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THE COMPUTATION OF JORDAN BLOCKS IN PARAMETER-DEPENDENT MATRICES

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Abstract. This paper extends the Implicit Determinant Method introduced by Spence & Poulton (J. Comput. Phys., 204 (2005), pp. 65–81) to obtain a numerical technique for the calculation of a 2-dimensional Jordan block in a parameter dependent matrix. An important feature of this technique is that the theory is straightforward to understand and an efficient numerical implementation is suggested naturally by the theory.

Three interesting physical problems are presented arising from the panel flutter problem in aerodynamics, the stability of electrical power systems and a problem in quantum mechanics.

Key words. Jordan block, eigenvalue coalescence, Newton's method.

AMS subject classifications. Primary 65F15, 15A18. Secondary 93B60.

1. Introduction. This paper describes a method for computing a 2-dimensional Jordan block in a parameter-dependent matrix based on the Implicit Determinant Method introduced in [24]. The need to compute Jordan blocks arises in a number of physical problems, for example, in aerodynamical stability [18, 19, 22, 23], the stability of electrical power systems [5, 20] and in quantum mechanics [13, 26].

Several types of parameter dependent matrices arise in applications (as we shall see in Section 5) but to give an illustration of the problems we examine, consider the simplest case of $A(\gamma)$ being a nonsymmetric real matrix depending on a real parameter γ. We consider the important question of finding the parameter γ such that two eigenvalues of $A(\gamma)$ coalesce at a Jordan block. Hence, we are looking for values of γ^* and λ^* such that $A(\gamma^*)$ has a defective eigenvalue λ^* corresponding to a Jordan block of dimension 2. This is precisely the type of behaviour that arises in supersonic panel flutter problems, see Examples 5.1 and 5.2, and references [18, 19, 22, 23].

The paper is organised as follows: We start with the most general case in Section 2, then restrict to the eigenvalue problem for a parameter dependent matrix in Sections 3, 4 and 5. More specifically, in Section 2 we consider the most general parameter dependent nonlinear matrix eigenvalue problem

$$T(\lambda, \gamma)x = 0, \quad x \neq 0,$$

where $T(\lambda, \gamma)$ is a matrix-valued function with range in $\mathbb{C}^{n \times n}$ and $\lambda, \gamma \in \mathbb{C}$. An alternative formulation is to seek solutions of $\det(T(\lambda, \gamma)) = 0$, and the main idea here is to obtain a simpler complex-valued function $f(\lambda, \gamma)$ such that

$$f(\lambda, \gamma) = 0 \iff \det(T(\lambda, \gamma)) = 0.$$

Hence, solutions of the nonlinear eigenvalue problem may be found by calculating solutions of $f(\lambda, \gamma) = 0$. In Section 3 we restrict the problem to

$$T(\lambda, \gamma)x = (A(\gamma) - \lambda I)x = 0, \quad x \neq 0,$$

a form that arises in many applications. Stated simply we seek pairs (λ, γ) where the parameter dependent matrix $A(\gamma)$ is defective, that is, it has a 2-dimensional

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Jordan block. We shall show that the required values (λ, γ) are found by solving the pair of nonlinear equations. In Section 4 we derive an efficient numerical procedure to implement the method suggested by the results of Theorem 3.1. This is based on the Implicit Determinant method [24] (see also [11]) for calculating the parameters (λ^*, γ^*) such that $A(\gamma^*) - \lambda^* I$ has a 2-dimensional Jordan block. Finally, in Section 5 we give examples from important applications such as calculating the critical dynamic pressure in supersonic panel flutter characteristics and parameters at which strong resonance occurs in power system dynamics.

2. Two parameter matrices and equivalence results. In this section we consider the general form of a two-parameter nonlinear matrix eigenvalue problem $T(\lambda, \gamma)x = 0$, $x \neq 0$, where $T(\lambda, \gamma)$ is a matrix-valued function with range in $\mathbb{C}^{n \times n}$ and where $\lambda, \gamma \in \mathbb{C}$. An alternative formulation is to seek solutions of $\det(T(\lambda, \gamma)) = 0$. The main idea in this section is to obtain an equivalent simpler scalar problem, namely, to derive a complex-valued function $f(\lambda, \gamma)$ such that

$$f(\lambda, \gamma) = 0 \iff \det(T(\lambda, \gamma)) = 0.$$

Hence, solutions of the nonlinear eigenvalue problem may be found by calculating solutions of $f(\lambda, \gamma) = 0$. The main theoretical results in this Section are Theorem 2.2 and Corollary 2.3.

Assume the matrix entries of $T(\lambda, \gamma)$ are analytic functions of $\lambda, \gamma \in \mathbb{C}$ in a neighbourhood of $\lambda^*, \gamma^* \in \mathbb{C}$, where

$$T(\lambda^*, \gamma^*)x^* = 0, \quad x^* \neq 0 \quad \text{and} \quad \dim \ker T(\lambda^*, \gamma^*) = 1. \tag{2.1}$$

Further, let y^* be the corresponding left null vector of $T(\lambda^*, \gamma^*)$ so that

$$y^{*H}T(\lambda^*, \gamma^*) = 0, \quad y^* \neq 0. \tag{2.2}$$

A natural example for $T(\lambda, \gamma)$ is $T(\lambda, \gamma) = A(\gamma) - \lambda I$, so that (λ^*, x^*) is a complex eigenpair of the parameter dependent matrix $A(\gamma^*)$ and y^* is the corresponding left eigenvector. Another example is the delay eigenvalue problem $T(\lambda, \gamma) = -\lambda I + A_0 + A_1 e^{-\gamma \lambda}$, where $A_i \in \mathbb{R}^{n \times n}$, $\lambda \in \mathbb{C}$ and $\gamma \in \mathbb{R}$ is a delay (see [14] and the references therein).

We first introduce a bordered matrix $M(\lambda, \gamma)$ and give conditions to ensure this matrix is nonsingular in the following theorem.

THEOREM 2.1. *Let $(\lambda^*, \gamma^*, x^*)$ satisfy (2.1) and y^* satisfy (2.2). For some $c \in \mathbb{C}^n$ and $b \in \mathbb{C}^n$ assume*

$$c^H x^* \neq 0 \quad \text{and} \quad b^H y^* \neq 0. \tag{2.3}$$

Then the bordered matrix

$$M(\lambda, \gamma) = \begin{bmatrix} T(\lambda, \gamma) & b \\ c^H & 0 \end{bmatrix} \tag{2.4}$$

is nonsingular at $\lambda = \lambda^*$, $\gamma = \gamma^*$.

Proof. This result follows from [16, Lemma 2.8] (see [10, Lemma 3.1] for a proof). □

Since $M(\lambda^*, \gamma^*)$ is nonsingular and the entries of $M(\lambda, \gamma)$ are analytic, we have that for (λ, γ) near (λ^*, γ^*), $M(\lambda, \gamma)$ is nonsingular, using, for example, [6, Theorem 2.3.4].

Now, define $x(\lambda, \gamma) \in \mathbb{C}^n$, $f(\lambda, \gamma) \in \mathbb{C}^n$ to be solutions to the linear system

$$\begin{bmatrix} T(\lambda, \gamma) & b \\ c^H & 0 \end{bmatrix} \begin{bmatrix} x(\lambda, \gamma) \\ f(\lambda, \gamma) \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{2.5}$$

for (λ, γ) near (λ^*, γ^*). From Theorem 2.1 $x(\lambda, \gamma)$, $f(\lambda, \gamma)$ are unique for (λ, γ) near (λ^*, γ^*). Further, Cramer's rule gives

$$f(\lambda, \gamma) = \frac{\det T(\lambda, \gamma)}{\det M(\lambda, \gamma)}. \tag{2.6}$$

Now $M(\lambda, \gamma)$ is nonsingular in the neighbourhood of (λ^*, γ^*) and since sums, products and quotients of holomorphic functions are holomorphic (whenever the denominator is not zero) we have that $f(\lambda, \gamma)$ is holomorphic near (λ^*, γ^*). Therefore $f(\lambda, \gamma)$ is an infinitely complex differentiable function and satisfies the Cauchy-Riemann conditions. This leads to the following equivalence results.

THEOREM 2.2. *Assume the conditions of Theorem 2.1 hold and let $f(\lambda, \gamma)$ be given by (2.6). Then*

$$f(\lambda, \gamma) = 0 \iff det\,(T(\lambda, \gamma)) = 0. \tag{2.7}$$

Furthermore, if $f(\lambda, \gamma) = 0$, then

$$f_\lambda(\lambda, \gamma) = 0 \iff \frac{\partial}{\partial \lambda} det\,(T(\lambda, \gamma)) = 0. \tag{2.8}$$

Proof. The equivalence (2.7) follows straight from (2.6). Now f is holomorphic and so differentiating (2.6) with respect to λ gives

$$f_\lambda(\lambda, \gamma) = \frac{(\det\,(T(\lambda, \gamma)))_\lambda \det\,(M(\lambda, \gamma)) - \det\,(T(\lambda, \gamma))(\det\,(M(\lambda, \gamma)))_\lambda}{(\det M(\lambda, \gamma))^2},$$

and, with (2.7), and $M(\lambda, \gamma)$ nonsingular, the equivalence (2.8) follows. $\square$

Theorem 2.2 gives equivalences between properties of the determinant $\det\,(T(\lambda, \gamma))$ (and its derivatives) of an $n \times n$ matrix and the scalar function $f(\lambda, \gamma)$ (and its derivatives). An immediate corollary is as follows (cf. [25, Theorem 2.1]).

