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Spectral causalities within dynamical effects framework

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Abstract – Spectral causalities are now widely used in physical and biological sciences to characterize directional couplings from time series. In particular, the Granger-Geweke spectrum is a frequency decomposition of a Wiener-Granger causality measure. However, there are considerable difficulties in their interpretation, so quite hot debates still arise. Here, the problem is studied within the dynamical effects framework: *spectral effects* are introduced as long-term effects of relevant parameter interventions. Quantitative relationships between the GG spectrum and certain spectral effects are established for linear stochastic differential equations. It is also argued that in general existing spectral causalities do not unambiguously relate to spectral effects. The latter are shown to be as estimable from time series, at least for some simple systems.

Introduction. – In the field of time series analysis, two recent decades have exhibited wide and strong and still rising interest in the problem of revealing directional (causal) couplings in complex systems, as discussed, *e.g.*, in the generalizing works [1–9]. The most widely used idea seems to be the Wiener-Granger causality (WGC) [10,11] which is, for a direction $Y \to X$, a kind of partial correlation [12,13] between the future of a system X and the past of a system Y, given the past of X. After the linear autoregression (AR) implementation [11], it has been developed in different ways including information-theoretic versions [14–20] and their analysis [12,21–25] with applications ranging from physics [19] to biomedicine [4,6,15,21] and climate [13,16,18,26–30]. In addition to a single value quantifying the influence $Y \to X$, it has been discovered [31,32] a very promising opportunity of its frequency decomposition which is now called the Granger-Geweke (GG) spectrum and represents a well-established technique, as discussed and applied, *e.g.*, in refs. [33–35]. Directed transfer function (DTF) [36] and partial directed coherence (PDC) [37] are somewhat similar, but simpler spectral causalities [38], also very popular in various applications ranging from neural systems [39] to nuclear reactors [40]. Impressively, the GG spectra have become so useful in neuroimaging studies that in a recent review [35] they are considered as an equally important tool along with basic fMRI, EEG, and MEG techniques.

It might then look surprising that these spectral causalities are often difficult to interpret and their meaning is still a subject of intense debate. Modifications of PDC are suggested, *e.g.*, to interpret it as true coherence [41] or to compare its values at various frequencies [42]. Even a hotter battle is occurring around the basic concept of the GG spectrum. Stokes and Purdon [43] have addressed difficulties of its interpretation: "causality measures . . . reflect a combination of dynamics from the different components of the system. How then do causality values relate to the underlying structure or dynamics of the generative system? . . . GG causality reflects only the dynamics of the transmitter node and channel, with no dependence on the dynamics of the receiver node. This suggests that, even in simple bivariate AR systems, GG causality may be prone to misinterpretation and may not reflect the intuitive notions of causality most often associated with these methods". Several authors have given justified replies [44–47] but their argument that the GG spectrum represents information transfer rate [46,47] has met the objection [48] that information transfer is then to be interpreted in its turn. Interpretation and "intuitive notion of causality" seemingly imply here that an abstract interdependence measure should be related to a more concrete quantity reflecting how some "cause" (a kind of independent intervention) produces some "effect" (a kind of dependent response). The non-finished character of these discussions suggests that the entire topic needs further investigation.

A novel contribution of this letter consists in considering the entire problem from the other side, within the dynamical effects framework [8] inspired by Pearl's interventional formalism [1], *i.e.*, in i) taking generative equations for the dynamics under study as known, ii) introducing "natural" frequency-domain coupling quantifiers of practical interest, and iii) studying which of them the GG spectra and other existing spectral causalities are close to. This opportunity has been briefly mentioned in ref. [8] (sects. IIC and IIIC). Somewhat similarly, the identification of generative equations has been used to estimate the GG spectra via dynamical causal modelling [38], but no wider use of the generative equations has been proposed and the GG spectra have remained a final goal. An important state-space approach has been developed to estimate the GG spectra [49–51] and allowed to define multiscale characteristics [52], but state space models have not been used to study effects of coupling variations. Generative equations have been used for causal couplings quantification in refs. [8,20,53], but not in the frequency domain.

I would note that the entire polemic about interpretations of causality spectra reminds that concerning "reality" of the spectral components (side bands) of a modulated radio signal, *i.e.*, the question of whether a Fourier series is only a formal decomposition, which occurred on the pages of *Nature* in 1930 [54,55]. That polemic found also a detailed response of Mandelshtam [56,57] who was together with his disciple A. A. Andronov a founder of the widest research direction in nonlinear oscillations theory called [58] "Russian school". His answer to that question is achieved via physical arguments based on how the signal is intended to be analysed. Similar arguments are given in the end of this letter for interpreting spectral causalities. In essence, the aim of this letter is to put the formal statistical problem under study into the oscillation-theoretic context, or to switch from the "logic of formal decompositions" to the "logic of dynamical effects".

Below, the spectral effects are first introduced for a simple, but general continuous-time stochastic system. The GG spectra are then recapitulated and compared to the spectral effects analytically and numerically, including accessibility from time series. Finally, other spectral causalities and oscillation-theoretic interpretations are discussed.

