AUGMENTED SYSTEMS FOR THE COMPUTATION OF SINGULAR POINTS IN BANACH SPACE PROBLEMS

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Abstract. We give a family of augmented systems as well as minimally extended systems which are suitable for the numerical detection and determination of singular points of Banach space problems. The systems are constructed in such a way that they only differ in a small part which must be adapted to the equivalence class to which the desired singular point belongs. The presented general results are specialized to the case of two-point boundary value problems.

Key words. Singular points, augmented systems, minimally extended systems, Lyapunov-Schmidt reduction, Fredholm operators, two-point boundary value problems.

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1. Introduction. In this paper, we consider the numerical determination of singular points of equations

$$T(x,\tau,\alpha)=0, \quad T: D \to Y, \quad D \subseteq X \times \mathbb{R}^p \times \mathbb{R}^q \text{ open}, \quad p,q \geq 0, \tag{1}$$

i. e., solutions $(x^0,\tau^0,\alpha^0) \in D$ where the Fréchet derivative $T_x(x^0,\tau^0,\alpha^0): X \to Y$ has a nontrivial corange. The last about fifteen years have seen a rapid development of so-called augmented systems and test functions for the detection and computation of such singular points. In the beginning, the main focus was on the treatment of special (simpler) singular points (see, e. g., [24, 27, 25, 26, 29, 30, 33]) whereas later general concepts of handling singular points became more important (see, e. g., [4, 5, 6, 13, 19, 21, 22, 28]). Most papers deal with (1) only in finite dimensional or Hilbert spaces although one can also find results for problems in Banach spaces (see, e. g., [1, 7, 8, 10, 11, 14]). In a simplified way one can state that the more general the approach is with respect to the kind of singular points the more restricted it is with respect to the kind of spaces. One may argue that any numerical approach will discretize (1) and solve the discrete problem. But the main problem will then be whether this discrete problem will catch the occurrence of singular points at least with some well-behaved perturbations. Typical results show convergence of the singular point of the discrete problem to the singular point of the true problem in a given sense provided a measure of the coarseness of the discretization tends to zero (see, e. g., [7]). This may not be a problem when we are just computing a singular point because we are then dealing with only one discrete problem. A more critical situation is when we follow a path of solutions and want to detect singular points. Using for example collocation for the solution of boundary value problems for ordinary differential equations, it is necessary to adapt the grid with respect to the actual solution in order to control the discretization error, see [3]. Therefore the normal situation during pathfollowing is that two successive solutions on the path correspond to two different grids. If one now computes the test functions that belong to the discrete problems, we cannot compare them because they

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are not related to the same discrete problem. Consequently, this would be a rather unreliable if not false method to detect singular points. On the other hand, trying to keep the grid for two successive points on the path and adapting the grid after the computation of the test function (and then adapting grid and recomputing the solution and the test function for the new grid) can lead to enormous discretization errors which would mean that we are far off the solution branch of the continuous problem and its bifurcation behaviour. The only way out of such problems is to construct test functions for the detection of special kinds of singular points and augmented systems for their computation (see [23] which shows in the finite dimensional case that the construction of augmented systems actually includes the construction of test functions) directly for Banach space problems and to include the evaluation of the test functions into the path following routine and therefore into the grid generation.

For these reasons we consider more specifically the following problem. Let X and Y in (1) be (real) Banach spaces and let T be infinitely often Fréchet differentiable (cf. [12]). Moreover, let $T_x(x,\tau,\alpha)$ be a Fredholm operator with index

$$l := \operatorname{ind} T_x(x,\tau,\alpha) \geq 0 \tag{2}$$

for all $(x,\tau,\alpha) \in D$. A singular point of (1) then is a solution (x^0,τ^0,α^0) of (1) where

$$k := \operatorname{codim} \operatorname{range} L \geq 1, \quad L := T_x(x^0,\tau^0,\alpha^0). \tag{3}$$

The aim of the present paper is now to develop augmented systems and test functions for the detection and determination of such singular points. In particular, we show that the approach of [23] given for finite dimensional problems can be extended to the above case. More specifically, we show that the main results of [23] based on a graph representation of derivatives can also applied here. For this we first outline the basic analytical concept for singular points in the form of the Lyapunov-Schmidt reduction in Section 2. In Section 3 we discuss a family of augmented systems and test functions. We then apply our approach to two-point boundary value problems for ordinary differential equations in Section 4.

2. Lyapunov-Schmidt reduction. In this section, we discuss the basic concept of the analytical treatment of singular points, namely the Lyapunov-Schmidt reduction, and by this way introduce the necessary notation. Since this paper heavily depends on results of [23] we try to mimic the notation used there as far as possible.

Utilizing that L is a Fredholm operator, the Lyapunov-Schmidt reduction allows for replacing the given problem (1) by a finite dimensional one. Let

$$X_0 := \operatorname{kernel} L, \quad Y_1 := \operatorname{range} L. \tag{4}$$

Since X_0 is finite dimensional and Y_1 is closed, there are closed complements X_1 and Y_0 such that

$$X_0 \oplus X_1 = X, \quad Y_0 \oplus Y_1 = Y. \tag{5}$$

Because of $\dim X_0 = k + l$ and $\dim Y_0 = k$, we can choose bases according to

$$X_0 = \operatorname{span}\{t_1^0, \ldots, t_{k+l}^0\}, \quad Y_0 = \operatorname{span}\{z_1^0, \ldots, z_k^0\}. \tag{6}$$

Since X_0 and Y_0 have closed complements, we can find linear forms $\varphi_1^0, \ldots, \varphi_{k+l}^0 \in X^*$ and $\psi_1^0, \ldots, \psi_k^0 \in Y^*$ satisfying

$$\begin{array}{lll} \varphi_i^0(t_{i'}^0) = \delta_{ii'}, & \varphi_i^0(X_1) = \{0\}, & i, i' = 1, \ldots, k+l, \\ \psi_j^0(z_{j'}^0) = \delta_{jj'}, & \psi_j^0(Y_1) = \{0\}, & j, j' = 1, \ldots, k. \end{array} \tag{7}$$

Here and in the sequel we use a superscript "*" to denote the dual space or the dual operator.

Following [23], we must show that there is a Lyapunov-Schmidt reduction leading to a special inverse involved in the determination of derivatives of the finite dimensional problem we aim at.