COROLLARY 2.3. *Under the conditions of Theorem 2.2, with $f(\lambda, \gamma) = 0$, we have*

$$f_\gamma(\lambda, \gamma) \neq 0 \iff \frac{\partial}{\partial \gamma} det\,(T(\lambda, \gamma)) \neq 0. \tag{2.9}$$

Furthermore, for $m \in \mathbb{N}$,

$$det\,(T(\lambda, \gamma)) = \frac{\partial}{\partial \lambda} det\,(T(\lambda, \gamma)) = \frac{\partial^2}{\partial \lambda^2} det\,(T(\lambda, \gamma)) = \ldots = \frac{\partial^{m-1}}{\partial \lambda^{m-1}} det\,(T(\lambda, \gamma)) = 0,$$

$$\frac{\partial^m}{\partial \lambda^m} det\,(T(\lambda, \gamma)) \neq 0$$

is equivalent to

$$f(\lambda, \gamma) = \frac{\partial}{\partial \lambda} f(\lambda, \gamma) = \frac{\partial^2}{\partial \lambda^2} f(\lambda, \gamma) = \ldots = \frac{\partial^{m-1}}{\partial \lambda^{m-1}} f(\lambda, \gamma) = 0, \quad \frac{\partial^m}{\partial \lambda^m} f(\lambda, \gamma) \neq 0.$$

Note that from the first row of (2.5) it also follows that

$$f(\lambda, \gamma) = 0 \iff x(\lambda, \gamma) \in \ker(T(\lambda, \gamma)). \tag{2.10}$$

The key theoretical concept here is that the zeros of $\det\,(T(\lambda, \gamma)) = 0$ and its derivatives are precisely the roots of $f(\lambda, \gamma) = 0$ and its derivatives. Moreover, from the computational viewpoint we shall see in Section 4 that there is a particularly

straightforward and efficient numerical procedure for the calculation of f and its derivatives.

Bordered matrices, like $M(\lambda, \gamma)$ in Theorem 2.1, provide a powerful tool in numerical bifurcation. They were first introduced by Griewank and Reddien [11], and the book by Govaerts [9] provides an extensive discussion of their application to the bifurcation analysis of dynamical systems. The extension to borderings of dimension greater than one is discussed in [8].

In the next section we consider the special case of $T(\lambda, \gamma) = A(\gamma) - \lambda I$, where we discover that the values of f and its derivatives at (λ^*, γ^*) give us an insight into the Jordan structure of $A(\lambda^*) - \gamma^* I$.

3. Analysis of Jordan blocks in $A(\gamma) - \lambda I$ using $f(\lambda, \gamma) = 0$. In this section we consider the case

$$T(\lambda, \gamma) = A(\gamma) - \lambda I, \tag{3.1}$$

so that solutions of $\det (T(\lambda, \gamma)) = 0$ correspond to eigenvalues of the parameter-dependent matrix $A(\gamma)$. In particular we consider the special case when $\lambda^* \in \mathbb{C}$ is a defective eigenvalue of $A(\gamma^*)$ of algebraic multiplicity 2, that is, λ^* corresponds to a 2-dimensional Jordan block of $A(\gamma^*)$, and x^*, y^* are the right and left eigenvectors corresponding to λ^*. Under these assumptions we have that (2.1) and (2.2) hold with $T(\lambda^*, \gamma^*) = A(\gamma^*) - \lambda^* I$. Furthermore, we assume

$$y^{*H} x^* = 0, \tag{3.2}$$

and, with the generalised eigenvector of the defective λ^* being denoted by $\hat{x}^*$ then

$$(A(\gamma^*) - \lambda^* I)\hat{x}^* = x^*, \tag{3.3}$$

and

$$y^{*H} \hat{x}^* \neq 0, \tag{3.4}$$

since we assume that the Jordan block has dimension 2. The following Theorem provides the theoretical basis for our numerical method for the computation of a 2-dimensional Jordan block (described in Section 4).

THEOREM 3.1. *Let $\lambda^* \in \mathbb{C}$ be a defective eigenvalue of $A(\gamma^*)$ of algebraic multiplicity 2, that is (2.1) and (2.2) hold for $T(\lambda^*, \gamma^*) = A(\gamma^*) - \lambda^* I$ and (3.2)-(3.4) hold where $x^* = x(\lambda^*, \gamma^*)$. Further, with $A(\gamma)$ analytic for γ near γ^*, assume that*

$$y^{*H} \frac{\partial}{\partial \gamma} A(\gamma^*)x^* = y^{*H} A_\gamma(\gamma^*)x^* \neq 0. \tag{3.5}$$

Then

$$(a) \qquad f_\lambda^* := f_\lambda(\lambda^*, \gamma^*) = 0, \tag{3.6}$$

$$(b) \qquad f_{\lambda\lambda}^* := f_{\lambda\lambda}(\lambda^*, \gamma^*) \neq 0, \tag{3.7}$$

$$(c) \qquad f_\gamma^* := f_\gamma(\lambda^*, \gamma^*) \neq 0. \tag{3.8}$$

Proof. We have that both $f(\lambda, \gamma)$ and $x(\lambda, \gamma)$ are analytic functions of (λ, γ) near (λ^*, γ^*), since the matrix elements of $A(\gamma)$ are analytic functions of γ in the neighbourhood of γ^*.
(a) Differentiating (2.5) with $T(\lambda, \gamma) = A(\gamma) - \lambda I$ with respect to λ gives

$$\begin{bmatrix} A(\gamma) - \lambda I & b \\ c^H & 0 \end{bmatrix} \begin{bmatrix} x_\lambda(\lambda, \gamma) \\ f_\lambda(\lambda, \gamma) \end{bmatrix} = \begin{bmatrix} x(\lambda, \gamma) \\ 0 \end{bmatrix}. \tag{3.9}$$

Evaluate at (λ^*, γ^*), multiply the first row from the left by y^{*H} and use $y^{*H}b \neq 0$ from Theorem 2.1 to get

$$f_\lambda^* := f_\lambda(\lambda^*, \gamma^*) = \frac{y^{*H}x(\lambda^*, \gamma^*)}{y^{*H}b} = 0,$$

using (3.2) since $x(\lambda^*, \gamma^*) = x^*$. Therefore, with (3.3), the first row of (3.9) evaluated at (λ^*, γ^*) gives

$$x_\lambda^* := x_\lambda(\lambda^*, \gamma^*) = \hat{x}^*, \tag{3.10}$$

so x_λ^* is a generalised eigenvector belonging to the defective eigenvalue λ^*.
(b) Differentiate the linear system (3.9) with respect to λ again to obtain

$$\begin{bmatrix} A(\gamma) - \lambda I & b \\ c^H & 0 \end{bmatrix} \begin{bmatrix} x_{\lambda\lambda}(\lambda, \gamma) \\ f_{\lambda\lambda}(\lambda, \gamma) \end{bmatrix} = \begin{bmatrix} 2x_\lambda(\lambda, \gamma) \\ 0 \end{bmatrix}. \tag{3.11}$$

Evaluate at (λ^*, γ^*), multiply the first row from the left by y^{*H} to get

$$f_{\lambda\lambda}^* := f_{\lambda\lambda}(\lambda^*, \gamma^*) = \frac{2y^{*H}x_\lambda^*}{y^{*H}b} \neq 0,$$

using (3.10) and (3.4).
(c) Differentiating (2.5) with respect to γ gives

$$\begin{bmatrix} A(\gamma) - \lambda I & b \\ c^H & 0 \end{bmatrix} \begin{bmatrix} x_\gamma(\lambda, \gamma) \\ f_\gamma(\lambda, \gamma) \end{bmatrix} = \begin{bmatrix} -A_\gamma(\gamma)x(\lambda, \gamma) \\ 0 \end{bmatrix}. \tag{3.12}$$

The same procedure as in parts (a) and (b) and using (3.5) yields

$$f_\gamma^* := f_\gamma(\lambda^*, \gamma^*) = -\frac{y^{*H}A_\gamma(\gamma^*)x^*}{y^{*H}b} \neq 0.$$

□

Theorem 3.1 tells us that if (λ^*, x^*) corresponds to a 2-dimensional Jordan block, then $f(\lambda^*, \gamma^*) = 0$ and $f_\lambda(\lambda^*, \gamma^*) = 0$ which immediately suggests a numerical technique for the computation of (λ^*, γ^*). We describe such a technique in the next section, but in this section explore further some theoretical aspects. From Theorem 3.1 we have the following result (see also [25]).

THEOREM 3.2. *Let the assumptions of Theorem 3.1 hold. Then $f(\lambda, \gamma)$ has a unique solution $\gamma(\lambda)$ in the neighbourhood of $\lambda = \lambda^*$ with $\gamma(\lambda^*) = \gamma^*$. This solution is analytic near λ^* and has a Taylor series expansion of the form*

$$\gamma(\lambda) = \gamma^* - \frac{1}{2}(\lambda - \lambda^*)^2 \frac{f_{\lambda\lambda}^*}{f_\gamma^*} + \sum_{k=3}^\infty c_k(\lambda - \lambda^*)^k, \tag{3.13}$$

where c_k, $k = 3, \ldots$ are complex coefficients.

