

ON THE BIRTH OF ISOLAS*

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Abstract. Isolals are isolated, closed curves of solution branches of nonlinear problems. They have been observed to occur in the buckling of elastic shells, the equilibrium states of chemical reactors and other problems. In this paper we present a theory to describe analytically the structure of a class of isolals. Specifically, we consider isolals that shrink to a point as a parameter τ of the problem, approaches a critical value τ_0 . The point is referred to as an isola center. Equations that characterize the isola centers are given. Then solutions are constructed in a neighborhood of the isola centers by perturbation expansions in a small parameter ε that is proportional to $(\tau - \tau_0)^\alpha$, with α appropriately determined. The theory is applied to a chemical reactor problem.

1. Introduction. Isolals are isolated, closed curves of solution branches of nonlinear problems. They have been determined numerically and experimentally in a variety of problems such as the equilibrium states of chemical reactors [1]–[4] and the buckling of elastic shells [5], [6], [7] and arches [8]. In this paper we present a theory to describe the mathematical structure of a class of isolals and a perturbation method to calculate them.

To motivate the analysis we first consider the elementary geometry of surfaces in \mathbb{R}^3 . Specifically, a surface Γ in (ξ, λ, τ) -space is given implicitly by,

$$(1.1) \quad f(\xi, \lambda, \tau) = 0.$$

If the normal to Γ at the point $\mathbf{p}_0 \equiv (\xi_0, \lambda_0, \tau_0)$ is in the direction of the τ -axis, then we have

$$(1.2) \quad f(\mathbf{p}_0) = f_\xi(\mathbf{p}_0) = f_\lambda(\mathbf{p}_0) = 0.$$

The level curves of Γ in planes parallel to and near to the plane $\tau = \tau_0$ are characterized by the Gaussian curvature of Γ at \mathbf{p}_0 , or equivalently by the sign of the discriminant

$$(1.3) \quad D_0 \equiv f_{\xi\xi}^0 f_{\lambda\lambda}^0 - f_{\xi\lambda}^0.$$

Here the superscript zero means that the quantity is evaluated at \mathbf{p}_0 . If $D_0 > 0 (< 0)$, the surface is elliptic (hyperbolic) at \mathbf{p}_0 and the level curves are, locally, ellipses (hyperbolas). Taylor expansions of f about \mathbf{p}_0 with $\tau = \tau_0 + \delta$ fixed yield, to leading order, the equations for these ellipses and hyperbolas.

Our characterization of isolals for the nonlinear problems considered below closely parallels this simple geometry. Specifically, the ellipses are isolals, and the point \mathbf{p}_0 is called the isola center. In the hyperbolic case the level curves for $\tau = \tau_0$ form two intersecting curves with distinct tangents, i.e., \mathbf{p}_0 is a bifurcation point of the level curves. For small $\tau - \tau_0 \neq 0$, the curves form hyperbolas so that the bifurcation is

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destroyed by the perturbation. Thus, for $D_0 \neq 0$ the point \mathbf{p}_0 is a critical point of the family of level curves. It is characterized as a root of (1.2). We also treat the case corresponding to $f_\tau^0 = 0$. Then the critical point \mathbf{p}_0 is also a singular point of the surface Γ , e.g., a cusp or a vertex of a cone; see Fig. 1.

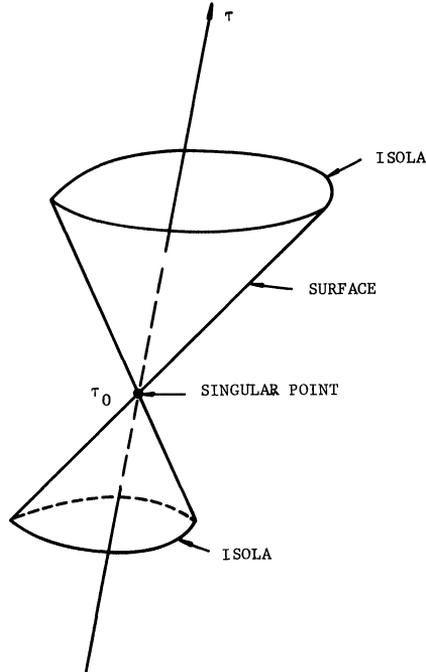


FIG. 1. Sketch of an isola surface, where the isola center is a singular point of the surface.