Spectral effects. – Stochastic linear differential equations represent a model which is appropriate for a variety of irregular real-world processes and widely used in physical community, *e.g.*, [59]. To define spectral effects of couplings and compare them to the GG spectrum, two continuous-time subsystems X and Y are used below:

$$\begin{aligned} L_x(\mathrm{d}/\mathrm{d}t)x &= K_{xy}(\mathrm{d}/\mathrm{d}t)y + \xi_x(t), \\ L_y(\mathrm{d}/\mathrm{d}t)y &= K_{yx}(\mathrm{d}/\mathrm{d}t)x + \xi_y(t), \end{aligned} \tag{1}$$

where x and y are observed variables, L_x, L_y, K_{xy}, and K_{yx} are symbolic polynomials in the derivative operator, their degrees are P_x, P_y, P_{xy}, and P_{yx}, respectively, with $P_x \geq 1$, $P_y \geq 1$, $P_{xy} < P_y$, $P_{yx} < P_x$. K_{xy} and K_{yx} describe directional couplings $Y \to X$ and $X \to Y$. Suppose that $L_x(i\omega)$ and $L_y(i\omega)$ as polynomials in ω have no roots in the low half of the complex plane (ω is the angular frequency, i is the imaginary unit), so the isolated subsystems X and Y are stable, *i.e.*, the isolated subprocesses x and y are stationary. The noises ξ_x and ξ_y with covariance functions $\langle \xi_x(t)\xi_x(t')\rangle = \Gamma_{xx}\delta(t-t')$ and $\langle \xi_y(t)\xi_y(t')\rangle = \Gamma_{yy}\delta(t-t')$ are taken below to be mutually independent without any loss for the development of the basic idea. The system (1) specifies a vector Markov process of the dimension $P_x + P_y$, whose state vector consists of x and y and their sequential derivatives. It describes stochastic damped oscillators at $P_x = P_y = 2$ and overdamped ones at $P_x = P_y = 1$.

Power spectral density (PSD) is a basic property of the stationary Gaussian processes x and y, especially in the oscillation-theoretic context, *e.g.*, [56,57,60]. An individual PSD is given by $W_x(\omega) = \lim_{T\to\infty}\langle \hat{x}_T(\omega) \cdot \hat{x}_T^*(\omega)\rangle/T$, where $\langle\cdot\rangle$ denotes the expectation and $\hat{x}_T(\omega) = \int_{-T/2}^{T/2} x(t)e^{-i\omega t}\mathrm{d}t$. The cross-PSD reads $W_{xy}(\omega) = \lim_{T\to\infty}\langle \hat{x}(\omega)\hat{y}^*(\omega)\rangle/T$ and the coherence $R_{xy}(\omega) = W_{xy}(\omega)/\sqrt{W_x(\omega)W_y(\omega)}$. In order to evaluate the importance of coupling $Y \to X$ in the frequency domain, it is natural to consider responses of $W_x(\omega)$ to changes in K_{xy} or parameters of Y. Since PSD describes stationary dynamics, any such quantifier belongs to the class of long-term [61] (or equilibrium [62]) dynamical effects of directional coupling [8].

The most direct and quite informative spectral effect, which is often desired in practice, seems to be the difference between W_x at given parameters and the PSD $W_{x|K_{xy}=0}$ under the condition of no coupling $Y \to X$. In case of two subsystems (1), $W_{x|K_{xy}=0}$ is just the "free" PSD of an isolated subsystem X. In convenient relative units, the suggested spectral effect reads

$$S_{y\to x}(\omega) = \frac{W_x(\omega) - W_{x|K_{xy}=0}(\omega)}{W_{x|K_{xy}=0}(\omega)}. \tag{2}$$

Thus, $S_{y\to x}$ evaluates the relative change of the PSD of x under switching the coupling $Y \to X$ on. Below, this coupling-on spectral effect is the main spectral causality measure within the framework of dynamical effects.

As soon as the coupling $Y \to X$ is "on", both the noise intensity Γ_{yy} and the functions K_{xy} and K_{yx} contribute to the PSD of x. Therefore, $S_{y\to x}$ combines effects of both factors. For a more detailed characterization, let us define "zero-noise coupling-on" spectral effect $C_{y\to x}$ to describe the coupling role when ξ_y is absent, *i.e.*, for $\Gamma_{yy} = 0$:

$$C_{y\to x}(\omega) = \frac{W_{x|\Gamma_{yy}=0}(\omega) - W_{x|K_{xy}=0}(\omega)}{W_{x|K_{xy}=0}(\omega)}, \tag{3}$$

where $W_{x|\Gamma_{yy}=0}$ is the PSD of x for zero noise ξ_y. Similarly, the "noise-on" spectral effect can be defined as the response of the PSD of x to switching the noise ξ_y on:

$$G_{y\to x}(\omega) = \frac{W_x(\omega) - W_{x|\Gamma_{yy}=0}(\omega)}{W_{x|\Gamma_{yy}=0}(\omega)}. \tag{4}$$

