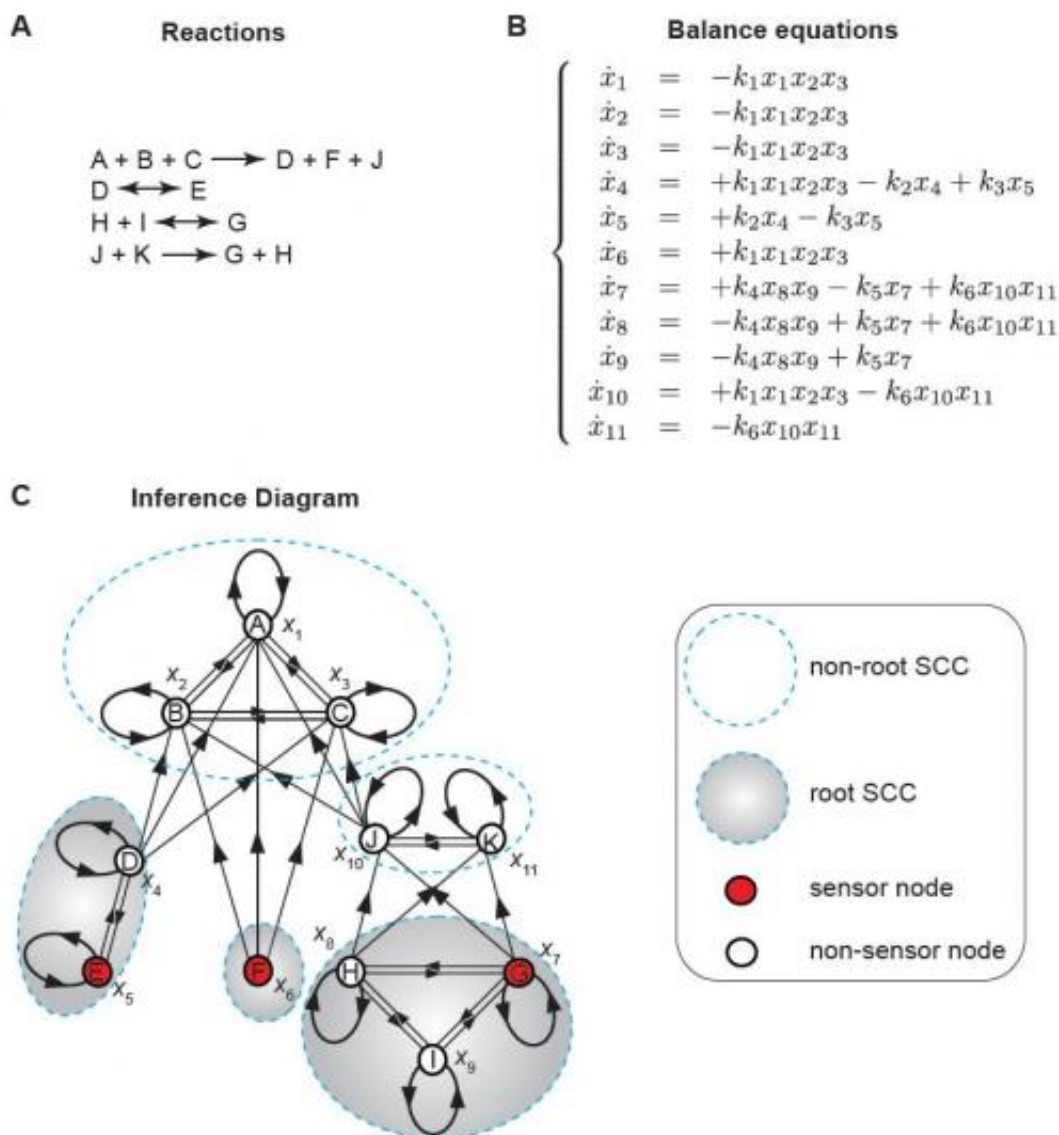


Through a sensor, clearly: Complex systems made observable

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Graphical approach. (A) Chemical reaction system with 11 species (A,B,..,J,K) involved in four reactions. Because two reactions are reversible, we have six

