Networks and
Time Series

Wednesday, Sept. 2: 11:00 – 13:00

Session 1: Audi Max

Contents

Bifurcation analysis of geophysical time series

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We propose a general synthetic framework, combining analytical and experimental techniques, for studying climatic bifurcations and transitions by means of the time series analysis. The method employs three major techniques: (i) derivation of potential from time series using unscented Kalman Filter (UKF); (ii) studying possible bifurcations and transitions of the obtained potential; (iii) projection of the time series according to the estimated perturbation. The method is tested on artificial data and then applied to observed records, in particular, a Greenland temperature proxy. We correctly detect potential changes in artificial series with a varied number of potential wells. In the case of Greenland data, the technique detects a change of the number of system states from two to one (double-well potential transforming into single-well) at about 20 kyr BP.

Nonlinear dynamics of modern power grids

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Reliable supply of electric power is a crucial pre-condition for everyday life in modern economy and society [1]. The generation of electric power is currently heavily dominated by relatively few but large power plants based on conventional energy (Figure 2.1a) but the contributions from renewable power sources become more and more significant (Figure 2.1b). Renewable sources such as wind- or solar-electric sources, however, come in much larger numbers, individually provide output powers that are typically orders of magnitude smaller than conventional ones, and are temporally less reliable and geographically much more distributed. Moreover, the entire power grid over time rearranges due to these developments. These features provide major challenges for the design and construction of reliable modern power grids - a multi-billion Euro market alone in Europe. One major question is how to ensure stable and robust synchronization of the entire grid given widely-distributed, dominantly small, and strongly fluctuating sources [3]. To date research strongly focused on so-called "smart grids", power grids that - in parallel to power transmission, enable the transfer of information about local load, storage, and control status throughout the grid; the impact of connection architecture on future grids performance, however, has received much less attention [4], [5] and is far from beeing understood.

Here we present and systematically study a class of oscillator networks [2] to characterize fundamental aspects of the synchronization dynamics of electric power distribution. Single units are modeled by two variables and the network is quantified by three key features: the strengths of power sources, the capac-

(a) Scheme of a power grid dominated by one large power plant (red) and lots of consumers (black)

(b) Scheme of a power grid with smaller, distributed power sources
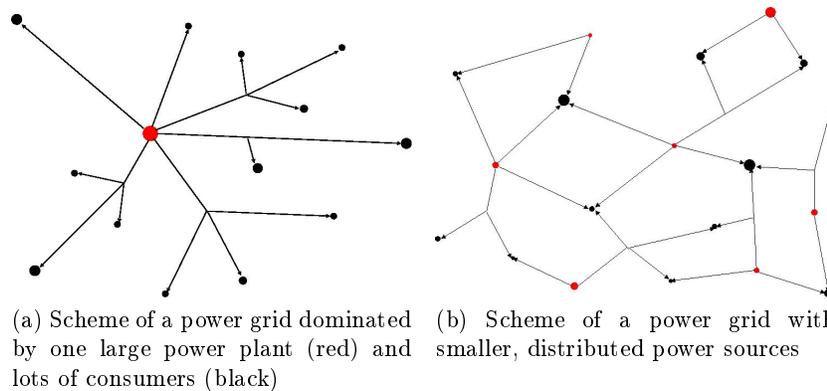
Fig. 2.1: Schematics of different power grid types

ities of transmission lines, and the maximum power used by consumer sinks. We find how replacing a low number of strong sources by a large number of small sources destabilizes synchronization and explain the mechanism underlying destabilization. We provide first hints how to circumvent destabilization by moderately restructuring local and connectivity features of the power grid.

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Wave localization in complex networks with high clustering

