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Bifurcation Structure of a Class of S_N-invariant Constrained Optimization Problems*

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In this paper we investigate the bifurcations of solutions to a class of constrained optimization problems. This study was motivated by annealing problems which have been used to successfully cluster data in many different applications. Solving these problems numerically is challenging due to the size of the space being optimized over, which depends on the size and the complexity of the data being analyzed. The type of constraints and the form of the cost functions make them invariant to the action of the symmetric group on N symbols, S_N, and we capitalize on this symmetry to describe the bifurcation structure. We ascertain the existence of bifurcating branches, address their stability, and compare the stability to optimality in the constrained problem. These theoretical results are used to explain numerical results obtained from an annealing problem used to cluster data.

1. INTRODUCTION

This paper analyzes bifurcations of solutions to constrained optimization problems of the form

$$\max_{q \in \Delta} F(q, \beta) = \max_{q \in \Delta} \left(\sum_{\nu=1}^{N} f(q^{\nu}, \beta) \right) \tag{1}$$

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* Dedicated to Professor Shui-Nee Chow on the occasion of his 60th birthday.

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as a function of a scalar parameter β. The scalar function f is sufficiently smooth, and the constraint space $\Delta \subset \mathbf{R}^{NK}$ is a convex set of valid discrete conditional probabilities. A vector $q \in \Delta$ can be decomposed into N subvectors $q^\nu \in \mathbf{R}^K$. The form of F implies that it is S_N-invariant: the value of $F(q,\beta)$ does not change under arbitrary permutations of the vectors q^ν.

This type of problem arises in Rate Distortion Theory [7, 20], the Deterministic Annealing approach to clustering [34], the Information Bottleneck approach to clustering [37, 41, 38], and the Information Distortion method [9, 10, 16] for determining neural coding schemes. In these cases, which originally motivated the study of (1), F has the form $F = G(q) + \beta D(q)$, giving the annealing problem

$$\max_{q \in \Delta}(G(q) + \beta D(q)), \tag{2}$$

where β is a homotopy or annealing parameter which is non-negative, and G and D are each of the form given in (1). We will motivate the importance of these annealing problems by presenting the Information Distortion approach to solving the neural coding problem in Section 1.1, and the Information Bottleneck approach to clustering in Section 1.2.

From the mathematical point of view, problem (2) represents an optimization problem with both equality and inequality constraints. It presents challenges numerically, since in applications it leads to optimization in hundreds to thousands of dimensions and is also very interesting from the theoretical point of view. In neural applications the problem one needs to solve is

$$\max_{q \in \Delta} D(q), \tag{3}$$

where $D(q)$ is the mutual information function. It has been shown that this problem is NP complete [28]. The problem (2) is used as a very effective scheme to get a (local) solution of the problem (3). The function $G(q)$ usually has a single maximum. Starting at this maximum when $\beta = 0$ and then continuing the solution as $\beta \to \infty$ produces a solution of (3). This procedure is common to all annealing problems. As β increases from 0 to ∞ the optimal solution undergoes a series of rapid changes, which we relate to bifurcations of the equilibria of a gradient flow of the corresponding Lagrangian of (1).

The general problem (1) has some special features. It has an integer parameter N, and the function F is S_N-invariant. The S_N symmetric vector fields on $\mathbf{R}^N$ were studied in Golubitsky and Stewart [18] and in a series of papers by Stewart [39], Stewart, Elmhirst and Cohen [5, 40], Elmhirst [14, 15], and Dias and Stewart [8] in a model of speciation in evolution. They have characterized expected symmetry breaking bifurcations and computed stability of the primary branches. There are several notable differences between our problems, which we will comment upon throughout the paper. Most importantly, the space on which the group S_N acts in our case, is essentially the vector space $\mathbf{R}^{NK}$, while in the speciation model it is $\mathbf{R}^N$. The immediate consequence is that the function f in (1) is not constrained in any way by the action of S_N. Therefore, the invariant theory for S_N, developed in Golubitsky and Stewart [18], is not applicable to our case. On the other hand, the form (1) of our functions rules out quadratic terms of the form $(q^\nu)^T q^\eta$, for $\nu \neq \eta$, in the function F, which are generically present in S_N-invariant vector fields on $\mathbf{R}^N$ [18, 40].

An additional difference is that our problem is constrained and therefore we will work with the Lagrangian which incorporates these constraints. There is an interesting parallel on this point with the speciation problem. If S_N acts on $\mathbf{R}^N$, then $\mathbf{R}^N$ admits an isotypic decomposition $V_0 \oplus V_1$ where V_0 is a one dimensional subspace consisting of multiples of $(1, 1, \dots, 1)$ and $V_1 = \{x \in \mathbf{R}^N | x_1 + \cdots + x_N = 0\}$. If at the bifurcation the kernel of the Jacobian lies in V_1, then one observes a symmetry breaking bifurcation. If this kernel lies in V_0 then one observes a symmetry preserving bifurcation. In our case, at a symmetry breaking bifurcation, we observe that all of the bifurcating directions u satisfy $u^1 + \cdots + u^N = 0$, but this time each $u^i \in \mathbf{R}^K$. This is a consequence of enforcing the constraint $q \in \Delta$. We will show that at a symmetry preserving bifurcation the constraints are active and so the bifurcating direction is in the span of vectors perpendicular to parts of the constraint space.

Our results differ in several aspects from those obtained by Stewart and collaborators. Most importantly, we show that the quadratic part of the Liapunov–Schmidt reduction at a symmetry breaking bifurcation vanishes, while in the speciation model, the quadratic part is generically nonzero [18, 40]. This implies that symmetry breaking bifurcations of (1) are generically degenerate and pitchfork-like. As explained above, since the restrictions imposed by the action of S_N on our system are less severe than in the speciation model, we did not obtain a stability result for bifurcating branches as general as that of Elmhirst [14, 15]. However, we provide a *bifurcation discriminator* in terms of the function f, which determines whether the pitchfork-like bifurcation is subcritical or supercritical. We also derive several results about the stability of these bifurcating branches.

Our numerical observations suggest that the stable branches of solutions follow a predictable pattern as the bifurcation parameter β increases. In particular, the symmetry of the stable branch follows the pattern $S_N \to S_{N-1} \to \cdots \to S_2 \to S_1$ as $\beta \to \infty$. More precisely, there are intervals $[a_n, b_n]$ for $n = 1, \dots, N$, such that $0 = a_N, a_n < a_{n-1}, b_n < b_{n-1}$ for all $n, b_1 = \infty$, with the property that if $\beta \in [a_n, b_n]$ then the branch of stable equilibria has symmetry S_n. Notice that two consecutive intervals $[a_n, b_n]$ and $[a_{n-1}, b_{n-1}]$ can overlap, since it is possible to have multiple branches stable for the same value of β due to existence of subcritical bifurcations. We do not observe numerically stable branches with symmetry $S_m \times S_n$ for $m > 1, n > 1$ and $m + n = N$, which play a crucial role in the speciation model, where they represent the assignment of m members of the original population to one new species and n members to another new species. We do not have an analytic explanation of this discrepancy since we do not have a complete characterization of the stability of the bifurcating branches for (1).

The paper is organized in the following way. In the rest of the introduction, we present problems from neuroscience and computer science which motivate our study. In Section 1.3 we illustrate an optimization procedure to solve problem (2) on a simple data set which exhibits the observed bifurcation structure. Preliminaries occupy Section 2. Section 3 is devoted to preparations for application of the theory of S_N-equivariant bifurcations. We define the generic class of problems which we investigate, introduce the gradient flow of the Lagrangian of (1), discuss the action of the group S_N on Δ, and perform the Liapunov–Schmidt reduction. Sections 4, 5, and 6 are the central part of the paper. In Section 4 we present existence theorems for bifurcating branches, and we derive a condition which determines whether branches with a given symmetry are supercritical or subcritical. In Section 5 we explain why we observe only a limited number of bifurcations. We will show that if an equilibrium of the gradient flow has trivial symmetry, then generically it can undergo only a saddle-node bifurcation. This result is a consequence of the interplay between the S_N-equivariant flow and the geometry of the space Δ. We put the results from Sections 4 and 5 together in Section 6. In Section 7 we present some numerical illustrations of our results.

1.1. The Neural Coding Problem

How does an organism's sensory system represent information about environmental stimuli? The Information Distortion method [9, 10, 16] attempts to decipher the neural code by solving a problem of the form (2). We consider the neural encoding process in a probabilistic framework [1, 25, 33]. Let X be a random variable (possibly continuous) of inputs or environmental stimuli. Let Y be a random variable of $K < \infty$ outputs or of neural responses, from either a single sensory neuron, or a neural ensemble. The relationship between the stimulus and response is given by the joint probability $p(X, Y)$, which we call a neural code. We seek to describe this probability distribution.

One of the major obstacles facing neuroscientists as they try to describe the neural code is that of having only limited data [24]. The limited data problem makes a nonparametric determination of $p(X, Y)$ impossible [30], and makes parametric estimations tenuous at best. One way to make parametric estimations more feasible is to optimally cluster the neural responses Y into N classes, $\mathscr{Z} = \{\nu_i\}_{i=1}^{N}$, and then to fit a Gaussian model to $p(X|\nu)$ for each class ν. This is the approach used by the Information Distortion method [9, 10, 16] to find a neural coding scheme [11, 12]. The optimal clustering $q^*(Z|Y)$ of the neural responses is obtained by minimizing the *information distortion measure* D_I,

$$\min_{q \in \Delta} D_I(q), \tag{4}$$

where Δ is the convex set of discrete conditional probabilities,

$$\Delta := \left\{ q(Z|Y) | \sum_{\nu \in \mathscr{Z}} q(\nu|y) = 1 \text{ and } q(\nu|y) \geqslant 0 \ \forall y \in \mathscr{Y} \right\}.$$

That is, the clustering of the neural responses Y to the classes Z is allowed to be stochastic, and it is defined by the $N \times K$ matrix $q(Z|Y)$. Before explicitly defining D_I, we first introduce the concept of the *mutual information* between X and Y, denoted by $I(X; Y)$, which is the amount of information that one can learn about X by observing Y [7],

$$I(X; Y) = E_{X,Y} \log \frac{p(X, Y)}{p(X)p(Y)},$$

where $E_{X,Y}$ denotes expectation with respect to *(X, Y)*. The information distortion measure can now be defined as

$$D_I(q) := I(X; Y) - I(X; Z),$$

which can be shown [16] to be the expected Kullback–Leibler divergence [26]

$$D_I(q(Z|Y)) = E_{Y,Z} KL(p(X|Y) \parallel p(X|Z)) > 0$$

when $X \leftrightarrow Y \leftrightarrow Z$ is a Markov chain.

Thus, to minimize D_I, one must assure that the mutual information between the stimuli X and the clusters Z is as close as possible to the mutual information between X and the original neural responses Y. Since $I(X; Y)$ is a fixed quantity, if we let $D_{\text{eff}} := I(X; Z)$, then the problem (4) can be rewritten as

$$\max_{q \in \Delta} D_{\text{eff}}(q). \tag{5}$$

Observe that we write D_{eff} as a function of the clustering q, where we write $q(Z=\nu|Y=y_k)$ as $q_{\nu k}$,

$$D_{\text{eff}}(q)=I(X;Z) = E_{X,Z} \log \frac{p(X,Z)}{p(X)p(Z)}$$
$$= \sum_{\nu,k,i} q_{\nu k} p(x_i, y_k) \log \left(\frac{\sum_k q_{\nu k} p(x_i, y_k)}{p(x_i) \sum_k p(y_k) q_{\nu k}} \right). \quad (6)$$

As we have mentioned in the introduction, the problem (5) is NP-complete [28]. Furthermore, since D_{eff} is convex and Δ is a convex domain [16], there are many local, suboptimal maxima on the boundary of Δ, which makes solving (5) difficult using many numerical optimization techniques. To deal with this issue, the Information Distortion method introduces a strictly concave function, *H(q)*, to maximize simultaneously with D_{eff}, which serves to regularize the problem (5) [34],

$$\max_{q \in \Delta} H(q) \quad \text{constrained by} \quad D_{\text{eff}}(q) \geqslant I_0, \quad (7)$$

where $I_0 > 0$ is some *minimal information rate*. The function $H(q) := H(Z|Y)$, *the conditional entropy* of the classes given the neural responses, is a function of $q(Z|Y)$

$$H(Z|Y) = -E_{Y,Z} \log_q (Z|Y)$$
$$= -\sum_{\nu,k} p(y_k) q_{\nu k} \log(q_{\nu k}). \quad (8)$$

Thus, of all the local solutions q^* to (5), we choose the ones which satisfy (7) and maximize the entropy. Using the entropy as a regularizer, as in the Deterministic Annealing approach to clustering [34], is justified by Jayne's maximum entropy principle, which states that among all clusterings that satisfy a given set of constraints, the maximum entropy clustering does not implicitly introduce additional constraints in the problem [23].

Using the method of Lagrange multipliers, the problem (7) is commonly rewritten as

$$\max_{q \in \Delta} (H(q) + \beta D_{\text{eff}}(q)), \quad (9)$$

for some $\beta \in [0, \infty)$, whose solutions are always solutions of (7). This is a problem of type (2), where $G = H(q)$ has a unique maximum.

1.2. Rate Distortion and Clustering

The second source of motivation for study of the problem (2) is from Rate Distortion Theory [7]. Rate Distortion Theory provides a rigorous way to determine how well a particular set of code words (or centers of clusters) $Z = \{\nu_i\}$ represents the original data $Y = \{y_i\}$ by defining a cost function, $D(Y; Z)$, called a *distortion function*. The basic question addressed by Rate Distortion Theory is that, when compressing the data Y, what is the minimum informative compression, Z, that can occur given a particular distortion $D(Y; Z) \leqslant D_0$[7]? This question is answered for independent and identically distributed data by the Rate Distortion Theorem [7], which states that the minimum compression is found by solving the *minimal information problem*

$$\min_{q\in\Delta} I(Y; Z) \quad \text{constrained by} \quad D(Y; Z) \leqslant D_0, \tag{10}$$

where $D_0 > 0$ is some maximum distortion level.

The Information Bottleneck method is a clustering algorithm which has used this framework for document classification, gene expression, neural coding [35], and spectral analysis [37, 38, 41]. It uses the information distortion measure D_I, defined in Section 1.1. This leads to an optimal clustering q^* of the data Y by solving

$$\min_{q\in\Delta} I(Y; Z) \quad \text{constrained by} \quad D_I \leqslant D_0.$$

Since $I(X; Y)$ is fixed, this problem can be rewritten as

$$\max_{q\in\Delta} -I(Y; Z) \quad \text{constrained by} \quad D_{\text{eff}} \geqslant I_0.$$

Now the method of Lagrange multipliers gives the problem

$$\max_{q\in\Delta}(-I(Y; Z) + \beta D_{\text{eff}}(q)), \tag{11}$$

for some $\beta \in [0, \infty)$, which is of the form given in (2). In this case, $G = -I(Y; Z)$ is not strictly concave, and has uncountably many maxima. In fact, the Hessian $\mathrm{d}^2 F(q, \beta) = \mathrm{d}^2(-I(Y; Z) + \beta D_{\text{eff}})$ is singular for every value of (q, β).

1.3. Annealing

In order to motivate our study of the bifurcation structure of (1) we now numerically illustrate the annealing procedure for a simple data set. These results [10, 16] served as the starting point of our effort to both improve the numerical algorithm used to obtain these solutions and to understand the underlying structure of the bifurcations.

A basic *annealing* algorithm, various forms of which have appeared in [10, 16, 34, 38, 41], can be used to solve (2) (which includes the cases (9) and (11)) for $\beta \in [0, \infty)$.

Algorithm 1 (Basic Annealing). Let *q_o be the maximizer of* $\max_{q\in\Delta} G(q)$ *and let* $\beta_0 = 0, \beta_{\max} > 0$. *For* $k \geqslant 0$, *let* (q_k, β_k) *be a solution to* (2). Iterate the following steps until $\beta_{\mathscr{K}} = \beta_{\max}$ for some $\mathscr{K}$.

(1) *Perform* β*-step*: Let $\beta_{k+1} = \beta_k + d_k$, *where* $d_k > 0$.
(2) *Take* $q_{k+1}^{(0)} = q_k + \eta$, *where* η *is a small perturbation, as an initial guess for the solution* q_{k+1} at β_{k+1}.
(3) *Optimization: solve*

$$\max_{q\in\Delta}(G(q) + \beta_{k+1} D(q))$$

to get the maximizer $q_k + 1$, *using initial guess* $q_{k+1}^{(0)}$.

The purpose of the perturbation in step 2 of the algorithm is due to the fact that a solution q_{k+1} may get "stuck" at a suboptimal solution q_k. The goal is to perturb $q_{k+1}^{(0)}$ outside of the basin of attraction of q_k.

The algorithm which we use to illustrate our results in Section 7 is more sophisticated [31, 32]. We use numerical continuation algorithms based on pseudo-arclength continuation [2, 13] applied to the gradient flow of the Lagrangian. While the basic algorithm can only find local maxima of (2), the continuation algorithm can track any stationary point of (2), which are equilibria of the gradient flow.

We now examine the results of the Basic Algorithm applied to (9) with the synthetic data set $p(X,Y)$, shown in Figure 1(a). This distribution was drawn from a mixture of four Gaussians as the authors did in [10, 16]. In this model, we may assume that $X = \{x_i\}_{i=1}^{52}$ represents a range of possible stimulus properties and that $Y = \{y_i\}_{i=1}^{52}$ represents a range of possible neural responses. There are four *modes* in $p(X,Y)$, where each mode corresponds to a range of responses elicited by a range of stimuli. For example, the stimuli $\{x_i\}_{i=1}^{11}$ elicit the responses $\{y_i\}_{i=39}^{52}$ with high probability, and the stimuli $\{x_i\}_{i=24}^{37}$ elicit the responses $\{y_i\}_{i=22}^{38}$ with high probability. One would expect that the maximizer q^* of (9) will cluster the neural responses $\{y_i\}_{i=1}^{52}$ into four classes, each of which corresponds to a mode of $p(X,Y)$. This intuition is justified by the Asymptotic Equipartition Property for jointly typical sequences [7]. For this analysis we used the joint probability $p(X,Y)$ explicitly to evaluate $H(q) + \beta D_{\text{eff}}(q)$, as opposed to modelling

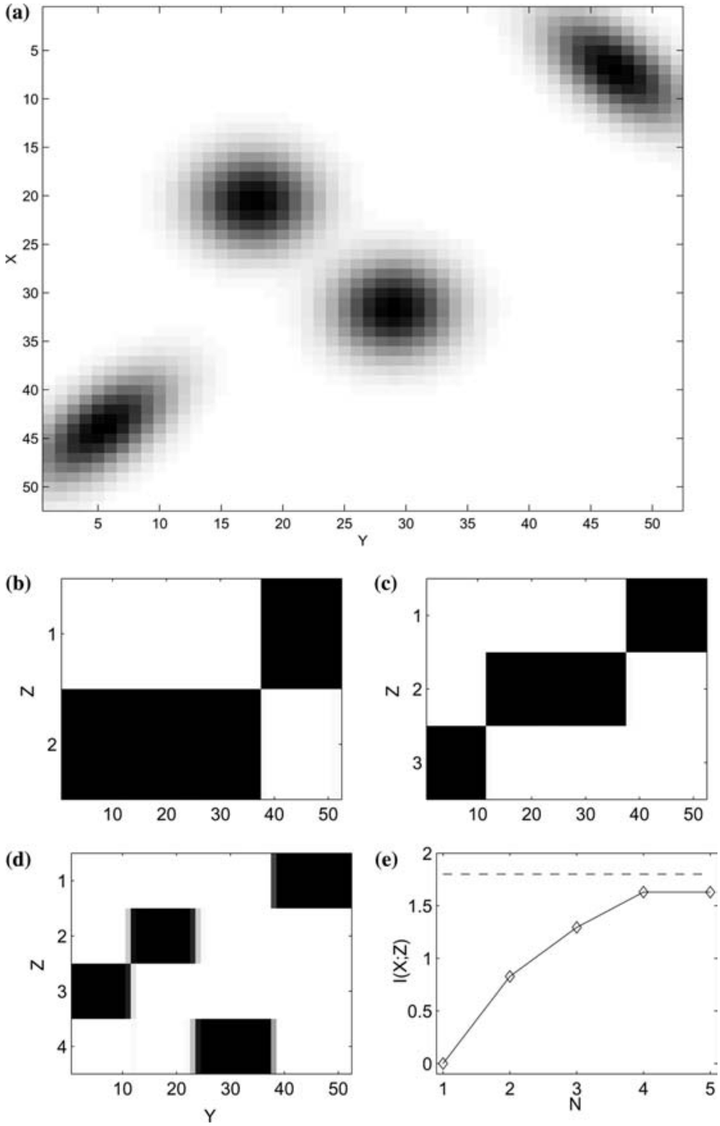

Figure 1. *The Four Blob Problem* from [10, 16]. (a) A joint probability $p(X,Y)$ between a stimulus set X and a response set Y, each with 52 elements (b–d). The optimal clusterings $q^*(Z|Y)$ for N = 2, 3, and 4 classes, respectively. These panels represent the conditional probability $q(\nu|y)$ of a response y being classified to class ν. White represents $q(\nu|y) = 0$, black represents $q(\nu|y) = 1$, and intermediate values are represented by levels of gray. Observe that the data naturally splits into four clusters because of the four modes of $p(X, Y)$ depicted in panel (a). The behavior of the effective distortion $D_{\text{eff}} = 1(X; Z)$ with increasing N can be seen in (e). The dashed line is $I(X; Y)$, which is the least upper bound of $I(X; Z)$.

