5 Parameter Dependent Systems: Continuation Methods

In typical scientific and engineering problems not only a single isolated nonlinear system is to be solved, but a family of problems depending on one or more *parameters* $\lambda \in \mathbb{R}^p, p \geq 1$. The subsequent presentation will be mainly restricted to the case $p = 1$ (with the exception of Section 4.4). In fact, parameter dependent *systems of nonlinear equations*

$$F(x, \lambda) = 0, \quad x \in D \subseteq \mathbb{R}^n, \quad \lambda \in [0, L] \tag{5.1}$$

are the basis for *parameter studies* in *systems analysis* and *systems design*, but can also be deliberately exploited for the *globalization of local Newton or Gauss-Newton methods*, if only poor initial guesses are available.

In order to understand the structure of this type of problem, assume that (5.1) has a locally unique solution $(x^*, \lambda^*) \in D \times [0, L]$. Let the (n, n)-matrix $F_x(x, \lambda)$ be *regular* in some neighborhood of this point. Then, by the implicit function theorem, there exists a unique *homotopy path* $\overline{x}$ defined by virtue of the *homotopy*

$$F\Big(\overline{x}(\lambda), \lambda\Big) \equiv 0\,, \ \lambda \in [0, L]$$

or, equivalently, by the linearly implicit ODE, often called the *Davidenko differential equation* (in memory of the early paper [48] by D. Davidenko),

$$F_x \dot{\overline{x}} + F_\lambda = 0 \tag{5.2}$$

with a selected solution x^* on the homotopy path as *initial value*, say

$$\overline{x}(\lambda^*) := x^*\,.$$

Note that the ODE (5.2) uniquely defines the *direction field* $\dot{\overline{x}}$ in terms of the λ-parametrization.

In order to avoid the specification of the parametrization, one may introduce the augmented variable

$$y := (x, \lambda) \in \mathbb{R}^{n+1}$$

and rewrite the above mapping (5.1) as

$$F(y) = 0$$

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and the direction field (5.2) as

$$F'(y)\, t(y) = 0\,.$$

Whenever the condition

$$\operatorname{rank} F'(y) = n$$

or, equivalently,

$$\dim \ker F'(y) = 1\,,$$

then $t(y)$ is uniquely defined up to some *normalization*, which might be fixed as

$$\|t\|_2 = 1\,.$$

In general, whenever the local condition

$$\operatorname{rank}\ F'(y) = n - k$$

or, equivalently

$$\dim \ker F'(y) = k + 1$$

holds, then a *singularity* of order k occurs. A special role is played by *turning points*, which, with respect to the selected parameter λ, can be characterized by $k = 0$ and

$$\operatorname{rank}\ F'(y^*) = n\,, \quad \operatorname{rank}\ F_x(x^*, \lambda^*) = n - 1\,,$$

so that they are, formally speaking, singularities of order $k = 0$. For $k > 0$ the local direction field is *not* unique, its actual structure depending on properties of higher derivatives up to order $k + 1$. For $k = 1$ *simple bifurcation points* may occur, which require, however, some second derivative discriminant D to be *positive*: in this case, two distinct branch directions are defined; if $D = 0$, a so-called *isola* occurs. For $k > 1$ there exists a hierarchy of critical points, which we cannot treat here in full beauty. The complete solution structure of parameter dependent mappings, usually represented within a *bifurcation diagram*, may turn out to be rather complicated. Here we will restrict our attention to turning points and simple bifurcation points.

Every now and then, the scientific literature contains the suggestion to just integrate the Davidenko differential equation (5.1) numerically, which is not recommended here for the following reasons:

- In most applications only *approximations* of the Jacobian (n, n)-matrix $F_x(x, \lambda)$ are available.
- The numerical integration of (5.1) requires some *implicit* or at least *linearly implicit* discretization, which, in turn, requires the solution of linear equations of the kind

$$\Big(F_x(y) - \beta \Delta\lambda F_{\lambda x}(y)\Big)\Delta x + \beta \Delta\lambda F_{xx}[\dot{\overline{x}}, \Delta x] = -\Delta\lambda F_\lambda(y)\,,$$

obviously requiring second order derivative information. Even though any stiff integrators will solve the ODE, they will not assure the basic condition $F = 0$ up to sufficient accuracy due to global error propagation—this is the well-known 'drift' of the global discretization error.

Rather so-called *discrete continuation methods* are the methods of choice: they concentrate on the solution of $F = 0$ directly and only require sufficiently accurate evaluation of the mapping F and approximations of F'. Such methods consist of two essential parts:

- a *prediction method* that, from given solution points $(\overline{x}_\nu, \overline{\lambda}_\nu)$ on the homotopy path, produces some 'new' point $(\widehat{x}_{\nu+1}, \widehat{\lambda}_{\nu+1})$ assumed to be 'sufficiently close' to the homotopy path,
- an iterative *correction method* that, from a given starting point $(\widehat{x}_\nu, \widehat{\lambda}_\nu)$, supplies some solution point $(\overline{x}_\nu, \overline{\lambda}_\nu)$ on the homotopy path.

For the prediction step, *classical* or *tangent continuation* are the canonical choices—see below. Needless to say that, for the iterative correction steps, we here concentrate on local Newton and quasi-Newton methods (see Sections 2.1.1 and 2.1.4 above) as well as (rank-deficient) Gauss-Newton methods (see Section 4.4.1 above).

Bibliographical Note. The principle of local continuation has been suggested in 1892 by H. Poincaré [168] in the context of *analytical continuation*. The idea of *discrete continuation* seems to date back to E. Lahaye [142] in 1934. As for the analysis of higher order singular points, the interested reader may want to look up, e.g., the textbooks [109, 110, 111] of M. Golubitsky and coauthors.

Since the underlying homotopy path is a mathematical object in the domain space of the nonlinear mapping F, we select the *affine covariant* framework. In Section 5.1 below, we derive an adaptive pathfollowing algorithm as a *Newton continuation* method, which terminates locally in the presence of *critical points including turning points*. In the next Section 5.2, based on the preceding Section 4.4, we treat an adaptive *quasi-Gauss-Newton continuation* method. This method is able to follow the path *beyond turning points*, but still terminates in the neighborhood of any other critical point. In order to overcome such points as well, we exemplify a scheme to construct *augmented systems*, whose solutions are just selected critical points of higher order—see Section 5.3. This scheme is an appropriate combination of Lyapunov-Schmidt reduction and topological universal unfolding. Details of numerical realization are only worked out for the computation of diagrams including simple bifurcation points.

Before we begin with a presentation of any algorithmic details, we want to point out that, quite often, there is a *choice of embedding* to be made in view of computational complexity.

Example 5.1 *Choice of embedding.* Consider the problem from [99]

$$G(x) := x - \phi(x) = 0,$$

with

$$\phi_i(x) := \exp(\cos(i \cdot \sum_{j=1}^{10} x_j)), \quad i = 1, \ldots, 10.$$

In [99], K. Georg treated the unspecific embedding

$$F(x, \lambda) = \lambda F(x) + (1 - \lambda)x = x - \lambda\phi(x)\,. \tag{5.3}$$

Assume that we know the solution at $\lambda = 0$, which is $x_i^0 = 0, i = 1, \ldots, 10$, and want to find the solution at $\lambda = 1$. The solution structure $x(\lambda)$ is given in Figure 5.1, left.

Alternatively, we might choose the more problem-oriented embedding (compare also [77, Section 4.4])

$$\tilde{F}_i(x, \lambda) := x_i - \exp(\lambda \cdot \cos(i \cdot \sum_{j=1}^{10} x_j)), \quad i = 1, \ldots, 10\,. \tag{5.4}$$

The solution at $\lambda = 0$ is now given by $x_i^0 = 1, i = 1, \ldots, 10$. The corresponding solution structure as given in Figure 5.1, right, is obviously much simpler.

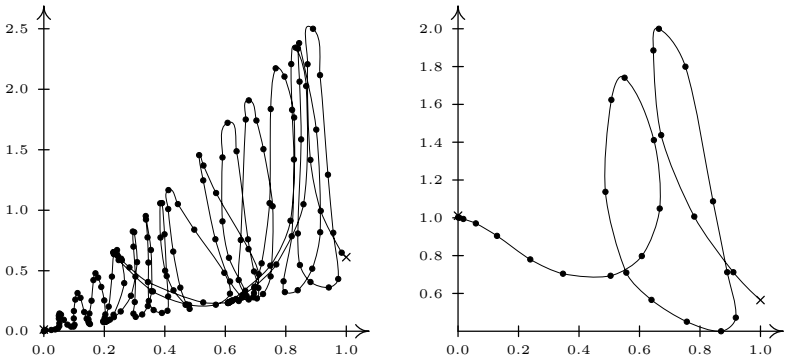

Fig. 5.1. Example 5.1. *Left:* unspecific embedding (5.3). *Right:* problem-oriented embedding (5.4).

All computations have been performed by the Gauss-Newton continuation code `ALCON1` to be described in Section 5.2 below. The dots in Figure 5.1 indicate the number of discrete continuation points as obtained from `ALCON1`: Observe that the computational complexity on the left is much higher than on the right. Look also at the quite different number of turning points. The cross-points arise from the projection $x_9(\lambda)$, not from bifurcations.

5.1 Newton Continuation Methods

This section deals with the situation that there exists a unique *homotopy path* $\overline{x}$ that can be explicitly parametrized with respect to λ over a finite interval of interest. A confirmation of this structure may often come directly from expert insight into the scientific or engineering problem to be solved. In this case the Jacobian (n,n)-matrix $F_x(x,\lambda)$ is known to be *nonsingular*, which excludes the occurrence of any type of critical points. As a consequence, *local Newton algorithms* may well serve as iterative correction methods within any discrete continuation method.

In order to treat the problem family (5.1), a *sequence of problems*

$$F(x,\lambda_\nu) = 0\,,\ \nu = 0,1\ldots\,, \tag{5.5}$$

is solved instead, where the interval $[0.L]$ is replaced by the subdivision

$$0 = \lambda_0 < \lambda_1 < \cdots < \lambda_N = L\,.$$

In order to solve each of the problems (5.5) by a local Newton method, 'sufficiently good' starting points are required, which should be supplied by some suitable *prediction method*. Formally speaking, any starting points will lie on some *prediction path* $\widehat{x}(\lambda)$ for $\lambda = \lambda_\nu$. The task therefore involves the choice of the prediction method (Section 5.1.1), the theoretical analysis of the coupling between prediction and Newton method (Section 5.1.2), which leads to a characterization of feasible stepsizes, and, on this theoretical basis, the adaptive choice of the stepsizes $\Delta\lambda_\nu = \lambda_{\nu+1} - \lambda_\nu$ in actual computation (Section 5.1.3). Since paths as mathematical objects live in the domain space of the mapping F, the *affine covariant* setting for both theory and algorithms is selected throughout Section 5.1.

5.1.1 Classification of continuation methods

As the first idea to choose a suitable *starting point* $\widehat{x}(\lambda_{\nu+1})$ one will just take the previous *solution point* $\overline{x}(\lambda_\nu)$. This so-called *classical continuation method* is represented schematically in Figure 5.2. For this continuation method the prediction path is defined as

$$\widehat{x}(\lambda) = \overline{x}(\lambda_\nu)\,,\ \lambda \geq \lambda_\nu\,.$$

A refinement of the above idea is to proceed along the tangent of the homotopy path in λ_ν. This is the so-called *tangent continuation method*, sometimes also called *method of incremental load* or *Euler continuation*, since it realizes the explicit Euler discretization of the ODE (5.2). The corresponding scheme is depicted in Figure 5.3. The associated prediction path is defined by

$$\widehat{x}(\lambda) = \overline{x}(\lambda_\nu) + (\lambda - \lambda_\nu)\,\dot{\overline{x}}(\lambda_\nu)\,,\ \lambda \geq \lambda_\nu\,,$$

wherein

$$\dot{\overline{x}}(\lambda_\nu) = -F_x\Big(\overline{x}(\lambda_\nu),\, \lambda_\nu\Big)^{-1} F_\lambda\Big(\overline{x}(\lambda_\nu),\, \lambda_\nu\Big)\,.$$

Note that both the classical and the tangent prediction paths are given in *affine covariant* terms, which suggests that a theoretical classification of prediction methods should also be formulated in such terms that match with the *error oriented* local convergence analysis of Newton's method from Section 2.1 above.

Definition. Let $\Delta\lambda := \lambda - \lambda_\nu$. A continuation method defined via the prediction path $\widehat{x}(\lambda)$ is said to be of order p, if a constant η_p exists such that

$$\|\overline{x}(\lambda) - \widehat{x}(\lambda)\| \le \eta_p \cdot \Delta\lambda^p\,. \tag{5.6}$$

In order to illustrate this definition, a few examples are given first. For simplicity, let $\lambda_\nu := 0$ and $\lambda = \Delta\lambda$.

Classical continuation method. For the method represented in Figure 5.2 one immediately derives

$$\|\overline{x}(\lambda) - \widehat{x}(\lambda)\| = \|\overline{x}(\lambda) - \overline{x}(0)\| \le \lambda \cdot \max_{s\in[0,L]} \big\|\dot{\overline{x}}(s)\big\|\,.$$

Hence, this method is of the order $p = 1$ with order coefficient

$$\eta_1 := \max_{s\in[0,L]} \big\|\dot{\overline{x}}(s)\big\|\,.$$

Actually, both H. Poincaré [168] and E. Lahaye [142] had just thought of this simplest type of continuation.

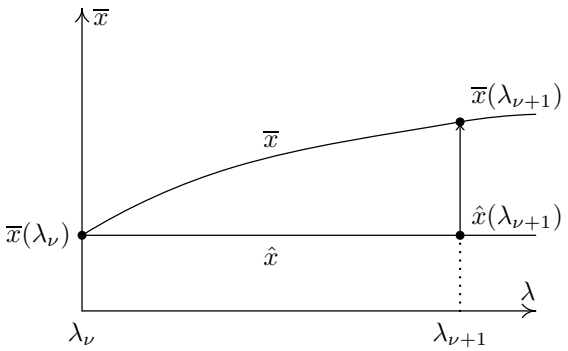

Fig. 5.2. Classical continuation method.

Tangent continuation method. For the method represented in Figure 5.3 one obtains

$$\|\overline{x}(\lambda) - \widehat{x}(\lambda)\| = \left\|\overline{x}(\lambda) - \overline{x}(0) - \lambda\dot{\overline{x}}(0)\right\| \leq \tfrac{1}{2}\lambda^2 \max_{s\in[0,L]} \left\|\ddot{\overline{x}}(s)\right\| . \tag{5.7}$$

So, this method is of the order $p = 2$ with order coefficient

$$\eta_2 := \tfrac{1}{2} \max_{s\in[0,L]} \left\|\ddot{\overline{x}}(s)\right\| . \tag{5.8}$$

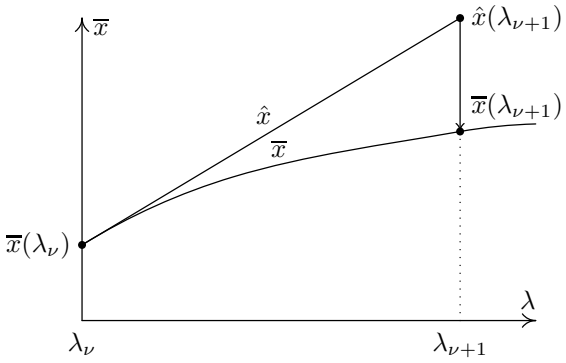

Fig. 5.3. Tangent continuation method.

