A Universal Route to Explosive Phenomena

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Phase transitions are observed in many physical systems. This includes the onset synchronization in a network of coupled oscillators or the emergence an epidemic state within a population. "Explosive" first-order transitions have caught particular attention in a variety of systems when classical models are generalized by incorporating additional effects. Here we give a mathematical argument that the emergence of such explosive phenomena is not surprising but rather a universally expected effect: Varying a classical model along a generic two-parameter family must lead to a change of the criticality. To illustrate our framework, we give three explicit examples of the effect: in a model of adaptive epidemic dynamics, for a generalization of the Kuramoto model, and for a percolation transition.

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Many nonlinear physical systems—ranging from epidemic spreading, synchronization of coupled oscillators to percolation on a network—undergo phase transitions as a system parameter is varied. These transitions can be continuous (second-order) at the transition point or discontinuous (first-order). Discontinuous first-order transitions typically lead to an "explosive" change of system properties; see [1] and references therein. For a wide variety of systems it has been observed that a variation of the model via additional features leads to the change from a continuous second-order to a discontinuous first-order phase transition. The emerging paradigm is as follows. First, many studies add an additional effect to a classical model. Second, these studies observe that a fundamental change in the phase transition (or bifurcation) structure occurs: Upon variation of a new parameter a previously second-order/soft transition becomes a first-order/hard transition. As an example consider the classical Kuramoto model, which shows a continuous synchronization transition. However, varying the distribution of intrinsic frequencies [2, 3] or generalizing the network to simplicial or higher-order coupling [4, 5] allows for discontinuous synchronization transitions. Similarly, adding adaptation [6] or higher-order coupling structures [7] to models of epidemic spreading can induce a discontinuous transition to the epidemic state.

In this paper, we give a mathematical argument that a transition from a continuous to a discontinuous phase transition is not surprising but a generically/universally expected effect if additional parameters are varied. Specifically, we show that a typical model variation along a two-parameter family of a classical model with a second-order transition must lead to a change of the criticality to first-order. To illustrate our results, we then demonstrate this effect in three explicit examples of physical systems: adaptive epidemic dynamics, synchronization in the Kuramoto model with non-additive higher-order interactions, and a model from percolation theory.

A universal mechanism that modulates transitions. We focus here on dynamical systems that have a mean-field or continuum limit model described near the phase transition by an ordinary differential equation (ODE)

$$x' := \frac{\mathrm{d}x}{\mathrm{d}t} = F(x,y), \quad x(0) = x_0, \tag{1}$$

where $x = x(t) \in \mathbb{R}^n$ is the unknown and $y \in \mathbb{R}^m$ are parameters. Suppose $x_* = x_*(y)$ is a smooth family of equilibrium points parametrized by y. For all models we have in mind, one trivial branch of solutions exists for all parameters so we may assume upon translation that $x_* = 0 := (0, 0, \dots, 0)^\top \in \mathbb{R}^n$, i.e., $F(0, y) = 0$ for all $y \in \mathbb{R}^m$. Furthermore, suppose that we have a bifurcation point [8] upon parameter variation generically given by a single eigenvalue of the Jacobian

$$A(y) := \mathrm{D}_x F(0, y) \in \mathbb{R}^{d\times d}$$

crossing the imaginary axis. Using a translation in parameter space and center manifolds [8] or Lyapunov–Schmidt reduction [9], we may assume without loss of generality that the main bifurcation parameter is $p = y_1$ and the one-dimensional ODE on the center manifold is given by

$$x' = f(x, p), \quad x \in \mathbb{R},\ p \in \mathbb{R}, \tag{2}$$

with bifurcation point at $p = 0$. Then it is well-known that the two typical bifurcation points encountered in applications are the transcritical bifurcation with local normal form

$$x' = px + ax^2, \tag{3}$$

where $a = \pm 1$ determines whether the bifurcation/transition upon varying p is second-order ($x \geq 0$, $a = -1$) or first-order ($x \geq 0$, $a = +1$). Similarly, if there is an equivariance given by a $\mathbb{Z}_2$-reflection symmetry in the model via $f(x, p) = -f(-x, p)$, then the generic transition is a pitchfork bifurcation

$$x' = px + ax^3. \tag{4}$$

The pitchfork is second-order if it is supercritical and $a = -1$, while it is first-order if it is subcritical and $a = +1$.