$p(X,Y)$ by $p(X,Z)$ as explained in Section 1.1. The Basic Annealing Algorithm was run for $0 \leqslant \beta \leqslant 2$.

The optimal clustering $q^*(Z|Y)$ for $N = 2$, 3, and 4 is shown in panels (b)–(d) of Figure 1. We denote Z by the natural numbers, $Z \in \mathscr{Z} = \{1, \ldots, N\}$. When $N = 2$ as in panel (b), the optimal clustering q^* yields an incomplete description of the relationship between stimulus and response, in the sense that the responses $\{y_i\}_{i=1}^{37}$ are in class 2 and the responses $\{y_i\}_{i=38}^{52}$ are in class 1. The representation is improved for the $N = 3$ case shown in panel (c) since now $\{y_i\}_{i=1}^{11}$ are in class 3, while the responses $\{y_i\}_{i=12}^{37}$ are still lumped together in the same class 2. When $N = 4$ as in panel (d), the elements of Y are separated into the classes correctly. The mutual information in (e) increases with the number of classes approximately as $\log_2 N$ until it recovers about 90% of the original mutual information (at $N = 4$), at which point it levels off.

The action of S_N on the clusterings q can be seen in Figure 1 in any of the panels (b)–(d). Permuting the numbers on the vertical axis just changes the labels of the classes $\mathscr{Z} = \{1, \ldots, N\}$, and does not alter the effective clustering of the data Y. The S_N-invariance of the cost function (9) is based upon the observation that the action of S_N on q does not affect the value of the cost function.

It has been observed that the solutions (q, β) of (2), which contain the sequence $\{(q_k, \beta_k)\}$ found in step 3 of Algorithm 1, undergo *bifurcations* as β increases [10, 16, 34, 38, 41]. The explicit form of some of these solutions about bifurcation points for the Information Distortion problem (9) are given in Figure 2. The behavior of D_{eff} as a function of β can be seen in the top panel. Some of the solutions $\{(q_k, \beta_k)\}$ for different values of β_k are presented on the bottom row (panels 1–6). Panel 1 shows the uniform clustering, denoted by $q_{\frac{1}{N}}$, which is defined componentwise by

$$q_{\frac{1}{N}}(\nu|y_k) := \frac{1}{N}$$

for every ν and k. One can observe the bifurcations of the solutions (1–5) and the corresponding transitions of D_{eff}. The abrupt transitions ($1 \to 2, 2 \to 3$) are similar to the ones described in [34] for a different distortion function. One also observes transitions ($4 \to 5$) which appear to be smooth in D_{eff} even though the solution from q_k to q_{k+1} seems to undergo a bifurcation.

Figure 2 illustrates the breakdown in symmetry, referred to in the introduction by the chain of subgroups

$$S_4 \to S_3 \to S_2 \to S_1,$$

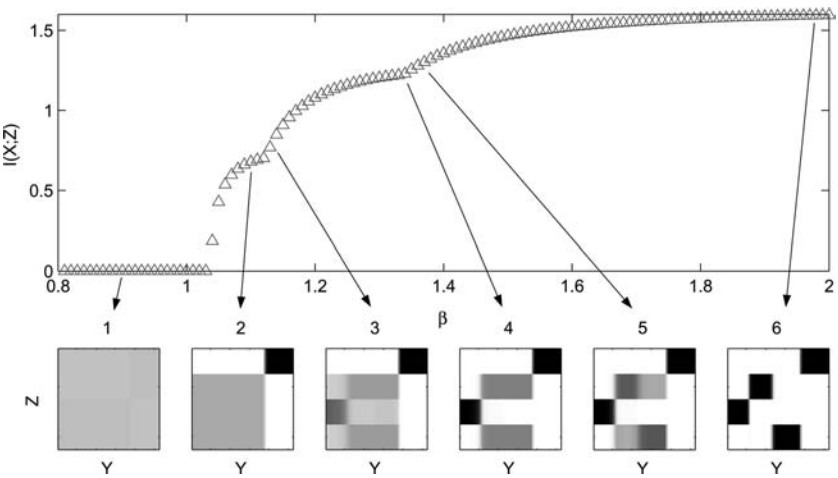

Figure 2. The bifurcations initially observed by Dimitrov and Miller in [10] of the solutions (q^*, β) to the Information Distortion problem (9). For the data set in Figure 1(a). the behavior of $D_{\text{eff}} = I(X; Z)$ as a function of β is shown in the top panel, and some of the solutions $q(Z|Y)$ are shown in the bottom panels.

which we tend to observe numerically when annealing with an algorithm which is affected by the stability of the solution branches. The first solution branch, $(q_{\frac{1}{N}}, \beta)$ shown in panel 1 of Figure 2, has symmetry of the full group S_4. In other words, $q_{\frac{1}{N}}$ is invariant to relabelling of all 4 classes. After bifurcation occurs on this branch, we see in panel 2 a solution with symmetry S_3. In panels 3 and 4, we illustrate solutions with symmetry S_2. The clusterings q depicted in panels 5 and 6 are no longer invariant to permutations of the class labels, and so we say that these have symmetry S_1.

The bifurcation structure outlined in Figure 2 raises some interesting questions. Why are there only three bifurcations observed? In general, are there only $N - 1$ bifurcations observed when one is clustering into N classes? In Figure 2, observe that $q \in \mathbf{R}^{4K} = \mathbf{R}^{208}$. Why should we observe only 3 bifurcations to local solutions of $H + \beta D_{\text{eff}}$ in such a large dimensional space? What types of bifurcations should we expect: pitchfork-like, transcritical, saddle-node, or some other type? At a bifurcation, how many bifurcating branches are there? What do the bifurcating branches look like: are they *subcritical or supercritical*? What is the stability of the bifurcating branches? In particular, from bifurcation of a solution, is there always a bifurcating branch which contains solutions of the original optimization problem?

These are the questions which motivated this paper.

2. PRELIMINARIES

2.1. Notation

The following notation will be used throughout the paper:

Y := a random variable with realizations from a finite set $\mathcal{Y} := \{y_1, y_2, \ldots, y_K\}$.
$K := |\mathcal{Y}| < \infty$, the number of elements of $\mathcal{Y}$, the realizations of the random variable Y.
Z := a random variable with realizations from the *set of classes* $\mathcal{Z} := \{1, 2, \ldots, N\}$.
$N := |\mathcal{Z}|$, the total number of classes.
$q(Z|Y)$:= the $K \times N$ matrix, $p(Z|Y)$, defining the conditional probability mass function of the random variable $Z|Y$, written explicitly as

$$\begin{pmatrix} q(1|y_1) & q(1|y_2) & q(1|y_3) & \ldots & q(1|y_K) \\ q(2|y_1) & q(2|y_2) & q(2|y_3) & \ldots & q(2|y_K) \\ \vdots & \vdots & \vdots & & \vdots \\ q(N|y_1) & q(N|y_2) & q(N|y_3) & \ldots & q(N|y_K) \end{pmatrix} = \begin{pmatrix} q(1|Y)^T \\ q(2|Y)^T \\ \vdots \\ q(N|Y)^T \end{pmatrix} = \begin{pmatrix} (q^1)^T \\ (q^2)^T \\ \vdots \\ (q^N)^T \end{pmatrix}. \tag{12}$$

where $q^\nu := q(Z = \nu|Y)$ is the transpose of the $1 \times K$ row of $q(Z|Y)$ corresponding to the class $\nu \in \mathcal{Z}$.
q := the vectorized form of $q(Z|Y)^T$, written as

$$q = ((q^1)^T (q^2)^T \ldots (q^N)^T)^T.$$

$q_{\nu k} := q(Z = \nu | Y = y_k)$, the component of q corresponding to the class $\nu \in \mathcal{Z}$ and the element $y_k \in \mathcal{Y}$.
$q_{\frac{1}{N}}$:= the uniform probability mass function on $Z|Y$ such that $q_{\frac{1}{N}}(\nu|y_k) = 1/N$ for every ν and k.
$\boldsymbol{x}^\nu$:= the νth $K \times 1$ vector component of $\boldsymbol{x} \in \mathbf{R}^{NK}$, so that $\boldsymbol{x} = ((\boldsymbol{x}^1)^T (\boldsymbol{x}^2)^T \ldots (\boldsymbol{x}^N)^T)^T$.
$I_n := n \times n$ identity matrix.

2.2. Equivariant Branching Lemma

In this section, we present the Equivariant Branching Lemma, an existence theorem for bifurcating branches from solutions of systems which have symmetry. Consider bifurcations of equilibria of some dynamical system,

$$\dot{\boldsymbol{x}} = \phi(\boldsymbol{x}, \beta), \tag{13}$$

where $\phi : V \times \mathbf{R} \to V$ for some Banach space V. If ϕ is G-equivariant for some compact Lie group G, then the Equivariant Branching Lemma relates the subgroup structure of G with the existence of bifurcating branches of equilibria of (13). This theorem is attributed to Vanderbauwhede [42] and Cicogna [3, 4].

Theorem 2. *(Equivariant Branching Lemma) ([19] p.83) Assume that*

(1) The smooth function $\phi : V \times \mathbf{R} \to V$ from (13) is G-equivariant for a compact Lie group G, and a Banach space V.
(2) The Jacobian $\mathrm{d}_{\boldsymbol{x}}\phi(\mathbf{0}, 0) = \mathbf{0}$.
(3) The group G acts absolutely irreducibly on ker $\mathrm{d}_{\boldsymbol{x}}\phi(\mathbf{0}, 0)$, so that $\mathrm{d}_{\boldsymbol{x}}\phi(\mathbf{0}, \beta) = c(\beta)I$ for some scalar valued function $c(\beta)$.
(4) The derivative $c'(0) \neq 0$.
(5) The subgroup H is an isotropy subgroup of G with dim $\mathrm{Fix}(H) = 1$.

Then there exists a unique smooth solution branch $(t\boldsymbol{x}_0, \beta(t))$ to $\phi = \mathbf{0}$ such that $\boldsymbol{x}_0 \in \mathrm{Fix}(H)$, and the isotropy subgroup of each solution is H.

Definition 3. [19]. The branch $(t\boldsymbol{x}_0, \beta(t))$ is transcritical if $\beta'(0) \neq 0$. If $\beta'(0) = 0$ then the branch is degenerate. The branch is subcritical if for all nonzero t such that $|t| < \epsilon$ for some $\epsilon > 0, t\beta'(t) < 0$. The branch is supercritical if $t\beta'(t) > 0$.

Definition 4. The branch $(t\boldsymbol{x}_0, \beta(t))$ is pitchfork-like if $\beta'(0) = 0$ and $\beta''0) \neq 0$.

3. A GRADIENT FLOW WITH SYMMETRIES

We now lay the groundwork necessary to determine the bifurcation structure of local solutions to (1). We first formally define the class of problems we investigate. The choice of this class is motivated by application to the Information Distortion method (9). In that problem, the variables are conditional probabilities. The collection of variables *q(Z|Y)*, which can be represented as a matrix (12), satisfies the constraints $\sum_\nu q(\nu|y_k) = 1$ for all y_k. These can be viewed as sums in the columns of *q(Z|Y)*. This motivates the following definitions.

Let $\sum$ be a unit positive simplex in $\mathbf{R}^N$

$$\sum := \{x \in \mathbf{R}^N | x_1 + \cdots + x_N = 0, x_i \geqslant 0\}$$

and let $\Delta = \sum^K$ be a product of K copies of $\sum$. We write $q = ((q^1)^T (q^2)^T \cdots (q^N)^T)^T$ where each $q^\nu \in \mathbf{R}^K$ represents a collection of ν components in all K copies of $\sum$.

Let $\mathscr{G}$ be the set of all maps from Δ to $\mathbf{R}$, at least C^4 on Int(Δ), and continuous on Δ, which factors as a sum of maps over $\sum$

$$\mathscr{G} := \{g \in C^4(\mathrm{Int}(\Delta) \times \mathbf{R}^+, \mathbf{R}) | g(q, \beta)\} = \sum_{\nu=1}^{N} f(q^\nu, \beta),$$

where $\mathbf{R}^+$ is the nonnegative real line and β is a scalar parameter. The problem (2) is a special case of (1) that is of great interest in applications. We formulate the genericity result below for both problems and therefore we need the following class of functions. Let $\mathscr{H}$ be a set of functions

$$\mathscr{H} := \{g \in C^4(\mathrm{Int}(\Delta), \mathbf{R}) | g(q) = \sum_{\nu=1}^{N} f(q^\nu)\},$$

where $f : \mathbf{R}^k \to \mathbf{R}$. Let $\mathscr{X} := \mathscr{H} \times \mathscr{H}$. Each pair of functions $(G, D) \in \mathscr{H} \times \mathscr{H}$ defines a function

$$F_0(q, \beta) := G(q) + \beta D(q), \quad \beta \geqslant 0. \tag{14}$$

Clearly, $F_0 \in \mathscr{G}$ and

$$\bigcup_{(G,D) \in \mathscr{X}} (G + \beta D) \subset \mathscr{G}.$$

In other words, the set of problems parameterized by $\mathscr{G}$ is larger than that parameterized by $\mathscr{X}$. Most of the results we prove holds for the class $\mathscr{G}$, but a few depend on the special dependence on β in (14).

For the problem (1)

$$\max_{q \in \Delta} \quad F(q, \beta),$$

where $F = \sum_{\nu=1}^{N} f(q^\nu, \beta)$, which includes as a special case the annealing problem (2), F has the following properties:

(1) $F(q, \beta)$ is an S_N-invariant, real valued function of q, where the action of S_N on q permutes the component vectors $q^\nu, \nu = 1, \ldots, N$, of q.

(2) The $NK \times NK$ Hessian $\mathrm{d}_q^2 F(q,\beta)$ is block diagonal, where each $K \times K$ block is $\mathrm{d}^2 f(q^\nu) = \mathrm{d}_{q^\nu}^2 F$, for some ν.

The Lagrangian of (1) with respect to the equality constraints from Δ is

$$\mathscr{L}(q,\lambda,\beta) = F(q,\beta) + \sum_{k=1}^{K} \lambda_k \left(\sum_{\nu=1}^{N} q_{\nu k} - 1 \right). \tag{15}$$

The scalar λ_k is the Lagrange multiplier for the constraint $\sum_{\nu=1}^{N} q_{\nu k} - 1 = 0$, and $\lambda \in \mathbf{R}^K$ is the vector of Lagrange multipliers $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_K)^T$. The gradient of the Lagrangian in (15) is

$$\nabla \mathscr{L} := \nabla_{q,\lambda} \mathscr{L}(q,\lambda,\beta) = \begin{pmatrix} \nabla_q \mathscr{L} \\ \nabla_\lambda \mathscr{L} \end{pmatrix},$$

where $\nabla_q \mathscr{L} = \nabla F(q,\beta) + \Lambda$ and $\Lambda = (\lambda^T, \lambda^T, \ldots, \lambda^T)^T \in \mathbf{R}^{NK}$. The gradient $\nabla_\lambda \mathscr{L}$ is a vector of K constraints

$$\nabla_\lambda \mathscr{L} = \begin{pmatrix} \sum_\nu q_{\nu 1} - 1 \\ \sum_\nu q_{\nu 2} - 1 \\ \vdots \\ \sum_\nu q_{\nu K} - 1 \end{pmatrix}. \tag{16}$$

Let J be the Jacobian of (16)

$$J := \mathrm{d}_q \nabla_\lambda \mathscr{L} = \mathrm{d}_q \begin{pmatrix} \sum_\nu q_{\nu 1} - 1 \\ \sum_\nu q_{\nu 2} - 1 \\ \vdots \\ \sum_\nu q_{\nu K} - 1 \end{pmatrix} = \underbrace{(I_K \quad I_K \quad \ldots \quad I_K)}_{N \text{ blocks}}. \tag{17}$$

Observe that J has full row rank. The Hessian of (15) is

$$d^2 \mathscr{L}(q) := \mathrm{d}^2 \mathscr{L}(q,\lambda,\beta) = \begin{pmatrix} d^2 F(q,\beta) & J^T \\ J & \mathbf{0} \end{pmatrix}. \tag{18}$$

where $\mathbf{0}$ is $K \times K$. The matrix $\mathrm{d}^2 F$ is the block diagonal Hessian of F,

$$\mathrm{d}^2 F(q) := \mathrm{d}_q^2 F(q,\beta) = \begin{pmatrix} B_1 & \mathbf{0} & \ldots & \mathbf{0} \\ \mathbf{0} & B_2 & \ldots & \mathbf{0} \\ \vdots & \vdots & & \vdots \\ \mathbf{0} & \mathbf{0} & \ldots & B_N \end{pmatrix}, \tag{19}$$

where $\mathbf{0}$ and $B_\nu = \mathrm{d}^2 f(q^\nu, \beta)$ are $K \times K$ matrices for $\nu = 1, \ldots, N$.