Standard embedding. The simple embedding

$$F_0(x,\lambda) := F(x) - (1-\lambda)F(x^0)$$

is rather popular. Note, however, that this homotopy 'freezes' the information of the starting point x^0. The least improvement, which can easily be realized, is to turn to a *damping* or *trust region strategy* (see Chapter 3), which may be understood as being formally based on the *homotopy chain* ($k = 0, 1, \ldots$)

$$F_k(x,\lambda) := F(x) - (1-\lambda)F(x^k)\,,$$

which brings in the information about the 'newest' iterate x^k. Observe, however, that this generally applicable homotopy does not exploit any special structure of the mapping.

Partial standard embedding. In the experience of the author the only sometimes successful variant has been the selection of only *one* component of the mapping, which leads to the so-called partial standard embedding

$$\overline{F}_0(x,\lambda) := PF(x) + P^\perp\Big(F(x) - (1-\lambda)F(x^0)\Big)\,, \tag{5.9}$$

where P is an orthogonal projector and $P^\perp$ its complement. In what follows we give some comparative results on the classical versus the tangent continuation method for this special kind of embedding.

Lemma 5.1 *Consider the partial standard embedding* (5.9)*. Notations as introduced in this section. Then, with the Lipschitz condition*

$$\left\| F'\Big(\widehat{x}(\lambda)\Big)^{-1}\Big(F'(x) - F'(\widehat{x}(\lambda))\Big)\right\| \le \widehat{\omega}_0 \|x - \widehat{x}(\lambda)\|\,,$$
$$x, \widehat{x}(\lambda) \in D\,, 0 \le \lambda \le L\,,$$

the order coefficient for the classical continuation method is

$$\eta_1 = \sup_{\lambda\in[0,\bar{\lambda}]} \left\| F'\Big(\overline{x}(\lambda)\Big)^{-1} P^\perp F(x^0)\right\|\,, \tag{5.10}$$

the one for the tangent continuation is closely related as

$$\eta_2 := \tfrac{1}{2}\widehat{\omega}_0\eta_1^2\,. \tag{5.11}$$

Proof. The extremely simple form of the embedding (5.9) leads to

$$\frac{\partial}{\partial x}\overline{F}_0(x,\lambda) = \frac{\partial}{\partial x}F(x) = F'(x)\,, \frac{\partial}{\partial\lambda}\overline{F}_0(x,\lambda) = P^\perp F(x^0)\,,$$

which implies

$$\dot{\overline{x}}(\lambda) = -F'(\overline{x})^{-1}P^\perp F(x^0)$$

and therefore (5.10). For the estimation of η_2, we must start with a Lipschitz condition for the directions

$$\begin{aligned}\|\dot{\overline{x}}(\lambda) - \dot{\overline{x}}(0)\| &= \left\|\Big(F'(\overline{x}(\lambda)\Big)^{-1} - F'\Big(\overline{x}(0)\Big)^{-1})P^\perp F(x^0)\right\| \\ &\le \left\| F'\Big(\widehat{x}(0)\Big)^{-1}\Big(F'(\overline{x}(\lambda)) - F'(\overline{x}(0))\Big)\right\| \|\dot{\overline{x}}(\lambda)\| \\ &\le \widehat{\omega}_0\,\|\overline{x}(\lambda) - \overline{x}(0)\|\,\eta_1 \le \widehat{\omega}_0\eta_1^2\lambda\,.\end{aligned}$$

Hence, with (5.8), one has the second result (5.11), which completes the proof. □

As for the consequence of this Lemma for the feasible stepsizes see Lemma 5.6 below.

It is an easy exercise to construct further refinements of prediction methods beyond the tangent continuation method, just based on higher derivative information of F. In view of complex real life problems, however, this is not very promising, since this would also require accurate higher order derivative information, which may be rarely available.

Polynomial continuation In order to classify such methods, the monomials $\Delta\lambda^p$ in (5.6) must be replaced by some *strictly monotone increasing function* $\varphi(\Delta\lambda)$ with $\varphi(0) = 0$ such that

$$\|\overline{x}(\lambda) - \widehat{x}(\lambda)\| \leq \eta \cdot \varphi(\Delta\lambda)\,. \tag{5.12}$$

In order to illustrate this definition, we consider two extrapolation methods (once more $\lambda_\nu := 0$ and $\lambda := \Delta\lambda$).

Standard polynomial extrapolation. Based on the data

$$\overline{x}(\lambda_{-q}), \ldots, \overline{x}(\lambda_{-1})\,,\ \overline{x}(0)$$

a prediction path can be defined as (with $\lambda_0 := 0$)

$$\widehat{x}_q(\lambda) := \sum_{m=-q}^{0} \overline{x}(\lambda_m) L_q^m(\lambda)$$

in terms of Lagrange polynomials $L(\cdot)$. Application of standard approximation error estimates then leads to

$$\|\overline{x}(\lambda) - \widehat{x}(\lambda)\| \leq C_{q+1} \cdot \lambda(\lambda - \lambda_{-1}) \cdot \ldots \cdot (\lambda - \lambda_{-q})\,,$$

which naturally defines

$$\varphi(\lambda) := \lambda(\lambda - \lambda_{-1}) \cdot \cdots \cdot (\lambda - \lambda_{-q})\,. \tag{5.13}$$

The numerical evaluation of the prediction path is, of course, done by the Aitken-Neville algorithm.

Hermite extrapolation. This type of polynomial extrapolation is based on the data

$$\overline{x}(\lambda_{-q})\,,\ \dot{\overline{x}}(\lambda_{-q}), \ldots, \overline{x}(0)\,,\ \dot{\overline{x}}(0)\,.$$

Evaluation of the prediction path $\widehat{x}_q(\lambda)$ is done here by a variant of the Aitken-Neville algorithm for pairwise confluent nodes. Proceeding as above leads to

$$\|\overline{x}(\lambda) - \widehat{x}(\lambda)\| \leq \overline{C}_{q+1} \cdot \lambda^2(\lambda - \lambda_{-1})^2 \cdot \cdots \cdot (\lambda - \lambda_{-q})^2\,,$$

which defines the monotone function

$$\varphi(\lambda) := \lambda^2(\lambda - \lambda_{-1})^2 \cdot \cdots \cdot (\lambda - \lambda_{-q})^2\,.$$

Note, however, that this prediction method requires quite accurate derivative information, which restricts its applicability.

Bibliographical Note. An affine contravariant definition of the order of a continuation method based on the residual F has been given in 1976 by R. Menzel and H. Schwetlick [150]. The here presented affine covariant alternative is due to the author [61] from 1979. Its extension to polynomial extrapolation is due to H.G. Bock [32]. For the standard embedding, convergence proofs were given by H.B. Keller [131] or M.W. Hirsch and S. Smale [119]; a general code has been implemented by A.P. Morgan et al. [154].

5.1.2 Affine covariant feasible stepsizes

Any of the discrete continuation methods are efficient only for 'sufficiently' small *local stepsizes*

$$\Delta\lambda_\nu := \lambda_{\nu+1} - \lambda_\nu \,,$$

which must be chosen such that the local Newton method starting at the predicted value $x^0 = \widehat{x}(\lambda_{\nu+1})$ can be expected to converge to the value $x^* = \overline{x}(\lambda_{\nu+1})$ on the homotopy path. In what follows, a theoretical analysis of *feasible stepsizes* is worked out, which will serve as the basis for an adaptive stepsize control to be presented in Section 5.1.3.

Among the *local Newton methods* to be discussed as correction methods are

- the *ordinary* Newton method with a new Jacobian at each iterate (cf. Section 2.1.1),
- the *simplified* Newton method with the initial Jacobian throughout (cf. Section 2.1.2), and
- the quasi-Newton method starting with an initial Jacobian based on 'good' Broyden Jacobian updates (cf. Section 2.1.4).

Ordinary Newton method. We begin with the ordinary Newton method as correction method within any discrete continuation method. The simplest theoretical framework is certainly given by Theorem 2.3.

Theorem 5.2 *Notation as introduced in this Section. Let $F_x(x,\lambda)$ be non-singular for all $(x,\lambda) \in D \times [0,L]$. Let a unique homotopy path $\overline{x}(\lambda)$ exist in a sufficiently large local domain. Assume the affine covariant Lipschitz condition*

$$\|F_x(x,\lambda)^{-1}\,(F_x(y,\lambda) - F_x(x,\lambda))\,(y-x)\| \le \omega\|y-x\|^2\,. \tag{5.14}$$

Let $\widehat{x}(\lambda)$ denote a prediction method of order p as defined in (5.6) *based on the previous solution point $\overline{x}(\lambda_\nu)$. Then the ordinary Newton method with starting point $\widehat{x}(\lambda_{\nu+1})$ converges towards the solution point $\overline{x}(\lambda_{\nu+1})$ for all stepsizes*

$$\Delta\lambda_\nu \le \Delta\lambda_{\max} := \left(\frac{2}{\omega\eta_p}\right)^{1/p} \tag{5.15}$$

within the interval $[0,L]$.

Proof. Upon skipping any fine structure of the local domains assumed to be sufficiently large, we must merely check the hypothesis of Theorem 2.3 for the ordinary Newton method with starting point $x^0 = \widehat{x}(\lambda)$ and solution point $x^* = \overline{x}(\lambda)$. In view of the local contractivity condition (2.9), we will estimate

$$\|x^* - x^0\| = \|\overline{x}(\lambda) - \widehat{x}(\lambda)\| \leq \eta_p \Delta\lambda^p \,.$$

Upon inserting the upper bound into (2.9), we arrive at the sufficient condition

$$\eta_p \Delta\lambda^p < 2/\omega \,,$$

which is essentially (5.15). □

The above theorem requires some knowledge about the 'rather global' Lipschitz constant ω. In order to permit a finer tuning within the automatic stepsize control to be derived in Section 5.1.3, we next apply the affine covariant Newton-Kantorovich theorem (Theorem 2.1), which requires 'more local' Lipschitz information.

Theorem 5.3 *Notation and assumptions essentially as just introduced. Compared to the preceding theorem replace the Lipschitz condition* (5.14) *by the condition*

$$\left\| F_x\left(\widehat{x}(\lambda), \lambda\right)^{-1} \Big(F_x(y, \lambda) - F_x(x, \lambda) \Big) \right\| \leq \widehat{\omega}_0 \, \|y - x\| \,, x, y \in D \,. \tag{5.16}$$

Then the ordinary Newton method with starting point $\widehat{x}(\lambda_{\nu+1})$ *converges towards the solution point* $\overline{x}(\lambda_{\nu+1})$ *for all stepsizes*

$$\Delta\lambda_\nu \leq \Delta\lambda_{\max} := \left(\frac{\sqrt{2} - 1}{\widehat{\omega}_0 \eta_p} \right)^{1/p} \,. \tag{5.17}$$

Proof. The above Lipschitz condition (5.16) permits the application of Theorem 2.1, which (with $\lambda = \Delta\lambda$) requires that

$$\alpha(\lambda)\widehat{\omega}_0 \leq \tfrac{1}{2} \,. \tag{5.18}$$

So an upper bound $\|\Delta x^0(\lambda)\| \leq \alpha(\lambda)$ for the first Newton correction needs to be derived. To obtain this, we estimate

$$\begin{aligned}
\|\Delta x^0(\lambda)\| &= \left\| F_x\left(\widehat{x}(\lambda), \lambda\right)^{-1} F\left(\widehat{x}(\lambda), \lambda\right) \right\| = \left\| F_x(\widehat{x}, \lambda)^{-1} \left(F(\widehat{x}, \lambda) - F(\overline{x}, \lambda) \right) \right\| \\
&= \left\| F_x(\widehat{x}, \lambda)^{-1} \int_{s=0}^{1} F_x(\overline{x} + s(\widehat{x} - \overline{x}), \lambda)(\widehat{x} - \overline{x}) ds \right\| \\
&\leq \|\widehat{x} - \overline{x}\| \left(1 + \tfrac{1}{2}\widehat{\omega}_0 \|\widehat{x} - \overline{x}\| \right) \,.
\end{aligned}$$

The application of the triangle inequality in the last step appears to be unavoidable.

With the definition of the order of a prediction method we are now able to derive the upper bound

$$\|\Delta x^0(\lambda)\| \le \eta_p \cdot \lambda^p \left(1 + \tfrac{1}{2}\widehat{\omega}_0 \eta_p \lambda^p\right) =: \alpha(\lambda)\,. \tag{5.19}$$

Finally, combination of (5.18) and (5.19) yields

$$\widehat{\omega}_0 \eta_p \lambda^p \left(1 + \tfrac{1}{2}\widehat{\omega}_0 \eta_p \lambda^p\right) \le \tfrac{1}{2}$$

or, equivalently

$$\widehat{\omega}_0 \eta_p \lambda^p \le \sqrt{2} - 1\,,$$

which confirms the result (5.17). □

Corollary 5.4 *If the characterization* (5.6) *of a prediction method is replaced by the generalization* (5.12) *in terms of a strictly monotone increasing function* $\varphi(\Delta\lambda)$*, then the maximum feasible stepsize* (5.17) *is replaced by*

$$\Delta\lambda_{\max} := \varphi^{-1}\left(\frac{\sqrt{2}-1}{\widehat{\omega}_0 \eta}\right) \tag{5.20}$$

with φ^{-1} *the mapping inverse to* φ*.*

Proof. Instead of (5.19), we now come up with (once again $\lambda := \Delta\lambda$)

$$\alpha(\lambda) := \eta\varphi(\lambda)\left(1 + \tfrac{1}{2}\widehat{\omega}_0 \eta \varphi(\lambda)\right)\,,$$

which directly leads to

$$\widehat{\omega}_0 \eta \varphi(\lambda) \le \sqrt{2} - 1$$

thus confirming (5.20). □

Simplified Newton method. In most applications, the *simplified* Newton method rather than the ordinary Newton method will be realized. For this specification, the following slight modifications hold.

Corollary 5.5 *Notation and assumptions as in Theorem* 5.3 *or Corollary* 5.4*, respectively. Let the ordinary Newton method therein be replaced by the simplified Newton method with the same starting point. Then, with the mere replacement of the Lipschitz constant* $\widehat{\omega}_0$ *via the slightly modified condition*

$$\left\| F_x\left(\widehat{x}(\lambda), \lambda\right)^{-1} \Big(F_x(x,\lambda) - F_x(\widehat{x}(\lambda), \lambda) \Big) \right\| \le \widehat{\omega}_0 \, \|x - \widehat{x}(\lambda)\|\,,$$

the maximum feasible stepsizes (5.17) *and* (5.20) *still hold.*

Proof. The above two proofs can be essentially copied: the contraction condition (2.3) of Theorem 2.1 needs to be formally replaced by condition (2.17) of Theorem 2.5, which means the mere replacement of the Lipschitz condition (2.2) by (2.16). □

Partial standard embedding. In order to illustrate what has been said at the end of Section 5.1.1 about the embedding (5.9), we now study the consequences of Lemma 5.1 for the associated feasible stepsizes.