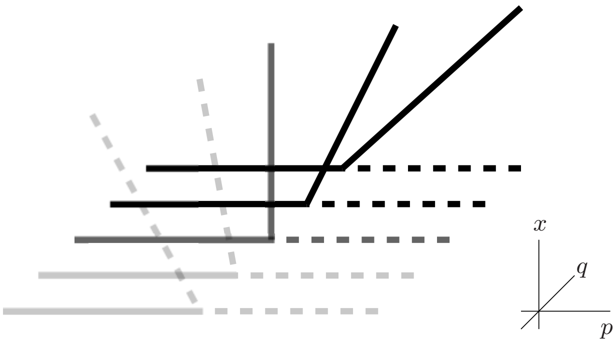

FIG. 1. Sketch for the variation of a transcritical bifurcation for the phase space $\{x \geq 0\}$ and parameters (p, q) with primary parameter p and second generic unfolding parameter q. Dashed lines indicate instability of the equilibrium and solid lines indicate stability. The grey cases are first-order (explosive, subcritical) transitions, while the black diagrams are second-order (non-explosive, supercritical) transitions.

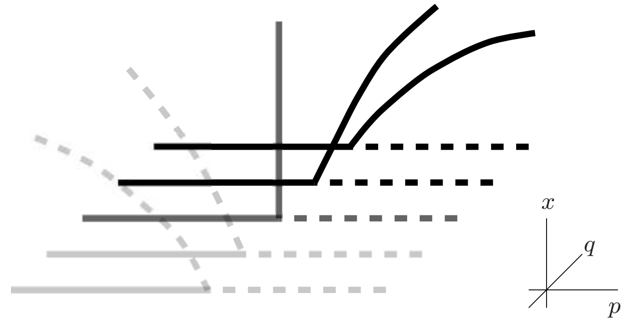

FIG. 2. Sketch for the variation of a pitchfork bifurcation for the phase space $\{x \geq 0\}$ and parameters (p, q) with primary parameter p and second generic unfolding parameter q. Dashed lines indicate instability of the equilibrium and solid lines indicate stability. The grey cases are first-order (explosive, subcritical) transitions, while the black diagrams are second-order (non-explosive, supercritical) transitions.

A generic model variation with at least one additional free parameter leads to a vector field f that allows for a change in criticality. Take a generic single-eigenvalue crossing and with the phase space $\{x \geq 0\}$. Upon variation of the model, the persistence of a single-eigenvalue crossing is generic within one-parameter families of the vector field f. Hence, without loss of generality suppose that the single eigenvalue crosses at $p = 0$. Furthermore, if we vary the model at least one additional free parameter, say $q = y_2$, generically appears. This parameter takes into account the additional effect for each model as indicated above. A Taylor expansion at the bifurcation point now yields

$$f(x, p, q) = \sum_{j,k,l=0}^{M} c_{jkl} x^j p^k q^l + \mathcal{O}(M+1),$$

where $\mathcal{O}(M+1)$ denotes terms of order $M+1$. The coefficients c_{jkl} are constrained: The existence of a trivial branch of equilibria, $f(0, p, q) = 0$, implies $c_{0kl} = 0$ for all $j, k \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$. Since a single eigenvalue crosses at $p = 0$, we must have $\partial_x f(0, 0, q) = 0$, where ∂_x denotes the partial derivative. Hence, we have $c_{10l} = 0$ for all $l \in \mathbb{N}_0$ and thus

$$f(x, p, q) = c_{110} xp + c_{200} x^2 + \sum_{j+k+l=3} c_{jkl} x^j p^k q^l + \mathcal{O}(4).$$

Now we have all the bifurcation conditions taken care of, one may use bifurcation theory to unfold the singular point into a generic family. In particular, the next derivatives of the vector field at the bifurcation point should not vanish. Hence, we must have $c_{102} = 0$ from above and for all other combinations of indices that $c_{jkl} \neq 0$ if $j \geq 1$ and $j + k + l = 3$, where the leading-order non-vanishing conditions are

$$\partial_{xxp} f(0) \neq 0, \qquad \partial_{xxq} f(0) \neq 0.$$

This yields the truncated lowest-order two-parameter unfolding normal form

$$f(x, p, q) = c_{110} xp + (c_{200} + c_{210} p + c_{201} q) x^2. \quad (5)$$

We now apply a scaling (or geometric desingularization, or renormalization) with a small parameter $\varepsilon > 0$ through the transformation

$$x \mapsto x\varepsilon^{\alpha}, \quad p \mapsto p\varepsilon^{\beta}, \quad q \mapsto q\varepsilon^{\gamma}.$$