The dynamical system whose equilibria are stationary points of (1) can now be posed as the gradient flow of the Lagrangian

$$\begin{pmatrix} \dot{q} \\ \dot{\lambda} \end{pmatrix} = \nabla \mathscr{L}(q, \lambda, \beta) \tag{20}$$

for $\mathscr{L}$ as defined in (15) and $\beta \in [0, \infty)$. The equilibria of (20) are points $\binom{q^*}{\lambda^*} \in \mathbf{R}^{NK+K}$, where

$$\nabla \mathscr{L}(q^*, \lambda^*, \beta) = 0.$$

The Jacobian of this system is the Hessian $d^2\mathscr{L}(q, \lambda, \beta)$ from (18). As in [17], we define a *singularity* of (20) to be an equilibrium $(q^*, \lambda^*, \beta^*)$ such that $\nabla \mathscr{L}(q^*, \lambda^*, \beta^*) = \mathbf{0}$ and $d^2\mathscr{L}(q^*, \lambda^*, \beta^*)$ is singular.

Remark 5. By the theory of constrained optimization [29], the equilibria (q^*, λ^*, β) of (20) where $d^2F(q^*, \beta)$ is negative definite, on ker J are local solutions of (1). Conversely, if (q^*, β) is a local solution of (1), then there exists a vector of Lagrange multipliers λ^* so that (q^*, λ^*, β) is an equilibrium of (20) (this necessary requirement is called the Karush-Kuhn-Tucker conditions) such that $d^2F(q^*, \beta)$ is non-positive definite on ker J.

3.1. A Generic Problem

The results of this paper are valid for a generic (i.e., open and dense) subset of the set $\mathscr{G}$ as well as for a generic subset of $\mathscr{X}$. Even though the set $\mathscr{G}$ is defined in terms of the function F, the nondegeneracy conditions, which define the generic set, are formulated in terms of the Hessian d^2F. Therefore we first define a set of admissible matrices and then require that the Hessian d^2F is in this class at every *critical point* of the Lagrangian $\mathscr{L}$: points where $\nabla \mathscr{L} = \mathbf{0}$, which correspond to equilibria of (20).

Let $\{\mathscr{U}_j\}_{j=l}^{l}$ be some partition (i.e., $\mathscr{U}_j \cap \mathscr{U}_i = \emptyset$ for $i \neq j$ and $\cup_{j=1}^{l} \mathscr{U}_j = \mathscr{Z}$) of the set of classes $\mathscr{Z} = \{1, \ldots, N\}$. Without loss of generality, we may assume that

$$\begin{aligned} \mathscr{U}_1 &= \{1, \ldots, M_1\}, \\ \mathscr{U}_2 &= \{M_1 + 1, \ldots, M_1 + M_2\}, \\ &\vdots \\ \mathscr{U}_1 &= \left\{ \sum_{j=1}^{l-1} M_j + 1, \ldots, \sum_{j=1}^{l} M_j \right\}, \end{aligned}$$

where $M_j := |\mathscr{U}_j|$ is the number of elements $\mathscr{U}_j$, so that $\sum_{j=1}^{l} M_j = N$.

Definition 6. Consider the class $\mathscr{T}$ of $NK \times NK$ block diagonal symmetric matrices U, where each square block $B_i, i = 1, \ldots, N$ has size K, and $B_i = B_k$, if and only if $i, k \in \mathscr{U}_j$ for some j. We denote by $\bar{B}_j$ a block common to the class $\mathscr{U}_j$, i.e., $\bar{B}_j = B_i$ for all $i \in \mathscr{U}_j$. If all matrices $\bar{B}_i$, for $i \neq j$ are nonsingular, we define the matrix A_j for each $j = 1, \ldots, l$ by

$$A_j := \bar{B}_j \sum_{i \notin \mathscr{U}_j} B_i^{-1} + M_j I_K. \tag{21}$$

If $\mathscr{U}_1 = \mathscr{Z}$, so that all of the blocks B_i are identical, then we define $A_1 = N I_K$.

Let $\mathscr{W} \subseteq \mathscr{T}$ be a class of matrices such that $U \in \mathscr{W}$ if and only if the following conditions are satisfied:

(1) At most one of the matrices $\bar{B}_1, \ldots, \bar{B}_l$ is singular.
(2) If $\bar{B}_j$ is singular then A_j is non-singular.
(3) If any matrix $\bar{B}_j$ is singular, or any matrix A_j is singular, the multiplicity of its zero eigenvalue is 1.

We are ready for our genericity result.

Theorem 7.

(1) There is an open and dense set $\mathscr{V} \subset \mathscr{X} = \mathscr{H} \times \mathscr{H}$ such that if $(G, D) \in \mathscr{V}$ then the Hessian

$$d^2 G(q) + \beta d^2 D(q) \in \mathscr{W}$$

for every critical point (q, λ, β) of $\mathscr{L}$, i.e., a point where $\nabla \mathscr{L} = \mathbf{0}$.

(2) There is an open and dense set $\mathscr{A} \subset \mathscr{G}$ such that if $F \in \mathscr{A}$ then the Hessian

$$d^2 F(q, \beta) \in \mathscr{W}$$

for every critical point (q, λ, β) of $\mathscr{L}$.

Proof. We first sketch the idea of the proof to part 1. We start by showing that the set $\mathscr{T} \backslash \mathscr{W}$ is a collection of manifolds of at least codimension 2 in $\mathscr{T}$. This implies that $(\mathscr{T} \backslash \mathscr{W}) \times [0, \infty)$ is a collection of manifolds of at least codimension 2 in $\mathscr{T} \times [0, \infty)$ Then we show that there is an open and dense set $\mathscr{O} \in \mathscr{X}$, such that if $(G, D) \in \mathscr{X}$, the critical points (q, λ, β) of the corresponding Lagrangian $\mathscr{L} = \mathscr{L}(G, D)$ form a finite collection of one dimensional manifolds in the space $\Delta \times [0, \infty)$. It follows that if $(G, D) \in \mathscr{O}$, then the set of matrices $\mathrm{d}^2 G(q) + \beta \mathrm{d}^2 D(q)$ that are evaluated at a critical point (q, λ, β) of the Lagrangian $\mathscr{L}$ forms a collection of one dimensional manifolds in the space $\mathscr{T} \times [0, \infty)$. For an open and dense subset $\mathcal{V} \subset \mathcal{O}$, these manifolds have an empty intersection with $(\mathcal{T} \backslash \mathcal{W}) \times [0, \infty)$, which consists of manifolds of at least codimension 2. This implies that for $(G, D) \in \mathcal{V} \subset \mathcal{X}$, the matrices $\mathrm{d}^2 G(q) + \beta \mathrm{d}^2 D(q)$ that are evaluated at a critical point (q, λ, β) of the Lagrangian $\mathcal{L}$, belong to $\mathcal{W}$.

To show that the set $\mathcal{T} \setminus \mathcal{W}$ is a collection of at least codimension 2 manifolds in $\mathcal{T}$, we start by characterizing the set $\mathcal{T} \setminus \mathcal{W}$. Let

$$\begin{aligned} J_{ij} &:= \{U \in \mathcal{T} \,|\, \bar{B}_j \text{ and } \bar{B}_i \text{ are singular}\}, \\ I_i &:= \{U \in \mathcal{T} \,|\, \bar{B}_i \text{ is singular and} A_i \text{ is singular}\}, \\ K_i &:= \{U \in \mathcal{T} \,|\, \bar{B}_i \text{ is singular with multiplicity } \geqslant 2\}, \\ L_i &:= \{U \in \mathcal{T} \,|\, A_i \text{ is singular with multiplicity} \geqslant 2\}. \end{aligned}$$

Clearly

$$\mathcal{T} \setminus \mathcal{W} \subset \bigcup_{ij} J_{ij} \cup \bigcup_{ij} I_{ij} \cup \bigcup_{i} K_i \cup \bigcup_{i} L_i .$$

Observe that $J_{ij} = \{U \in \mathcal{T} | \det(\bar{B}_j) = 0 \text{ and } \det(\bar{B}_i) = 0\}$ and $I_i = \{U \in \mathcal{T} | \det(\bar{B}_i) = 0 \text{ and } \det(A_i) = 0\}$ and so for any pair *i,j* these are at least codimension 2 submanifolds in $\mathcal{T}$. Similarly, $K_i = \{A \in \mathcal{T} \,|\, \bar{B}_i$ has a two-dimensional kernel$\}$ and L_i are at least codimension 2 submanifolds of $\mathcal{T}$. Therefore $\mathcal{T} \setminus \mathcal{W}$ is a subset of a collection of at least codimension 2 submanifolds of $\mathcal{T}$.

Let $\Upsilon : \mathcal{X} \to C^3(\mathbf{R}^{NK+K+1}, \mathbf{R}^{NK+K})$ be a continuous function associating

$$(G, D) \mapsto \nabla_{q,\lambda} \mathcal{L},$$

where $\nabla_{q,\lambda} \mathcal{L}$ is a function of (q, λ, β) and so the extra dimension in the domain of the map is the domain of β. By the Transversality theorem [21], for a typical (i.e., one which belongs to an open and dense set in a strong topology) $f \in C^3(\mathbf{R}^{NK+K+1}, \mathbf{R}^{NK+K})$, the inverse image $f^{-1}(0)$ is a collection of one-dimensional manifolds. Since Υ is continuous, the inverse image of an open and dense set in $C^3(\mathbf{R}^{NK+K+1}, \mathbf{R}^{NK+K})$ is open and dense in $\mathcal{X}$. We call this set $\mathcal{O}$. Taking $(G, D) \in \mathcal{O}$ and $f = \Upsilon(G, D)$ then $f^{-1}(0)$ is the set of critical points of the Lagrangian $\mathcal{L}$ and this set forms a collection of one-dimensional manifolds in $\Delta \times [0, \infty)$. Therefore for $(G, D) \in \mathcal{O}$ the set of matrices $\mathrm{d}^2 G(q) + \beta \mathrm{d}^2 D(q)$, evaluated at a critical point (q, λ, β) of the Lagrangian $\mathcal{L}$, forms a finite collection of one dimensional manifolds in the space $\mathcal{T} \times [0, \infty)$.

Note that $\mathcal{T} \setminus \mathcal{W} \times [0, \infty)$ is at least codimension 2 in $\mathcal{T} \times [0, \infty)$ and for $(G, D) \in \mathcal{O}$ and the set of matrices $\mathrm{d}^2 G(q) + \beta \mathrm{d}^2 D(q)$, evaluated at a critical point (q, λ, β) of the Lagrangian $\mathscr{L}$, is a collection of one-dimensional manifolds in $\mathscr{T} \times [0, \infty)$. Hence there is an open and dense subset $\mathscr{V} \subset \mathscr{O}$ such that for $(G, D) \in \mathscr{V}$, the intersection of $\mathscr{T} \setminus \mathscr{W} \times [0, \infty)$ and the set of matrices $d^2 G(q) + \beta d^2 D(q)$, evaluated at a critical point (q, λ, β) of the Lagrangian $\mathscr{L}$, is empty.

The proof of 2 is analogous to the proof of 1. We replace the set $\mathscr{X}$ by the set $\mathscr{G}$ and instead of $(G, D) \in \mathscr{O}$ we need to consider $F \in \mathscr{O}$. □

From this point on we will use the term "generic" always to refer to the set $\mathscr{A}$ in Theorem 7, unless otherwise noted.

We now consider bifurcations of equilibria of the gradient flow (20) for a generic function $F(q, \beta)$. The potential bifurcation points are singularities: points $(q^*, \lambda^*, \beta^*)$, where $\nabla \mathscr{L}(q^*, \lambda^*, \beta^*) = \mathbf{0}$ and $d^2 \mathscr{L}(q^*, \lambda^*, \beta^*)$ is singular.

Assume that (q, λ) is an equilibrium with a partition $\{\mathscr{U}_j\}_{j=1}^{l}$ of the set $\mathscr{Y}$ such that $q^i = q^k$ if and only if i and k belong to same partition set $\mathscr{U}_j$. For example, in panel 2 of Figure 2, $\mathscr{U}_1 = \{1\}, \mathscr{U}_2 = \{2, 3, 4\}$, and $q^2 = q^3 = q^4$. The Hessian $d^2 F(q^*)$ evaluated at such a point q has equal blocks, $B_i = B_k$, if $i, k \in \mathscr{U}_j$. What happens if such an equilibrium becomes a singularity of (20)? By Theorem 7, then there are two cases:

(1) Either there is exactly one j such that $\bar{B}_j$ is singular; or
(2) All $\bar{B}_j$ are nonsingular.

We assume without loss of generality that $j = 1$. We will show that in the first case, when $\bar{B}_1$ is singular and $|\mathscr{U}_1| > 1$, we get a symmetry breaking bifurcation (Theorem 17). Generically, $|\mathscr{U}_1| \neq 1$ at a singularity (Corollary 12). In the second case we get a symmetry preserving bifurcation (Theorem 29).

We start considering the first case. To ease the notation we set

$$\mathscr{U} := \mathscr{U}_1, \quad M := M_1, \quad \mathscr{R} := \bigcup_{j=2}^{l} \mathscr{U}_j.$$

Thus,

$$\mathscr{U} = \{1, \ldots, M\} \quad \text{and} \quad \mathscr{R} = \{M+1, \ldots, N\}.$$

We need to distinguish between singular blocks $B_\nu, \nu \in \mathscr{U}$ and non-singular blocks $B_\nu, \nu \in \mathscr{R}$. We will write

$$B := \overline{B}_1 = B_\nu \quad \text{for} \quad \nu \in \mathscr{U}. \tag{22}$$

$$R_\nu := B_\nu \quad \text{for} \quad \nu \in \mathscr{R}. \tag{23}$$

The type of symmetry breaking bifurcation we get from a singularity $(q^*, \lambda^*, \beta^*)$ only depends on the number of blocks B which are singular. This motivates the following definition.

Definition 8. An equilibrium of (20) (q, λ, β), where $q^1 = q^2 = \cdots = q^M$, is M-singular if $|\mathcal{U}| = M$ and B is singular.

If (q, λ, β) is an M-singular equilibrium of (20), we will say that q is M singular. By Theorem 7, for a generic F, the following properties hold if q is M-singular:

(1) $q^1 = q^2 = \cdots = q^M$.
(2) For B, the M block(s) of the Hessian defined in (22),

$$\ker B \text{ has dimension 1 with basis vector } \boldsymbol{\upsilon} \in \mathbf{R}^K. \tag{24}$$

(3) The $N - M$ block(s) of the Hessian $\{R_\nu\}_{\nu \in \mathcal{R}}$, defined in (23), are nonsingular.
(4) The matrix $A = B \sum_\nu R_\nu^{-1} + M I_K$ is nonsingular. When $M = N$, then $\mathcal{R}$ is empty, and $A = N I_K$.

3.2. The Kernel of the Hessian $d^2\mathcal{L}(q^*)$at an M-singular q^*

We first determine a basis for $\ker d^2 F(q^*)$ at an M-singular q^*. Recall that in the preliminaries, when $\boldsymbol{x} \in \mathbf{R}^{NK}$, we defined $\boldsymbol{x}^\nu \in \mathbf{R}^K$ to be the ν^{th} vector component of $\boldsymbol{x}$. We now define the linearly independent vectors $\{\boldsymbol{v}_i\}_{i=1}^M$ in $\mathbf{R}^{NK}$ by

$$\boldsymbol{\upsilon}_i^\nu := \begin{cases} \boldsymbol{\upsilon} & \text{if } \nu = i \in \mathcal{U}, \\ \mathbf{0}, & \text{otherwise,} \end{cases} \tag{25}$$

where $\mathbf{0} \in \mathbf{R}^K$, and $\boldsymbol{\upsilon}$ is defined in (24). For example, if $N = 3$ with $\mathcal{U} = \{1, 2\}$ and $\mathcal{R} = \{3\}$, then $\boldsymbol{\upsilon}_1 := (\boldsymbol{\upsilon}^T, \mathbf{0}, \mathbf{0})^T$and $\boldsymbol{\upsilon}_2 := (\mathbf{0}, \boldsymbol{\upsilon}^T, \mathbf{0})^T$. This shows the following:

Lemma 9. *If q^* is M-singular, then $\{\boldsymbol{\upsilon}_i\}_{i=1}^M$ as defined in (25) is a basis for* $\ker d^2 F(q^*)$.

Now, let

$$\boldsymbol{w}_i = \begin{pmatrix} \boldsymbol{\upsilon}_i \\ \mathbf{0} \end{pmatrix} - \begin{pmatrix} \boldsymbol{\upsilon}_M \\ \mathbf{0} \end{pmatrix} \tag{26}$$

for $i = 1, \ldots, M - 1$, where $\mathbf{0} \in \mathbf{R}^K$. From (18), it is easy to see that $\{\boldsymbol{w}_i\}$ are in $\ker d^2\mathcal{L}(q^*)$, which proves the following lemma.

Lemma 10. *If* $\mathrm{d}^2F(q^*)$ *is singular at an* M*-singular* q^* *for* $1<M\leqslant N$, *then* $\mathrm{d}^2\mathscr{L}(q^*)$ *is singular.*

Next we give an explicit basis for $\ker \mathrm{d}^2\mathscr{L}(q^*)$.

Theorem 11. *If* q^* *is* M*-singular for* $1<M\leqslant N$, *then* $\{\boldsymbol{w}_i\}_{i=1}^{M-1}$ *from (26) are a basis for* $\ker \mathrm{d}^2\mathscr{L}(q^*)$.