THEOREM 2.1. *Let $\tilde{X} := X \times \mathbb{R}^k$ and $\tilde{Y} := Y \times \mathbb{R}^{k+l}$ and let the linear operator $\tilde{L}\colon \tilde{X} \to \tilde{Y}$ be defined by*

$$\tilde{L}(x,u) := (Lx + \tilde{z}u, \tilde{\varphi}(x)) = (Lx + \sum_{j=1}^{k} u_j \tilde{z}_j, (\tilde{\varphi}_1(x), \ldots, \tilde{\varphi}_{k+l}(x))), \tag{8}$$

where $\tilde{\varphi}_1, \ldots, \tilde{\varphi}_{k+l} \in X^*$ and $\tilde{z}_1, \ldots, \tilde{z}_k \in Y$. Furthermore, let

$$\tilde{\varphi}(t^0) = (\tilde{\varphi}_i(t_{i'}^0))_{i,i'=1,\ldots,k+l},\ \psi^0(\tilde{z}) = (\psi_j^0(\tilde{z}_{j'}))_{j,j'=1,\ldots,k} \text{ nonsingular} \tag{9}$$

hold. Then $\tilde{L}$ is a linear homeomorphism and $L^-\colon Y \to X$ defined by

$$L^- y := P_X \tilde{L}^{-1}(y,0) = P_X \tilde{L}^{-1} I_Y y, \tag{10}$$

where P_X and I_Y are the canonical projection and inclusion connected with the above direct products defining $\tilde{X}$ and $\tilde{Y}$, is a generalized inverse of L satisfying

$$LL^-L = L, \quad L^-LL^- = L^- \tag{11}$$

and

$$L^-\tilde{z} = 0, \quad \tilde{\varphi}L^- = 0. \tag{12}$$

Proof. Since continuity of $\tilde{L}$ is trivial, it is sufficient for the first part of the claim to show bijectivity of $\tilde{L}$. For this let $(y,v) \in \tilde{Y}$. We now must solve

$$Lx + \tilde{z}u = y, \quad \tilde{\varphi}(x) = v \tag{13}$$

for (x,u). With $t^0 = (t_1^0, \ldots, t_{k+l}^0)$ and $s \in \mathbb{R}^{k+l}$ the element $x \in X$ can be represented in the form

$$x = t^0 s + x_1, \tag{14}$$

where $x_1 \in X_1$. Substituting (14) into (13) yields

$$Lx_1 = y - \tilde{z}u, \quad \tilde{\varphi}(t^0)s = v - \tilde{\varphi}(x_1). \tag{15}$$

The first equation is solvable if

$$\psi^0(y - \tilde{z}u) = 0.$$

Since $\psi^0(\tilde{z})$ is nonsingular, we obtain

$$u = \psi^0(\tilde{z})^{-1}\psi^0(y).$$

Thus, there exists a unique solution $x_1 = L_1^{-1}(y - \tilde{z}u)$, where L_1^{-1} denotes the inverse of $L_1 : X_1 \to Y_1$ with $L_1 w := Lw$ for $w \in X_1$. The vector s is uniquely determined by the second equation in (15) as

$$s = \tilde{\varphi}(t^0)^{-1}(v - \tilde{\varphi}(x_1)).$$

Substituting x_1 and s into equation (14), we find

$$(x,u) = \tilde{L}^{-1}(y,v) \Longleftrightarrow \begin{cases} x = t^0\tilde{\varphi}(t^0)^{-1}(v - \tilde{\varphi}(L_1^{-1}(y - \tilde{z}u))) + L_1^{-1}(y - \tilde{z}u) \\ u = \psi^0(\tilde{z})^{-1}\psi^0(y) \end{cases}$$

and

$$x = L^- y \Longleftrightarrow x = L_1^{-1}(y - \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0(y)) - t^0\tilde{\varphi}(t^0)^{-1}\tilde{\varphi}(L_1^{-1}(y - \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0(y))).$$

Since the projection P_X and the inclusion I_Y are related to a product of closed spaces, they are continuous and so is L^-. Applying L^- on $\tilde{z}_j$ gives $u = e_j^{(k)}$, where $e_j^{(k)}$ denotes the j-th canonical basis vector of of $\mathbb{R}^k$, and therefore $x = 0$, hence $L^-\tilde{z}_j = 0$. Applying $\tilde{\varphi}_i$ on $L^- y$ with arbitrary $y \in Y$ gives $\tilde{\varphi}_i(L^- y) = 0$, hence $\tilde{\varphi}_i L^- = 0$. Because of

$$LL^- y = y - \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0(y)$$

we have $LL^-Lx = Lx$ for arbitrary $x \in X$ implying L^- is an inner inverse of L, i. e., $LL^-L = L$. Applying L^- on $LL^- y$ yields

$$u = \psi^0(\tilde{z})^{-1}\psi^0(y - \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0(y)) = 0$$

and therefore

$$L^-LL^- y = L_1^{-1}(y - \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0(y)) - t^0\tilde{\varphi}(t^0)^{-1}\tilde{\varphi}(L_1^{-1}(y - \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0(y))) = L^- y$$

for arbitrary $y \in Y$ implying L^- to be an outer inverse of L, i. e., $L^-LL^- = L^-$. □

Thus we want to choose the Lyapunov-Schmidt reduction in such a way that the inverse involved is given by L^- with some selected $\tilde{\varphi}$ and $\tilde{z}$ satisfying (9).

LEMMA 2.2. *Let $\hat{P}: X_1 \to X$ and $\hat{Q}: Y \to Y_1$ be defined by*

$$\hat{P} := (\mathrm{id}_X - t^0\tilde{\varphi}(t^0)^{-1}\tilde{\varphi})I_{X_1}, \quad \hat{Q} := P_{Y_1}(\mathrm{id}_Y - \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0) \tag{16}$$

where P_{Y_1} and I_{X_1} are the canonical projection and inclusion connected with the direct sums (5). Then the operators

$$\hat{U}: Y \to Y_1 \times \mathbb{R}^k, \quad y \mapsto (\hat{Q}y, \psi^0(y)) \tag{17}$$

and

$$\hat{V}: X_1 \times \mathbb{R}^{k+l} \to X, \quad (\hat{\xi}, \xi) \mapsto \hat{P}\hat{\xi} + t^0\xi \tag{18}$$

are linear homeomorphisms.

