NBA Lecture 2

Continuation problems. Numerical continuation of equilibria and limit cycles of ODEs

Yu.A. Kuznetsov (Utrecht University, NL)

March 15, 2011

Contents

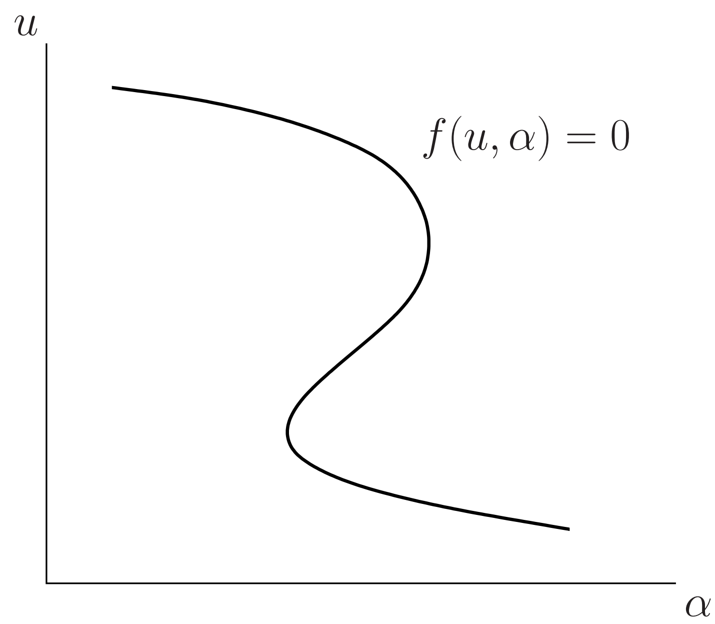
1. Equilibria of autonomous ODEs

- Consider a family of autonomous ODEs:

$$\dot{u} = f(u, \alpha), \qquad u \in \mathbb{R}^n, \alpha \in \mathbb{R},$$

where $f : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ is smooth.

- Equilibrium manifold:



2. Algebraic continuation problems

- **Def. 1 ALCP**: *Find a* **curve** $M \subset \mathbb{R}^{N+1}$ *defined by*

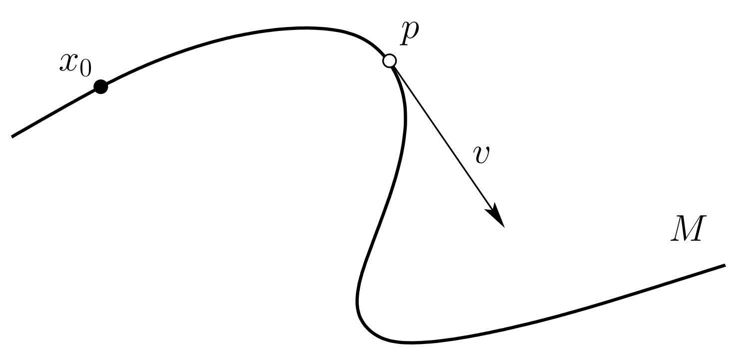
$$F(x) = 0, \quad F : \mathbb{R}^{N+1} \to \mathbb{R}^N,$$

starting from a point $x_0 \in M$.

Finding an equilibrium manifold is an example of ALCP with $N = n$,

$$x = (u, \alpha) \equiv \begin{pmatrix} u \\ \alpha \end{pmatrix} \in \mathbb{R}^{n+1}, \quad F(x) = f(u, \alpha).$$

- **Def. 2** *A point* $p \in M$ *is called* **regular** *for ALCP if* rank $F_x(p) = N$.



- Near any regular point p, the ALCP defines a solution curve M that passes through p and is locally unique and smooth.

- If $p \in M$ is a regular point, then the linear equation

$$Jv = 0, \quad J = F_x(p),$$

has a unique (modulus scaling) solution $v \in \mathbb{R}^{N+1}$.