Proof. To show that $\{\boldsymbol{w}_i\}$ span $\ker \mathrm{d}^2\mathscr{L}(q^*)$, let $\boldsymbol{k}\in\ker \mathrm{d}^2\mathscr{L}(q^*)$ and decompose it as

$$\boldsymbol{k}=\begin{pmatrix}\boldsymbol{k}_F\\ \boldsymbol{k}_J\end{pmatrix}, \tag{27}$$

where $\boldsymbol{k}_F$ is $NK\times 1$ and $\boldsymbol{k}_J$ is $K\times 1$. Hence

$$\begin{aligned}\mathrm{d}^2\mathscr{L}(q^*,\lambda^*,\beta)\boldsymbol{k} &= \begin{pmatrix}\mathrm{d}^2F(q^*,\beta^*) & J^T\\ J & \mathbf{0}\end{pmatrix}\begin{pmatrix}\boldsymbol{k}_F\\ \boldsymbol{k}_J\end{pmatrix}=0\\ &\Rightarrow \mathrm{d}^2F(q^*,\beta)\boldsymbol{k}_F=-J^T\boldsymbol{k}_J\\ &\quad\; J\boldsymbol{k}_F=0.\end{aligned} \tag{28}$$

Now, from (17) and (19), we have

$$\begin{pmatrix}B_1 & \mathbf{0} & \dots & \mathbf{0}\\ \mathbf{0} & B_2 & \dots & \mathbf{0}\\ \vdots & \vdots & & \vdots\\ \mathbf{0} & \mathbf{0} & \dots & B_N\end{pmatrix}\boldsymbol{k}_F=-\begin{pmatrix}\boldsymbol{k}_J\\ \boldsymbol{k}_J\\ \vdots\\ \boldsymbol{k}_J\end{pmatrix}. \tag{29}$$

We set

$$\boldsymbol{k}_F:=(\boldsymbol{x}_1^T\,\boldsymbol{x}_2^T\cdots\boldsymbol{x}_N^T)^T \tag{30}$$

and using the notation from (22) and (23), then (29) implies

$$\begin{aligned}B\boldsymbol{x}_\eta&=-\boldsymbol{k}_J\quad \text{for } \eta\in\mathscr{U},\\ R_\nu\boldsymbol{x}_\nu&=-\boldsymbol{k}_J\quad \text{for } \nu\in\mathscr{R}.\end{aligned} \tag{31}$$

It follows that $\boldsymbol{x}_\nu=R_\nu^{-1}B\boldsymbol{x}_\eta$ for any $\eta\in\mathscr{U}$. By (28), we have that $\sum_{i=1}^N\boldsymbol{x}_i=\mathbf{0}$ and so

$$\begin{aligned}&\sum_{\nu\in\mathscr{R}}\boldsymbol{x}_\nu+\sum_{\eta\in\mathscr{U}}\boldsymbol{x}_\eta=\mathbf{0}\\ &\quad\Rightarrow\sum_{\nu\in\mathscr{R}}R_\nu^{-1}B\boldsymbol{x}_{\hat\eta}+\sum_{\eta\in\mathscr{U}}\boldsymbol{x}_\eta=\mathbf{0},\end{aligned} \tag{32}$$

where $\hat{\eta}$ is some fixed class in $\mathscr{U}$. By (31), for every $\eta \in \mathscr{U}$, $\boldsymbol{x}_\eta$ can be written as $\boldsymbol{x}_n = \boldsymbol{x}_p + \mathrm{d}_\eta \boldsymbol{\upsilon}$ where $\boldsymbol{x}_p \in \{0\} \cup (\mathbf{R}^K \setminus \ker B)$, $\mathrm{d}_\eta \in \mathbf{R}$, and $\boldsymbol{\upsilon}$ is the basis vector of $\ker B$ from (24). Thus,

$$\begin{aligned} & B \sum_{\nu \in \mathscr{R}} R_\nu^{-1} B(\boldsymbol{x}_p + d_{\hat{\eta}} \boldsymbol{\upsilon}) + B \sum_{\eta \in \mathscr{U}} (\boldsymbol{x}_p + d_\eta \boldsymbol{\upsilon}) = \mathbf{0} \\ & \Leftrightarrow \left(B \sum_{\nu \in \mathscr{R}} R_\nu^{-1} + M I_K \right) B \boldsymbol{x}_p = \mathbf{0} \\ & \Leftrightarrow B \boldsymbol{x}_p = \mathbf{0}, \end{aligned}$$

since $A = B \sum_{\nu \in \mathscr{R}} R_\nu^{-1} + M I_K$ is nonsingular. This shows that $\boldsymbol{x}_p = \mathbf{0}$. Therefore, $\boldsymbol{x}_\eta = d_\eta \boldsymbol{\upsilon}$ for every $\eta \in \mathscr{U}$. Now (31) shows that $\boldsymbol{k}_J = \mathbf{0}$ and so

$$\boldsymbol{x}_\nu = \mathbf{0} \quad \text{for } \nu \in \mathscr{R}. \tag{33}$$

Hence $\boldsymbol{k} = \binom{\boldsymbol{k}_F}{\mathbf{0}}$, where

$$\boldsymbol{k}_F^\nu = \begin{cases} \mathrm{d}_\nu \boldsymbol{\upsilon} & \text{if } \nu \in \mathscr{U}, \\ \mathbf{0} & \text{if } \nu \in \mathscr{R}, \end{cases}$$

from which it follows that $\boldsymbol{k}_F \in (\ker \mathrm{d}^2 F(q_{\frac{1}{N}})) \cap (\ker J)$ and so Lemma 9 gives

$$\boldsymbol{k}_F = \sum_{i=1}^{M} c_i \boldsymbol{\upsilon}_i \quad \text{and} \quad J \boldsymbol{k}_F = J(c_1 \boldsymbol{\upsilon}^T, c_2 \boldsymbol{\upsilon}^T, \ldots, c_M \boldsymbol{\upsilon}^T)^T = \mathbf{0}.$$

Thus, $\sum_i c_i \boldsymbol{\upsilon} = \boldsymbol{\upsilon} \sum_i c_i = \mathbf{0}$, and so $\boldsymbol{k}_F = \sum_{i=1}^{M-1} c_i (\boldsymbol{\upsilon}_i - \boldsymbol{\upsilon}_M)$. Therefore, the linearly independent vectors

$$\{\boldsymbol{w}_i\} = \left\{ \begin{pmatrix} \boldsymbol{\upsilon}_i - \boldsymbol{\upsilon}_M \\ \mathbf{0} \end{pmatrix} \right\}$$

span $\ker \mathrm{d}^2 \mathscr{L}(q^*)$. □

Observe that the dimensionality of $\ker \mathrm{d}^2 \mathscr{L}(q^*)$ is one less than $\ker \mathrm{d}^2 F(q^*)$. This insight suggests that when $\dim \ker \mathrm{d}^2 F(q^*) = 1$, then $\mathrm{d}^2 \mathscr{L}(q^*)$ is nonsingular. This is indeed the case.

Corollary 12. *If q^* is 1-singular, then $d^2 \mathscr{L}(q^*)$ is nonsingular.*

Proof. By Lemma 9, $\dim \ker \mathrm{d}^2 F(q^*) = 1$ and we need to compute the dimension of $\ker \mathrm{d}^2 \mathscr{L}(q^*, \lambda, \beta)$. To that end, following the Proof of Theorem 11, we take an arbitrary $\boldsymbol{k} \in \ker \mathrm{d}^2 \mathscr{L}(q^*, \lambda, \beta)$, and then decompose $\boldsymbol{k}$ as in (27) and (30). The proof to Theorem 11 holds for the present case up until, and including (33), $\boldsymbol{x}_{\boldsymbol{\upsilon}} = \boldsymbol{0}$ for $\nu \in \mathscr{R}$. Since q^* is 1-singular, we have $|\mathscr{U}| = 1$ and so (32) becomes $\sum_{\nu \in \mathscr{R}} \boldsymbol{x}_\nu + \boldsymbol{x}_\eta = \boldsymbol{x}_\eta = \boldsymbol{0}$ which implies that $\boldsymbol{k} = \boldsymbol{0}$. □

3.3. Liapunov–Schmidt Reduction

To show the existence of bifurcating branches from a bifurcation point $(q^*, \lambda^*, \beta^*)$ of equilibria of (20), the Equivariant Branching Lemma requires that the bifurcation is translated to $(\boldsymbol{0},\boldsymbol{0},0)$, and that the Jacobian vanishes at bifurcation. To accomplish the former, consider

$$\mathscr{F}(q, \lambda, \beta) := \nabla \mathscr{L}(q + q^*, \lambda + \lambda^*, \beta + \beta^*).$$

To assure that the Jacobian vanishes, we restrict and project $\mathscr{F}$ onto $\ker d^2\mathscr{L}(q^*)$ in a neighborhood of $(\boldsymbol{0},\boldsymbol{0},0)$. This is the Liapunov–Schmidt reduction of $\mathscr{F}$ [17],

$$\begin{aligned} r &: \mathbf{R}^{M-1} \times \mathbf{R} \to \mathbf{R}^{M-1}, \\ r(\boldsymbol{x}, \beta) &= W^T (I - E) \mathscr{F}(W\boldsymbol{x} + U(W\boldsymbol{x}, \beta), \beta), \end{aligned} \tag{34}$$

where

$$W\boldsymbol{x} + U(W\boldsymbol{x}, \beta) = \begin{pmatrix} q \\ \lambda \end{pmatrix}.$$

The $(NK + K) \times (NK + K)$ matrix $I - E$ is the projection matrix onto $\ker \mathscr{F}(\boldsymbol{0}, 0) = \ker d^2\mathscr{L}(q^*)$ with $\ker\ (I–E) = \text{range } d^2\mathscr{L}(q^*)$. W is the $(NK + K) \times (M - 1)$ matrix whose columns are the basis vectors $\{\boldsymbol{w}_i\}$ of $\ker d^2\mathscr{L}(q^*)$ from (26) so that $W\boldsymbol{x}$ is a vector in $\ker d^2\mathscr{L}(q^*)$. The vector function $U(W\boldsymbol{x}, \beta)$ is the component of (q, λ) which is in range $d^2\mathscr{L}(q^*)$ such that $E\mathscr{F}(W\boldsymbol{x} + U(\mathrm{x}, \beta), \beta) = \boldsymbol{0}$, $U(\boldsymbol{0}, 0) = \boldsymbol{0}$, and

$$d_{\boldsymbol{x}} U(\boldsymbol{0}, 0) = \boldsymbol{0}. \tag{35}$$

The system defined by the Liapunov–Schmidt reduction, $\dot{\boldsymbol{x}} = r(\boldsymbol{x}, \beta)$, has a bifurcation of equilibria at $(\boldsymbol{x} = \boldsymbol{0}, \beta = 0)$, which are in $1 - 1$ correspondence with equilibria of (20): $(t\boldsymbol{x}, \beta(t))$ is a bifurcating solution of $r(\boldsymbol{x}, \beta) = \boldsymbol{0}$ if and only if

$$\begin{pmatrix} q^* \\ \lambda^* \\ \beta^* \end{pmatrix} + \begin{pmatrix} tW\boldsymbol{x} \\ \beta(t) \end{pmatrix}$$

is a bifurcating solution of $\nabla \mathscr{L}(q, \lambda, \beta) = \boldsymbol{0}$. However, the stability of these associated equilibria is not necessarily the same.

It is straightforward to verify the following derivatives ([17] p. 32), which we will require in the sequel. The Jacobian of (34) is

$$d_{\boldsymbol{x}} r(\boldsymbol{x}, \beta) = W^T (I-E) d^2_{q,\lambda} \mathscr{L}(q+q^*, \lambda+\lambda^*, \beta+\beta^*)(W + d_x U(W\boldsymbol{x}, \beta)), \tag{36}$$

which shows that

$$d_{\boldsymbol{x}} r(\boldsymbol{0}, 0) = \boldsymbol{0} \tag{37}$$

since ker*(I–E)* = range $d^2\mathscr{L}(q^*)$. The derivative with respect to the bifurcation parameter is

$$d_\beta r(\boldsymbol{0}, 0) = W^T d_\beta \nabla \mathscr{L}(q^*, \lambda^*, \beta^*). \tag{38}$$

The three dimensional array of second derivatives of r is

$$\begin{aligned}
\frac{\partial^2 r_i}{\partial x_j \partial x_k}(\boldsymbol{0}, 0) &= d^3 \mathscr{L}(q^*, \lambda^*, \beta^*)[\boldsymbol{w}_i, \boldsymbol{w}_j, \boldsymbol{w}_k] \\
&= \sum_{\nu,\delta,\eta,\in \mathscr{Z}} \sum_{l,m,n \in \mathscr{Y}} \frac{\partial^3 F(q^*, \beta^*)}{\partial q_{\nu l} \partial q_{\delta m} \partial q_{\eta n}} \\
&\quad \times [\boldsymbol{\upsilon}_i - \boldsymbol{\upsilon}_M]_{\nu l} [\boldsymbol{\upsilon}_j - \boldsymbol{\upsilon}_M]_{\delta m} [\boldsymbol{\upsilon}_k - \boldsymbol{\upsilon}_M]_{\eta n} \\
&= \sum_{l,m,n \in \mathscr{Y}} \frac{\partial^3 F(q^*, \beta^*)}{\partial q_{\nu l} \partial q_{\nu m} \partial q_{\nu n}} (\delta_{ijk} [\boldsymbol{\upsilon}]_l [\boldsymbol{\upsilon}]_m [\boldsymbol{\upsilon}]_n - [\boldsymbol{\upsilon}]_l [\boldsymbol{\upsilon}]_m [\boldsymbol{\upsilon}]_n),
\end{aligned} \tag{39}$$

where $\boldsymbol{\upsilon}$ is defined in (24). An immediate consequence of (39) is that

$$\frac{\partial^2 r_i}{\partial x_i \partial x_i}(\boldsymbol{0}, 0) = 0$$

for each i, and that

$$\frac{\partial^2 r_i}{\partial x_i \partial x_k}(\boldsymbol{0}, 0) = \frac{\partial^2 r_{i'}}{\partial x_{j'} \partial x_{k'}}(\boldsymbol{0}, 0) \quad \text{if } (i, j, k) \neq (i', j', k').$$

The four dimensional array of third derivatives of r is

$$\begin{aligned}
\frac{\partial^3 r_i}{\partial x_j \partial x_k \partial x_l}(\boldsymbol{0}, 0) = \; & d^4 \mathscr{L}[\boldsymbol{w}_i, \boldsymbol{w}_j, \boldsymbol{w}_k, \boldsymbol{w}_l] - d^3 \mathscr{L}[\boldsymbol{w}_i, \boldsymbol{w}_j, L^- E d^3 \mathscr{L}[\boldsymbol{w}_k, \boldsymbol{w}_l]] \\
& - d^3 \mathscr{L}[\boldsymbol{w}_i, \boldsymbol{w}_k, L^- E d^3 \mathscr{L}[\boldsymbol{w}_k, \boldsymbol{w}_l]] \\
& - d^3 \mathscr{L}[\boldsymbol{w}_i, \boldsymbol{w}_l, L^- E d^3 \mathscr{L}[\boldsymbol{w}_j, \boldsymbol{w}_k]],
\end{aligned} \tag{40}$$

where the derivatives of $\mathscr{L}$ are evaluated at $(q^*, \lambda^*, \beta^*)$, and L^- is the Moore–Penrose generalized inverse [36] of $d^2\mathscr{L}(q^*)$. Thus, $E = LL^-$, so that

$$L^- E = L^- L L^- = L^-. \tag{41}$$

The explicit basis (26) shows that ker $d^2\mathscr{L}(q^*) \cong \{\boldsymbol{x} \in \mathbf{R}^M : \sum[\boldsymbol{x}]_i = 0\} \cong \mathbf{R}^{M-1}$ is absolutely irreducible [18]. Thus,

$$d_{\boldsymbol{x}} r(\mathbf{0}, \beta) = c(\beta) I_{M-1}, \tag{42}$$

which assures that we can use Theorem 2.

3.4. The Action of S_N

In this section we give the explicit representation of the action of S_N on the dynamical system (20).

Let $\mathscr{P}$ be a subgroup of $O(NK)$, the group of orthogonal matrices in $\mathbf{R}^{NK}$. We define $\mathscr{P}$ to be the group of *block permutation* matrices which act on $q \in \mathbf{R}^{NK}$ by permuting the vector components, q^ν, of q. For example, for $N = 3$, the element ρ_{13} (which permutes classes 1 and 3) and the element ρ_{123} (which maps class 1 to 2, class 2 to 3, and class 3 to 1) in $\mathscr{P}$ are

$$\rho_{13} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & I_K \\ \mathbf{0} & I_K & \mathbf{0} \\ I_K & \mathbf{0} & \mathbf{0} \end{pmatrix}, \qquad \rho_{123} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & I_K \\ I_K & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & I_K & \mathbf{0} \end{pmatrix},$$

where $\mathbf{0}$ is $K \times K$. The group $\Gamma \subset O(NK + K)$ that acts on $(q, \lambda) \in \mathbf{R}^{NK} \times \mathbf{R}^K$, and on $\nabla\mathscr{L}$ is

$$\Gamma := \left\{ \begin{pmatrix} \rho & \mathbf{0}^T \\ \mathbf{0} & I_K \end{pmatrix} \mid \text{for } \rho \in \mathscr{P} \right\},$$

where $\mathbf{0}$ is $K \times NK$. Observe that $\gamma \in \Gamma$ acts on $\nabla\mathscr{L}$ by

$$\gamma \nabla_{q,\lambda} \mathscr{L}(q, \lambda) = \begin{pmatrix} \rho & \mathbf{0}_T \\ \mathbf{0} & I_K \end{pmatrix} \begin{pmatrix} \nabla_q \mathscr{L} \\ \nabla_\lambda \mathscr{L} \end{pmatrix} = \begin{pmatrix} \rho \nabla_q \mathscr{L} \\ \nabla_\lambda \mathscr{L} \end{pmatrix}$$

and on

$$\begin{pmatrix} q \\ \lambda \end{pmatrix} \quad \text{by} \quad \gamma \begin{pmatrix} q \\ \lambda \end{pmatrix} = \begin{pmatrix} \rho q \\ \lambda \end{pmatrix}.$$

Thus, $\gamma \in \Gamma$ acts on $q \in \mathbf{R}^{NK}$ as defined by $\rho \in \mathscr{P}$ but leaves the Lagrange multipliers $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_K)^T$ fixed.

Lemma 13, which follows easily from the form of F given in (1), establishes S_N-equivariance for the gradient system (20).

Lemma 13. *$\mathscr{L}(q,\lambda,\beta)$ is Γ-invariant, $\nabla\mathscr{L}(q,\lambda,\beta)$ is Γ-equivariant, and ∇F is $\mathscr{P}$-equivariant.*

Given an equilibrium q with $q^1=q^2=\cdots=q^M$, we write that $q\in \mathrm{Fix}(S_M)$, which really implies that (q,λ) is in the fixed point space of

$$\Gamma_{\mathscr{U}} := \left\{ \begin{pmatrix} \rho & \mathbf{0}^T \\ \mathbf{0} & I_k \end{pmatrix} | \rho \in \mathscr{P}_{\mathscr{U}} \right\},$$

where $\mathbf{0}$ is $K\times NK$. The subgroup $\mathscr{P}_{\mathscr{U}}\subset\mathscr{P}$ fixes the subvectors q^ν if $\nu\in\mathscr{R}$ and freely permutes the subvectors q^η if $\eta\in\mathscr{U}=\{1,\ldots,M\}$, so that $\mathscr{P}_{\mathscr{U}}$ and $\Gamma_{\mathscr{U}}$ are isomorphic to S_M. Observe that if $\mathscr{U}=\mathscr{Y}$, then we are back to the case where $q^*=q_{\frac{1}{N}}$ and $\Gamma_{\mathscr{U}}=\Gamma$.

Similarly, when we write that (q,λ) has isotropy group S_M, this refers to the group $\Gamma_{\mathscr{U}}$.

3.5. Isotropy Subgroups of S_M

The isotropy groups of (q,λ) for the clusterings q pictured in Figure 2 are clear. In panel 2, the isotropy group is S_3, and in panels 3 and 4, the isotropy group is S_2. It turns out that, restricted to $\ker \mathrm{d}^2\mathscr{L}(q^*)$, the fixed point spaces of these groups is one dimensional. In this section, we give all of the isotropy subgroups of S_M which, acting on $\ker d^2\mathscr{L}(q^*)$, have fixed point spaces of dimension 1.

For arbitrary M, the full lattice of subgroups is unknown [6, 27]. By [22, 27], the subgroups $S_m\times S_n$ are maximal in S_M when $m+n=M$ and $m\neq n$, which makes them possible maximal isotropy subgroups of S_M. Golubitsky and Stewart ([18] p. 18) show that all of the isotropy subgroups in S_M with one dimensional fixed point spaces are of the form $S_m\times S_n$, where $m+n=M$ (in this case, m can be equal to n). The following Lemma which follows from this result will enable us to use the Equivariant Branching Lemma to show the existence of explicit bifurcating solutions, with isotropy group $S_m\times S_n$, from an M-singular solution q^* of (20) for any $1<M\leqslant N$.