All these spectral effects follow certain relationships. To present them briefly, let us define the (unidirectional) transfer function from Y to X as $H_{xy}(\omega) = K_{xy}(i\omega)/L_x(i\omega)$, where $K_{xy}(i\omega)$ is in fact the transfer function from input to output of an isolated coupling element $Y \to X$ (all the same for H_{yx}). Let us denote the characteristic determinant of the system (1) as $D(\omega) = L_x(i\omega)L_y(i\omega) - K_{xy}(i\omega)K_{yx}(i\omega)$, that of the uncoupled system as $D_0(\omega) = L_x(i\omega)L_y(i\omega)$, and $\tilde{D}(\omega) = D(\omega)/D_0(\omega) = 1 - H_{xy}(\omega)H_{yx}(\omega)$. The free PSDs read $W_{x|K_{xy}=0}(\omega) = \Gamma_{xx}/|L_x(i\omega)|^2$ and $W_{y|K_{yx}=0}(\omega) = \Gamma_{yy}/|L_y(i\omega)|^2$. The PSD of x is then expressed as

$$W_x(\omega) = \frac{W_{x|K_{xy}=0}(\omega) + |H_{xy}(\omega)|^2 W_{y|K_{yx}=0}(\omega)}{|\tilde{D}(\omega)|^2}. \quad (5)$$

Then, one readily obtains the PSD of x for zero noise ξ_y as $W_{x|\Gamma_{yy}=0} = W_{x|K_{xy}=0}/|\tilde{D}|^2$ and the PSD of x for unidirectional coupling $Y \to X$ (*i.e.*, for zero coupling $X \to Y$) as $W_{x|K_{yx}=0} = W_{x|K_{xy}=0} + |H_{xy}|^2 W_{y|K_{yx}=0}$. It follows that the noise-on effect is $G_{y\to x} = |H_{xy}|^2 W_{y|K_{yx}=0}/W_{x|K_{xy}=0}$ which is equal to the "unidirectional" coupling-on effect $S_{y\to x}$, *i.e.*, to that obtained for $K_{yx} = 0$. Thus, the relative contribution of ξ_y to W_x is independent of the coupling $X \to Y$. For bidirectional coupling, $G_{y\to x}$ differs from the coupling-on effects $C_{y\to x} = 1/|\tilde{D}|^2 - 1$ and $S_{y\to x} = C_{y\to x} + G_{y\to x}/|\tilde{D}|^2$. Further algebra gives

$$S_{y\to x}(\omega) = (1 + G_{y\to x}(\omega))(1 + C_{y\to x}(\omega)) - 1. \quad (6)$$

Hence, $G_{y\to x}(\omega) \approx S_{y\to x}(\omega)$ if $|C_{y\to x}(\omega)| \ll 1$ which is the case for a weak mutual coupling $|K_{xy}(i\omega)K_{yx}(i\omega)| \ll |L_x(i\omega)L_y(i\omega)|$, *i.e.*, for $|\tilde{D}(\omega)| \approx 1$. As $|\tilde{D}(\omega)| \to 0$, the system (1) gets close to instability having $C_{y\to x}(\omega) \gg 1$ and $S_{y\to x}(\omega) \gg G_{y\to x}(\omega)$. If $|\tilde{D}(\omega)| \gg 1$, $G_{y\to x}(\omega)$ and $S_{y\to x}(\omega)$ can be even of different signs. Thus, different spectral effects reflect different aspects of the coupling role.

Granger-Geweke spectrum. – Based on the WGC idea and spectral decompositions of the prediction error [60,63] and mutual information [64], the GG spectrum has been introduced [31] for the AR process,

$$\begin{aligned} l_x(b)x_n &= k_{xy}(b)y_n + \zeta_{x,n}, \\ l_y(b)y_n &= k_{yx}(b)x_n + \zeta_{y,n}, \end{aligned} \quad (7)$$

where n is the discrete time (denote one time step as Δt in units of the above continuous time), $bx_n = x_{n-1}$ is the lag operator, l_x, l_y, k_{xy}, and k_{yx} are polynomials with $k_{xy}(0) = 0$ and $k_{yx}(0) = 0$. White noise (ζ_x, ζ_y) is the zero mean with component variances γ_{xx}, γ_{yy} and covariance γ_{xy}. If $\gamma_{xy} = 0$, the system (7) is completely analogous to eqs. (1) with mutually independent noises, so all the above spectral measures can be defined via the same formulas with $e^{-i\omega\Delta t}$ instead of $i\omega$ as the argument of the polynomials and $[-\pi/\Delta t, \pi/\Delta t]$ instead of the entire real axis as the domain of ω. Small letters are used here to denote characteristics of the discrete-time system. Being sampled at intervals Δt, the process (1) can be exactly represented in the form (7), *e.g.*, [51], where in general the degrees of l_x, l_y, k_{xy}, and k_{yx} are infinite and $\gamma_{xy} \neq 0$ [24,51].