For the transcritical normal form (5) we choose $\alpha = 1$, $\beta = -1$, $\gamma = -2$ to obtain (upon a suitable time rescaling)

$$f(x, p, q) = c_{110} xp + (c_{200} \varepsilon^2 + c_{210} p\varepsilon + c_{201} q) x^2. \quad (6)$$

Hence, one easily checks that there is a sign change of $\partial_{xx} f(0, p, q)$ upon varying q in an interval $[-q_0, q_0]$ for some $q_0 > 0$ as long as $c_{201} \neq 0$, which we expect generically. Even if $c_{201} = 0$, we can expand to higher order in q and may thereby eventually change the sign of $\partial_{xx} f(0, p, q)$ so only certain situations with e.g. symmetries and/or non-generic smooth functions could lead to the preservation of the sign for all $q \in \mathbb{R}$. Once the sign of $\partial_{xx} f(0, p, q)$ changes, this implies that generically the second parameter is able to change the transition from second to first order or vice versa. Of course, from the viewpoint of the geometry of the bifurcation diagram, this is quite intuitive as shown in Fig. 1 that a second generic parameter may change criticality.

The situation for the pitchfork works very similarly except that an additional symmetry $f(x, p, q) = -f(-x, p, q)$ has to be respected. This further constrains the coefficients of the Taylor expansion. Note that if this symmetry is broken then we are in the transcritical case if there is still a trivial branch for all values of the parameters. Hence, we now assume that the symmetry holds. Taylor expansion as above gives for a bifurcation point with a single eigenvalue crossing

$$f(x, p, q) = c_{110} xp + c_{300} x^3 + \sum_{j+k+l=4} c_{jkl} x^j p^k q^l + \mathcal{O}(5).$$

The same steps as above lead to leading-order to the two-parameter normal form

$$f(x, p, q) = c_{110} xp + (c_{300} + c_{310} p + c_{301} q) x^3. \quad (7)$$

Again, this shows that a second parameter can generically change second-order to first-order phase transitions; cf. Fig. 2.

We now give three examples of complex systems where a generalization leads to a change from a first-order to a second-order phase transition. We explicitly relate each of the examples to the abstract framework above.

Transitions in adaptive epidemics. We consider the adaptive epidemic model by Gross et al. [6], which is microscopically modeled as a Markov chain on networks with nodes being in two states, either susceptible $\mathcal{S}$ or infected $\mathcal{I}$. Infections take place at rate ρ, recovery at rate r (which we set to $r = 1$ without loss of generality here), and adaptive re-wiring of an $\mathcal{SI}$-link to an $\mathcal{SS}$-link at rate q. Direct numerical simulations show that the bifurcation at the epidemic threshold $\rho = \rho_{\mathrm{c}}$ is a second-order transition if $q = 0$. It becomes a first-order transition if q is increased sufficiently, i.e., the network becomes more strongly adaptive. Based upon our considerations above, it is natural to expect that allowing for general network topologies via re-wiring is a sufficiently generic breaking mechanism to allow the second-to-first order change via the parameter q. In fact, this is what is verified implicitly in [6] by using a moment-closure expansions [10] of the network dynamics. The following moment-closed ODEs describe the dynamics for large networks

$$\begin{aligned}
I' &= \rho(\frac{\mu}{2} - l_{\mathcal{II}} - l_{\mathcal{SS}}) - I,\\
l'_{\mathcal{II}} &= \rho(\frac{\mu}{2} - l_{\mathcal{II}} - l_{\mathcal{SS}}) \left(\frac{\frac{\mu}{2} - l_{\mathcal{II}} - l_{\mathcal{SS}}}{1-I} + 1\right) - 2l_{\mathcal{II}},\\
l'_{\mathcal{SS}} &= (1+q)(\frac{\mu}{2} - l_{\mathcal{II}} - l_{\mathcal{SS}}) - \frac{2\rho(\frac{\mu}{2} - l_{\mathcal{II}} - l_{\mathcal{SS}})l_{\mathcal{SS}}}{1-I},
\end{aligned}$$

where I and $l_{\mathcal{II}}$, $l_{\mathcal{SS}}$ are a normalized infected density and two similarly normalized link densities respectively [6]; note that conservation laws allow for the elimination of S and $l_{\mathcal{SI}}$. We fix μ arising from a connectivity assumption [6] of the network to $\mu = 20$. This is a standard assumption [11], as we only want to demonstrate the principal effect of adding re-wiring via q. It can be checked, see [6, 11], that a first-order transition is possible upon varying q.