Lemma 14. *Let $M = m + n$ such that $M > 1$ and $m, n > 0$. Let $\mathscr{U}_m$ be a set of m classes, and let $\mathscr{U}_n$ be a set of n classes such that $\mathscr{U}_m\cap\mathscr{U}_n=\emptyset$ and $\mathscr{U}_m\cup\mathscr{U}_n=\mathscr{U}$. Now define $\hat{\boldsymbol{u}}_{(m,n)}\in\mathbf{R}^{NK}$ such that*

$$\hat{\boldsymbol{u}}^\nu_{(m,n)} = \begin{cases} \frac{n}{m}\boldsymbol{v} & if\ \nu\in\mathscr{U}_m, \\ -\boldsymbol{v} & if\ \nu\in\mathscr{U}_n, \\ \mathbf{0} & otherwise, \end{cases}$$

where $\mathfrak{v}$ is defined as in (24), and let

$$\boldsymbol{u}_{(m,n)} = \begin{pmatrix} \hat{\boldsymbol{u}}_{(m,n)} \\ \mathbf{0} \end{pmatrix}, \tag{43}$$

where $\mathbf{0} \in \mathbf{R}^K$. Then the isotropy subgroup of $\boldsymbol{u}_{(m,n)}$ is $\sum_{(m,n)} \subset \Gamma_{\mathscr{U}}$ such that $\sum_{(m,n)} \cong S_m \times S_n$, where S_m acts on $\boldsymbol{u}^\nu$ when $\nu \in \mathscr{U}_m$ and S_n acts $\boldsymbol{u}^\nu$ when $\nu \in \mathscr{U}_n$. The fixed point space of $\sum_{(m,n)}$ restricted to $\ker \mathrm{d}^2 \mathscr{L}(\mathrm{q}^*)$ *is one dimensional.*

It is straightforward to verify that

$$\boldsymbol{u}_{(m,n)} = -\sum_{i=1}^{n} \boldsymbol{w}_i + \frac{n}{m} \sum_{j=n+1}^{M-1} \boldsymbol{w}_j,$$

confirming that $\boldsymbol{u}_{(m,n)} \in \ker \mathrm{d}^2 \mathscr{L}(q^*)$ as claimed. Without loss of generality, one can assume that $\mathscr{U}_m = \{1, 2, \ldots, m\}$ and $\mathscr{U}_n = \{m+1, \ldots, M\}$. This is because if $\mathscr{U}'_m$ and $\mathscr{U}'_n$ is another partition of $\mathscr{U}$ into m and n classes respectively, and if the vector $\boldsymbol{u}'_{(m,n)}$ has isotropy group $\Sigma'_{(m,n)} \cong S_m \times S_n$ which acts on the subvector components $\boldsymbol{u}'^{\nu}$ for ν in $\mathscr{U}'_m$ and $\mathscr{U}'_n$, then $\boldsymbol{u}'_{(m,n)} = \gamma \boldsymbol{u}_{(m,n)}$ for some element $\gamma \in \Gamma$. The vectors $\boldsymbol{u}'_{(m,n)}$ and $\boldsymbol{u}_{(m,n)}$ are said to be in the same *orbit* of Γ [19],

$$\Gamma u_{(m,n)} := \{\gamma u_{(m,n)} | \gamma \in \Gamma\}.$$

Furthermore, $\boldsymbol{u}'_{(m,n)}$ and $\boldsymbol{u}_{(m,n)}$ have conjugate isotropy subgroups,

$$\Sigma'_{(m,n)} = \gamma \Sigma_{(m,n)} \gamma^{-1}.$$

This is why we use the notation $\Sigma_{(m,n)}$ to specify the isotropy subgroups in Lemma 14 instead of the precise, but elaborate notation $\Sigma_{(\mathscr{U}_m, \mathscr{U}_n)}$.

Letting $m = 1$ and $n = M - 1$ yields the following corollary.

Corollary 15. *Let $\hat{\boldsymbol{u}} \in \mathbf{R}^{NK}$ such that*

$$\hat{\boldsymbol{u}}^\nu = \begin{cases} (M-1)\mathfrak{v} & if \;\; \nu = 1, \\ -\mathfrak{v} & if \;\; \nu = 2, \ldots, M, \\ \mathbf{0} & otherwise, \end{cases}$$

where $\mathfrak{v}$ is defined as in (24), and let

$$\boldsymbol{u} = \begin{pmatrix} \hat{\boldsymbol{u}} \\ \mathbf{0} \end{pmatrix},$$

where $\mathbf{0} \in \mathbf{R}^K$. Then the isotropy subgroup of $\boldsymbol{u}$ is $\Sigma \subset \Gamma_{\mathscr{U}}$, such that $\Sigma \cong S_{M-1}$. The fixed point space of Σ restricted to $\ker \mathrm{d}^2 \mathscr{L}(q^*)$ *is one dimensional.*

Remark 16. We want to pause and collect information about our notation. Assume q^* is an M-singular point for $M>1$ so that $(q^*, \lambda^*, \beta^*)$ is a singularity of the flow (20) for a generic choice of F. Thus, the Hessian $d^2F(q^*)$ has M blocks which are singular. The vector $\boldsymbol{v} \in \mathbf{R}^K$ is in the kernel of the singular block B of d^2F. The vectors $\boldsymbol{w}_i \in \mathbf{R}^{NK+K}$ are constructed from the vector $\boldsymbol{v}$, and they form a basis for $\ker d^2\mathscr{L}$ which has dimension $M-1$. The vectors $u_{(m,n)} \in \mathbf{R}^{NK+K}$ are particular vectors in $\ker d^2\mathscr{L}$ which have isotropy group $S_m \times S_n$. Since these belong to $\ker d^2\mathscr{L}$ they are in the span of the vectors $\boldsymbol{w}_i$ and hence are constructed using the vector $\boldsymbol{v}$.

4. SYMMETRY BREAKING BIFURCATIONS

We have laid the groundwork so that in this section, we may ascertain the existence of explicit bifurcating branches from a symmetry breaking bifurcation of an M-singular q^* at some β^* and vector of Lagrange multipliers λ^* (Theorem 17). To accomplish this, the Equivariant Branching Lemma is applied to the Liapunov–Schmidt reduction $r(\boldsymbol{x}, \beta)$ (34) of $\nabla\mathscr{L}$ at a singularity $(q^*, \lambda^*, \beta^*)$, where $\nabla\mathscr{L}$ defines the dynamical system (20)

$$\begin{pmatrix} \dot{q} \\ \dot{\lambda} \end{pmatrix} = \nabla\mathscr{L}(q, \lambda, \beta).$$

We will show that these symmetry breaking bifurcations are degenerate (Theorem 18), that is, $\beta'(0)=0$. If $\beta''(0) \neq 0$, which is a generic assumption, then symmetry breaking bifurcations are pitchfork-like. We will provide a condition, called the bifurcation discriminator, which ascertains whether the bifurcating branches with isotropy group $S_m \times S_n$ are pitchfork-like and either subcritical or supercritical (Theorem 20). We also provide a condition which determines whether branches are stable or unstable (Theorem 21). Lastly, we determine when unstable bifurcating branches contain no solutions to (1) (Theorem 26).

4.1. Explicit Bifurcating Branches

In this section we use the Equivariant Branching Lemma to ascertain the existence of explicit bifurcating branches from a symmetry breaking bifurcation of an M-singular equilibrium of (20).

Theorem 17. *Let $(q^*, \lambda^*, \beta^*)$ be an equilibrium of (20) such that q^* is M-singular for $1 < M \leqslant N$, and the crossing condition $c'(0) \neq 0$ (see (42)) is satisfied. Then there exists bifurcating solutions,*

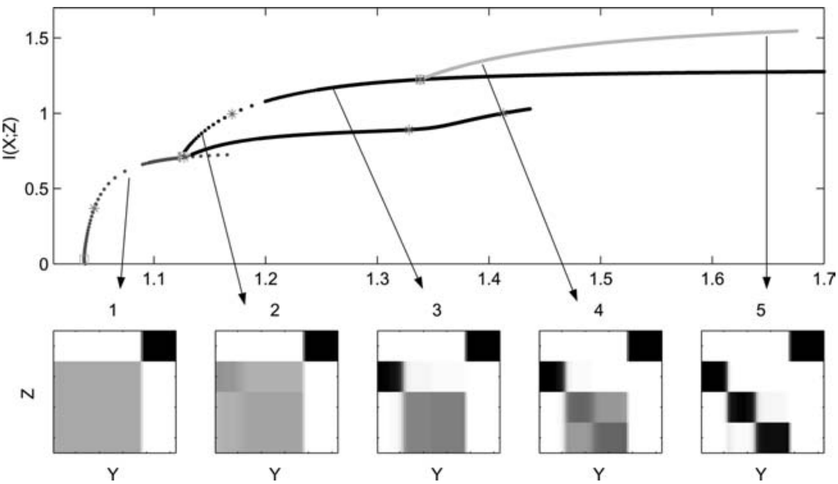

Figure 3. The bifurcation structure of stationary points of (9) when $N=4$. Figure 2 showed an incomplete bifurcation structure for this same scenario since the algorithm in that case was affected by the stability of the branches. The panels illustrate the sequence of symmetry breaking bifurcations from the branch $(q_{\frac{1}{N}}, \lambda, \beta)$ with symmetry S_4, to a branch with symmetry S_3, then to S_2, and finally, to S_1.

$$\begin{pmatrix} q^* \\ \lambda^* \\ \beta^* \end{pmatrix} + \begin{pmatrix} t\boldsymbol{u}_{(m,n)} \\ \beta(t) \end{pmatrix},$$

where $\boldsymbol{u}_{(m,n)}$ *is defined in (43), for every pair of positive integers (m,n) such that* $M = m+n$, *each with isotropy group isomorphic to* $S_m \times S_n$.

Proof. Lemma 14, and Eqs. (37) and (42) show that the requirements of the Equivariant Branching Lemma are satisfied, whose application proves the theorem. □

Figure 3 shows some of the bifurcating branches guaranteed by Theorem 17 when $N = 4$ (see Section 7). The symmetry of the clusterings shown depict symmetry breaking from $S_4 \to S_3 \to S_2 \to S_1$. Figure 4 depicts symmetry breaking from S_4 to $S_2 \times S_2$. The first bifurcation in the figure, which occurs at $\beta^* = 1.0387$, coincides with the break from S_4 to S_3 symmetry given in Figure 3. The subsequent two bifurcating branches given in Figure 4 correspond to bifucations at β^*=1.1339 and β^*=1.3910.

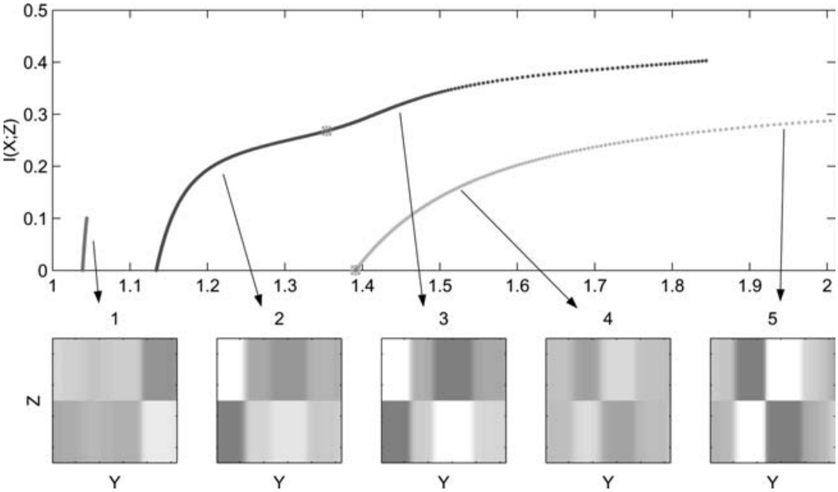

Figure 4. Symmetry breaking bifurcations from the branch $(q_{\frac{1}{N}}, \lambda, \beta)$ with symmetry S_4 to branches which have symmetry $S_2 \times S_2$.

4.2. Subcritical and Supercritical Bifurcating Branches

Suppose that a bifurcation occurs at $(q^*, \lambda^*, \beta^*)$ where $(q^*$ is M-singular. This section examines the structure of the bifurcating branches

$$\left(\begin{pmatrix} q^* \\ \lambda^* \end{pmatrix} + t\boldsymbol{u}, \beta^* + \beta(t)\right), \tag{44}$$

whose existence is guaranteed by Theorem 17.

The next theorem shows that symmetry breaking bifurcations of equilibria of (20) are degenerate.

Theorem 18. *If q^* is M-singular for $1 < M \leqslant N$, then all of the bifurcating branches (44) guaranteed by Theorem 17 are degenerate, i.e., $\beta'(0) = 0$.*

Proof. By Definition 4, we need to show that $\beta'(0) = 0$. Let $\boldsymbol{x}_0$ be defined so that $\boldsymbol{u} = W\boldsymbol{x}_0$ is a bifurcating direction given in (43). Thus, the isotropy subgroup of $\boldsymbol{x}_0$, Σ, has a one dimensional fixed point space. Since $r(\text{Fix}(\Sigma)) \subseteq \text{Fix}(\Sigma)$, then $r(t\boldsymbol{x}_0, \beta) = h(t, \beta)\boldsymbol{x}_0$, where r is the Liapunov–Schmidt reduction (34) and h is a polynomial in t. By absolute irreducibility, $r(\mathbf{0}, \beta) = \mathbf{0}$, and so $h(0, \beta) = 0$ ([19] p.84), from which it follows that $h(t, \beta) = tk(t, \beta)$. Thus

$$r(t\boldsymbol{x}_0, \beta) = tk(t, \beta)\boldsymbol{x}_0.$$

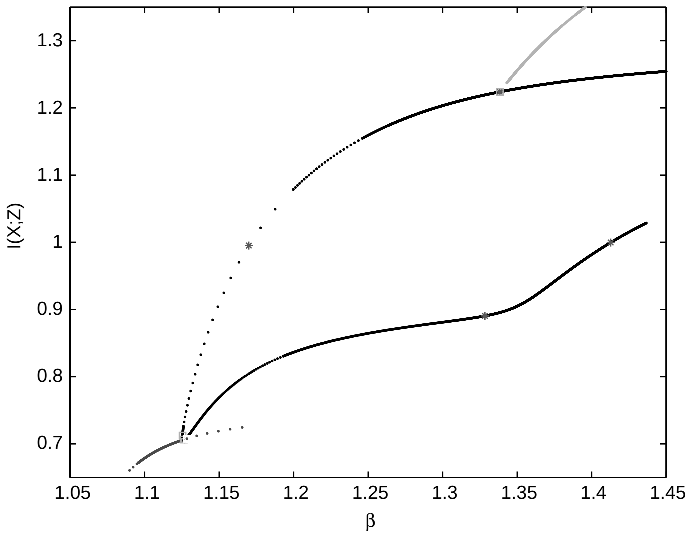

Figure 5. A close up, from Figure 3, of the branch with S_2 symmetry which connects the S_3 symmetric branch below to the S_1 symmetric solution above. By Theorem 18, the symmetry breaking bifurcations from $S_3 \to S_2$ and from $S_2 \to S_1$ are degenerate, and, since $\beta''(0) \neq 0$, pitchfork-like.

Differentiating this equation with respect to t yields

$$d_{\boldsymbol{x}} r(t\boldsymbol{x}_0, \beta)\boldsymbol{x}_0 = (k(t, \beta) + t\, d_t k(t, \beta))\boldsymbol{x}_0. \tag{45}$$

Using absolute irreducibility, this equation shows that $k(0, 0) = c(0) = 0$ and $d_\beta k(0, 0) = c'(0) \neq 0$. By the Implicit Function theorem, we can take the total derivative of $k(t, \beta) = 0$,

$$d_t k(t, \beta(t)) + d_\beta k(t, \beta(t))\beta'(t) = 0, \tag{46}$$

so that

$$\beta'(0) = -\frac{d_t k(t, \beta(t))}{c'(0)}.$$

Differentiating (45) with respect to t and then evaluating at $t = 0$ shows that

$$\beta'(0) = \frac{-d_x^2 r(\mathbf{0}, 0)[\boldsymbol{x}_0, \boldsymbol{x}_0, \boldsymbol{x}_0]}{2\|\boldsymbol{x}_0\|^2 c'(0)}, \tag{47}$$

where

$$\mathrm{d}^2_{\boldsymbol{x}} r(\mathbf{0},0)[\boldsymbol{x}_0,\boldsymbol{x}_0,\boldsymbol{x}_0] = \sum_{i,j,k} \frac{\partial^2 r}{\partial[\boldsymbol{x}]_i \partial[\boldsymbol{x}]_j \partial[\boldsymbol{x}]_k}(\mathbf{0},0)[\boldsymbol{x}_0]_i[\boldsymbol{x}_0]_j[\boldsymbol{x}_0]_k$$

(see (39)).
This expression is similar to the one given in [19] p. 90. To show that $\mathrm{d}^2_{\boldsymbol{x}} r(\mathbf{0},0)=\mathbf{0}$, expand r_i, the ith component of r, about $\boldsymbol{x}=0$,

$$r_i(\boldsymbol{x},\beta)=r_i(\mathbf{0},\beta)+\mathrm{d}_{\boldsymbol{x}} r_i(\mathbf{0},\beta)^T\boldsymbol{x}+\boldsymbol{x}^T d^2_{\boldsymbol{x}} r_i(\mathbf{0},\beta)\boldsymbol{x}+\mathcal{O}(\boldsymbol{x}^3).$$

Absolute irreducibility gives

$$r_i(\boldsymbol{x},0)=c(0)x_i+\boldsymbol{x}^T \mathrm{d}^2_{\boldsymbol{x}} r_i(\mathbf{0},0)\boldsymbol{x}+\mathcal{O}(\boldsymbol{x}^3).$$

By (39),

$$\frac{\partial^2 r_i}{\partial x_i \partial x_j}(\mathbf{0},0)=0 \quad \text{for each } i.$$

Applying the equivariance relation $Ar(\boldsymbol{x},0)=r(A\boldsymbol{x},0)$, where A is any element of the group isomorphic to S_M which acts on r in $\mathbf{R}^{M-1}$, shows that

$$\frac{\partial^2 r_i}{\partial x_j \partial x_k}(\mathbf{0},0)=0 \quad \text{for every } i,j,k. \qquad \square$$

If $\beta''(0)\neq 0$, which we expect to be true generically, then Theorem 18 shows that the bifurcation guaranteed by Theorem 17 is pitchfork-like. We next show how to determine the sign of $\beta''(0)$.

Definition 19. The *bifurcation discriminator* of the bifurcating branches (44) with isotropy group $S_m \times S_n$ is

$$\zeta(q^*,\beta^*,m,n):=3\Xi-\mathrm{d}^4 f[\boldsymbol{\upsilon},\boldsymbol{\upsilon},\boldsymbol{\upsilon},\boldsymbol{\upsilon}],$$

where

$$\Xi := \boldsymbol{b}^T B^- \left(I_K - \frac{mn(m+n)}{m^2-mn+n^2}A^{-1}\right)\boldsymbol{b},$$
$$\boldsymbol{b} := \mathrm{d}^3 f[\boldsymbol{\upsilon},\boldsymbol{\upsilon}].$$

The matrix B^- is the Moore–Penrose generalized inverse of a block of the Hessian (22), A is defined in (21), and $\boldsymbol{\upsilon}$ is defined in (24).

When $q^* = q_{\frac{1}{N}}$ is N-singular, then $A^{-1} = (1/N)I_K$, and so the bifurcation discriminator in this case simplifies to

$$\zeta(q_{\frac{1}{N}}, \beta^*, m, n) = 3\left(1 - \frac{mn}{m^2 - mn + n^2}\right)\boldsymbol{b}^T B^- \boldsymbol{b} - \mathrm{d}^4 f[\boldsymbol{\upsilon}, \boldsymbol{\upsilon}, \boldsymbol{\upsilon}, \boldsymbol{\upsilon}].$$

We want to note that the discriminator $\zeta(q^*, \beta^*, m, n)$ is defined purely in terms of the constitutive functions f of $F(q, \beta) = \Sigma_{\nu=1}^N f(q^\nu, \beta)$ (see (1)). This follows since the blocks of $\mathrm{d}^2F(q^*)$ are $B_\nu = \mathrm{d}^2 f(q^\nu)$ for $\nu = 1, \ldots, N$, A is a function of these blocks, and $B = B_\nu$ for $\nu = 1, \ldots, M$.