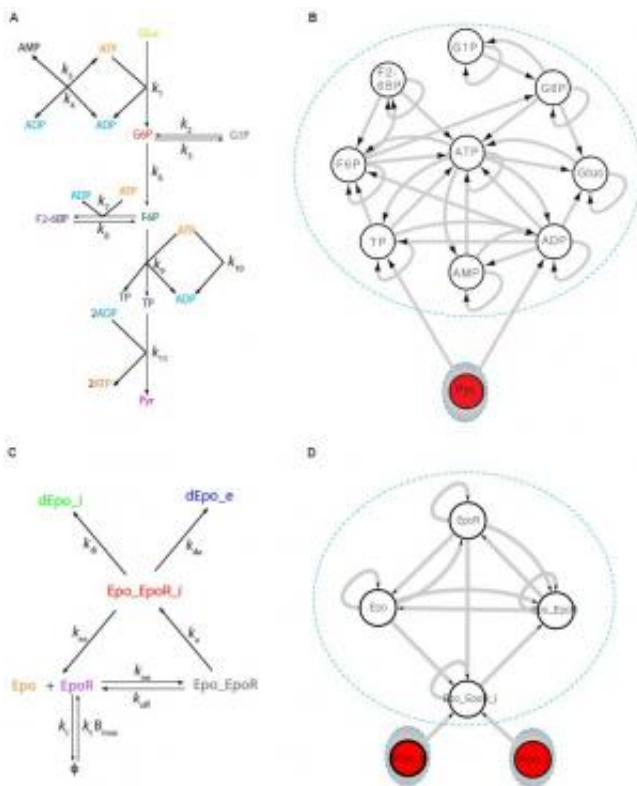
elementary reactions. (B) Balance equations of the chemical reaction system shown in A. Concentrations of the 11 species are denoted by $x_1, x_2, \dots, x_{10}, x_{11}$, respectively. Rate constants of the six elementary reactions are given by k_1, k_2, \dots, k_6 , respectively. Balance equations are derived using the mass-action kinetics. (C) Inference diagram is constructed by drawing a directed link ($x_i \rightarrow x_j$) if x_j appears in the right-hand side of x_i 's balance equation shown in B. SCCs, which are the largest subgraphs chosen such that there is a directed path from each node to every other node in the subgraph, are marked with dashed circle; root SCCs, which have no incoming links, are shaded in gray. A potential minimum set of sensor nodes, whose measurements allow us to reconstruct the state of all other variables (metabolite concentrations), is shown in red. Copyright © PNAS, doi:10.1073/pnas.1215508110

(Phys.org) —A complex system can, in principle, be *observable* – that is, the system's complete internal state can be reconstructed from its outputs, which would ostensibly involve describing in complete quantitative detail all of its internal state variables at once. In an actual experiment, however, such measurement is typically beyond our reach, and so is limited to a smaller number of those variables. Referred to as *sensors* (or *sensor nodes*), these key variables can be used to make the complete system observable. Recently, scientists at Northeastern University and MIT devised a graphical approach that first derives the mathematical equations describing a complex system's dynamics, and then determines the key sensors for that system. Moreover, when applying their approach to biochemical reaction systems, the researchers discovered that the derived sensors were both *necessary* and *sufficient* to describe the complete system. The scientists conclude that their findings allow a systematic exploration of many diverse natural, technological and socioeconomic systems.

Dr. Yang-Yu Liu comments on the research he, Prof. Albert-László Barabási and Prof. Jean-Jacques Slotine performed, starting with the

three main challenges they faced. "The primary challenge is that for many [nonlinear systems](#), we don't know the system parameters," Liu tells *Phys.org*. "However, conceptually it is quite straightforward to adopt a graphical approach derived from the dynamical laws that govern a system to determine the sensors that are necessary to reconstruct the full internal state of a complex system."

In fact, control theorists have been working on the concept of system digraphs some time. Liu and his associates used this approach to study the observability problem for highly nonlinear systems, which he says that to his knowledge has not been previously addressed. "The surprise," Liu adds, "was that, except for some pathological cases which almost never occur in real systems, the sensors we identified are not only necessary but also sufficient: Usually, we expect that to observe the system we'd need to monitor more sensors than just the necessary nodes, since if the topology of a dynamic system's inference diagram is very complex, it's hard to have any symmetries. However, the complicated topology somehow helped us achieve system observability." An inference diagram reveals the underlying structure of information flow or casualty when the measurements are performed.