We now formally show that the change of criticality is a special case of our more general results above. One checks that there always exists the invariant trivial branch of steady states $\{I = 0, l_{\mathcal{II}} = 0, l_{\mathcal{SS}} = \frac{\mu}{2}\}$. The epidemic threshold bifurcation point is given by

$$\rho_{\mathrm{c}} = \frac{1+q}{\mu} = \frac{1+q}{20}.$$

Now we employ a lengthy, yet very direct and general, center manifold calculation to find the normal form, which we outline here. First, we shift coordinates $I = X_1$, $l_{\mathcal{II}} = X_2$, $l_{\mathcal{SS}} = X_3 + 10$, $\rho = p + \rho_c$, to obtain a vector field $X' = F(X, p, q)$. Then we transform the linear part $A = \mathrm{D}_X F(0, 0, q)$ into Jordan canonical form

$$M^{-1}AM = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & \frac{1}{20}(-q-41) \end{pmatrix}$$

for a transformation matrix $X = M\tilde{x}$ that can be calculated from the eigenvectors of A. We augment the new ODEs $\tilde{x}' = M^{-1}F(M\tilde{x}, p, q)$ by $p' = 0$ and $q' = 0$ to calculate a the three-dimensional center manifold $\{(\tilde{x}_2, \tilde{x}_3) = h(\tilde{x}_1, p, q)\}$ as there are three zero eigenvalues. The manifold is parametrized over the center directions $(\tilde{x}_1, p, q)$. Using the invariance equation [8] and a quadratic ansatz for h, one obtains after equating coefficients

$$\begin{aligned}
\tilde{x}_2 &= h_1(\tilde{x}_1, p, q) = -\frac{4}{35301}\tilde{x}_1^2,\\
\tilde{x}_3 &= h_2(\tilde{x}_1, p, q) = \frac{3364}{206763}\tilde{x}_1^2 + \frac{280}{1681}\tilde{x}_1 p.
\end{aligned}$$

Plugging this back into the equation for $\tilde{x}_1'$ and writing $x := \tilde{x}_1$ gives the flow on the center manifold to leading order as

$$x' = \frac{800}{q+41}xp + \frac{80\left(\frac{2(q+1)^2}{q+41} - \frac{1}{10}(q+1)\right)}{q+41}x^2 + \cdots$$

Now one easily checks from the coefficients of xp and x^2, as above, that the parameter q indeed yields a change in the criticality from a second-order to a first-order transition at $q = 21/19$. Hence, from this perspective we can clearly see that a change in criticality is not surprising: The re-wiring q appears in the reduced center manifold as a sufficiently generic second unfolding parameter as in the universal route described above.

Synchronization in phase oscillator networks. The Kuramoto model [12] describes the evolution of a network of N phase oscillators, where the state of oscillator $k \in \{1, \ldots, N\}$ is given by the phase $\theta_k \in \mathbb{R}/(2\pi\mathbb{Z})$. Kuramoto oscillators interact additively, so a natural generalization is to consider the effect of non-additive interactions [13–15] since they arise naturally in phase reductions of coupled nonlinear oscillators [16]. For example, Skardal and Arenas [4] considered the synchronization transition in such a variation of the Kuramoto model with triplet interactions. Specifically, the phase of oscillator k evolves according to

$$\begin{aligned}
\theta_k' = \omega_k &+ \frac{K_2}{N}\sum_{j=1}^{N}\sin(\theta_j - \theta_k)\\
&+ \frac{K_3}{N}\sum_{j,l=1}^{N}\sin(2\theta_l - \theta_j - \theta_k),
\end{aligned} \tag{8}$$

with intrinsic frequencies ω_k sampled from a Lorentzian distribution with mean 0 and width 1 [17]. The parameter K_2 determines the strength of the additive interactions and K_3 the strength of the triplet interactions; for $K_3 = 0$ we recover the classical Kuramoto model.

