

$$\times e^{[(\alpha^N+\alpha^T)A^+_{it}+(\beta^N+\beta^T)A^-_{it}+(\gamma^N+\gamma^T)w^+_{it}+(\sigma^N+\sigma^T)w^-_{it}]}$$

$$= \prod_{i=1}^{N} \prod_{t=1}^{T} \sum_{\{(A^k, A^\gamma) = (1,0)\}}^{(0,1)} \left( e^{-(\alpha^N+\alpha^T)\frac{A^+_{it}}{\gamma^N+\gamma^T}} e^{-(\beta^N+\beta^T)\frac{A^-_{it}}{\sigma^N+\sigma^T}} \right)^{A^k_{it}}$$

$$= \prod_{i=1}^{N} \prod_{t=1}^{T} \left[ 1 + e^{-(\alpha^N+\alpha^T)\frac{A^+_{it}}{\gamma^N+\gamma^T}} + e^{-(\beta^N+\beta^T)\frac{A^-_{it}}{\sigma^N+\sigma^T}} \right]$$

where we have defined the following quantities in order to make apparent the analogy with the two species fermionic gas introduced in the main text:

$$T_{ij} = \frac{1}{kT} \log (\sigma_{ij}^T + \sigma_{ij}^T e^{\epsilon_{ij}}) + \log (\gamma_{ij}^T + \gamma_{ij}^T e^{\epsilon_{ij}}),$$

$$\epsilon_{ij} = \frac{1}{2} + \frac{T_{ij}}{2} (\alpha_{ij}^T + \alpha_{ij}^T + \beta_{ij}^T + \beta_{ij}^T),$$

$$\mu_{ij}^2 = \frac{kT_{ij}}{2} (\alpha_{ij}^T + \alpha_{ij}^T - \beta_{ij}^T - \beta_{ij}^T - \log (\gamma_{ij}^T + \gamma_{ij}^T e^{\epsilon_{ij}})) = -\mu_{ij}^1.$$  \hspace{1cm} (A8)

From the above partition function, via Eq. (A6) we can derive the probability density function in Eq. (5) of the main text, which quantifies the probability of drawing a specific instance $W$ from the ensemble. The quantities defining such probability distribution have a well defined physical meaning, and read as follows:

$$P_{it}^+ = \frac{e^{-\epsilon_{it}^N}}{z_{it}^w} \text{Probability of observing a positive value in the } i\text{-th time series at time } t$$

$$P_{it}^- = \frac{e^{-\epsilon_{it}^N}}{z_{it}^w} \text{Probability of observing a negative value in the } i\text{-th time series at time } t$$

$$1 - P_{it}^- - P_{it}^- \text{Probability of observing a missing value in the } i\text{-th time series at time } t$$

$$Q_{it}^+(w) = (\gamma_{it}^N + \gamma_{it}^T) e^{-(\gamma_{it}^N + \gamma_{it}^T)w} \text{Probability distribution of a positive value } w \text{ for the } i\text{-th time series at time } t$$

$$Q_{it}^-(w) = (\sigma_{it}^N + \sigma_{it}^T) e^{-(\sigma_{it}^N + \sigma_{it}^T)w} \text{Probability distribution of a negative value } w \text{ for the } i\text{-th time series at time } t$$

When no data are missing, i.e. $(A^+_{it}, A^-_{it}) \neq (0,0)$, the sum defined in Eq. (A7) changes and, as a result, the partition function (A8) becomes:

$$Z = \prod_{i,t=1}^{N,T} z_{it} \left[ \frac{e^{-\epsilon_{it}^N}}{z_{it}^w} + \frac{1}{z_{it}^w} \right].$$

After noticing that $A^+_{it} = 0 \Rightarrow w^+_{it} = 0 \land w^-_{it} > 0$, the probability of drawing from the ensemble an instance $W$ can be easily found:

$$P(W) = \prod_{i,t=1}^{N,T} \left[ P_{it}^+ \ Q_{it}^+(w^+_{it}) \right] A^-_{it}^+ \left[ P_{it}^- \ Q_{it}^-(w^-_{it}) \right]^{1-A^-_{it}}.$$  \hspace{1cm} (A9)

Looking at Eq. (A9), we can understand how we have obtained Eq. (6) in the main text. In order to simulate a drawing of a set of time series $W$ from the ensemble, we first need to construct a “topology” of positive events by placing a positive event in entry $W_{it}$ with probability $P_{it}^+$.
and a negative event otherwise. Then we need to place a weight \( W_{it} = x \) using one of the two exponential distributions \( Q^x_{it} \) defined above, depending on the type of event that was assigned to \( W_{it} \). This procedure is encompassed by the hyperexponential distribution in Eq. (6) of the main text, which can be obtained via the standard generating function approach, and whose parameters read \( \lambda^+_i = (\gamma_i^N + \gamma_i^T)^{-1} \), and \( \lambda^-_i = (\sigma_i^N + \sigma_i^T)^{-1} \).

**Appendix B: Application to a set of temperature time series**

We now apply the framework introduced in the main text to sets of time series featuring temperatures recorded at different frequencies (week/day/8 hours) in \( N = 30 \) different North American cities [34] (weekly data range from July 2013 to July 2018, daily data range from July 2016 to July 2018, 8 hours data range from January 2017 to July 2018). We do so in order to test the ability of our ensemble approach to capture the main features of time series whose most relevant statistical properties are markedly different from those of financial returns, which we instead studied in the main paper. In particular, our main focus will be on the ability of the ensemble to capture the periodicities that characterize temperature data at different time scales.