Since the kernel of B is spanned by the vector $\boldsymbol{\upsilon}$, the expression $B^- x$ in Definition 19 is not uniquely determined. However, we made a choice of L^- to be the Moore-Penrose inverse of $\mathrm{d}^2\mathscr{L}$ which leads to the simplification in (41) by selecting $L^- x$ to be in the image of the projection E. Since $\mathrm{d}^2\mathscr{L}$ has the blocks B on its diagonal, the choice of the inverse B^- is affected by the requirement that L^- satisfies (41). It follows from the computation (48) that in order for (41) to hold, we must take B^- to also be the Moore-Penrose inverse of the block B.

The term $\mathrm{d}^4 f[\boldsymbol{\upsilon}, \boldsymbol{\upsilon}, \boldsymbol{\upsilon}, \boldsymbol{\upsilon}]$ in $\zeta(q^*, \beta^*, m, n)$ can be expressed as

$$\mathrm{d}^4 f[\boldsymbol{\upsilon}, \boldsymbol{\upsilon}, \boldsymbol{\upsilon}, \boldsymbol{\upsilon}] := \sum_{r,s,t,u \in Y} \frac{\partial^4 F(q^*, \beta^*)}{\partial q_{\nu r} \partial q_{\nu s} \partial q_{\nu t} \partial q_{\nu u}} [\boldsymbol{\upsilon}]_r [\boldsymbol{\upsilon}]_s [\boldsymbol{\upsilon}]_t [\boldsymbol{\upsilon}]_u.$$

Notice that $\boldsymbol{b}$ is a vector, whose tth component is

$$[\boldsymbol{b}]_t = \sum_{r,s \in Y} \frac{\partial^3 F(q^*, \beta^*)}{\partial q_{\nu r} \partial q_{\nu s} \partial q_{\nu t}} [\boldsymbol{\upsilon}]_r [\boldsymbol{\upsilon}]_s.$$

Theorem 20. *Suppose q^* is M-singular for $1 < M \leqslant N$ and $c'(0) > 0$ (see (42)). Then*

$$\operatorname{sgn}\beta''(0) = \operatorname{sgn}\zeta(q^*, \beta^*, m, n).$$

In particular, if $\zeta(q^*, \beta^*, m, n) < 0$, then the bifurcating branches (44) guaranteed by Theorem 17, are pitchfork-like and subcritical. If $\zeta(q^*, \beta^*, m, n) > 0$, then the bifurcating branches are pitchfork-like and supercritical.

Proof. Since $\beta'(0) = 0$ (Theorem 18), then we need to compute $\beta''(0)$ to determine whether a branch is subcritical or supercritical. Differentiating (46) shows that

$$\beta''(0) = -\frac{\mathrm{d}_t^2 k(0, 0)}{\mathrm{d}_\beta k(\mathbf{0}, 0)}.$$

Twice differentiating (45) and solving for $d_t^2 k(0,0)$ shows that

$$\beta''(0) = -\frac{d_{\boldsymbol{x}}^3 r(\mathbf{0},0)[\boldsymbol{x}_0,\boldsymbol{x}_0,\boldsymbol{x}_0,\boldsymbol{x}_0]}{3\|\boldsymbol{x}_0\|^2 c'(0)},$$

where $W\boldsymbol{x}_0 = \boldsymbol{u} = \boldsymbol{u}_{(m,n)}$. Since $c'(0) > 0$, we need only determine the sign of the numerator. By (40) and (41),

$$d_x^3 r(\mathbf{0},0)[\boldsymbol{x}_0,\boldsymbol{x}_0,\boldsymbol{x}_0,\boldsymbol{x}_0] = d^4\mathscr{L}[\boldsymbol{u},\boldsymbol{u},\boldsymbol{u},\boldsymbol{u}] - 3d^3\mathscr{L}[\boldsymbol{u},\boldsymbol{u},L^- d^3\mathscr{L}[\boldsymbol{u},\boldsymbol{u}]],$$

where the derivatives of $\mathscr{L}$ are evaluated at (q^*,λ^*,β^*). Using (43), the first term can be simplified as

$$\begin{aligned}
&\sum_{i,s,t,u\in\mathscr{Y}}\ \sum_{\nu,\delta,\eta,\omega\in\mathscr{Z}} \frac{\partial^3 F(q^*,\beta^*)}{\partial q_{\nu i}\partial q_{\delta s}\partial q_{\eta t}\partial q_{\omega u}}[\hat{\boldsymbol{u}}]_{\nu i}[\hat{\boldsymbol{u}}]_{\delta s}[\hat{\boldsymbol{u}}]_{\eta t}[\hat{\boldsymbol{u}}]_{\omega u}\\
&= \sum_{i,s,t,u\in\mathscr{Y}} \left(\left(\frac{n}{m}\right)^4 \sum_{\nu\in\mathscr{U}_m} \frac{\partial^3 F(q^*,\beta^*)}{\partial q_{\nu i}\partial q_{\nu s}\partial q_{\nu t}\partial q_{\nu u}}[\boldsymbol{v}]_i[\boldsymbol{v}]_s[\boldsymbol{v}]_t[\boldsymbol{v}]_u \right.\\
&\qquad \left. + \sum_{\nu\in\mathscr{U}_n} \frac{\partial^3 F(q^*,\beta^*)}{\partial q_{\nu i}\partial q_{\nu s}\partial q_{\nu t}\partial q_{\nu u}}[\boldsymbol{v}]_i[\boldsymbol{v}]_s[\boldsymbol{v}]_t[\boldsymbol{v}]_u\right)\\
&= \left(\frac{n^4}{m^3} + n\right) d^4 f[\boldsymbol{v},\boldsymbol{v},\boldsymbol{v},\boldsymbol{v}].
\end{aligned}$$

To simplify the second term $-3d^3\mathscr{L}[\boldsymbol{u},\boldsymbol{u},L^- d^3\mathscr{L}[\boldsymbol{u},\boldsymbol{u}]]$, let

$$y := d^3\mathscr{L}[\boldsymbol{u},\boldsymbol{u}],$$

so that by (43),

$$\boldsymbol{y}^\nu = \begin{cases} \left(\frac{n}{m}\right)^2 d^3 f[v,v] & \text{if } \nu\in\mathscr{U}_m \\ d^3 f[v,v] & \text{if } \nu\in\mathscr{U}_n \\ 0 & \text{otherwise} \end{cases} = \begin{cases} \frac{n}{m}^2 \boldsymbol{b} & \text{if } \nu\in\mathscr{U}_m, \\ \boldsymbol{b} & \text{if } \nu\in\mathscr{U}_n, \\ 0 & \text{otherwise.} \end{cases}$$

The vector $\boldsymbol{k} := L^- d^3\mathscr{L}[\boldsymbol{u},\boldsymbol{u}] = L^-\boldsymbol{y}$ is a solution to the linear equation

$$L\boldsymbol{k} = d^2\mathscr{L}\boldsymbol{k} = \boldsymbol{y}.$$

We decompose $\boldsymbol{k}$ as

$$\boldsymbol{k} = \begin{pmatrix}\boldsymbol{k}_F\\ \boldsymbol{k}_J\end{pmatrix}$$

so that $\boldsymbol{k}_F := (\boldsymbol{x}_1^T \boldsymbol{x}_2^T \cdots \boldsymbol{x}_N^T)^T$. Now (18) shows that $L\boldsymbol{k} = \boldsymbol{y}$ is equivalent to

$$\begin{aligned} B\boldsymbol{x}_\nu &= \left(\frac{n}{m}\right)^2 \boldsymbol{b} - \boldsymbol{k}_J \quad \text{for } \nu \in \mathscr{U}_m, \\ B\boldsymbol{x}_\nu &= \boldsymbol{b} - \boldsymbol{k}_J \quad \text{for } \nu \in \mathscr{U}_n, \\ R_\nu \boldsymbol{x}_\nu &= -\boldsymbol{k}_J \quad \text{for } \nu \in \mathscr{R}, \\ \sum_{\nu=1}^{N} \boldsymbol{x}_\nu &= \boldsymbol{0}. \end{aligned} \tag{48}$$

The first three equations can be solved to get $\boldsymbol{k}_F$ in terms of $\boldsymbol{k}_J$, so that

$$\begin{aligned} \boldsymbol{x}_\nu &= \left(\frac{n}{m}\right)^2 B^- \boldsymbol{b} - B^- k_J \quad \text{for } \nu \in \mathscr{U}_m, \\ \boldsymbol{x}_\nu &= B^- \boldsymbol{b} - B^- \boldsymbol{k}_J \quad \text{for } \nu \in \mathscr{U}_n, \end{aligned}$$

and that

$$\boldsymbol{x}_\nu = -R_\nu^{-1} \boldsymbol{k}_J \quad \text{for } \nu \in \mathscr{R}.$$

To get $\boldsymbol{k}_J$, we now use the last equation,

$$B \sum_{\nu=1}^{N} \boldsymbol{x}_\nu = \sum_{\nu \in \mathscr{U}} B\boldsymbol{x}_\nu + \sum_{\nu \in \mathscr{R}} B\boldsymbol{x}_\nu = 0,$$

and then substitute in from the first three equations to get

$$A\boldsymbol{k}_J = \left(B \sum_{\nu \in \mathscr{R}} R_\nu^{-1} + M I_K \right) \boldsymbol{k}_J = \left(\frac{n^2}{m} + n \right) \boldsymbol{b},$$

since $A = B \sum_{\nu \in \mathscr{R}} R_\nu^{-1} + M I_K$. This yields

$$\boldsymbol{k}_J = \left(\frac{n^2}{m} + n \right) A^{-1} \boldsymbol{b},$$

since A from (21) is generically nonsingular (Theorem 7).

Now we are ready to compute

$$\mathrm{d}^3 \mathscr{L}[\boldsymbol{u}, \boldsymbol{u}, L^- \mathrm{d}^3 \mathscr{L}[\boldsymbol{u}, \boldsymbol{u}]] = \boldsymbol{y}^T \boldsymbol{k} = \mathrm{d}^3 \mathscr{L}[\boldsymbol{u}, \boldsymbol{u}]^T \begin{pmatrix} \boldsymbol{k}_F \\ \boldsymbol{k}_J \end{pmatrix}$$

which is equal to

$$\left(\frac{n^4}{m^3} + n \right) \boldsymbol{b}^T B^- \boldsymbol{b} - \left(\frac{n^2}{m} + n \right) \boldsymbol{b}^T B^- \boldsymbol{k}_J.$$

Substituting in this expression for $\mathbf{k}_J$ shows that

$$d^3\mathscr{L}[\boldsymbol{u},\boldsymbol{u},L^- d^3\mathscr{L}[\boldsymbol{u},\boldsymbol{u}]] = \boldsymbol{b}^T B^- \left(\left(\frac{n^4}{m^3} + n \right) I_K - \left(\frac{n^2}{m} + n \right)^2 A^{-1} \right) \boldsymbol{b}.$$

We have shown that

$$\begin{aligned}
\operatorname{sgn}\beta''(0) &= -\operatorname{sgn}\, d_x^3 r(\mathbf{0},0)[\boldsymbol{x}_0,\boldsymbol{x}_0,\boldsymbol{x}_0,\boldsymbol{x}_0] \\
&= \operatorname{sgn}(3d^3\mathscr{L}[\boldsymbol{u},\boldsymbol{u},L^- d^3\mathscr{L}[\boldsymbol{u},\boldsymbol{u}]] - d^4\mathscr{L}[\boldsymbol{u},\boldsymbol{u},\boldsymbol{u},\boldsymbol{u}]) \\
&= \operatorname{sgn}\left(3\boldsymbol{b}^T B^- \left(\left(\frac{n^4}{m^3} + n \right) I_K - \left(\frac{n^2}{m} + n \right)^2 A^{-1} \right) \boldsymbol{b} \right. \\
&\qquad \left. - \left(\frac{n^4}{m^3} + n \right) d^4 f[\upsilon,\upsilon,\upsilon,\upsilon] \right).
\end{aligned}$$

Dividing by $\left(\frac{n^4}{m^3} + n\right)$ completes the proof. □

Consider the bifurcation at $(q_{\frac{1}{N}}, \lambda^*, \beta^* = 1.0387)$ in Figure 3 where symmetry breaks from S_4 to S_3. The value of the discriminator at this bifurcation is $\zeta(q_{\frac{1}{N}}, 1.0387, 1, 3) = -.0075$ (see Section 7 for details), which predicts that this bifurcation is subcritical. Figure 6, a close up of the bifurcation structure at this bifurcation, illustrates the subcritical bifurcating branch.

The following result discusses stability of the bifurcating branches. Here we compare our results to those of Golubitsky *et al.*, in [19]. They showed that if $d_{\boldsymbol{x}} Q(\mathbf{0},0)[\boldsymbol{x}_0]$ has eigenvalues with a nonzero real part, where $Q(\boldsymbol{x},\beta) := \frac{1}{2} d_{\boldsymbol{x}}^2 r(\mathbf{0},\beta)[\boldsymbol{x},\boldsymbol{x}]$ is the quadratic part of the Liapunov–Schmidt reduction r, then, generically, all bifurcating branches guaranteed by the Equivariant Branching Lemma are unstable, regardless of the value of $\beta'(0)$. We cannot use this result in the present case since $d_{\boldsymbol{x}} Q(\mathbf{0},0)[\boldsymbol{x}_0] = d_{\boldsymbol{x}}^2 r(\mathbf{0},0)[\boldsymbol{x}_0]$, which we showed in the proof of Theorem 18, is identically zero.

Theorem 21. *Suppose q^* is M-singular for $1 < M \leqslant N$ and that $c'(0) >$ 0. All of the subcritical bifurcating branches (44) guaranteed by Theorem 17 are unstable. If*

$$\theta(q^*,\beta^*,m,n) := \sum_{k=1}^{M-1} (\theta_1 - 2\theta_2 - \theta_3) > 0,$$

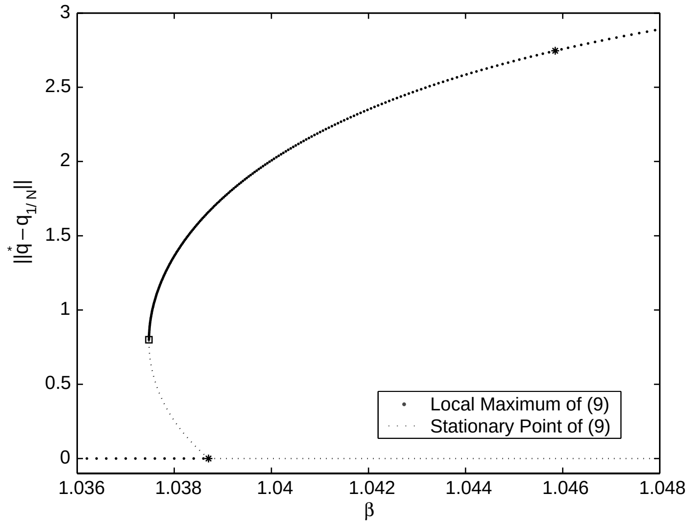

Figure 6. The subcritical bifurcation from the solution branch $(q_{\frac{1}{4}}, \beta)$ with symmetry S_4 to a branch with symmetry S_3 at $\beta^* = 1.0387$. This was predicted by the fact that $\zeta(q_{\frac{1}{4}}, 1.0387, 1, 3) < 0$. The bifurcation diagram is shown with respect to $\| q^* - q_{\frac{1}{N}} \|$. It is at the saddle node that this branch changes from being composed of stationary points to local solutions of the problem (9).

then the supercritical bifurcating branch consists of unstable solutions. The component functions of θ *are*

$$\begin{aligned}
\theta_1 &= \mathrm{d}^4\mathscr{L}[\boldsymbol{w}_k, \boldsymbol{w}_k, \boldsymbol{u}, \boldsymbol{u}],\\
\theta_2 &= \mathrm{d}^3\mathscr{L}[\boldsymbol{w}_k, \boldsymbol{u}, L^{-}\mathrm{d}^3\mathscr{L}[\boldsymbol{w}_k, \boldsymbol{u}]],\\
\theta_3 &= \mathrm{d}^3\mathscr{L}[\boldsymbol{w}_k, \boldsymbol{w}_k, L^{-}\mathrm{d}^3\mathscr{L}[\boldsymbol{u}, \boldsymbol{u}]],
\end{aligned}$$

where all of the derivatives are taken with respect to (q, λ)*, and* $\boldsymbol{w}_k$ *is a basis vector from (26).*

Proof. Subcritical bifurcating branches are unstable ([19] p. 91). To determine the stability of supercritical branches, consider the Taylor series of $r(\boldsymbol{x}, \beta)$ about $\boldsymbol{x} = 0$ up to cubic order

$$r(\boldsymbol{x}, \beta) = c(\beta)\boldsymbol{x} + Q(\boldsymbol{x}, \beta) + T(\boldsymbol{x}, \beta) + \mathcal{O}(\boldsymbol{w}^4),$$

where Q and T are the quadratic and cubic terms respectively. Thus

$$\begin{aligned}
\mathrm{trace}(\mathrm{d}_{\boldsymbol{x}} r(t\boldsymbol{x}_0, \beta)) = (M-1)c(\beta) &+ \mathrm{trace}(\mathrm{d}_{\boldsymbol{x}} Q(t\boldsymbol{x}_0, \beta))\\
&+ \mathrm{trace}(\mathrm{d}_{\boldsymbol{x}} T(t\boldsymbol{x}_0, \beta)) + \mathcal{O}(t^3).
\end{aligned}$$

Golubitsky *et al.* ([19] p. 93) show that trace($d_{\boldsymbol{x}}Q(t\boldsymbol{x}_0,\beta)$) = 0 for all β. Now substituting in the Taylor expansion for $c(\beta) = c(\beta(t))$ about $t = 0$ shows that trace($d_{\boldsymbol{x}}$r(t$\boldsymbol{x}_0$, β(t))) is

$$
\begin{aligned}
&= (M-1)\left(c'(0)\beta'(0)t + c''(0)\beta'(0)^2 + c'(0)\beta''(0)\frac{t^2}{2}\right) \\
&\quad + \text{trace}(d_{\boldsymbol{x}}T(t\boldsymbol{x}_0,\beta)) + \mathcal{O}(t^3) \\
&= (M-1)c'(0)\beta''(0)\frac{t^2}{2} + \text{trace}(d_{\boldsymbol{x}}T(t\boldsymbol{x}_0,\beta)) + \mathcal{O}(t^3)
\end{aligned}
$$

Since $c'(0) > 0$ and for supercritical branches $\beta''(0) > 0$, then we have that $d_{\boldsymbol{x}}r(t\boldsymbol{x}_0, \beta(t))$ must have an eigenvalue with positive real part for sufficiently small t if trace($d_x T(t\boldsymbol{x}_0,\beta)$) > 0. Since $T(\boldsymbol{x},\beta) = \frac{1}{6}d^3_{\boldsymbol{x}}r(\boldsymbol{0},\beta)[\boldsymbol{x},\boldsymbol{x},\boldsymbol{x}]$, then $d_{\boldsymbol{x}}T(t\boldsymbol{x}_0,\beta) = \frac{1}{2}t^2 d^3 r(\boldsymbol{0},\beta)[\boldsymbol{x}_0,\boldsymbol{x}_0]$, so

$$
\text{trace}(d_{\boldsymbol{x}}T(t\boldsymbol{x}_0,\beta)) = \sum_{i,j,k} \frac{\partial^3 r_k(0,0)}{\partial \boldsymbol{x}_i \partial \boldsymbol{x}_j \partial \boldsymbol{x}_k}[\boldsymbol{x}_0]_i[\boldsymbol{x}_0]_j = \theta(q^*,\beta^*,m,n),
$$

where the last equality follows from (40). □

Remark 22. The expression $\theta(q^*,\beta^*,m,n)$ from Theorem 21 can be simplified to a form which only uses derivatives of the constituent functions f of F,

$$
\begin{aligned}
\theta_1 &= \left(\frac{n^2}{m} + n\right) d^4 f[\boldsymbol{v},\boldsymbol{v},\boldsymbol{v},\boldsymbol{v}], \\
\theta_2 &= \boldsymbol{b}^T B^-(a_1 I_K + a_2 A^{-1})\boldsymbol{b}, \\
\theta_3 &= \boldsymbol{b}^T B^-(a_3 I_K + a_4 A^{-1})\boldsymbol{b},
\end{aligned}
$$

where a_i are scalars which depend only on m and n.