A sufficiently large triplet coupling strength K_3 can now change the nature of the synchronization transition. Write $\mathrm{i} := \sqrt{-1}$ and let $Z = R\mathrm{e}^{\mathrm{i}\phi} = \frac{1}{N}\sum_{j=1}^{N}\mathrm{e}^{\mathrm{i}\theta_j}$ denote the Kuramoto order parameter. In the mean-field limit of $N \to \infty$ oscillators, the Ott–Antonsen reduction [18] of (8) yields the effective dynamics

$$R' = \left(\frac{K_2}{2} - 1\right)R + \left(\frac{K_3}{2} - \frac{K_2}{2}\right)R^3 - \frac{K_3}{2}R^5,$$

which describe the evolution of the system; see also [19]. Set $p = \frac{K_2}{2} - 1$, $q = \frac{K_3}{2}$ and $x = R$ to read off the normal form expansion (7). There is a critical transition at the bifurcation $p = 0$, that is $K_2 = 2$ for any K_3. For the Kuramoto model $K_3 = 0$, the bifurcation is always supercritical (second-order). However, for $K_3 > 2$ the synchronization transition becomes subcritical and discontinuous. Hence, a discontinuous synchronization transition in phase oscillators with higher-order interactions is another special case of the universal route described above.

Discontinuous percolation transitions. Change from a continuous to a discontinuous transition have also been observed in percolation problems. Consider the q-state Potts model on a Bethe-lattice with coordination number 3 [20]. For $q = 2$ this gives the Ising model. Now suppose that the bonds are occupied occupied independently with homogeneous density $\hat{p} \in [0, 1]$. Evaluating the percolation probabilities recursively [21], one obtains the percolation probability for the lattice as a fixed point of the iteration

$$P_{n+1} = \frac{2\hat{p}P_n + (q-2)\hat{p}^2 P_n^2}{1 + \hat{p}^2(q-1)P_n^2} =: H(P_n). \tag{9}$$

The percolation transition of the fixed point $P_* = 0$ of H happens at the critical bond density $\hat{p} = \frac{1}{2}$; whether this transition is continuous or discontinuous depends on the number of states q of the Potts model [21].

The change of criticality of the percolation transition can be understood within the general framework introduced above. Set $p := \hat{p} - \frac{1}{2}$ and consider the ODE

$$x' = f(x, p, q) := H(x) - x \tag{10}$$

obtained by seeing (9) as a difference equation. By definition, the fixed points of H in (9) correspond to equilibria of f in (10). Moreover, since $\partial_x f = \partial_x H - 1$ and $\partial_x H > 0$ in a neighborhood of $(x, p) = 0$, linear stability of stationary states coincides as well. Thus, the behavior of the percolation transition of (9) is completely determined by the bifurcations of the equilibrium $x = 0$ of (10) at $p = 0$. A Taylor expansion of $f(x, p, q)$ yields

$$f(x, p, q) = 2xp + \frac{1}{4}(g(p)q - 2g(p))x^2 + \cdots$$

with $g(p) = 4p^2 + 4p + 1$. Thus, the change of criticality of the percolation transition at $q = 2$ corresponds to a change from a super- to a subcritical transcritical bifurcation in the universal route described above.

How the the percolation probability changes with the bond density is also directly related to discontinuous transitions in the expected maximal cluster size of a random graph. Specifically, random graphs with an underlying hierarchical self-similar structure allow to calculate the percolation probability through recursive relations [22] as in the Potts model discussed above. By calculating the corresponding generating functions [23], one can observe a discontinuous transition in the expected size of the largest cluster.

Discussion. Our argument shows that from the perspective of bifurcation theory, one can expect a change from a continuous transition to a discontinuous transition as additional effects are added to a classical model. Here, we gave three explicit network dynamics examples to illustrate this universal route. Our formalism not only shows that a transition to an explosive change of system properties is not surprising but also has the same underlying dynamical mechanism. In particular, our framework links explosive percolation, explosive synchronization, and explosive epidemic spreading explicitly.

Many other variations are possible that fit into our framework. First, the effect of numerous generalizations of the Kuramoto model on the synchronization transition have been explored in the literature. This includes varying the properties of the intrinsic frequencies [2, 3] or generalized coupling structures that encode higher-order effects [4, 5]. Second, we anticipate our theory to be relevant in neural networks. For example, networks of quadratic-integrate-and-fire neurons can be described by low-dimensional equations using a reduction closely related to the Ott–Antonsen approach [19, 24]. These equations show transcritical bifurcation in a limiting case [25] that could shed light on the emergence of discontinuous transitions between low- and high firing dynamics [26]. Finally, we expect our theory to apply also in further physical systems, for example, chemical reaction networks, where the same type of mechanism is bound to be relevant.

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