More generally, we consider nonlinear problems

$$(1.4) \quad F[u, \lambda, \tau] = 0$$

depending on two scalar parameters λ and τ . Here F is a nonlinear operator and $u(\lambda, \tau)$ is a solution vector. For a fixed value of τ , an isola is a closed "curve" in (u, λ) -space. As τ varies we obtain a one-parameter family of isolas which are the level curves of a "surface" in (u, λ, τ) -space. We refer to this as an isola surface. Furthermore, we assume that the isola surface shrinks to a point $\mathbf{p}_0 \equiv (u_0, \lambda_0, \tau_0)$ as τ approaches a critical value τ_0 . Alternatively, we may think of the isola as growing out of this point, its birthpoint. We refer to the point as an isola center. It is a critical point of the family of level curves of the solution surface of (1.4). To aid in geometrical visualization, an appropriate scalar amplitude of u is defined in § 2. We denote it by $\xi(\lambda, \tau)$. For each solution of (1.4) and for each fixed value of τ , $\xi(\lambda, \tau)$ defines a response curve in the (ξ, λ) -plane. We consider problems (1.4) which possess closed response curves. The amplitude ξ is defined so that each closed response curve corresponds to a closed curve in (u, λ) -space, i.e., to an isola.

Our method for determining isola solutions of (1.4) is to first find the critical points \mathbf{p}_0 of (1.4) which are analogous to those defined by (1.2). Then we determine approximations to the solutions of (1.4) near \mathbf{p}_0 by a perturbation expansion in a small parameter ε . The parameter is proportional to $(\tau - \tau_0)^\alpha$, where α is an appropriately determined positive integer. If isola solutions exist in the neighborhood of \mathbf{p}_0 , then

\mathbf{p}_0 is an isola center and the isolas are locally ellipses. The perturbation expansion gives an explicit representation of the isola solutions. Thus, our theory displays the birth of isolas from isola centers as ε increases.

Of course, not all the critical points are elliptic. For example, bifurcation points correspond to hyperbolic critical points, or saddles. As ε increases the bifurcation point may disappear, and the perturbations of bifurcation analyzed in [9]–[11] occur. Then τ is interpreted as an imperfection parameter. Other perturbations of bifurcation, which have been studied in [12], lead to the phenomenon of secondary bifurcation of solutions. It is shown in [12] that isolas may arise by the splitting of multiple bifurcation points into their constituent simple bifurcation points and secondary bifurcation points as a splitting parameter τ is varied. The secondary bifurcation branches may then form an isola. A preliminary discussion of some of these ideas is given in [13].

This work is related to the study of singular points of maps where information on the structure of the solutions of algebraic equations is obtained by studying their unfoldings. However, singularity theory does not give methods for obtaining approximations to the solutions of more general equations (1.4). In our method we present specific perturbation expansions to determine approximations to the isolas. Higher order corrections are easily obtained. Our method is developed in § 2 for general operator equations in a Hilbert space. An application is given in § 3 to determine isola solutions for the steady response of continuous stirred tank chemical reactors.

2. A general theory. We consider a general nonlinear operator equation

$$(2.1) \quad F[u, \lambda, \tau] = 0,$$

where the solutions $u(\lambda, \tau)$ are elements of a real Hilbert space. F is a nonlinear operator on that space, and λ and τ are real-valued scalar parameters. For simplicity, the dependence of F and u on other parameters and variables, such as space and time coordinates, is suppressed. We employ the bracket notation $\langle f, g \rangle$ for the inner product of two vectors f and g of the Hilbert space.