Lemma 5.6 *Notation and assumptions as in Lemma* 5.1. *Let* $\Delta\lambda_{\max}^{(1,2)}$ *denote the maximum feasible stepsizes for the classical continuation method* ($p = 1$) *and for the tangent continuation method* ($p = 2$). *Then the following results hold:*

$$\Delta\lambda_{\max}^{(2)} = \sqrt{2(\sqrt{2}+1)}\,\Delta\lambda_{\max}^{(1)} \approx 2.2\,\Delta\lambda_{\max}^{(1)}\,.$$

Proof. We merely insert the results (5.10) for $p = 1$ and (5.11) for $p = 2$ into the maximum stepsize formula (5.17) to verify the above results. □

Obviously, in this rather unspecific embedding, tangent continuation seems to require roughly double the number of continuation steps compared to classical continuation. This theoretically backed expectation has actually been observed in large scale problems. At the same time, however, an efficient implementation of the tangent continuation method will roughly require double the amount of work per step (see Section 5.1.3). Hence, there is no clear advantage on either side. In sensitive examples, however, smaller stepsizes increase robustness and reliability of the numerical pathfollowing procedure. That is why for this type of embedding *classical continuation* is generally recommended.

5.1.3 Adaptive pathfollowing algorithms

In the preceding section we analyzed discrete continuation methods with the simplified Newton method as correction method. In its actual realization in the code `CONTI1`, this is extended to some quasi-Newton correction method.

Simplified Newton method. This method keeps the Jacobian matrix $F'(x^0)$ fixed for all iterative steps, which implies that a single matrix decomposition at the beginning is sufficient throughout the iteration. As a convergence monitor, the *contraction factors* Θ_k in terms of the simplified Newton corrections are used. From (2.21) we require the local convergence criterion

$$\Theta_0 \le \overline{\Theta} = \tfrac{1}{4}\,,$$

which is easily tested after the first Newton step.

Quasi-Newton method. After the first iterative step, we substitute the simplified Newton iteration by the quasi-Newton method based on 'good' Broyden updates, as documented by algorithm `QNERR` in Section 2.1.4. Let Θ_k denote the corresponding contraction factors in terms of the quasi-Newton

corrections. In agreement with the convergence analysis in Theorem 2.7 we require that $\Theta_k \leq 1/2$. Hence, whenever the condition

$$\Theta_k > \tfrac{1}{2} \tag{5.21}$$

occurs, then the continuation step $\lambda_\nu \to \lambda_\nu + \Delta\lambda_\nu$ is repeated with reduced stepsize $\Delta\lambda_\nu$.

Discrete continuation method. The *classical continuation method* is certainly most simple to realize and needs no further elaboration. The *tangent continuation method* additionally requires the numerical solution of a linear system of the kind

$$F_x(\overline{x}(\lambda_\nu), \lambda_\nu)\dot{\overline{x}}(\lambda_\nu) = -F_\lambda(\overline{x}(\lambda_\nu), \lambda_\nu)\,,$$

which has the same structure as the systems arising in Newton's method. Note, however, that in order to realize a continuation method of *actual* order $p = 2$, *sufficiently accurate* Jacobian approximations $(F_x,\ F_\lambda)$ need to be evaluated not only at the starting points $\widehat{x}$, but also at the solution points $\overline{x}$. In large scale problems, this requirement may roughly *double* the amount of work per continuation step compared to the classical method $(p = 1)$.

Adaptive stepsize control. In the globalization of local Newton methods by continuation, adaptive trust region strategies come up as adaptive stepsize strategies. Colloquially, the construction principle is as follows: choose stepsizes such that the initial guess $\widehat{x}(\lambda_\nu)$ stays within the 'Newton contraction tube' around the homotopy path—see the theoretical stepsize results like (5.17) containing the unavailable theoretical quantities $\widehat{\omega}_0$ and η_p.

Following once more our paradigm of Section 1.2.3, we replace the unavailable theoretical quantities by computationally available estimates $[\widehat{\omega}_0] \leq \widehat{\omega}_0$ and $[\eta_p] \leq \eta_p$—thus arriving at stepsize estimates

$$[\Delta\lambda_{\max}] := \left(\frac{\sqrt{2}-1}{[\widehat{\omega}_0][\eta_p]}\right)^{1/p} \geq \Delta\lambda_{\max}\,. \tag{5.22}$$

Again both a *prediction strategy* and a *correction strategy* will be needed. Of course, all formulas will be invariant under *rescaling or shifting* of the continuation parameter.

Suppose that, for given $\lambda_{\nu+1}$, the value Θ_0 has already been computed. From the convergence analysis of the simplified Newton method we know that

$$\Theta_0(\lambda) \leq \tfrac{1}{2}\widehat{\omega}_0\|\overline{\Delta x}^0(\lambda)\| \leq \tfrac{1}{2}\widehat{\omega}_0\alpha(\lambda)\,. \tag{5.23}$$

Insertion of $\alpha(\lambda)$ from (5.19) yields

$$\Theta_0 \leq \tfrac{1}{2}\widehat{\omega}_0\eta_p\Delta\lambda^p\left(1 + \tfrac{1}{2}\widehat{\omega}_0\eta_p\Delta\lambda^p\right)$$

or, equivalently,

$$\widehat{\omega}_0 \eta_p \Delta\lambda^p \geq g(\Theta_0)$$

in terms of the monotone increasing function

$$g(\Theta) := \sqrt{1 + 4\Theta} - 1 \,.$$

From this, we may obtain the *a-posteriori estimate*

$$[\widehat{\omega}_0 \eta_p] := \frac{g\Big(\Theta_0(\lambda)\Big)}{\Delta\lambda^p} \leq \widehat{\omega}_0 \eta_p$$

and the associated stepsize estimate

$$[\Delta\lambda_{\max}] := \left(\frac{g\left(\overline{\Theta}\right)}{[\widehat{\omega}_0 \eta_p]} \right)^{1/p} .$$

Note that $g\left(\overline{\Theta}\right) = \sqrt{2} - 1$ as in formula (5.17)—a mere consequence of the fact that both formulas are based on the Kantorovich condition. Let $\Delta\lambda'_\nu$ denote some desirable stepsize corresponding to $\Theta_0 = \overline{\Theta}$, whereas the actual stepsize $\Delta\lambda_\nu$ corresponds to the actually computed value of Θ_0. Then the above derivation leads to the *stepsize correction* formula

$$\Delta\lambda'_\nu := \left(\frac{g\left(\overline{\Theta}\right)}{g(\Theta_0)} \right)^{1/p} \Delta\lambda_\nu \,. \tag{5.24}$$

For $\Theta_0 < \overline{\Theta}$ the actual stepsize $\Delta\lambda_\nu$ is acceptable, since $\Delta\lambda'_\nu > \Delta\lambda_\nu$. If, however, the termination criterion (5.21) is activated by some $\Theta_k > 1/2$, then the last continuation step should be repeated with stepsize

$$\Delta\lambda'_\nu := \left(\frac{g\left(\overline{\Theta}\right)}{g(\Theta_k)} \right)^{1/p} \Delta\lambda_\nu \,,$$

which is a clear reduction, since

$$\Delta\lambda'_\nu < \left(\frac{\sqrt{2} - 1}{\sqrt{3} - 1} \right)^{1/p} \Delta\lambda_\nu \approx 0.57^{1/p} \Delta\lambda_\nu \,.$$

In order to derive *a-priori estimates*, we may exploit (5.23) again to obtain

$$[\widehat{\omega}_0] := \frac{2\Theta_0(\lambda_\nu)}{\|\overline{\Delta x}^0(\lambda_\nu)\|} \leq \widehat{\omega}_0$$

and just use the definition of the order of a prediction method in the form

$$[\eta_p] := \frac{\|\widehat{x}(\lambda_\nu) - \overline{x}(\lambda_\nu)\|}{|\Delta\lambda_{\nu-1}|^p} \leq \eta_p \,.$$

Upon inserting these quantities into (5.22), a *stepsize prediction strategy* is defined via

$$\Delta\lambda_\nu^0 := \left(\frac{\|\overline{\Delta x}^0(\lambda_\nu)\|}{\|\widehat{x}(\lambda_\nu) - \overline{x}(\lambda_\nu)\|} \cdot \frac{g\left(\overline{\Theta}\right)}{2\Theta_0} \right)^{1/p} \Delta\lambda_{\nu-1} \,. \tag{5.25}$$

Note that this estimate is not sensitive to the computational accuracy of $\overline{x}$. Even if only a single Newton step is performed, which means that

$$\overline{x} \to \widetilde{x} := \widehat{x}(\lambda_\nu) + \overline{\Delta x}^0(\lambda_\nu) \,,$$

then the predicted value degenerates to

$$\Delta\lambda_\nu^0 := \left(\frac{g\left(\overline{\Theta}\right)}{2\Theta_0} \right)^{1/p} \Delta\lambda_{\nu-1} \,,$$

which, compared with (5.24), is seen to be still a reasonable estimate. Precaution must be taken in the *nearly linear* case, characterized by

$$\Theta_0 \leq \Theta_{\min} \ll 1 \,.$$

In this case, the stepsize estimate (5.25) should be replaced by

$$\Delta\lambda_\nu^0 := \left(\frac{g\left(\overline{\Theta}\right)}{2\Theta_{\min}} \right)^{1/p} \Delta\lambda_{\nu-1} \,.$$

to avoid exponential overflow.

Polynomial continuation. Both the correction and the prediction strategy carry over to the more general case of continuation by polynomial extrapolation. Upon recalling definition (5.12), formula (5.24) must be modified such that

$$\Delta\lambda'_\nu = \varphi^{-1}\left(\frac{g\left(\overline{\Theta}\right)}{g\left(\Theta_0\right)} \varphi(\Delta\lambda_\nu) \right) \,.$$

A comparable formula holds instead of (5.25). The above required evaluation of φ^{-1} is easily performed: since the typically arising functions φ are convex (see, e.g., (5.13)), both the ordinary and the simplified Newton method in $\mathbb{R}^1$ converge certainly monotonically; good starting guesses are available from the dominant monomial so that the methods converge even fast.

Graphical output. The automatically selected points typically give a really good representation on the basis of comparably few data—which is a nice side effect of any efficient stepsize control.

Classical continuation. In this case the data $\overline{x}(\lambda_\nu)$ are available, so that in the interactive mode only linear interpolation is possible, whereas in the batch mode cubic spline interpolation will be preferable. For details the reader may check, e.g., Section 7.4 in the textbook [77].

Tangent continuation. In this case both the nodal values $\overline{x}(\lambda_\nu)$ and the associated tangents $\dot{\overline{x}}(\lambda_\nu)$ are available data so that Hermite interpolation will be the method of choice—compare, e.g., Section 7.1.2 in [77].

Detection of critical points. Any critical point (x^*, λ^*) is characterized by the fact that $F_x(x^*, \lambda^*)$ is singular, which will show up as a convergence failure of the local Newton method for iterates sufficiently close to (x^*, λ^*). As a consequence, *turning points* with respect to λ are safely detected: beyond these points, the local Newton iteration will repeatedly activate the termination criterion (5.21). Generally speaking, the feasible stepsizes $\Delta\lambda_{\max}$ will shrink as $(x, \lambda) \to (x^*, \lambda^*)$. On the other hand, due to $[\Delta\lambda_{\max}] \geq \Delta\lambda_{\max}$, an equivalent behavior for the computational estimates cannot be guaranteed: since these estimates are only based on *pointwise sampling* of F and F' possible 'jumps beyond critical points without notice' cannot be excluded. Fortunately, extensive computational experience has demonstrated that the stepsize control derived herein is quite sensitive, typically exhibiting *marked stepsize reductions* in the neighborhood of critical points. Summarizing, critical points of order $k > 0$ are rather often, but not safely detected in continuation methods with explicit parametrization.

Jacobian ill-conditioning. When approaching a critical point on the homotopy path, the Jacobian condition number is known to increase, which might support the idea of estimating it along the continuation process. In connection with QR-decomposition, the *subcondition number* $\mathrm{sc}(F_x)$ is cheaply at hand [83]. Further condition number estimates may be found within `Matlab`. In the experience of the author, the most reliable technique for general linear equations has been found to be based on *iterative refinement with the same mantissa length* (cf. I. Jankowsky/H. Woźniakowski [122]): Let δx denote the correction computed from the linear residual equation and let ε denote the relative machine precision. Then a rough estimate of the condition number is

$$\mathrm{cond}\,(F_x) \doteq \mathrm{cd}\,(F_x) = \frac{\|\delta x\|_\infty}{\varepsilon \|x\|_\infty}\,.$$

Bibliographical Note. The stepsize control presented here is based on the author's habilitation thesis [61], there in the context of optimal control problems attacked by multiple shooting techniques—compare [71, Section 8.6.2]. In Section 7.1.3 below, the success of these methods is documented at a space shuttle problem (Example 7.1).

Explicit reparametrization beyond turning points. The mathematical reason, why turning points with respect to the parameter λ cannot be computed via Newton continuation is that in the neighborhood of these points the parametrization with respect to λ breaks down. In order to be able to pass beyond turning points, W.C. Rheinboldt and J.V. Burkardt [178] suggested a technique that selects any of the components $x_1, \ldots, x_{n+1}$ (identifying $\lambda = x_{n+1}$) for local parametrization, if only the curve can be locally parametrized by that component. This approach is rather popular in computational science and engineering, whenever the basic structure of a bifurcation diagram is known from insight into the problem at hand.

In the absence of such insight, explicit parametrization can also be automated: the selection may be based on the occurrence of 'small' pivots within Jacobian LU-decompositions during the Newton continuation process. If QR-decomposition with column permutation is realized, then the last column will be selected. Apart from the choice of a corresponding single component of x, any norm of x can be chosen likewise. The selected artificial parameter will then be used for discrete continuation, while the local Newton method runs over the remaining n components (code `PITCON`, which realizes the strategy of [178]).

Note, however, that this approach requires some switching between components of x, which introduces an element of *nondifferentiability* into the algorithm and, as a consequence, may cause some lack of robustness.

5.2 Gauss-Newton Continuation Method

In this section we again study the numerical solution of parameter dependent systems of nonlinear equations

$$F(y) = 0$$

in terms of the extended variable $y = (x, \lambda), x \in \mathbb{R}^n, \lambda \in \mathbb{R}^1$. In contrast to Section 5.1, however, local Newton methods are now replaced by local Gauss-Newton methods (see Section 4.4.1), which open the possibility to some smooth *pathfollowing beyond turning points*—as will be shown next.

5.2.1 Discrete tangent continuation beyond turning points

Throughout the present section we assume that a numerical solution $y^* = (x^*, \lambda^*)$ is at hand—either gained directly from insight into the problem or computed via a local or global Gauss-Newton method for underdetermined equations (see Section 4.4). As already discussed earlier, Newton methods with explicit λ-parameterization are bound to fail in the neighborhood of turning points, since there this parameterization breaks down.

Pseudo-arclength continuation. As a first idea to overcome this difficulty we may resort to *differential geometry*, where the smooth parametrization with respect to the *arclength* s is usually recommended: in addition to the n equations

$$F(y(s)) = 0$$

this parameterization includes the normalizing condition

$$\left\| \frac{dy}{ds} \right\|_2^2 = \left\| \frac{dx}{ds} \right\|_2^2 + \left(\frac{d\lambda}{ds} \right)^2 = 1\,,$$

which after discretization eventually leads to the *pseudo-arclength parametrization*

$$\|\Delta y\|_2^2 - \Delta s^2 = 0$$

as normalizing condition.

Bibliographical Note. The idea of pseudo-arclength continuation has been suggested and worked out in first details by H.B. Keller in [130]. Its most mature and popular implementation is in the code `AUTO` due to E. Doedel [89], a code known to be rather robust and reliable. Since a sound theoretically backed control of the above stepsize parameter Δs is hard to design, the code realizes some empirical stepsize control. From the invariance point of view, the concept of arclength is not even invariant under *rescaling* of the parameter λ—see Exercise 5.1, where an interesting limiting case is discussed.