Proof. Again continuity is trivially given and it remains to show bijectivity. For $\hat{U}$ we must solve

$$\hat{Q}y = w, \quad \psi^0(y) = u$$

for arbitrary $w \in Y_1$ and $u \in \mathbb{R}^k$. With the splitting $y = z^0 r + y_1$ with some $r \in \mathbb{R}^k$ and $y_1 \in Y_1$ we obtain

$$\hat{Q}(z^0 r + y_1) = w, \quad \psi^0(z^0)r + \psi^0(y_1) = u,$$

hence $r = u - \psi^0(y_1)$. It therefore remains

$$\hat{Q}(y_1 - z^0\psi^0(y_1) + z^0 u) = w.$$

Inserting the definition of $\hat{Q}$ gives

$$P_{Y_1}(\mathrm{id}_Y - \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0)(y_1 - z^0\psi^0(y_1) + z^0 u) = w$$

or

$$P_{Y_1}(y_1 - z^0\psi^0(y_1) + z^0 u - \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0(z^0)u) = w.$$

This finally reduces to

$$y_1 - P_{Y_1}\tilde{z}\psi^0(\tilde{z})^{-1}u = w$$

with the unique solution

$$y_1 = w + P_{Y_1}\tilde{z}\psi^0(\tilde{z})^{-1}u \in Y_1$$

showing bijectivity of $\hat{U}$. For $\hat{V}$ we must solve

$$\hat{P}\hat{\xi} + t^0\xi = x$$

for arbitrary $x \in X$. Applying $\tilde{\varphi}$ yields $\tilde{\varphi}(t^0)\xi = \tilde{\varphi}(x)$ or $\xi = \tilde{\varphi}(t^0)^{-1}\tilde{\varphi}(x)$. It remains

$$\hat{P}\hat{\xi} = x - t^0\tilde{\varphi}(t^0)^{-1}\tilde{\varphi}(x)$$

or

$$Lx = L\hat{P}\hat{\xi} = LI_{X_1}\hat{\xi} = L_1\hat{\xi}$$

with the unique solution $\hat{\xi} = L_1^{-1}Lx \in X_1$ showing bijectivity of $\hat{V}$ as well. □

The preceeding lemma states that (1) in the simplified form

$$T(x, \lambda) = 0$$

with $\lambda := (\tau, \alpha)$ is equivalent to

$$\hat{Q}T(\hat{P}\hat{\xi} + t^0\xi, \lambda) = 0, \quad \psi^0 T(\hat{P}\hat{\xi} + t^0\xi, \lambda) = 0. \tag{19}$$

The Fréchet derivative $J: X_1 \to Y_1$ of the first equation with respect to $\hat{\xi}$ in (x^0, λ^0) is given by

$$J = \hat{Q} L \hat{P} = P_{Y_1}(\mathrm{id}_Y - \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0) L (\mathrm{id}_X - t^0\tilde{\varphi}(t^0)^{-1}\tilde{\varphi}) I_{X_1} = \tag{20}$$

Hence J is a linear homeomorphism. Due to the implicit function theorem we can locally solve the first equation for $\hat{\xi}$ obtaining a unique solution of the form

$$\hat{\xi} = \hat{\xi}^0(\xi, \lambda). \tag{21}$$

Inserting into the second equation yields the so-called reduced function

$$h: \tilde{D} \to \mathbb{R}^k, \quad h(\xi, \lambda) := \psi^0 T(\hat{P}\hat{\xi}^0(\xi, \lambda) + t^0\xi, \lambda), \quad \tilde{D} \subseteq \mathbb{R}^{k+l} \times \mathbb{R}^{p+q} \text{ open.} \tag{22}$$

Hence we have indeed reduced (1) to a finite dimensional problem $h(\xi, \lambda) = 0$ which is completely singular, because of $h_\xi(\xi^0, \lambda^0) = 0$ where $(\hat{\xi}^0, \xi^0) := \hat{V}^{-1}(x^0)$.

Since there is no unique reduced function h associated with the original function T due to the choice of the splitting, there is a second concept called contact equivalence such that all reduced functions of T belong to the same equivalence class. The aim of singularity theory is then to decide to what class a given reduced function belongs. This is done with the help of the values of some combinations of derivatives of h evaluated at (ξ^0, λ^0). Here it also becomes important to distinguish between bifurcation parameters τ and unfolding parameters α. For details see [12] and [23].

To apply the results of [23] we must now show that the derivatives of h at (ξ^0, λ^0) have the same structure as in the finite dimensional case. To determine the derivatives of h at (ξ^0, λ^0) we set $x^0(\xi, \lambda) := \hat{P}\hat{\xi}^0(\xi, \lambda) + t^0\xi$ and obtain

$$\begin{aligned} x^0_\xi(\xi, \lambda)(a_1) &= \hat{P}\hat{\xi}^0_\xi(\xi, \lambda)(a_1) + t^0 a_1, \\ x^0_\lambda(\xi, \lambda)(b_1) &= \hat{P}\hat{\xi}^0_\lambda(\xi, \lambda)(b_1) \end{aligned} \tag{23}$$

and so on. Here and in the following we write down the derivative tensors as multilinear mappings. Because of $\tilde{\varphi}\hat{P} = 0$, we in general have for a derivative v of x^0 evaluated at (ξ^0, λ^0)

$$\tilde{\varphi}(v) = r_d \tag{24}$$

with a residual r_d which is nontrivial only for $v = x^0_\xi(\xi, \lambda)(a_1)$. To proceed we set $\overline{T}(\xi, \lambda) := T(x^0(\xi, \lambda), \lambda)$ and compute

$$\begin{aligned} \overline{T}_\xi(\xi, \lambda)(a_1) &= T_x(x^0(\xi, \lambda), \lambda)(x^0_\xi(\xi, \lambda)(a_1)), \\ \overline{T}_\lambda(\xi, \lambda)(b_1) &= T_x(x^0(\xi, \lambda), \lambda)(x^0_\lambda(\xi, \lambda)(b_1)) + T_\lambda(x^0(\xi, \lambda), \lambda)(b_1) \end{aligned} \tag{25}$$

and so on. Evaluating at (ξ^0, λ^0) yields relations of the form

$$\hat{Q} L v = \hat{Q} r_v \tag{26}$$

with some residual r_v since v occurs in (25) for the first time together with the operator $L = T_x(x^0(\xi^0, \lambda^0), \lambda^0)$.

Setting

$$d := \psi^0(\tilde{z})^{-1}\psi^0(r_v)$$

yields

$$Lv + \tilde{z}d - r_v = Lv + \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0(r_v) - r_v.$$

Applying $\hat{U}$ on the right hand side gives

$$\hat{U}(Lv + \tilde{z}\psi^0(\tilde{z})^{-1}\psi^0(r_v) - r_v) = (\hat{Q}Lv - \hat{Q}r_v, \psi^0(r_v) - \psi^0(r_v)).$$

The equation $\hat{Q}Lv = \hat{Q}r_v$ is therefore equivalent to $Lv + \tilde{z}d = r_v$ such that v and d satisfy

$$Lv + \tilde{z}d = r_v, \quad \tilde{\varphi}(v) = r_d$$

or

$$\tilde{L}(v,d) = (r_v, r_d) \tag{27}$$

with the solution

$$v = t^0\tilde{\varphi}(t^0)^{-1}(r_d - \tilde{\varphi}(L_1^{-1}(r_v - \tilde{z}d))) + L_1^{-1}(r_v - \tilde{z}d).$$