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Complex networks can exhibit a transition from a phase with metallic transport properties to a phase with insulating behavior, i. e., no transport across the network. The simplest cause of such a transition is the breaking of the cluster spanning the network, akin to the classical percolation transition. Quantum phase transitions (Anderson-like transitions), on the other hand, are relevant in complex networks with long-range coherent wave transport, e. g., in optical networks. In this case, quantum localization can be caused by backscattering and interference due to disorder in the network.
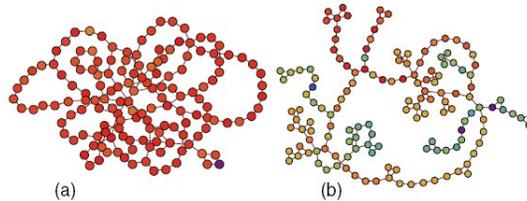
Fig. 3.1: Representative pictures of the giant component of scale-free networks ($\lambda = 5$) (a) without and (b) with clustering ($C_0 = 0.6$). Both networks have giant components of similar size ($N \sim 150$); the size of the whole network being $N = 150$ for (a) and $N = 200$ for (b). The logarithmically scaled coloring presents the intensity of a mode with $E \approx 0.2$, red indicating the highest and violet the lowest probability.

We show that strong clustering of links, i. e., a high probability of triadic closure, can induce a localization-delocalization quantum phase transition of coherent excitations [1]. Figure 3.1 illustrates how the network structure changes upon increasing the clustering index and how the localization properties of a wave function change. Clustering represents a new degree of freedom that can be used to induce and study phase transitions in complex networks. Comparing systems with different clustering properties might enable one to find the most relevant cause of quantum localization.

For example, the propagation of light wave-packets between two distant nodes of an optical network (composed of fibers and beam splitters) will be absent if the fraction of closed triangles exceeds a certain threshold. We suggest that such an experiment is feasible with current optics technology.

Numerically studying level statistics we determine the localization phase diagram as a function of the clustering coefficient C and the on-site disorder
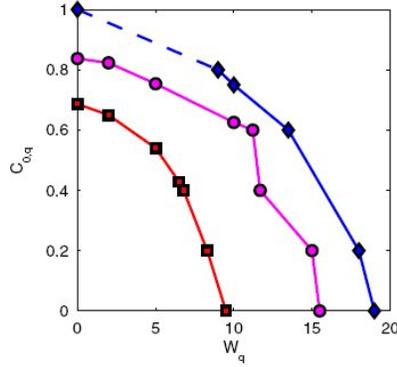
Fig. 3.2: Phase diagram for transitions from localized optical modes (upper right) to extended modes in parts of the spectrum (lower left) for different degree distribution exponents λ, $\lambda = 4$ (blue diamonds), 4.25 (magenta circles), and 5 (red squares). Data for $C_0 > 0.9$ are not reliable for network generation reasons, and the error bar for the point at $C_0 = 1$ is about 0.1.

W for scale-free networks of different degree distributions $P(k) \sim k^{-\lambda}$. Here, k denotes the number of neighbors per node.

We find that (i) a localization-delocalization transition is induced by increasing C even in the absence of on-node (on-site) disorder W for $\lambda > 4$; (ii) the quantum transition point C_q moves to lower values when W is increased (continuous phase diagram, see Fig. 3.2); and (iii) the scaling exponent ν is very close to the mean-field value $\nu = 0.5$ for all values of λ and C_q, as may be expected for a system with high spatial dimension. We have also verified that similar results hold for networks with homogeneous or Erdös-Renyi type degree distribution $P(k)$. For $P(k) \sim k^{-\lambda}$ with $\lambda > 4.5$ (approximately) there is an additional distinct classical transition at a clustering coefficient $C_c > C_q$.

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Generic long-range correlations in music rhythms

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Music rhythms performed by humans will always fluctuate to a certain amount around the exact rhythm (e.g. given by the steady beat of a metronome). We refer to these fluctuations as temporal deviations e_n from the metronome clicks. It is believed that the task of synchronizing the movement of one's finger to a periodic environmental signal (*finger tapping*) shows deviations from the signal which exhibit long-range correlations ($1/f^\beta$-type) [1, 2]. But musicians do not restrict themselves to finger tapping.

We present preliminary results on generic long-range correlations in simple as well as in complex music rhythms [3]. The fact that long-memory processes arise in a broad variety of complex rhythmic tasks suggests that a common basic neurophysical mechanism accounts for the timing in human music rhythms. Moreover, we investigate the question: Does the rhythmic structure of a piece of music sound better to listeners, when it is as exact as possible or are long-range correlations more favorable?

