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**PATH-FOLLOWING METHODS FOR
BOUNDARY VALUE PROBLEMS AND
THEIR APPLICATIONS TO
COMBUSTION EQUATIONS**

A thesis presented in partial fulfilment of the
requirements for the degree of
Master of Science in Mathematics
at Massey University

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Abstract

This thesis is primarily concerned with the numerical techniques involved in bifurcation analysis, in particular with the software package AUTO developed by Eusebius Doedel which performs this analysis on dynamical systems.

The techniques of AUTO are investigated and applied to a steady state heat equation. The chosen equation can be solved by analytical methods for some boundary conditions. Initially AUTO was successfully applied to such problems, which have analytical solutions confirming its reliability. The software was then used to solve dynamical system problems which do not have known analytical solutions. These problems necessitated a modification to AUTO for non-autonomous systems. The modified version of AUTO was shown to be successful in finding solutions to these problems.

ACKNOWLEDGEMENTS

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1 INTRODUCTION

1.1 BIFURCATION ANALYSIS

Bifurcation theory allows the analysis of a system (or model) with a *control parameter* which is fixed (in any single instance) but can vary depending on the system which is been modelled. For example, if the load on a vertical beam is greater than a certain amount, the beam will buckle causing a deflection (see figure 1.1). At the point of buckling, the solution structure changed. There is a solution branch where there is buckling, and a solution branch where there is none. The solution branch has *bifurcated* into two branches. The *control parameter* (λ) for this system is the load on the beam. It is fixed for any particular set of physical parameters, but if varied, the solution structure may change. This system could have many other variable parameters (for example the elasticity modulus of the beam); however if only one parameter is varied at a time then its effects may be seen without other parameter variation influencing the results. This is the technique used in *bifurcation analysis*.

DEFLECTION

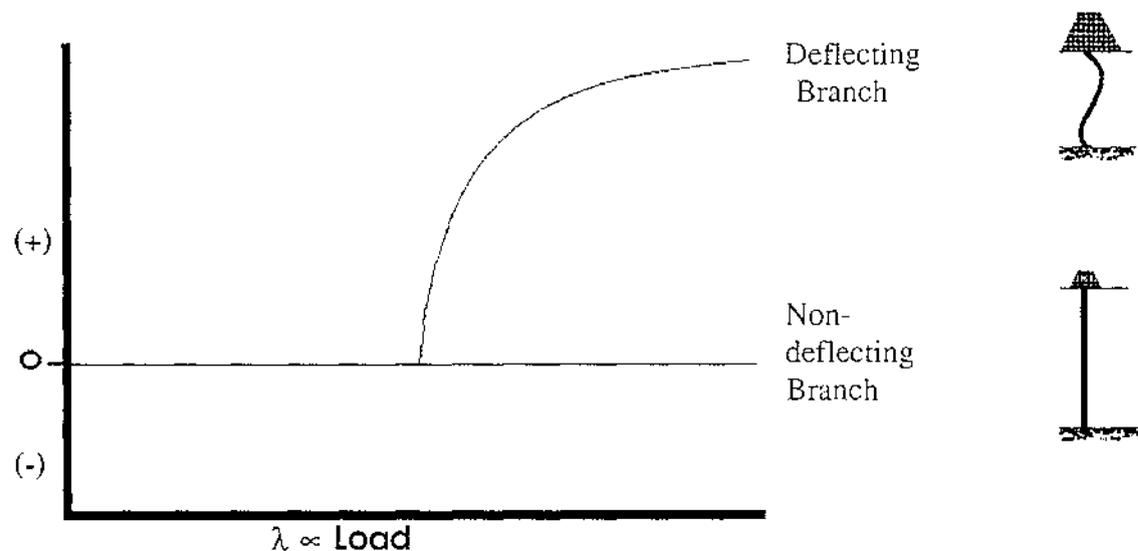


Figure 1.1: A bifurcation Graph for the load on a beam

The control parameter for a system is usually called the *distinguishing parameter*, *principle parameter*, or the *bifurcating parameter*, and will be denoted by λ . As the previous example has shown, changing λ changes the structure of the solution set.

BIFURCATION POINTS

Bifurcation analysis is the process of finding critical values of λ which change the solution structure. A *bifurcation graph* is generated to aid this task. A *bifurcation graph* plots λ against some *norm* of the solution (see figure 1.2). Solutions to the system are represented on this graph as curves or *branches*, where a *branch* is defined as a curve which can be parameterised by a single parameter. If, in a small neighbourhood of λ , there is a point λ_0 at which the number of solutions change (in every small neighbourhood), then this point is described as a *bifurcation point*. These points are important as a change in the number of solutions indicates a change in the state of the system.

The system will be defined as:

$$(1.1) \quad F(u, \lambda) = 0$$

where $u = [u_1, u_2, \dots, u_n]^t$, λ is a scalar and $F = [F_1, F_2, \dots, F_n]^t$ is a system of equations.

The *Jacobian* operator F_u for this system is defined as:

$$(1.2) \quad F_u = \begin{bmatrix} \frac{\partial F_1}{\partial u_1} & \frac{\partial F_1}{\partial u_2} & \dots & \frac{\partial F_1}{\partial u_n} \\ \frac{\partial F_2}{\partial u_1} & \frac{\partial F_2}{\partial u_2} & \dots & \frac{\partial F_2}{\partial u_n} \\ \dots & \dots & \dots & \dots \\ \frac{\partial F_n}{\partial u_1} & \frac{\partial F_n}{\partial u_2} & \dots & \frac{\partial F_n}{\partial u_n} \end{bmatrix}$$

This system has a solution set:

$$(1.3) \quad S_\lambda = \{u \in \mathfrak{R}^n \mid F(u, \lambda) = 0\}$$

for a particular value of λ . A point λ_0 is a *bifurcation point* if $S_{\lambda_0} \neq \emptyset$, and there is

a $u_0 \in S_{\lambda_0}$ such that, for all sufficiently small neighbourhoods

$$U = \{u_x \in \mathfrak{R}^n \mid \|u_x - u_0\| < \varepsilon\} \text{ and } V = \{\lambda_x \in \mathfrak{R} \mid |\lambda_x - \lambda_0| < \delta\}:$$

there are two distinct solutions (u_1, λ_x) and $(u_2, \lambda_x) \in U \times V$ (see reference [3]). That

is there is more than one solution of x for a particular value of λ .

