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Directed and Undirected Network Evolution from Euler-Lagrange Dynamics

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ABSTRACT

In this paper, we investigate both undirected and directed network evolution using the Euler-Lagrange equation. We use the Euler-Lagrange equation to develop a variational principle based on the von Neumann entropy for time-varying network structure. Commencing from recent work to approximate the von Neumann entropy using simple degree statistics, the changes in entropy between different time epochs are determined by correlations in the degree difference in the edge connections. Our Euler-Lagrange equation minimises the change in entropy and allows to develop a dynamic model to simulate the changes of node degree with time. We first explore the effect of network dynamics on the three widely studied complex network models, namely a) Erdős-Rényi random graphs, b) Watts-Strogatz small-world networks, and c) Barabási-Albert scale-free networks. Our model effectively captures both undirected and directed structural transitions in the dynamic network models. We apply our model to a network time sequence representing the evolution of stock prices on the New York Stock Exchange(NYSE) and sequences of Drosophila gene regulatory networks containing different developmental phases of the organism from embryo to adult. Here we use the model to differentiate between periods of stable and unstable stock price trading and to detect periods of anomalous network evolution. Our experiments show that the presented model not only provides an accurate simulation of the degree statistics in time-varying networks but also captures the topological variations taking place when the structure of a network changes violently.

1. Introduction

The study of network evolution plays an increasingly crucial role in modelling and predicting the structural variance of complex networks (Wolstenholme and Walden, 2015). Previous studies have addressed this problem from the perspectives of both the local and the global characterization of network structure. At the local level, the aim is to model how the detailed connectivity structure changes with time (Lacasa et al., 2008). Specifically, networks grow and evolve with the addition of new components and connections, or the rewiring of connections from one component to another (Barabasi and Albert, 1999; Ernesto and Naomichi, 2008). On the other hand, at the global level, the aim is to model the evolution of characteristics which capture the structure and hence the function of a network and allow different types of network function to be distinguished from one to another. Thermodynamic analysis of network structure allows the macroscopic properties of network structure to be described in terms of variables such as temperature, associated with the internal structure (Wang et al., 2017b). There are also models developed to learn the patterns of network evolution. Examples here include generative and autoregressive models which allow the detailed evolution of edge connectivity structure to be estimated from noisy or uncertain input data (Han et al., 2015).

However, both the global and the local methods require to us to develop models that can be fitted to the available data by estimating their parameters, which describe how vertices interact through edges and how this interaction evolves with time (Wu and Yang, 2013). There are few methods that are both simple and effectively predict the evolution of network structure (Tambo et al., 2016). Motivated by the need to fill this gap in the literature and to augment the methods available for understanding the evolution of time-varying networks, there have been a number of attempts to extend the scope of probabilistic genera-

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tive models using various forms of regressive or autoregressive models (Han et al., 2015; Andreas et al., 2015). However, these essentially local models are parameter intensive and a simpler approach is to coach the model in terms of how different node degree configurations co-occur on the edges connecting them (Wang et al., 2017b).

In recent work we have addressed the problem by detailing a generative model of graph-structure (Han et al., 2015) and have shown how it can be applied to network time series using an autoregressive model (Andreas et al., 2015). One of the key elements of this model is a means of approximating the von Neumann entropy of both directed and undirected graphs (Han et al., 2012). von Neumann entropy is the extension of the Shannon entropy defined over the re-scaled eigenvalues of the normalised Laplacian matrix. A quadratic approximation of the von Neumann entropy gives a simple expression for the entropy associated with the degree combinations of nodes forming edges (Wang et al., 2017a). In accordance with intuition, those edges that connect high degree vertices have the lowest entropy, while those connecting low degree vertices have the highest entropy (Aytekin et al., 2016; Wang et al., 2017b). Making connections between low degree vertices is thus entropically unfavourable. Moreover, the fitting of the generative model to dynamic network structure involves a description length criterion which describes both the likelihood of the goodness of fit to the available network data together with the approximate von Neumann entropy of the fitted network. This latter term regulates the complexity of the fitted structure (Wolstenholme and Walden, 2015; Andreas et al., 2015), and mitigates against over-fitting of the irrelevant or unlikely structure. Moreover, the change in entropy of the two vertices forming an edge between different epochs depends on the product of the degree of one vertex and the degree change of the second vertex. In other words, the change in entropy depends on the structure of the degree change correlations.

The aim of this paper is to explore whether our model of network entropy can be extended to model the way in which the node degree distribution evolves with time, taking into account the effect of degree correlations caused by the degree structure of edges. We exploit this property by modelling the evolution of network structure using the Euler-Lagrange equations. Our variational principle is to minimise the changes in entropy during the evolution (Wang et al., 2017b). Using our approximation of the von Neumann entropy, this leads to update equations for the node degree which include the effects of the node degree correlations induced by the edges of the network (Ye et al., 2014). It is effectively a type of diffusion process that models how the degree distribution propagates across the network. In fact, it has elements similar to preferential attachment (Barabasi and Albert, 1999), since it favours edges that connect high degree nodes (Wang et al., 2017a,b).

This model can also be extended to directed graphs. In prior work we have developed approximate expressions for the von Neumann entropy of directed graphs (Ye et al., 2014), considering the cases where there is a) a mixture of unidirectional and bidirectional edges, b) where the unidirectional edges dominate (strongly directed graphs) and c) where the bidirectional edges outnumber the unidirectional edges (weakly directed graphs). Here we focus on the strongly directed graphs, where edges are purely unidirectional and there are no bi-directional edges. Our model distinguishes between the in and out degrees of vertices, and we develop Euler-Lagrange equations for how the distributions quantities evolve with time.

The remainder of the paper is organized as follows. In Sec.2, we provide a detailed analysis of entropy changes in dynamic networks and develop models for degree statistics by minimising the von Neumann entropy change using the Euler-Lagrange equations. We theoretically analyse both undirected and directed networks separately. In Sec.3, we conduct numerical experiments on the synthetic and real-world time-varying networks and apply the resulting characterization of network evolution. Finally, we conclude the paper and make suggestions for future work.

2. Variational Principle on Graphs

2.1. Preliminaries

Let $G(V, E)$ be an undirected graph with node set V and edge set $E \subseteq V \times V$, and let $|V|$ represent the total number of nodes on graph $G(V, E)$. The adjacency matrix A of a graph is defined as

$$A = \begin{cases} 1 & \text{if } (u, v) \in E \\ 0 & \text{otherwise.} \end{cases} \quad (1)$$

Then the degree of node u is $d_u = \sum_{v \in V} A_{uv}$.