For the system (7), the GG spectrum in the direction $Y \to X$ is defined [31] as $\log(1 + g_{y\to x}(\omega))$, where

$$g_{y\to x}(\omega) = \frac{W_x(\omega)}{W_x(\omega) - \gamma_{yy}\left(1 - \frac{\gamma_{xy}^2}{\gamma_{xx}\gamma_{yy}}\right)|h_{xy}(\omega)|^2} - 1, \quad (8)$$

and $h_{xy}(\omega) = k_{xy}\left(e^{-i\omega\Delta t}\right)/l_x\left(e^{-i\omega\Delta t}\right)$. Integrating $\log(1 + g_{y\to x}(\omega))$ over frequency, one gets the WGC as logarithm of the ratio of prediction error variances for the univariate and bivariate AR models [31]. However, any decomposition of a single number into an integral is obviously non-unique, so the second requirement underlying the definition is that $g_{y\to x}(\omega)$ relates to a decomposition of the PSD of x into a sum of two terms each related to one of the subsystems. Indeed, the PSD of x takes directly such form at $\gamma_{xy} = 0$: $w_x(\omega) = w_{x|k_{xy}=0}(\omega)(1 + g_{y\to x}(\omega))$, where $g_{y\to x}(\omega) = |h_{xy}(\omega)|^2 w_{y|k_{yx}=0}(\omega)/w_{x|k_{xy}=0}(\omega)$. For convenience, $g_{y\to x}$ itself is called GG spectrum below.

The quantity $\log(1 + G_{y\to x})$ integrated over ω gives the WGC rate for the system (1) with $P_x = P_y = 1$ [51]. For higher-order systems such a proof has not been provided, but due to the separation of two terms in W_x (5), the quantity $G_{y\to x} = |H_{xy}|^2 W_{y|K_{yx}=0}/W_{x|K_{xy}=0}$ is conceptually a direct analogue to $g_{y\to x}$ in any case. Therefore, for the continuous-time system (1) with mutually independent noises, $G_{y\to x}(\omega)$ is called below the GG spectrum which thus represents the noise-on spectral effect.

For that system, the relationship between $G_{y\to x}$ and $S_{y\to x}$ is not simple (6), and one can further derive $|\tilde{D}|^2 = (1 - |R_{xy}|^2)(1 + G_{x\to y})(1 + G_{y\to x})$, so eq. (6) gives

$$S_{y\to x}(\omega) = \frac{1}{(1 + G_{x\to y}(\omega))(1 - |R_{xy}(\omega)|^2)} - 1. \quad (9)$$

Thus, the GG spectrum in the other direction and the coherence $|R_{xy}(\omega)|$ can be used to compute $S_{y\to x}(\omega)$. Let us further check how strongly $G_{y\to x}$ and $S_{y\to x}$ can differ.

Minimal example. – The simplest system (1) widely used in mathematical modelling and statistical testing consists of overdamped oscillators, *i.e.*, $L_x x = \alpha_x x + \dot{x}$, $L_y y = \alpha_y y + \dot{y}$, $K_{xy}y = c_{xy}y$, $K_{yx}x = c_{yx}x$. In this case, all spectral measures are found explicitly. In particular, the characteristic determinant is $D(\omega) = (\alpha_x + i\omega)(\alpha_y + i\omega) - c_{xy}c_{yx}$ and the condition of weak coupling $|1 - \tilde{D}(\omega)| \ll 1$ becomes $|c_{xy}c_{yx}| \ll \alpha_x\alpha_y$. Figure 1 illustrates two typical situations for $\alpha_x = \alpha_y = 1$ and $\Gamma_{xx} = \Gamma_{yy}$.

At weak symmetric coupling $c_{xy} = c_{yx} = 0.1$ (fig. 1(a)), the GG spectrum $G_{y\to x}$ and the spectral effect $S_{y\to x}$ are both maximal at 0, differing three times in their values. The difference rises as $c_{xy}c_{yx} \to \alpha_x\alpha_y$ and so $|\tilde{D}(0)| \to 0$. Figure 1(b) shows that $S_{y\to x}(0) \approx 50$ (W_x rises 50 times due to coupling) for $c_{xy} = c_{yx} = 0.9$, while $G_{y\to x}(0)$ is only 0.8. The coupling-on effect on the variance of x [61] equals

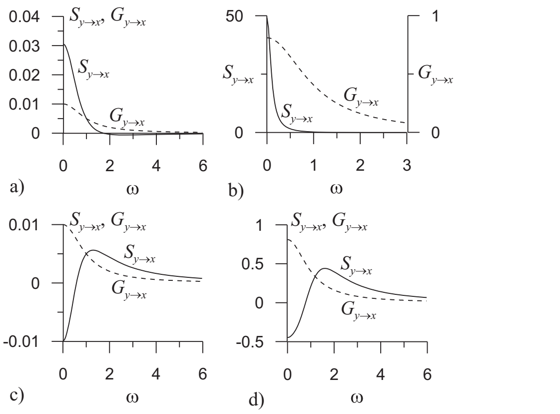

Fig. 1: Spectral effects (solid lines) and GG spectra (dashed lines) for the system (1) with $L_x x = \alpha_x x + \dot{x}$, $L_y y = \alpha_y y + \dot{y}$, $K_{xy} y = c_{xy} y$, $K_{yx} x = c_{yx} x$, $\alpha_x = \alpha_y = 1$: (a) $c_{xy} = c_{yx} = 0.1$, (b) $c_{xy} = c_{yx} = 0.9$, (c) $c_{xy} = -c_{yx} = 0.1$, (d) $c_{xy} = -c_{yx} = 0.9$.

