An Introduction to fast-Super Paramagnetic Clustering

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We map stock market interactions to spin models to recover their hierarchical structure using a simulated annealing based Super-Paramagnetic Clustering (SPC) algorithm. This is directly compared to a modified implementation of a maximum likelihood approach to fast-Super-Paramagnetic Clustering (f-SPC). The methods are first applied standard toy test-case problems, and then to a dataset of 447 stocks traded on the New York Stock Exchange (NYSE) over 1249 days. The signal to noise ratio of stock market correlation matrices is briefly considered. Our result recover approximately clusters representative of standard economic sectors and mixed clusters whose dynamics shine light on the adaptive nature of financial markets and raise concerns relating to the effectiveness of industry based static financial market classification in the world of real-time data-analytics.

A key result is that we show that the standard maximum likelihood methods are confirmed to converge to solutions within a Super-Paramagnetic (SP) phase. We use insights arising from this to discuss the implications of using a Maximum Entropy Principle (MEP) as opposed to the Maximum Likelihood Principle (MLP) as an optimization device for this class of problems.

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I. INTRODUCTION

We consider the problem of unsupervised statistical learning for the classification of financial trading and investment strategies. Concretely, we consider Potts model [51] based [6, 7] methods optimized for performance [17, 21, 22, 32] using a Maximum Likelihood Estimation (MLE) approach based on the ground-state Noh Ansatz [37] compared to the finite-temperature approach using a cooling schedule to select configurations based on the susceptibility [6, 7].

We compare the cluster configuration from the fast clustering algorithms based on the ground state configurations [21, 22] (Sec. A 2) with those based on finite temperature Simulated Annealing (SA) based Monte-Carlo Markov-Chain (MCMC) [24, 47] (see Sec. A 1) to generate the full dendrogram of cluster configurations [6, 7]. It was shown that the clustering structure of financial assets are time horizons dependent in [9], and given a proper translation of correlations into the euclidean distance can be represented using Minimal Spanning Trees (MST) [27].

The Super-Paramagnetic Clustering (SPC) method originally developed in the early 90s is a universal data clustering method [6] and has acquired a certain popularity for its implementation of the Maximum Entropy Principle (MEP) [20] where no assumptions are made about the distributions found in the data, and the number of clusters is revealed rather than predefined. It can be used in any environment as long as the features are

A. The Algorithms

1. SPC Algorithms
2. f-SPC Algorithms

References

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The Super-Paramagnetic Clustering (SPC) method originally developed in the early 90s is a universal data clustering method [6] and has acquired a certain popularity for its implementation of the Maximum Entropy Principle (MEP) [20] where no assumptions are made about the distributions found in the data, and the number of clusters is revealed rather than predefined. It can be used in any environment as long as the features are
embedded in an appropriate similarity metric. SPC has
tested applied to chemical data using a sequential method
and the Tanimoto similarity measure [41], the detection
and classification of spiking activity in neuronal tissue in
[42], the identification of regions of the brain with shared
functionality in [43], yeast genes profiles in [16], histone
modification data [29], and image segmentation in [1].

Marsili and Giada [17] were able to develop an ef-
ficient maximum likelihood clustering method for high
dimensional data using the same spin-model inspired
approach used in the SPC method. However, given the
ill-posed nature of clustering they chose to evaluate the
likelihood model $L_c$ for robustness relative to different
optimization methods in [18]. The method is then ap-
piled to the detection of clusters of assets, and financial
markets states in [32] to uncover collective behavior of
agents in a complex systems. Hendricks, Gebbie, and
Wilcox created a GPU based Parallel Genetic Algorithm
(PGA) implementation to maximize $L_c$ in near real time
clustering of market states in for quantitative trading ap-
plications [21].

In this work we explore the relationship between the
SPC method of Domany-Wiseman-Blatt [6] as compared
to that of Giada-Marsili [17] and we are able to confirm
that the likelihood method is super-paramagnetic and
conforms well to the entropy method when dimension-
ality is sufficiently high (see Sec. V). We are also able
to further optimize the PGA implementation [21]. How-
ever, what we really demonstrate is the variety of cluster-
ing problems that the SPC can quickly and easily han-
dle, but with the advantage of leveraging a mature and
well-understood foundational theoretical framework from
statistical mechanics that has many, if not most, viable
alternative algorithms, as special cases. We are of the
view that SPC type models grounded in the maximum
entropy principle and within the general framework of
energy-based machine learning offer a variety of research
and development opportunities for building better and
faster unsupervised learning algorithms.

The paper is organized as follows: Section II discusses a
brief overview of Erdos-Renyi’s Random Graphs (see Sec.
II A), and their connection to the Potts models as special
cases. We describe the inhomogeneous Potts Model as a
data-clustering engine (see Sec. II B). In Section II C the implementa-
tions with the SPC algorithm (Sec. II C 1) followed by Marsili’s maximum likelihood methods
(see Sec. II C 2). Section III goes over our choice of similarity
metric (Sec. III A), data-preprocessing (Sec. III B), and
time-series noise filtering (Sec. III C). Section IV provides
toy test cases, and stock market applications. In Section V a summary analysis of the results and their im-
lications, and finally in Section VI the conclusion, and
potential directions for further research on similar topics
are mentioned.

We promote the idea that a promising future research
direction would be quantized spin-models and ultimately
building unsupervised learning algorithms that more ef-
effectively accommodate state-interference and phase in-
formation within some likelihood method.

II. POTTS CLUSTERING

A. Random Graphs

A graph is a mathematical model which formalizes
pairwise relationships between objects [45]. Graphs are
popular in complexity sciences because they provide a
framework to model large systems of interacting com-
ponents by representing the system directly through the
pair-wise relationships between the components. The
field has seen the rise of many models, each with their
own assumptions and various nuance, almost all are of
the generative form based on the premise of bottom-up
causation. One feature that is useful in our context is
that one can observe certain types of emergent dynamics
i.e. “phase transitions” [10].

A general class of models called the Random Cluster
model was developed by Fortuin-Kasteleyn in 1972 [15].
It is a “random” graph generated by a probability distri-
bution

$$W(N) = \frac{CN}{Z} \prod_{\{i,j\}} P_{ij}^{n_{ij}} (1 - P_{ij})^{(1-n_{ij})}$$

where $N$ is a given edge configuration (or adjacency ma-
trix of $n_{ij}$), $C_N$ is the number of clusters given $N$, $P_{ij}$ is
the probability of nodes $i$ and $j$ being connected, and
$Z$ is the normalization constant (also called the partition
function in statistical mechanics [45 ]). The adjacency
matrix is linked to the probabilities $P_{ij}$ by picking a value
$P$ such that if $P_{ij} > P$ then $n_{ij} = 1$ or 0 otherwise. $W$ is
essentially the probability of the graph being connected
given an adjacency matrix $N$.

If we now set $q = 1$, the random cluster model reduces to
an Erdos-Renyi’s random graph [12]. Given the exis-
tence of only one class on the graph, bonds are linked
independently from their respective states (i.e. they all
have the same state) with equal probability $P_{ij} = \frac{1}{n}$ with
$n$ the number of nodes on the graph [12]. An important
generalization of this idea is the Barabsi-Albert model
[4]; this model works slightly differently: it starts with a
low number of connected nodes $m_0$, adds new nodes one
at a time, one new node is able to connect to $m < m_0$
nodes, and every time a node $i$ is connected its degree
$k_i$ increases. The probability of a node connecting to
another is $P_{ij} = \frac{k_i}{\sum k_j}$. This means as a node $i$ makes
connections it becomes “popular” and succeeding nodes
have a higher likelihood of connecting to that same node:
this is the principle of “preferential attachment” which
hopes to explains how some social networks are formed.

1 See Grimmett [20] and references therein.
These models are all based on a generative model that builds on microscopic causal relationships from the system components to the bulk.

The Fortuin-Kasteleyn random cluster model is closely related to the Potts model via its distribution

\[
P(S, N) = \prod_{(i,j)} \left[ (1 - P_{ij})(1 - n_{ij}) + P_{ij}n_{ij}\delta_{s_i,s_j} \right]
\]  

which is the conditional probability of the spin configuration \( S \) given the edge configuration \( N \). The marginal probability \( W \) is recovered by summing over all edge configurations \( \int_d P(S, N) dn \). The major difference the Potts model brings is entropy maximization which assumes an exponential Boltzmann distribution of edges connections \( P_{ij} = 1 - e^{-J_{ij}/T} \) where not only \( J_{ij} \) defines the pairwise probabilities, but \( T \) modulates the whole distribution.

The strength \( J_{ij} \) captures the closeness between nodes, and, with the clusters membership, defines the topology of the graph. It’s a central variable of the model. This is similar to the Bianconi-Barabsi model [5] which introduces a fitness \( q \) which plays a related role as an add-on to the Barabasi-Albert model [4].