A bifurcation point on a solution branch can be sub-divided into one of two categories, a *limit point* and a *branching point* (see figure 1.2).

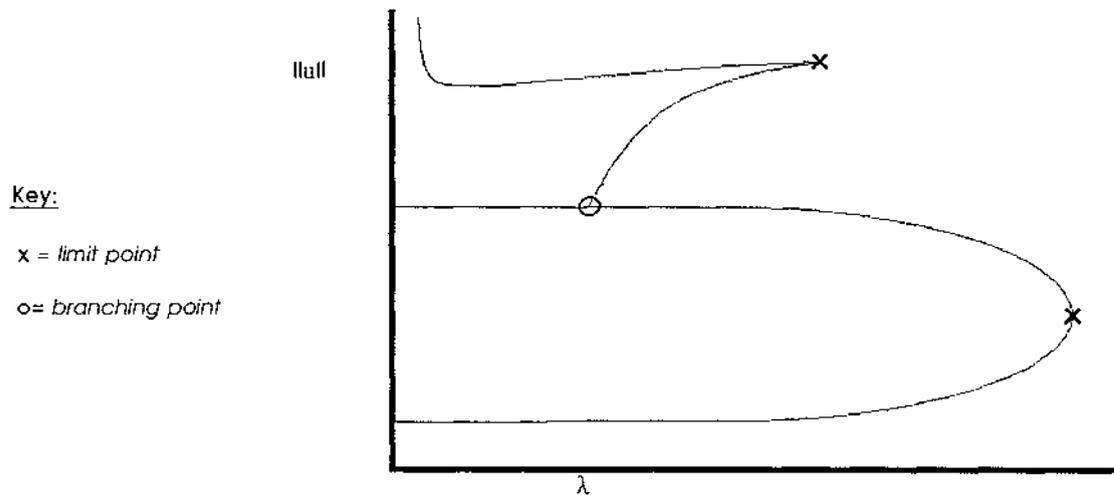


Figure 1.2: A Bifurcation Diagram

Limit point:

This is when the solution curve folds back on itself.

A *limit point* (λ_0, u_0) is defined to be a bifurcation point which has solutions

(λ_x, u_x) in the neighbourhood $U \times V$ such that :

either $\lambda_x \leq \lambda_0$ for all $\lambda_x \in V$, or $\lambda_x \geq \lambda_0$ for all $\lambda_x \in V$.

Branching Point:

This can be defined as a bifurcation point which is not a *limit point*.

Note that any single branch can be parameterised using a single parameter t , giving a solution space $\{ (u(t), \lambda(t)) \mid a < t < b \}$. So an alternative definition of a limit point is a point $(u(t_0), \lambda(t_0))$ such that $\lambda'(t_0) = 0$.

Other conditions for bifurcation points can be found by introducing the Implicit Function Theorem:

Theorem 1.1: The Implicit Function Theorem (see [12], Page 78)

If

- (i) F is continuously differentiable and
- (ii) F_u has a continuous inverse at a point (u_a, λ_a) in solution space (1.3)

then for the neighbourhoods:

$$U = \{ u_x \in \mathfrak{R}^n \mid \|u_x - u_a\| < \varepsilon \} \text{ and } V = \{ \lambda_x \in \mathfrak{R} \mid \|\lambda_x - \lambda_a\| < \delta \};$$

- (a) F_u has a bounded inverse for all points $(u_x, \lambda_x) \in U \times V$.
- (b) for all fixed $\lambda_x \in V$, the equation $F(u_x, \lambda_x) = 0$ has a unique solution $u_x \in U$. ■

This implies that, when F_u is non-singular, there are no bifurcation points. So a necessary (but not sufficient) condition for a bifurcation point is that F_u is singular.

If Theorem 1.1 holds then a branch B of solutions can be defined:

$$(1.4) \quad B = \{(u(\lambda), \lambda) \mid a < \lambda < b, F(u(\lambda), \lambda) = 0\}, \text{ where } a, b \in \mathfrak{R}$$

The solution $(0, \lambda)$ is called the *trivial branch*. This happens when $F(0, \lambda) = 0$ for all values of λ (i.e. $u(\lambda) = 0$).

Theorem 1.2: (see [12] page 79)

If the *trivial branch* exists and $\lambda_0 = 0$ is an eigenvalue of the Jacobian F_u , then if λ_0 is an eigenvalue of odd multiplicity, λ_0 is a branching point from the trivial branch,

i.e. $\lambda_0 = 0$ is a root of $\det(F_u(0) - \lambda_0 I) = 0$ which is of odd multiplicity (where $F_u(0)$ is the Jacobian evaluated at $u=0$). ■

Note: λ_0 and λ are different variables.

This is a **sufficient** condition for a bifurcation point. Note that if the multiplicity of the eigenvalue is not odd then it is still not known whether the point is a bifurcation point. If the trivial solution does not exist, or bifurcation points from other branches are wanted, then Theorem 1.2 cannot be applied. So this theorem only locates bifurcation points which are on the trivial branch. To find bifurcation points from other branches, the system has to be converted into this form by linearisation:

If a solution branch $(U = u(\lambda), \lambda)$ is **known** then equation (1.1) can be linearised such that:

$$(1.5) \quad H(h, \mu) = F(U + h, \mu) = 0$$

where h is a vector $[h_1, h_2, \dots, h_n]^t$, and $\mu = \lambda$ is the new bifurcation parameter (it is given a different symbol as λ is fixed by the solution branch U).