The normalized Laplacian matrix $\tilde{L}$ of the graph G is defined as $\tilde{L} = D^{-\frac{1}{2}} L D^{\frac{1}{2}}$, where $L = D - A$ is the Laplacian matrix and D denotes the degree diagonal matrix whose elements are given by $D(u, u) = d_u$ and zeros elsewhere. The element-wise expression of $\tilde{L}$ is

$$\tilde{L}_{uv} = \begin{cases} 1 & \text{if } u = v \text{ and } d_u \neq 0 \\ -\frac{1}{\sqrt{d_u d_v}} & \text{if } u \neq v \text{ and } (u, v) \in E \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

2.2. Network Entropy

Severini et al. (Passerini and Severini, 2008) exploit the concept of density matrix ρ from quantum mechanics in the network domain. They obtain the density matrix for a network by re-scaling the combinatorial Laplacian matrix by the reciprocal of the number of nodes in the graph, i.e. $\boldsymbol{\rho} = \frac{\tilde{L}}{|V|}$. The von Neumann entropy of the network is then defined as the Shannon entropy of the scaled Laplacian eigenvalues $\lambda_1, \ldots.., \lambda_V$ and is given by

$$S = -Tr[\boldsymbol{\rho} \log \boldsymbol{\rho}] = -\text{Tr}(\boldsymbol{\rho} \log \boldsymbol{\rho}) = -\sum_{i=1}^{|V|} \frac{\hat{\lambda}_i}{|V|} \log \frac{\hat{\lambda}_i}{|V|} \quad (3)$$

Because of the overheads involved in computing the Laplacian eigensystem (which is cubic in the number of nodes), Han et al.(Han et al., 2012) render the computation of entropy more tractable by making a second order approximation to the Shannon entropy. In so -doing they re-express the entropy it in terms of the traces of the normalised Laplacian and its square. The resulting approxminate von Neumann entropy depends on the degrees of pairs of nodes forming edges, and is given by

$$S = 1 - \frac{1}{|V|} - \frac{1}{|V|^2} \sum_{(u,v)\in E} \frac{1}{d_u d_v} \tag{4}$$

The approximation of von Neumann entropy avoids the cubic complexity of computing the Laplacian eigensystem and gives a formula for computing the von Neumann entropy which is at most quadratic in the number of nodes. This allows it to be used to efficiently compute the entropy of networks. It has been shown to be an effective tool for characterizing structural properties of networks, with extremal values for the cycle and fully connected graphs (Han et al., 2015).

For directed graphs on the other hand, the approximate von Neumann entropy is related to the in-degree and out-degree of the nodes (Ye et al., 2014). First, the edge set E is divided into two subsets E_1 and E_2, where $E_1 = \{(u, v)|(u, v) \in E$ and $(v, u) \notin E\}$ is the set of unidirectional edges, $E_2 = \{(u, v)|(u, v) \in E$ and $(v, u) \in E\}$ is the set of bidirectional edges. The two edge-sets satisfy the conditions $E_1 \cup E_2 = E, E_1 \cap E_2 = \emptyset$. With this distinction between unidirectional and bidirectional edges, the analogous approximation for the von Neumann entropy of a directed graph is,

$$S_d = 1 - \frac{1}{|V|} - \frac{1}{2|V|^2} \left\{ \sum_{(u,v)\in E} \frac{d_u^{in}}{d_v^{in} d_u^{out^2}} + \sum_{(u,v)\in E_2} \frac{1}{d_u^{out} d_v^{out}} \right\} \tag{5}$$

To simplify the expression according to the relative importance of the sets of unidirectional and bidirectional edges E_1 and E_2, the von Neumann entropy can be further approximated to distinguish between weakly and strongly directed graphs. For weakly directed graphs, i.e., $|E_1| \ll |E_2|$ most of the edges are bidirectional, and we can ignore the summation over E_1 in Eq.(5), rewriting the remaining terms in curly brackets as

$$S_{wd} = 1 - \frac{1}{|V|} - \frac{1}{2|V|^2} \left\{ \sum_{(u,v)\in E} \frac{\frac{d_u^{in}}{d_u^{out}} + \frac{d_v^{in}}{d_v^{out}}}{d_u^{out} d_v^{in}} \right\} \tag{6}$$

For the strongly directed graph the unidirectional edges dominate, i.e., $|E_1| \gg |E_2|$, there are few bidirectional edges, and we can ignore the summation over E_2 in Eq.(5), giving the approximate entropy as

$$S_{sd} = 1 - \frac{1}{|V|} - \frac{1}{2|V|^2} \left\{ \sum_{(u,v)\in E} \frac{d_u^{in}}{d_v^{in} d_u^{out^2}} \right\} \tag{7}$$

Thus, both the strongly and weakly directed graph entropies depend on the graph size and the in-degree and out-degree statistics of edge connections (Ye et al., 2014).

2.3. Euler-Lagrange Equation

We would like to understand the dynamics of a network which evolves so as to minimise the entropy change between different sequential epochs. To do this we cast the evolution process into a variational setting of the Euler-Lagrange equation (Wang, 2013), and consider the system which optimises the functional

$$\mathcal{E}(q) = \int_{t_1}^{t_2} \mathcal{G}\left[t, q(t), \dot{q}(t)\right] dt \tag{8}$$

where t is time, $q(t)$ is the variable of the system as a function of time, and $\dot{q}(t)$ is the time derivative of $q(t)$. Then, the Euler-Lagrange equation is given by

$$\frac{\partial \mathcal{G}}{\partial q}\left[t, q(t), \dot{q}(t)\right] - \frac{d}{dt}\frac{\partial \mathcal{G}}{\partial \dot{q}}\left[t, q(t), \dot{q}(t)\right] = 0 \tag{9}$$

Here we consider an evolution which changes just the edge connectivity structure of the vertices and does not change the number of vertices in the graph (Nuno et al., 2011). As a result, the factors $1 - \frac{1}{|V|}$ and $\frac{1}{|V|^2}$ are constants and do not affect the solution of the Euler-Lagrange equation.

2.4. Undirected Graphs

Suppose that two undirected graphs $G_t = (V_t, E_t)$ and $G_{t+\Delta t} = (V_{t+\Delta t}, E_{t+\Delta t})$ represent the structure of a time-varying complex network at two consecutive epochs t and $t + \Delta t$ respectively. Then the change of approximate von Neumann entropy between two sequential undirected graphs can be written a

$$\Delta S = S(G_{t+\Delta t}) - S(G_t) = \frac{1}{|V|^2} \sum_{(u,v)\in E,E'} \frac{d_u\Delta_v + d_v\Delta_u + \Delta_u\Delta_v}{d_u(d_u + \Delta_u)d_v(d_v + \Delta_v)} \tag{10}$$

where Δ_u is the change of degree for node u, i.e., $\Delta_u = d_u^{t+\Delta t} - d_u^t$; Δ_v is similarly defined as the change of degree for node v, i.e., $\Delta_v = d_v^{t+\Delta t} - d_v^t$. The entropy change is sensitive to degree correlations for pairs of nodes connected by an edge.

We aim to study evolutions that minimise the entropy change associated with the structure of the degree change correlations, i.e. minimise the entropy change between time intervals. In order to represent the change of entropy more accurately, here, we approximate the denominator in Eq.(10) to the quadratic term and apply the Euler-Lagrange equation $\mathcal{G} = \Delta S$ with the entropy change to obtain

$$\mathcal{G}\left[t, d_u(t), \Delta_u(t), d_v(t), \Delta_v(t)\right] = \frac{d_u\Delta_v + d_v\Delta_u + \Delta_u\Delta_v}{d_u^2 d_v^2} \tag{11}$$

For the vertex indexed u with degree d_u the Euler-Lagrange equation in Eq.(9) gives,

$$\frac{\partial \mathcal{G}}{\partial d_u} - \frac{d}{dt}\frac{\partial \mathcal{G}}{\partial \Delta_u} = 0 \tag{12}$$

First, solving for the partial derivative of the degree d_u, we find

$$\frac{\partial \mathcal{G}}{\partial d_u} = -\frac{d_u\Delta v + 2d_v\Delta u + 2\Delta u\Delta v}{d_u^3 d_v^2} \tag{13}$$

The detailed analysis above not only involves the terms to first order in the node degree change but also those of second order, i.e. degree difference correlations of the form $\Delta u\Delta v$.