If (2.1) is a single algebraic equation for the scalar u , then we have the elementary results of § 1 about the critical points of the level curves $\tau = \text{constant}$ on a surface in \mathbb{R}^3 . We now generalize the conditions (1.2) to define critical points of the level curves of the solutions of the nonlinear operator equation (2.1). As a generalization of (1.2), we require the critical points to satisfy the linearized problem

$$(2.2) \quad F_u[u(\lambda, \tau), \lambda, \tau]\varphi = 0, \quad \langle \varphi, \varphi \rangle = 1,$$

where $u(\lambda, \tau)$ is a solution of (2.1), and we impose the condition

$$(2.3) \quad \langle F_\lambda[u(\lambda, k), \lambda, \tau], \Psi \rangle = 0, \quad \langle \Psi, \Psi \rangle = 1.$$

The linear operator $F_u[u, \lambda, \tau]$ is the Fréchet derivative of F evaluated at u, λ, τ . The subscript u on F denotes a functional derivative. We assume that this operator has a one-dimensional null space. The vector Ψ spans the null space of the adjoint operator of F_u , also assumed to be one-dimensional. The critical points are then among the solutions $\mathbf{p}_0 = (u_0, \lambda_0, \tau_0)$ of (2.1)–(2.3).

We now consider the behavior of the solutions of (2.1) near \mathbf{p}_0 . To do this we introduce a small parameter ε by

$$(2.4a) \quad \tau = \tau_0 + \tau_1\varepsilon + \tau_2\frac{\varepsilon^2}{2}.$$

Here τ_1 and τ_2 are constants to be determined. For τ near τ_0 we seek solutions as asymptotic expansions in ε of the form:

$$(2.4b) \quad u = \sum_{j=0}^{\infty} u_j \frac{\varepsilon^j}{j!},$$

$$(2.4c) \quad \lambda = \sum_{j=0}^{\infty} \lambda_j \frac{\varepsilon^j}{j!}.$$

The leading terms in (2.4b, c) are the ‘‘coordinates’’ of the critical point. Substituting (2.4) into (2.1) and equating to zero the coefficient of each power of ε , we obtain a sequence of equations to determine the coefficients in (2.4). The first two of these equations are

$$(2.5) \quad F_u^0 u_1 = -\{F_\lambda^0 \lambda_1 + F_\tau^0 \tau_1\},$$

$$(2.6) \quad F_u^0 u_2 = -\{(F_{uu}^0 u_1)u_1 + 2\lambda_1 F_{u\lambda}^0 u_1 + \lambda_1^2 F_{\lambda\lambda}^0 + \lambda_2 F_\lambda^0 + 2\tau_1 F_{u\tau}^0 u_1 + 2\lambda_1 \tau_1 F_{\lambda\tau}^0 + \tau_1^2 F_{\tau\tau}^0 + \tau_2 F_\tau^0\}.$$

Subscripts on F denote either ordinary or functional derivatives. The superscript zero on F denotes evaluation of the operator at the critical point.

The operator F_u^0 is not invertible at \mathbf{p}_0 . Therefore, the solvability condition requires that the right sides of (2.5) and (2.6) must be orthogonal to the null space of the adjoint of F_u^0 . Applying the solvability condition to (2.5) and employing the condition (2.3) gives

$$(2.7) \quad \langle F_\tau^0, \Psi \rangle \tau_1 = 0.$$

Thus, we have either

$$(2.8) \quad \langle F_\tau^0, \Psi \rangle \neq 0 \quad \text{and} \quad \tau_1 = 0$$

or

$$(2.9) \quad \langle F_\tau^0, \Psi \rangle = 0 \quad \text{with } \tau_1 \text{ arbitrary.}$$

If (2.1) is a single algebraic equation, then a geometric interpretation of the condition (2.8), i.e., $F_\tau^0 \neq 0$, is that the surface has a tangent plane at the critical point. The normal to this plane is parallel to the τ -axis, so that the surface is ‘‘bowl’’ shaped for τ near τ_0 . Similarly the condition (2.9), i.e., $F_\tau^0 = 0$, implies that the critical point is also a singular point of the surface. That is, the surface has no unique normal at \mathbf{p}_0 , see Fig. 1.