Proof. Using the results of Theorem 3.1, i.e. $f(\lambda^*, \gamma^*) = 0$ and $f_\gamma^* \neq 0$, the Holomorphic Implicit Function Theorem (see, for example [17]) shows that near (λ^*, γ^*) we have a unique $\gamma = \gamma(\lambda)$ such that $f(\lambda, \gamma(\lambda)) = 0$ and $\gamma = \gamma(\lambda)$ is locally analytic. Hence there is a smooth path of solutions to $f(\lambda, \gamma(\lambda)) = 0$. Differentiating this last equation with respect to λ and setting $\lambda = \lambda^*$ yields

$$\frac{\partial \gamma}{\partial \lambda}(\lambda^*) = -\frac{f_\lambda^*}{f_\gamma^*} = 0,$$

by Theorem 3.1. Differentiating $f(\lambda, \gamma(\lambda)) = 0$ twice with respect to λ yields

$$\frac{\partial^2 \gamma}{\partial \lambda^2}(\lambda^*) = -\frac{f^*_{\lambda\lambda}}{f^*_\gamma} \neq 0,$$

where the last inequality follows from Theorem 3.1, i.e. the fact that $A(\gamma^*)$ has an eigenvalue of algebraic multiplicity 2. Simple calculus then shows that near (λ^*, γ^*) with $\gamma^* = \gamma(\lambda^*)$ the Taylor series expansion of $\gamma(\lambda)$ has the required form (3.13). $\square$

Following on from Theorem 3.2 we can express, for γ sufficiently close to γ^*, two of the eigenvalues of $A(\gamma)$ near λ^* as convergent Puiseux series, i.e. a convergent series in fractional powers of γ (see, for example, [3, 15]). So, if $A(\gamma^*)$ has a 2-dimensional Jordan block we have the following Theorem (cf. [25]).

THEOREM 3.3. *Let the assumptions of Theorem 3.1 hold, i.e. let $\lambda^* \in \mathbb{C}$ be a defective eigenvalue of $A(\gamma^*)$ of algebraic multiplicity 2. Then there exists a convergent Puiseux series whose branches are given by*

$$\lambda_1(\gamma) = \lambda^* + a_1(\gamma - \gamma^*)^{\frac{1}{2}} + \sum_{k=2}^{\infty} a_k \left((\gamma - \gamma^*)^{\frac{1}{2}} \right)^k, \tag{3.14}$$

$$\lambda_2(\gamma) = \lambda^* - a_1(\gamma - \gamma^*)^{\frac{1}{2}} + \sum_{k=2}^{\infty} a_k \left(-(\gamma - \gamma^*)^{\frac{1}{2}} \right)^k, \tag{3.15}$$

where $a_1 = \left(-\dfrac{2f^*_\gamma}{f^*_{\lambda\lambda}} \right)^{\frac{1}{2}} \neq 0$, a_k, $k = 2, \ldots$ are complex coefficients, such that the value of the branches are the eigenvalues of $A(\gamma)$ for (λ, γ) sufficiently close to (λ^*, γ^*).

Proof. From Theorem 3.2 we have that $\gamma(\lambda) - \gamma^*$ has a zero of order 2 at $\lambda = \lambda^*$. Rewrite (3.13) as

$$\gamma(\lambda) - \gamma^* = (\lambda - \lambda^*)^2 \left(-\frac{1}{2} \frac{f^*_{\lambda\lambda}}{f^*_\gamma} + \sum_{k=3}^{\infty} c_k (\lambda - \lambda^*)^{k-2} \right).$$

Following the proof of [25, Theorem 2.1] we take the square root of this equation, with the branch of the square root fixed. Set $h(\lambda) = (\gamma(\lambda) - \gamma^*)^{\frac{1}{2}}$ and obtain

$$h(\lambda) = (\lambda - \lambda^*) \left(-\frac{1}{2} \frac{f^*_{\lambda\lambda}}{f^*_\gamma} + \sum_{k=3}^{\infty} c_k (\lambda - \lambda^*)^{k-2} \right)^{\frac{1}{2}}.$$

For λ near λ^* the function $h(\lambda)$ is analytic and $h(\lambda^*) = 0$ as well as $\frac{\partial h}{\partial \lambda}(\lambda^*) = \left(-\frac{1}{2} \frac{f^*_{\lambda\lambda}}{f^*_\gamma} \right)^{\frac{1}{2}} \neq 0$, since $f^*_{\lambda\lambda} \neq 0$ from Theorem 3.1. By the inverse function theorem for analytic functions we have that for λ close to λ^* the function $h(\lambda)$ has an analytic inverse h^{-1} in the neighbourhood of 0 and $h^{-1}(0) = \lambda^*$. Hence we can define a multivalued function $\lambda(\gamma) := h^{-1}((\gamma - \gamma^*)^{\frac{1}{2}})$, where $(\gamma - \gamma^*)^{\frac{1}{2}}$ means all branches of the square root of $\gamma - \gamma^*$. Hence, since h^{-1} is analytic $\lambda(\gamma)$ is a Puiseux series for γ close enough to γ^*. Furthermore

$$\frac{\partial h^{-1}}{\partial \gamma}(0) = \left(\frac{\partial h}{\partial \lambda}(\lambda^*) \right)^{-1} = \left(-\frac{1}{2} \frac{f^*_{\lambda\lambda}}{f^*_\gamma} \right)^{-\frac{1}{2}} \neq 0,$$

where the last inequality follows from Theorem 3.1. Hence

$$\lambda(\gamma) = h^{-1}((\gamma - \gamma^*)^{\frac{1}{2}}) = \lambda^* + a_1(\gamma - \gamma^*)^{\frac{1}{2}} + \sum_{k=2}^{\infty} a_k \left((\gamma - \gamma^*)^{\frac{1}{2}} \right)^k,$$

where $a_1 = \left(\frac{-2f_\gamma^*}{f_{\lambda\lambda}^*}\right)^{\frac{1}{2}} \neq 0$. When including all branches of the square root we obtain the solution branches given by $\lambda_1(\gamma)$ and $\lambda_2(\gamma)$. $\square$

From equations (3.14) and (3.15) we see that at $\gamma = \gamma^*$ the two eigenvalues $\lambda_1(\gamma^*)$ and $\lambda_2(\gamma^*)$ coalesce. To explain a typical solution behaviour, let us assume for the moment that γ is real. In this case, for an increasing value of $\gamma > \gamma^*$ the two eigenvalues $\lambda_1(\gamma)$ and $\lambda_2(\gamma)$ move away from λ^* in opposite directions with the same speed. For $\gamma < \gamma^*$ the eigenvalues change direction by a right angle (compared to $\gamma > \gamma^*$) and are also moving away from each other in opposite directions with the same speed. This behaviour can be observed in the example in Figure 5.3.

A sketch of what happens when two complex eigenvalues coalesce at a 2-dimensional Jordan block is drawn in Figure 3.1 Note that for this figure we assumed that f and γ are real. If complex eigenvalues $\lambda = \alpha + i\beta$ collide at $\lambda^* = \alpha^* + i\beta^*$ to form a Jordan block one also speaks of "strong coupling", see [21].

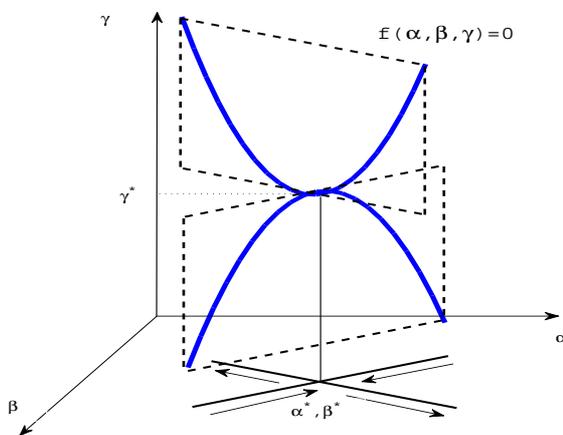
Fig. 3.1: Strong coupling of eigenvalues at a saddle point of f.

If λ is real and both A and γ are real we have from (2.7) that $f(\lambda, \gamma)$ is a real function of two real variables and $f(\lambda, \gamma) = 0$ represents a smooth curve in the (λ, γ)-plane. The solution structure of $f(\lambda, \gamma) = 0$ near (λ^*, γ^*) depends on the sign of $\frac{f_{\lambda\lambda}^*}{f_\gamma^*} = -\frac{2y^{*H}x_\lambda^*}{y^{*H}A'(\gamma^*)x^*}$ and is plotted in Figure 3.2. We see that at the point $(\lambda, \gamma) = (\lambda^*, \gamma^*)$ both $f(\lambda, \gamma) = 0$ and $f_\lambda(\lambda, \gamma) = 0$. For the case $\frac{f_{\lambda\lambda}^*}{f_\gamma^*} < 0$, if $\gamma > \gamma^*$ there are two real eigenvalues λ_1 and λ_2. They coalesce at $\lambda = \lambda^*$ and for $\gamma < \gamma^*$ there are no real solutions to $f(\lambda, \gamma) = 0$. A similar discussion follows for the case $\frac{f_{\lambda\lambda}^*}{f_\gamma^*} > 0$. We see that $A(\gamma^*) - \lambda^*I$ has a 2-dimensional Jordan block when (λ^*, γ^*) is a quadratic turning point of $f(\lambda, \gamma) = 0$.

4. A technique to compute a 2-dimensional Jordan block of $A(\gamma) - \lambda I$. Though the theory in Sections 2 and 3 is given for the purely complex case, the physical examples often involve real parameters. Hence, we discuss four common cases separately in the next four subsections.