**B. The Potts Model**

The Ising model [10] simulates the existence of phase transitions in large systems of interacting particles. The model consists in the representation of a n-Dimensional plane. Ising’s PhD Thesis [10] solved the 1D problem, which showed no phase transition, while Onsager provided an analytical solution using a transfer-matrix method [39] for the 2D case. If we consider observations in our data sets as nodes with edges which link nodes together it becomes natural to consider the data-set in the context of a Potts model [51]. An edge is active or inactive with probability dependent on the distance between two nodes. The collection of nodes and edges form the graph which is navigated for clustering. Every node can be assigned, for example, a +1 or -1 spin (for the Ising model). Interactions are permitted by randomly changing the spin values in the graph, and then accepting or rejecting new configurations is implemented using the Swendsen-Wang MCMC algorithm (See Appendix 2 ) at every step [44].

The Potts model [51] is a generalization of the Ising [10] model allowing the system to accept a higher \( q \) spin values instead of 2. The parameter \( q \) can be compared to the \( K \) value in K-means used to fix the number of clusters. \( q \) is the maximum number of classes: it must be chosen to be big enough to avoid clusters forcefully merged together. The only inconvenience to a relatively high \( q \) is the additional computational cost needed to perform the statistics after the system reaches thermal equilibrium.

The model is governed by a Hamiltonian Energy [2] equation [51]

\[
H_S = \sum_{(i,j)} J_{ij}(1 - \delta_{s_i,s_j})
\]  

with: \( S = [s_1, ..., s_N] \) the spin vector assigned to our data, spins \( s_i \in [1, ..., q] \), and \( N \) nodes. The Kronecker delta which is 1 for equal spins and 0 otherwise. For data embedded in a metric space the Euclidean distance function \( d_{ij} = ||x_i - x_j|| \) is computed between two nodes.

\( d_{ij} \) is fed to the strength function which, in turn, measures similarity. Many models for strength exist but their central feature is they must decrease with distance. This is typically achieved with a function of the type \( e^{-d_{ij}} \) or a power law as seen in [6]:

\[
J_{ij} = \frac{1}{K} \exp \left\{ -\frac{1}{2} \left[ \frac{d_{ij}}{a} \right]^2 \right\}
\]  

where \( \hat{K} \) is the average number of neighbors per node, and \( a \) is a local length scale: the average \( d_{ij} \) of all nearest-neighbors.

There are alternative choices for local characteristic length scale [6]. We only report the results obtained with the previous definition, and note that the adjustments to \( a \) are problem dependent: higher values of \( a \) ensure the 1st phase of the simulation is ferromagnetic while lower values start the simulation in the super-paramagnetic (SP) phase.

The objective is to compute averages of thermodynamic quantities after simulating the system at a given temperature for a set number of MCMC iterations \( M \) until thermal equilibrium.

The first simulation serves to uncover the existence of a critical temperature \( T_c \) at which a first transition occurs. At \( T \leq T_c \) all spins are strongly correlated, \( \langle m \rangle \approx 1 \) and all have the same state: It is called spontaneous magnetization (ferromagnetic phase). At \( T = T_c \) the single cluster breaks down into smaller ones (SP-phase). Furthermore, inside the temperature range where the SP-phase exists, a system can go through additional transitions: These reflect the different hierarchical structures present in the data. Finally at \( T \geq T_c \) we go through a final transition into complete disorder (Paramagnetic phase): The energy \( H_S \) is high, all clusters dissolve, and \( \langle m \rangle \approx 0 \).

The magnetization \( m \) of the system is given by

\[
m(S) = \frac{q N_{max}(S) - N}{(q - 1)N}
\]
This quantity, which ranges from 0 to 1, expresses how dominated the system is by the largest cluster. The order parameter of the system is the average magnetization \( \langle m \rangle \), and its variance \( \chi^2 \) is \( (m^2) - (m) \) is called the susceptibility density. Both can be used to detect a phase transition: \( (m) \) dives down while \( \chi \) peaks at every transition.

For a quantity \( A \) the thermal average will be

\[
\langle A(S) \rangle = \sum A(S) P(S).
\]

Here each \( S \) represents a single MCMC step. If \( M \) is large enough, Eqn. (5) is equivalent to the arithmetic mean

\[
\langle A(S) \rangle \approx \frac{1}{M} \sum_{i=1}^{M} A(S).
\]

The probability of a system being in a particular state (referring to the energy of the system \( H_S \)) is:

\[
P(S) = \frac{e^{-H_S/T}}{Z}
\]

where \( e^{-H_S/T} \) is the Boltzmann factor, \( Z \) is the partition function \( Z = \sum_S e^{-H_S/T} \) and the normalization constant of the Gibbs-Boltzmann distribution.

Numerically, we use a mean-field mode of the Hamiltonian such that \( H_S = \frac{1}{N} \sum_{i,j} J_{ij} (1 - \delta_{s_i s_j}) \). The motivation being that high levels of \( H \) lead to Boltzmann factors close to 0, \( Z \) also \( \approx 0 \) which by definition makes the computation of \( P(S) \) impossible, also the value of \( H_S \) impacts the cooling schedule, and the temperature range explored.

1. Maximum Entropy

We briefly remind ourselves of the MEP [26]. We define a statistical mechanical system as an ensemble of objects each in their respective micro-states (spin values \( s_i \)) so that the resulting in microscopic state of the entire system \( S = \{ s_1, ..., s_N \} \) can be used to derive parameters which characterize the distributions for macroscopic variables of interests (here the internal energy \( H_S \)). We assume that at equilibrium, thermodynamic systems obey conservation of energy which sets the constraints of the system such that on average \( H_S \) is a constant, and then from Eqn. (6) it follows that:

\[
\langle H_S \rangle = \sum H_S P(H_S), \quad \sum P(H_S) = 1.
\]

We then consider that the distribution representative of the energy of the system as the one which incorporates our constraints and assumes nothing else. This maximizes the Shannon’s Entropy as defined by:

\[
H = -\sum P(H_S) \ln(P(H_S)) \quad 3
\]

The problem can then be reduced to a Lagrange optimization task for which the exponential family of distributions is a well known solution (see Eqn. (9)) with the inverse temperature as its Lagrange multiplier [20].

C. Super-Paramagnetic Clustering (SPC)

1. Maximum Entropy Method

We define a neighbor on a lattice to be a node located in the vicinity of another node such that a node \( s_{i,j} \) will have neighbors \( s_{i+1,j}, s_{i-1,j}, s_{i,j+1}, \) and \( s_{i,j-1} \). A neighborhood generated using these rules is valid for a 2D lattice with a fixed \( J \) for all nodes (the interaction strength is said to be homogeneous). This is the original method used in simulating Ising/Potts models of ferromagnets. As a generalization to the problem of data clustering, we will consider a neighborhood which emerges from the inhomogeneous interaction strength \( J_{ij} \). Every neighborhood is a mini-graph, and their aggregation constitutes a graph whose topology is determined by the matrix \( J_{ij} \): For two nodes to be neighbors they, each, must be included in their respective K-nearest neighbors.

We first define the neighborhood of size \( K \). This is implemented following steps in Table (A) below.

| TABLE A: Setting the neighborhood size \( K \) |
|--------------------------------------------------|
| The graph is traveled via nodes, and edges can be set active or inactive with probability |
| \( p_{ij} = 1 - e^{-\frac{J_{ij}}{T} \delta_{s_i s_j}} \) |

The next array is called \( \text{links} \). It is the adjacency matrix where the activation status of edges is stored such that \( \text{links}_{ij} = 1 \) if \( p_{ij} > \text{rand} \), and 0 otherwise.

The original Hoshen-Kopelman (HK) algorithm [23] is the standard for labeling clusters in many statistical mechanics problems. The 2D version is mostly restricted to two neighbors per node: \( s_{i-1,j} \) and \( s_{i,j-1} \). SPC (Sec. A1) deals with problems where \( J_{ij} \) is not fixed, and \( K \) can be large so we apply the extension of HK to non-lattice environments found in [9].

The clusters are labeled using the extended HK algorithm (See Table B below).
B.1. Initialize the label counter at 0, create two arrays: node, a 1xN array which stores the labels, and nodep, an empty list where the roots are recorded. HK is inspired by the Union-Find algorithm which, like its name says, “finds” the root class of nodes, and “unites” nodes belonging to the same class. The concept is applied similarly in SPC, nodes’ labels are stored in node, and once clustering is done, nodep is used to re-assign every nodes to its root class.

B.2a. Check for activated edges, if none or if any are occupied but none of those link to already labeled nodes: start a new cluster by storing the current label counter in node, and nodep, then increase the label counter.

B.2b. On the other hand if active edges link to labeled nodes: Find the root of the node, and its labeled neighbors. This is achieved by first locating the labels stored in node, then using nodep to recover the root associated with these labels. We then pick the smallest root, store it as the label of the present node in node, and we replace the other roots in nodep.

B.3. Sequentialize nodep

B.4. Relabel node with the true roots using nodep

TABLE C: Flipping Clusters using Swendsen-Wang MCMC with Acceptance-Rejection Cooling Schedule (See Appendix 2)

Finally, the spin-spin correlation $G_{ij}$ is the average probability of two spins being in the same cluster is computed in two steps (See Table (D)).