The solution of (2.5) is given by

$$(2.10) \quad u_1 = \xi\varphi + \lambda_1 Z_1 + \tau_1 Z_2,$$

where Z_1 and Z_2 are the unique solutions of

$$(2.11) \quad \begin{aligned} F_u^0 Z_1 &= -F_\lambda^0, & \langle Z_1, \varphi \rangle &= 0, \\ F_u^0 Z_2 &= -F_\tau^0, & \langle Z_2, \varphi \rangle &= 0. \end{aligned}$$

The amplitude ξ is the projection of u_1 onto the null space of F_u^0 . It is determined by applying the solvability condition to the right side of (2.6). The resulting amplitude equation is given by

$$(2.12) \quad a\xi^2 + 2b\lambda_1\xi + c\lambda_1^2 + 2\tau_1(p\xi + q\lambda_1) + r\tau_1^2 + d\tau_2 = 0.$$

We set $\tau_1 = 0$ when (2.8) holds and $d = 0$ when (2.9) holds. Here we have introduced the notation

$$\begin{aligned}
 a &\equiv \langle \Psi, (F_{uu}^0 \varphi) \varphi \rangle, & p &\equiv \langle \Psi, (F_{uu}^0 \varphi) Z_2 + F_{u\tau}^0 \varphi \rangle, \\
 b &\equiv \langle \Psi, (F_{uu}^0 \varphi) Z_1 + F_{u\lambda}^0 \varphi \rangle, & q &\equiv \langle \Psi, (F_{uu}^0 Z_1) Z_2 \\
 & & & + F_{u\lambda}^0 Z_2 + F_{u\tau}^0 Z_1 + F_{\lambda\tau}^0 \rangle, \\
 c &\equiv \langle \Psi, (F_{uu}^0 Z_1) Z_1 + 2F_{u\lambda}^0 Z_1 + F_{\lambda\lambda}^0 \rangle, & r &\equiv \langle \Psi, (F_{uu}^0 Z_2) Z_2 + 2F_{u\tau}^0 + F_{\tau\tau}^0 \rangle. \\
 d &\equiv \langle \Psi, F_{\tau}^0 \rangle,
 \end{aligned}
 \tag{2.13}$$

Equation (2.12) can be written in the centered form

$$a[\xi - \tau_1 h]^2 + 2b[\xi - \tau_1 h][\lambda_1 - \tau_1 k] + c[\lambda_1 - \tau_1 k]^2 = \rho,
 \tag{2.14}$$

where

$$\begin{aligned}
 \Delta &\equiv ac - b^2, \quad k \equiv \frac{bp - aq}{\Delta}, \quad h \equiv \frac{bq - cp}{\Delta}, \\
 \rho &\equiv [ah^2 + 2bhk + ck^2 - r]\tau_1^2 - d\tau_2 = -[ph + qk + r]\tau_1^2 - d\tau_2.
 \end{aligned}
 \tag{2.15}$$

We thus see that (2.14) has a family of real solutions $[\xi, \lambda_1]$ which lie on an ellipse centered at $(\xi, \lambda_1) = (\tau_1 h, \tau_1 k)$ in the (ξ, λ_1) -plane, provided that the isola conditions

$$(a) \quad \Delta > 0 \quad (b) \quad a\rho > 0
 \tag{2.16}$$

are satisfied. The principal axes of the ellipse make an angle of β with the ξ and λ_1 axis, where β is defined by

$$\beta = \frac{1}{2} \cot^{-1} \left(\frac{a - c}{2b} \right).
 \tag{2.17}$$

When (2.16) are satisfied, the solution given by

$$\begin{aligned}
 u(\varepsilon) &= u_0 + \varepsilon[\xi\varphi + \lambda_1 Z_1 + \tau_1 Z_2] + O(\varepsilon^2), \\
 \lambda(\varepsilon) &= \lambda_0 + \varepsilon\lambda_1 + O(\varepsilon^2)
 \end{aligned}
 \tag{2.18}$$

forms an isola to first order in ε . When (2.8) holds and we set $\tau_1 = 0$, condition (2.16b) can be satisfied by using the value

$$\tau_2 = \text{sign}(-ad).
 \tag{2.19}$$

Higher order perturbations can be determined in a straightforward manner. However, now only linear equations result so that the isola is distorted by the higher order terms.