4.1. Complex λ and complex γ. Following the development of the theory in Section 3 (especially Theorem 3.1) it is clear that to compute the values λ^*, γ^* such that $A(\gamma^*) - \lambda^*I$ has a 2-dimensional Jordan block, we should set up the 2×2
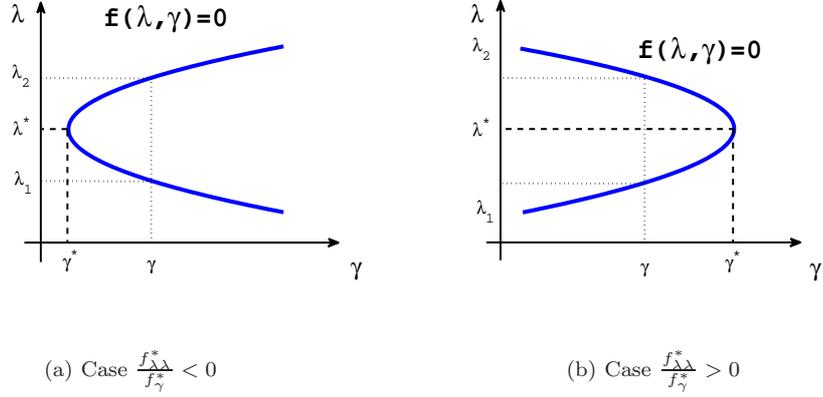
(a) Case $\frac{f^*_{\lambda\lambda}}{f^*_\gamma} < 0$ (b) Case $\frac{f^*_{\lambda\lambda}}{f^*_\gamma} > 0$

Fig. 3.2: Curve $f(\lambda, \gamma) = 0$ in the (λ, γ)-plane depending on the sign of $\frac{f^*_{\lambda\lambda}}{f^*_\gamma}$

complex nonlinear system

$$g(\lambda, \gamma) = \left[\begin{array}{c} f(\lambda, \gamma) \\ f_\lambda(\lambda, \gamma) \end{array} \right] = 0, \tag{4.1}$$

At the root (λ^*, γ^*) the Jacobian matrix of $g(\lambda, \gamma)$ is

$$G(\lambda^*, \gamma^*) = \left[\begin{array}{cc} f^*_\lambda & f^*_\gamma \\ f^*_{\lambda\lambda} & f^*_{\lambda\gamma} \end{array} \right] = \left[\begin{array}{cc} 0 & f^*_\gamma \\ f^*_{\lambda\lambda} & f^*_{\lambda\gamma} \end{array} \right],$$

which is nonsingular iff $f^*_\gamma \neq 0$ and $f^*_{\lambda\lambda} \neq 0$. The first condition holds from the nondegeneracy condition (3.5) and the second one from (3.7), which holds since the Jordan block has precise dimension 2.

Problem (4.1) is two nonlinear complex analytic equations with two complex unknowns, hence, we can apply Newton's method. For a given starting guess $(\lambda^{(0)}, \gamma^{(0)})$ we need to update

$$\left[\begin{array}{c} \lambda^{(i+1)} \\ \gamma^{(i+1)} \end{array} \right] = \left[\begin{array}{c} \lambda^{(i)} \\ \gamma^{(i)} \end{array} \right] + \left[\begin{array}{c} \Delta\lambda^{(i)} \\ \Delta\gamma^{(i)} \end{array} \right],$$

where $i = 0, 1, 2 \ldots$ until convergence and $\left[\begin{array}{c} \Delta\lambda^{(i)} \\ \Delta\gamma^{(i)} \end{array} \right]$ is obtained from solving

$$G(\lambda^{(i)}, \gamma^{(i)}) \left[\begin{array}{c} \Delta\lambda^{(i)} \\ \Delta\gamma^{(i)} \end{array} \right] = -g(\lambda^{(i)}, \gamma^{(i)}), \tag{4.2}$$

with

$$G(\lambda^{(i)}, \gamma^{(i)}) = \left[\begin{array}{cc} f_\lambda(\lambda^{(i)}, \gamma^{(i)}) & f_\gamma(\lambda^{(i)}, \gamma^{(i)}) \\ f_{\lambda\lambda}(\lambda^{(i)}, \gamma^{(i)}) & f_{\lambda\gamma}(\lambda^{(i)}, \gamma^{(i)}) \end{array} \right] =: G^{(i)}. \tag{4.3}$$

The values $f^{(i)}$, $f^{(i)}_\lambda$, $f^{(i)}_\gamma$ and $f^{(i)}_{\lambda\lambda}$ are calculated from (2.5), (3.9), (3.11) and (3.12). $f^{(i)}_{\lambda\gamma}$ can be obtained from differentiating (3.9) with respect to γ:

$$\left[\begin{array}{cc} A(\gamma) - \lambda I & b \\ c^H & 0 \end{array} \right] \left[\begin{array}{c} x_{\lambda\gamma}(\lambda, \gamma) \\ f_{\lambda\gamma}(\lambda, \gamma) \end{array} \right] = \left[\begin{array}{c} -A_\gamma(\gamma)x_\lambda(\lambda, \gamma) + x_\gamma(\lambda, \gamma) \\ 0 \end{array} \right]. \tag{4.4}$$

Therefore, in order to calculate $g(\lambda^{(i)}, \gamma^{(i)})$ and $G(\lambda^{(i)}, \gamma^{(i)})$ we need to solve five linear systems which all use the same nonsingular system matrix $M(\lambda^{(i)}, \gamma^{(i)})$ and hence, only one LU factorisation is needed per iteration. Newton's method itself is only carried out in two complex dimensions. For completeness we now give the algorithm that is used.

ALGORITHM 4.1 (Newton's method). *Given $(\lambda^{(0)}, \gamma^{(0)})$ and $c, b \in \mathbb{C}^n$ such that $M(\lambda^{(0)}, \gamma^{(0)})$ is nonsingular; set $i = 0$:*
  (i) *Solve (2.5) and (3.9) in order to evaluate $g(\lambda^{(i)}, \gamma^{(i)})$*
  (ii) *Solve (3.11), (3.12) and (4.4), in order to evaluate the Jacobian $G(\lambda^{(i)}, \gamma^{(i)})$ given by (4.3).*
  (iii) *Newton update: Solve (4.2) in order to get $(\lambda^{(i+1)}, \gamma^{(i+1)})$.*
  (iv) *Repeat until convergence.*

The Newton method is well-defined, that is the Jacobian $G(\lambda^{(i)}, \gamma^{(i)})$ is nonsingular for a starting guess that is close enough to the solution, since $G(\lambda^*, \gamma^*)$ is nonsingular under the conditions of Theorem 3.1 as noted at the beginning of this subsection. In many physical applications, including the ones discussed in Section 5 later, good starting values for Algorithm 4.1 are likely to be available by solving the physical problem for a value of γ near the critical value. Under these circumstances, as shown in Section 5, Algorithm 4.1 performs well. The choice of b and c in (2.4) is also relevant and we discuss this aspect further in Section 4.5.

4.2. Real λ and real γ. If λ and γ are real and $A(\gamma)$ is a real $n \times n$ matrix then b and c are chosen to be real. Hence

$$g(\lambda, \gamma) = \left[\begin{array}{c} f(\lambda, \gamma) \\ f_\lambda(\lambda, \gamma) \end{array} \right] = 0 \tag{4.5}$$

is real and Algorithm 4.1 can be implemented in real arithmetic.

4.3. Real γ and complex λ. When $A(\gamma)$ and γ are real but λ^* is complex, as is the case in Example 5.3 in the next section, then there are two options. One can simply apply Algorithm 4.1 with a real starting value for γ or we can write (4.1) as a system of 4 real equations with 3 real unknowns as we now describe. It may appear that there is no gain in studying this case separately from that in Section 4.1, but there may be cases where it is convenient to work in real arithmetic (see [1]) and also results obtained in the next paragraph are needed for the theory in the following section.

If $\lambda = \alpha + i\beta$ then (4.1) can be written as

$$g(\alpha, \beta, \gamma) = \left[\begin{array}{c} f(\alpha, \beta, \gamma) \\ f_\alpha(\alpha, \beta, \gamma) \\ f_\beta(\alpha, \beta, \gamma) \end{array} \right] = 0, \tag{4.6}$$

where f, f_α and f_β are complex and hence, if we consider real and imaginary part of g in (4.6) separately we obtain six nonlinear equations for three real unknowns. We can reduce this to a system of four nonlinear equations in three real unknowns using the fact that $f(\lambda, \gamma)$ satisfies the Cauchy-Riemann equations, which show that

$$f_\beta(\alpha, \beta, \gamma) := i f_\alpha(\alpha, \beta, \gamma), \quad \forall \alpha, \beta, \gamma, \tag{4.7}$$

$$f_{\beta\beta}(\alpha, \beta, \gamma) := -f_{\alpha\alpha}(\alpha, \beta, \gamma), \quad \forall \alpha, \beta, \gamma, \tag{4.8}$$

$$f_{\alpha\beta}(\alpha, \beta, \gamma) := i f_{\alpha\alpha}(\alpha, \beta, \gamma), \quad \forall \alpha, \beta, \gamma. \tag{4.9}$$

and hence (a) and (b) in Theorem 3.1 reduce to

$$f_\alpha^* := f_\alpha(\alpha^*, \beta^*, \gamma^*) = 0, \tag{4.10}$$

$$f_{\alpha\alpha}^* := f_{\alpha\alpha}(\alpha^*, \beta^*, \gamma^*) \neq 0. \tag{4.11}$$

Hence, the three complex equations given by (4.6) reduce to four real equations in three real unknowns

$$g(\alpha, \beta, \gamma) = \begin{bmatrix} \mathrm{Re}f(\alpha, \beta, \gamma) \\ \mathrm{Im}f(\alpha, \beta, \gamma) \\ \mathrm{Re}f_\alpha(\alpha, \beta, \gamma) \\ \mathrm{Im}f_\alpha(\alpha, \beta, \gamma) \end{bmatrix} = 0. \tag{4.12}$$

Thus, we obtain an overdetermined system that can be solved using the Gauss-Newton method (see [4, Section 10.2]) which solves the nonlinear least squares problem

$$\min_{(\alpha,\beta,\gamma)\in\mathbb{R}^3} \|g(\alpha, \beta, \gamma)\|.$$

The Gauss-Newton method uses the Jacobian $G(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)})$ of $g(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)})$ given by

$$G(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)}) = \begin{bmatrix} \mathrm{Re}f_\alpha^{(i)} & -\mathrm{Im}f_\alpha^{(i)} & \mathrm{Re}f_\gamma^{(i)} \\ \mathrm{Im}f_\alpha^{(i)} & \mathrm{Re}f_\alpha^{(i)} & \mathrm{Im}f_\gamma^{(i)} \\ \mathrm{Re}f_{\alpha\alpha}^{(i)} & -\mathrm{Im}f_{\alpha\alpha}^{(i)} & \mathrm{Re}f_{\alpha\gamma}^{(i)} \\ \mathrm{Im}f_{\alpha\alpha}^{(i)} & \mathrm{Re}f_{\alpha\alpha}^{(i)} & \mathrm{Im}f_{\alpha\gamma}^{(i)} \end{bmatrix} := G^{(i)}, \tag{4.13}$$

where we have used (4.7), (4.8) and (4.9).