Then computing the partial time derivative to the first order degree difference Δ_u, we obtain

$$\frac{\partial \mathcal{G}}{\partial \Delta_u} = \frac{d_v + \Delta v}{d_u^2 d_v^2} \tag{14}$$

Substituting Eq.(13) and Eq.(14) into Eq.(12),

$$\frac{\partial \mathcal{G}}{\partial d_u} - \frac{d}{dt}\frac{\partial \mathcal{G}}{\partial \Delta_u} = \frac{2\Delta^2 u - d_u \dot{\Delta u}}{d_u^3 d_v^2} = 0 \tag{15}$$

The solution for Euler-Lagrange equation in terms of node degree difference is

$$\Delta_u = \left(\frac{d_u}{d_v}\right)^2 \Delta_v + C \tag{16}$$

where C is the constant term coming from the integral of the differential equation. This leads to a detailed degree update equation which involves a square term of d_u/d_v and plus a constant C. Since it considers the effects of second order terms in the change of von Neumann entropy, this solution is accurate in predicting the degree distribution

As a result, solving the Euler-Lagrange equation which minimises the change in entropy over time gives a relationship between the degree changes of nodes connected by an edge. Since we are concerned with understanding how network structure changes with time, the solution of the Euler-Lagrange equation provides a way of modelling the effects of these structural changes on the degree distribution across nodes in the network. The update equation for the node degree is at time epochs t and $t + \Delta t$ is

$$d_u^{t+\Delta t} = d_u^t + \sum_{v\sim u} \dot{\Delta}_v \Delta_t = d_u^t + \sum_{v\sim u} \left(\frac{\Delta_u}{\Delta_t}\right)_v \Delta_t \tag{17}$$

In other words by summing over all edges connected to node u, we increment the degree at node u due to changes associated with the degree correlations on the set of connecting edges. We then leverage the solution of the Lagrange equation to simplify the degree update equation, to give the result

$$d_u^{t+\Delta t} = d_u^t + \sum_{v\sim u} \left(\frac{d_u}{d_v}\right)^2 \Delta_v + C \tag{18}$$

This can be viewed as a type of diffusion process, which updates edge degree so as to satisfy constraints on degree change correlation so as to minimise the entropy change between time epochs. Specifically, the update of degree reflects the effects of correlated degree changes between nodes connected by an edge.

2.5. Directed Graphs

2.5.1. Weakly Directed Graphs

In order to accommodate directed edges, we consider the node u and let d_u^{in} be the number of edges incident on vertex u or in-degree and d_u^{out} be the number of edges leaving vertex u or out-degree. The ratio of in-degree to out-degree is $r_u = \frac{d_u^{in}}{d_u^{out}}$ and $r_v = \frac{d_v^{in}}{d_v^{out}}$. We use this ratio to re-write the directed graph entropies in terms of the node in-degree and the in/out degree ratio. As a result the weakly directed graph entropy is

$$S_{wd} = 1 - \frac{1}{|V|} - \frac{1}{2|V|^2}\left\{\sum_{(u,v)\in E} \frac{r_u(r_u + r_v)}{d_u^{in} d_v^{in}}\right\} \tag{19}$$

For two weakly directed graphs $G_{wd}^t = (V_t, E_t)$ and $G_{wd}^{t+\Delta t} = (V_{t+\Delta t}, E_{t+\Delta t})$, representing the structure of a time-varying complex network at two consecutive epochs t and $t+\Delta t$ respectively, the change of von Neumann entropy is given by

$$\begin{aligned} \Delta S_{wd} &= S(G_{wd}^{t+\Delta t}) - S(G_{wd}^t) \\ &= -\frac{1}{2|V|^2}\sum_{(u,v)\in E,E'}\Big\{\frac{(2r_u + r_v)\Delta r_u + r_u \Delta r_v}{d_u^{in} d_v^{in}} \\ &\quad - \frac{r_u(r_u + r_v)(d_u^{in}\Delta_v^{in} + d_v^{in}\Delta_u^{in})}{(d_u^{in} d_v^{in})^2}\Big\} \end{aligned} \tag{20}$$

where Δ_u^{in} is the change of in-degree for node u, i.e., $\Delta_u^{in} = d_u^{in}(t + \Delta t) - d_u^{in}(t)$; Δ_v^{in} is similarly defined as the change of in-degree for node v, i.e., $\Delta_v^{in} = d_v^{in}(t + \Delta t) - d_v^{in}(t)$. Δr_u and Δr_v are the change of degree ratio for the node u and node v respectively.

The Euler-Lagrange equation for r_u gives

$$\frac{\partial \Delta S_{wd}}{\partial r_u} - \frac{d}{dt}\frac{\partial \Delta S_{wd}}{\partial \Delta r_u} = -\frac{2(2r_u + r_v)(d_u^{in}\Delta_v^{in} + d_v^{in}\Delta_u^{in})}{(d_u^{in} d_v^{in})^2} = 0 \tag{21}$$

and similarly for r_v gives

$$\frac{\partial \Delta S_{wd}}{\partial r_v} - \frac{d}{dt}\frac{\partial \Delta S_{wd}}{\partial \Delta r_v} = -\frac{2r_u(d_u^{in}\Delta_v^{in} + d_v^{in}\Delta_u^{in})}{(d_u^{in} d_v^{in})^2} = 0 \tag{22}$$

Combining the Eq.(21) and Eq.(22), the relationship between d_u^{in} and d_v^{in} is

$$\frac{\Delta_u^{in}}{d_u^{in}} = -\frac{\Delta_v^{in}}{d_v^{in}} \tag{23}$$

Thus, for the weakly directed graph, there exists a linear correlation between Δ_u^{in}/d_u^{in} and Δ_v^{in}/d_v^{in}.

2.5.2. Strongly Directed Graphs

For a strongly directed graph the von Neumann entropy in Eq.(6) can be expressed in terms of in-degree and in.our degree ratio as

$$S_{sd} = 1 - \frac{1}{|V|} - \frac{1}{2|V|^2}\left\{\sum_{(u,v)\in E} \frac{r_u^2}{d_u^{in} d_v^{in}}\right\} \tag{24}$$

For two strongly directed graphs $G_{sd}^t = (V_t, E_t)$ and $G_{sd}^{t+\Delta t} = (V_{t+\Delta t}, E_{t+\Delta t})$, the change of von Neumann entropy is

$$\begin{aligned} \Delta S_{sd} &= S(G_{sd}^{t+\Delta t}) - S(G_{sd}^t) \\ &= -\frac{1}{2|V|^2}\sum_{(u,v)\in E,E'} \frac{d_u^{in} d_v^{in}\Delta r_u - r_u(d_v^{in}\Delta_u^{in} + d_u^{in}\Delta_v^{in})}{(d_u^{in} d_v^{in})^2} \end{aligned} \tag{25}$$

where Δ_u^{in} is the change of in-degree for node u; Δ_v^{in} is similarly defined as the change of in-degree for node v.