Because of

$$L^- r_v = L_1^{-1}(r_v - \tilde{z}d) - t^0\tilde{\varphi}(t^0)^{-1}\tilde{\varphi}(L_1^{-1}(r_v - \tilde{z}d))$$

we finally obtain

$$v = L^- r_v + t^0\tilde{\varphi}(t^0)^{-1}r_d. \tag{28}$$

This shows that the tree-based representation of the derivatives of h evaluated at (ξ^0, λ^0), which has been developed in [23], can be applied with the pure notational replacements

$$f \to T,\ x^* \to x^0,\ \lambda^* \to \lambda^0,\ t^* \to t^0,\ z^{*T} \to \psi^0,\ \tilde{t}^T \to \tilde{\varphi}. \tag{29}$$

3. Augmented systems. In [23] the tree-based representation of the derivatives of a reduced function is used to show that a certain augmented system is suitable for the computation of every singular point whose reduced problem belongs to a certain equivalence class. In this section we are going to show that this procedure can be carried over to Banach space problems of the form (1). The augmented systems of choice are

$$\begin{array}{l} T_x(x,\lambda)t_i + \tilde{z}\beta_i = 0, \quad \tilde{\varphi}(t_i) = e_i^{(k+l)}, \quad i = 1,\ldots,k+l, \\ \psi_j T_x(x,\lambda) + \tilde{\varphi}\gamma_j = 0, \quad \psi_j(\tilde{z}) = e_j^{(k)}, \quad j = 1,\ldots,k, \\ T(x,\lambda) = 0, \\ b(x,\lambda,t,\psi) = 0 \end{array} \tag{30}$$

or briefly $F(u) = 0$ with the unknowns $u := (x, \lambda, t, \psi, \beta, \gamma)$ and F maps an open subset of $X \times \mathbb{R}^{p+q} \times X^{k+l} \times Y^{*k} \times \mathbb{R}^{k,k+l} \times \mathbb{R}^{k+l,k}$ into $Y^{k+l} \times \mathbb{R}^{(k+l)^2} \times Y^{*k} \times \mathbb{R}^{k^2} \times Y \times \mathbb{R}^{l+p+q}$. The condition given by b depends on the equivalence class associated with the singular point to be computed.

We first must derive a condition when a solution of (30) is regular.

THEOREM 3.1. *Let $u^0 := (x^0, \lambda^0, t^0, \psi^0, \beta^0, \gamma^0)$ be a perfect solution of $F(u) = 0$, i. e., $\beta^0 := 0$, $\gamma^0 := 0$, and let $\tilde{\varphi}$ and $\tilde{z}$ satisfy (9). Furthermore, let M be the Fréchet derivative of F at u^0. Then M is a linear homeomorphism if and only if the square matrix*

$$W := \begin{bmatrix} 0 & \psi^0 P \\ B & R \end{bmatrix} \tag{31}$$

of size $k + l + p + q$ is nonsingular where

$$P := T_\lambda(x^0, \lambda^0), \quad B := \overline{B} t^0, \quad R := \overline{R} - \overline{B} L^- P \tag{32}$$

and $\overline{B}\colon X \to \mathbb{R}^{l+p+q}$, $\overline{R}\colon \mathbb{R}^{p+q} \to \mathbb{R}^{l+p+q}$ are given by

$$\begin{aligned}
\overline{B}\,\overline{x} := {} & \frac{\partial b}{\partial x}(x^0, \lambda^0, t^0, \psi^0)(\overline{x}) - \sum_{i=1}^{k+l} \frac{\partial b}{\partial t_i}(x^0, \lambda^0, t^0, \psi^0)(L^- T_{xx}(x^0, \lambda^0)(t_i^0, \overline{x})) - \\
& - \sum_{j=1}^{k} \psi_j^0 T_{xx}(x^0, \lambda^0)(L^- \frac{\partial b}{\partial \psi_j}(x^0, \lambda^0, t^0, \psi^0)^*(\cdot), \overline{x}), \\
\overline{R}\,\overline{\lambda} := {} & \frac{\partial b}{\partial \lambda}(x^0, \lambda^0, t^0, \psi^0)(\overline{\lambda}) - \sum_{i=1}^{k+l} \frac{\partial b}{\partial t_i}(x^0, \lambda^0, t^0, \psi^0)(L^- T_{x\lambda}(x^0, \lambda^0)(t_i^0)(\overline{\lambda})) - \\
& - \sum_{j=1}^{k} \psi_j^0 T_{x\lambda}(x^0, \lambda^0)(L^- \frac{\partial b}{\partial \psi_j}(x^0, \lambda^0, t^0, \psi^0)^*(\cdot))(\overline{\lambda}).
\end{aligned} \tag{33}$$

Proof. Without loss of generality we can assume that

$$\begin{array}{lll}
L t_i^0 = 0, & \tilde{\varphi}(t^0) \text{ nonsingular}, & \varphi^0(t^0) = I_{k+l}, \\
L^* \psi_j^0 = 0, & \psi^0(\tilde{z}) \text{ nonsingular}, & \psi^0(z^0) = I_k.
\end{array}$$

The Fréchet derivative M is given by

$$\begin{aligned}
M\overline{u} = {} & (\operatorname{row}(\tilde{L}(\overline{t}_i, \overline{\beta}_i) + (T_{xx}(x^0, \lambda^0)(t_i^0, \overline{x}), 0) + (T_{x\lambda}(x^0, \lambda^0)(t_i^0)(\overline{\lambda}), 0)), \\
& \operatorname{row}((\overline{\psi}_j, \overline{\gamma}_j)\tilde{L} + (\psi_j^0 T_{xx}(x^0, \lambda^0)(\cdot, \overline{x}), 0) + (\psi_j^0 T_{x\lambda}(x^0, \lambda^0)(\cdot)(\overline{\lambda}), 0)), \\
& L\overline{x} + P\overline{\lambda}, \\
& \frac{\partial b}{\partial x}(x^0, \lambda^0, t^0, \psi^0)(\overline{x}) + \frac{\partial b}{\partial \lambda}(x^0, \lambda^0, t^0, \psi^0)(\overline{\lambda}) + \\
& \quad + \sum_{i=1}^{k+l} \frac{\partial b}{\partial t_i}(x^0, \lambda^0, t^0, \psi^0)(\overline{t}_i) + \sum_{j=1}^{k} \frac{\partial b}{\partial \psi_j}(x^0, \lambda^0, t^0, \psi^0)(\overline{\psi}_j)).
\end{aligned}$$

Since continuity of M is trivial, it is sufficient to show that $M\overline{u} = r$ is uniquely solvable for arbitrary right hand sides r. Let

$$r =: (\operatorname{row}(r_{t_i}, r_{m_i}), \operatorname{row}(r_{\psi_j}, r_{n_j}), r_f, r_b).$$