Biochemical reaction systems and their inference diagrams. (A) Simplified glycolytic reaction map (20), where the symbols denote G6P, F6P, TP, F2-6BP, ATP (adenosine 5'-triphosphate), and ADP (adenosine 5'-diphosphate). Source (glucose) and sinks (G1P and Pyr) are also included in this model. Different chemical species are shown in different colors. (B) Inference diagram of the reaction system shown in A consists of a nonroot SCC of nine species (marked with dashed circle) and a root SCC of one species—the pure product Pyr (shaded in gray), hence indicating that the system can be observed through monitoring the concentration of Pyr only. (C) Simple model of ligand binding (23). The symbols denote Epo, EpoR, Epo_EpoR, Epo_EpoR_i, dEpo_i, and dEpo_e, marked with different colors. Bmax is the maximal amount of receptor at the cell membrane. (D) Inference diagram of the reaction system shown in C consists of a nonroot SCC of four species (marked with dashed circles) and two root SCCs (shaded in gray). Each root SCC contains one pure product. The system can be observed through monitoring the concentrations of the two pure products, dEpo_i and dEpo_e. Copyright © PNAS, doi:10.1073/pnas.1215508110

Lastly, Liu addressed the challenge of reconstructing selected state variables from appropriately chosen outputs using their graphical approach. "The reconstruction of other state variables is highly nontrivial task," Liu explains. This is the so-called *observer design problem*, which can be defined as the problem of designing observers which are insensitive to nonlinear behavior, sensor noise, modeling errors, and other effects. "For [biochemical reaction](#) systems, or any general nonlinear systems, the observer design problem is very difficult. In this paper, we were concerned only with observability, rather than the observer design."

Since the team's graphical approach relies only on the dynamics equations, notes Liu, their findings offer avenues to systematically explore the dynamics of a wide range of natural, technological and socioeconomic systems. "For any nonlinear systems, as long as we can come up with a suitable set of nonlinear dynamic equations, we should be able to construct the inference diagram. We can then use strongly connected component, or SCC, analysis to get the necessary sensors that need to be monitored. This approach is applicable to any nonlinear system."

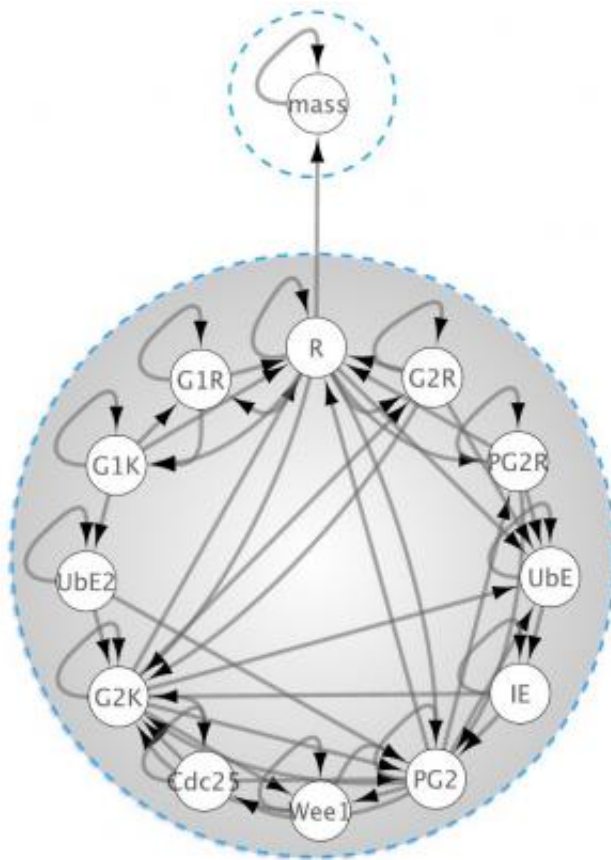


Fig. S3. Inference diagram of the cell cycle control model in fission yeast (18). Strongly connected components (SCCs) are marked with dashed circles. The root SCC, which has no incoming links, is shaded in gray. Copyright © PNAS, doi:10.1073/pnas.1215508110

This idea alone is tremendously important, since the statistical rules describing different classes of [complex systems](#) (for example, biological systems vs. large-city urbanization) vary significantly. However, to address the observability problem Liu and his colleagues propose a general framework – so once the complex system's dynamics equations are derived, the inference diagram can be constructed and the key sensors identified. "For example," Liu illustrates, "in addition to the biological systems discussed in our paper, one can apply this approach to social dynamic system such as opinion or social influence dynamics. "

Moving forward, Liu describes other innovations the researchers might develop and apply to the current experimental design. "We may want to also infer all system parameters, which can be viewed as a special type of state variables with time derivative 0. This is a rather challenging question, but without knowing the system parameters, we can never design a real observer to completely construct the system's internal state. We'd also like to get more biological implications and applications from the biological systems [sensors](#) we identified."

More information: Observability of complex systems, *PNAS* February 12, 2013 vol. 110 no. 7 2460-2465, [doi:10.1073/pnas.1215508110](https://doi.org/10.1073/pnas.1215508110)

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