Now we apply the Euler-Lagrange equation to the changes of entropy for strongly directed graph. The partial derivative of the ratio r_u is

$$\frac{\partial \Delta S_{sd}}{\partial r_u} = -\frac{d_u^{in}\Delta_v^{in} + d_v^{in}\Delta_u^{in}}{(d_u^{in} d_v^{in})^2} \tag{26}$$

And the partial time derivative to the first order ratio difference Δr_u is

$$\frac{\partial \Delta S_{sd}}{\partial \Delta r_u} = \frac{2}{d_u^{in} d_v^{in}} \tag{27}$$

Then, the solution of the Euler-Lagrange equation for r_u can be computed as

$$\frac{\partial \Delta S_{sd}}{\partial \Delta r_u} - \frac{d}{dt}\frac{\partial \Delta S_{sd}}{\partial \Delta r_u} = -\frac{2(d_u^{in}\Delta_v^{in} + d_v^{in}\Delta_u^{in})}{(d_u^{in}d_v^{in})^2} = 0 \quad (28)$$

Similarly, applying the Euler-Lagrange equation on the in-degree d_u^{in}, we get

$$\frac{\partial \Delta S_{sd}}{\partial d_u^{in}} - \frac{d}{dt}\frac{\partial \Delta S_{sd}}{\partial \Delta_u^{in}} = \frac{r_u(d_u^{in}\Delta_v^{in} + d_v^{in}\Delta_u^{in}) + d_v^{in}(r_u\Delta_u^{in} - 2d_u^{in}\Delta r_u)}{(d_u^{in})^3(d_v^{in})^2} = 0 \quad (29)$$

Substituting Eq.(28) into Eq.(29), the relationship between d_u and r_u can be obtained

$$\frac{\Delta_u^{in}}{d_u^{in}} = 2\frac{\Delta r_u}{r_u} \quad (30)$$

Therefore, the Euler Lagrange dynamics leads to a linear relationship between $\frac{\Delta_u^{in}}{d_u^{in}}$ and $\frac{\Delta r_u}{r_u}$ for strongly directed graphs. This should be compared to the analogous relationship which arises from the incremental analysis of the ratio $r_u = \frac{d_u^{in}}{d_u^{out}}$,

$$\Delta r_u = \frac{\Delta_u^{in}}{d_u^{out}} - \frac{d_u^{in}\Delta_u^{out}}{(d_u^{out})^2} \quad (31)$$

and as a result

$$\frac{\Delta r_u}{r_u} = \frac{\Delta_u^{in}}{d_u^{in}} - \frac{\Delta_u^{out}}{d_u^{out}} \quad (32)$$

Combining with Eq.(30) gives the growth equation

$$\frac{\Delta_u^{out}}{d_u^{out}} = \frac{1}{2}\frac{\Delta_u^{in}}{d_u^{in}} \quad (33)$$

which is the out-degree grows at half the rate of the in-degree. In the next section we explore empirically how well this relationship is observed.

3. Experimental Evaluation

3.1. Data Sets

Synthetic Networks: We generate three kinds of complex network models, namely, a) Erdős-Rényi random graph model, b) Watts-Strogatz small-world model (Watts and Strogatz, 1998), and c) Barabási-Albert scale-free model (Barabasi and Albert, 1999; Barabasi et al., 1999). These are created with a fixed number of vertices with changing the parameters with the network structure evolution. For the Erdős-Rényi random graph, the connection probability is monotonically increasing at the uniform rate of 0.005. Similarly, the link rewiring probability in the small-world model(Watts and Strogatz, 1998) increases uniformly between 0 to 1 as the network evolves. For the scale-free model (Barabasi et al., 1999), one vertex is added to the connection at each time step.

Drosophila Gene Regulatory Networks: The time-evolving network represents the DNA microarrays expressed at different developmental stages from fertilization to adulthood during the life cycle of Drosophila melanogaster. The developmental process has four stages, namely, the embryonic (1-30), larval (31-40), pupal (41-58) and adulthood (59-66). The vertices in the network are gene identities which vary in number from 588 to 4028 at different time epochs. This hence tests the ability of our method to deal with networks of variable size. The gene expression patterns are modelled as a binary Markov random field (Song et al., 2009) which allow the edge connections to be determined.

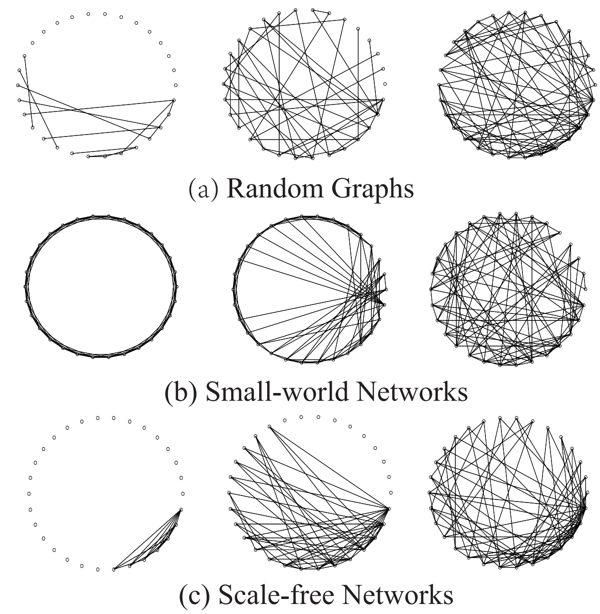
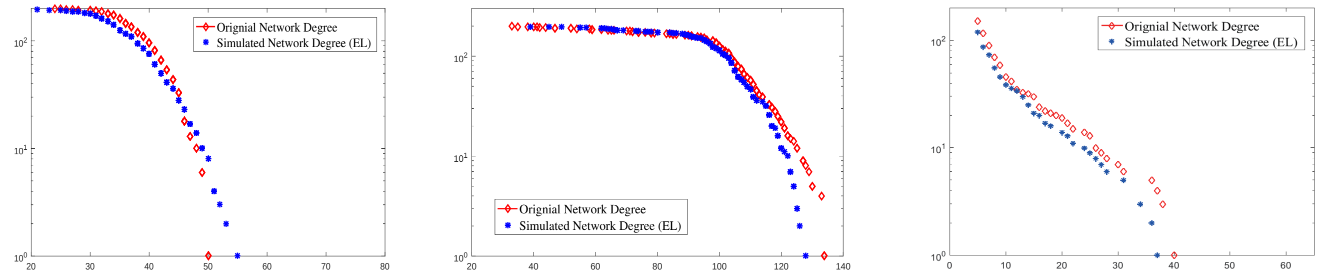


Fig. 1. Visualization of dynamic network structures in time evolution for three network models (Erdős-Rényi random graphs, Watts-Strogatz small-world networks, Barabási-Albert scale-free networks)

Financial Networks: The financial networks consist of the daily prices of 3,799 stocks traded continuously on the New York Stock Exchange over 6000 trading days. The stock prices were obtained from the Yahoo! financial database (Silva et al., 2015). A total of 347 stock were selected from this set, for which historical stock prices from January 1986 to February 2011 are available. In our network representation, the nodes correspond to stock and the edges indicate that there is a statistical similarity between the time series associated with the stock closing prices (Silva et al., 2015). To establish the edge-structure of the network we use a time window of 20 days is to compute the cross-correlation coefficients between the time-series for each pair of stock. Connections are created between a pair of stock if the cross-correlation exceeds an empirically determined threshold. In our experiments, we set the correlation coefficient threshold to the value to $\xi = 0.85$. This yields a time-varying stock market network with a fixed number of 347 nodes and varying edge structure for each of 6,000 trading days. The edges of the network, therefore, represent how the closing prices of the stock follow each other.