$H(0, \mu) = 0$, for all μ , so Theorem 1.2 can be used to find bifurcation points.

A bifurcation point $\mu_0 = g(U)$ in system H can be related back to F by substituting μ_0 with λ and solving $\lambda = g(U)$ for λ .

Note that this requires an existing solution branch U .

Example 1.1:

Define F to be the system:

$$\begin{aligned} f_1(u_1, u_2, \lambda) &= u_1^3 + u_2 - \lambda u_1 = 0 \\ f_2(u_1, u_2, \lambda) &= u_1^2 u_2 - u_1^3 - \lambda u_2 = 0 \end{aligned}$$

This system has the trivial solution branch $(u^t, \lambda) = (0, 0, a)$, $a \in \mathfrak{R}$. But does it have any other branches? The implicit function theorem can be used to find **possible** bifurcation points along this branch.

The Jacobian F_u along the trivial branch is:

$$F_u = \begin{bmatrix} -\lambda & 1 \\ 0 & -\lambda \end{bmatrix}$$

This is singular when the determinant is zero, i.e when $\lambda=0$. So by Theorem 1.1 $\lambda=0$ is a possible bifurcation point. At that point F_u has a zero eigenvalue of multiplicity 2, which is even, so that Theorem 1.2 does not prove whether it is a bifurcation point or not.

However if some algebraic manipulation is done on the system, one finds that $\{(a, 0, \lambda), a > 0\}$ is **not** a solution and also $\{(0, b, \lambda), b > 0\}$ is not a solution so non-trivial solutions only exist if $u_1, u_2 \neq 0$. Eliminating λ gives:

$$u_2^2 = -u_1^4$$

which has only the trivial solution. So as there are no non-trivial solutions, $\lambda=0$ is not a bifurcation point. ■

Example 1.2:

Define F to be:

$$f_1(u_1, u_2, \lambda) = u_1^2 - \lambda u_1 = 0$$

$$f_2(u_1, u_2, \lambda) = u_2^2 - \lambda u_2 = 0$$

This system has the trivial solution branch. The Jacobian F_u is:

$$F_u = \begin{bmatrix} 2u_1 - \lambda & 0 \\ 0 & 2u_2 - \lambda \end{bmatrix}$$

The trivial branch $(0,0,a)$ has a possible bifurcation point when $\lambda=0$.

$F_u(0)$ has an eigenvalue of multiplicity 2 at that point, which is even, so Theorem 1.2 does not prove whether it is a bifurcation point or not. Clearly $\lambda=u_1$ and $\lambda=u_2$ are non-trivial solutions. So solution branches $(a,0,a)$ $(0,a,a)$ and (a,a,a) exist for $a \in \mathfrak{R}$, and $(0,0,0)$ is a bifurcation point. F_u is not singular along any of the non-trivial branches, so by Theorem 1.1, there are no **new** bifurcation points coming off these branches. The bifurcation graph for this system is shown in figure 1.3.