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Cross-modulated amplitudes and frequencies characterize interacting components in complex systems

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The dynamics of complex systems is characterized by oscillatory components on many time scales. To study the interactions between these components we analyze the cross-modulation of their instantaneous amplitudes and frequencies, separating synchronous and anti-synchronous modulation. Our approach is a direct and systematic way to screen simultaneously recorded time series for linear and non-linear interactions. Specifically, we can observe how amplitude or frequency of one emergent oscillator in a specific location affects amplitude or frequency of another oscillator in a different place and/or operating at a different frequency. The approach is stable for non-stationary data — a major advantage for slow dynamics.

Applying our novel technique to brain-wave oscillations in the human electroencephalogram (EEG) we show that interactions between the α wave and the δ or β wave oscillators as well as spatial interactions can be quantified and related with physiological conditions (e. g., sleep stages).

The method begins with the separation of signals into specific frequency bands. Then, instantaneous amplitudes and frequencies for each band are calculated via a Hilbert transform. The final step is an analysis of synchronous and anti-synchronous variation of these signals involving a second Hilbert transform. The corresponding synchronization and anti-synchronization indices are averaged in time windows of 30 seconds and presented in matrix format in Fig. 5.1 for (a) amplitude-amplitude modulation, (b,c) amplitude-frequency cross-modulation, and (d) frequency-frequency modulation.

The calculation of instantaneous amplitudes and frequencies in time series characterizing the dynamics of a complex system is useful in at least two aspects. Firstly, it yields amplitude and frequency series showing long-term scaling in some physiological states. Secondly, these signals can be used to study and characterize in detail linear and nonlinear interactions between the corresponding oscillators with very different characteristic frequencies and hence support modeling. Furthermore, the approach could be helpful in finding the origin of scaling behavior in complex systems in biology, geoscience and financing.

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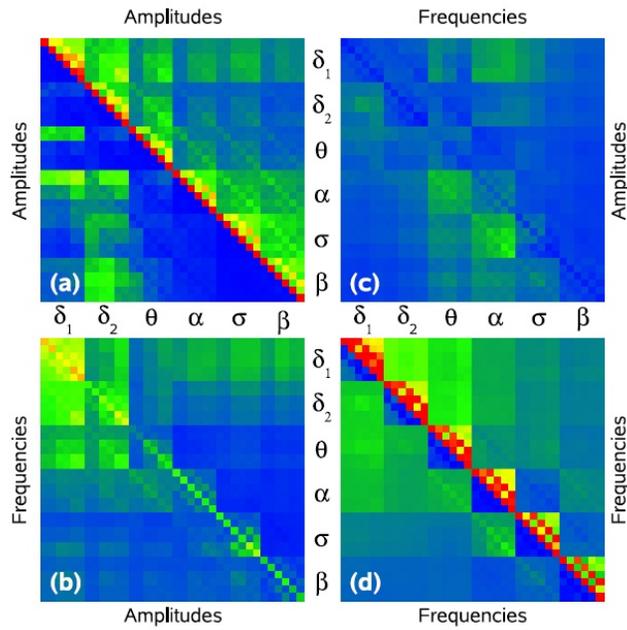
Fig. 5.1: Results of modulation analysis of instantaneous amplitudes (a) and frequencies (d) as well as amplitude-frequency cross-modulation analysis (b,c). The four 36×36 matrices show the modulation coefficients γ_+ [(c) and upper triangles in (a,d)] and γ_- [(b) and lower triangles in (a,d)] with modulation degrees increasing from blue to green, yellow and red. The six first rows and columns refer to the δ_1 band of the EEG electrodes O1-M2 (occipital left), O2-M1 (occipital right), C3-M2 (central left), C4-M1 (central right), Fp1-M2 (frontal left), and Fp2-M1 (frontal right); repeated for each band.

Elastic network modeling of molecular motor HCV helicase: Inchworm translocation and DNA unzipping cycles

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Protein machines that operate as mechanical motors play a fundamental role in biological cells. Prominent examples are kinesin that transports cargo along microtubules through the cell or myosin that generates muscle contractions through its interaction with actin filaments. To execute their functions, protein motors need energy provided with ATP molecules. Binding and hydrolysis of ATP induce large-scale conformational changes essential for the operation of motor proteins. One of the key problems is to gain insight into cyclic conformational motions of protein motors and understand how they are coupled to the actual function in the cells.