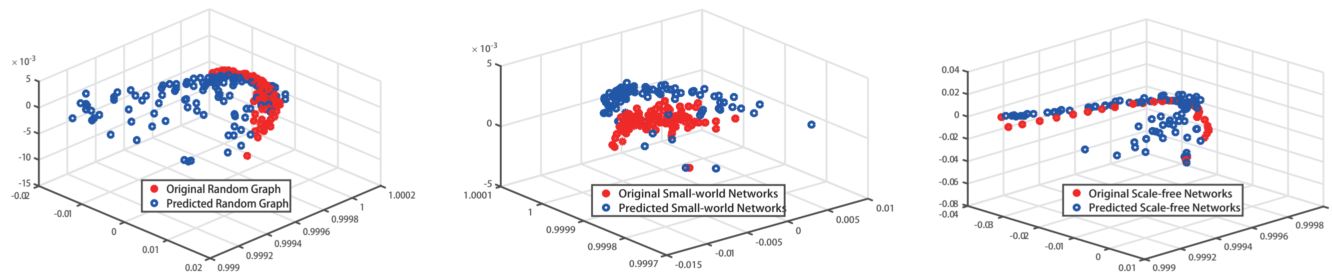
3.2. Synthetic Experiments

We first conduct experiments on the synthetic networks. We generate three kinds of time-evolving network models from Erdős-Rényi random graphs, Watts-Strogatz small-world net-



(a) Random Graphs (b) Small-world Networks (c) Scale-free Networks

Fig. 2. Degree distribution of original networks and simulated networks for three network models. The red line is for the originally observed networks and the blue line is for the results simulated with the Euler-Lagrange analysis. (Erdős-Rényi random graphs, Watts-Strogatz small-world networks, Barabási-Albert scale-free networks.)



(a) Random Graphs (b) Small-world Networks (c) Scale-free Networks

Fig. 3. Visualization of degree distribution in network evolution with principle component analysis (Erdős-Rényi random graphs, Watts-Strogatz small-world networks, Barabási-Albert scale-free networks).

works, and Barabási-Albert scale-free networks to evaluate our theoretical analysis.

Using the degree update equation derived from the principle of minimum entropy change and the Euler-Lagrange equation in Eq.(18), we turn our attention to synthetic network data to characterize the structural variance in network models. Fig.1 shows the visualization of the time evolution for three complex networks. We fix the number of vertices to 200, for the random graphs and evolve the networks from an initially sparse set of edges with a low value of the connection probability. As the connection probability increases, the structure of the random graph exhibits a phase transition to a state with a high density of connection and a giant connected component. A phase transition can also be observed for the Watts-Strogatz small-world model, as the rewiring probability evolves with time. Commencing from a regular ring lattice, the network structure evolves to a small-world network with high rewiring probability, and then to an Erdős-Rényi random graph structure with unit rewiring probability. For the scale-free network, the evolution takes place via preferential attachment. The nodes with the highest degree have the largest probability to receive new links. This process produces several high degree nodes or hubs in the network structure.

Now we explore whether the Euler-Lagrange equation can capture structural properties in the time evolution. We use our model to predict the network structure at subsequent time steps and simulate the degree distribution. We then to compare the predicted degree distribution with that from the original time se-

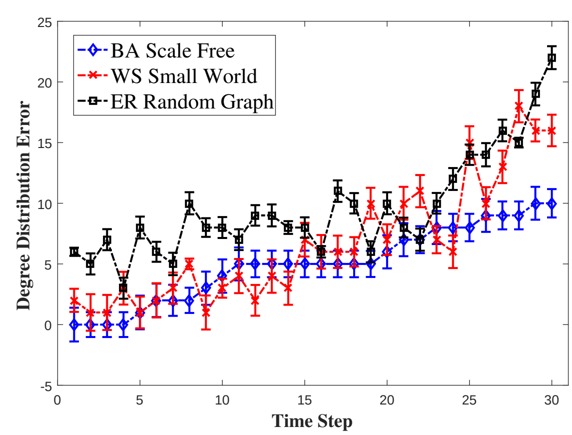


Fig. 4. The degree distribution error with the different value of time steps for three network models (Erdős-Rényi random graphs, Watts-Strogatz small-world networks, Barabási-Albert scale-free networks). The degree prediction error increases quickly after time step $\Delta t = 20$.

ries. Fig.2 shows the simulation results and degree distribution comparisons. The predicted degree distribution resulting from Euler-Lagrange dynamics for the simulated networks fit quite well to the observed distributions. This provides empirical evidence that the Euler-Lagrange equation accurately predicts the short-term evolution of the different network models.

To visualise how the different networks evolve over extended time intervals, we apply the principal component analysis of the degree distribution to project the degree distribution sequences for the networks into a low dimensional space. To commence, we normalize the degree distributions so that the bin contents sum to unity, and then we construct a long vector from the normalised bin contents. We then construct the covariance matrix for the set of long vectors representing the observed degree distributions for the sample of networks. Finally, we apply principal component analysis to the sample covariance matrix for the sample of observed vectorised network degree distributions. We project both the observed and predicted distributions into the principal component space spanned by the leading three eigenvectors of the covariance matrix. In this way, we visualise the evolution of the observed and predicted degree distributions in the principal component space. The results are shown in Fig.3. The red points are the original network distributions and the blue ones are the predicted ones. Fig.3 clearly shows that for all three network models the predicted network degree distribution evolves in a similar manner to the observed network degree distribution.

Then, we explore the effect of length of time step on the performance of the degree distribution prediction accuracy. Fig.4 shows the degree distribution error with a different value of the time step for the three different network models. The prediction error shown is the standard error over the normalised bin contents (the standard deviation of the difference in observed and predicted bin contents, divided by the square root of the number of bins). The longer the time intervals Δt, the higher the prediction error in the degree distribution. For the random graph, the errors sharply increase around the step $\Delta t = 20$. This is because, during the evolution, the random graph undergoes a phase transition from being sparsely connected to containing a giant connected component. At large time intervals, the predictions fail because of the presence of this giant component.