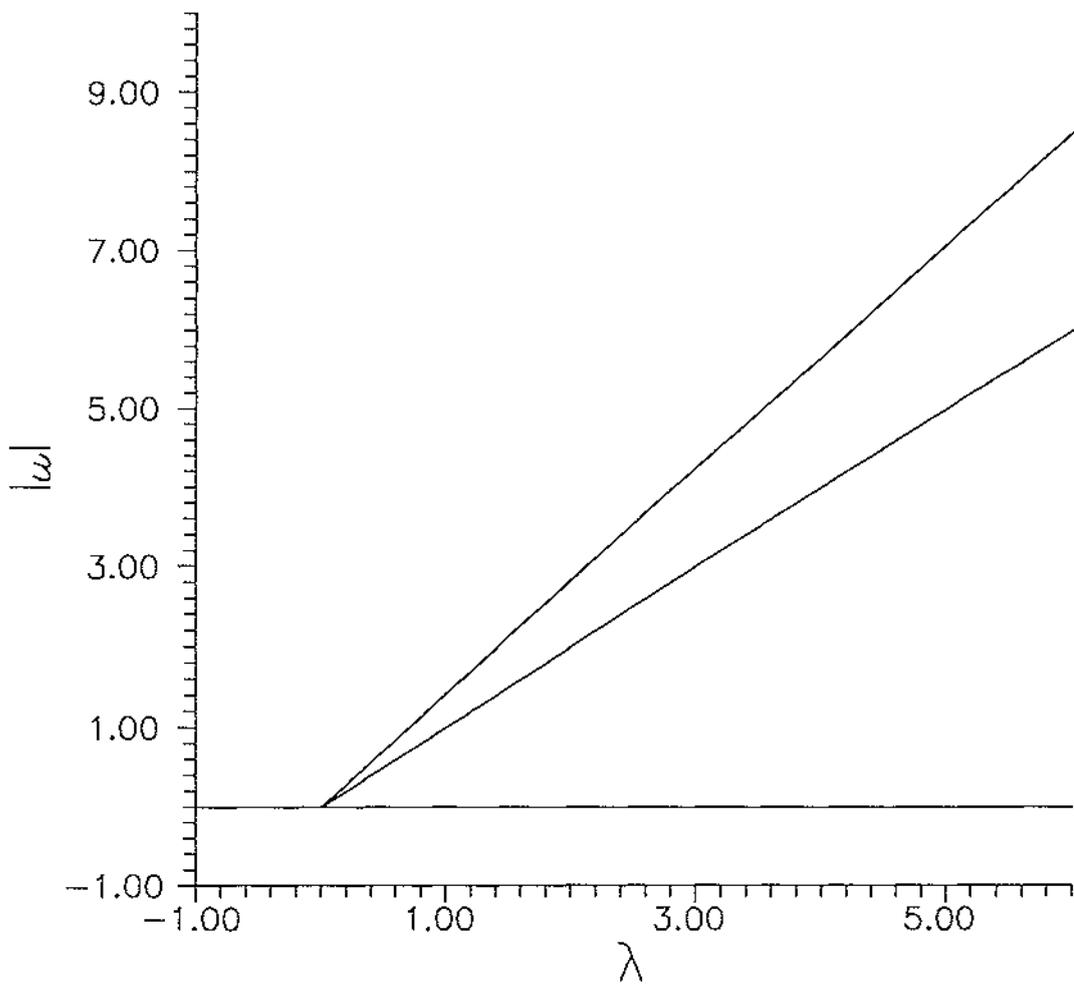


Figure 1.3: Bifurcation diagram for Example 1.2



Example 1.3:

Define F to be:

$$f_1(u_1, u_2, \lambda) = 16u_1 + 12u_1^3 + 24u_1u_2^2 - \lambda u_1 = 0$$

$$f_2(u_1, u_2, \lambda) = 12u_2 + 9u_2^3 + 18u_2u_1^2 - \lambda u_2 = 0$$

This system has the *trivial branch* as a solution.

For points along this branch, the Jacobian F_u becomes:

$$\begin{bmatrix} 16-\lambda & 0 \\ 0 & 12-\lambda \end{bmatrix}$$

This is singular when $\lambda=16$ and $\lambda=12$ where the nullspace is one-dimensional. So by Theorem 1.2 these points are bifurcation points. As λ has values both before and after these points (in their respective neighbourhoods) and also by Theorem 1.2, they can be sub-categorised as branching points (using the definition of a branching point defined earlier).

The branches can be found analytically and are:

$$u_a = \left[0, \pm \sqrt{\frac{1}{9}(\lambda - 12)} \right]^t \text{ and } u_b = \left[\pm \sqrt{\frac{1}{12}(\lambda - 16)}, 0 \right]^t$$

To find bifurcation points along non-trivial branches, the system needs to be linearised about each solution branch by defining the system: $H(h, \mu) = F(U+h, \mu)$, where U is a non-trivial solution branch $u(\lambda)$. The Jacobian H_h along the solution branch ($h=0$) is:

$$(1.6) \quad H_h(0) = \begin{bmatrix} 16 + 36U_1^2 + 24U_2^2 - \mu & 48U_1U_2 \\ 36U_2U_1 & 12 + 27U_2^2 + 18U_1^2 - \mu \end{bmatrix}$$

For the first branch u_a (inserting it in the system H and making $\mu=\lambda$) the determinant is zero when:

$$16 + 24U_2(\lambda) = \lambda, \text{ and } 12 + 27U_2(\lambda) = \lambda \quad (\text{as } U_1(\lambda)=0)$$

This corresponds to $\lambda=12$ and $\lambda=9.6$. The first point is the existing bifurcation point from the trivial solution. The second point is not in the range of the solution space (of $\lambda>12$). So by theorem 1.1, there are no more bifurcation points along this branch.

The second branch u_b makes the determinant zero when $\lambda=16$ and when $\lambda=24$. The first eigenvalue is the point where this branch connects to the trivial solution. The second point is a possible bifurcation point. By theorem 1.2, $\lambda=24$ is a branching point from the branch u_b .

This new branch is:

$$\left[\pm \sqrt{\frac{(\lambda - 9.6)}{21.6}}, \pm \sqrt{\frac{(\lambda - 24)}{54}} \right]^t$$

It is more difficult to find branching points from this branch as U_1 and U_2 are both not zero.

So the analysis stops here, and a bifurcation graph of the results can be seen in figure 1.4.