In order to calculate $g(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)})$ and $G(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)})$ we need to solve five linear systems that all use the same bordered system matrix

$$M(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)}) = \begin{bmatrix} A(\gamma^{(i)}) - (\alpha^{(i)} + i\beta^{(i)})I & b \\ c^H & 0 \end{bmatrix} \tag{4.14}$$

therefore only one LU factorisation is needed per iteration. The Gauss-Newton method is carried out in three dimensions only and the algorithm is noted below.

ALGORITHM 4.2 (Gauss-Newton method, [4, Section 10.2]). *Given* $(\alpha^{(0)}, \beta^{(0)}, \gamma^{(0)})$ *and* $c, b \in \mathbb{C}^n$ *such that* $M(\alpha^{(0)}, \beta^{(0)}, \gamma^{(0)})$ *is nonsingular; set* $i = 0$:
  (i) *Evaluate* $g(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)})$ *given by (4.12) and the Jacobian* $G(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)})$ *given by (4.13) by solving bordered systems with system matrix* $M(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)})$ *from (4.14) and different right hand sides.*
 (ii) *Find the QR factorisation of* $G(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)}) = QR$.
(iii) *Solve* $R \begin{bmatrix} \Delta\alpha^{(i)} \\ \Delta\beta^{(i)} \\ \Delta\gamma^{(i)} \end{bmatrix} = -Q^T g(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)})$ *and update the solution.*
(iv) *Repeat until convergence.*

The Gauss-Newton method is well-defined, that is the Jacobian has full rank, for a starting guess that is close enough to the solution, as, in the limit, we have

$$G(\alpha^*, \beta^*, \gamma^*) = \begin{bmatrix} \mathrm{Re}f_\alpha^* & -\mathrm{Im}f_\alpha^* & \mathrm{Re}f_\gamma^* \\ \mathrm{Im}f_\alpha^* & \mathrm{Re}f_\alpha^* & \mathrm{Im}f_\gamma^* \\ \mathrm{Re}f_{\alpha\alpha}^* & -\mathrm{Im}f_{\alpha\alpha}^* & \mathrm{Re}f_{\alpha\gamma}^* \\ \mathrm{Im}f_{\alpha\alpha}^* & \mathrm{Re}f_{\alpha\alpha}^* & \mathrm{Im}f_{\alpha\gamma}^* \end{bmatrix} = \begin{bmatrix} 0 & 0 & \mathrm{Re}f_\gamma^* \\ 0 & 0 & \mathrm{Im}f_\gamma^* \\ \mathrm{Re}f_{\alpha\alpha}^* & -\mathrm{Im}f_{\alpha\alpha}^* & \mathrm{Re}f_{\alpha\gamma}^* \\ \mathrm{Im}f_{\alpha\alpha}^* & \mathrm{Re}f_{\alpha\alpha}^* & \mathrm{Im}f_{\alpha\gamma}^* \end{bmatrix}.$$

The determinant of the left lower block is given by $(\mathrm{Re}f_{\alpha\alpha}^*)^2 + (\mathrm{Im}f_{\alpha\alpha}^*)^2$ and is non-zero by (4.11). Furthermore, at least one of $\mathrm{Re}f_\gamma^*$ and $\mathrm{Im}f_\gamma^*$ is non-zero by (3.8). Hence $G(\alpha^*, \beta^*, \gamma^*)$ has full rank.

REMARK 4.3. *Note that for a complex parameter* $\gamma = \gamma_R + i\gamma_I$ *we can also work in real arithmetic. In this case* $g(\alpha, \beta, \gamma_R, \gamma_I) = 0$ *is a system of four real nonlinear equations and four unknowns and we can apply Newton's method.*

The Cauchy-Riemann equations lead to $f_{\gamma_I}(\alpha, \beta, \gamma_R, \gamma_I) := if_{\gamma_R}(\alpha, \beta, \gamma_R, \gamma_I)$ and $f_{\alpha\gamma_I}(\alpha, \beta, \gamma_R, \gamma_I) := if_{\alpha\gamma_R}(\alpha, \beta, \gamma_R, \gamma_I)$ for all α, β, γ_R and γ_I. In fact, it is straightforward to show that the Jacobian in this case is formed by the Jacobian (4.13) with an extra column, namely,

$$G(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)}) = \begin{bmatrix} Ref_\alpha^{(i)} & -Imf_\alpha^{(i)} & Ref_{\gamma_R}^{(i)} & -Imf_{\gamma_R}^{(i)} \\ Imf_\alpha^{(i)} & Ref_\alpha^{(i)} & Imf_{\gamma_R}^{(i)} & Ref_{\gamma_R}^{(i)} \\ Ref_{\alpha\alpha}^{(i)} & -Imf_{\alpha\alpha}^{(i)} & Ref_{\alpha\gamma_R}^{(i)} & -Imf_{\alpha\gamma_R}^{(i)} \\ Imf_{\alpha\alpha}^{(i)} & Ref_{\alpha\alpha}^{(i)} & Imf_{\alpha\gamma_R}^{(i)} & Ref_{\alpha\gamma_R}^{(i)} \end{bmatrix} := G^{(i)}. \quad (4.15)$$

Newton's method can then be applied in real arithmetic and the nonsingularity of $G^{(i)}$ in the limit is straightforward and similar to the case for a real γ, with the determinant of $G^{(i)}$ in the limit being given by $|f_{\alpha\alpha}^*|^2 |f_{\gamma_R}^*|^2$, which is non-zero using (4.11) and (3.8).

REMARK 4.4. *Note that in the computations for the complex case, Example 5.3, we observe no difference (up to machine precision) between using Newton's method in complex arithmetic, Newton's method in real arithmetic, and the Gauss-Newton method for an overdetermined system if one of the parameters is real, see Tables 5.3-5.5, which is to be expected.*

Lastly, in this section about real γ and complex λ, we note that a related approach, but with a Hermitian T so that f is real, can be used to calculate the distance to a nearby defective matrix, with λ representing a complex defective eigenvalue and γ the distance (see [1] for more details).

4.4. Complex λ and two real parameters γ_1 and γ_2. From the overdetermined system (4.12) in the previous subsection it is easy to see that we can extend the method to deal with the case when A depends on two independent real parameters, say γ_1 and γ_2, as in the case in Example 5.4 in the next section. In this case system (4.12) becomes four real equations in four unknowns, namely

$$g(\alpha, \beta, \gamma_1, \gamma_2) = \begin{bmatrix} \mathrm{Re}f(\alpha, \beta, \gamma_1, \gamma_2) \\ \mathrm{Im}f(\alpha, \beta, \gamma_1, \gamma_2) \\ \mathrm{Re}f_\alpha(\alpha, \beta, \gamma_1, \gamma_2) \\ \mathrm{Im}f_\alpha(\alpha, \beta, \gamma_1, \gamma_2) \end{bmatrix} = 0, \quad (4.16)$$

where, again $\lambda = \alpha + i\beta$. Such problems arise in power system dynamics, where, under two-parameter variation two complex eigenvalues coalesce (see Examples 5.3 and 5.4). We apply Newton's method to (4.16), with the Jacobian being given by

$$G(\alpha^{(i)}, \beta^{(i)}, \gamma_1^{(i)}, \gamma_2^{(i)}) = \begin{bmatrix} \mathrm{Re}f_\alpha^{(i)} & -\mathrm{Im}f_\alpha^{(i)} & \mathrm{Re}f_{\gamma_1}^{(i)} & \mathrm{Re}f_{\gamma_2}^{(i)} \\ \mathrm{Im}f_\alpha^{(i)} & \mathrm{Re}f_\alpha^{(i)} & \mathrm{Im}f_{\gamma_1}^{(i)} & \mathrm{Im}f_{\gamma_2}^{(i)} \\ \mathrm{Re}f_{\alpha\alpha}^{(i)} & -\mathrm{Im}f_{\alpha\alpha}^{(i)} & \mathrm{Re}f_{\alpha\gamma_1}^{(i)} & \mathrm{Re}f_{\alpha\gamma_2}^{(i)} \\ \mathrm{Im}f_{\alpha\alpha}^{(i)} & \mathrm{Re}f_{\alpha\alpha}^{(i)} & \mathrm{Im}f_{\alpha\gamma_1}^{(i)} & \mathrm{Im}f_{\alpha\gamma_2}^{(i)} \end{bmatrix} := G^{(i)}. \quad (4.17)$$

Note that this Jacobian is similar to (4.15), however, here γ_1 and γ_2 are independent of each other (and not the real and imaginary part of the same parameter). Following the same derivation as in the previous subsection, the Jacobian is nonsingular in the limit if and only if (4.11) holds and

$$\mathrm{Re}f_{\gamma_1}^* \mathrm{Im}f_{\gamma_2}^* - \mathrm{Re}f_{\gamma_2}^* \mathrm{Im}f_{\gamma_1}^* \neq 0.$$

This holds essentially if (3.8) is satisfied for both γ_1 and γ_2, and both parameters are independent of each other.