Gauss-Newton continuation idea. Here we will follow an alternative idea: at any point $y \in \mathbb{R}^{n+1}$ *including turning points*, the *local tangent* is well-defined via the underdetermined system of equations

$$F'(y)t(y) = 0\,.$$

As long as rank $F'(y) = n$, the mapping $t(y)$ is known to vary smoothly along the parameter curve also beyond turning points. Suppose now we parameterize the curve $\overline{y}$ locally with respect to some coordinate $s > 0$ along the unique tangent direction t starting at the previous solution point $\overline{y}_\nu = \overline{y}(0)$. Continuation along t then defines some *prediction path* (for $\nu = 0, 1, \ldots$)

$$\widehat{y}_{\nu+1}(s) = \overline{y}_\nu + s_\nu t(\overline{y}_\nu), \quad s_\nu > 0\,. \tag{5.26}$$

The prediction path supplies possible starting points $y^0 = \widehat{y}_{\nu+1}$ for the *local quasi-Gauss-Newton iteration* towards the next solution point $\overline{y}_{\nu+1}$.

As derived in Section 4.4.1, we may construct a quasi-Gauss-Newton method, equivalent to a *local quasi-Newton method* in the n-dimensional hyperplane

$$H := \widehat{y}(s) \oplus \mathcal{N}^\perp\Big(F'(\widehat{y}(s))\Big)\,.$$

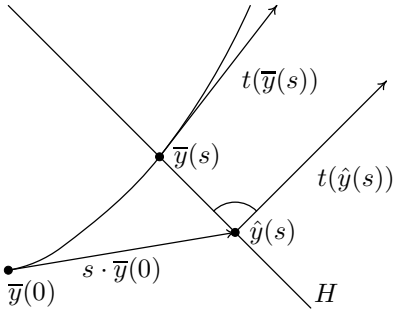

Fig. 5.4. Discrete tangent continuation in $y = (x, \lambda)$.

The geometric situation is represented in Figure 5.4. Observe that $\overline{y}_{\nu+1}$ is just defined as the intersection of H with the solution curve. A natural coordinate frame for this setting is $y = \widehat{y}(s) + (u, \sigma), u \in H(s) = \mathbb{R}^n, \sigma \in \mathbb{R}^1$.

In view of the straightforward estimate

$$\|\overline{y}_\nu(s) - \widehat{y}_\nu(s)\| \leq \tfrac{1}{2} \max_{\delta \in [0,s]} \|\ddot{\overline{y}}_\nu(\delta)\| s^2 \tag{5.27}$$

the discrete tangent continuation method is seen to be of order 2—compare (5.7) and definition (5.6). In order to implement the *actual order* $p = 2$, tangent continuation requires a *sufficiently accurate* approximation of the Jacobian *both* at each solution point $\overline{y}_\nu$ *and* at each starting point $\widehat{y}_\nu$.

Tangent computation via *QR*-decomposition. Assume that we realize the rank-deficient pseudoinverse J^+ of the Jacobian $(n, n+1)$-matrix J through the QR-Cholesky algorithm (4.77) as given in Section 4.4.1. Then, using the vector $w = R^{-1}S$ and the permutation Π as defined therein, we can compute the *normalized* kernel vector t as

$$t := \pm \Pi \begin{pmatrix} -w \\ 1 \end{pmatrix} \Big/ \sqrt{1 + w^T w}\,.$$

One method of fixing the arbitrary sign is to require the last component of $t(\overline{y}_\nu)$, say t_ξ, to have the same sign as $\widehat{\xi}_\nu - \overline{\xi}_{\nu-1}$—thus defining a natural orientation also around turning points.

Tangent computation via *LU*-decomposition. In large sparse problems a *direct sparse solver* based on LU-decomposition will be applied. During the actual decomposition of the $(n, n+1)$-matrix J, the pivoting strategy with possible column permutations Π will give rise to a zero pivot. Upon dropping the associated column of J and setting the corresponding component to zero, say $\tilde{z}_\xi = 0$, a *particular* solution $\tilde{z}$ satisfying

$$J\tilde{z} = -F \tag{5.28}$$

can be computed. In order to solve $Jt = 0$ for some (unnormalized) kernel vector t, we may set the component of t associated with the zero pivot column to some nonzero value, say $t_\xi = 1$. Upon using the relations

$$z := -J^+F = J^+J\tilde{z} = \left(I - \frac{t\,t^T}{t^T t}\right)\tilde{z}$$

we arrive at the computationally attractive representation

$$z = \tilde{z} - \frac{(t,\tilde{z})}{(t,t)}t \tag{5.29}$$

in terms of the Euclidean inner product $(\cdot,\cdot)$.

Computation of quasi-Gauss-Newton corrections. The actual computation of the quasi-Gauss-Newton corrections

$$\Delta y^k = -J_k^+ F(y^k)$$

requires the computation of the Moore-Penrose pseudo-inverse of the Jacobian updates J_k. Since this quasi-Gauss-Newton update preserves the nullspace component, we can use a simple variant of the recursive quasi-Newton method, given as algorithm `QNERR` in Section 2.1.4: with $J_0 = F'(y^0)$, we only need to formally replace J_0^{-1} by J_0^+, wherever this term arises.

5.2.2 Affine covariant feasible stepsizes

In order to develop an adaptive stepsize control (see Section 5.2.3 below), theoretical feasible stepsizes are studied first. As in the case of the Newton continuation method, an *affine covariant* setting appears to be natural, since the path concept is the dominating one in continuation. Since the local *quasi-Gauss-Newton* iteration has been shown to be equivalent to a *quasi-Newton* iteration in H (see Figure 5.4), we may proceed as in the simpler Newton continuation method (Section 5.1.2) and model the situation just by the *simplified Newton* iteration in H.

Theorem 5.7 *Consider the discrete tangent continuation method* (5.26) *in combination with the simplified local Gauss-Newton iteration starting at* $y^0 := \widehat{y}(s) = \widehat{y}_\nu$ *and with Jacobian approximations* $J_k := F'(y^0)$ *for* $k \geq 0$. *Let* $F : D \subset \mathbb{R}^{n+1} \to \mathbb{R}^n$ *denote some* C^1*-mapping with* D *open, convex, and sufficiently large. Then, under the assumption of the affine covariant Lipschitz conditions*

$$\left\| F'(y^0)^+ \Big(F'(y) - F'(y^0) \Big) \right\| \leq \omega_H \|y - y^0\|\,,\ y, y^0 \in H$$

and

$$\Big\|F'(y)^+\Big(F'(u+\delta_2 t(u),\,-F'(u)\Big)t(u)\Big\|_2 \le \delta_2\omega_t\|t(u),\,\|_2^2$$

with the (normalized) kernel vector $t(u) = \ker F'(u)$ *and*

$$y, u+\delta_2 t(u) \in D\,, 0 \le \delta_2 \le 1\,,$$

the simplified Gauss-Newton iteration converges for all

$$s \le s_{\max} := 1/\sqrt{\omega_H\omega_t}\,. \tag{5.30}$$

Proof. For the simplified Newton iteration in H we may apply Theorem 2.5, which here requires the verification of the *sufficient* condition

$$\|\Delta y^0(s)\|\omega_H \le \alpha_0(s)\omega_H \le \tfrac{1}{2}\,. \tag{5.31}$$

For simplification, we introduce the notation

$$J(s) := F'(\widehat{y}(s))\,,\;\; F(s) := F(\widehat{y}(s))\,,\;\; t(s) := t(\widehat{y}(s))$$

so that

$$F(0) = 0\,,\;\; J(0)t(0) = 0\,.$$

Then the derivation of an appropriate $\alpha_0(s)$ may proceed as follows:

$$\begin{aligned}\big\|\Delta y^0(s)\big\| &= \|J(s)^+F(s)\| = \Big\|J(s)^+\Big(F(s)-F(0)\Big)\Big\| \\ &= \Big\|\; J(s)^+ \int_{\delta=0}^{s} J(\delta)t(0)d\delta\;\Big\| \le \int_{\delta=0}^{s} \Big\|\; J(s)^+J(\delta)t(0)\;\Big\|\,d\delta \\ &= \int_{\delta=0}^{s} \Big\|\; J(s)^+\Big(J(\delta)-J(0)\Big)t(0)\;\Big\|\,d\delta \le \tfrac{1}{2}\omega_t s^2\,.\end{aligned}$$

Hence

$$\alpha_0(s) := \tfrac{1}{2}\omega_t s^2\,, \tag{5.32}$$

which inserted above directly leads to the maximum feasible stepsize $s_{\max}$. □

As an extension of the simpler Newton continuation case treated in Section 5.1.2 we next study the 'movement' of H along the parameter curve.

Theorem 5.8 *Assumptions and notation as in the preceding Theorem* 5.7. *Let*

$$\widehat{y}(s) := \overline{y}(0) + st\Big(\overline{y}(0)\Big)$$

denote a short-hand notation for the discrete tangent continuation (5.26)*. Let* $t := t(\overline{s}) = t\Big(\widehat{y}(\overline{s})\Big)$*,* $\overline{s}$ *fixed. Define* $\overline{y}(s)$ *as the intersection of* $H(s)$ *with the solution curve and let*

$$c_s := t(\overline{s})^T t\Big(\overline{y}(s)\Big).$$

Then, for $c_s \neq 0$*, one has*

$$\left\|\ddot{\overline{y}}(s)\right\|_2 \leq \omega_t \frac{c_0^2}{|c_s|^3}\,. \tag{5.33}$$

Proof. For simplification we introduce

$$z(s) := \overline{y}(s) - \widehat{y}(s)$$

so that

$$\begin{aligned} \dot{z}(s) &= \dot{\overline{y}}(s) - t(0)\,, && (5.34)\\ \ddot{z}(s) &= \ddot{\overline{y}}(s)\,. && (5.35) \end{aligned}$$

For fixed $\overline{s}$ and $t(\overline{s}) = t(\widehat{y})$, we obtain

$$\begin{aligned} t(\overline{s})^T z(s) &\equiv 0\,,\\ t(\overline{s})^T \dot{z}(s) &\equiv 0\,, && (5.36)\\ t(\overline{s})^T \ddot{z}(s) &\equiv 0 && (5.37) \end{aligned}$$

for $0 \leq s \leq \overline{s}$. Variation of s defines $\overline{y}(s)$ by virtue of

$$F\Big(\overline{y}(s)\Big) \equiv 0\,,$$

which implies

$$\begin{aligned} F'\Big(\overline{y}(s)\Big)\dot{\overline{y}}(s) &\equiv 0\,, && (5.38)\\ F''\Big(\overline{y}(s)\Big)\left[\dot{\overline{y}}(s)\right]^2 + F'(\overline{y}(s))\ddot{\overline{y}}(s) &\equiv 0\,. \end{aligned}$$

Next, from rank $F'(y) = n$ for all $y \in D$ and (5.38), we may write

$$\dot{\overline{y}}(s) = \gamma(s) t\Big(\overline{y}(s)\Big)$$

in terms of some coefficient γ to be determined. From this we obtain

$$\ddot{z}(s) = \beta(s) t\Big(\overline{y}(s)\Big) - \eta(s) \tag{5.39}$$

in terms of some coefficient β and some vector

$$\eta \perp t\Big(\overline{y}(s)\Big)\,.$$

Upon collecting these relations, we arrive at the expression

$$\eta(s) = F'\Big(\overline{y}(s)\Big)^{+} F''\Big(\overline{y}(s)\Big)\left[\gamma(s)t\Big(\overline{y}(s)\Big)\right]^2 . \tag{5.40}$$

The determination of $\beta(s)$, $\gamma(s)$ starts from

$$\|\ddot{z}(s)\|_2^2 = \|\eta(s)\|_2^2 + \beta^2(s)\,,$$

since t is normalized. Upon combining (5.34) and (5.36) we obtain

$$0 = t^T\dot{z}(s) = t^T\Big(\gamma(s)t(\overline{y}(s)) - t(0)\Big)\,,$$

from which

$$\gamma(s) = \frac{c_0}{c_s} \quad \text{for} \quad c_s \neq 0\,.$$

Application of the same procedure with (5.35), (5.39) and (5.37) yields

$$0 = t^T\ddot{z}(s) = t^T\Big(\beta(s)t(\overline{y}(s)) - \eta(s)\Big)$$

or, equivalently

$$\beta(s) = \frac{t^T\eta(s)}{c_s} \quad \text{for} \quad c_s \neq 0\,. \tag{5.41}$$

As $t = t\Big(\widehat{y}(\overline{s})\Big)$, we may continue

$$t\Big(\widehat{y}(s)\Big)^T\eta(s) = 0\,.$$

Hence

$$\begin{aligned}
|t^T\eta(s)| &= \Big|\; t^T\eta(s) - c_s t\Big(\overline{y}(s)\Big)^T\eta(s)\;\Big| \\
&= \Big|\; t^T\eta(s) - t^T t\Big(\overline{y}(s)\Big)t\Big(\overline{y}(s)\Big)^T\eta(s)\;\Big| \\
&= \Big|\; t^T\Big(I - t(\overline{y}(s))t^T(\overline{y}(s))\Big)\eta(s)\;\Big| \\
&\leq \Big\|\Big(I - t(\overline{y}(s))t^T(\overline{y}(s))\Big)t\Big\|_2 \cdot \|\eta(s)\|_2 \\
&= \sqrt{1-c_s^2}\,\|\eta(s)\|_2\,.
\end{aligned}$$

Insertion into (5.41) yields

$$\Big|\;\beta(s)\;\Big| \leq \frac{\sqrt{1-c_s^2}}{|c_s|}\;\Big\|\;\eta(s)\;\Big\|_2\,,$$

which leads to

$$\|\ddot{z}(s)\|_2^2 \le \|\eta(s)\|_2^2 + \frac{1-c_s^2}{c_s^2}\|\eta(s)\|_2^2 = \frac{\|\eta(s)\|_2^2}{c_s^2}\,.$$

Finally, estimation of $\|\eta(s)\|$ in (5.40) supplies

$$\|\eta(s)\|_2 \le \omega_t(\gamma(s))^2$$

and, therefore

$$\|\ddot{z}(s)\|_2 \le \omega_t \cdot \left(\frac{c_0}{c_s}\right)^2 \cdot \frac{1}{|c_s|}\,,$$

which with (5.35) completes the proof. □

The result (5.33) shows that the Lipschitz constant ω_t just measures the *local curvature* $\ddot{\bar{y}}(s)$ of the parameter curve. Insertion into (5.27) specifies the second order coefficient. In view of actual computation we may eliminate the variation of c_s via the additional *turning angle restriction*

$$c_0 = \min_{\delta\in[0,\bar{s}]} c_\delta > 0\,,$$

which, in turn, yields a *stepsize restriction*, of course. Then the bound (5.33) can be replaced by the corresponding expression

$$\left\|\ddot{\bar{y}}(s)\right\|_2 \le \omega_t/c_0\,. \tag{5.42}$$

For an *affine contravariant* derivation of feasible stepsizes see Exercise 5.2.