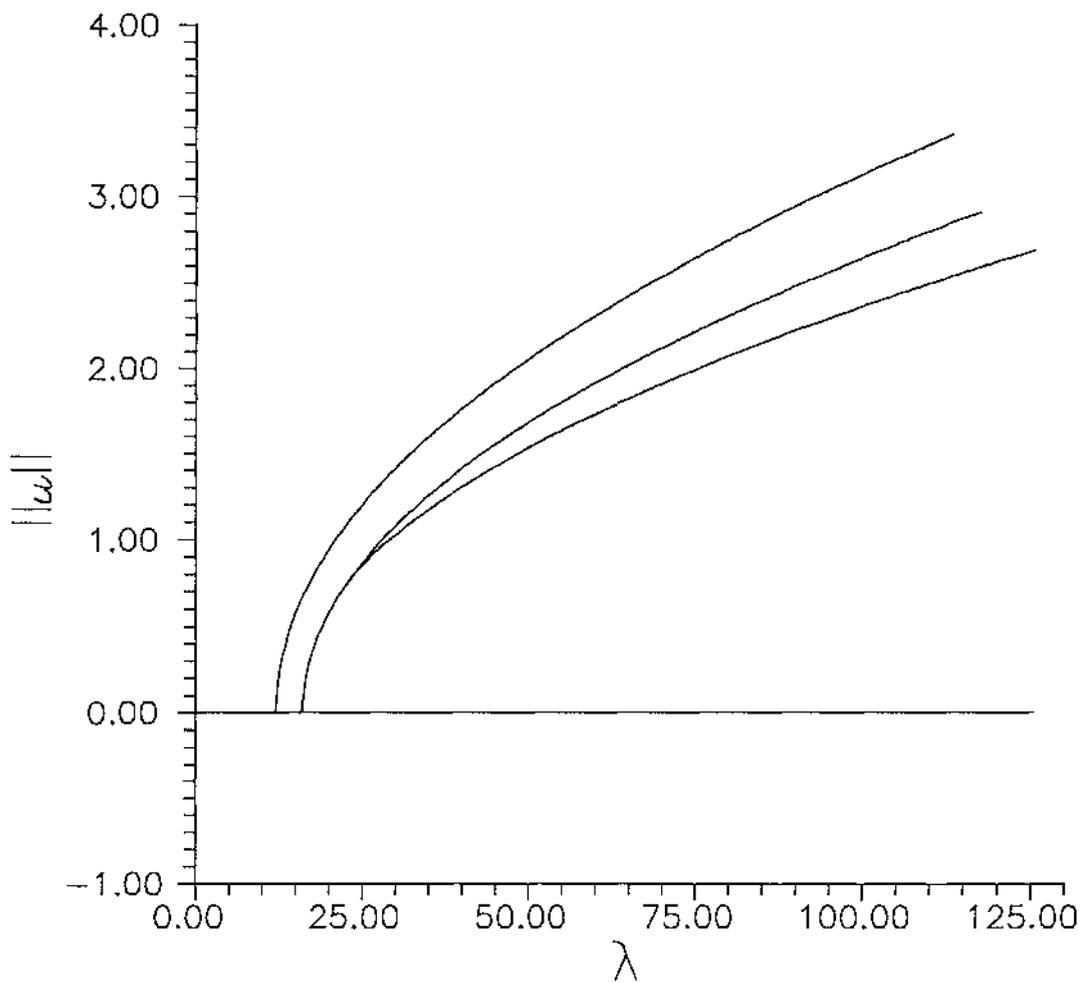


Figure 1.4: Bifurcation diagram for example 1.3



NORMS

Bifurcation graphs require a single value from a vector of many solution values to plot against the distinguishing parameter λ . The most commonly used value is the *Euclidean norm*:

$$\|u\|_2 = \sqrt{u_1^2 + u_2^2 + \dots + u_n^2}, \text{ where } u = [u_1 \ u_2 \ \dots \ u_n]^T$$

If a particular variable u_a is of interest, then $\|u\| = |u_a|$ can be used. If a bound is wanted on the variables the ∞ -norm ($\|u\|_\infty$) can be used where:

$$\|u\|_\infty = \max\{|u_i| : i = 1, \dots, n\}.$$

Each definition will give a different bifurcation diagram. Some may not show bifurcation points, or may show branching points which do not exist.

For example, the point $u=(1,2)$ has the same *Euclidean norm* and ∞ -norm as the point $u=(2,1)$, so the two solutions from different branches will *appear* to be intersecting on a bifurcation graph. However the norm $\|u\| = |u_1|$ will graph the two points differently. Another example considers the curves $u_1 = (\lambda, \lambda+1)$ and $u_2 = (1-\lambda, \lambda+1)$ which intersect when $\lambda=1/2$. $\|u\|_\infty = \lambda+1$ for all positive λ on **both** solution curves. A bifurcation graph of λ versus $\|u\|_\infty$ will show an intersection of the two curves at all values of λ greater than zero. This problem is due to the difference between the dimension of the bifurcation graph, which is 2-dimensional, and the dimension of the system which it graphs. These two examples show that care must be taken when choosing a norm to ensure the solution curve is represented clearly on its bifurcation graph.

SYSTEMS OF DIFFERENTIAL EQUATIONS

The previous analysis is for algebraic systems of the form $F(u,\lambda)=0$. Now consider the situation when the model is a system of differential equations. i.e. $F(D(u),\lambda)=0$ where $D(u)$ is a $n \times n$ matrix of all the derivatives of u with respect to t , where u is a vector of independent variables, and t is a vector of dependent variables.

The solution space is:

$$\{ (u(t),\lambda) \mid u \in \mathfrak{R}^n, t \in \mathfrak{R}^{Tn}, \lambda \in \mathfrak{R} \},$$

For each value of λ , there exists one or more vector fields $u(t)$ of solutions.

The definitions for bifurcation points, limit points and branching points can still be applied to this system by defining a fixed point $u=u(t)$ which must satisfy the definitions for all values of $t \in \mathfrak{R}^{Tn}$.

Theorems 1.1 and 1.2 are not easily applied to F as the Jacobian F_u is undefined.

There is an analytical method for transforming a D.E. system into an algebraic system using an appropriate Green's integral, in which case the theorems can be used. This method will not be covered in any detail other than to say that it is very difficult to do for all systems except very simple ones. (see Gomez' thesis [5] and [9]), and then one still needs to find the function H from (1.5).

The existing norms can be applied at any fixed point u (usually the maximum). If there is only one dependent variable t defined over a fixed range $[0, T]$, then there is another norm which can be applied:

$$\|u\| = \sqrt{\frac{1}{T} \int_0^T [u_1(t)^2 + u_2(t)^2 + \dots + u_n(t)^2] dt}$$

This gives a *Euclidean*-type norm which encompasses the value for u over the whole interval, rather than just a single value, so all points have an 'effect' on the norm.

To make use of these theorems, one needs analytical solutions, which are only found in a very small subset of non-linear systems. Solution branches can be determined numerically, and Chapter 2 presents methods for doing this.

1.2 COMBUSTION MODELS

Cellulosic materials such as wood chips (or shavings or sawdust), hay or bagasse are stored in large piles under conditions which may vary in temperature and humidity. Under certain conditions, the material spontaneously combusts, possibly causing substantial damage.