4.5. Computational aspects. It is readily seen that Algorithms 4.1 and 4.2 are extraordinarily straightforward to understand and implement. For each function evaluation f all that is required is the solution of a linear system with a nonsingular bordered matrix of the form (2.4). Any (first, second or mixed) derivative of the function f with respect to λ or γ requires a solve with *the same* bordered matrix - so any factorisation of that matrix will have to be done only once. In particular, we can choose any numerical method to solve the linear systems - and thereby also take into account any sparsity structure of the $(1,1)$ block of the bordered matrix if n is large. In particular, in Example 5.1 in the following section we use the Block Elimination Method for bordered systems (see [7]) in order to exploit the special sparse structure of the $(1,1)$ block of the bordered matrix.

In applications one has to make the choice of the bordering vector b and c in (2.4). If $T(\lambda^*, \gamma^*)$ is singular it is easy to prove that good choices for b and c are normalised left and right kernel vectors of $T(\lambda^*, \gamma^*)$, respectively. In this, theoretical, case it is easy to prove by direct calculation, that the condition number of M, say $\kappa(M)$, satisfies the following result: if the singular values of $T(\lambda^*, \gamma^*)$ are $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{n-1} > \sigma_n = 0$, then $\kappa(M) = \frac{\max\{\sigma_1, 1\}}{\min\{\sigma_{n-1}, 1\}}$. However, in applications the kernel vectors won't be known, but if estimates are available, these can be used, which we do in our examples in the next section. A bound on the spectral condition number of the bordered matrix $M(\lambda^*, \gamma^*)$ for general values of b and c can be found in [2], in which it is shown that $\kappa(M)$ is bounded by a term that is inversely proportional to $\cos(\bar{c}, x^*) \cos(b, \bar{y}^*)$ (see [2, Theorem 10.2]). Clearly poor choices of b and c in (2.4) might result in a large condition number of M and possible loss of significant digits in the computation of f and its derivatives. Poor performance is also likely if there is a nearby 3-dimensional Jordan block, as would be indicated by a small value of $f_{\lambda\lambda}$, though this would be easily detected, say by monitoring the $(2,1)$-component of the matrix in (4.3).

5. Numerical examples. In this section we describe several numerical examples for the case of real and complex coalescing eigenvalues. For all our examples we choose c to be the normalised eigenvector of $A(\gamma^{(0)})$ corresponding to the eigenvalue of smallest real part (so that (2.3) holds) and, as suggested by (3.5), choose $b = A_\gamma(\gamma^{(0)})c$ (where $\gamma^{(0)}$ is the starting guess for γ^*).

5.1. The real case. In our first example, under a variation of the real parameter γ, two real eigenvalues collide on the real axis and then change direction perpendicular to the real axis. This case occurs for example in supersonic panel flutter computations where eigenvalues are known to be real for a certain parameter γ and approach each other, collide (at a Jordan block) and become complex for an increasing value of γ (see, for example [18, 19, 22, 23]). We consider this behaviour in Examples 5.1 and 5.2.

EXAMPLE 5.1. *Consider a problem arising from the supersonic flutter prediction of a functionally graded panel [18]. The finite difference discretisation of the problem*

$$\frac{\partial^4 U}{\partial x^4} + R_x \frac{\partial^2 U}{\partial x^2} + \gamma \frac{\partial U}{\partial x} - \pi^4 \lambda U = 0 \tag{5.1}$$

with boundary conditions $U(0) = U(1) = \frac{\partial^2 U}{\partial x^2}(0) = \frac{\partial^2 U}{\partial x^2}(1) = 0$ gives a matrix eigenvalue problem

$$\frac{1}{\pi^4}(A_1 + R_x A_2 + \gamma B)x = \lambda x,$$

where A_1 and A_2 are real symmetric $n \times n$ matrices, R_x is a scalar, B is an $n \times n$ nonsymmetric matrix and γ a real parameter corresponding to the non-dimensional

aerodynamic pressure. For $\gamma = 0$ the problem is symmetric and all the eigenvalues λ are real. Since λ and γ are real, we solve the two real equations (4.5). For increasing γ the eigenvalues coalesce. For Algoritm 4.1 we therefore choose $\gamma^{(0)} = 0$ and the exact smallest eigenvalue of $(A(\gamma^{(0)}))$ is taken for $\lambda^{(0)}$. The finite difference discretisation of (5.1) leads to a pentadiagonal matrix and hence the $(1,1)$ block of the bordered system is sparse. We exploit this sparsity by solving the bordered system in the Implicit Determinant Method using the Block Elimination Method by Govaerts [7] and applying a Thomas algorithm to the banded pentadiagonal matrix in the $(1,1)$ block. The cost of solving the system reduces to $\mathcal{O}(n)$ (instead of the usual $\mathcal{O}(n^3)$ for an LU factorisation).

Figure 5.1 shows the coalescence of eigenvalues for $R_x = 0$ and $R_x = \pi^2$. For the finite difference discretisation we choose $n = 200$. We observe from Figure 5.1
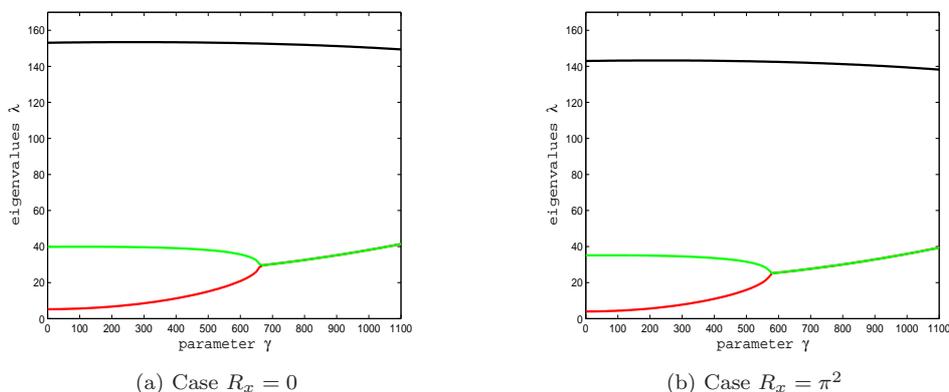

(a) Case $R_x = 0$ (b) Case $R_x = \pi^2$

Fig. 5.1: Coalescence of smallest eigenvalues for Example 5.1.

that $\gamma^* \approx 670$ ($R_x = 0$) and $\gamma^* \approx 580$ ($R_x = \pi^2$). The plots are constructed by calculating the smallest eigenvalues for several values of γ. As a means of estimating the point of coalescence, this is a very costly computation. Using the new approach we quickly obtain the critical values of λ^* and γ^* corresponding to coalescence, see Tables 5.1. Both tables show fast (and eventually quadratic) convergence to the

Table 5.1: Results for Example 5.1, $n = 200$, $R_x = 0$ (left) and $R_x = \pi^2$ (right).

i	$\gamma^{(i)}$	$\lambda^{(i)}$	$\|g(\lambda^{(i)},\gamma^{(i)})\|$	i	$\gamma^{(i)}$	$\lambda^{(i)}$	$\|g(\lambda^{(i)},\gamma^{(i)})\|$
0	0	5.2435e+00	-	0	0	3.9763e+00	1.4142e+00
1	9.2692e+00	5.2465e+00	3.1192e+03	1	8.2778e+00	3.9790e+00	3.0794e+03
2	2.7809e+01	5.2643e+00	1.5598e+03	2	2.4835e+01	3.9951e+00	1.5399e+03
3	6.4833e+01	5.3474e+00	7.8008e+02	3	5.7896e+01	4.0702e+00	7.7009e+02
4	1.3817e+02	5.6999e+00	3.9063e+02	4	1.2337e+02	4.3890e+00	3.8547e+02
5	2.7839e+02	7.0968e+00	2.0032e+02	5	2.4835e+02	5.6517e+00	1.9663e+02
6	5.1155e+02	1.1903e+01	1.3237e+02	6	4.5474e+02	9.9829e+00	1.2482e+02
7	7.4861e+02	2.2922e+01	1.5294e+02	7	6.5666e+02	1.9758e+01	1.3819e+02
8	7.3081e+02	3.1155e+01	1.5591e+02	8	6.2544e+02	2.6427e+01	1.4011e+02
9	6.5595e+02	2.9221e+01	6.9977e+01	9	5.7169e+02	2.4925e+01	5.5255e+01
10	6.6071e+02	2.9441e+01	5.0929e+00	10	5.7430e+02	2.5064e+01	2.9709e+00
11	6.6072e+02	2.9443e+01	7.4594e-03	11	5.7430e+02	2.5065e+01	2.6925e-03
12	6.6072e+02	2.9443e+01	2.5449e-06	12	5.7430e+02	2.5065e+01	4.9050e-07

desired value of $\gamma^* = 660.72$ (for $R_x = 0$) and $\gamma^* = 574.30$ (for $R_x = \pi^2$).