D.1a. At every MCMC step $c_{ij}$, the two-point connectedness, is incremented if i and j are clustered together.

D.1b. Once the simulation ends for the temperature explored we compute

$$G_{ij} = \frac{(q - 1)c_{ij} + 1}{q}$$

TABLE D: Compute the Spin-Spin Correlation $G_{ij}$

The spin-spin correlation $G$ is probably the most important quantity as it is used to build the final clusters. The threshold $\theta$ for which two nodes are members of the same cluster is picked to be higher than $\frac{1}{q}$ but less than $1 - \frac{2}{q}$. The bounds on that range are explained by the distribution of $G_{ij}$ which peaks at those two values: They are respectively the peak inter and intra cluster correlations. It is typical to use $\theta = 0.5$ as it does not significantly affect the results in previous examples.

2. A Maximum-Likelihood Method

Based on an analysis of the spectral properties of stock market correlations matrices, Noh makes the following statistical ansatz: let’s assume an existing market hierarchy where individual stocks dynamics are dependent on clusters of similar stocks. This can be illustrated by a simple model as follows:

$$x_i = f_i + \epsilon_i$$  \hspace{1cm} (10)

where $x_i$ are the stock’s features, $f_i$ the cluster-related influence, and $\epsilon_i$ the node’s specific effect.

In Giada, and Marsili formally develop a Potts model using Noh’s idea, and in Hendricks, Gebbie, and Wilcox solved the optimization problem using a PGA for unsupervised learning for quantitative trading. Let’s consider a group of $N$ observations, embedded in a space with dimensionality $D$ as the features, and as with SPC (Sec. A 1), every observation is assigned a spin value. One version of the ansatz models the observation features such that

$$x_i = g_s \eta_s + \sqrt{1 - g_s^2} \epsilon_i$$  \hspace{1cm} (11)

For $q = 20$ results in $\rho_{ss} = 0.05$, and $\rho_{sb} = 0.9$. Uncorrelated nodes have $\rho_{ij} \approx \rho_{ss}$, and correlated nodes $\rho_{ij} \approx \rho_{sb}$.
where $x_i$ is one feature, $g_{s_i}$ the intra-cluster coupling parameter $^5$, $\eta_{s_i}$ the cluster-related influence, and $\epsilon_i$ the observation’s specific effect, and measurement error. A covariance analysis yields additional terms such as $n_s$ the size of cluster $s$, and $c_s$ the intra-cluster correlation $^6$.

We explicitly mention that $n_s < c_s < n_s^2$ must be enforced: the lower bound is required because $g_s$ is undefined for values of $c_s < n_s$, and the upper bound requires a strict inequality because Eqn. (13) is undefined when $c_s = n_s^2$. We introduce a Dirac-delta function $^7$ to model the probability of observing data in a configuration $S$ close to criticality:

$$P = \prod_{d=1}^{D} \prod_{i=1}^{N} \left( \delta(x_i - g_s \eta_{s_i} + \sqrt{1 - g_s^2 \epsilon_i}) \right). \tag{12}$$

This joint likelihood is the probability of a cluster configuration matching the observed data for every observation, and for every feature. The log-likelihood derived from $P$ can be thought of the Hamiltonian of this Potts system:

$$L_c = \frac{1}{2} \sum_{s,n_s > 1} \ln n_s \frac{n_s}{c_s} + (n_s - 1) \ln \frac{n_s^2 - n_s}{n_s^2 - c_s}. \tag{13}$$

The sum is computed for every feature, and represents the amount of structure present in the data. The value of $L_c$ is indirectly dependent on spins via the terms $n_s$, and $c_s$.

A-priori advantages of this method over industry standard alternatives: First, that $L_c$ is completely dependent on $C_{ij}$, and the dimensionality of the dataset only plays a part in computing $C_{ij}$, and Second, it is unsupervised: There are no preset number of clusters. Clustering configurations are randomly generated, and that which maximizes $L_c$ provides us with the number of clusters, and their compositions.

Further modification of the model can be made to reduce the Hamiltonian to that of the standard K-means algorithm $^30$:

$$H_{KM} = \sum_{s,n_s > 0} (n_s - \frac{n_s}{c_s}) \tag{14}$$

The f-SPC algorithm (Sec. 4) uses a PGA to find the global optimum of the likelihood $L_c$ $^{13}$.

The principles of our GA are given in Table (E) below.

---

E.1. Generate Populations: Generate the populations as a set of randomly generated Potts configuration with spin values ranging form 0 to $N$, 2.)

E.2. Evaluate Fitness: Use the computation of $L_c$

E.3. Select the Best Individuals

E.4. Mutate: A set number of individuals in the populations are mutated

E.5. Recombine: The parent and child generations are recombined and again selection of the best individuals takes place.

E.6. Iterative Convergence: Repeat 2.) to 5.) until sufficient convergence has been achieved.

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The original PGA algorithm implemented in $^{21}$ contained a mating step involving a bespoke cross-over function, and a restriction: Only parents with the same number of clusters could be mated, and the resulting children should maintain the same characteristic. The enforcement of this rule restricted clusters merging and splitting through mutations only. Our f-SPC implementation removes this intermediary step. This was implemented in order to decrease the computational cost $^8$.

In addition to the diversity of individuals present in the population, mutations serve as GA diversity operators: They increase the genetic diversity, and send the system onto another path toward higher local maxima. We used six equally weighted types of mutations: i) New: A complete new individual, ii) Split: a random cluster split into two, iii) Merge: two clusters merged at random, iv) Swap: two spin labels are exchanged, v) Scramble: where a sequence of spins have their labels re-assigned in reverse order, and, vi) Flip: cluster (spin) labels are randomly re-assigned using the total cluster number (See SW Table C).

At last, the simulation has converged once the fitness of the best individual hasn’t increased for a pre-determined number of iterations called “Stall Generations”. It should also be noted that although we did not recode a CUDA implementation for direct GPU implementation of our refined PGA algorithm this can be implemented using a modified version of the original CUDA implementation $^{21}$.

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$^5$ The thermal average $\langle g_s \rangle$ can be used to reconstruct datasets sharing identical statistical features of the original time-series by using Eqns. $^{14}$ $^{17}$

$^6$ Here $n_s = \sum_{i=1}^{N} \delta_{s_i,s}$, $c_s = \sum_{i=1}^{N} \sum_{j=1}^{N} C_{ij} \delta_{s_i,s} \delta_{s_j,s}$, and $g_s = \sqrt{\frac{\sum_{i=1}^{N} n_s}{n_s^2 - n_s}} \frac{n_s}{c_s}$ $^{17}$ $^{24}$.

$^7$ Let $y_i = x_i - (g_s \eta_{s_i} + \sqrt{1 - g_s^2 \epsilon_i})$, and $\delta(y)$ a Dirac delta function of $y$ which is 1 when $y = 0$, and 0 otherwise.

$^8$ The algorithm is able to double the number of generations from 250 to 500 for a 5 mins simulation (Iris see Sec. IV D: $L_c = 100$, and without the cross-over function $L_c = 105$.)
III. DATA PRE-PROCESSING

A. The Distance Function

The wide variety of problems our clustering methods can tackle necessitates a careful choice of pairwise distances if we are to properly identify shared behavior. We will proceed by using the Euclidean distances whenever we assume independence of the features, and the Pearson correlations otherwise especially for problems where the features consist of time-series.

This has implications for both algorithms such that we use the Euclidean distance or the Pearson correlation distance for SPC, and for f-SPC, we use the Pearson correlation matrix, and the similarity matrix, which is the Euclidean distance matrix on $[0, 1]$, and subtracted from 1.

We note that from [28] that our Eqn. (4) can be modified to incorporate negative correlations, but the authors explain this only affects the results at the ground state (i.e. $T \approx 0$).

B. Scaling

Raw data sets often contain features on different order of magnitude of scales, outliers, and missing data which can have significant impact on Machine Learning algorithms. One way to deal with these issues is through normalization of the features. This was achieved using the Min-Max Scaling technique which puts all features on a 0 to 1 scale by performing the following operation:

$$x_{scaled} = \frac{x - x_{min}}{x_{max} - x_{min}}.$$  

(15)

Scaling has significant effects on the feature space: one example is seen in Fig. (5a), and Fig. (5b) which respectively show the unscaled and scaled plots of the 3 wines problem. The unscaled data set has two classes completely inseparable whereas scaling the data effectively dissociates all three classes with minimal overlap.

C. Noise

The next and final pre-processing task consist in removing any noise present in our data. This is especially important for financial market time-series which exhibit extreme randomness and possibly chaotic behavior. Stock market correlation matrices are noisy, and positively skewed Fig. (1a) which translates into what is referred as the “Market Mode”. We consider an intermediary step which consist in “removing” the market mode, thus ensuring we are able to recover the underlying correlation structures, if any, present in the system.