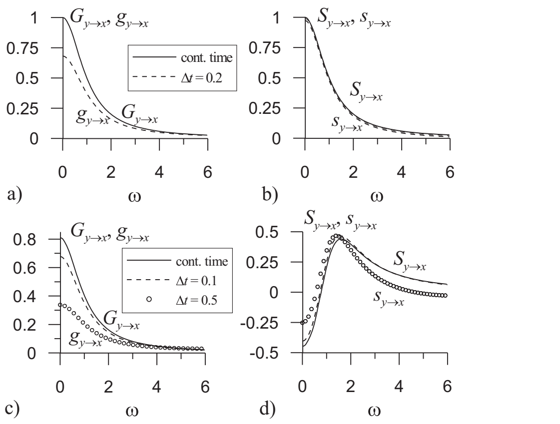

Fig. 2: Spectral effects and GG spectra for the system (1) with $L_x x = \alpha_x x + \dot{x}$, $L_y y = \alpha_y y + \dot{y}$, $K_{xy} y = c_{xy} y$, $K_{yx} x = c_{yx} x$, $\alpha_x = \alpha_y = 1$, $\Gamma_{xx} = \Gamma_{yy}$ (solid lines) and for its AR version (dashed lines, circles): (a), (b): $c_{xy} = 1$, $c_{yx} = 0$, $\Delta t = 0.2$; (c), (d): $c_{xy} = -c_{yx} = 0.9$, dashed lines for $\Delta t = 0.1$, circles for $\Delta t = 0.5$.

$1/(\alpha_x^2/c_{xy}^2 - 1) \approx 4$, *i.e.*, large $S_{y\to x}$ at low frequencies are partly compensated by negative $S_{y\to x}$ at higher ones.

For "anti-symmetric" coupling $c_{xy} = -c_{yx}$, fig. 1(c), (d) shows that $S_{y\to x}$ is negative at low frequencies and positive at higher ones contrary to the above case, the coupling-on effect on the variance of x being zero. This coupling gives birth to a peak in the PSD of x at some frequency ω_0 (in the noise-free case the frequency of decaying oscillations would be $\sqrt{|c_{xy}c_{yx}|}$), so $S_{y\to x}(\omega_0)$ is positive and large. $S_{y\to x}(0)$ tends to -1 as the coupling increases indicating that such coupling suppresses power of x at low frequencies. The GG spectrum does not exhibit such behaviour, being maximal at 0 and always positive.

To generalize, strong differences between $G_{y\to x}$ and $S_{y\to x}$ occur under one of the two conditions: i) the system (1) approaches the boundary of its stability domain, *i.e.*, $|\tilde{D}(\omega)| \ll 1$ at some ω (at $\omega = 0$ above), where $S_{y\to x}(\omega) \gg G_{y\to x}(\omega)$; ii) a new characteristic oscillation frequency ω_0 arises as a result of the "stable node-stable focus" transition occurring when the coupling coefficient increases from zero to a given value, so $S_{y\to x}(\omega_0) \gg G_{y\to x}(\omega_0)$, while $S_{y\to x}(0) \approx -1$ and $G_{y\to x}(0) \approx 1$ since $|\tilde{D}(0)| \gg 1$.

Finite sampling rate. – In practice, a system is typically analysed from a time series $x_n = x(n\Delta t)$. Probably, the basic reason why the suggested spectral effects have not yet attracted much attention is that the generative equations are usually supposed to be necessarily known for their estimation. However, the GG spectrum $G_{y\to x}$ is also not directly estimable from a time series, only its discrete-time counterpart $g_{y\to x}$ being readily available [49,50]. As for $S_{y\to x}$, two approximations can be suggested. First, by computing the PSD of x for the AR process (7) and for this AR process with $k_{xy} = 0$ and substituting these PSDs into eq. (2), one gets the spectral effect $s_{y\to x}$ which is a proxy for $S_{y\to x}$. Second, eq. (9) can be used where the continuous-time quantities are replaced with their discrete-time counterparts giving the proxy $s'_{y\to x}$. A practical question is whether $S_{y\to x}$ can be estimated from sampled data with errors not much greater than those for $G_{y\to x}$. To check inevitable influence of finite Δt, it is helpful to find analytically for the above overdamped oscillators how strongly $s_{y\to x}$ and $g_{y\to x}$ diverge from $S_{y\to x}$ and $G_{y\to x}$ with the rise of Δt.