In case (2.8), where $\tau_1 = 0$, the center of the ellipse is at the origin $(\xi, \lambda_1) = (0, 0)$. We observe that in this case τ can take on values $\tau > \tau^0$ or $\tau < \tau^0$ but not *both*. Thus, isolas are formed in this case when τ is perturbed in the proper way from τ_0 , i.e., τ_2 satisfies (2.19).

In case (2.9) we have, with no loss of generality, $\tau_1 = 1, \tau_2 = 0$. Then isolas exist for both $\tau > \tau^0$ and $\tau < \tau^0$ if the isola condition (2.16b), which is now given by

$$a(ph + qk + r) < 0,
 \tag{2.20}$$

is satisfied. Furthermore, the center of the ellipse in the (ξ, λ_1) -plane is at the point $\xi = h, \lambda_1 = k$. Thus, the origin may lie inside, on or outside the ellipse. For the special case $h = k = 0$, the center of the ellipse coincides with the coordinate origin.

3. Continuous stirred tank reactors. Isola solutions have been discovered both experimentally and numerically for continuous stirred tank chemical reactors. A brief historical account is given in [1]. An elementary "lumped model" theory that describes the reactor states consists of a pair of first order, nonlinear ordinary differential equations in time; see, e.g., [1]. The dependent variables are the reactor temperature and the reactant concentration. The equilibrium states are then determined as the roots of a system of two nonlinear algebraic equations. By eliminating the temperature from these two equations, we obtain the following single nonlinear equation for a dimensionless reactant concentration u ,

$$(3.1) \quad \tau\lambda - \frac{u}{1-u} \exp \left\{ \frac{-[Bu + \lambda\eta]}{(1+\lambda) + \frac{1}{\gamma}[Bu + \lambda\eta]} \right\} = 0.$$

The five dimensionless parameters in (3.1), τ , λ , B , η and γ , are proportional to: a reference value of the Damköhler number of the reactor, the reactant flow rate, the heat of reaction, the cooling temperature and the activation energy. All these parameters are positive, and only positive solutions of (3.1) are considered because u is a concentration.

For simplicity of presentation we analyze (3.1) for isola solutions in the special case that $\eta = 0$ and $\gamma = 0$, since for many specific chemicals γ is large. Thus, we consider the nonlinear equation

$$(3.2) \quad F[u, \lambda, \tau] = \tau\lambda - \frac{u}{1-u} e^{-\Gamma} = 0, \quad \Gamma \equiv \frac{Bu}{1+\lambda},$$

where the reference Damköhler number is taken as the isola parameter τ .

The critical points of the solution curves of (3.2) are determined by simultaneously solving (3.2) and

$$(3.3) \quad F_u = -\frac{e^{-\Gamma}}{(1-u)^2} \left[1 - \frac{Bu(1-u)}{1+\lambda} \right] = 0,$$

$$(3.4) \quad F_\lambda = \tau - \frac{e^{-\Gamma} Bu^2}{(1-u)(1+\lambda)^2} = 0.$$

By elementary manipulations of (3.2)–(3.4) it can be shown that for each positive root λ_0 of

$$(3.5) \quad B\lambda = (1+\lambda)^3$$

we obtain a corresponding value for u_0 and τ_0 from

$$(3.6) \quad u_0 = \frac{1}{1+\lambda_0}, \quad \tau = \frac{e^{-\Gamma_0}}{\lambda_0^2}, \quad \Gamma_0 \equiv \frac{1+\lambda_0}{\lambda_0}.$$

These give the critical points (u_0, λ_0, τ_0) of the response curves of (3.2).