1. Random Matrix Theory (RMT)

We follow the predictions of RMT in [49] by assuming that stock market returns are IID random variables with zero mean and unit variance. These assumptions lead us to the conclusion that stock market correlations should all be zeros, and if the assumptions are indeed true, RMT predicts that the eigenvalues of the random matrices are Wishart distributed such that:

$$P(\lambda) = \frac{Q}{2\pi} \sqrt{(\lambda_{max} - \lambda)(\lambda - \lambda_{min})} \lambda \quad \quad (16)$$

where $Q = \frac{D}{N}$, and $\lambda_{min/max} = 1 + \frac{1}{Q} \pm 2\sqrt{\frac{1}{Q}}$.

FIG. 2: The Eigenvalue distribution of the Correlation Matrix of 1249 daily returns for 447 publicly traded companies in the S&P500 (Sec. IVF). The two vertical red lines delimit the wishart range $\lambda_{min} = 0.16$ and $\lambda_{max} = 2.55$: The eigenvalues located inside the Wishart range (see Sec. III C 1) are noise whereas the ones outside aren’t. Inset: (red curve) We show that the computed Wishart PDF of a random matrix (using Eqn. (16)) fits well the eigenvalue distribution of our correlation matrix only inside the wishart range.

Shown in Fig. (2) is the distribution of eigenvalues of the correlation matrix of our stock market data Sec. IVF. As can be observed the eigenvalues inside the Wishart range are responsible for the noise whereas those outside of the range are potentially correlated signal which shouldn’t be discarded.
FIG. 1: Distribution of Pearson correlations of daily returns for 447 publicly traded companies on the S&P 500 stock exchange from 8/13/2012 to 8/11/2017 (Sec. IV F). The “Market Mode” (Sec. III C): Noisy markets like in (a) are highly correlated with most $\rho_{ij} > 0$. The noise is cleaned by removing the “Market Mode” either by IMN (Sec. III C 2) in (b) or RMT methods (Sec. III C 1) in (c), and produces distributions centered around 0.

TABLE F: Implementation of RMT Noise removal methods

We consider the eigenvalues $\lambda > \lambda_{\text{max}}$ represent the linear, and 1st order relations between time-series while it is unclear what those on the left side ($\lambda < \lambda_{\text{min}}$) of the Wishart distribution are. The linear signals are the signals shared by assets at the sectoral level.

The RMT “Market Mode” removal method is implemented in the five following steps bellow in F:

F.1. Compute the correlation matrix $C_{ij}$
F.2. Extract the eigenvalues and eigenvectors from $C_{ij}$
F.3. Select the eigenvalues (and the corresponding eigenvectors) found outside the Wishart Range.
F.4. Reconstruct the data using the compressed signal: Let $X$ be our data, $W$ the matrix of eigenvectors found outside the Wishart Range, and $Z = W'X$ the compressed data. The reconstructed data is then $X = WZ$.
F.5. Re-compute the correlations $C_{ij}$ from the reconstructed data.

TABLE G: Implementation of Noise Removal via Iterative Matrix Normalization

G.1. Compute the Covariance Cov
G.2. Standardize Cov across rows then columns for a set number of iterations (i.e. 500) or until a convergence criteria is met.
G.3. Extract the correlation matrix $C_{ij}$ from Cov

noise-less data reconstruction. An example of a cleaned correlation matrix resulting from this method Fig. (1c).

2. Iterative Matrix Normalization (IMN)

Another “Market Mode” removal method IID random variables with zero mean and unit variances.

The Iterative Matrix Normalization “Market Mode” removal method is implemented in the three following steps bellow in G:

We observe in Fig. (1b) that the distribution of correlations is now centered around 0.

9 In [17], The authors achieve a similar result by using the model in Sec. II C 2 confirming that “noise cleaning” mainly affects the small eigenvalues of stock market correlation matrices.
IV. THE DATA TEST-CASES

The following examples are used as a stress test for both methods. We obtained both synthetic, and real data which enabled us to discuss the features of each models.

As a comparison tool we use the Adjusted Rand Index (ARI) which gives two classifications measures their similarity. The ARI operates on a $[-1, 1]$ scale with positive values signifying increasing similarity. Where a true classification exists we will use the ARI to measure the quality of clustering of both methods but also industry standards such as “K-Means” and “DBSCAN”. Using SPC (Sec. A) we cluster a temperature range which we then compare against the $L_c$ solution recovered. We then select the SPC temperature with the highest ARI for a closer comparison with the $L_c$ solution in the stock market case where a true classification is not available.

For visualization, where possible, we provide the plots or we make use of a nonlinear dimensionality reduction package called UMAP. The graph of the MST is also provided as it is a faithful representation of clusters on a 2D plane. The MST takes in the graph of our data, and find the unique shortest path linking every nodes.

A. Sci-Kit learn: Concentric Circles

Our first problem is the identification of two concentric circles on a 2D plane using Sci-Kit learn samples generator with $N = 500, 0.5$ for the noise parameter, and the 2 dimensions represent the X and Y coordinates of the observations.

Judging by observing Fig. (3b), and we see no overlap between the two clusters present in the data, and we expect to recover close to perfect clusters after applying the algorithms.

We obtained the susceptibility as a function of temperature in Fig. (5a). Within the SP-phase at $T = 0.01$ we observe two clusters in figure Fig. (4a) both contain 250 nodes with an ARI of 1. Once the temperature gets relatively high, near $T \approx 0.15$, the system is deemed at “high energy”, and the clusters dissolve almost simultaneously. Unlike this particular example, this does not generally happen with real data where clusters have different densities.

On this data, f-SPC runs for 100000 generations maximizing $L_c$ to 639 while the real classification scores 317. The f-SPC configuration is presented in Fig. (4b) with an ARI of 0.855. In comparison K-Means and DBSCAN respectively achieve 0.16, and 1. K-Means has low clustering quality despite specifying the correct number of clusters. This is due to its inability to deal with nonspherical and non-Gaussian shaped clusters. Despite the high likelihood, Fig. (4b) shows a high number of clusters. The clusters are not mixed and ultimately we fail to recover the initial two clusters.

B. Sci-Kit learn: Wine data

The second problem consists of a data set containing three clusters: $N = 178$, and $D = 13$. It is a reputed easy problem illustrating the importance of Normalizing/Standardizing features. There are 59, 71, and 48 samples respectively for class 1, 2 and 3, and the data is generated using Sci-kit learn loader. The 13 features are quantities extracted from a chemical analysis of 3 types of Italian wines: One Alcohol, Malic acid, Ash, Alkalinity of ash, Magnesium, Total phenols, Flavanoids, Nonflavanoid phenols, Proanthocyanins, Color intensity, Hue, OD280/OD315 of diluted wines, and Proline.

At first sight in Fig. (5a), 2 clusters are merged whereas once the features have been normalized Fig. (5b) the 3 clusters occupy separate regions of the space. Each cluster has one extremity close to its neighboring cluster which may induce some misclassification error, and because of this we expect to recover 3 imperfect clusters.

Between $T = 0.147$ and $T \approx 0.22$ we observe three clusters, and the best classification recovered in Fig. (6a) provides the MST of the SPC’s solution with an ARI of 0.82.

Figure Fig. (6b) presents $L_c$’s solution with a likelihood of 83.94, an ARI of 0.51, and an expected likelihood of 66.97. As with the circle problem our solution’s $L_c$ is higher than our expectation, and it has 7 clusters instead of 3. 1 cluster contains observations of cluster 0, while clusters 1 and 2 are split in smaller ones without much misclassification. In comparison K-Means and DBSCAN respectively achieve ARI of 0.85, and 0.42.

C. Sci-Kit learn: Varying Density Clusters

The third problem consists of 3 clusters using Sci-kit learn samples generator with $N = 500, \sigma =$

10 B. Thirion, G. Varoquaux, A. Gramfort, V. Michel, O. Grisel, G. Louppe, J. Nothman, ’make_circles’, 2017. [Online]. Available: [Accessed: 12-Jun-2018]

11 D. Cournapeau, F. Pedregosa, O. Grisel ’load_wine’, 2007-2010. [Online]. Available: [Accessed: 12-Jun-2018]

12 B. Thirion, G. Varoquaux, A. Gramfort, V. Michel, O. Grisel, G. Louppe, J. Nothman, ’make_blobs’, 2017. [Online]. Available: [Accessed: 12-Jun-2018]
FIG. 3: in a) Two circle (Sec. IV A) shaped 2D clusters each of size $N = 250$ such that the blue points have higher density than the red ones. in b) Cluster size vs Temperature $T$ using SPC (Sec. II C 1). As $T$ increases, the giant component successively breaks down: at $T = 0.007$ we can observe 2 clusters which remain stable until $T = 0.10$. Inset: (in a) above right ) Susceptibility $\chi(T)$ at $T = 0.01$. $\chi$ peaks around $T = 0.007$, remains stable until $T \approx 0.10$ inside the SP-phase, then dives down toward 0 for $T > 0.10$. (in a) below right) The Average Magnetization $\langle M \rangle(T)$ at $T = 0.01$. $\langle M \rangle$ starts at 1 for $T = 0$ then remains stable at $\langle M \rangle = 0.5$ inside the SP-phase from $T = 0.01$ to $T = 0.10$. This stability only occurs when clusters have uniform or identical densities, and are linearly separable. Once $T > 0.10$, $\langle M \rangle$ goes down to 0 inside the Paramagnetic Phase.