A similar behaviour can be observed in the sample of small-world networks. As the time step interval increases, there are two instants in time separating three different evolution models. The first event occurs around $\Delta t = 15$ and the second at $\Delta t = 25$. The reason is that, during the evolution, the structure of network changes from a regular lattice at the beginning to a small-world network, and then finally takes on a similar structure to a random graph. These three epochs and the associated with a structural transitions impact on the performance of degree distribution prediction. Finally, the degree prediction error for the scale-free network grows slowly and smoothly with the time step, since there are no significant structure transitions during the evolution. As a result, the topology of the scale-free network remains stable. Overall, increasing the value of the time interval results in a reduction of the prediction accuracy. Our new model is capable of capturing the local trends arising from the structural changes during the evolution.

3.3. Real-world Networks

For real-world network evaluation, we test our method on data provided by the Drosophila genes and the New York Stock Exchange. We first evaluate the undirected networks with the life cycle of Drosophila genes dataset. Then we construct the time sequential undirected and directed networks which consist of the daily prices of 3,799 stocks traded continuously on the New York Stock Exchange over 6000 trading days.

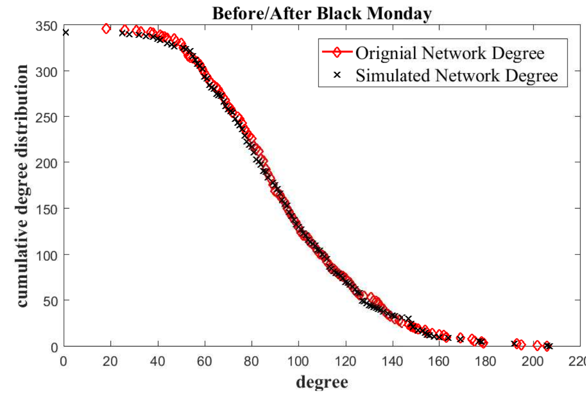


Fig. 5. Degree distribution of originally observed networks and simulated networks before/after Black Monday.

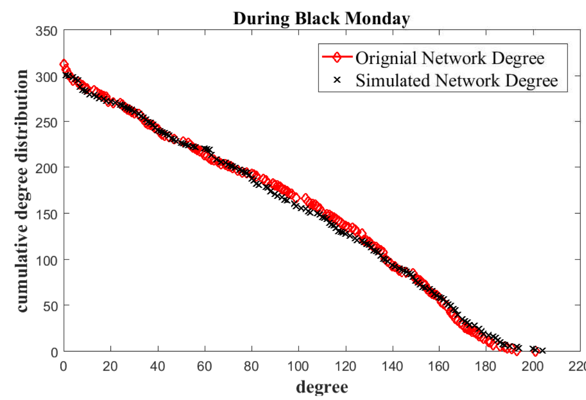


Fig. 6. Degree distribution of originally observed networks and simulated networks during Black Monday. The network becomes disconnected and most vertices are disjoint, which results in the degree distribution following the power-law.

3.3.1. Undirected Drosophila Gene Regulatory Networks

To commence, we represent the Drosophila gene regulatory networks as undirected graphs evolving from the embryonic stage to the adulthood stage. The four phases of the Drosophila life cycle in genes represent the structural variations in the gene regulatory network connections.

We compare the computed von Neumann entropy of the network with that computed from the degree evolution predicted by the Euler-Lagrange model in Eq.(18). Fig.7 plots the two entropies for the entire life cycle of Drosophila development. The four developmental phases, namely, embryonic (red line), larval (black line), pupal (blue line), and adulthood (green line) are represented by different colours. The entropy predicted by the Euler-Lagrange model exhibits a similar time series compared to that obtained with the von Neumann entropy computed from the observed degree distribution. In other words, the degree distribution predicted by the Euler-Lagrange equation effectively captures the changes in structure due to developmental changes in the gene regulatory networks.

3.3.2. Undirected Financial Networks

Now we simulate the behaviour of the financial market networks. Here we focus on how the degree distribution evolves

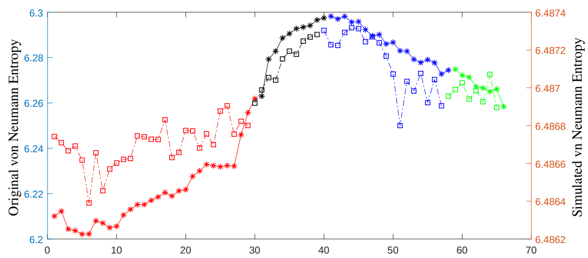


Fig. 7. Comparison of the evolution of the entropy of Drosophila gene regulatory networks using von Neumann entropy and the simulation with the Euler-Lagrange model. The four developmental phases are embryonic (red line), larval (black line), pupal (blue line), and adulthood (green line).

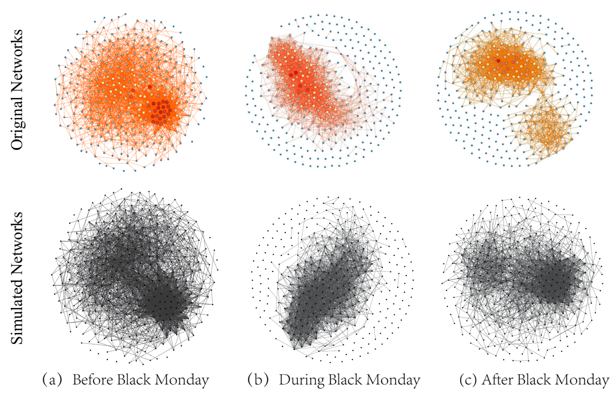


Fig. 8. The visualization of network structure at three specific days in Black Monday financial crisis. The red line corresponds to the entropy difference for the original networks and the grey line is the Euler-Lagrange model.

with time. We compare the simulated structure and the observed network properties and provide a way to identify the consequence of structural variations in time-evolving networks.

Our procedure is as follows. We first select a network at a particular epoch from the time series and simulate its evolution using the degree update equation in Eq.(18). Then we compare the degree distributions for the real network sampled at a subsequent time and the simulation of the degree distribution after an identical elapsed time. One of the most salient events in the NYSE is Black Monday. This event occurred on October 19, 1987, during which the world stock markets crashed, dropping in value in a very short time.

We compare the prediction of consecutive time steps at different epochs, before/after and during the Black Monday crisis. The results are shown in Fig.5 and Fig.6. The most obvious feature is that the degree distribution for the networks before and after Black Monday is quite different to that during the crisis period. During the Black Monday crisis, a large number of vertices in the network is disconnected. This results in a power-law degree distribution. However, for time epochs before and after Black Monday, the disconnected nodes recover their interactions to one another. This increases the number of connections among vertices and causes departures from the power law distribution. This phenomenon is also observed in the networks simulated networks using our degree update equation. This is an important result that shows empirically that the simulated networks reflect the structural properties of the original networks from which they are generated. Moreover, our dynamic model can reproduce the topological changes that occur during the financial crisis.

In Fig.8, we show network visualizations corresponding to three different instants of time around the Black Monday crisis. In order to compare the simulated network structures resulting from the current model, we show the connected components (community structures) at three-time epochs. As the network approaches the crisis, the network structure changes violently, and the community structure substantially vanishes. Only a single highly connected cluster at the centre of the network persists. These features can be observed in both the simulations and original time evolution of the networks. At the crisis epoch, most stocks are disconnected, meaning that the prices evolve independently without strong correlations to the remaining stock. During the crisis, the persistent connected component exhibits a more homogeneous structure as shown in Fig.8. Compared to the first order model (Wang et al., 2017a), our new second order network prediction gives structures that more closely resemble the original network structure. After the crisis, the network preserves most of its existing community structure and begins to reconnect again. This result also agrees with findings in other literature concerning the structural organization of financial market networks (Silva et al., 2015).