4.3. Application to Annealing

We now give some results which hold when F is an annealing problem as in (2)

$$
F(q,\beta) = H(q) + \beta D(q).
$$

First, we show that the crossing condition $c'(0) \neq 0$ in Theorem 17 can be checked in terms of the Hessian of the function D. Furthermore, when G is strictly concave, then $c'(0)$ is positive at any singularity of (20), so that every singularity is a bifurcation. Lastly, we show how to explicitly compute the discriminator $\zeta(q,\beta,m,n)$ for the Information Distortion problem (9).

A singularity of (20) at $(q^*, \lambda^*, \beta^*)$ results in a bifurcation when $\mathrm{d}^2 D(q)$ is positive definite on $\ker \mathrm{d}^2 F(q^*)$. In particular, this condition holds when $\mathrm{d}^2 G(q^*)$ is negative definite on $\ker \mathrm{d}^2 F(q^*)$.

Lemma 23. *Let* $\mathrm{d}^2 F(q^*, \beta^*)$*, at* $\beta^* \neq 0$*, be singular, and such that* $\mathrm{d}^2 G(q^*)$ *is negative definite on* $\ker \mathrm{d}^2 F(q^*)$*. Then* $\mathrm{d}^2 D(q^*)$ *is positive definite on* $\ker \mathrm{d}^2 F(q^*)$*.*

Proof. If $\boldsymbol{u} \in \ker \mathrm{d}^2 F(q^*)$, then $\boldsymbol{u}^T \mathrm{d}^2 G(q^*) \boldsymbol{u} + \beta^* \boldsymbol{u}^T \mathrm{d}^2 D(q^*) \boldsymbol{u} = 0$. Since $\boldsymbol{u}^T \mathrm{d}^2 G(q^*) \boldsymbol{u} < 0$, then we get $\mathbf{u}^T \mathrm{d}^2 D(q^*) \boldsymbol{u} > 0$. □

Now we show that if $\mathrm{d}^2 D(q^*)$ is positive definite on $\ker \mathrm{d}^2 F(q^*)$, then every singularity is a bifurcation point.

Lemma 24. *Suppose that* q^* *is* M*-singular for* $1 < M \leqslant N$*. If* $(q^*, \lambda^*, \beta^*)$ *is a singularity such that* $d^2 D(q^*)$ *is positive definite on* $\ker d^2 F(q^*)$*, then* $c'(0) > 0$*.*

Proof. By (42), $\mathrm{d}_{\boldsymbol{x}} r(\mathbf{0}, \beta) = c(\beta) I_{M-1}$. Now (36) gives

$$\boldsymbol{k}^T \mathrm{d}^2_{q,\lambda} \mathscr{L}(q^*, \lambda^*, \beta + \beta^*)(I_{NK+K} + \mathrm{d}_{\boldsymbol{w}} U(\mathbf{0}, \beta))\boldsymbol{k} = c(\beta) \|\boldsymbol{k}\|^2 \tag{49}$$

for some $\boldsymbol{k} \in \ker \mathrm{d}^2 \mathscr{L}(q^*)$. By Theorem 11, an arbitrary $\boldsymbol{k} \in \ker \mathrm{d}^2 \mathscr{L}(q^*)$ can be written as

$$\boldsymbol{k} = \begin{pmatrix} \boldsymbol{k}_F \\ \mathbf{0} \end{pmatrix},$$

where $\boldsymbol{k} \in \ker \mathrm{d}^2 F(q^*, \beta^*)$. Substituting this into (49), differentiating with respect to β, and using (35) yields

$$c'(0) = \frac{\boldsymbol{k}_F^T \mathrm{d}^2 D(q^*) \boldsymbol{k}_F}{\|\boldsymbol{k}_F\|^2}, \tag{50}$$

which must be positive since $\mathrm{d}^2 D(q^*)$ is positive definite on $\ker \mathrm{d}^2 F(q^*)$. Thus an eigenvalue of $\mathrm{d}_x r(\mathbf{0}, \beta)$ changes sign. □

For-the Information Distortion problem (9), $G(q) = H(Z|Y)$ is strictly concave and so $\mathrm{d}^2 G$ is negative definite on Δ. By Lemmas 23 and 24, every singularity is a bifurcation point. Therefore the bifurcation discriminator and Theorem 20 can always be applied to bifurcations of equilibria for the Information Distortion problem (9). For the Information Bottleneck problem (11), $G(q) = -I(Y:Z)$ is concave, but not strictly concave. In fact, $\mathrm{d}^2 F(q, \beta) = \mathrm{d}^2(-I(Y:Z) + \beta D_{\mathrm{eff}})$ is singular for every value of (q, β) [32].

The following Lemma provides an explicit expression for the discriminant $\zeta(q^*, \beta^*, m, n)$ for the Information Distortion problem (9), $F = H(q) + \beta D_{\text{eff}}(q)$, which we use for numerical calculations in Section 7.

Lemma 25. *For the Information Distortion problem (9).*

$$\frac{\partial^3 F}{\partial q_{\nu r} \partial q_{\nu s} \partial q_{\nu t}} = \frac{1}{\ln 2}\left(\delta_{rst}\frac{p(y_r)}{q_{\nu r}^2} + \beta\left(\frac{p(y_r)p(y_s)p(y_t)}{\left(\sum_j p(y_j)q_{\nu j}\right)^2} - \sum_i \frac{p(x_i, y_r)p(x_i, y_s)p(x_i, y_t)}{\left(\sum_j p(x_i, y_j)q_{\nu j}\right)^2}\right)\right).$$

The expression

$$\frac{\partial^4 F}{\partial q_{\nu r} \partial q_{\nu s} \partial q_{\nu t} \partial q_{\nu u}} = \frac{2}{In2}\left(\beta\left(\sum_i \frac{p(x_i, y_r)p(x_i, y_s)p(x_i, y_t)p(x_i, y_u)}{\left(\sum_j p(x_i, y_j)q_{\nu j}\right)^3} - \frac{p(y_r)p(y_s)p(y_t)p(y_u)}{\left(\sum_j p(y_j)q_{\nu j}\right)^3}\right) - \delta_{rstu}\frac{p(y_r)}{q_{\nu r}^3}\right).$$

Proof. Direct computation using (6) and (8). □

4.4. Stability and Optimality

In this subsection we relate the stability of equilibria $(q^*, \lambda^*, \beta^*)$ in the flow (20) with optimality of q^* in the problem (1). In particular, if a bifurcating branch corresponds to an eigenvalue of $d^2\mathscr{L}(q^*)$ changing from negative to positive, then the branch consists of stationary points (q^*, β^*) which are not solutions of (1). Positive eigenvalues of $d^2\mathscr{L}(q^*)$ do not necessarily show that q^* is not a solution of (1) (see Remark 5). For example, consider the Information Distortion problem (9) and the Four Blob problem presented in Figure 1. In this scenario, for the equilibria (q^*, λ^*, β) of (20) such that (q^*, β^*) is a solution of (9), $d^2\mathscr{L}(q^*)$ always has at least 52 positive eigenvalues, even when $d^2F(q^*)$ is negative definite.

Theorem 26. *For the bifurcating branch (44) guaranteed by Theorem 17,* $\boldsymbol{u}$ *is an eigenvector of*

$$d^2\mathscr{L}\left(\begin{pmatrix} q^* \\ \lambda^* \end{pmatrix} + t\boldsymbol{u}, \beta^* + \beta(t)\right)$$

for sufficiently small t. Furthermore, if the corresponding eigenvalue is positive, then the branch consists of stationary points which are not solutions to (1).

Proof. We first show that $\boldsymbol{u}$ is an eigenvector of $\mathrm{d}^2\mathscr{L}(q^*+t\hat{\boldsymbol{u}}, \lambda^*, \beta^*+\beta(t))$ for small t. Let $Q=\begin{pmatrix} q \\ \lambda \end{pmatrix}$ so that

$$\mathscr{F}(Q,\beta) := \nabla\mathscr{L}(q^*+q, \lambda^*+\lambda, \beta^*+\beta).$$

Thus, a bifurcation of solutions to $\mathscr{F}(Q,\beta)=\mathbf{0}$ occurs at $(\mathbf{0}, 0)$. For $\gamma \in \sum := \sum_{(m,n)}$, $\mathscr{F}(t\boldsymbol{u},\beta) = \mathscr{F}(t\gamma\boldsymbol{u},\beta) = \gamma\mathscr{F}(t\boldsymbol{u},\beta)$, where the first equality follows from Lemma 14, and the second equality follows from equivariance. Hence, $\mathscr{F}(t\boldsymbol{u},\beta)$ is in Fix($\sum$), which is one dimensional with basis vector $\boldsymbol{u}$, showing that $\mathscr{F}(t\boldsymbol{u},\beta)=h(t,\beta)\boldsymbol{u}$ for some scalar function $h(t,\beta)$. Taking the derivative of this equation with respect to t, we get

$$\mathrm{d}_Q\mathscr{F}(t\boldsymbol{u},\beta)\boldsymbol{u} = \mathrm{d}_t h(t,\beta))\boldsymbol{u}, \tag{51}$$

which shows that $\boldsymbol{u}$ is an eigenvector of $\mathrm{d}^2\mathscr{L}(q^*+t\hat{u}, \lambda^*, \beta+\beta(t))$, with corresponding eigenvalue $\xi = \mathrm{d}_t h(t,\beta)$. Using (18) and letting $\widehat{\mathrm{d}^2 F} := \mathrm{d}^2 F(q^*+t\hat{\boldsymbol{u}}, \lambda^*, \beta+\beta(t))$, we see that (51) can be rewritten as

$$\begin{pmatrix} \widehat{\mathrm{d}^2 F} & J^T \\ J & \mathbf{0} \end{pmatrix}\begin{pmatrix} \hat{\boldsymbol{u}} \\ \mathbf{0} \end{pmatrix} = \xi \begin{pmatrix} \hat{\boldsymbol{u}} \\ \mathbf{0} \end{pmatrix},$$

which shows that $\widehat{\mathrm{d}^2 F}\hat{\boldsymbol{u}} = \xi\hat{\boldsymbol{u}}$ and $J\hat{\boldsymbol{u}}=\mathbf{0}$. Thus, $\hat{\boldsymbol{u}} \in \ker\ J$ is an eigenvector of $\mathrm{d}^2 F(q^*+t\hat{\boldsymbol{u}}, \beta+\beta(t))$ with corresponding eigenvalue ξ. If $\xi>0$, the desired result now follows from Remark 5. □

We used Theorem 26 to show that the subcritical bifurcating branch depicted in Figure 6 is not composed of solutions to the constrained problem (9).

5. SADDLE-NODE BIFURCATIONS

We now turn our attention to bifurcations which are not symmetry breaking bifurcations of equilibria of (20),

$$\begin{pmatrix} \dot{q} \\ \dot{\lambda} \end{pmatrix} = \nabla\mathscr{L}(q,\lambda,\beta).$$

We show that, generically, these bifurcations are saddle-node bifurcations, which we have illustrated numerically in Figure 6 for the Information

Distortion problem (9). A bifurcation which is not a symmetry breaking bifurcation will be called a *symmetry preserving bifurcation*.

To analyze symmetry breaking bifurcations, we exploited the singular blocks of $d^2F(q^*)$. For the symmetry preserving case, we have the following relationship with $d^2F(q^*)$.

Lemma 27. *At a generic symmetry preserving bifurcation* $(q^*, \lambda^*, \beta^*)$*, the Hessian* $d^2F(q^*)$ *is nonsingular.*

Proof. Assume that $d^2F(q^*)$ is singular. We will show that this assumption leads to the conclusion that q^* undergoes a symmetry breaking bifurcation or no bifurcation at all. If $d^2F(q^*)$ is singular, then at least one of the blocks B_i is singular. If the corresponding partition set $|\mathcal{U}_j| > 1$ (see Definition 6), then there are multiple blocks equal to B_i, and so Theorem 17 implies that q^* undergoes a symmetry breaking bifurcation. If the corresponding partition set $|\mathcal{U}_j| = 1$, then B_i is the only block that is singular by genericity, so $d^2\mathcal{L}$ is nonsingular by Corollary 12. This leads to a contradiction since we assume that bifurcation takes place at q^*. □

Theorem 28. *Consider a singularity* $(q^*, \lambda^*, \beta^*)$ *of* (20) *such that* $d^2F(q^*)$ *is nonsingular. Then*

(1) The matrices A_j *are singular for all* j.
(2) The spaces $\ker A_i = \ker A_j$ *for all* i *and* j. *Generically. these spaces are one dimensional.*
(3) Generically, $\dim \ker d^2\mathcal{L}(q^*) = 1$.
(4) The basis vector for $\ker A_i$ *is* $\mathbf{v}$ *if and only if the basis vector for* $\ker d^2\mathcal{L}(q^*)$ *is*

$$\boldsymbol{w} = \left((B_1^{-1}\mathbf{v})^T, (B_2^{-1}\mathbf{v})^T, \ldots, (B_N^{-1}\mathbf{v})^T, -\mathbf{v}^T\right)^T. \tag{52}$$

Proof. By assumption $d^2\mathcal{L}(q^*)$ is singular, but all of the blocks B_i are nonsingular. Take $\boldsymbol{k} \in \ker d^2\mathcal{L}(q^*)$ and decompose it as $\boldsymbol{k} = (\boldsymbol{k}_F^T, \boldsymbol{k}_J^T)^T$ as in the proof to Theorem 11. Since $d^2F(q^*)$ is non-singular, we must have $\boldsymbol{k}_J \neq 0$. We follow the argument of Theorem 11 up until (31), which gets replaced by

$$B_\eta \boldsymbol{x}_\eta = -\boldsymbol{k}_J \quad \text{for all } \eta. \tag{53}$$

It follows that $\boldsymbol{x}_\eta = -B_\eta^{-1}\boldsymbol{k}_J$ for any η. By (28), we have that

$$\sum_{i=1}^{N} \boldsymbol{x}_i = -\sum_\eta B_\eta^{-1}\boldsymbol{k}_J = 0. \tag{54}$$

Select now an index j of some block B_j of the Hessian $\mathrm{d}^2F(q^*)$. Recall that for all $\nu \in \mathcal{U}_j$ we have $B_\nu = \bar{B}_j$. Let $|\mathcal{U}_j| = M$. Then (54) can be written as

$$\sum_{\eta \notin \mathcal{U}_j} B_\eta^{-1} \boldsymbol{k}_J + \sum_{\nu \in \mathcal{U}_j} B_\nu^{-1} \boldsymbol{k}_J = \sum_{\eta \notin \mathcal{U}_j} B_\eta^{-1} \boldsymbol{k}_J + M \bar{B}_j^{-1} \boldsymbol{k}_J = 0.$$

This is equivalent to

$$\left(\bar{B}_j \sum_{\eta \notin \mathcal{U}_j} B_\eta^{-1} + MI \right) \boldsymbol{k}_j = 0. \tag{55}$$

Since $A_j = \bar{B}_j \sum_{\eta \notin \mathcal{U}_j} B_\eta^{-1} + MI$ we conclude that A_j has a nontrivial kernel spanned by $\boldsymbol{k}_J$. Since j was arbitrary, this proves (1). By genericity (Theorem 7), the kernel of A_j is one dimensional, which proves (2). It follows from (53) that given $\boldsymbol{k}_J$, the vector $\boldsymbol{k}_F$ is determined uniquely. This proves (3). Finally, (53) and (55) show that $\boldsymbol{k}$ has the form in (4). □

Next, we provide a sufficient condition for the existence of saddle-node bifurcations. Observe that the first assumption given in the following theorem is satisfied generically at any symmetry preserving bifurcation (Lemma 27), the second assumption is a crossing condition, and the third condition assures that $\beta'' \neq 0$.

Theorem 29. *Suppose that $(q^*, \lambda^*, \beta^*)$ is a sinqularity of (20) such that:*

(1) The Hessian $\mathrm{d}^2F(q^*)$ is nonsingular.
(2) The dot product $\boldsymbol{w}^T \begin{pmatrix} \mathrm{d}_\beta \nabla F(q^*, \beta^*) \\ \mathbf{0} \end{pmatrix} \neq 0$ for $\boldsymbol{w}$ defined in (52).
(3) $\sum_{\nu=1}^N \mathrm{d}^3 f \left[B_\nu^{-1} \boldsymbol{v}, B_\nu^{-1} \boldsymbol{v}, B_\nu^{-1} \boldsymbol{v} \right] \neq 0.$

Then, generically, $(q^*, \lambda^*, \beta^*)$ is a saddle-node bifurcation.