We observed two cases of this problem: a 3D case, and a 500D case.

Figure Fig. (7a) respectively show the susceptibility, and the clusters size as a functions of temperature. At $T = 0.01$, in the SP-phase, we observe 3 clusters in Fig. (7a) of size 167, 166, and 166 with an ARI of 1.

We follow this with $L_c$’s solution which scores 1460.47, an ARI of 0.20, while the expected likelihood was 599.91. Yet again our solution’s likelihood is higher than our expectation, and the real clusters are divided in smaller ones. In comparison K-Means and DBSCAN respectively achieve ARI of 1, and 0.8. In light of this, we decided to try again the same problem but with the dimensionality set to $D = 500$. As expected SPC’s results do not change. However in this instance f-SPC’s solution quickly converges to the best classification. A further investigation was done by simulating both the 3D, and 500D cases using SPC, and computing the likelihood $L_c$ for every configurations. The assumption being that the maximum likelihood should be found within the temperature range where the system is in the SP-phase.

Figures (7b) and (7c) respectively show the likelihood as functions of temperature. We notice that in the 500D case in Fig. (7c), the maximum likelihood is found at temperatures $T < 0.15$ within the SP-phase, and the $L_c$ monotonously decreases at higher temperatures. The opposite happens in Fig. (7b) where the best classification doesn’t correspond to the maximum likelihood of $L_c$ which in this case is found at high temperatures $T \approx 0.25$ which by looking at $\chi$ in Fig. (7a) means we are effectively in the paramagnetic phase. We provide additional comments in the discussion section of this paper.

D. Sci-Kit learn: Fishers Iris data

Fisher’ Iris Data using Sci-kit learn loader which includes individuals from 3 species: Iris Setosa, Virginica, and Versicolor. $N = 150$, $D = 4$, and there are 50 nodes per cluster.

As we can see in Fig. (8b), It’s one of the more challenging toy problems because two of the three clusters,
FIG. 4: in a) 2 Circles (Sec. IV A): The MST of the (SPC Sec. II C 1) Solution at $T = 0.01$ shows two subtrees each representing the two clusters in the data, and in b) with the f-SPC (Sec. II C 2) Solution, a high number of clusters are found: There is no misclassification however the 2 original clusters are pieced apart.

FIG. 5: in a) 3 wines (Sec. IV B), 2D plot of dimensionality reduction of the 13 features using UMAP [34]. No scaling and/or normalizing done to the features produces 3 clusters: Wines of type 1 and 2 are found in the same clusters while Wines in cluster 0 remain isolated. in b) we rescaled the 11 features using the MinMax method Sec. III B. The MinMax Scaler spreads out the original clusters, and the Wine 1 and 2 clusters are now linearly separable. in c) Clusters size vs Temperature $T$. From $T = 0$ to $T \approx 0.14$, The ferromagnetic Phase with one giant cluster, then from $T \approx 0.14$ to $T \approx 0.20$, the SP-phase with 3 clusters which all start dissolving once $T > 0.20$. Insets: (in a) above right) Susceptibility $\chi(T)$, and (in a) below right) Average Magnetization $\langle M \rangle$ at $T \approx 0.15$. $\chi$ peaks at $T = 0.12$ into the SP-phase, decreases, and peaks one last time at $T \approx 0.17$ to transition into the Paramagnetic Phase.
FIG. 6: In a) 3 wines (Sec. IV B) MST of SPC’s solution at $T = 0.147$: The 3 largest clusters respectively contain most of the observations from the original wine groups except for few unclassified or misclassified samples. in b) f-SPC’s solution: There are 7 clusters: 1 for Wine 0, 4 for Wine 1, and 2 for Wine 2.

FIG. 7: in a) 3D blobs (Sec. IV C): Cluster sizes vs Temperature $T$ using SPC (Sec. II C 1). 1 giant cluster at $T = 0$, and 3 stable clusters from $T = 0.007$ to $T \approx 0.05$. The transition into the Paramagnetic Phase is asynchronous for each clusters because of their differing densities: At $T \approx 0.05$ cluster 1 starts dissolving, followed by cluster 2 at $T \approx 0.11$, and finally, cluster 3 at $T \approx 0.19$. Insets: (in a) above right) Susceptibility $\chi(T)$, and (in a) below right) Average Magnetization $\langle M \rangle$ at $T = 0.01$. $\chi$ peaks at $T = 0.007$ into the SP-phase, remains stable until $T \approx 0.09$, and then slowly decreases to 0 into the Paramagnetic Phase. in b) the likelihood $L_c(T)$ of SPC solutions for 3D clusters, and 500D in c). When D is low, $L_c$ is stable until $T \approx 0.05$ which is the temperature at which the transition into the Paramagnetic Phase occurs. Where we would expect a decrease in $L_c$, we see an increase as $T$ goes up, a maximum is reached around $T \approx 0.20$ which as can be seen from a) $\chi \approx 0$ which signals the Paramagnetic Phase of the system. The 500D case in c), on the other hand, peaks within the SP-phase until $T \approx 0.10$ which is the temperature at which the transition into the Paramagnetic Phase occurs. Once $T > 0.10$, a net decrease in $L_c$ happens, and as $T$ goes up the slope of $L_c$ remains negative as expected.
Virginica, and Versicolor, are not linearly separable. We set \( K = 7 \), and observe two phases in Fig. 8a: for \( 0.05 < T < 0.137 \) there are 2 clusters. The largest contains the Virginica, and Versicolor nodes while the smaller one includes most Seratosa nodes. The 2nd phase transition occurs at right before \( T = 0.137 \), and is followed by the separation of most Virginica nodes into their own cluster. This SPC solution Fig. 9a has an ARI of 0.65.

The \( L_c \) solution in Fig. 9b has an ARI of 0.627, a likelihood of 132, and our expected \( L_c \) is 104. In comparison K-Means and DBSCAN respectively achieve ARI of 0.73, and 0.52. Similarly to the precedent examples, we recover five large clusters: Cluster 1 contains Seratosa individuals, while the Virginica, and Versicolor clusters are split into 4 smaller ones with minimal misclassification.

### E. Sci-Kit learn: MNIST digits

The hand-written digits dataset, generated with Sci-kit learn loader 14, is mainly used to test classification algorithms in supervised learning but we are interested in how well both SPC, and f-SPC deal with the nonlinear nature of hand-writing. The data contains 10 classes of digits ranging from 0 to 9. The full set has close to 2000 nodes from which we select 500, and 50 of each class. The images are 8 by 8, and \( D = 64 \).

The MST in Fig. 10a, and the UMAP 24 plot in Fig. 10b show us all digit classes are linearly separable, the data contains outliers especially “1”s and “9”s which may be the result of different writing styles.

We see that the big cluster breaks down in multiple steps Fig. 10c due to the differing densities of clusters present in the data. Fig. 10c shows that at \( T = 0.178 \) right after the final \( y \) peak the configuration’s clusters in Fig. 11a has an ARI = 0.75, and show no significant misclassification. \( L_c \)’s solution in Fig. 11b, after 25000 generations, has a likelihood of 149.47, an ARI of 0.747, and an expected \( L_c \) of 135. Once again we encounter similar results as with the previous cases with the higher likelihood, and the number of clusters. The \( L_c \) solution has close to 20 clusters, and while there is one main cluster per digit which is the case for digits 0 and 6, and mostly for 3, 7, 8, and 9, the digits 1, 2, 4, and 5 are all split in two clusters. We explain this by the inconsistent nature of hand-writing which produces different writing styles. In comparison K-Means and DBSCAN respectively achieve ARI of 0.56, and 0. There are many reasons why DBSCAN fails this problem: DBSCAN classifies some observations as noise into one cluster, it also has issues tackling problems with clusters of different densities.

### F. Kaggle: NYSE Data

We obtained publicly available NYSE stock market data on Kaggle 15. The original data contains daily open, high, low, closing prices, and volume from 8/13/2012 to 8/11/2017. Because not all stocks traded for the whole duration we only select the stocks which did for the last 1250 days (\( \approx 5 \) years) which left us with 447 stocks, and furthermore we, in this case, were interested in a time horizon of 5 years in trading days from 8/23/2012 to 8/11/2017. We consider the daily trading closing prices which are use to compute the daily returns such that:

\[
r(t) = \ln(P_{t+1}) - \ln(P_t)
\]

The final data set has a time-series Length \( D = 1249 \). Using Eqn. 17 we consider three cases for the correlation matrix: i.) the full correlations, ii.) denoising using IMN (See Sec. III C 2), and iii.) cleaning the matrix using a RMT method (See Sec. III C 1).