For the unidirectional coupling $K_{xy} y = c_{xy} y$, $K_{yx} = 0$, one has $S_{y\to x} = G_{y\to x}$. Already for moderate $\Delta t = 0.2$, less than the characteristic time $1/\alpha_x = 1$, $g_{y\to x}$ is not an accurate approximation of $G_{y\to x}$ as shown in fig. 2(a). This is because in the AR representation, which is here a first-order AR process, the coupling term $c_{xy} y$ is partly "transferred" to the noise covariance γ_{xy} leading to underestimation of the coupling role. This is not as notable for $s_{y\to x}$ which is a much more accurate proxy (fig. 2(b)). Indeed, one can show that $s_{y\to x}$ is of the second-order accuracy in Δt, while $g_{y\to x}$ is only of the first-order accuracy. The proxy $s'_{y\to x}$ coincides with $s_{y\to x}$ in fig. 2(b), (d).

For the antisymmetric coupling, where $G_{y\to x}$ and $S_{y\to x}$ strongly differ, the error $|G_{y\to x} - g_{y\to x}|$ is still greater than $|S_{y\to x} - s_{y\to x}|$ as shown by the dashed line in fig. 2(c), (d). The circles in fig. 2(c), (d) show that even at large $\Delta t = 0.5$ the spectral effect $S_{y\to x}$ around its maximum (and even minimum) is reasonably well approximated with $s_{y\to x}$, while $g_{y\to x}$ as a proxy for $G_{y\to x}$ is stronger biased. Thus, here the spectral effect should be estimable from a time series with even higher accuracy than the GG spectrum.

Weakly damped oscillators. – The overdamped oscillators are a system with completely observed state space (x, y) and, in this sense, a singular case. Let us check a more general situation of subsystems X and Y with higher state space dimensions $P_x > 1$ and $P_y > 1$, where the full state of $P_x + P_y$ coordinates cannot be precisely computed from the observables x and y. The simplest example is the damped oscillators (1) with $L_x x = \omega_x^2 x + 2\delta_x \dot{x} + \ddot{x}$, $L_y y = \omega_y^2 y + 2\delta_y \dot{y} + \ddot{y}$. Let us specify couplings again as $K_{xy} y = c_{xy} y$, $K_{yx} x = c_{yx} x$, set $\omega_x = \omega_y = 1$, $\Gamma_{xx} = \Gamma_{yy}$, and let the damping to be weak $\delta_x = \delta_y = 0.1$.

The exact AR representation (7) is not available here. Therefore, to compute spectral measures for the sampled processes, two numerical techniques are used: i) covariance functions for the system (1) are computed, *e.g.*, [8,24], the Yule-Walker equations are solved to derive coefficients in the AR equations (7) of a trial order (increased until saturation of the results) and the above formulas are applied to get $g_{y\to x}$, $s_{y\to x}$, and $s'_{y\to x}$; ii) the algebraic Riccati equation is solved [49,50] to get $g_{y\to x}$ and $s'_{y\to x}$.

For moderate $\Delta t = 0.6 < 2\pi/\omega_x$ and couplings $c_{xy} = c_{yx} = 0.1$ which are weak relative to ω_x^2, the spectral effect $S_{y\to x}$ is quite non-trivial (fig. 3(a)). This is because eigenfrequencies of the coupled system (1) diverge from the natural frequency of an isolated subsystem ω_x when the coupling increases. Two positive peaks of $S_{y\to x}$ in fig. 3(a), (b) point to these eigenfrequencies, while the negative trough corresponds to ω_x where the PSD decreases. These features are not revealed by the GG spectrum, which is positive and maximal at ω_x. Figure 3(b) exhibits even stronger differences between $S_{y\to x}$ and $G_{y\to x}$ for stronger coupling $c_{xy} = c_{yx} = 0.9$. Figure 3(c), (d) shows that $S_{y\to x}$ is recovered using both $s_{y\to x}$ and $s'_{y\to x}$ with accuracy not worse than that for $G_{y\to x}$ recovered using $g_{y\to x}$. Similar results are observed for many other sampling rates and coupling strengths. Thus, the spectral effect estimates again should not be less accurate than the GG spectrum estimates.

Three subsystems. – Here, the definition of the GG spectrum is more complex [32] and its interpretation is far more troublesome. As an exemplary system, consider discrete-time overdamped oscillators with generative equations

$$\begin{aligned} x_n &= a_x x_{n-1} + c_{xy} y_{n-1} + c_{xz} z_{n-1} + \zeta_{x,n}, \\ y_n &= a_y y_{n-1} + c_{yx} x_{n-1} + c_{yz} z_{n-1} + \zeta_{y,n}, \\ z_n &= a_z z_{n-1} + c_{zx} x_{n-1} + c_{zy} y_{n-1} + \zeta_{z,n}. \end{aligned} \quad (10)$$

For mutually independent white noises ζ_x, ζ_y, and ζ_z, the conditional GG spectrum $g_{y\to x|z}(\omega)$ reads [32,49]

$$g_{y\to x|z} = \frac{\gamma'_{xx}}{\gamma'_{xx} - \gamma_{yy}|\tilde{h}_{xy}(\omega)|^2 - \gamma_{zz}|\tilde{h}_{xz}(\omega)|^2} - 1, \quad (11)$$

where γ'_{xx} is the noise variance in the bivariate AR model without y, *i.e.*, $\gamma'_{xx} = \mathrm{var}(x_n|x_{n-1}, z_{n-1}, x_{n-2}, z_{n-2}, \ldots)$, $\tilde{h}_{xy}(\omega)$ and $\tilde{h}_{xz}(\omega)$ are the components of the matrix product of the inverse transfer function of the bivariate AR model and the sub-matrix of the transfer function of eq. (10) [49]. Namely, $\log(1 + g_{y\to x|z})$ is a frequency decomposition of the logarithmic prediction improvement of x achieved with the use of y, $g_{y\to x|z} \neq 0$ if and only if $c_{xy} \neq 0$. Spectral effects can be defined via the same formulae (2) and (4).