5.2.3 Adaptive stepsize control

On the basis of the theoretical results above, we are now ready to derive computational estimates for feasible stepsizes s_ν according to (5.26). Recall again that the first quasi-Gauss-Newton step may be interpreted as an ordinary Newton step in H, whereas further quasi-Gauss-Newton steps are just quasi-Newton steps in H. Let $\overline{\Delta y}^1$ denote the first simplified Gauss-Newton correction, which is cheaply available in the course of the computation of the first quasi-Gauss-Newton correction. Then a first contraction factor Θ_0 must satisfy

$$\Theta_0 := \frac{\|\overline{\Delta y}^1\|}{\|\Delta y^0\|} \le \tfrac{1}{2}\omega_H\alpha_0\,, \tag{5.43}$$

which with (5.31) implies that

$$\Theta_0 \le \overline{\Theta} := \tfrac{1}{4}\,.$$

In the spirit of our paradigm in Section 1.2.3, we construct computational stepsize estimates $[\cdot]$ on the basis of the theoretical stepsizes (5.30) as

$$[s_{\max}] := 1/\sqrt{[\omega_H]\,[\omega_t]}\,. \tag{5.44}$$

As usual, since

$$[s_{\max}] \geq s_{\max}$$

both a prediction and a correction strategy need to be designed.

Correction strategy. From (5.43) we may obtain

$$[\omega_H] := \frac{2\Theta_0}{\|\Delta y^0\|} \leq \omega_H \tag{5.45}$$

and similarly from (5.32)

$$[\omega_t] := \frac{2\,\|\Delta y^0\|}{s^2} \leq \omega_t\,.$$

Upon inserting these estimates into (5.44), we are led to the stepsize suggestion

$$s'_\nu := \sqrt{\frac{\overline{\Theta}}{\Theta_0}}\, s_\nu\,.$$

This estimate requires the knowledge of an actual stepsize s_ν, which means that it may only serve within a correction strategy. Whenever the termination criterion (for $k \geq 0$)

$$\Theta_k > \tfrac{1}{2}$$

holds, then the quasi-Gauss-Newton iteration is terminated and the previous continuation step (5.26) is repeated supplying the new starting point

$$\widehat{y}'_{\nu+1} = \overline{y}_\nu + s'_\nu t(\overline{y}_\nu)\,,$$

wherein roughly

$$s'_\nu < 0.7 s_\nu$$

is guaranteed.

Prediction strategy. For the construction of a prediction strategy, we may combine the relations (5.42) and (5.27) to obtain

$$\|\overline{y}_\nu - \widehat{y}_\nu\| \leq \tfrac{1}{2}\omega_t s_{\nu-1}^2 \frac{1}{c_0}\,.$$

This naturally defines the computational estimate

$$[\omega_t] := \frac{2c_0\|\overline{y}_\nu - \widehat{y}_\nu\|_2}{s_{\nu-1}^2} \leq \omega_t\,.$$

Together with $[\omega_H]$ from (5.45), the general formula (5.44) leads to the stepsize suggestion

$$s_\nu^0 := \left(\frac{\|\Delta y^0\|}{\|\overline{y}_\nu - \widehat{y}_\nu\|} \frac{\overline{\Theta}}{\Theta_0} \frac{1}{c_0} \right)^{1/2} s_{\nu-1} \,. \tag{5.46}$$

Clearly, this is a direct extension of the prediction formula (5.25) for the Newton continuation method. Recalling that $g(\overline{\Theta}) \approx 2\overline{\Theta}$, the main new item appears to be the trigonometric factor

$$c_0 = t^T(\widehat{y}_\nu) t\left(\overline{y}_{\nu-1}\right) \,,$$

which roughly measures the 'turning angle' of the hyperplane $H_{\nu-1} \supset \overline{y}_{\nu-1}$ to $H_\nu \supset \overline{y}_\nu$—see again Figure 5.4.

Finally, as in the Newton continuation scheme, precaution must be taken for the *nearly linear* case

$$\Theta_0 \leq \Theta_{\min} \ll 1 \,,$$

in which case $\Theta_0 \to \Theta_{\min}$ in (5.46).

Detection of critical points. In the described tangent continuation *turning points* (as critical points of order $k = 0$) do not play any exceptional role. The occurrence of critical points of order $k \geq 1$, however, needs to be carefully monitored. For this purpose, we define by

$$d_\lambda := \det\left(F_x\right)$$

the determinant of the (n, n)-submatrix of the Jacobian $F'(y)$ that is obtained by dropping the λ-column, which is F_x, of course. Similarly, let d_ξ denote the determinant of the submatrix, where the last column has been dropped—which corresponds to the *internal parameter* ξ, in general different from the *external parameter* λ, when column permutations based on pivoting are involved. For the safe detection of critical points, we compute the *determinant pair* (d_ξ, d_λ) along the solution curve. The computation of d_ξ is easily done via $\det(R)$—with a possible sign correction, by $(-1)^n$ for n Householder reflections or for the actually performed permutations in the LU-decomposition. If $\lambda \neq \xi$, then the computation of d_λ requires the evaluation of the determinant of a Hessenberg matrix, which means $\mathcal{O}(n^2)$ operations only. Sign changes of this pair clearly indicate the occurrence of both turning points and simple (possibly unfolded) bifurcation points—see Figure 5.5 for an illustration of the typical situations. This device has a high degree of reliability in detecting turning and simple bifurcation points and a good chance of detecting higher order critical points. Safety,of course, cannot be guaranteed as long as only pointwise sampling is used.

Computation of turning points. Assume that the discrete continuation method has supplied some *internal embedding parameter* ξ (associated with the last column in the matrix decomposition) and some *interval* $\left[\underline{\xi}, \overline{\xi}\right]$ supposed to contain a turning point, say ξ^*. Then the implicit mapping $\lambda(\xi)$ will have a minimum or maximum value within that interval so that

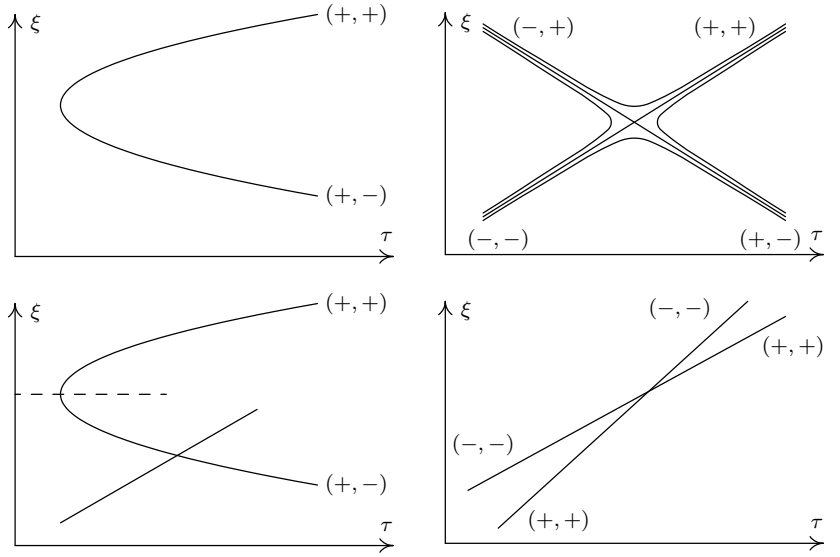

Fig. 5.5. Sign structure of determinant pair (d_ξ, d_λ)**.** *Upper left*: turning point, *upper right*: detected simple bifurcation and unfoldings, *lower left*: pair of turning and bifurcation point or pitchfork bifurcation, *lower right*: possibly undetected bifurcation point due to too small branch angle.

$$\dot{\lambda}(\xi^*) = 0\,. \tag{5.47}$$

On this basis, the following algorithm for the determination of turning points is recommended:

(I) Construct the *cubic Hermite polynomial* $p(\xi)$, $\xi \in \left[\underline{\xi}, \overline{\xi}\right]$ such that

$$\begin{aligned} p\left(\underline{\xi}\right) &= \lambda\left(\underline{\xi}\right), \quad p\left(\overline{\xi}\right) = \lambda\left(\overline{\xi}\right), \\ \dot{p}\left(\underline{\xi}\right) &= \dot{\lambda}\left(\underline{\xi}\right), \quad \dot{p}\left(\overline{\xi}\right) = \dot{\lambda}\left(\overline{\xi}\right). \end{aligned}$$

As an approximation of the unknown implicit equation (5.47), we solve the quadratic equation

$$\dot{p}(\xi) = 0\,. \tag{5.48}$$

The usual bisection assumption

$$\dot{\lambda}\left(\underline{\xi}\right)\dot{\lambda}\left(\overline{\xi}\right) \leq 0\,, \tag{5.49}$$

then assures that equation (5.48) has a real root $\widehat{\xi} \in \left[\underline{\xi}, \overline{\xi}\right]$.

(II) Perform a Gauss-Newton iteration of standard type with starting point $y^0 = \widehat{y}\left(\widehat{\xi}\right) = \left(\overline{x}\left(\widehat{\xi}\right), \widehat{\xi}\right)$. Let $\widehat{y}^*$ denote the point obtained on the solution curve.

(III) As soon as

$$\|\widehat{y} - \widehat{y}^*\| \leq \varepsilon$$

holds for some prescribed (relative) accuracy ε, then $\widehat{y}^*$ is accepted as turning point approximation. Otherwise, $\widehat{\xi}^*$ replaces either $\underline{\xi}$ or $\overline{\xi}$ such that (5.49) holds and step (I) is repeated.

The above algorithm fits into the frame of a class of algorithms, for which *superlinear convergence* has been proved by H. Schwetlick [183].

Graphical output. Here both nodal data $\{\overline{y}_\nu\}$ and their local tangents $t(\{\overline{y}_\nu\})$ are usually given in different parametrizations corresponding to the different internal parameters ξ_ν. As a consequence, Bezier-Hermite splines appear to be the method of choice for the graphical output—compare, e.g., Section 7.3 in the textbook [77] or any book on computer aided design.

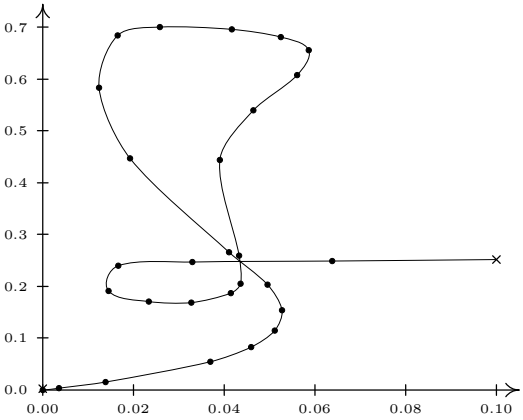

Fig. 5.6. Chemical reaction problem: $x_2(\lambda)$. Crosspoint just by projection.

Example 5.2 *Chemical reaction problem.* This model due to M. Kubiček [137] reads (see Figure 5.6):

$$\begin{aligned}
\lambda(1-x_3)\exp(10x_1/(1+0.01x_1)) - x_3 &= 0\\
22\lambda(1-x_3)\exp(10x_1/(1+0.01x_1)) - 30x_1 &= 0\\
x_3 - x_4 + \lambda(1-x_4)\exp(10x_2/(1+0.01x_2)) &= 0\\
10x_1 - 30x_2 + 22\lambda(1-x_4)\exp(10x_2/(1+0.01x_2)) &= 0\,.
\end{aligned}$$

Example 5.3 *Aircraft stability problem.* In [149] R.G. Melhem and W.C. Rheinboldt presented the following problem:

$$\begin{aligned}
-3.933x_1 + 0.107x_2 + 0.126x_3 - 9.99x_5 - 45.83\lambda & \\
-0.727x_2x_3 + 8.39x_3x_4 - 684.4x_4x_5 + 63.5x_4\lambda &= 0 \\
-0.987x_2 - 22.95x_4 - 28.37u + 0.949x_1x_3 + 0.173x_1x_5 &= 0 \\
0.002x_1 - 0.235x_3 + 5.67x_5 - 0.921\lambda - 0.713x_1x_2 & \\
-1.578x_1x_4 + 1.132x_4\lambda &= 0 \\
x_2 - x_4 - 0.168u - x_1x_5 &= 0 \\
-x_3 - 0.196x_5 - 0.0071\lambda + x_1x_4 &= 0\,.
\end{aligned}$$

Herein x_1, x_2, x_3 are the roll rate, pitch rate, and yaw rate, respectively, x_4 is the incremental angle of attack, and x_5 the sideslip angle. The variable u is the control for the elevator, λ the one for the aileron. The rudder deflection is set to zero. For $u = 0$ this problem is symmetric: $F(x, \lambda) = F(x, -\lambda)$. For $u = -0.008$ the perturbed symmetry is still visible, see Figure 5.7.

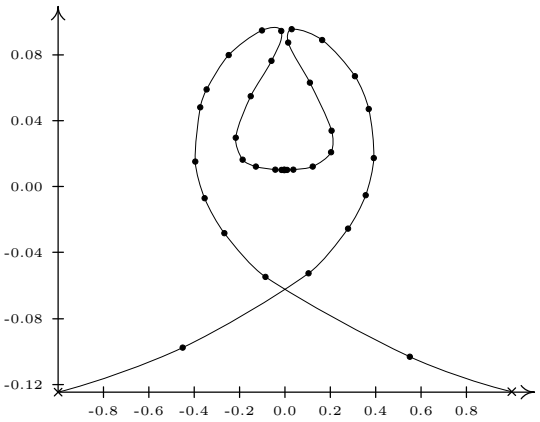

Fig. 5.7. Aircraft stability problem: $x_4(\lambda)$, perturbed symmetry.

Bibliographical Note. The adaptive pathfollowing algorithm, as worked out here, has been implemented in the code `ALCON1` due to P. Deuflhard, B. Fiedler, and P. Kunkel [72].

5.3 Computation of Simple Bifurcations

Suppose that the numerical pathfollowing procedure described in Section 5.2 has produced some guess y^0 of an expected close-by simple bifurcation point y^*—see, e.g., the double determinant detection device presented in Section 5.2.3. Then the task is to either compute a bifurcation point y^* iteratively from the starting point y^0 or to decide that there is none in the neighborhood of y^0. In Section 5.3.1, we will first study the basic construction of *augmented systems* that have certain critical points of order $k > 0$ as locally unique solutions—excluding turning points ($k = 0$), which can be computed easier as shown in the preceding section. The general construction scheme for augmented systems will be based on the theory of *universal unfolding of singularities*, which in the case of simple bifurcations specifies to the system of G. Moore. In Section 5.3.2, certain *Newton-like algorithms* for an efficient solution of that augmented system will be worked out in some detail. On the basis of *structure preserving* block elimination techniques for each Newton step, details of the *branching-off algorithm* are elaborated in Section 5.3.3—involving the computation of entering and emanating semi-branches as well as the restart of discrete tangent continuation on the new semi-branches.

5.3.1 Augmented systems for critical points

Let y^* denote a *perfect* or *unperturbed* singularity of order $k \geq 1$ with

$$F(y^*) = 0$$

and

$$\operatorname{rank} F'(y^*) = n - k\,. \tag{5.50}$$

Even though we will later only work out an algorithm for simple bifurcations ($k = 1$), we include the more general case $k > 1$ here as well—to make the general construction of augmented systems transparent.