Financial markets are perpetually evolving living ecosystems, and this is illustrated in the lack of available true sectoral classification of publicly traded companies. In the process of clustering stock market data, 16, we wanted to compare the results of our algorithms with industry standard classification but we faced the following difficulties:

We consider the following industry classifications 17:

- The New York Stock Exchange (NYSE) uses the Global Industry Classification Standard (GICS) 18 (which we use here). The National Association of Securities Dealers Automated Quotations (NASDAQ) and the London Stock Exchange (LSE) both use the Industry Classification Benchmark (ICB) 19. Industry classifications have sectoral, industrial and sub-industrial levels. Although

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14 D. Cournapeau, F. Pedregosa, O. Grisel ‘load_digits’, 2007-2010. [Online]. Available: http://scikit-learn.org/stable/modules/generated/sklearn.datasets.load_digits.html [Accessed: 12-Jun-2018]

15 C. Nugent ‘S&P 500 stock data - Historical stock data for all current S&P 500 companies’, 2017-2018. [Online]. Available: https://www.kaggle.com/camnugent/sandp500 [Accessed: 01-Dec-2017]

16 A very nice review of clustering methods applied to financial datasets is available at [33]

17 There is no consensus industry classification used in the financial services industry.

18 The GICS counts 11 sectors, 24 industry groups, 68 industries, 157 sub-industries, and is updated annually. For more details on their hierarchical industry classification system https://www.msci.com/documents/10199/4547797/GICS+Structure+effective+Sep+1%2C+2016.xls

19 The ICB counts 10 industries, 19 supersectors, 41 sectors, 114 subsectors, and is For details on their hierarchical industry classification system https://www.ftse.com/products/downloads/ICS_Rules.pdf
commonalities exists one is left to determine the equivalences when information aggregation is required across different markets.

GICS, and ICB are static classifications which are updated at irregular intervals (i.e. GICS every year, ICB from weekly to yearly updates). The focus of these companies is to provide long term structural trends of financial markets. As such they lose their usefulness if one wants to consider the impact of rare events such as financial crashes which significantly alter the behavior of businesses. They also do not consider how the diversification of investments and activities affect their respective classifications. The case of Amazon can be argued to illustrate the idea behind the Adaptive Market Hypothesis (AMH) [31]: Amazon’s GICS’ sector is Consumer Discretionary. GICS uses this sector to classify companies whose activity they deem “most sensitive to economic cycles” 20. It is unclear what is meant by “sensitive” in this instance as there are many possible interpretations, and this sector is very heterogeneous. Perhaps it highlights the adaptive nature of Amazon’s business interests which started first as an order-to-delivery e-commerce bookstore but based on Fig. (12a) is now closest to the Information Technology sector.

The life cycle of publicly traded companies can be short. Firms go public and private at relatively high frequency when compared to biological evolution on a human timescale as motivated by Farmer in [14]. The inclusion or exclusion of individuals in an ecosystem can and should have an impact on its structure based on how important the individuals are to the groups. When we looked for GICS data for our time-series, a number of companies had gone private since Aug 2017, and GICS classification had been updated without reflecting these new changes for these companies. Gathering data on these companies which translated into the newer nomenclatures was thus rendered more difficult. Yet again illustrating the need for expert-free unsupervised methods.

Finally, while as previously stated, GICS and ICB intend on providing data which capture long term trends. Financial markets are populated with participants (i.e. pension funds, high frequency trader, asset managers etc...) each holding a diverse set of objectives, who do not necessarily operate on the same time scales or have the

20 A description of GICS sector is available at [https://www.msci.com/documents/10199/4547797/GICS+Sector+definitions-Sep+2016.pdf](https://www.msci.com/documents/10199/4547797/GICS+Sector+definitions-Sep+2016.pdf)
FIG. 9: in a) Iris 3 species (Sec. IV D) : MST of SPC’s solution at $T = 0.137$. 3 large clusters representing the original Iris species (Cluster 0 for “Setosa”, 1 for “Versicolor”, and 2 for “Virginica”), and 6 smaller ones. in b) $t$-SPC’s solution after 10000 generations. 5 large clusters: 1 for Setosa, 2 for Versicolor, and 2 for Virginica.

FIG. 10: in a) MNIST hand-written digits (Sec. IV E) : 2D plot of dimensionality reduction of the 64 features using UMAP [34]. $N = 500$. 10 classes from 0 to 9. in b) the MST: Overall numbers of the same digit class are close. in c) Cluster sizes vs Temperature $T$ using SPC (Sec. II C 1) at $T \approx 0.18$. Insets: (in a) above right) Susceptibility $\chi(T)$, and (in a) below right) Average Magnetization $\langle M \rangle$ at $T \approx 0.18$.

same investment horizons. If one goal is to provide comprehensive analyses of the multiple existing dynamics in markets, tools which capture these trends, and methods which subsequently find relations between them should be prioritized.

This motivates us to argue that the highly dynamic nature of financial markets renders the use of static classifications problematic to a certain extent.

We use GICS’s 11 sectors as the “true” economic sectors of the US financial market. These include Consumer Discretionary (74 stocks), Consumer Staples (31 stocks), Energy (28 stocks), Financials (62 stocks), Health Care
FIG. 11: in a) MNIST hand-written digits (Sec. IV E): MST of SPC’s solution at $T \approx 0.18$. 10 classes recovered: Cluster 8 is split in two, and some observations from cluster 9 & 1 are found in one mixed cluster. There are nonlinearities in how digits are drawn which may explain the closeness of 9s and 1s. in b) f-SPC’s solution: 10 classes recovered: 1 cluster for 0s and 6s, 3 for 1s, 2 for 2s, 3s, 4s, 5s, 7s, 8s and 9s.

(51 stocks), Information Technology (IT) (59 stocks), Industrials (58 stocks), Materials (26 stocks), Real Estate (26 stocks), Telecoms (4 stocks), and Utilities (28 stocks). Although as previously mentioned we do not believe this classification to be valid, here we make use of it as benchmark.

Looking at MSTs in figures (12a), (12b), and (12c), and aided by the GICS classification as legend, we notice nodes belonging to the same economic sectors are mostly located in proximity of each other as one would expect in a static world or over time-scales where the static model is a reasonable approximation.

We report SPC results in figures (13a), (13c), and (13e) respectively at $T = 0.081, T = 0.071$, and $T = 0.129$ for the full (K=5), normalized, and RMT cases.

We briefly mention again one of SPC’s features which consists in linking a node to its closest neighbor based on the spin-spin correlations. Using the condition $\theta > 0.5$ we construct a graph but in the case where a node has no correlations meeting our condition, it is linked to its neighbor of highest spin-spin correlation. This feature forces SPC to produce graphs without isolated nodes. At the same time, and because of this fact, we consider small size clusters are equivalent to noisy, insufficiently correlated, or unclassified observations.

SPC solutions recover GICS information as seen by their respective ARI: 0.317, 0.479, and 0.33. The solution with highest number of noisy or unclustered stocks is Fig. [13a], The financial sector is merged with many other stocks from other sectors, whereas most industries are found in one or two clusters. The complexity goes down when we move to Fig. [13b] where every sector have mostly separated into their own unique cluster, and Fig. [13c] which gives a similar picture although with more smaller unclassified clusters present.

$L_c$ results were simulated for 25000 generations, and we obtained $L_c$ values of 113.92, 54.13, and 367.93 respectively for the Full Fig. (13b), the Normalized Fig. (13d), and the RMT Correlations Fig. (13f). Their economic GICS information recovered via the ARI were, following the same order, 0.25, 0.35 and 0.41. While Fig. (13b) has the smallest number of clusters 15, we find clusters which mostly contain firms from single industries such as the financial, utilities, Real Estate, and Energy sectors. The other clusters more or less mixed including a very large one which we could refer to as the “market”. Recall that Fig. (1a) shows the correlations of the “Market Mode” are mostly positive, and one can easily infer this kind of result. Fig. (13d) and Fig. (13f) provide a cleaner pictures of the market: in Fig. (13d) there is no large “market” cluster and every industry is mostly represented in their own respective clusters. Firms, previously found in the “market” are now for most of them located in clusters representative of their respective industries. Similar situation in Fig. (13f) except the industry sectors have a better definition while a large mixed cluster remains
FIG. 12: in a) S&P500: Market Mode Correlation-based MST of 447 stocks over 1249 trading days (Sec. IV F). in b) The Market Mode was removed using IMN Sec. III C 2 of the correlation matrix, and in c) using the eigenvalues of the correlation matrix of daily returns, located outside the Wishart range Sec. III C 1.

Th neighborhood search SPC performs constrains the scope of the optimization. In SPC’s case, SA can only minimize the Hamiltonian $H_S$ over the neighborhoods necessitates an additional decision in picking the neighborhood size $K$ which acts as a hyper-parameter. The likelihood $L_c$ is optimized over the whole range of observations effectively removing such need, and making the optimization fully unsupervised. This also means that there exists a possibility that nodes which wouldn’t cluster together, because of neighborhood limitation, would in this particular case. It is unclear which is the best way to proceed.