Proof. To prove the theorem, we show that there is a unique solution branch $\left(\begin{pmatrix} q^* \\ \lambda^* \end{pmatrix} + t\boldsymbol{u}, \beta^* + \beta(t) \right)$ in a neighborhood of $(q^*, \lambda^*, \beta^*)$ with $\beta'(0) = 0$ and $\beta''(0) \neq 0$[2]. By Theorem 28, generically, $\ker \mathrm{d}^2\mathcal{L}(q^*)$ has a single basis vector $\boldsymbol{w}$ of the form (52), so that any vector $\boldsymbol{u} \in \ker \mathrm{d}^2\mathcal{L}(q)$ can be written as $\boldsymbol{u} = x_0 \boldsymbol{w}$ for some nonzero scalar $\boldsymbol{x}_0 \in \mathbf{R}$. The Liapunov–Schmidt reduction in this case is (compare with (34)),

$$\begin{aligned} r &: \mathbf{R} \times \mathbf{R} \to \mathbf{R} \\ r(x, \beta) &:= \boldsymbol{w}^T (I - E) \mathcal{F}(\boldsymbol{w}x + U(\boldsymbol{w}x, \beta), \beta), \end{aligned} \tag{56}$$

where $\mathscr{F}(q,\lambda,\beta) = \nabla\mathscr{L}(q+q^*,\lambda+\lambda^*,\beta+\beta^*)$ and $q = \boldsymbol{w}x + U(\boldsymbol{w}x,\beta)$. Thus

$$r(tx_0,\beta) = h(t,\beta)x_0$$

for some scalar function $h(t,\beta)$, which can not be factored as we did in the proof to Theorem 18 since $(t=0,\beta)$ is not a critical point of r: by assumption 2 above

$$\mathrm{d}_\beta r(0,0) = \mathrm{d}_\beta h(0,0)x_0 = \boldsymbol{w}^T \mathrm{d}_\beta \nabla\mathcal{L}(q^*,\lambda^*,\beta^*) = \boldsymbol{w}^T \begin{pmatrix} \mathrm{d}_\beta \nabla F(q^*,\beta^*) \\ \mathbf{0} \end{pmatrix}$$

is nonzero (see (38)). Thus, the Implicit Function Theorem can be used to solve $h(t,\beta)=0$ uniquely for $\beta=\beta(t)$ in a neighborhood of $(t=0,\beta=0)$. This shows that there is a unique solution branch in a neighborhood of (q^*,λ^*,β^*). Analogous to how we computed $\beta'(0)$ in (47), we have that

$$\beta'(0) = -\frac{\mathrm{d}_t h(0,0)}{\mathrm{d}_\beta h(0,0)} = -\frac{\mathrm{d}_x r(0,0)}{\mathrm{d}_\beta h(0,0)} = 0.$$

Similar to the computations we did in the proof to Theorem 20 we see that

$$\beta''(0) = -\frac{\mathrm{d}_t^2 h(0,0)}{\mathrm{d}_\beta h(0,0)} = -\frac{\mathrm{d}_x^2 r(0,0)[x_0,x_0,x_0]}{x_0^2 \mathrm{d}_\beta h(0,0)}.$$

Calculating the derivative $\mathrm{d}_x^2 r(0,0))[x_0,x_0,x_0]$ as we did in (39), and the explicit form of $\boldsymbol{w}$ given in Theorem 28 show that $\beta''(0) = \mathrm{sgn}\left(-\sum_\nu \mathrm{d}^3 f[B_\nu^{-1}\boldsymbol{v}, B_\nu^{-1}\boldsymbol{v}, B_\nu^{-1}\boldsymbol{v}]\right)$, which we assumed was nonzero. □

6. BIFURCATION STRUCTURE

We have described the generic bifurcation structure of problems of the form (1)

$$\max_{q\in\Delta} F(q,\beta) = \max_{q\in\Delta}\left(\sum_{\nu=1}^N f(q^\nu,\beta)\right).$$

The type of bifurcation which occurs depends on three types of singular points of $\mathrm{d}^2\mathscr{L}(q^*)$ and $\mathrm{d}^2F(q^*)$, which we have depicted in Figure 7.

The first type of singular point is where the $M>1$ blocks B_i of d^2F, for $i\in\mathscr{U}$, are singular. By Lemma 10, $\mathrm{d}^2\mathscr{L}$ must be singular. Generically, the blocks, $\{B_\nu\}_{\nu\notin\mathscr{U}}$ of d^2F are nonsingular, and $A_i = B_i\Sigma_{\nu\notin\mathscr{U}}B_\nu^{-1} + MI_K$ is nonsingular. Theorem 17 shows that this is the type of singularity that exhibits symmetry breaking bifurcation.

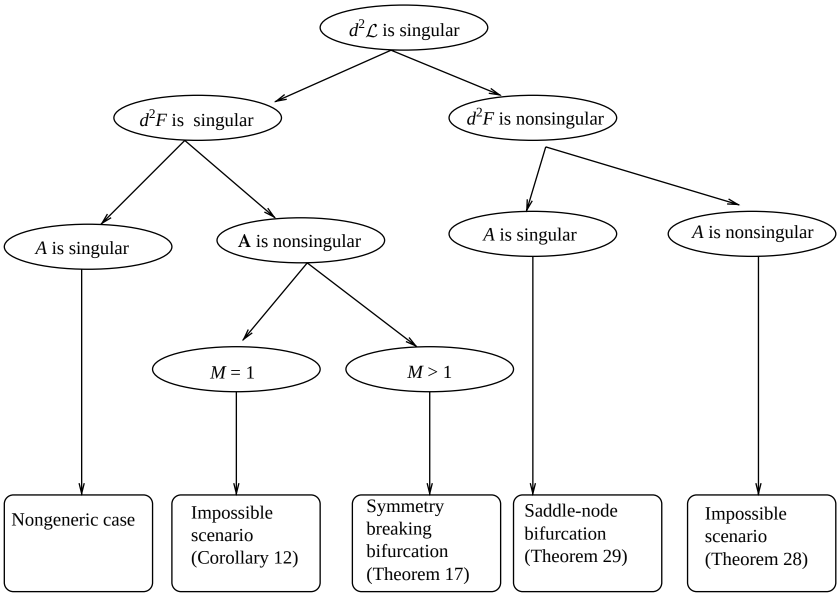

Figure 7. A hierarchical diagram showing how the singular points of $d^2\mathscr{L}$ and d^2F affect the bifurcation structure of equilibria of (20).

The second type of singular point is a special case in which no bifurcation occurs. If only a single block, B_i, of d^2F is singular (i.e., $M = 1$), and if the generic condition that the corresponding A_i is nonsingular holds, then we show in Corollary 12 that $d^2\mathscr{L}$ is nonsingular. Thus, generically, no bifurcation occurs for this case.

The third type of singular point is when $d^2\mathscr{L}$ is singular, but when d^2F is nonsingular. By Theorem 28, it must be that all of the matrices A_i are singular. This singular point manifests itself as a saddle-node bifurcation (Theorem 29). Figure 7, which summarizes the preceding discussion, indicates how the singular points of $d^2\mathscr{L}$ and d^2F affect the bifurcations of equilibria of (20).

7. NUMERICAL RESULTS

We created software in MATLAB which implemented pseudo-arclength continuation [2, 13] to numerically illustrate the bifurcation structure guaranteed by the theory of Sections 4 and 5. All of the results presented here are for the Information Distortion problem (9).

$$\max_{q \in \Delta}(H(q) + \beta D_{\text{eff}}(q))$$

and for the Four Blob Problem introduced in Figure 1.

Figure 3 is analogous to Figure 1. It uses the same data set and the same cost function. The difference is that Figure 1 was obtained using the Basic Annealing Algorithm, while we used the continuation algorithm in Figure 3. The continuation algorithm shows that the bifurcation picture is richer than shown in Figure 1. Panels 1–5 in Figure 3 show that the clusterings along the branches break symmetry from S_4 to S_3 to S_2, and, finally, to S_1. An "*" indicates a point where $d^2F(q^*)$ is singular, and a square indicates a point where $d^2\mathscr{L}(q^*)$ is singular. Notice that there are points denoted by "*" from which emanate no bifurcating branches. At these points a single block of d^2F is singular, and, as explained by Corollary 12, $d^2\mathscr{L}(q^*)$ is nonsingular. Notice that there are also points where both $d^2\mathscr{L}(q^*)$ and $d^2F(q^*)$ are singular (at the symmetry breaking-bifurcations) and points where just $d^2\mathscr{L}(q^*)$ is singular (at the saddle-node bifurcations). These three types of singular points are depicted in Figure 7.

Figure 4 illustrates symmetry breakdown from S_4 to $S_2 \times S_2$. The clusterings depicted in the panels are not found when using an algorithm which is affected by the stability of the equilibria (such as the Basic annealing Algorithm).

Theorem 20 shows that the bifurcation discriminator, $\zeta(q^*, \beta^*, m, n)$, can determine whether the bifurcating branches guaranteed by Theorem 17 are subcritical ($\zeta < 0$) or supercritical ($\zeta > 0$). We considered the bifurcating branches from $(q_{\frac{1}{N}}, \lambda^*, \beta^* = 1.0387)$ with isotropy group S_{N-1}. The numerical results obtained by calculating $\zeta(q_{\frac{1}{N}}, \beta^*, 1, N-1)$ for $N = 2, 3, 4, 5$ and 6 at $\beta^* = 1.0387$ are shown in Table 1. The subcritical bifurcation predicted by the discriminator for the Information Distortion problem (9) for $N = 4$ is shown in Figure 6.

Figure 8 explores some of the clusterings on one of the secondary branches after symmetry breaks from S_3 to S_2.

Table I. The bifurcation discriminator: Numerical evaluations of the bifurcation discriminator $\zeta(q_{\frac{1}{N}}, \beta^* \approx 1.038706, m = 1, n = N-1)$ as a function of N for the four blob problem (see Figure 1a) when F is defined as in (9). A supercritical bifurcation is predicted when $N = 2$, and subcritical bifurcations for $N \in \{3, 4, 5, 6\}$.

N	2	3	4	5	6
$\zeta(q_{\frac{1}{N}}, \beta^*, m, n)$	0.0006	−0.0010	−0.0075	−0.0197	−.0391

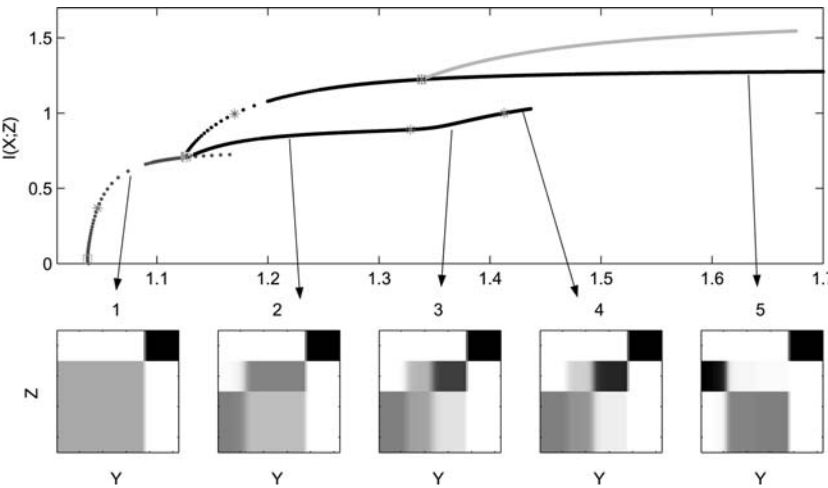

Figure 8. The symmetry breaking bifurcations branches from the solution branch $(q_{\frac{1}{N}}, \lambda, \beta)$ (which has symmetry S_4) at $\beta^* = 1.087$, as in Figure 3, but now we investigate further the branches which have S_2 symmetry.

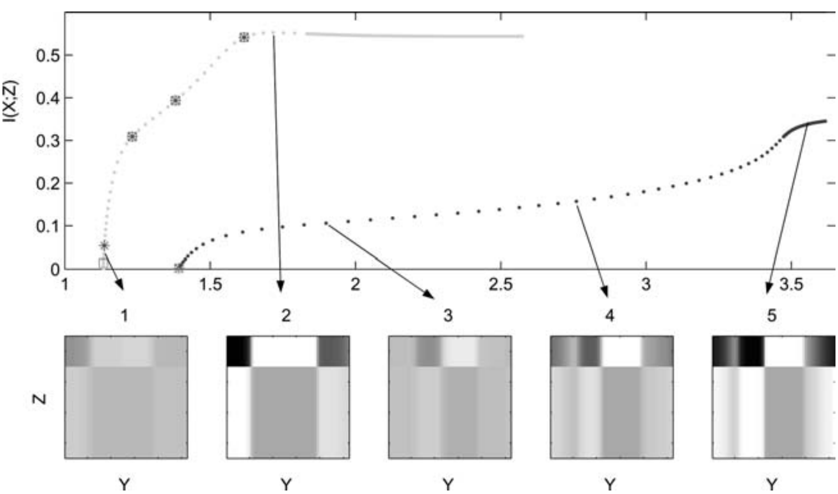

Figure 9. Depicted here are bifurcating branches with S_3 symmetry from the $q_{\frac{1}{N}}$ branch at the β values 1.133929 and 1.390994 which occur after the bifurcation shown in Figure 3. The bottom panels show some of the particular clusterings along these branches.

Figure 9 illustrates clusterings along branches which emanate from $q^* = q_{\frac{1}{N}}$ at larger β than the value of $\beta = 1.0387$ at the first bifurcation.

These branches are locally unstable at bifurcation, and do not give solutions of (9). However, we cannot at the moment reject the possibility that these branches continue to a branch that leads to a global maximum of (3) as $\beta \to \infty$.

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REFERENCES

1. Barlow, H. B. (1961). Possible principles underlying the transformation of sensory messages. In Rosenblith, W. A. (ed.), *Sensory Communications*, MIT Press. Cambridge. MA.
2. Beyn, W. J., Champneys, A., Doedel, E., Govaerts, W., Kuznetsov, Y. A., and Sandstede, B. (1999). Numerical continuation and computation of normal forms, In *Handbook of Dynamical System III*. World Scientific, Singapore.
3. Cicogna, G. (1981). Symmetry breakdown from bifurcation. *Lett. Al Nuevo Cimento* **31**, 600–602.
4. Cicogna, G. (1982). Bifurcation and symmetries. *Bollettino Un. Mat. ltal.* 787–796.
5. Cohen, J., and Stewart, I. (2000). Plymorphism viewed as phenotypic symmetry-breaking. In Malik, S. K., Chandrashekaran, M. K., and Pradhan, N. (eds.), *Non-linear Phenomena in Biological and Physical Sciences*. Indian National Science Academy, New Delhi, pp. 1–63.
6. Conway, J., Curtis, R. T., Norton, S. P., Parker, R. A., and Wilson, R. (1985). *Atlas of Finite Groups.* Clarendon Press, Oxford, p. 236.
7. Cover, T., and Thomas, J. (1991). *Elements of Information Theory. Wiley Series in Communication*, New York.
8. Dias, A. P. S., and Stewart, I. (2003). Secondary bifurcations with all-to-all coupling. *Proc. R. Soc. Land.* **459**.
9. Dimitrov, A. G., and Miller, J. P. (2000). Analyzing sensory systems with the information distortion function. In Altman, R. B. (ed.), *Pacific Symposium on Biocomputing 2001*, World Scientific Publishing Co., Singapore.
10. Dimitrov, A. G., and Miller, J. P. (2001). Neural coding and decoding: communication channels and quantization. *Netw.: Comput. in Neural Syst.* **12**(4), 441–472.
11. Dimitrov, A. G., Miller, J. P., Aldworth, Z., Gedeon, T., and Parker, A. E. (2003). Analysis of neural coding through quantization with an information-based distortion measure. *Netw.: Comput. Neural Syst.* **14**, 151–170.
12. Dimitrov, A. G., Miller, J. P., Aldworth, Z., and Parker, A. (2002). Spike pattern-based coding schemes in the cricket cereal sensory system. *Neurocomput.* 373–379.
13. Doedel, E., Keller, H. B., and Kernevez, J. P. (1991). Numerical analysis and control of bifurcation problems in finite dimensions. *Int. J. Bifurcation Chaos* **1**, 493–520.
14. Elmhirst, T. (1998). Symmetry-breaking bifurcations of S_n-equivariant vector fields and polymorphism. MSc thesis, Mathematics Institute, University of Warwick.
15. Elmhirst, T. (2001). Symmetry and emergence in polymorphism and sympiatic speciation. PhD thesis. Mathematics Institute, University of Warwick.

16. Gedeon, T., Parker, A. E., and Dimitrov, A. G. (2003). Information distortion and neural coding. *Can. Appl. Math. Q.* **10**(1), 33–70.
17. Golubitsky, M., and Schaeffer, D. G. (1985). *Singularities and Groups in Bifurcation Theory I*. Springer-Verlag, New York.
18. Golubitsky, M., and Stewart, I. (2002). *The Symmetry Perspective: From Equilibrium to Chaos in Phase Space and Physical Space*. Birkhauser Verlag, Boston.
19. Golubitsky, M., Stewart, I., and Schaeffer, D. G. (1988). *Singularities and Groups in Bifurcation Theory II*. Springer-Verlag, New York.
20. Gray, R. M. (1990). *Entropy and Information Theory*. Springer-Verlag, New York.
21. Hirsch, M. W. (1976). *Differential Topology*. Springer-Verlag, New York.
22. James, G., and Kerber, A. (1981). *The Representation Theory of the Symmetric Group*. The Encyclopedia of Mathematics and Applications, Vol. 16, Addison-Wesley, Reading, Massachusetts.
23. Jaynes, E. T. (1982). On the rationale of maximum-entropy methods. *Proc. IEEE* **70**, 939–952.
24. Johnson, D. H., Gruner, C. M., Baggerly, K., and Seshagiri, C. (2001). Information-theoretic analysis of the neural code. *J. Comp. Neurosci.* **10**(1), 47–70.
25. Kjaer, T. W., Hertz, J. A., and Richmond, B. J. (1994). Decoding cortical neuronal signals: Network models, information estimation and spatial tuning. *J. Comp. Neurosci*. **l**(l–2), 109–139.
26. Kullback, S. (1959). *Information Theory and Statistics*. Wiley, New York.
27. Liebeck, M. W., Praeger, C. E., and Saxl, J. (1987). A classification of the maximal subgroups of the finite alternating and symmetric groups. *J. Algebra* 365–383.
28. Mumey, B., and Gedeon, T. (2003). *Optimal Mutual Information Quantization is NP-complete*. Neural Information Coding (NIC) workshop, Snowbird UT.
29. Nocedal, J., and Wright, S. J. (2000). *Numerical Optimization*. Springer, New York.
30. Paninski, L. (2003). Estimation of entropy and mutual information. *Neural Computation*.
31. Parker, A., Gedeon, T., and Dimitrov, A. (2003). Annealing and the rate distortion problem. In Becker, S. T. S., and Obermayer, K. (eds.), *Advances in Neural Information Processing Systems*, Vol. 15, MIT Press, Cambridge, MA, pp. 969–976.
32. Parker, A. E. (2003). Symmetry breaking bifurcations of the information distortion. PhD Thesis. Montana State University.
33. Rieke, F., Warland, D., de Ruyter van Steveninck, R. R., and Bialek, W. (1997). *Spikes: Exploring the neural code*. The MIT Press, Cambridge, USA.
34. Rose, K. (1998). Deteministic annealing for clustering, compression, classification, regression, and related optimization problems. *Proc. IEEE* **86**(ll), 2210–2239.
35. Schneidman, E., Slonim, N., Tishby, N., de Ruyter van Steveninck, R. R., and Bialek, W. (2003). Analyzing neural codes using the information bottleneck method. In *Advances in Neural Information Processing Systems*, Vol. 15, MIT Press, Cambridge, USA.
36. Schott, J. R. (1997). *Matrix Analysis for Statistics*. Wiley, New York.
37. Slonim, N. (2002). The information bottleneck: Theory and applications. Doctoral Thesis. Hebrew University, Jerusalem.
38. Slonim, N., and Tishby, N. (2000). Agglomerative information bottleneck. In Solla, S. A. Leen, T. K., and Müller, K. (eds.), *Advances in Neural Information Processing Systems*, Vol. 12, MIT Press, Cambridge, USA, pp. 617–623.
39. Stewart, I. (2003). Self-organization in evolution: A mathematical perspective. *Philos. Trans. R. Soc.* **361**, 1101–1123.
40. Stewart, I., Elmhirst, T., and Cohen, J. (2003). Symmetry-breaking as an origin of species. In Buescu, J. Castro, S. B., Dias, A., and Labouriau, I. S. (eds.), *Trends in Mathematics: Bifurcations, Symmetry and Patterns*, Birkhauser Verlag Basel/Switzerland, pp. 3–54.

41. Tishby, N., Pereira, P. C., and Bialek, W. (1999). The information bottleneck method. The 37th Annual Allerton Conference on Communication, Control, and Computing.
42. Vanderbauwhede, A. (1980). Local bifurcation and symmetry. Habilitation Thesis. Rijksuniversiteit Gent.