For inert isotropic bodies obeying the Arrhenius Law the Fourier heat balance equation becomes (see [7] and [11]):

$$k\nabla^2 T + q\sigma A.e^{\left(\frac{-E}{RT}\right)} = C\frac{\partial T}{\partial t} \quad \text{in the region } \hat{r} \in \hat{\Omega} \subset \mathcal{R}^3, t > 0$$

with boundary conditions:

$$k\frac{\partial T}{\partial n} + h(T - T_a) = 0 \quad \text{on } \partial\hat{\Omega} \quad (\text{assuming Newtonian Cooling})$$

$$\frac{\partial T}{\partial x_i} = 0, \quad \text{when } x_i = 0 \quad \forall i$$

where $T(x,t)$ is the absolute temperature of a body at position vector x and time t , k is the thermal conductivity, and q , σ , and A are exothermicity/unit mass, density and frequency factors respectively. E is the activation energy of the oxidation reaction, C is the specific heat capacity, and R is the gas constant. $\nabla^2 T$ is the Laplacian operator. In the boundary conditions, h is the heat transfer coefficient, and T_a is the absolute ambient temperature.

The first boundary condition ensures that the temperature at the surface of the reactant is equal to the ambient temperature minus the effects of Newtonian cooling at the surface. In a symmetrically heated system, it is assumed that the temperature gradient at the centre is zero, resulting in the second boundary condition.

The steady state model for this system is:

$$\begin{aligned} k\nabla^2 T + q\sigma A \cdot e^{\left(-\frac{E}{RT}\right)} &= 0 \\ k\frac{\partial T}{\partial n} + h(T - T_a) &= 0 \text{ on boundary } \partial\hat{\Omega} \\ \frac{dT}{dx_i} &= 0, \text{ when } x_i = 0 \quad \forall i \end{aligned}$$

This system in symmetrical shapes can be converted to the dimensionless form (see [7] and [11]):

$$(1.7) \quad \begin{aligned} \frac{d^2 u}{dr^2} + \frac{j}{r} \frac{du}{dr} + \lambda(a_0) e^u &= 0 \\ \frac{du}{dr}(0) = 0, \quad \frac{du}{dr}(1) + \text{Bi}u(1) &= 0 \end{aligned}$$

where $u = \frac{E(T - T_a)}{RT_a^2}$ is the dimensionless temperature excess, $r = \frac{\hat{r}}{a_0}$ is a

dimensionless length-scale (same for objects of any size) in the interval $[0,1]$, with a_0 representing an appropriate characteristic length such as the half-width of the body, $\text{Bi} = ha_0/k$ (> 0) is the surface heat transfer coefficient (denoted as the Biot number), and λ is the Frank-Kamenetskii parameter [1] given by:

$$\lambda(a_0) = \frac{a_0^2 q \sigma A \cdot e^{\left(-\frac{E}{RT_a}\right)}}{k \left(\frac{RT_a^2}{E}\right)}$$

The value for λ is crucial. Solutions only exist for certain values of λ . The maximum value of λ occurs at the point where the substance will combust spontaneously.

In physical terms if, for a given ambient temperature the substance radius is larger than a critical size, then there are no steady states for temperature in the substance, and it will combust spontaneously over time. This critical value for λ is denoted by λ_{crit} .

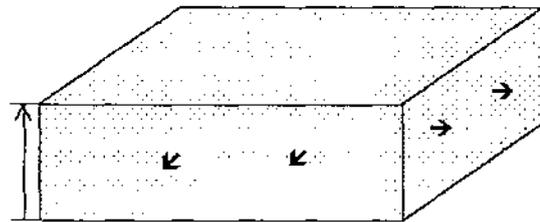
$\frac{d^2u}{dr^2} + \frac{j}{r} \frac{du}{dr}$ is the Laplacian Δu for *Class A* geometries in dimension $j+1$. i.e.

geometries which have a single unit of measurement.

EXAMPLES

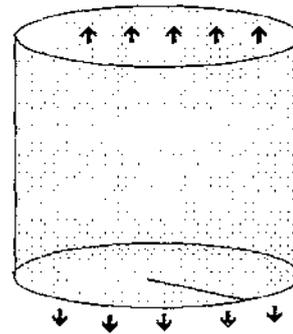
An infinite Slab ($j=0$):

$$\frac{d^2u}{dr^2} + \lambda e^u = 0$$



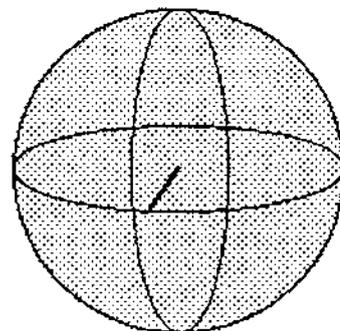
An infinite Cylinder ($j=1$)

$$\frac{d^2u}{dr^2} + \frac{1}{r} \frac{du}{dr} + \lambda e^u = 0$$



A Sphere ($j=2$):

$$\frac{\partial^2 u}{\partial r^2} + \frac{2}{r} \frac{\partial u}{\partial r} + \lambda e^u = 0$$



There exists a well known analytical general solution to equation (1.7) when $j=0$ (see [7]):

$$(1.8) \quad u(r) = \ln(A) - 2 \ln \left[\cosh \left(\sqrt{\frac{\lambda A}{2}} r + C \right) \right], \quad A > 0$$

where A and C are constants. C must be zero to satisfy the first boundary condition.

The norm, which will be plotted in the bifurcation diagram against λ , is the maximum value of u over $0 \leq r \leq 1$ denoted by u_{max} . Over this range the maximum value of u occurs when $r = 0$, so the norm u_{max} is:

$$u_{max} = u_0 = u(0) = \ln(A)$$

An implicit solution relating u_0 to λ , for $\lambda > 0$ is found by replacing $\ln(A)$ by the norm u_0 , and using the other boundary condition:

$$(1.9) \quad \ln(\lambda) = \ln(2\alpha^2) - 2 \ln \cosh(\alpha) - \frac{2\alpha \tanh(\alpha)}{\text{Bi}}, \quad \text{where } \alpha = \sqrt{\lambda \frac{e^{u_0}}{2}} \text{ and } \lambda > 0.$$

When $\lambda=0$, u is the trivial solution $u(r)=0$ for all r . As u_0 and λ are unique for each value of α , the solution curve can be parameterised by α , giving a branch $(u_0(\alpha), \lambda(\alpha))$ of solutions.