From the first two blocks we obtain

$$\begin{aligned}
(\overline{t}_i, \overline{\beta}_i) &= \tilde{L}^{-1}(r_{t_i} - T_{xx}(x^0, \lambda^0)(t_i^0, \overline{x}) - T_{x\lambda}(x^0, \lambda^0)(t_i^0)(\overline{\lambda}), r_{m_i}), \\
(\overline{\psi}_j, \overline{\gamma}_j) &= (\tilde{L}^*)^{-1}(r_{\psi_j} - \psi_j^0 T_{xx}(x^0, \lambda^0)(\cdot, \overline{x}) - \psi_j^0 T_{x\lambda}(x^0, \lambda^0)(\cdot)(\overline{\lambda}), r_{n_j})
\end{aligned}$$

using that the dual operator $\tilde{L}^*: Y^* \times \mathbb{R}^{k+l} \to X^* \times \mathbb{R}^k$ of the linear homeomorphism $\tilde{L}$ given by

$$\tilde{L}^*(\psi, v) = (L^*\psi + \tilde{\varphi}v, \psi(\tilde{z}))$$

is a linear homeomorphism as well. Projecting onto the first components yields

$$\begin{aligned}\overline{t}_i &= \hat{r}_{t_i} - P_X \tilde{L}^{-1} I_Y (T_{xx}(x^0, \lambda^0)(t_i^0, \overline{x}) + T_{x\lambda}(x^0, \lambda^0)(t_i^0)(\overline{\lambda})),\\ \overline{\psi}_j &= \hat{r}_{\psi_j} - P_{Y^*}(\tilde{L}^*)^{-1} I_{X^*}(\psi_j^0 T_{xx}(x^0, \lambda^0)(\cdot, \overline{x}) + \psi_j^0 T_{x\lambda}(x^0, \lambda^0)(\cdot)(\overline{\lambda}))\end{aligned}$$

with

$$\hat{r}_{t_i} := P_X \tilde{L}^{-1}(r_{t_i}, r_{m_i}), \quad \hat{r}_{\psi_j} := P_{Y^*}(\tilde{L}^*)^{-1}(r_{\psi_j}, r_{n_j}).$$

Hence the system under consideration reduces to a system of the form

$$L\overline{x} + P\overline{\lambda} = r_f, \quad \overline{B}\overline{x} + \overline{R}\,\overline{\lambda} = \hat{r}_b$$

when we in addition use the fact that

$$(P_{Y^*}(\tilde{L}^*)^{-1} I_{X^*})^* \mid_Y = P_X \tilde{L}^{-1} I_Y = L^-.$$

Writing $\overline{x}$ in the form $\overline{x} = t^0\overline{s} + \overline{x}_1$ with $\overline{s} \in \mathbb{R}^{k+l}$ and $\overline{x}_1 \in X_1$ yields

$$L\overline{x}_1 + P_{Y_1} P\overline{\lambda} = P_{Y_1} r_f, \quad \psi^0 P\overline{\lambda} = \psi^0(r_f), \quad \overline{B}\overline{x}_1 + \overline{B}t^0\overline{s} + \overline{R}\,\overline{\lambda} = \hat{r}_b.$$

With $\overline{x}_1 = L_1^{-1} P_{Y_1}(r_f - P\overline{\lambda})$ from the first equation we obtain

$$\psi^0 P\overline{\lambda} = \psi^0(r_f), \quad \overline{B}t^0\overline{s} + (\overline{R} - \overline{B}L_1^{-1}P_{Y_1}P)\overline{\lambda} = \hat{r}_b - L_1^{-1}P_{Y_1}r_f.$$

Shifting according to $\overline{s} = \overline{s}_c + C\overline{\lambda}$ replaces this system by

$$\psi^0 P\overline{\lambda} = \psi^0(r_f), \quad \overline{B}t^0\overline{s}_c + (\overline{R} - \overline{B}(L_1^{-1}P_{Y_1}P - t^0C))\overline{\lambda} = \hat{r}_b - L_1^{-1}P_{Y_1}r_f.$$

Because of the special shape of L^- we can choose the matrix C in such a way that the system takes the form

$$\psi^0 P\overline{\lambda} = \psi^0(r_f), \quad \overline{B}t^0\overline{s}_c + (\overline{R} - \overline{B}L^-P)\overline{\lambda} = \hat{r}_b - L_1^{-1}P_{Y_1}r_f.$$

The claim is now evident. □

We observe that the structure of $\overline{B}$ and $\overline{R}$ is the same as in the finite dimensional case. The only differences are the replacements (29). This yields that the tree-based theory of [23] can be directly applied on the augmented systems (30) for Banach space problems. Again only the replacements (29) have to be executed.

REMARK 3.2. We obtain suitable minimally extended systems

$$T(x, \lambda) = 0, \quad \hat{b}(x, \lambda) = 0 \tag{34}$$

when we take b from a suitable augmented system (30) and define the test function $\hat{b}: X \times \mathbb{R}^{p+q} \to \mathbb{R}^{l+p+q}$ by

$$\hat{b}(x, \lambda) := b(x, \lambda, t(x, \lambda), \psi(x, \lambda)) \tag{35}$$

with

$$t_i(x,\lambda) := P_X \tilde{L}(x,\lambda)^{-1} I_{\mathbb{R}^{k+l}} e_i^{(k+l)}, \quad \psi_j(x,\lambda) := P_{Y^*}(\tilde{L}(x,\lambda)^*)^{-1} I_{\mathbb{R}^k} e_j^{(k)} \tag{36}$$

and

$$\tilde{L}(x,\lambda)(\overline{x},\overline{u}) := (T_x(x,\lambda)\overline{x} + \tilde{x}\,\overline{u}, \tilde{\varphi}(\overline{x})). \tag{37}$$

EXAMPLE 3.3. Applying (29) on the function b obtained in [23] as part of a suitable augmented system for the computation of turning points, we obtain (with $k=1$, $l=0$, $p=1$, $q=0$)

$$b(x,\tau,t,\psi) = \psi T_x(x,\tau)t. \tag{38}$$

Because $b(x,\tau,t,\psi)=0$ implies $\beta=\gamma=0$, the augmented system (30) can be reduced to

$$T_x(x,\tau)t = 0, \quad \tilde{\varphi}(t) = 1, \quad T(x,\tau) = 0, \tag{39}$$

which is due to Seydel [29]. The corresponding test function reads

$$\hat{b}(x,\tau) = (P_{Y^*}(\tilde{L}(x,\tau)^*)^{-1}(0,1))T_x(x,\tau)(P_X\tilde{L}(x,\tau)^{-1}(0,1)). \tag{40}$$

4. Application to boundary value problems. In this section we want to apply the theory of the previous section on two-point boundary value problems

$$\frac{dx(s)}{ds} =: x' = f(s,x,\lambda), \quad a \le s \le b, \quad r(x(a),x(b),\lambda) = 0 \tag{41}$$

with f and r sufficiently smooth. In particular we want to specialize the structure of the augmented system (30) to (41) such that we may apply standard numerical methods for its solution. To avoid a conflict in the notation of the right boundary of the integration interval and the additional equations in the augmented systems, we denote the latter ones by $\hat{b}$ throughout this section.