Finally, we explore the anomaly detection in dynamic networks. We validate our framework by analysing the entropy differences between simulated networks and actual stock market networks in the New York Stock Exchange (NYSE). In order to quantitatively investigate the relationship between a financial crisis and network entropy changes, we analyse a set of well-documented crisis periods. These crisis periods are marked alongside the curve of the first order entropy difference in Fig.9, for all business days in our dataset.

The literature in the financial domain usually identifies the potential crashes using either a) the trading volumes (Chesney et al., 2015), b) the variation of expected returns (Bali and Hovakimian, 2009) or c) Spearman's rank correlation (Alanyali et al., 2013). Recently, machine learning techniques, such as conditional random fields, support vector machines and artificial neural networks, have been used to identify trading patterns using various criteria on specific financial datasets (Choudhry and Garg, 2008). Unfortunately, the complexity of these data-driven methods is generally high due to the combination of multiple techniques. By contrast, our entropy based analysis is easily effected using our dynamic model which clearly indicates the financial crises.

3.3.3. Directed Financial Networks

We extend our study to directed graph representations of the New York Stock Exchange data. To extract directed graphs from the stock times series data we compute the correlation with a time lag. We measure the correlation over 30-day windows separated by a time and then select the lag that results in the maximum correlation. As with undirected graphs we threshold the correlation to establish edges representing interactions between stock. We determine the directionality of the edges using the sign of the lag. All the resulting edges are unidirectional. We, therefore, explore how the time evolution follows our model for strongly directed graphs.

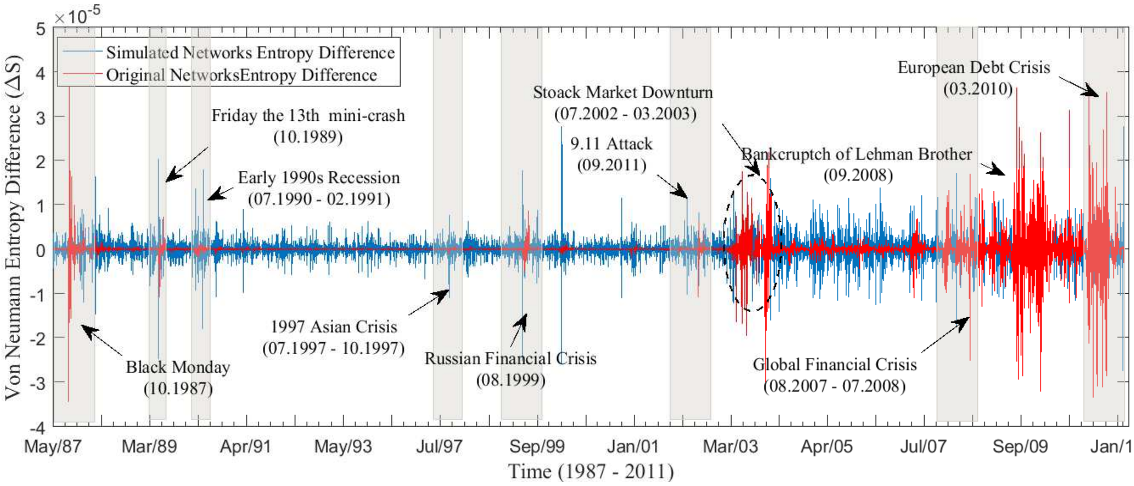


Fig. 9. The von Neumann entropy difference in NYSE (1987-2011) for original financial networks and simulated networks. Critical financial events, i.e., Black Monday, Friday the 13th mini-crash, Early 1990s Recession, 1997 Asian Crisis, 9.11 Attacks, Downturn of 2002-2003, 2007 Financial Crisis, the Bankruptcy of Lehman Brothers and the European Debt Crisis, are associated with large entropy differences.

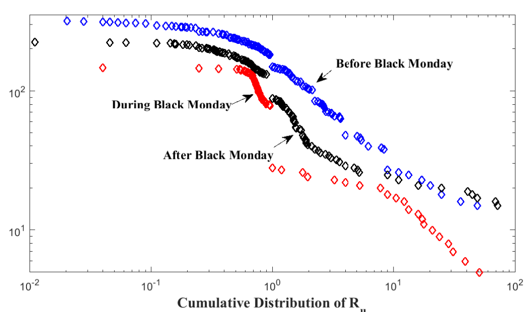


Fig. 10. The cumulative distribution of parameter $r_u = d_u^{in}/d_u^{out}$ in directed financial networks before/during/after the Black Monday. The distribution shrinks during the Black Monday crisis.

First, we investigate how the distribution of r_u evolves with the time. Fig.10 shows the distribution at three different time epochs, i.e., before, during and after Black Monday. Here, the parameter r_u reveals the relationship between in-degree and out-degree for each vertex. As shown in Fig.10, during the Black Monday, the cumulative distribution becomes concentrated over a small range of values around unity. This reflects the fact that a substantial fraction of vertices become isolated during the Black Monday, without the out-edges. The remaining connections exist with a balance between in-degree and out-degree. After Black Monday, the network structure begins to recover as the cumulative distribution widens to return to its previous shape.

From the analysis leading to Eq.(23), there is a linear relationship between the quantities $\frac{\Delta r_u}{r_u}$ and $\frac{\Delta_u^{in}}{d_u^{in}}$. In order to test whether this relationship holds in practice, Fig.12 shows scatter plots of $\frac{\Delta r_u}{r_u}$ versus $\frac{\Delta_u^{in}}{d_u^{in}}$ for epochs before, during and after the Black Monday crisis. This provides evidence that there exists a linear relationship between the fractional in-degree change and the degree ratio change. By fitting a linear regression to the sequence of scatter plots for the time series, we explore how the slope parameters of the regression line and the regression error evolve with time. Fig.13 shows the linear regression errors, as well as the fitted slope, during the period around Black Monday. Here we provide the regression error, for a) the flexible fitting of the slope and b) the regression for a fixed value of the slope. In the time interval around Black Monday, both the linear regression parameter and its error changes abruptly. This is because there are substantial structural differences in the network evolution. During the Black Monday, many nodes become disconnected and the connected components of vertices become small and fragmented. Only a small number of community structures remain highly inter-connected. During Black Monday itself, although the slope of the regression line is zero, the scatter about the line is relatively small.

Furthermore, the linear regression error sequence for the entire directed financial network time series is shown in Fig.11. The peaks in the regression error correspond closely to the occurrence of the financial crisis. Our analysis in the directed graph is effective and efficient to detect the abnormal structure in dynamic networks. The most striking observation is that the largest peaks of regression can be used to identify the corresponding financial crisis. This shows that the theoretical analysis of minimising the change of directed entropy is sensitive to significant structural changes in networks. The financial crises are characterized by significant entropy changes, whereas outside these critical periods remains stable.