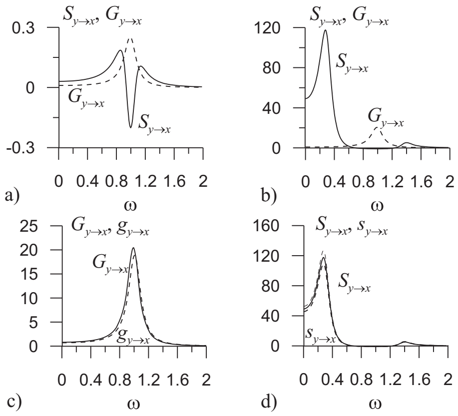

Fig. 3: Spectral effects and GG spectra for the system (1) with $L_x x = \omega_x^2 x + 2\delta_x \dot{x} + \ddot{x}$, $L_y y = \omega_y^2 x + 2\delta_y \dot{y} + \ddot{y}$, $K_{xy} y = c_{xy} y$, $K_{yx} x = c_{yx} x$, $\omega_x = \omega_y = 1$, $\delta_x = \delta_y = 0.1$, $\Gamma_{xx} = \Gamma_{yy}$: (a) $c_{xy} = c_{yx} = 0.1$, (b)–(d) $c_{xy} = c_{yx} = 0.9$. (a), (b): Spectral effects (solid lines) and GG spectra (dashes); (c), (d): spectral measures for the system (1) (solid lines) and for its AR representation at $\Delta t = 0.6$ (thick dashed lines for $s_{y\to x}$, thin dashed lines for $s'_{y\to x}$, obtained with the technique i), see the main text).

Interpretation of $g_{y\to x|z}$ as a spectral effect is possible only under strong restrictions on the coupling structure even for this simple example. Namely, take the simplest structure without loops: $c_{zx} = c_{zy} = c_{yx} = 0$ and $c_{xy} = c_{xz} = c_{yz} = C > 0$. Specify $a_x = a_y = a_z = A > 0$ and $\gamma_{xx} = \gamma_{yy} = \gamma_{zz}$. Compare $g_{y\to x|z}$ to the spectral effect (2) given by $s_{y\to x} = (W_x(\omega) - W_{x|c_{xy}=0}(\omega))/W_{x|c_{xy}=0}(\omega)$. It can be shown that for weak couplings $C \ll 1 - A$, the GG spectra approach the respective coupling-on spectral effects: $g_{y\to x|z} \approx g_{y\to x} \approx s_{y\to x}$ and $g_{z\to x|y} \approx g_{z\to x} \approx s_{z\to x}$. However, stronger couplings change the situation drastically. For $A = 0.9$ and $C = 1 - A = 0.1$, two of the GG spectra exhibit counterintuitive closeness to the spectral effect from another subsystem: $g_{z\to x} = s_{y\to x}$ (fig. 4(a)) and $g_{y\to x|z} = s_{z\to x}$ (fig. 4(b)). The other two GG spectra are even less clear: $g_{y\to x}$ is roughly close to $s_{z\to x}$ (fig. 4(b)), while $g_{z\to x|y}$ is far from any spectral effect (fig. 4(a)). Hence, under the increase of C from 0 to $1-A$, some GG spectra transit from one kind of spectral effect to another kind, while some mix takes place in between.

For the above simplest structure, $g_{y\to x|z}$ appears equal to $s_{y\to x}$ obtained for $c_{xz} = c_{yz} = 0$, *i.e.*, for an isolated pair (X, Y). However, for bidirectional coupling between Y and Z and especially for loops involving X, the interpretation of any GG spectrum in the direction of X in terms of dynamical effects directly becomes impossible. Under an increase of the number of subsystems and interconnections, difficulties of interpreting the GG spectra only rise. In contrast, the spectral effects possess the same unambiguous interpretation discussed in more detail below.