Setting $X = C^1([a,b],\mathbb{R}^n)$ and $Y = C^0([a,b],\mathbb{R}^n)\times\mathbb{R}^m$ (i. e., n differential equations and m boundary conditions), we obtain (41) in the operator form $T(x,\lambda)=0$ with $T\colon D \to Y$, $D \subseteq X \times \mathbb{R}^{p+q}$ open, defined by

$$T(x,\lambda) := (x' - f(s,x,\lambda), r(x(a),x(b),\lambda)). \tag{42}$$

Here the term $x' - f(s,x,\lambda)$ for given (x,λ) shall stand for the function with values $x'(s) - f(s,x(s),\lambda)$. Similar notations are also used in the sequel.

The Fréchet derivative $T_x(x,\lambda)\colon X \to Y$ of T at $(x,\lambda)\in D$ is given by

$$T_x(x,\lambda)v := (v' - f_x(s,x,\lambda)v, r_{x_a}(x(a),x(b),\lambda)v(a) + r_{x_b}(x(a),x(b),\lambda)v(b)). \tag{43}$$

where r_{x_a} and r_{x_b} shall denote the partial derivatives of r with respect to the first and second argument, respectively.

To investigate the special properties of $T_x(x,\lambda)$, we must have a closer look at linear two-point boundary value problems. For this, we consider (with a new, more appropriate notation) the linear operator $L: X \to Y$ defined by

$$Lx := (g,r) := (x' - J(s)x, Ax(a) + Bx(b)), \tag{44}$$

where $J:[a,b] \to \mathbb{R}^{n,n}$ is continuous and $A, B \in \mathbb{R}^{m,n}$.

THEOREM 4.1. *The operator $L: X \to Y$ defined by (43) is a Fredholm operator with index* $\operatorname{ind} L = n - m$.

Proof. Although the stated result is well-known (see, e. g., [18, 31]), we present here the explicit construction of the kernel and range of L for later use omitting as usual the trivial proof of continuity and also the proof of the closedness of the range.

For the kernel we must determine all solutions of $Lx = 0$ or

$$x' - J(s)x = 0, \quad Ax(a) + Bx(b) = 0.$$

Let $W(s,s_0)$ denote the Wronskian matrix (or fundamental solution matrix) of the homogeneous differential equation defined by $W'(s,s_0) = J(s)W(s,s_0)$, $W(s_0,s_0) = I$, $s_0 \in [a,b]$ (see, e.g., [2, 32]). Then, all solutions of this equation have the form $x(s) = W(s,a)x(a)$. Inserting this expression into the boundary condition yields

$$Ex(a) = 0, \quad E := A + BW(b,a))$$

such that E is a matrix of size (m,n). Hence we have

$$\operatorname{kernel} L = \{t \in X \mid t(s) = W(s,a)t(a),\ t(a) \in \operatorname{kernel} E\}$$

and

$$\dim \operatorname{kernel} L = \dim \operatorname{kernel} E < \infty.$$

The range of L consists of all pairs $(g,r) \in Y$, for which

$$x' - J(s)x = g, \quad Ax(a) + Bx(b) = r$$

has a solution. With the help of the Wronskian matrix all solutions of the inhomogeneous differential equation are given by

$$x(s) = W(s,a)x(a) + \int_a^s W(s,u)g(u)\,du.$$

Inserting this expression into the boundary condition yields

$$Ew(a) = r - \int_a^b BW(b,s)g(s)\,ds.$$

Hence, there can only be a solution if the right hand side lies in the range of E. Thus we have

$$\operatorname{range} L = \{(g,r) \in Y \mid r \in v + \operatorname{range} E, \quad v := \int_a^b BW(b,s)g(s)\,ds\}.$$

Given $(g,r) \in Y$, we can write r uniquely as

$$r = v + e_0 + e_1$$

with v as above and $e_0 \in \operatorname{corange} E := \operatorname{kernel} E^T$ and $e_1 \in \operatorname{range} E$. With this, the decomposition

$$(g, r) = (g, v + e_1) + (0, e_0)$$

implies $Y = Y_0 \oplus Y_1$ where

$$Y_0 := \{0\} \times \operatorname{corange} E, \quad Y_1 := \operatorname{range} L.$$

In particular, we have

$$\operatorname{codim} \operatorname{range} L = \dim \operatorname{corange} E < \infty.$$

Both parts together yield

$$\operatorname{ind} L = \dim \operatorname{kernel} L - \operatorname{codim} \operatorname{range} L = (n - \operatorname{rank} E) - (m - \operatorname{rank} E) = n - m.$$

□

Thus we have for (41) the setting

$$l = \operatorname{ind} L = n - m, \quad k = \operatorname{codim} \operatorname{range} L = \dim \operatorname{corange} E. \tag{45}$$

The problem of the general form (30) of the augmented systems for a numerical treatment lies in the occurrence of the k linear forms ψ_j. To bring them into a more suitable form we use the theory of the adjoint problems, see, e. g., [9, Ch. 11]. Consider the homogeneous boundary value problem

$$x' - J(s)x = 0, \quad Ax(a) + Bx(b) = 0 \tag{46}$$

with $A, B \in \mathbb{R}^{m,n}$ and $\operatorname{rank}(A, B) = m$. If $C, D \in \mathbb{R}^{2n-m,n}$ satisfy $\operatorname{rank}(C, D) = 2n-m$ and $AC^T = BD^T$, the homogeneous boundary value problem

$$y' + J(s)^T y = 0, \quad Cy(a) + Dy(b) = 0 \tag{47}$$

is said to be adjoint to (46). The central property of the adjoint problem is the following. If (46) possesses exactly $k + l$ linearly independent solutions, then the adjoint problem (47) possesses exactly k linearly independent solutions. To utilize this property, we try to construct the desired linear forms ψ in the form

$$\psi(g, r) := \int_a^b y(s)^T g(s)\, ds + w^T r \tag{48}$$

with some well-chosen $y \in X$ and $w \in \mathbb{R}^m$. The first requirement is that ψ vanishes on $\operatorname{range} L$. Taking a solution of the adjoint problem for y, we obtain for arbitrary $x \in X$

$$\begin{aligned}
\psi(Lx) &= \int_a^b y(s)^T (x'(s) - J(s)x(s))\, ds + w^T (Ax(a) + Bx(b)) \\
&= y(b)^T x(b) - y(a)^T x(a) - \int_a^b x(s)^T (y'(s) + J(s)^T y(s))\, ds \\
&\qquad + w^T (Ax(a) + Bx(b)) \\
&= (w^T A - y(a)^T) x(a) + (w^T B + y(b)^T) x(b).
\end{aligned}$$