Next, we consider an example arising in the computation of supersonic flutter characteristics of composite cylindrical panels [23].

EXAMPLE 5.2. *Consider*

$$(K_F + \gamma A_F)d = \lambda M_F d \quad where \quad \lambda = \omega^2,$$

K_F, M_F are symmetric positive definite mass and stiffness matrices of size $n \times n$, and A_F is the nonsymmetric aerodynamic load matrix arising from the finite element discretisation of the supersonic panel flutter problem for composite cylindrical panels, and γ represents the dynamic pressure (see [23]). The eigenfrequencies of the system, given by ω, which are real for $\gamma = 0$ and will approach each other as γ increases from zero, coalesce at $\gamma = \gamma^*$ and become complex conjugate pairs for $\gamma > \gamma^*$. Substitute $x = L^T d$, where $M_F = LL^T$ is the Cholesky factorisation of M_F and obtain

$$(L^{-1} K_F L^{-T} + \gamma L^{-1} A_F L^{-T}) x = \lambda x. \tag{5.2}$$

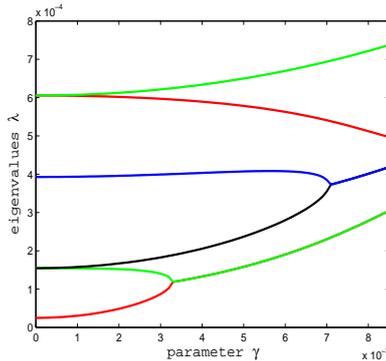*Hence, we again have a real problem of the form (4.5). Figure 5.2 shows the be-*

Fig. 5.2: Coalescence of smallest eigenvalues for Example 5.2.

haviour of the smallest eigenvalues λ of (5.2) depending on the parameter γ. We see that for $\gamma \approx 0.003$ the two smallest real eigenvalues coalesce and for $\gamma \approx 0.007$ the third and fourth smallest eigenvalues coalesce. For our new method we choose $\gamma^{(0)} = 0.001$ and the exact smallest eigenvalue of $(A(\gamma^{(0)}))$ is taken for $\lambda^{(0)}$. Applying Algoritm 4.1 we obtain the results in Table 5.2, that is, quadratic convergence to the critical values $\gamma^* = 3.2813e - 03$ with $\lambda^* = 1.1855e - 04$, the coalescing eigenvalue is achieved.

Table 5.2: Results for Example 5.2, $n = 200$.

i	$\gamma^{(i)}$	$\lambda^{(i)}$	$\|g(\lambda^{(i)}, \gamma^{(i)})\|$
0	1.0000e-03	3.0561e-05	-
1	2.6117e-03	4.8976e-05	8.7525e+01
2	3.9623e-03	1.0029e-04	4.3102e+01
3	3.6232e-03	1.2775e-04	1.5257e+01
4	3.2661e-03	1.1755e-04	1.4444e+00
5	3.2815e-03	1.1855e-04	4.3606e-01
6	3.2813e-03	1.1855e-04	2.5904e-03
7	3.2813e-03	1.1855e-04	8.8329e-08

Note that the main cost for our algorithm is the LU factorisation of the matrix $M(\lambda^{(i)}, \gamma^{(i)})$ from (2.4) at each step of the Newton method. The cost of this operation will be $\frac{2}{3}(n+1)^3 \approx \frac{2}{3}n^3$, where n is the size of the matrix $A(\gamma)$. If we carry out m Newton steps we get an algorithm cost of about $m \times \frac{2}{3}n^3$, where m is usually small.

5.2. The complex case. We consider two examples where complex eigenvalues coalesce arising in the stability analysis of electric power systems. As γ is increased two eigenvalues approach each other, at a specific value of γ^* the eigenvalues coincide (this is know as "strong resonance") and as γ is increased further the eigenvalues change direction by a right angle.

EXAMPLE 5.3. *Consider the following parameter dependent matrix*

$$A(\gamma) = \begin{bmatrix} -1 & 1 & 2 & 1 \\ \gamma & -1 & 0 & 2 \\ -2 & -1 & -1 & 1 \\ 0 & -2 & \gamma & -1 \end{bmatrix},$$

that arises from a model problem to illustrate strong resonance, see [5, Section III]. Eigenvalues coalesce at $\lambda^* = -1 + 2i$ for $\gamma^* = 0$. Figure 5.3 shows the behaviour
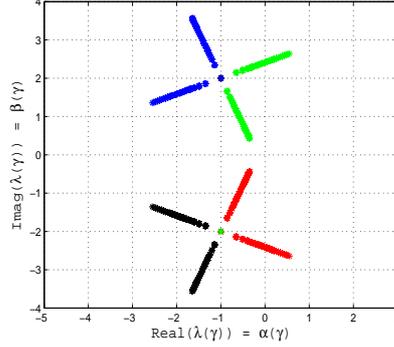

Fig. 5.3: Coalescence of complex eigenvalues for Example 5.3.

of the four eigenvalues of $A(\gamma)$ for a variation of γ from -2 to 2 (with coalescence for $\gamma^* = 0$). The results for starting guesses $\gamma^{(0)} = 1$ and $\alpha^{(0)}$ and $\beta^{(0)}$ the real

Table 5.3: Results for Example 5.3 for Newton method applied to system (4.1) in complex arithmetic (Algorithm 4.1).

i	$\gamma^{(i)}$	$\lambda^{(i)}$	$\|g(\lambda^{(i)}, \gamma^{(i)})\|$
0	1.0000e+00	-2.0987e+00 - 1.5449e+00i	1.4142e+00
1	-2.4142e+00 + 3.8892e-15i	-2.2311e-01 - 2.3218e+00i	1.6818e+00
2	-2.9651e-01 - 2.5565e-16i	-3.8120e-01 - 2.2563e+00i	1.8750e+01
3	-1.8175e-01 - 2.9771e-16i	-6.7791e-01 - 2.1334e+00i	4.7390e+00
4	-9.0875e-02 + 6.8438e-16i	-9.1335e-01 - 2.0359e+00i	1.6015e+00
5	-1.0510e-02 + 2.0742e-16i	-9.9312e-01 - 2.0029e+00i	3.9185e-01
6	-8.5287e-05 + 2.4642e-18i	-9.9995e-01 - 2.0000e+00i	3.4067e-02
7	-4.6223e-09 - 1.8475e-20i	-1.0000e+00 - 2.0000e+00i	2.5846e-04
8	-1.3011e-17 - 1.0723e-24i	-1.0000e+00 - 2.0000e+00i	1.3839e-08
9	-1.5407e-33 + 1.4269e-35i	-1.0000e+00 - 2.0000e+00i	2.6885e-17

Table 5.4: Results for Example 5.3 for Gauss-Newton method (Algorithm 4.2).

i	$\gamma^{(i)}$	$\alpha^{(i)}$	$\beta^{(i)}$	$\|g(\alpha^{(i)}, \beta^{(i)}, \gamma^{(i)})\|$
0	1.0000e+00	-2.0987e+00	1.5449e+00	2.0000e+00
1	-2.4142e+00	-2.2311e-01	2.3218e+00	1.6818e+00
2	-2.9651e-01	-3.8120e-01	2.2563e+00	1.8750e+01
3	-1.8175e-01	-6.7791e-01	2.1334e+00	4.7390e+00
4	-9.0875e-02	-9.1335e-01	2.0359e+00	1.6015e+00
5	-1.0510e-02	-9.9312e-01	2.0029e+00	3.9185e-01
6	-8.5287e-05	-9.9995e-01	2.0000e+00	3.4067e-02
7	-4.6223e-09	-1.0000e+00	2.0000e+00	2.5846e-04
8	-1.3011e-17	-1.0000e+00	2.0000e+00	1.3839e-08
9	-1.5407e-33	-1.0000e+00	2.0000e+00	2.6885e-17

and imaginary parts of the eigenvalue of $A(\gamma^{(0)})$ with smallest real part are given in Tables 5.3 (for Newton's method applied to system (4.1) in complex arithmetic), 5.4 (for the Gauss-Newton method) and 5.5 (for the Newton method in real arithmetic). All tables show the quadratic convergence of the algorithm (and the results are in fact the same up to machine precision).

Table 5.5: Results for Example 5.3 for Newton method in real arithmetic (Remark 4.3).

i	$\gamma_R^{(i)}$	$\gamma_I^{(i)}$	$\alpha^{(i)}$	$\beta^{(i)}$	$\|g(\alpha^{(i)}, \beta^{(i)}\gamma^{(i)})\|$
0	1.0000e+00	0	-2.0987e+00	1.5449e+00	2.0000e+00
1	-2.4142e+00	-3.1235e-15	-2.2311e-01	2.3218e+00	1.6818e+00
2	-2.9651e-01	2.1701e-14	-3.8120e-01	2.2563e+00	1.8750e+01
3	-1.8175e-01	5.2083e-15	-6.7791e-01	2.1334e+00	4.7390e+00
4	-9.0875e-02	2.4649e-16	-9.1335e-01	2.0359e+00	1.6015e+00
5	-1.0510e-02	-4.2022e-17	-9.9312e-01	2.0029e+00	3.9185e-01
6	-8.5287e-05	-2.6004e-18	-9.9995e-01	2.0000e+00	3.4067e-02
7	-4.6223e-09	7.9440e-21	-1.0000e+00	2.0000e+00	2.5846e-04
8	-1.3011e-17	4.3973e-25	-1.0000e+00	2.0000e+00	1.3839e-08
9	0	-1.4269e-35	-1.0000e+00	2.0000e+00	2.6885e-17