Our second goal is to explore clustering differences
FIG. 13: S&P 500: $N = 447$ stocks traded over 1249 days (Sec. IV F). 11 GICS economic sectors: Consumer Discretionary (royal blue), Consumer Staples (sky blue), Energy (orange), Financials (beige), Health Care (dark green), Information Technology (light green), Industrials (red), Materials (pink), Real Estate (purple), Telecom (magenta), Utilities (brown). In (a), (c), and (e) SPC’s solution at $T = 0.081$, $T = 0.071$, and $T = 0.119$ respectively for the Full “Market Mode” sample Correlation Matrix, the Noise cleaned and iteratively normalized (Sec. III C 2) , and Noise cleaned RMT (Sec. III C 1) cases. And in (b), (d), and (f) the f-SPC’s solutions after 25000 generations.
which arise in our 3 cases. In Fig. (13a), and Fig. (13b) The biggest clusters have significant overlap with economic sectors except for a few large ones such as the financials cluster which also houses stocks from other sectors. The picture gets cleaner once we look at Fig. (13c), and Fig. (13d) where we now have less mixing in most clusters, and finally in Fig. (13e), and Fig. (13f) some of the clusters such as the Real Estate, Utilities, Health Care, and Consumer Staples found in the Normalized case are split. We noticed a similar result in Sec. [IV] where the $L_c$ solution had a higher number of clusters, but they were essentially subgroup within the ones found by SPC. 

Shown in Fig. (14a), Fig. (14b), and Fig. (14c) are the Adjusted Rand Indices as functions of temperature for our three cases. We compute the ARIs at every temperature taking f-SPC as the true classification, and SPC as the candidates. Maximal ARI values are respectively 0.175, 0.6, and 0.05 for temperatures $T = 0.068$, $T = 0.071$, and $T = 0.08$. These temperature values are all located in the SP-phase where the susceptibility is non-zero confirming the claim in [17] that the maximization of $L_c$ should recover a clustering configuration of the a system in the vicinity of the phase transition. We also note that despite SPC neighborhood search restrictions the Normalized f-SPC solution has the highest similarity to its SPC’s counterparts. The “Market Mode” case of f-SPC has a large mixed cluster, and the RMT one has its largest cluster mixed with securities from every economic sector. This would require further analysis but we think the main difference between that and SPC’s equivalent is this cluster which could be of low correlation. 

We push further the analysis by considering $L_c$ as a clustering quality evaluator. As was demonstrated in [18] $L_c$ is a consistent objective function which if maximized can discriminate between clustering algorithms. Similarly to the “Silhouette Coefficient”, and the “Calinski-Harabaz Index” which are methods used to evaluate the clusters definition when the ground truth class is not known, $L_c$ plays a similar role. 

We test for this by evaluating all SPC candidates for their $L_c$ values, and we add a horizontal line on each plot indicating the respective f-SPC’s $L_c$. In every case, SPC’s $L_c$ start low at low T, reaches a maximum at intermediate T and decreases slowly at T increases into Paramagnetic territory. This is yet another confirmation that higher $L_c$ values are located in a intermediate temperature regime which coincides with the SP-phase when the system is critical. SPC’s $L_c$ maxima are 105, 43, and 170 respectively in Fig. (15a) Fig. (15b) Fig. (15c), and we observe that solutions recovered using f-SPC all have higher likelihoods than SPC’s. Based on the result in this paper, and in [18] one could argue that f-SPC produces better clustering candidates than SPC at least in this case.

V. DISCUSSION

In this paper, we were able to successfully implement SPC, and f-SPC, and we tested those methods on synthetic, and real data. If there exists significantly different structures within the data, SPC will exhibit multiple transitions within the SP-phase. As the temperature is varied, the couple Susceptibility $\chi$ and Average Magnetization $\langle m \rangle$ signal the occurrence of phase transitions. The spin-spin correlation $G$ is indirectly linked to the interaction strength $J$ and the distributions found in the data. The method has the advantage of being unsupervised for the most part, it does not necessitate $a$-priori knowledge of the number of clusters, and makes no assumption about the distributions of the data. While SPC performs a neighborhood search, which requires picking a value for $K$, it does not affect the simulation significantly for large data sets; as was previously seen in [4]. The parameter $\theta$ is set to 0.5 and helps decide clusters membership. We clustered at every temperature within a pre-determined range such that we do not need to identify “clustering temperatures $T_{clus}$” like in [6] but we do so at the expense of additional computational cost. We note that in the literature there are modifications of the Potts model clustering which automate parameter selections for the clustering temperature $T_{clus}$, the local length scale $a$, and the cluster membership threshold $\theta$ through validation based calibration. [35].

Once we have a hierarchy of configurations, such as in Fig. (10c), one needs to select appropriate clusters representative of the different regimens of the SP-phase. This is an easy task as can be seen in Fig. (5c) when the number of cluster is low, and the clusters have similar densities which establishes a stable phase for a relatively wide temperature range. On the other hand if the number of clusters is high, and the data is composed of clusters of different densities, the susceptibility, which tracks the variance of biggest cluster has its limitations [28]. As the size of the dataset increases the susceptibility is a useful as a tool to locate the final transition and lowest clustering level. 

f-SPC’s GA only requires the correlation matrix and is completely unsupervised. The randomly generated population is diversified at every iteration by applying as many as 7 different mutations. It’s a fast algorithm that can be easily parallelized while SPC is sequential due to it’s Markovian nature. The computation time is affected by the order of the observations in the data [8]. We noticed that ordering our data based on the order of one of the observations’ closest “neighbors” produced better results which should motivate further exploration of potential heuristics dealing with this issue. $L_c$ measures the quality of cluster configurations: its value is computed from the clusters sizes $n_i$ and the intra-cluster correlations $c_r$. The optimization is global which, as opposed to SPC, avoids the need to determine a neighborhood size $K$. There exist problems where choosing a sufficiently big $K$ has an non-trivial impact on SPC’s
FIG. 14: In figures (a), (b) and (c) find the ARI (See Sec. IV) for the following cases: (a), with a market mode (See Sec. III C), (b) de-noising with IMN (see Sec. III C 2) and (c) when a RMT method is used to clean the covariance matrix (See Sec. III C 1). The ARI index expresses configuration similarity on $[0,1]$ [25]. Blue dots represent ARI values, and the red line the curve linking them all. We looked at NYSE S&P500 447 Stocks Data. In all three cases we compare the f-SPC method (See Sec. II C 2) to each of the estimated SPC candidates estimated at each temperature $T$ (See Sec. IV F). This demonstrated that in all three cases the maximum likelihood candidates are close to solutions recovered within the super-paramagnetic phase.

FIG. 15: S&P 500 (Sec. IV F) $N = 447$ Stocks, $D = 1249$ trading days: We computed the Likelihood $L_{c}$ (13) of every SPC solutions for all temperatures (red curve, and blue dots), and Likelihood $L_{c}$ of f-SPC’s solution (blue horizontal line) in a) the Market Mode case, in b) the Normalized case, and in c) the RMT case. Every f-SPC solutions has higher likelihood than the SPC entire temperature range in every case. f-SPC solutions are composed of clusters with higher correlation than SPC candidates.

solutions. One such example would be the existence of a relatively low density and sparse cluster in a data set mostly composed of high density clusters. Low values of $K$ would fail to recover the low density clusters which would remain unclassified whereas this isn’t an issue for f-SPC which would perform much better.

f-SPC results are consistent for high dimensionality datasets. If we consider the metric used to evaluate the noise in correlation matrices $q = \frac{N}{D}$ as the ratio of the dimension over the number of observations in the limit of $N \to \infty$. We recall that in [49], $q$ encodes the noise level of the eigenvalues of the sample covariance matrix. $q$ values for our problems are 250 for the two circles, 13.69 for the wines, 166.66 for the 3D blobs, 1 for the 500D blobs, 37.5 for Fisher’s Iris, 7.81 for the MNIST digits, and 0.35 for the NYSE Kaggle data. The $L_{c}$ results consistent
with SPC were the 500D blobs, MNIST, and the NYSE stock data which all confirm that a low $q$ is necessary to compute appropriate correlation matrices. We want $q$ to be as small as possible, and if possible close to 0. This is not always the case, and we have tested ways to de-noise the correlation matrix (Sec. III C 2 and III C 1) in the case of financial time-series but it is unclear at this time what would the solutions be in other cases. In Marsili and Giada derive $L_c$, and along the way they assume that $D \to \infty$ which in turn means one has to consider the finite size effects of the method. Fig. (7b) and Fig. (7e) tell us that if we were to visualize the $L_c$’s objective surface, depending on dimensionality of the problem we could face a “rough” space. One could consider $L_c$ as a sort of modularity function just like in the Network Science literature. One major Network Science problem is the efficient detection of communities inside networks. Similar to our work, cluster configurations are the input of the modularity function $Q$ which, through diverse heuristics, is maximized. However it is well known to Network Scientists that modularity objective surfaces are degenerate: many significantly different clustering results have similar modularity, or in our case, higher likelihood than the true clustering.