Thus we must choose w such that

$$\begin{pmatrix} A^T \\ B^T \end{pmatrix} w = \begin{bmatrix} I_n & 0 \\ 0 & -I_n \end{bmatrix} \begin{pmatrix} y(a) \\ y(b) \end{pmatrix}. \tag{49}$$

Since

$$\begin{pmatrix} y(a) \\ y(b) \end{pmatrix} \in \text{kernel}(C, D) = \text{range} \begin{pmatrix} A^T \\ -B^T \end{pmatrix} \tag{50}$$

and (A, B) has full row rank, we find k linearly independent solutions w_j of (49) for the k linearly independent solutions y_j of (47). Hence we have k linear forms ψ_j given by

$$\psi_j(g, r) = \int_a^b y_j(s)^T g(s)\, ds + w_j^T r \tag{51}$$

satisfying $\psi_j L = 0$. Moreover $(\psi_j(0, w_{j'})) = (w_j^T w_{j'})$ is nonsingular. This at once implies that the orthogonal projections e_j of w_j onto corange E form a basis of corange E and $(\psi_j(0, e_{j'})) = (w_j^T e_{j'})$ is nonsingular as well. Thus the determination of the linear forms ψ_j can be replaced by the determination of a maximum set of linearly independent solutions of the adjoint problem and the computation of matching vectors w_j via (49).

As possible candidates for the quantities $\tilde{\varphi}_i$ and $\tilde{z}_j$ in (30) we can take for example

$$\tilde{\varphi}_i(x) = \tilde{t}_i(a)^T x(a) + \tilde{t}_i(b)^T x(b), \quad \tilde{z}_j = (0, \tilde{e}_j) \tag{52}$$

where the quantities with tilde on the right hand side may represent first approximations of the quantities without tilde. Consequently the equation in (30) determining ψ_j becomes

$$\int_a^b y_j(s)^T (x'(s) - J(s)x(s))\, ds + w^T (Ax(a) + Bx(b)) + \gamma_j^T (\tilde{t}(a)^T x(a) + \tilde{t}(b)^T x(b)) = 0$$

which must hold for all $x \in X$. As above, this leads to

$$A^T w_j = y_j(a) - \tilde{t}(a)\gamma_j, \quad B^T w_j = -y_j(b) - \tilde{t}(b)\gamma_j. \tag{53}$$

Solvability for w_j requires

$$\begin{pmatrix} y_j(a) - \tilde{t}(a)\gamma_j \\ y_j(b) + \tilde{t}(b)\gamma_j \end{pmatrix} \in \text{range} \begin{pmatrix} A^T \\ -B^T \end{pmatrix} = \text{kernel}(C, D)$$

which gives the boundary condition

$$C y_j(a) + D y_j(b) + (-C\tilde{t}(a) + D\tilde{t}(b))\gamma_j = 0.$$

Applying these results to the special situation of the Fréchet derivative(43), i. e., setting

$$A := r_{x_a}(x(a), x(b), \lambda), \quad B := r_{x_b}(x(a), x(b), \lambda), \quad J(s) := f_x(s, x(s), \lambda), \tag{54}$$

we have been led to augmented systems of the form

$$
\begin{aligned}
& t_i' - f_x t_i = 0, \quad A t_i(a) + B t_i(b) + \tilde{e}\beta_i = 0, \\
& \qquad \tilde{t}(a)^T t_i(a) + \tilde{t}(b)^T t_i(b) = e_i^{(k+l)}, \\
& y_j' + f_x^T y_j = 0, \quad C y_j(a) + D y_j(b) + (-C\tilde{t}(a) + D\tilde{t}(b))\gamma_j = 0 \\
& \qquad \tilde{e}^T w_j = e_j^{(k)}, \quad w_j \text{ from (53)}, \\
& x' - f(x,\lambda) = 0, \quad r(x(a), x(b), \lambda) = 0, \\
& \overline{b}(x,\lambda,t,\psi) = 0
\end{aligned}
\tag{55}
$$

for the determination of singular solutions of two-point boundary value problems. To avoid a conflict in the notation of the right boundary of the integration interval and the additional equations in the augmented systems, we denote here the latter ones by $\overline{b}$ throughout the rest of this section. At this point, it is clear that $\overline{b}$ must still be adapted for the use of y and w instead of ψ.

EXAMPLE 4.2. To rewrite (38) along the lines of the above construction for use in (55), we observe

$$
\begin{aligned}
\psi T_x(x,\tau)t &= \psi(t' - J(s)t, At(a) + Bt(b)) \\
&= \int_a^b y(s)^T (t'(s) - J(s)t(s))\, ds + w^T(At(a) + Bt(b)) \\
&= (w^T A - y(a)^T)t(a) + (w^T B + y(b)^T)t(b),
\end{aligned}
$$

the latter expression replacing $\overline{b}(x,\lambda,t,\psi)$ in (55). For the test function (40) we first must solve

$$
\tilde{L}(x,\tau)(\overline{x},\overline{u}) = (T_x(x,\tau)\,\overline{x} + \tilde{z}\,\overline{u}, \tilde{\varphi}(\overline{x})) = (0,1)
$$

for $(\overline{x},\overline{u})$. This is equivalent to the boundary value problem

$$
\begin{aligned}
& \overline{x}' - J(s)\,\overline{x} = 0, \\
& A\,\overline{x}(a) + B\,\overline{x}(b) + \tilde{e}\,\overline{u} = 0, \\
& \tilde{t}(a)^T \overline{x}(a) + \tilde{t}(b)^T \overline{x}(b) = 0
\end{aligned}
$$

where the additional (scalar) boundary condition corresponds to the additional (scalar) unknown $\overline{u}$. Thus the above system fixes $(\overline{x},\overline{u})$. Application of $T_x(x,\tau)P_X$ according to (40) yields

$$
T_x(x,\tau)P_X(\overline{x},\overline{u}) = T_x(x,\tau)\,\overline{x} = (\overline{x}' - J(s)\,\overline{x}, A\,\overline{x}(a) + B\,\overline{x}(b)) = (0, -\tilde{e}\,\overline{u}).
$$

A more lengthy computation in the spirit of the previous discussion then shows that the term $P_{Y^*}(\tilde{L}(x,\tau)^*)^{-1}(0,1)$ reproduces $\overline{u}$ up to a nonzero factor. Thus a possible test function is given by $\overline{u}$ itself as part of the solution of the above linear boundary value problem which of course still depends on (x,τ).

EXAMPLE 4.3. Let us continue the discussion of the last section by studying a specific and very simple example (see [20]), which, however, already displays the essential features of our approach.