While the structure of many motor proteins is known, modeling of dynamics of their operation cycles presents substantial difficulties. Because the cycles of molecular motors are slow and typically lie in the range from tens of milliseconds to a second, they cannot be followed in all-atom molecular dynamics simulations. On the other hand, phenomenological models such as mechanical ratchets or stochastic oscillators provide an oversimplified view of motor operation, reducing it to effective motions along a single mechanical coordinate. More realistic coarse-grained descriptions are therefore needed to fill the gap between simple phenomenology and full atomic dynamics. Elastic network models, picturing the protein as a network made up of beads connected by elastic springs provide such a middle-level description. Elastic network methods are broadly used (see [1, 2]) to study protein dynamics around the equilibrium conformation (the normal mode analysis). Recently, large conformational motions with nonlinear elastic dynamics have been studied [3] for two classical motor proteins (myosin and F1-ATPase).

Helicases are generally involved when transient unwinding and separation of duplex DNA or RNA substrates is needed, in such processes as viral replication, DNA repair or removal of secondary structures in RNA. The HCV helicase is not only an important drug target for viral infection treatments, it is also considered as a characteristic example for a broad class of helicase motors. Based on experimental studies, the inchworm operation mechanism of this protein machine has been proposed [4]. According to it, two mobile domains of the HCV helicase are translocating along the upper strand of the double DNA, with each translocation step accompanied by binding and hydrolysis of an ATP molecule. The third domain is attached to the lower DNA strand. It unzips the DNA, separating the two strands in every third translocation step, through the accumulation of elastic strains [5]. While some evidence, supporting the inchworm mechanism and based on single-molecule experiments, is available [6], its action has never been theoretically described. *We have developed an elastic network model of the molecular motor Hepatitis*

C virus (HCV) helicase and used it to follow, for the first time, the entire operation cycle of this motor and its interaction with DNA molecules.

In the first part of our study, responses of HCV helicase to global and local (near the ATP binding site) conformational perturbations have been determined in numerical simulations. We have shown that this protein can perform ordered internal mechanical motions, which are robust against noise and variations of initial conditions. Essentially, in such motions the protein behaves as if it were consisting of several rigid domains connected by flexible joints. These motions are closely related to the soft relaxation mode of the elastic network of the HCV helicase. They are in agreement with the experimentally known conformational changes, induced in the protein by ATP binding.

At the next stage, binding of ATP and its hydrolysis have been incorporated into the elastic network model. The ATP molecule has been modeled as an additional particle placed inside the ATP binding domain and forming a number of new links inside it. We could show that conformational motions in each cycle (consuming one ATP molecule) can lead to an effective translocation by one nucleotide unit along the single DNA strand, in agreement with experimental findings [5]. Monitoring conformational dynamics in the region of the DNA binding cleft, we could conclude that the protein possesses alternating tight and weak grip states on the nucleotide chain at different parts of the cleft, as assumed in the proposed inchworm mechanism.

Finally, numerical simulations of interactions between the protein and the duplex DNA have been performed to verify the DNA unzipping mechanism. It is assumed that during its progressive translocation along the single strand, the protein generates the force applied to the complementary strand at the replication fork. Thus the protein motor should act as a wedge pressed into the space between the two strands and mechanically separating them. To run the respective simulations, we have additionally modeled the duplex DNA as a semi-flexible polymer, with the links that connect the two strands breaking down when the critical force is applied. We could demonstrate that unzipping of DNA takes place as the two mobile protein domains are translocating along its upper strand, powered by the energy brought with the ATP molecules.

In our study, it became possible to realistically follow the entire cycles of a particular molecular motor — the hepatitis C virus helicase — by using coarse-grained elastic network models for the protein and similar descriptions for the DNA molecule. While providing the first direct dynamical simulation of the entire cycles of this specific machine, our investigations also demonstrate how the analysis can be performed for other important molecular motors.

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Self-tuned dynamical criticality and self-organized statistical criticality together in an evolving network.