Lyapunov-Schmidt reduction. In the notation from above, let $A := F'(y^*)$, $\mathcal{N}(A) = \ker(A)$ its $(k+1)$-dimensional nullspace, and $\mathcal{R}^\perp(A)$ its k-dimensional corange. If we again introduce the orthogonal projectors $P := A^+A$, $\overline{P} := AA^+$, we have that $P^\perp$ projects onto $\mathcal{N}(A)$ and $\overline{P}^\perp$ onto $\mathcal{R}^\perp(A)$. With this notation we may define the natural splitting

$$y = y^* + v + w\,, \quad w := P(y - y^*)\,, \quad v := P^\perp(y - y^*)$$

in the space of the unknowns. From assumption (5.50) and the implicit function theorem, we know that there exists a function w^* such that

$$\overline{P}F(y^* + v + w) = 0 \Longleftrightarrow w = w^*(v)\,.$$

Replacement of the variable w by the function w^* then leads to a *reduced system* of k equations in $k+1$ unknowns

$$f(v) := \overline{P}^{\perp} F(y^* + v + w^*(v)) = 0\,. \tag{5.51}$$

This is the well-known Lyapunov-Schmidt *reduction*, which stands at the beginning of every mathematical treatment of singularities—see, e.g., the classical book edited by P.H. Rabinowitz [173]. For actual computation we need to define *orthogonal bases* for both $\mathcal{N}$ and $\mathcal{R}^{\perp}$ as

$$\mathcal{N}(A) =: \langle t_1, \ldots, t_{k+1} \rangle \quad \mathcal{R}^{\perp}(A) =: \langle z_1, \ldots, z_k \rangle$$

or, in equivalent matrix notation, as

$$t := [t_1, \ldots, t_{k+1}]\,, \quad z := [z_1, \ldots, z_k]\,,$$

so that

$$\begin{aligned} At = 0, \quad & t^T t = I_{k+1},\ P^{\perp} = tt^T, \\ A^T z = 0, \quad & z^T z = I_k,\ \overline{P}^{\perp} := zz^T\,. \end{aligned} \tag{5.52}$$

Note that t and z are only specified up to orthogonal transformations—which leaves $\dim O(k+1) = \frac{1}{2}k(k+1)$ degrees of freedom for t and $\dim O(k) = \frac{1}{2}k(k-1)$ degrees of freedom for z.

Upon introducing *local coordinates* $\xi \in \mathbb{R}^{k+1}$, $\gamma \in \mathbb{R}^k$ by virtue of

$$v = \sum_{i=1}^{k+1} \xi_i t_i = t\xi\,, \qquad f(v) = \sum_{j=1}^{k} \gamma_j z_j = z\gamma\,,$$

the reduced equations (5.51) can be rewritten in the form

$$\gamma(\xi) := z^T f(t\xi) = z^T F(y^* + t\xi + w^*(t\xi)) = 0\,. \tag{5.53}$$

For the actual determination of singularities, higher order derivatives of both sides will play an important role.

Lemma 5.9 *Assumptions as just introduced. Let $y^* := 0$ for convenience and $a_i \in \mathbb{R}^{k+1}$. Then the following relations hold:*

$$\dot{\gamma}(0)a_1 = 0 \tag{5.54}$$

$$\ddot{\gamma}(0)[a_1, a_2] = z^T F''[ta_1, ta_2] \tag{5.55}$$

$$\begin{aligned} \dddot{\gamma}\,(0)[a_1, a_2, a_3] = {} & z^T F'''[ta_1, ta_2, ta_3] \\ & -z^t F''[ta_1, A^+ F''[ta_2, ta_3]] \\ & -z^T F''[ta_2, A^+ F''[ta_3, ta_1]] \\ & -z^T F''[ta_3, A^+ F''[ta_1, ta_2]] \end{aligned} \tag{5.56}$$

Proof. As a consequence of $y^* = 0$ we have $v^* = 0$, $w^*(0) = 0$ and $\xi^* = 0$. We start from

$$\gamma(\xi) = z^T F(t\xi + w^*(t\xi)) \tag{5.57}$$

and

$$\overline{P} F(t\xi + w^*(t\xi)) \equiv 0\,. \tag{5.58}$$

Differentiation of (5.57) with respect to ξ yields

$$\dot{\gamma}(\xi) a_1 = z^T F'(t\xi + w^*(t\xi))(ta_1 + w^*_\xi(t\xi)a_1)$$

and, after insertion of $z^T A = 0$

$$\dot{\gamma}(0) a_1 = z^T A(ta_1 + w^*_\xi(0)a_1) = 0\,,$$

which confirms (5.54). Differentiation of (5.58) yields

$$\overline{P} A(ta_1 + w^*_\xi(0)a_1) = 0\,.$$

which, with $\overline{P}A = A$, $At = 0$ and $w^*_\xi(0)a_1 \in \mathcal{N}^\perp$, can be solved by

$$w^*_\xi(0)a_1 = 0\,. \tag{5.59}$$

Upon differentiating (5.57) once more and inserting the expression above we obtain

$$\ddot{\gamma}(0)[a_1, a_2[= z^T F''(0)[ta_1, ta_2]\,,$$

which confirms (5.55). Differentiation of (5.58) once more leads to

$$\overline{P} F''(0)[ta_1, ta_2] + \overline{P} A w^*_{\xi\xi}(0)[a_1, a_2] = 0\,.$$

With arguments as just used before, the latter equation can be solved to yield

$$w^*_{\xi\xi}(0)[a_1, a_2] = -A^+ F''(0)[ta_1, ta_2]\,. \tag{5.60}$$

Upon differentiating (5.57) for a third time, we eventually arrive at

$$\begin{aligned}
\dddot{\gamma}\,(0)[a_1, a_2, a_3] \;=\; & z^T F'''(0)[ta_1, ta_2, ta_3] \\
& + z^T F''(0)[ta_1, w^*_{\xi\xi}(0)[a_2, a_3]] \\
& + z^T F''(0)[ta_2, w^*_{\xi\xi}(0)[a_3, a_1]] \\
& + z^T F''(0)[ta_3, w^*_{\xi\xi}(0)[a_1, a_2]]\,.
\end{aligned}$$

Insertion of $w^*_{\xi\xi}(0)$ then finally confirms (5.56). □

Universal unfolding. It is clear from the above derivation that the function $\gamma : \mathbb{R}^{k+1} \to \mathbb{R}^k$ contains all essential information needed to classify the local structure of a singularity. Since only derivatives of γ up to a certain order are required, it suffices to study simple polynomial *germs* $g(\xi)$, which then may stand for the whole function class

$$\Gamma(g) := \{\gamma(\xi) = \beta(\xi)g(h(\xi)) \mid \beta, h\ C^\infty\text{-diffeomorphism},\ \ h(0) = 0\}$$

called the *contact equivalence class*. From a geometrical point of view all germs within one equivalence class show a similar solution structure around $\xi = 0$. We may say that the reduced mapping γ is contact equivalent to a representative germ $g \in \Gamma(\gamma)$ or, vice versa, $\gamma \in \Gamma(g)$. As examples, the germ

$$g_s(\xi) := \xi_1^2 - \xi_2^2 \quad (k = 1)$$

represents a *simple bifurcation*, whereas the germ

$$g_c(\xi) := \xi_1^2 - \xi_2^3 \quad (k = 1)$$

characterizes an *asymmetric cusp*. We then obtain

$$\beta(\xi)g(h(\xi)) = z^T F(y^* + t\xi + w^*(t\xi)) = 0$$

in terms of certain diffeomorphisms β, h.

Up to now, our analytical presentation has only covered *perfect* singularities. An efficient algorithm will have to deal with *imperfect* or *unfolded* singularities y^* as well—even without knowing in advance about the structure of the perturbations. As an immediate consequence, we will encounter $\gamma(0) \neq 0$ and the associated Jacobian matrix $F'(y^*)$ may no longer be exactly rank-deficient, but still 'close to' a rank-deficient matrix. In this situation, the structure of *topological perturbations* is important, which are known to lead to an *unfolding of nongeneric singularities*. In the just introduced framework, such perturbations may be written as polynomial perturbations $p(\xi, \alpha)$ of the germs g replacing them by the *perturbed germs*

$$G(\xi, \alpha) := g(\xi) + p(\xi, \alpha)\,, \tag{5.61}$$

wherein $p(\xi, 0) \equiv 0$ and the parameters α denote the *unfolding parameters*. The *minimal number of unfolding parameters* is a characteristic of each type of singularity and is called its *codimension* q. In case of this minimal parameterization, the representation (5.61) is called *universal unfolding*. A special feature of any universal unfolding is that monomials arising in p are *at least 2 orders less* than corresponding monomials arising in g. As examples again, g_s for the *simple bifurcation* is replaced by

$$G_s(\xi, \alpha) := \xi_1^2 - \xi_2^2 + \alpha\,, \quad (k = 1,\, q = 1)\,,$$

whereas g_c for the *asymmetric cusp* is replaced by

$$G_c(\xi, \alpha_1, \alpha_2) := \xi_1^2 - \xi_2^3 + \alpha_1 + \alpha_2\xi_2\,, \quad (k = 1,\, q = 2)\,. \tag{5.62}$$

Bibliographical Note. For a general thorough treatment of unfolded singularities, the reader may refer to M. Golubitsky and D. Schaeffer [109] and their textbooks [110, 111]. Since these authors treat dynamical systems $\dot{x} = F(x, \lambda)$ with state variables x, they give the *explicit parameter* λ an extra role—in contrast to the present section here, which treats all $n + 1$ components of $y = (x, \lambda)$ the same.

Construction of augmented systems. Summarizing, we may assume that specific diffeomorphisms β, h exist such that

$$\beta(\xi)G(h(\xi), \alpha) = z^T F(y^* + t\xi + w^*(t\xi)) \tag{5.63}$$

with, in general,

$$G(h(0), \alpha) = G(0, \alpha) = p(0, \alpha) \neq 0\,.$$

Therefore, for perturbed singularities, the reduced system (5.53) must be replaced by

$$z^T F(y^*) = p(0, \alpha)\,.$$

These k equations, together with the $n - k$ equations $\overline{P}F = 0$, then lead to the n equations

$$F(y^*) = z\, p(0, \alpha)$$

in terms of the $(k + 1)n + q + 1$ unknowns (y, z, α).

Simple bifurcation. Let us now return to the special case $k = 1, q = 1$. Here we arrive at the *augmented system* of G. Moore [103]:

$$F'(y)^T z = 0\,, \tag{5.64}$$

$$F(y) + \alpha z = 0\,, \tag{5.65}$$

$$\tfrac{1}{2}(z^T z - 1) = 0\,. \tag{5.66}$$

It comprises $(2n+2)$ nonlinear equations for the $(2n+2)$ unknowns (y, z, α). The Jacobian $J(y, z, \alpha)$ of this mapping is *nonsingular* for sufficiently small perturbation parameter α. The proof of this fact is postponed to Section 5.3.2 below, since it stimulates an algorithmic idea for the iterative solution of the above augmented system.

In order to make sure that a geometrical bifurcation really exists locally, we must impose the additional *second derivative* condition

$$z^T F''(y^*)[t, t] \qquad \text{nondegenerate, indefinite}\,. \tag{5.67}$$

This condition assures the existence of two local *branch directions* as will be shown next. In most of the established analysis treatise—compare, e.g., M.G. Crandall and P.H. Rabinowitz [46]—one of the intersecting branches is

assumed to be the trivial one—which is acceptable for a merely analytical treatment, but unsatisfactory for the construction of efficient numerical algorithms. Therefore we here include a theorem that treats both branches as indistinguishable.

Theorem 5.10 *Assumptions and notation as just introduced. Let* $F \in C^k$, $k \geq 3$. *Then, in a neighborhood of* y^*, *the solution set* $F + \alpha z = 0$ *consists of two one-dimensional* C^{k-2}*-branches* $\gamma_1(s)$, $\gamma_2(s)$ *such that*

$$\gamma_i(0) = y^*\,,\ i = 1, 2\,,$$
$$\mathcal{N} = \langle \dot\gamma_1(0), \dot\gamma_2(0) \rangle\,,$$
$$z^T F''(y^*)\Big[\dot\gamma_i(0), \dot\gamma_i(0)\Big] = 0\,.$$

Proof. (*Sketch*) For convenience, assume again that $y^* = 0$. Let a standard Lyapunov-Schmidt reduction have been performed in terms of a parametrization of the two-dimensional nullspace $\mathcal{N}$. It is then sufficient to study the mapping $\overline{F} = \overline{P}^{\perp} F : \mathcal{N} \to \mathbb{R}$. Introducing polar coordinates, define a blow-up version of $\overline{F}$ by

$$\Phi(r, \Theta) := \begin{cases} 2\overline{F}\Big(r\, e(\Theta)\Big) \,\Big/\, r^2 & r > 0 \\ \overline{F}''(0)\Big[e(\Theta),\, e(\Theta)\Big] & r = 0\,, \end{cases}$$

where $e(\Theta) := (\cos\Theta,\ \sin\Theta)$ denotes the unit vector in the direction $\Theta \in [0,\ \pi]$. Obviously, $\Phi = 0$ holds if $\overline{F} = 0$. Moreover, $\overline{F} \in C^k$ implies $\Phi \in C^{k-2}$ and Φ can also be formally continued to $r < 0$. By assumption (5.67) there exist directions $\Theta_i (i = 1, 2)$ such that

$$\begin{aligned} \Phi(0, \pm\Theta_i) &= 0\,, \\ \Phi_\Theta(0, \pm\Theta_i) &= F''(0)\Big[e_\Theta(\Theta_i),\, e_\Theta(\Theta_i)\Big] \neq 0\,. \end{aligned}$$

Hence, by the implicit function theorem, there are four C^{k-2}–semi-branches

$$\gamma_i^{\pm}(r) = r\, e(\Theta_i^{\pm}(r))\,,\ i = 1, 2 \quad r \geq 0$$

for sufficiently small r. At $r = 0$, the functions $\gamma_i^+(r)$ and $\gamma_i^-(-r)$ have the same derivatives up to order $k - 2$. Therefore, combining $\gamma_i^+(r)$ and $\gamma_i^-(-r)$, $i = 1, 2$, yields two C^{k-2}-branches, which completes the proof. □

From this result, the desired local tangent directions

$$t_i^* = \dot\gamma_i(y^*)\,, \qquad i = 1, 2\,,$$

are seen to be defined from the *quadratic equation*

$$z^T F''(y^*)\,[t_i^*, t_i^*] = 0\,,$$

which, under the assumption (5.67) has the two distinct real roots t_1^*, t_2^*.