An elementary analysis reveals that (3.5) has no positive roots for B in $0 \leq B < B_0 \equiv \frac{27}{4}$, and it has two positive roots $\lambda_0^{(j)}(B)$, $j = 1, 2$, for $B > B_0$. These roots satisfy: $\lambda_0^{(1)}(B) \rightarrow 0$ and $\lambda_0^{(2)}(B) \rightarrow \infty$ as $B \rightarrow \infty$; $\lambda_0^{(1)}(B_0) = \lambda_0^{(2)}(B_0) = \frac{1}{2}$, and they lie in the intervals

$$(3.7) \quad 0 < \lambda_0^{(1)}(B) \leq \frac{1}{2}, \quad \frac{1}{2} \leq \lambda_0^{(2)}(B) < \infty, \quad B \geq B_0.$$

The corresponding values $u_0^{(j)}$ and $\tau_0^{(j)}$ are obtained by inserting $\lambda_0^{(j)}$ in (3.6) to obtain

$$(3.8) \quad u_0^{(j)} = \frac{1}{1 + \lambda_0^{(j)}}, \quad \tau_0^{(j)} = \frac{e^{-(1+1/\lambda_0^{(j)})}}{\lambda_0^{(j)}}, \quad j = 1, 2.$$

To classify the critical points $\mathbf{p}_0^{(j)} \equiv (u_0^{(j)}, \lambda_0^{(j)}, \tau_0^{(j)})$, $j = 1, 2$, we evaluate the discriminant Δ (2.15) to get

$$(3.9) \quad \Delta = \frac{[1 + \lambda_0^{(j)}]^2 [1 - 2\lambda_0^{(j)}]}{[\lambda_0^{(j)}]^6} e^{-2\tau_j}.$$

Since $\lambda_0^{(2)} \cong \frac{1}{2}$, the corresponding value of Δ is negative and $\mathbf{p}_0^{(2)}$ is hyperbolic for all $B > B_0$. It follows from (3.9) that $\mathbf{p}_0^{(1)}$ is elliptic when $\lambda_0^{(1)}$ is in the interval $0 < \lambda_0^{(1)} < \frac{1}{2}$. Since isola centers are among the elliptic critical points, we shall confine our attention to $\mathbf{p}_0^{(1)}$.

Since $F_\tau = \lambda$ and $0 < \lambda_0^{(1)} < \frac{1}{2}$, $\mathbf{p}_0^{(1)}$ corresponds to the case (2.8). In this case we have $\tau_1 = 0$, and it follows from (2.19) that $\tau_2 = 1$. Thus the isola solutions exist for $\tau > \tau_0^{(1)}$. Since $Z_1 = Z_2 = 0$, they are obtained from (2.12)–(2.20) as

$$(3.10) \quad \begin{aligned} \tau &= \tau_0^{(1)} + \varepsilon^2, \\ \lambda &= \lambda_0^{(1)} + \varepsilon \lambda_1 + O(\varepsilon^2), \\ u &= u_0^{(1)} + \varepsilon \xi + O(\varepsilon^2), \end{aligned}$$

where (ξ, λ_1) ranges over the ellipse

$$(3.11) \quad (1 + \lambda_0^{(1)})^4 \xi^2 + 2 \frac{(1 + \lambda_0^{(1)})^2 \lambda_0^{(1)}}{1 - \lambda_0^{(1)}} \xi \lambda_1 + \lambda_1^2 = \lambda_0^{(1)4} \frac{(1 + \lambda_0^{(1)})}{(1 - \lambda_0^{(1)})} e^{(1+1/\lambda_0^{(1)})}.$$

This ellipse is centered at the origin, and its principal axes make an angle

$$(3.12) \quad \beta = \frac{1}{2} \cot^{-1} \left\{ \frac{(1 - \lambda_0^{(1)}) [(1 + \lambda_0^{(1)})^4 - 1]}{2 \lambda_0^{(1)} (1 + \lambda_0^{(1)})^2} \right\}$$

with the ξ and λ_1 axes.

4. Concluding remarks. The principal computational difficulty in the application of our method to a specific problem is to solve (2.1)–(2.3) for the critical points \mathbf{p}_0 . Then, as we have shown, the isolas are determined by an elementary perturbation analysis. For some problems, (2.1) may depend on an additional small parameter, which we denote by δ . Then the critical points are functions of δ , and it may be possible to solve (2.1)–(2.3) for \mathbf{p}_0 using asymptotic and perturbation methods in the small parameter δ .

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