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Dynamical systems theory holds that systems of interest should be *structurally stable*. This would imply that High-order criticality, the *simultaneous* presence of several critical features such as Hopf bifurcations, is not expected to be observed in a natural system. However, not infrequently natural systems do exhibit such kind of criticality: neuroscience examples include *dynamically critical* systems such as line attractors [1] in motor control [2] and decision making [3], *self-tuned* Hopf bifurcations in the auditory periphery [4] and olfactory system [5], and "regulated criticality" models [6]. There are also many examples of *statistically critical* [7] systems with spontaneous heavy-tailed or scale-free fluctuations, such as neuronal avalanches [8], anomalous correlations in the retina [9,10] and in functional imaging [11], nonlinear dynamics models of networked spiking elements, [12,13], etc. There is, however, no real understanding of the relation between these different concepts of criticality and although a well-studied physical system displays both statistical [14] and dynamical (extensive number of zero Lyapunovs [15]), criticality little effort has been devoted to study possible connections.

We present a simple abstract model, an anti-Hebbian [16] network which spontaneously poises itself at a *dynamically critical state*: an extensive number of degrees of freedom approach Hopf bifurcations, becoming arbitrarily sensitive to external perturbations. As the dynamics controlling this state has itself a marginal fixed point, the eigenvalues do not converge but fluctuate, close to the imaginary axis; when they become slightly unstable, the corresponding mode "breaks out" and becomes more prominent, and as they become slightly stable the mode slowly damps out. This breakout dynamics displays avalanche-like activity bursts whose sizes may be power-law distributed. Within these epochs the neurons of our model are slightly correlated; yet, as the number of small but significant correlations is high, the model has strongly correlated network states [9]. This system is, on the short time-scale, sensitive in bulk to any outside input, even if applied only to a small subset of the neurons. However, it does not learn — being anti-Hebbian, it constantly forgets. We can achieve learning by adding another plasticity term "positively" Hebbian to directed correlations, i.e., those causal in the sense of Granger [17]. Then the network may learn "predictable" stimuli and will display timing-dependent synaptic changes reminiscent of spike-timing dependent plasticity (STDP, [18]).

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Complex network approach for earthquake science

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The seismic data taken from California and Japan are mapped to growing random networks [1, 2]. Vertices and edges of such networks correspond to coarse-grained events and event-event correlations, respectively. Yet unknown microscopic dynamics governing event-event correlations and fault-fault interactions is replaced by these edges. Global physical properties of seismicity can then be explored by examining its geometric (e.g., topological etc.), statistical and dynamical properties. Firstly, we show that the earthquake network is scale free, being characterized by the power-law connectivity distribution (see Fig. 8.1) [3, 4]. We give a physical interpretation to this result based
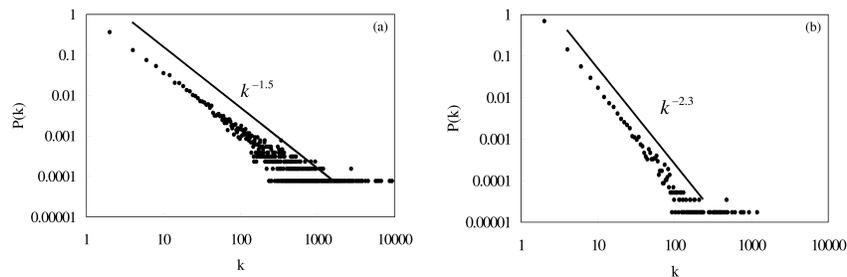
Fig. 8.1: The log-log plots of the connectivity distributions of the earthquake networks P(k) in California (a) and Japan (b).

on network growth with the preferential attachment rule together with the Gutenberg-Richter law. Secondly, we study the small-world structure of the earthquake network reduced to an undirected simple network [4]. The value of the clustering coefficient is found to be much larger than that of the classical random network. In addition, the average path length is very small. Thirdly, we show that the earthquake network possesses hierarchical organization [5]. We interpret this fact in terms of vertex fitness and vertex deactivation by the process of stress release at faults. Fourthly, We find that the earthquake network has the property of assortative mixing. This point is an essential difference of the earthquake network from the Internet that has disassortative mixing. Finally, we report the discovery of a scale-invariant law of the period distribution in the directed earthquake network [6], which indicates that after how many earthquakes an earthquake returns to the initial location. This result manifests a fundamental difficulty in statistically estimating the value of

period. Combined with other dynamical properties [7], the present results imply that yet unknown mechanism governing seismicity may be so-called glassy dynamics on a growing complex network. These observations have obvious importance for constructing and improving physical models of seismicity such as the ones exhibiting self-organized criticality.

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