4. Conclusion

In this paper, we explore how to model the time evolution of networks using a variational principle. We use the Euler-Lagrange equations to model the evolution of undirected and directed networks that undergo changes in structure by minimising the change in von Neumann entropy. This treatment leads to the model of how the node degree varies with time and captures the effects of degree change correlations introduced by the edge-structure of the network. In other words, because of these correlations, the variety of one degree determines the translation in connected nodes.

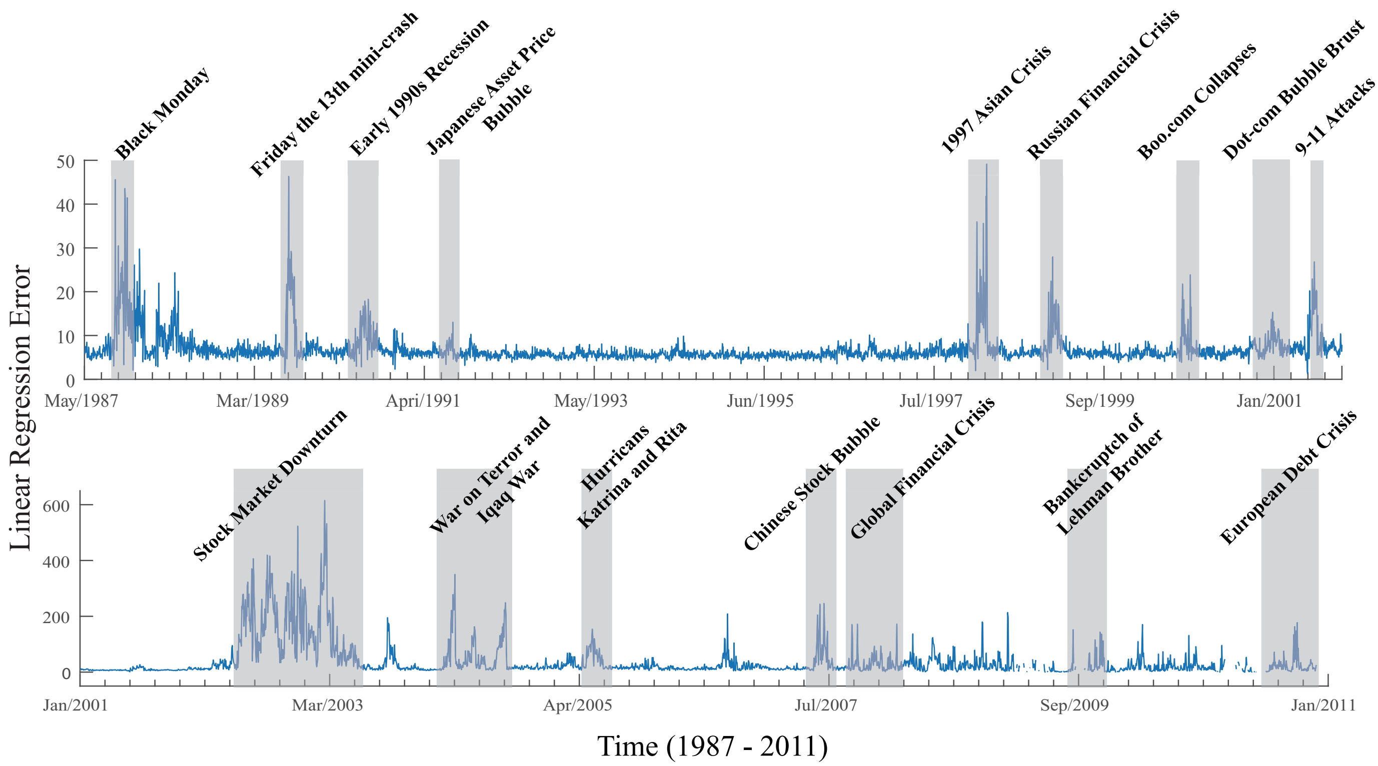


Fig. 11. The linear regression error for the whole sequential financial data in NYSE (1987-2011). Critical financial events, i.e., Black Monday, Friday the 13th mini-crash, Early 1990s Recession, 1997 Asian Crisis, 9.11 Attacks, Downturn of 2002-2003, 2007 Financial Crisis, the Bankruptcy of Lehman Brothers and the European Debt Crisis, are associated with significant error peaks.

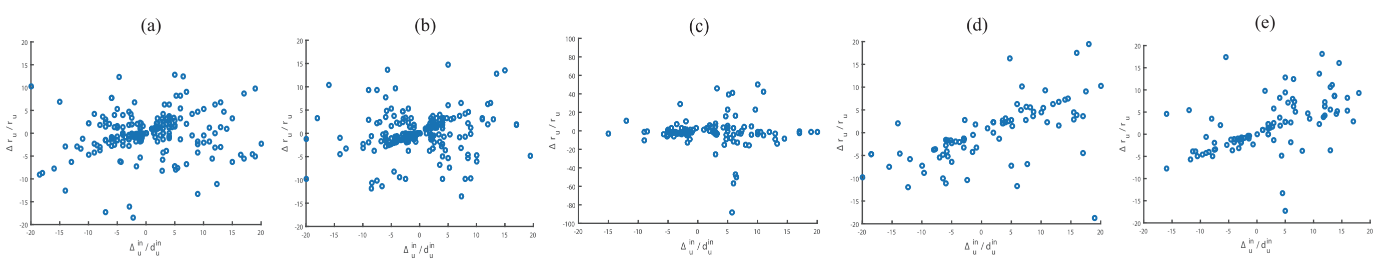


Fig. 12. The scatter plots of Δ_u^{in}/d_u^{in} versus $\Delta r_u/r_u$ during the epoch of Black Monday (a)-(e). Before Black Monday: (a) October 1, 1987; (b) October 10, 1987. During Black Monday: (c) October 19, 1987. After Black Monday: (d) October 29, 1987; (e) November 10, 1987

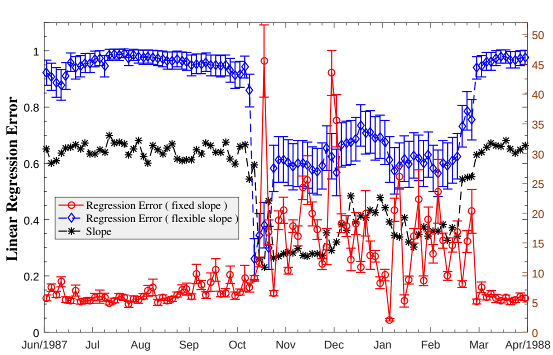


Fig. 13. The linear regression error and standard deviation during Black Monday (June 1987 - April 1988). The blue diamond curve is the error bar with the flexible slope in the regression. Red circle line is the errorbar with the fixed slope in the regression. Black star curve is the value of the slope.

We conduct the experiments on a time-series of networks representing life cycle of Drosophila and the stock trades on the NYSE. Our model is capable of predicting how the degree distribution evolves with time. Moreover, it can also be used to detect abrupt changes in network structure.

In the future, it would be interesting to study different variational models for the network evolution, based on minimising different physical quantities or different forms of the entropy. It would also be interesting to understand the dynamics of quantities such as the edge density and its variance.

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