EXAMPLE 5.4. *Consider a small power system with one infinite bus and one motor, modelled by a 4×4 system of differential equations [5, 12, 20]. The Jacobian $A(\gamma_1, \gamma_2)$ at a fixed point of this dynamical system depends on the parameters γ_1 and γ_2 which represent the mechanical power delivered to the motor and the damping in the swing equation respectively. For certain values of $\gamma_1 = \gamma_1^*$ and $\gamma_2 = \gamma_2^*$ two complex eigenvalues of $A(\gamma_1^*, \gamma_2^*)$ coalesce. Figure 5.4 shows the behaviour of the*
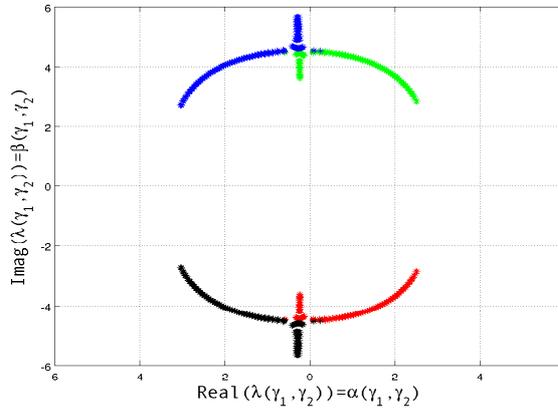

Fig. 5.4: Coalescence of complex eigenvalues for Example 5.4.

four eigenvalues of $A(\gamma_1, \gamma_2)$ for a variation of γ_1 from 1 to 2 and γ_2 from 5.5 to 6.5. Coalescence of two complex eigenvalues occurs within that box.

For the computation of the entries of the Jacobian (4.17) for this example we need the derivatives $A_{\gamma_1}(\gamma_1, \gamma_2)$ and $A_{\gamma_2}(\gamma_1, \gamma_2)$ (the calculation of f_{γ_1} requires the derivative $A_{\gamma_1}(\gamma_1, \gamma_2)$, see for example (3.12)). Since $A(\gamma_1, \gamma_2)$ is only given implicitly we use a finite difference approximation in order to calculate the derivatives, that is

$$A_{\gamma_1}(\gamma_1, \gamma_2) = \frac{A(\gamma_1 + h, \gamma_2) - (\gamma_1, \gamma_2)}{h} \quad and \quad A_{\gamma_2}(\gamma_1, \gamma_2) = \frac{A(\gamma_1, \gamma_2 + h) - (\gamma_1, \gamma_2)}{h},$$

for $h > 0$. For our computations we choose $h = 0.1$ and $h = 0.001$. With these approximations to the derivative we only calculate an approximate Jacobian, which therefore leads to a quasi-Newton method which is only linear convergent. For the two-parameter problem we choose c to be the normalised eigenvector of $A(\gamma_1^{(0)}, \gamma_2^{(0)})$ corresponding to the eigenvalue of smallest real part and for $b = A_{\gamma_1}(\gamma_1^{(0)}, \gamma_2^{(0)})c$. The results for starting guesses $\gamma_1^{(0)} = \gamma_2^{(0)} = 1$ and $\alpha^{(0)}$ and $\beta^{(0)}$ the real and imaginary part of the eigenvalue of $A(\gamma_1^{(0)}, \gamma_2^{(0)})$ with smallest real part are given in Tables 5.6 (for $h = 0.1$) and 5.7 (for $h = 0.001$). We see linear convergence for

Table 5.6: Results for Example 5.4 for Quasi-Newton method in real arithmetic and $h = 0.1$.

i	$\gamma_1^{(i)}$	$\gamma_2^{(i)}$	$\alpha^{(i)}$	$\beta^{(i)}$	$\|g(\alpha^{(i)}, \beta^{(i)}, \gamma_1^{(i)}, \gamma_2^{(i)})\|$
0	1.0000e+00	1.0000e+00	-2.9435e-01	3.6089e+00	2.0000e+00
1	1.3580e+00	9.3734e+00	-3.3565e-01	4.3229e+00	5.1469e-01
2	1.1871e+00	5.4962e+00	-2.5118e-01	4.5431e+00	2.8713e-01
3	1.1815e+00	5.8387e+00	-2.5450e-01	4.5137e+00	2.2050e-02
4	1.1811e+00	5.8448e+00	-2.5445e-01	4.5135e+00	7.1324e-04
5	1.1811e+00	5.8448e+00	-2.5445e-01	4.5135e+00	2.4057e-05
6	1.1811e+00	5.8448e+00	-2.5445e-01	4.5134e+00	7.1697e-07
7	1.1811e+00	5.8448e+00	-2.5445e-01	4.5134e+00	2.1327e-08
8	1.1811e+00	5.8448e+00	-2.5445e-01	4.5134e+00	6.3432e-10
9	1.1811e+00	5.8448e+00	-2.5445e-01	4.5134e+00	1.8865e-11
10	1.1811e+00	5.8448e+00	-2.5445e-01	4.5134e+00	5.6179e-13

Table 5.7: Results for Example 5.4 for Quasi-Newton method in real arithmetic and $h = 0.001$.

i	$\gamma_1^{(i)}$	$\gamma_2^{(i)}$	$\alpha^{(i)}$	$\beta^{(i)}$	$\|g(\alpha^{(i)}, \beta^{(i)}, \gamma_1^{(i)}, \gamma_2^{(i)})\|$
0	1.0000e+00	1.0000e+00	-2.9435e-01	3.6089e+00	2.0000e+00
1	1.3675e+00	9.3836e+00	-3.3725e-01	4.3343e+00	5.1984e-01
2	1.1815e+00	5.4584e+00	-2.4917e-01	4.5347e+00	3.0778e-01
3	1.1812e+00	5.8410e+00	-2.5449e-01	4.5135e+00	1.3113e-02
4	1.1811e+00	5.8448e+00	-2.5445e-01	4.5134e+00	1.6457e-04
5	1.1811e+00	5.8448e+00	-2.5445e-01	4.5134e+00	4.2743e-08
6	1.1811e+00	5.8448e+00	-2.5445e-01	4.5134e+00	1.2700e-11
7	1.1811e+00	5.8448e+00	-2.5445e-01	4.5134e+00	2.8891e-15

$h = 0.1$ *in Table 5.6 and for $h = 0.001$ in Table 5.7 to the coalescing eigenvalue pair* $-0.2545 \pm 4.5134i$ *for $\gamma_1 = 1.1811$ and $\gamma_2 = 5.8448$, where the linear convergence is considerably faster for the smaller value of $h = 0.001$.*

Finally, in this section, we consider an application in quantum mechanical perturbation theory, where both the coalescing λ and the parameter γ are complex.

EXAMPLE 5.5. *A problem in computational quantum mechanics is to find the complex eigenvalue λ^* and the complex parameter γ^* of the Hermitian pencil $A(\gamma) = A + \gamma B$, such that λ^* is a double eigenvalue of $A + \gamma^* B$. This example was discussed in [13] and we refer to that article for details of the problem. For our computations we use $\gamma^{(0)} = 0.1 + 0.1i$ (in fact, most nonzero random complex values work) and $\lambda^{(0)} = 1$, the smallest eigenvalue of A, and c is the eigenvector of A corresponding to $\lambda^{(0)} = 1$. For $b = A_\gamma(\gamma)c = Bc$. Numerical results are given for the application of Algorithm 4.1.*

Table 5.8: Results for Example 5.5 for Newton method in complex arithmetic.

i	$\gamma^{(i)}$	$\lambda^{(i)}$	$\|g(\lambda^{(i)}, \gamma^{(i)})\|$
0	1.0000e-01 + 1.0000e-01i	1.0000e+00	-
1	-3.8234e+00 - 4.1328e-02i	-3.6686e+00 + 5.8178e-02i	8.3106e-01
2	-2.0764e+00 - 7.6612e-02i	8.0332e-01 - 7.1998e-02i	1.1649e+01
3	-1.5136e+00 - 2.0318e-01i	8.8234e-01 - 7.2653e-01i	3.3350e+00
4	-4.8852e-01 - 4.4049e-01i	1.5413e+00 - 8.6548e-01i	1.8256e+00
5	-9.9141e-01 - 2.6578e+00i	1.2507e+00 - 4.2478e+00i	9.0023e-01
6	-6.4764e-01 - 1.8447e+00i	2.4672e+00 - 2.5170e+00i	1.3801e+00
7	-6.3326e-01 - 1.6747e+00i	1.9311e+00 - 2.4494e+00i	4.3842e-01
8	-5.5418e-01 - 1.6079e+00i	2.0360e+00 - 2.0715e+00i	1.4943e-01
9	-5.6993e-01 - 1.6104e+00i	2.0146e+00 - 2.1329e+00i	5.1938e-02
10	-5.7108e-01 - 1.6109e+00i	2.0142e+00 - 2.1371e+00i	2.9410e-03
11	-5.7108e-01 - 1.6109e+00i	2.0142e+00 - 2.1371e+00i	1.0027e-05
12	-5.7108e-01 - 1.6109e+00i	2.0142e+00 - 2.1371e+00i	1.2551e-10

Table 5.8 shows the results for Example 5.5 and eventually quadratic convergence to the coalescing double eigenvalue $\lambda^* = 2.0142 - 2.1371i$ at $\gamma^* = -0.57108 - 1.6109i$.

6. Conclusions. We have extended the approach of the Implicit Determinant Method introduced in [24] (see also [11]) to produce a technique for the computation of a 2-dimensional Jordan block in a parameter-dependent matrix. We have tested

the algorithm on some physical problems, namely panel flutter, a simple power system, and a problem in quantum mechanics.

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