We consider the nonlinear parametrized two-point boundary value problem

$$x''(s) + 2\tau q(\tau) + \pi^2 \tau (z + z^2) = 0, \qquad x(0) = x(1) = 0, \tag{56}$$

where $q(\tau) := \tau \exp(-\tau/2)$ and $z := z(s,\tau) := x(s) - \tau q(\tau) s(1-s)$. It can analytically be shown that

1. there is a trivial solution curve $\Gamma = \{x_1(s,\tau) := q(\tau)s(1-s),\ \tau \in \mathbb{R}\}$, and
2. bifurcation from this trivial curve occurs at the critical parameter values $\tau_i = i^2, \quad i = 1, 2, \ldots$.

In order to study the solution manifold of (56) numerically, we have transformed (56) into a system of first order differential equations. Then, we have used the code RWPKV (see, e.g., [17]) for pathfollowing, detecting of singular points and determining a first approximation of the bifurcation points by an indirect method. The bifurcation diagram computed with this code is shown in Figure 1. To improve the approximations

Figure 1: Part of the solution field of problem (56); Γ - trivial solution curve, $*$ - simple secondary bifurcation points, $\circ$ - simple turning point

of the simple secondary bifurcation points we have adapted the augmented system technique as follows.

Let

$$T(x, \lambda) = 0 \tag{57}$$

be the operator form of (56). Then, the main part of the augmented system (30) reads

$$\tilde{L}(x,\tau) \begin{pmatrix} t \\ \beta \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{58}$$

$$\tilde{L}^*(x,\tau)\begin{pmatrix}\psi\\ \gamma\end{pmatrix}-\begin{pmatrix}0\\ 1\end{pmatrix}=\begin{pmatrix}0\\ 0\end{pmatrix}, \tag{59}$$

$$T(x,\tau)+\tilde{z}\alpha=0. \tag{60}$$

Note, to simplify the notation we have used the same symbol "T" in the equations (57) and (60).
The function $b(x,\lambda,t,\psi)$ has to reflect the conditions $h_\xi=0$ and $h_\tau=0$ which are necessary for a simple secondary bifurcation point (see, e.g., [19]). Thus, we write the last operator equation of formula (30) in the form

$$\tilde{L}(x,\tau)\begin{pmatrix}w_\xi+t\\ h_\xi\end{pmatrix}=\begin{pmatrix}0\\ 0\end{pmatrix}, \tag{61}$$

$$\tilde{L}(x,\tau)\begin{pmatrix}w_\tau\\ h_\tau\end{pmatrix}+\begin{pmatrix}T(x,\tau)\\ 0\end{pmatrix}=\begin{pmatrix}0\\ 0\end{pmatrix}, \tag{62}$$

$$h_\xi=0, \tag{63}$$

$$h_\tau=0. \tag{64}$$

Substituting $h_\xi=h_\tau=0$ into (61), (62) and considering $T_x(x,\tau)t=-\tilde{z}\beta$ as well as $w_\xi=0$, the equations (58)–(62) are reduced to

$$\begin{aligned}
&T_x(x,\tau)t=0,\\
&\tilde{\phi}t-1=0,\\
&T(x,\tau)+\tilde{z}\alpha=0,\\
&T_x(x,\lambda)w_\tau+T_\tau(x,\tau)=0,\\
&\tilde{\phi}w_\tau=0.
\end{aligned} \tag{65}$$

Thus, Weber's well-known determining system for simple secondary bifurcation points (see [34]) comes out as a special case of our general theory of augmented systems. Applying this augmented system to the boundary value problem (56), we obtain (with $\dot{q}:=dq(\tau)/d\tau$):

$$\begin{aligned}
t_1' &= t_2,\\
t_2' &= -\pi^2\tau(1+2z)t_1,\\
\xi' &= t_1^2+t_2^2,\\
x_1' &= x_2,\\
x_2' &= -2\tau q(\tau)-\pi^2\tau(z+z^2)-t_1\alpha,\\
w_{\tau,1}' &= w_{\tau,2}',\\
w_{\tau,2}' &= -\pi^2\tau(1+2z)w_{\tau,1}-2q(\tau)-2\tau\dot{q}(\tau)-\pi^2(z+z^2)\\
&\quad +\pi^2\tau s(1-s)(q\tau+\tau\dot{q}(\tau))(1+2z),\\
\zeta' &= t_1w_{\tau,1}+t_2w_{\tau,2},\\
\tau' &= 0,\\
\alpha' &= 0,
\end{aligned} \tag{66}$$

$$\begin{aligned}
t_1(0) &= \xi(0)=x_1(0)=w_{\tau,1}(0)=\zeta(0)=0,\\
t_1(1) &= x_1(1)=w_{\tau,1}(1)=\xi(1)=0,\quad \zeta(1)=1.
\end{aligned}$$

Here, we have used t instead of $\tilde{z}$ since the linearized boundary value problem is self-adjoint.
To determine the bifurcation points drawn in Figure 1 (symbol "$*$") at $\tau_1 = 1$, $\tau_2 = 4$ and $\tau_3 = 9$, we have computed the corresponding isolated solutions of the augmented system (66) with the multiple shooting code RWPM (see, e.g., [15]). We obtained the starting trajectories by solving an initial value problem for the differential equations (66). The associated initial vectors

$$(t_1, t_2, \xi, x_1, x_2, w_{\tau,1}, w_{\tau,2}, \zeta, \tau, \alpha)^T(0)$$

have been chosen as follows. For x_1, x_2 and τ, we used the values computed by the indirect method during the pathfollowing process (executing RWPKV):

bifurcation point	1	2	3
$x_1(0)$	0	0	0
$x_2(0)$	0.6095443	2.165934	0.927900
$\tau(0)$	0.9992720	4.000132	8.888919

From the boundary conditions in (66), it follows $t_1(0) = 0$, $\xi(0) = 0$, $w_{\tau,1}(0) = 0$ and $\zeta(0) = 0$. Since there is no information about the second component of w_τ, we have set $w_{\tau,2}(0) = 1$. The unfolding parameter α vanishes in a bifurcation point which implies that $\alpha(0) = 0$ is a good choice. With an eigenfunction t, $\|t\| \neq 0$, all multiples ct, $c \in \mathbb{R}\backslash\{0\}$, are eigenfunctions. Therefore, we have chosen $t_2(0) = 1$.
With these starting trajectories, the multiple shooting method required 4 iterations to compute the following approximations of the simple bifurcation points (with a defect of the nonlinear algebraic shooting equations of order 10^{-19}):

bifurcation point	1	2	3
$x_1(0)$	0	0	0
$x_2(0)$	0.60653066	2.1653645	0.89982872
$\tau(0)$	1.00000000	4.0000000	9.00000000

In each computation, we have started the code RWPM with 11 equidistributed shooting points and a Runge-Kutta method of order 8. Finally, it should be mentioned that we could not observe a turning point for $\tau \in [0.5, 1]$ as it is shown in the corresponding bifurcation diagram in [20].

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