Discussion. – The GG spectrum is interpreted as information transfer rate [46,47], since it is a frequency decomposition of the WGC quantified as conditional

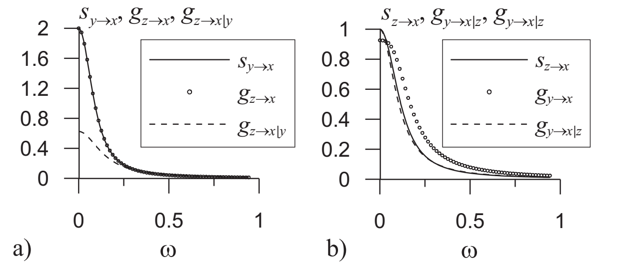

Fig. 4: Spectral effects (solid lines) and GG spectra (circles for bivariate and dashed lines for conditional ones) for the system (10) with $c_{zx} = c_{zy} = c_{yx} = 0$, $c_{xy} = c_{xz} = c_{yz} = 0.1$, and $a_x = a_y = a_z = 0.9$. The technique ii) is used, see main text.

mutual information [12,14,23,31,32]. However, as shown above, such formal decompositions generally do not reflect spectral effects of parameter interventions (2), (3), and (4). Thus, when one calls the GG spectrum "an effect, not mechanism" (title of ref. [65]), even this modest formulation seems to be exact in a rather restricted sense. Namely, the GG spectrum is non-zero if and only if the coupling $Y \to X$ is non-zero in a model equation and, hence, it directly reflects the presence of coupling and is a result of it. However, its further quantitative interpretation as a spectral effect requires special conditions and efforts.

The debates around interpretations remind those initiated by a famous radio engineer, J. A. Fleming [54]. He claimed that spectral components (side bands) of an amplitude-modulated radio signal are just formal and do not "really exist", only modulation depth being real. If so, one should not reserve a minimal frequency bandwidth for a radio channel. The incorrectness of this view was pointed out by several authors [55] and discussed in detail by Mandelshtam in his 1930–1932 lectures on oscillations which were published much later [56]. He stresses that this question is ill-posed, since one should say which systems are used to analyse the radio signal. Spectral components are quite real, if one uses the signal as an input to a narrow-band filter which gives at its output a narrow-band component of the original signal. Summed outputs of a set of filters covering the entire frequency axis give the total power of the original signal and, thereby, its PSD is directly visible and actual. Still, the reality of spectral components was often discussed again, *e.g.*, in [57]. In our case, due to the linearity of the system (1), the spectral effect $S_{y\to x}(\omega')$ represents the response of W_x to inserting/removing a narrow-band ($\omega' \pm \Delta\omega$) rejecting filter on/out of the way $Y \to X$. If such a filter is removed, the relative change of $W_x(\omega')$ is given by $S_{y\to x}(\omega')$. Similarly, $G_{y\to x}$ is the spectral effect of removing a narrow-band rejecting filter out of the way $\xi_y \to y$. Such interpretations are valid for an arbitrary number of subsystems, but generally not for the GG spectra.

As for the DTF, its interpretation is straightforward. For an arbitrary number N of subsystems, the DTF is defined via factorization of the PSD matrix [36]: $\mathbf{W}(\omega) = \mathbf{H}(\omega)\mathbf{\Gamma}\mathbf{H}^{*\mathrm{T}}(\omega)$, where T means transposition and $\mathbf{\Gamma}$ is the noise intensity matrix. For mutually independent noises, the normalized DTF in the direction $m \to n$ defined as $\Gamma_{mm}|H_{nm}|^2/\sum_{j=1}^{N}\Gamma_{jj}|H_{nj}|^2$ (called informational DTF [41] or directed coherence [37]) is equivalent to the noise-on spectral effect $G_{m\to n}$ (4). Such a relation was also outlined in ref. [43]. As for the PDC, it is defined via a similar factorization of the partial coherence matrix [37] and has no direct interpretation as a spectral effect. But the non-normalized PDC [43] in the direction $m \to n$ is just $K_{nm}(\omega)$, a transfer function of an isolated coupling element $m \to n$. Thus, any PDC relates to the spectral effect of the input of a coupling element on its output, without more detailed interpretation. Only for $N = 2$ the informational DTF and generalized PDC [41] coincide with the GG spectrum and, hence, with the noise-on spectral effect.

The suggested approach to studying spectral effects of couplings can be generalized to i) cross-correlated noises in subsystems, ii) arbitrary state vectors rather than only sequential derivatives, iii) larger ensembles of subsystems, iv) nonlinear systems with the use of relevant parameter estimation (*e.g.*, [3,66]) and identification (*e.g.*, [38,52,67]) procedures. Another useful line of research seems to be the study of quantitative conditions under which the spectral effect estimation is reliable. All that will allow to understand better the meaning of the GG spectra (and DTF and PDC) and to more reliably estimate spectral effects.

Conclusions. – It is shown that the spectral effects introduced within the dynamical effects framework may well be more desirable for coupling characterization than the GG spectrum and other spectral causalities, though probably less accessible from data. Thus, further studies of the relationships between the two types of characteristics should improve the interpretation of the latter and accessibility of the former. To a significant extent, the suggested view resolves the interpretational difficulties debated in refs. [43–48]. This step has appeared possible because the formal statistical problem under study has been considered in the oscillation-theoretic spirit, via switching from the logic of formal decompositions to the logic of dynamical effects. The suggested view does not replace the GG spectra and other existing spectral causalities, but complements them and may serve to develop a more diverse set of spectral characteristics capable of answering quite different questions about the coupling role in dynamics.

* * *

The work is done within the framework of a state task.

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