Asymmetric cusp. This possibly unfolded singularity has also rank-deficiency $k = 1$, but codimension $q = 2$. Recall the perturbed germ $G_c = G$ from (5.62) to derive the characterization (with $h(0) = 0$):

$$G_(0, \alpha) = \alpha_1 , \tag{5.68}$$

$$\begin{aligned} G_{\xi_1}(0, \alpha) &= 0 , \\ G_{\xi_2}(0, \alpha) &= \alpha_2 , \end{aligned} \tag{5.69}$$

$$\begin{aligned} G_{\xi_2\xi_2}(0, \alpha) &= 0 , \\ G_{\xi_1\xi_2}(0, \alpha) &= 0 . \end{aligned} \tag{5.70}$$

Note that all nonvanishing derivatives beyond (5.69) and (5.70) such as

$$G_{\xi_1\xi_1}(0, \alpha) = 2$$

do not show up, since they are arbitrary due to the arbitrary C^∞-diffeomorphic transformation $\beta(\xi)$ in (5.63). Upon differentiating the right-hand side of (5.63) with $h(\xi) = \xi$ and $\beta(\xi) = 1$, we may obtain (as in the simple bifurcation)

$$z^T F(y^*) = \alpha_1$$

from (5.68), which leads to

$$F(y^*) = \alpha_1 z . \tag{5.71}$$

From (5.69) and (5.59) we may verify that

$$F'(y^*)t_1 = 0 , \ F'(y^*)t_2 = \alpha_2 z . \tag{5.72}$$

Finally, from (5.70), (5.60) and $z^T \overline{P}^\perp = z^T$ we arrive at

$$\begin{aligned} z^T F''(y^*)[t_2, t_2] &= 0 , \\ z^T F''(y^*)[t_1, t_2] &= 0 . \end{aligned}$$

Of course, we will add the perturbed corange condition

$$F'(y^*)^T z = \alpha_2 t_2 \tag{5.73}$$

to be compatible with (5.72). For normalization we will choose the four equations

$$z^T z = 1 , \ t_1^T t_1 = t_2^T t_2 = 1 , \ t_1^T t_2 = 0 . \tag{5.74}$$

Upon combining (5.71) up to (5.74) we would arrive at an overdetermined system, $4n + 8$ equations in $4n + 5$ unknowns. Careful examination for general $h(\xi)$ (with still $\beta(\xi) = 1$ w.l.o.g) leads to a replacement of (5.72) and (5.73) by the *perturbed Lyapunov-Schmidt reduction* (originally suggested by R. Menzel)

$$\begin{aligned} F'(y^*)^T z &= \gamma_{11} t_1 + \gamma_{21} t_2 \,, \\ F'(y^*) t_1 &= \beta_{11} z \,, \\ F'(y^*) t_2 &= \beta_{21} z \,. \end{aligned} \tag{5.75}$$

Thus we end up with the following *augmented system* for the asymmetric cusp

$$\begin{aligned} &F(y) = \alpha z \,, \\ &F'(y)^T z = \gamma_{11} t_1 + \gamma_{21} t_2 \,, \\ &F'(y) t_1 = \beta_{11} z_1 \,, \\ &F'(y) t_2 = \beta_{21} z_2 \,, \\ &z^T F''(y)[t_2, t_2] = 0 \,, \\ &z^T F''(y)[t_1, t_2] = 0 \,, \\ &z^T z = 1 \,, \\ &t_1^T t_1 = t_2^T t_2 = 1, \quad t_1^T t_2 = 0 \,. \end{aligned}$$

This system comprises $4n + 7$ equations in the $4n + 8$ unknowns y, z, t_1, t_2, α_1, γ_{11}, γ_{21}, β_{11}, β_{21}—which means that the system is *underdetermined*.

The associated augmented Jacobian can be shown to have full row rank for sufficiently small perturbation parameters α_1, γ_{11}, γ_{21}, β_{11}, β_{21}.

Higher order critical points. The perturbed system (5.75) is a special case of the general perturbed Lyapunov-Schmidt reduction, wherein $A = F'(y^*)$ has rank-deficiency $k > 0$:

$$\begin{aligned} A^T z_j &= \sum_{i=1}^{k+1} \gamma_{ji} t_i \,, \\ A t_i &= \sum_{j=1}^{k} \beta_{ij} z_j \,, \\ z_j z_l &= \delta_{j,l} \,, \qquad l \le j = 1, \ldots, k \,, \\ t_i t_m &= \delta_{i,m} \,, \qquad m \le i = 1, \ldots, k+1 \,. \end{aligned} \tag{5.76}$$

This *underdetermined* system comprises $(2k+1)(n+k+1) - k^2$ equations in $(2k+1)(n+k+1)$ unknowns. It has been suggested by P. Kunkel in his thesis [138, 139, 140] and worked out using tree structures in [141]. The extended Jacobian has full row rank at a *perfect* singularity, where

$$\beta_{ij}^* = \gamma_{ij}^* = 0 \,.$$

Note that, also for an *imperfect* singularity y^*, we can verify that

$$\gamma_{ij} = \beta_{ij} = z_j^T A t_i \,, \qquad i = 1, \ldots k, \quad j = 1, \ldots, k+1 \,.$$

However, had we identified $\gamma_{ij} = \beta_{ij}$ from the start, then the system would no longer be uniquely solvable.

The missing k^2 degrees of freedom come from $\frac{1}{2}k(k-1)$ arbitrary degrees in z and $\frac{1}{2}k(k+1)$ arbitrary degrees in t due to orthogonal transformation—compare (5.76) and (5.52) and the discussion thereafter.

Generally speaking, for *higher order* singularities the number of equations and of dependent variables does not agree as nicely as in the simple bifurcation case. Consequently, quite complicated augmented systems may arise, usually *underdetermined* as in the *cusp* case. Part of such systems are still under investigation including the problem of their automatic generation by means of computer algebra systems—see, e.g., D. Armbruster [6]. In principle, a general bifurcation algorithm would need to represent a whole *hierarchy of augmented systems*—which, however, will be limited for obvious reasons.

5.3.2 Newton-like algorithm for simple bifurcations

We return to the augmented system (5.64) of G. Moore. The associated *extended Jacobian* has the block structure

$$J(y,z,\alpha) := \begin{bmatrix} C & A^T & 0 \\ A & \alpha I_n & z \\ 0 & z^T & 0 \end{bmatrix}$$

in terms of the submatrices

$$C := \left(F'(y)^T z\right)' = \sum_{i=1}^{n} f_i''(y) z_i\,,\ A := F'(y)\,.$$

Note that C and therefore J are symmetric matrices.

Theorem 5.11 *At a simple (possibly perturbed) bifurcation point y^* with sufficiently small perturbation parameter α^* the extended Jacobian $J(y^*, z^*, \alpha^*)$ is nonsingular.*

Proof. First $J(y,z,0)$ is shown to be nonsingular. We start with applying the singular value decomposition

$$A = U \sum V^T\,,\ \sum = \begin{bmatrix} \sum' & 0 \\ 0 & 0 \end{bmatrix},$$
$$\begin{array}{lcl} U & : & \text{orthogonal } (n,n)\text{-matrix}, \\ V^T & : & \text{orthogonal } (n+1,n+1)\text{-matrix}, \\ \sum' & = & \text{diag}\,(\sigma_1,\ldots,\sigma_{n-1})\,,\ \sigma_i > 0\,. \end{array}$$

Inserting this decomposition into $J(y,z,0)$ yields after proper transformation

$$J = \begin{bmatrix} C & A^T & 0 \\ A & 0 & z \\ 0 & z^T & 0 \end{bmatrix} \to \begin{bmatrix} \overline{C} & \sum^T & 0 \\ \sum & 0 & \overline{z} \\ 0 & \overline{z}^T & 0 \end{bmatrix} =: \overline{J}$$

with $\overline{z} := U^T z$, $\overline{C} := VCV^T = \overline{C}^T$. In the above notation, the equations $F'(y)^T z = 0$ now read

$$\Sigma^T \overline{z} = 0\,,$$

which implies that $\overline{z}^T = (0, \ldots, 0, 1)$. If, in addition, we introduce the corresponding partitioning

$$\overline{C} = \begin{bmatrix} \overline{C}_{11} & \overline{C}_{12} \\ \overline{C}_{12}^T & \overline{C}_{22} \end{bmatrix}\,,\ \overline{C}_{22} = \overline{C}_{22}^T \quad (2,2)\text{-matrix}\,,$$

then

$$\overline{J} = \begin{bmatrix} \overline{C}_{11} & \overline{C}_{12} & \sum' & 0 & 0 \\ \overline{C}_{12} & \overline{C}_{22} & 0 & 0 & 0 \\ \sum' & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}\,.$$

Hence

$$\operatorname{rank}(J) = \operatorname{rank}\left(\overline{J}\right) = 2n + \operatorname{rank}\left(\overline{C}_{22}\right)\,.$$

Upon recalling assumption (5.67), we obtain here

$$\left(z^T F'\right)'[t,t] = \overline{C}_{22}\,,$$

which assures that $\overline{C}_{22}$ is certainly nonsingular and

$$\operatorname{rank}\Big(J(y^*, z^*, 0)\Big) = 2n + 2\,.$$

Finally, by the usual perturbation lemma for symmetric matrices with symmetric perturbation, $J(y^*, z^*, \alpha^*)$ is nonsingular for α^* 'sufficiently small', which completes the proof. □

The above Theorem 5.11 assures that the *ordinary* Newton method (dropping the iteration index)

$$\begin{bmatrix} C & A^T 0 & \\ A & \alpha I & z \\ 0 & z^T & 0 \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta z \\ \Delta\alpha \end{bmatrix} = - \begin{bmatrix} F'^T z \\ F + \alpha z \\ \frac{1}{2}(z^T z - 1) \end{bmatrix}$$

is well-defined in a neighborhood of the simple bifurcation point. In the special situation a *Newton-like* method characterized by the replacement

$$\begin{array}{lcl} J(y,z,\alpha) & \rightarrow & J(y,z,0)\,, \\ A = F'(y) & \rightarrow & \widetilde{A} \approx F'(y^*) \end{array}$$

seems to be preferable, since the associated linear block system (again dropping the iteration index)

$$\begin{bmatrix} C & \widetilde{A}^T & 0 \\ \widetilde{A} & 0 & z \\ 0 & z^T & 0 \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta z \\ \Delta\alpha \end{bmatrix} = - \begin{bmatrix} A^T z \\ F + \alpha z \\ \frac{1}{2}(z^T z - 1) \end{bmatrix} \tag{5.77}$$

is easier to solve. On the basis of the theory of Section 2.1, the thus defined iteration will converge *superlinearly* for *perfect* bifurcations ($\alpha^* = 0$), but only *linearly* for *imperfect* bifurcations. Since excellent starting points are available in the present setting, one may even keep the *initial* Jacobian approximation—thus implementing a variant of the *simplified* Newton method. This method permits even further computational savings per iteration step.

Distinction between perfect and imperfect bifurcations. Whenever a *perfect bifurcation* arises, then the Newton-like iterates $\{\alpha^k\}$ will approach *zero* superlinearly so that the criterion

$$\left|\alpha^{k+1}\right| \leq \tfrac{1}{4}\left|\alpha^k\right|$$

will be passed. Otherwise, leading digits of α^* will show up.

In order to compute the two branch directions t_1^*, t_2^* easily, the above extended Jacobian matrix needs to be decomposed in some *structure preserving* way. We work out two possibilities.

Implementation based on QR-decomposition. Let $A = F'(y)$ denote the Jacobian $(n, n+1)$-matrix to be decomposed according to

$$A = Q \begin{bmatrix} R & S \\ 0 & \varepsilon^T \end{bmatrix} \Pi^T \,, \text{where} \quad \begin{array}{ll} Q: & \text{orthogonal } (n,n)\text{-matrix}, \\ \Pi: & \text{permutation } (n+1,n+1)\text{-matrix}, \\ R: & \text{upper triangular } (n-1,n-1)\text{-matrix}, \\ S: & (n-1,2)\text{-matrix}, \\ \varepsilon: & \text{2-vector}. \end{array}$$

For y 'close to' y^*, R will be nonsingular and ε 'small'. Hence, the approximation

$$\widetilde{A} := Q \begin{bmatrix} R & S \\ 0 & 0 \end{bmatrix} \Pi^T$$

will be appropriate within a Newton-like iteration.

Starting points for Newton-like iteration. A starting guess y^0 is available from the path-following procedure, typically from linear interpolation between the

two points $\overline{y}_1, \overline{y}_2$ on the solution curve (see Figure 5.8) that had activated the device for the detection of critical points (see Figure 5.5). A starting guess z^0 can be obtained from solving

$$\widetilde{A}^T z = 0\,, \qquad \|z\|_2^2 = 1\,,$$

which, upon inserting the QR-decomposition directly leads to

$$z^0 = Qe_n\,,\ e_n = (0,\ldots,0,1)\,.$$

From this, a natural choice of α^0 can be seen to be

$$\alpha^0 = -\Big(Q^T F(y^0)\Big)_n\,.$$

Block elimination. Insertion of the above QR-decomposition into the block system (5.77) suggests the following partitioning

$$\begin{aligned}
&\widehat{C} := \Pi^T C \Pi = \begin{pmatrix} C_{11} & C_{12} \\ C_{12} & C_{22} \end{pmatrix}\,, && C_{22} : (2,2)\text{-matrix}\,,\\
&\overline{z} := Q^T z = \begin{pmatrix} w \\ \zeta \end{pmatrix}\,, && w \in \mathbb{R}^{n-1}\,,\ \zeta \in \mathbb{R}\,,\\
&\Pi^T \Delta y = \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix}\,, && \Delta u \in \mathbb{R}^{n-1}\,,\ \Delta v \in \mathbb{R}^2\,,\\
&\Delta\overline{z} = Q^T \Delta z = \begin{pmatrix} \Delta w \\ \Delta\zeta \end{pmatrix}\,, && \Delta w \in \mathbb{R}^{n+1}\,,\ \Delta\zeta \in \mathbb{R}\,,\\
&\Pi^T A^T z = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}\,, && f_1 \in \mathbb{R}^{n-1}\,,\ f_2 \in \mathbb{R}^2\\
&Q^T(F + \alpha z) = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}\,, && g_1 \in \mathbb{R}^{n-1}\,,\ g_2 \in \mathbb{R}\\
&h := \tfrac{1}{2}(z^T z - 1)\,.
\end{aligned}$$

In this notation, (5.77) now reads

$$\begin{bmatrix} C_{11} & C_{12} & R^T & 0 & 0 \\ C_{12}^T & C_{22} & S^T & 0 & 0 \\ R & S & 0 & 0 & w \\ 0 & 0 & 0 & 0 & \zeta \\ 0 & 0 & w^T & \zeta & 0 \end{bmatrix} \begin{bmatrix} \Delta u \\ \Delta v \\ \Delta w \\ \Delta\zeta \\ \Delta\alpha \end{bmatrix} = - \begin{bmatrix} f_1 \\ f_2 \\ g_1 \\ g_2 \\ h \end{bmatrix}\,.$$

Simplified Newton iteration. The initial guess z^0 is equivalent to

$$w^0 = 0\,,\ \zeta^0 = 1\,,$$

which may be used to decouple the last two equations. In this simplified Newton method the last two equations then yield (dropping the index k):

$$\Delta\alpha = -g_2\,, \quad \Delta\zeta = -h\,.$$

In order to solve the remaining three equations, we compute once

$$R\overline{S} = S\,, \tag{5.78}$$

$$\overline{C}_{22} := C_{22} - (C_{12}^T\overline{S} + \overline{S}^T C_{12}) + \overline{S}^T C_{11}\overline{S} \tag{5.79}$$

and repeatedly for each new right-hand side

$$\begin{aligned} R\overline{g}_1 &= g_1\,, \\ \overline{C}_{22}\Delta v &= -f_2 + \left(C_{12}^T - \overline{S}^T C_{11}\right)\overline{g}_1 + \overline{S}^T f_1\,, \\ \Delta u &= -\overline{g}_1 - \overline{S}\Delta v\,, \\ R^T\Delta w &= -f_1 - C_{11}\Delta u - C_{12}\Delta v\,. \end{aligned}$$

Note that the symmetric $(2,2)$-matrix $\overline{C}_{22}$ is just the one used in the proof of Theorem 5.11—which means that $\overline{C}_{22}$ may be assumed to be nonsingular in a neighborhood of a simple bifurcation point. If it appears to be singular when decomposed, then there will be *no bifurcation point* locally. Finally, back substitution yields

$$\Delta y = \Pi \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix}\,, \quad \Delta z = Q \begin{pmatrix} \Delta w \\ \Delta\zeta \end{pmatrix}\,.$$

Implementation based on LU-decomposition. Assume that we start with the decomposition

$$A(\varepsilon) := L \begin{bmatrix} R & S \\ 0 & \varepsilon^T \end{bmatrix} \Pi^T\,,$$

where L is a lower triangular matrix obtained from some sparse elimination technique. Due to conditional pivoting within a sparse solver, say, the entries ε may be 'small'. Then A may be replaced according to

$$\widetilde{A} := A(0)\,.$$

For reasons to be understood below, it is advisable to modify the *normalizing condition* $z^T z = 1$ such that

$$h := \tfrac{1}{2}(\|L^T z\|_2^2 - 1) = 0\,.$$

Starting points for Newton-like iteration. With y^0 given, initial guesses z^0 are easily derived from

$$\begin{aligned} \widetilde{A}^T z &= 0\,, \\ \|L^T z\|_2^2 &= 1\,. \end{aligned}$$

which, with $L = (l_{ij})$, leads to

$$\begin{aligned} L^T z^0 &:= e_n\,, \\ \alpha^0 &:= (F(y^0))_n / l_{nn}\,. \end{aligned}$$