The solution when $Bi = 1$ is plotted in figure 1.5.

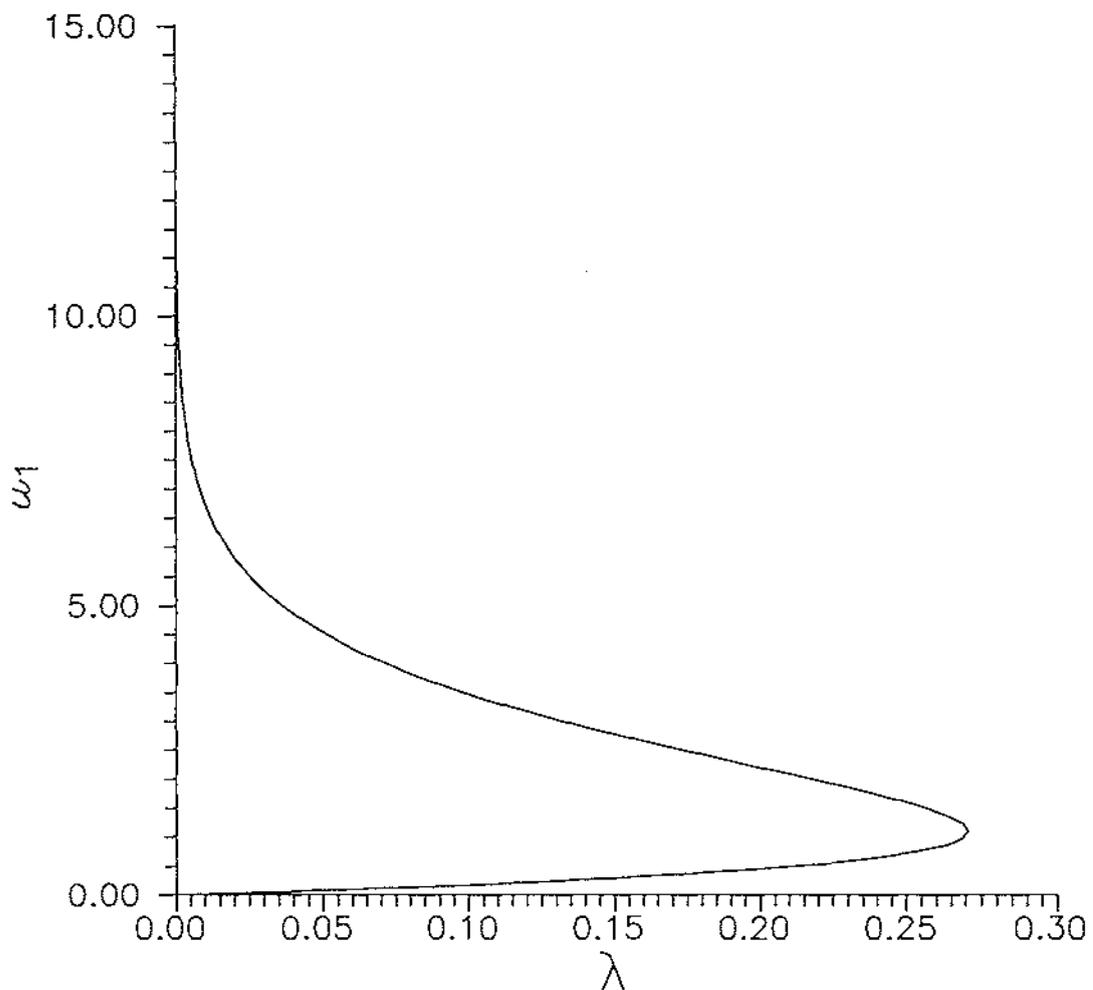


Figure 1.5: Bifurcation graph of system (1.7) with $j=0$ and $Bi=1$.

The maximum value of λ is at a limit point, $\lambda_{\text{crit}} = 0.270671$.

By the definition of a limit point (see section 1.1), a limit point is a point when

$\lambda'(\alpha) = 0$, or equivalently $\frac{d(\ln \lambda)}{d\alpha} = 0$. Also as the entire solution space is parameterised

by **one** parameter, there are no other branches, and therefore no branching points.

This gives an implicit equation for the co-ordinates of the limit point, for any given Biot number Bi:

$$(1.10) \quad \text{Bi} = \frac{\alpha_{\text{crit}} \sinh(\alpha_{\text{crit}}) \cosh(\alpha_{\text{crit}}) + \alpha_{\text{crit}}^2}{[1 - \alpha_{\text{crit}} \tanh(\alpha_{\text{crit}})] \cosh^2(\alpha_{\text{crit}})}$$

where α_{crit} is the value of α when it is a limit point, from which the corresponding values $(u_0)_{\text{crit}}$ and λ_{crit} can be attained by using (1.9).

A singular solution of (1.10) occurs when the denominator is zero and $\text{Bi} = \infty$. This is called the Frank-Kamenetskii boundary condition, and corresponds to perfect heat transfer at the surface of the object. The last term of (1.9) becomes zero when $\text{Bi} = \infty$, and λ can be defined explicitly in terms of u_0 :

$$\lambda = \frac{2}{e^{u_0}} \left[\cosh^{-1} \left(e^{\frac{u_0}{2}} \right) \right]^2$$

The limit point (when $\frac{d\lambda}{du_0} = 0$) is 0.87846.