We compare this to the modus operandi of SPC: The generative model of the SPC is the Gibbs-Boltzmann distribution which not only validates clusters locally using Eqm. (9), and globally using a cooling schedule. It is a bottom up approach as opposed to global optimization methods which are top down. One assumes that there exists multiple realizations (micro-states) of the generative model, the so called “equivalence classes” which are valid representation of the data. In order to link micro and macro-state one could pick any one micro-state translating into the desired macro-state: Maximum Likelihood methods essentially achieve this feature by searching the space of solutions for any candidates meeting the global objective. We argue that in complex systems, the existence of equivalence classes as illustrated by the degeneracy of clustering objective surfaces leads to the Maximum Entropy principle [26] as an alternative optimization device. The generative model generates equivalence classes (among which are included maximum likelihood candidates) each with differing probabilities, and one then needs to probabilistically combine them to achieve some sort of representative weighted average.

We suspect a way to deal with cases where $D$ is small compared to $N$, and indirectly $q \gg 1$, would be a modification of $L_c$ by adding an additional term acting as a regularizer which could account for the number of clusters. Our rationale follows that $L_c$ as an objective function is degenerate with multiple spin configurations whose likelihood are equal or very close. This degeneracy comes from, if we assume the minimum number size of clusters to be 2 (no singletons), the number of possible configurations $(\frac{N}{2})^N$ which for a case $N = 100$ would be on the other of $10^{169}$.

Finally one is left to decide which de-noising method is deemed optimal and as a consequence which clustering one prefers. The assumptions in both methods have their validity and should be carefully considered. Whereas IMN (Sec. III C 2) of the covariance matrix makes assumption on the nature of covariances as IID normally distributed random variables, RMT (Sec. III C 1) predicts a spectrum of random matrices eigenvalues exists which is pure noisy signal. The noise is removed by reconstructing the data without the noisy eigenvalues whose number increases with dimensionality. We suspect a proper way of deciding which method is optimal is the implementation of such methods as bases of trading strategies.

VI. CONCLUSION

In this paper we have presented two unsupervised data clustering algorithms inspired by the Potts Model [51]. Using SA (SPC Sec. II C 1) optimizes the Hamiltonian of a thermodynamics systems, and the ground state energy solution recovered provides the best clustering structure present in our data. We show that the parameter-free Marsili and Giada’s (Sec. II C 2) maximum likelihood methods implemented with a modified version of Hendricks et al. Parallelized Genetic Algorithm recover solutions similar to those found in the SP-phase Fig. (14). This was done by comparing the SPC solutions to the f-SPC one using the ARI [29]. By comparing the Likelihood of SPC solutions to f-SPC one we showed that f-SPC have higher likelihood which prompted an additional discussion on implication for statistical inference in complex systems. The methods were tested both on toy test cases, and real stock market time-series data illustrating their universality provided an appropriate similarity metric is selected such as the euclidean distance of the Pearson correlation coefficient. We showed that the results are similar to the 11 standard GICS economic sectors however the differences in the number of clusters, and their composition should be cause for concerns with respect to the use of GICS classification for risk management purposes.

Building on the work presented in this paper we would like to perform cluster analysis of stock market intra-day time-series. The last thirty years have seen a magnificent increase in technological power which enabled simultaneous trading on multiple time scales. The so called “High Frequency Trading” paradigm increased tenfold the amount of stock market data, and has significantly impacted the market participants behaviors at shorter time scales. It is therefore natural to consider new species of market participants to exist, and that they come with different objectives to fulfill than longer timescales participants. We conjecture this would be reflected in clusters of stocks disconnected from their economic sectors. We assume traders use all information available to make decisions however the rate of economic information released about publicly traded firms can range from once a month...
to once a year. This rate is significantly lower than that of high frequency trading which leads us to think it is therefore impossible for high frequency traders to trade based solely on economic information alone, and we suspect different objectives may be at play.

One logical next step is what we call Dynamical Cluster Analysis (DCA): Events such as financial crises like the one which preceded the 2008 Great Recession can be investigated at the intra-day scale. Here again we conjecture shocks to the system irremediably affect strategies, and clustering structures are less persistent with time as in [30]. Ultimately some sort of quantification of clustering on different temporal scales could be useful towards probing potential hierarchical causal affects given that different effective theories may dominate at different scales [50].

We have so far worked with changes in price returns as our factor model. The derivation and formulation of the Giada-Marsili $L_c$ allows for multivariate clustering: We can use F by N by N Correlation matrices where $F$ is the number of factors we want to include. Another challenge however would be that at this time we are not aware of an implementation of multi-factor correlation based SPC.

It is notoriously difficult to obtain trading data linked to individual market participants accounts. This kind of data would be extremely useful to directly, not only study traders’ behavior, but begin to understand the kind of ecosystem a financial market is. Unfortunately one is only left with the possibility proxy studies through the dynamics of the traded securities. One alternative approach is to create simulated trading agents, and cluster them using our unsupervised methods using technical trading strategies available in the literature.

Finally, one should consider a complete rewrite of f-SPC as a GPU-based Parallelized Genetic Algorithm to take advantage of modern computing power available at our disposal and further reduce the computation time.

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Appendix A: The Algorithms

The algorithms implemented in this paper have been coded in python and are available on a github repository at [52].

1. SPC Algorithms

We provide a pseudo-code for the SPC [6] algorithm introduced in Sec. II C. Given a distance matrix, and a neighborhood of size K, the algorithm uses the Swendsen-Wang [47] MCMC method to optimize the thermodynamic system.

**TABLE 1**

**Algorithm 1 SPC (Sec. II C and [6])**

| Line | Description |
|------|-------------|
| 1:   | for $k = 0$ to $k = M$ do |
| 2:   | Create edge configuration matrix “link” |
| 3:   | Create Swendsen-Wang clusters |
| 4:   | Compute, and store thermodynamic quantities i.e. $m, c_{ij}$ |
| 5:   | end for |

Swendsen-Wang flips clusters at each iteration, allowing the quick convergence toward a local maxima by conditioning the acceptance of every MCMC move with a cooling schedule.

**TABLE 2**

**Algorithm 2 Swendsen-Wang (Table C and [47])**

| Line | Description |
|------|-------------|
| 1:   | Create new spin configuration using Hoshen-Kopelman |
| 2:   | Flip all clusters |
| 3:   | if Energy of new configuration is higher than precedent then |
| 4:   | if Boltzmann factor of new configuration is lower than rand() then |
| 5:   | Reject new configuration |
| 6:   | end if |
| 7:   | end if |

Hoshen-Kopelman [3] is the mechanism behind clusters discovery in SPC. It allows for the graph to be traveled via its nodes and neighborhoods while clustering the system locally.
Algorithm 3

Extended Hoshen-Kopelman (Table B and [3])

1: Initialize cluster label counter to 0
2: Initialize node1, 1xN array filled with inf
3: Create nodelp, an empty array
4: for i = 0 to i = N do
5:   if The adjacency array of node i is 0 everywhere then
6:     Set the label of i to the label counter
7:     Store the label of i to nodelp
8:     Increase the label counter by 1
9:   else
10:      Find location of 1s in link of i
11:      Store all i neighbors’ labels in t
12:      if All elements of t are equal inf then
13:         Set the label of i to the label counter
14:         Store the label of i to nodelp
15:         Increase the label counter by 1
16:      else
17:         Create an empty array w
18:         for h = 0 to h = len(t) do
19:            Store label t[h] in w if different from inf
20:         end for
21:         Create empty array z
22:         for h in w do
23:            In i’s neighbor, find corresponding neighbor to h
24:            Find the corresponding cluster label in node1
25:            Find the corresponding root to the label
26:            Store the root to z
27:         end for
28:         Set min the minimum of z
29:         Set the node1 of i to min
30:         Find index of the labeled neighbors of i using w
31:         In nodelp, use index, and change label roots to min
32:      end if
33:   end if
34: { Make nodelp sequential }
35: for y = 0 to y = len(nodelp) do
36:   n = y
37:   while The root of n is less than n do
38:      Set n to the root of n
39:   end while
40: for i = 0 to i = len(nodelp) do
41:   Find the labels in node1 equal to i
42:   Update those labels with their root in nodelp
43: end for
44: end for

2. f-SPC Algorithms

We discussed f-SPC in Sec. [1C2] and here we provide a pseudo-code for the implementation of the parallelized genetic algorithm which generates clustering candidates, evaluates their likelihood $L_c$ [17] using Eqn. [13], selects the best candidates and discards the others.

Algorithm 4

f-SPC implementation of Marsili and Giada Maximum likelihood methods (Sec. [1C2] and [17])

1: Produce an initial population of N individuals
2: for (In parallel ) All individuals do
3:   evaluate fitnesses
4: end for
5: for G number of generations do
6:   Create offsprings by copying the entire population
7:   Mutate the offsprings
8: for (In parallel ) All offsprings do
9:   Evaluate fitnesses
10: end for
11: Recombine parents and offsprings
12: Select the N individuals as next population
13: end for
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