As done in the main text, we indicate as \( \mathbf{W} \) the \( N \times T \) data matrix (with \( T = 264,730,2321 \) in the case of temperatures recorded at the weekly, daily, and 8 hour frequency, respectively) with values rescaled to have zero mean, and we indicate as \( W \) any generic instance drawn from the corresponding ensemble. We also redefine here for convenience the matrices \( A^\pm = \Theta(\pm W), w^\pm = \pm W\Theta(\pm W) \). The ensemble we are going to use is fully specified by the \( 6(N + T) \) constraints enforced in the following Hamiltonian (there are no missing data, which leads to \( 2(N + T) \) fewer constraints with respect to the general formulation outlined in the main paper):

\[
H(W) = \sum_{i=1}^{N} \sum_{t=1}^{T} \left[ (\alpha_i^N + \alpha_i^T) A^+_{it} + (\gamma_i^N + \gamma_i^T) w^+_{it} + (\sigma_i^N + \sigma_i^T) w^-_{it} \right],
\]

leading to the partition function:

\[
Z = \prod_{i=1}^{N} \prod_{t=1}^{T} Z_{it} = \prod_{i=1}^{N} \prod_{t=1}^{T} \left[ e^{-\frac{(\alpha_i^N + \alpha_i^T)}{\gamma_i^N + \gamma_i^T}} + \frac{1}{\sigma_i^N + \sigma_i^T} \right].
\]

In Figure 6 we show that, independently from the frequency at which temperatures are sampled, the average ensemble power spectral density captures remarkably well the relevant frequencies that characterize the empirical time series of each city. Indeed, as can be seen from panels a and b, the ensemble power spectra based on the data recorded at the weekly and daily frequency perfectly capture the six-months periodicity associated with the seasons’ cycle. Panel c shows that the same frequency is also captured in the data recorded every 8 hours, and that when calibrating the ensemble on such data, the power spectrum also perfectly captures the daily frequency associated with the day-night cycle (see inset).

In Fig. 6 we expand the above analysis to the periodicities of moments. Panel a shows the empirical daily variance of temperatures recorded across the 30 cities mentioned above against the corresponding ensemble average. At first sight, the latter seems to be largely uncorrelated from the former. Yet, the corresponding power spectrum shown in panel b highlights that the relevant frequencies in the data (six months and one day) are captured very well, although the ensemble places additional power on such frequencies.

A somewhat similar phenomenon is shown in panels c and d, which show the daily skewness computed across all cities and its corresponding power spectra. Once again, the average ensemble spectrum places more power on the six-months and daily frequencies with respect to the empirical one. This results in a clearly discernible oscillating pattern, which significantly deviates from the empirical behavior. Nevertheless, these results are interesting. Indeed, as it can be seen in panel c positive (negative) skewness values take place during the summer (winter) months, as a reflection of higher (lower) average temperatures. Although this is a fairly trivial example, it highlights how the ensemble approach can reveal stylized trends that are genuinely informative about the dynamics of the system under study.

**Code availability**

The MATLAB code used to implement the ensemble methodology described in this paper is available at [mathworks.com/matlabcentral/fileexchange/72000-canonical-ensemble-for-time-series](http://mathworks.com/matlabcentral/fileexchange/72000-canonical-ensemble-for-time-series).

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FIG. 5: Ability of the ensemble to preserve periodicities in the data. a) Empirical power spectrum of weekly temperatures against the average ensemble spectrum for two different cities (city 1 is Boston and city 2 is Los Angeles). b) Same plot for daily temperatures. c) Same plot for 8 hours temperatures.

FIG. 6: Ability of the ensemble to preserve periodicities in the data. a) Variance of the temperatures recorded at 8 hour intervals across all 30 cities (the blue line denotes empirical values, the orange one denotes the ensemble average). b) Comparison between the empirical spectrum of the 8-hours temperature variance across cities (dashed line) and the ensemble spectrum (blue line). c) Skewness of the temperatures recorded at 8 hour intervals across all 30 cities (the blue line denotes empirical values, the orange one denotes the ensemble average). d) Comparison between the empirical spectrum of the 8-hours temperature skewness across cities (dashed line) and the ensemble spectrum (blue line).

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[32] It should be noted that in some cases this does not necessarily leads to the distribution $P(W)$ being peaked around the values $\mathcal{O}_t$.

[33] We compute the empirical variance of the $i$-th variable as $\text{Var}[W_i] = T^{-1} \sum_t (W_{it} - \langle W_{it} \rangle_T)^2$, and the cross-sectional variance at time $t$ as $\text{Var}[\mathcal{W}_t] = N^{-1} \sum_i (W_{it} - \langle W_{it} \rangle_N)^2$. The skewness and kurtosis are computed as $\text{Skew}[\mathcal{W}_t] = T^{-1} \sum_t (W_{it} - \langle W_{it} \rangle_T)^3/\text{Var}[W_i]^{3/2}$ and $\text{Kurt}[\mathcal{W}_t] = T^{-1} \sum_t (W_{it} - \langle W_{it} \rangle_T)^4/\text{Var}[W_i]^2$, with analogous definitions in the cross-sectional case. The same estimators are used to numerically compute these quantities on the time series generated from the ensemble.