A general solution also exists for equation (1.7) when $j=1$ (the infinite cylinder):

$$(1.11) \quad u(r) = \ln \left[\frac{8A}{\lambda} (1 + Ar^2)^2 \right]$$

where A is a constant of integration. Similar analysis may be used on this to give an implicit equation for λ and u_0 . From (1.11), $u_0 = u_{\text{max}} = \ln(8A/\lambda)$ and introducing $G = A$ results in:

$$\ln(\lambda) = \ln \left[\frac{8G}{(G+1)^2} \right] - \left[\frac{4G}{\text{Bi}(G+1)} \right], \quad \text{where } G = \frac{\lambda}{8} e^{u_0}$$

The limit point $(u_0)_{crit}, \lambda_{crit}$ occurs when $\frac{d(\ln \lambda)}{dG} = 0$, and results in the implicit equation:

$$Bi = \frac{4G_{crit}}{(1-G_{crit}^2)}$$

When $Bi = \infty$, an explicit solution for λ in terms u_0 exists:

$$\lambda = 8 \left(e^{-\frac{u_0}{2}} - e^{-u_0} \right)$$

and λ_{crit} is 2.

A general solution for $j=2$ (or more generally for $j \neq \{0 \text{ or } 1\}$) has not been found.

Chapter 3 discusses a numerical approach for solving (1.7) for any j and Bi .

THE SHAPE FACTOR

The examples so far are *Class A* shapes which have Laplacians which are of the form

of equation (1.7). The Laplacian $\nabla^2 u = \frac{d^2 u}{dr^2} + \frac{j}{r} \frac{du}{dr}$ can also be used to approximate

non-*Class A* geometries. Boddington, Gray and Harvey [1] developed a technique for using (1.7) to model **any** shape possessing a point of symmetry by defining j as a *shape factor*:

$$(1.12) \quad j = 3 \frac{R_0^2}{R_s^2} - 1$$

where R_s is the Seminov radius [1], and R_o is the harmonic root-mean-square radius of the body:

$$R_s = 3 \frac{\text{volume}}{\text{surface area}}, \quad \frac{1}{R_o^2} = \frac{1}{4\pi} \iint \frac{d\omega}{a^2}$$

where $d\omega$ is the solid angle subtended at the

centre O and a is the radius from O to the edge for given angle co-ordinates.

For example, a cube of volume $(2a)^3$ has $R_s = \frac{3(2a)^3}{6(2a)^2} = a$, and

$$R_o = a \sqrt{\frac{3}{1 + \frac{2\sqrt{3}}{\pi}}} = 1.194a$$

so the shape factor j for a cube of any size (as the a 's cancel)

is 3.280 (using (1.12)).

The harmonic root-mean-square radius RA_o for any **unit Class A** shape is defined (see [1]) as:

$$RA_o^{-2} = \frac{1}{3}(j+1)$$

A shape X is modelled by a *Class A* shape of radius $\frac{1}{3}(j+1)$, where j is defined using R_s and R_o from the original shape X . This results in solving a modified version of (1.7) which has a new parameter $\lambda(R_o)$ (see [1]):

$$\frac{d^2u}{dr^2} + \frac{j}{r} \frac{du}{dr} + \frac{1}{3}(j+1)\lambda(R_o)e^u = 0$$

$$\frac{du}{dr}(0) = 0, \quad \frac{du}{dr}(1) + Bi u(1) = 0$$

This system gives an approximate value of λ for shape X .

λ can be found for the **unit** shape X by scaling $\lambda(R_0)$ by R_0^{-2} .

So (1.7) can model a shape of unit size by:

- 1 -> Calculating the shape factor j from (1.12)
- 2 -> Solving (1.7) to get solution points (u_i, λ_i)
- 3 -> Scaling λ_i :

$$\lambda_i^* = \frac{3\lambda_i}{(j+1)RA_0^2}$$

Table 1.1 has some more examples of shape factors. RA_s is easy to find, but RA_0 is not.

(There is list of formulae of R_0 for simple geometries in [1]).

Table 1.1: Example Shape factors

Geometry	RA_0	RA_s	j
Infinite Slab	3	3	0
Rectangular Parallelepiped (ratio 1:10:10)	1.731	5/2	0.438
Infinite Cylinder	1.225	3/2	1
Infinite Square Rod	1.354	3/2	1.444
Rectangular Parallelepiped (ratio 1:1:10)	1.354	10/7	1.694
Sphere	1	1	2
Equicylinder	1.115	1	2.729
Cube	1.194	1	3.280
Regular Tetrahedron	0.537	0.408	4.178

Boddington, Gray and Harvey [1] showed that, for convex bodies, the shape parameter has values lying between 0 (the infinite slab) and 4.178 (the regular tetrahedron).

If $N = j + 1$ is defined as the dimension of a sphere, then $\frac{d^2\theta}{dr^2} + \frac{N-1}{r} \frac{d\theta}{dr}$ can be thought

of as the Laplacian of the N -dimensional sphere in spherical co-ordinates. So, using the shape factor j , an object can be modelled as a $j+1$ dimensional sphere, where j is a positive real number.

RESULTS FOR ARBITRARY j

A *phase plane analysis* of (1.7) by Wake [14], has shown that for $1 < j < 9$, as u increases, λ converges to λ_∞ where :

$$(1.14) \quad \lambda_\infty = 2(j-1)e^{-\frac{2}{Bi}}$$

He also showed that there are an infinite number of solutions to (1.7) when $\lambda = \lambda_\infty$. This implies that the bifurcation curve has a damped oscillation about the line $\lambda = \lambda_\infty$, with amplitude decreasing as u increases. As there are infinitely many oscillations about a vertical line, there are also infinitely many limit points.

No analytical solution to (1.7) has been found for arbitrary j and Bi . The rest of this thesis discusses techniques for numerically solving (1.7) to generate bifurcation graphs for any j or Bi value. The analytical results of this Chapter are used to test the accuracy of the numerical results.