Block elimination. The above LU-decomposition is now inserted into the block system (5.77) with the slight change of normalization as just described. In comparison with the QR-variant we can keep the notation for $\widehat{C}$, Δu, Δv, f_1, f_2 unchanged and introduce the following modified quantities:

$$\begin{aligned} \widehat{z} := L^{-1} z &= \begin{pmatrix} \widehat{w} \\ \widehat{\zeta} \end{pmatrix}, && \widehat{w} \in \mathbb{R}^{n-1},\ \widehat{\zeta} \in \mathbb{R}\,, \\ \overline{z} := L^T z &= \begin{pmatrix} w \\ \zeta \end{pmatrix}, && w \in \mathbb{R}^{n-1},\ \zeta \in \mathbb{R}\,, \\ L^T \Delta z &= \begin{pmatrix} \Delta w \\ \Delta \zeta \end{pmatrix}, && \Delta w \in \mathbb{R}^{n+1},\ \Delta\zeta \in \mathbb{R}\,, \\ L^{-1}(F + \alpha z) &= \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}, && g_1 \in \mathbb{R}^{n-1},\ g_2 \in \mathbb{R}\,. \end{aligned}$$

In this notation, (5.77) now reads

$$\begin{bmatrix} C_{11} & C_{12} & R^T & 0 & 0 \\ C_{12}^T & C_{22} & S^T & 0 & 0 \\ R & S & 0 & 0 & \widehat{w} \\ 0 & 0 & 0 & 0 & \widehat{\zeta} \\ 0 & 0 & w^T & \zeta & 0 \end{bmatrix} \begin{bmatrix} \Delta u \\ \Delta v \\ \Delta w \\ \Delta\zeta \\ \Delta\alpha \end{bmatrix} = - \begin{bmatrix} f_1 \\ f_2 \\ g_1 \\ g_2 \\ h \end{bmatrix}.$$

Simplified Newton iteration. In order to implement this variant, just verify that the choice of z^0 is again equivalent to

$$w^0 = 0\,,\ \zeta^0 = 1\,,$$

which once more implies that

$$\Delta\alpha = -g_2\,,\ \Delta\zeta = -h\,.$$

With $\overline{S}$ and $\overline{C}_{11}$ from equations (5.78) and (5.79) the remaining system can be solved as follows

$$\begin{aligned} R\overline{g}_1 &= g_1 + \widehat{w}\Delta\alpha\,, \\ \overline{C}_{22}\Delta v &= -f_2 + \left(C_{12}^T - \overline{S}^T C_{11}\right)\overline{g}_1 + \overline{S}^T f_1\,, \\ \Delta u &= -\overline{g}_1 - \overline{S}\Delta v\,, \\ R^T \Delta w &= -f_1 - C_{11}\Delta u - C_{12}\Delta v\,. \end{aligned}$$

Finally, back substitution yields

$$\Delta y = \Pi \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix} L^T \Delta z = \begin{pmatrix} \Delta w \\ \Delta \zeta \end{pmatrix} .$$

5.3.3 Branching-off algorithm

Suppose that a simple bifurcation point y^* has been computed. Then y^* is the intersection of exactly two solution branches associated with the mapping $F + \alpha z$. In order to continue the numerical pathfollowing beyond bifurcations, one will need to first compute the directions of these branches and second to design an efficient restart strategy along each new semi-branch.

Computation of branch directions. As described above, the local tangent directions t_i^*, $i = 1, 2$ are computed from the quadratic equation (5.67). Starting from any of the two presented decompositions, the following parametrization of $\mathcal{N}$ is natural:

$$t_i^* := \Pi \begin{pmatrix} -\overline{S}\, e_i \\ e_i \end{pmatrix} , \qquad e_i := (\cos \Theta_i,\ \sin \Theta_i)$$

with $\overline{S}$ as defined by (5.78). In the present notation this equation can be rewritten as

$$t_i^{*T} C\, t_i^* = 0 ,$$

which reduces to

$$e_i^T \overline{C}_{22} e_i = 0$$

in terms of the symmetric $(2,2)$-matrix $\overline{C}_{22}$ known to be nonsingular when a simple bifurcation point exists locally. This is again a quadratic equation in either $\tan \Theta_i$ or $\cot \Theta_i$ with two different real roots under the assumption (5.67). In case $\overline{C}_{22}$ turns out to be semi-definite or degenerate, then a *nonsimple* bifurcation point is seen to occur. Complex conjugate roots indicate an *isola* (which, however, would be hard to detect by just pathfollowing with respect to one parameter!).

Stepsize control restart. Suppose we have the situation of one *entering* semi-branch (already computed) and three *emanating* semi-branches (to be computed next) as depicted in Figure 5.8.

Let, formally, $t_3^* := -t_2^*$. In order to start the path-following procedure along each emanating semi-branch, one is required to define starting points $\widehat{y}$ for the quasi-Gauss-Newton iteration ($i = 1, 2, 3$):

$$\widehat{y}_i(s) := y^* + s \cdot t_i^* .$$

Herein an efficient control of the stepsize s requires some care. Two antagonistic conditions are to be matched:

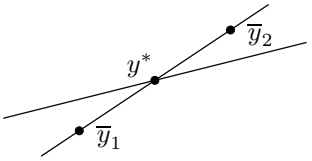

Fig. 5.8. Simple bifurcation point: branch situation.

- The Jacobian $F'(\widehat{y}(s))$ must have full (numerical) rank, which leads to a lower bound $s > s_{\min}$.
- The local quasi-Gauss-Newton iteration starting at $\widehat{y}(s)$ should converge sufficiently fast, which leads to an upper bound $s \leq s_{\max}$.

Prediction strategy. If we use the fact that the Gauss-Newton iteration had converged on the entering semi-branch towards some point $\overline{y}_{\text{old}}$, we are led to the choice

$$s_0 := \rho \frac{\|y^* - \overline{y}_{\text{old}}\|}{\|t_1^*\|}\,,\ \rho < 1$$

with some safety factor ρ. With $\widehat{y}(s_0)$, the Jacobian $F'(\widehat{y}(s_0))$ and the contraction factors $\Theta(s_0)$ are available in the course of the Gauss-Newton iteration. Therefore, numerical estimates $[s_{\min}]$, $[s_{\max}]$ can be computed.

In view of (I) above, we require that

$$\overline{\varepsilon}\,\text{cond}\left(F'(\widehat{y}(s))\right) < 1$$

with some prescribed $\overline{\varepsilon} > \mathit{eps}$, the relative machine precision. Near y^* all determinants (such as d_ξ, d_λ) are $O(s)$. So we have

$$\text{cond}\Big(F'(\widehat{y}(s))\Big) > \frac{\gamma}{s}\,,$$

which leads to

$$s > \overline{\varepsilon}\gamma =: s_{\min}\,.$$

As γ is unknown, a numerical condition number estimate $[\text{cond}\,(\cdot)]$ is required to derive the estimate

$$[s_{\min}] := \overline{\varepsilon}\left[\text{cond}\Big(F'(\widehat{y}(s_0))\Big)\right] \cdot s_0\,.$$

In view of (II) above, a careful analysis shows that the contraction factor

$$\Theta_0(s) = O(s)$$

close to y^* instead of $O(s^2)$ in the neighborhood of a regular point $\overline{y}$. As a consequence of the Newton-Kantorovich theorem, we require

$$\Theta_0 \leq \overline{\Theta} = \tfrac{1}{4}\,,$$

which leads to the stepsize estimate

$$[s_{\max}] = \frac{\overline{\Theta}}{\Theta_0(s_0)} \cdot s_0\,.$$

In case we had obtained

$$[s_{\min}] > [s_{\max}]$$

the computation would have to be terminated suggesting higher precision arithmetic—thus lowering $[s_{\min}]$.

In the author's experience, such a situation has never occurred up to now. In the standard situation

$$[s_{\min}] \ll [s_{\max}]$$

some initial steplength $\overline{s}_0$ can be selected. A typical choice will be

$$\overline{s}_0 := \rho \cdot [s_{\max}]$$

for some sufficiently large $\rho < 1$.

Construction of complete bifurcation diagrams. The implementation of the whole algorithm—as described in the previous Section 5.2 and the present Section 5.3—requires careful book-keeping of critical points and of entering and emanating semi-branches to avoid endless cycling. As an example, *before* actually iterating towards some conjectured bifurcation point y^*, the corresponding starting point y^0 should be tested: if it is within the Kantorovich neighborhood of some formerly computed bifurcation point, then identity of old and new bifurcation point can be assumed; as usual, the test is based on the local contraction factor criterion $\Theta_0 \leq 1/4$ in agreement with the sufficient Kantorovich condition ($h_0 \leq 1/2$). Whenever $\Theta_0 > 1/4$, i.e., when the Kantorovich condition is locally violated, then a possible local nonuniqueness of a solution is indicated.

Bibliographical Note. The computation of simple bifurcations via the QR-implementation of Moore's extended system has been worked out in the paper [72] by P. Deuflhard, B. Fiedler, and P. Kunkel. The here presented algorithm with quasi-Gauss-Newton method, adaptive stepsize control, computation of turning points and simple bifurcation points has been implemented in the code `ALCON2`. An advanced descendant of `ALCON2` is the code `SYMCON` due to K. Gatermann and A. Hohmann [95] for equivariant parameter dependent nonlinear systems. In this algorithm, symmetries are exploited such that along each branch symmetry transformations are performed based on Schur's lemma. As a consequence, symmetry breaking or symmetry preserving *higher order* bifurcations often just show up as *simple* generic or non-generic bifurcations and can be treated as such. Due to this property the algorithm is

considerably more robust than its predecessor ALCON2. In passing, dynamical stability of the solutions along each branch can be identified. In order to illustrate the kind of additional results available from SYMCON, we give a rather challenging illustrative example.

Example 5.4 *Hexagonal lattice dome.* This well-known challenging equivariant bifurcation problem from continuum mechanics is due to T.J. Healey [117]. It is known to contain a large number of all kinds of higher order singularities connected with symmetries of the mechanical construction, the most dominant of which is the symmetry D_6. The problem has been tackled by SYMCON [95] and is documented in detail in [94]. Figure 5.9 gives parts of the rather complex total bifurcation diagram associated with two different subsymmetries. As it turned out, the bifurcation diagram computed by SYMCON revealed hitherto unknown parts.

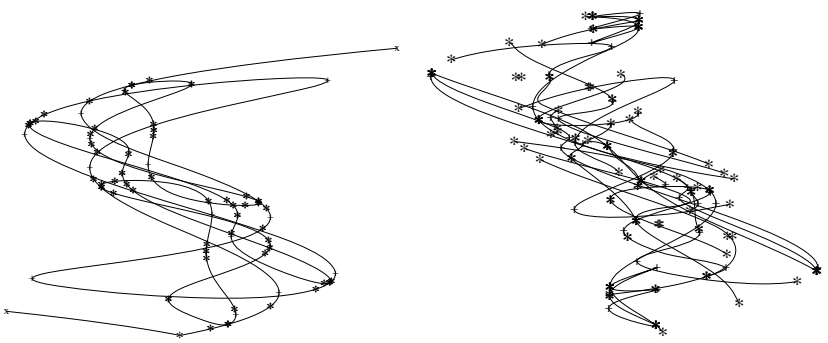

Fig. 5.9. Hexagonal lattice dome: Bifurcation subdiagrams associated with partial symmetries. *Left:* Kleinian group and D_6. *Right:* D_3 and Z_2^4.

Exercises

Exercise 5.1 Consider the *pseudo-arclength* continuation method as discussed at the beginning of Section 5.2.1. Study the effect of rescaling of the parameter

$$\lambda \longrightarrow \sigma = \lambda\kappa\,.$$

What kind of continuation method is obtained in the limiting case $\kappa \to 0$?

Exercise 5.2 Derive feasible stepsize bounds for the classical and the tangent Newton-continuation method using

a) the affine contravariant Newton-Mysovskikh theorem for the ordinary Newton method (Theorem 2.12),

b) the affine contravariant Newton-Kantorovich theorem for the simplified Newton method (Theorem 2.13).

c) On this theoretical basis, design computational estimates for use within an adaptive stepsize control strategy.

Exercise 5.3 *Classical continuation method for nonlinear least squares problems.* For given real parameter λ, let the prediction path be $\hat{x}(\lambda) = \overline{x}(0)$. In the residual based formulation of the Gauss–Newton method as given in Section 4.2, we write the homotopy for the path $\overline{x}(\lambda)$ as

$$\overline{P}(\overline{x}(\lambda), \lambda) F(\overline{x}(\lambda), \lambda) \equiv 0\,,$$

where

$$\overline{P}(x, \lambda) = F'(x, \lambda) F'(x, \lambda)^-\,, \quad \overline{P}^{\perp}(x, \lambda) = I_m - \overline{P}(x, \lambda)$$

are the corresponding projectors, assumed to be orthogonal.

a) Show that the classical continuation method is of order $p = 1$.

b) Derive an affine contravariant formula for the feasible stepsize.

c) Design an affine contravariant computational estimate for the order coefficient and consider details for the corresponding *adaptive* continuation algorithm.

Exercise 5.4 *Tangent continuation method for nonlinear least squares problems.* The notation is the same as in Exercise 5.3. The only new aspect is that the prediction path now reads

$$\hat{x}(\lambda) = \overline{x}(0) + \lambda \dot{\overline{x}}(0)\,.$$

a) We need an expression for the local path direction $\dot{\overline{x}}(0)$. Verify the result

$$F'(\overline{x}(0), 0)\dot{\overline{x}}(0) + F'(\overline{x}(0), 0)^{-T} F''(\overline{x}(0), 0)[\overline{P}^{\perp}(\overline{x}(0), 0) F(\overline{x}(0), 0), \dot{\overline{x}}(0)] =$$
$$- \left(\overline{P}(\overline{x}(0), 0) F_{\lambda}(\overline{x}(0), 0) + F'(\overline{x}(0), 0)^{-T} F'_{\lambda}(\overline{x}(0), 0)[\overline{P}^{\perp}(\overline{x}(0), 0) F(\overline{x}(0), 0) \right).$$

Hint: For the symmetric projector $\overline{P} = AA^-$ in terms of the generalized (inner) inverse A^- apply the formula

$$D\overline{P} = \overline{P}^{\perp}(DA)A^- + \left(\overline{P}^{\perp}(DA)A^-\right)^T$$

and, in addition, use special properties at $(\overline{x}(0), 0)$.

b) Show that under the assumption

$$\overline{P}^{\perp}(\overline{x}(\lambda),\lambda)F(\overline{x}(\lambda),\lambda) \equiv 0$$

the above equation shrinks to

$$\|F'(\overline{x}(0),0)\dot{\overline{x}}(0) + \overline{P}(\overline{x}(0),0)F_\lambda(\overline{x}(0),0)\| = \min\,,$$

which can be satisfied by

$$\dot{\overline{x}}(0) = -F'(\overline{x}(0),0)^- F_\lambda(\overline{x}(0),0)\,.$$

c) Discuss the necessary steps to be taken toward an *adaptive* tangent continuation algorithm.