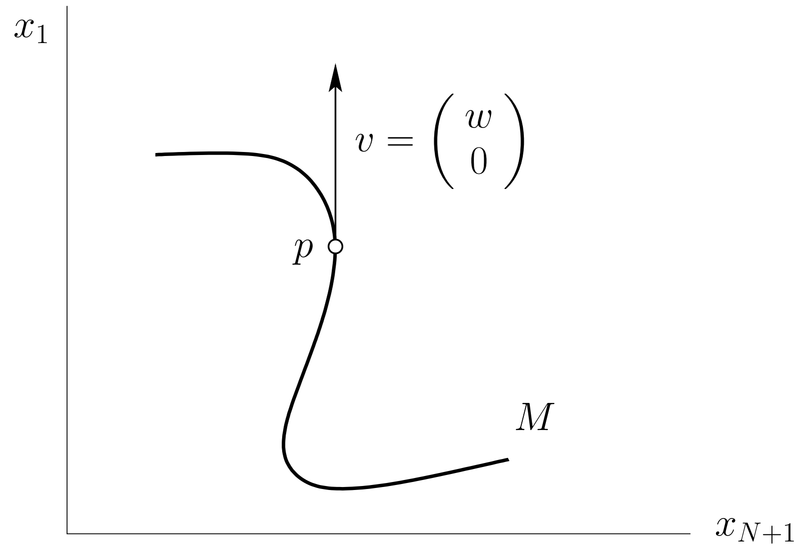
- **Lemma 1** *A tangent vector v to M at p satisfies*

$$Jv = 0.$$

Indeed, let $x = x(s)$ be a smooth parametrization of M, such that $x(0) = p$ and $\dot{x}(0) = v$. The differentiation of $F(x(s)) = 0$ yields at $s = 0$:

$$\frac{d}{ds} F(x(s))\Big|_{s=0} = F_x(x(0))\dot{x}(0) = Jv = 0$$

- **Def. 3** *A regular point $p \in M$ is a* **limit point** *for ALCP with respect to a coordinate x_j if $v_j = 0$.*



If p is a limit point w.r.t. x_{N+1}, then the $N \times N$ matrix

$$A = \left(\frac{\partial F_i(p)}{\partial x_j} \right)_{i,j=1,\ldots,N}$$

has eigenvalue $\lambda = 0$. Indeed, let $x = x(s)$ be a smooth parametrization of M, such that $x(0) = p$ and $\dot{x}(0) = v$ with

$$v = \begin{pmatrix} w \\ 0 \end{pmatrix} \neq 0, \quad w \in \mathbb{R}^N.$$

Then

$$Jv = Aw + \frac{\partial F(p)}{\partial x_{N+1}} v_{N+1} = Aw = 0.$$

- **Def. 4** *A point* $p \in M$ *is called a* **branching point** *for ALCP if* rank $F_x(p) < N$.

  Let $p = 0$ be a branching point. Write

$$F(x) = Jx + \frac{1}{2}B(x,x) + O(\|x\|^3),$$

  where $J = F_x(p)$. Introduce the null-spaces

$$\mathcal{N}(J) = \{v \in \mathbb{R}^{N+1} : Jv = 0\}$$

  and

$$\mathcal{N}(J^\mathsf{T}) = \{w \in \mathbb{R}^{N} : J^\mathsf{T} w = 0\}.$$

- Assume that rank $J = N - 1$, so that

$$\dim \mathcal{N}(J) = 2 \quad \text{and} \quad \dim \mathcal{N}(J^\mathsf{T}) = 1.$$

  Let q_1 and q_2 span $\mathcal{N}(J)$ and φ span $\mathcal{N}(J^\mathsf{T})$. Then

$$v = \beta_1 q_1 + \beta_2 q_2, \quad w = \alpha\varphi,$$

  where $(\beta_1, \beta_2) \in \mathbb{R}^2, \alpha \in \mathbb{R}$.

- Suppose we have a solution curve $x = x(s)$ passing through the branching point $p = 0$: $x(0) = 0$, $\dot{x}(0) = v$.

- By differentiating $F(x(s)) = 0$ twice with respect to s at $s = 0$, taking the scalar product with φ, and using $J^{\mathsf{T}}\varphi = 0$, one proves:

  Lemma 2 *Any tangent vector $v \in \mathbb{R}^{N+1}$ to M at $p = 0$ satisfies the equation*

$$\langle \varphi, B(v, v) \rangle = 0.$$

- Substituting here $v = \beta_1 q_1 + \beta_2 q2$, we obtain the **Algebraic Branching Equation**:

$$b_{11}\beta_1^2 + 2b_{12}\beta_1\beta_2 + b_{22}\beta_2^2 = 0,$$

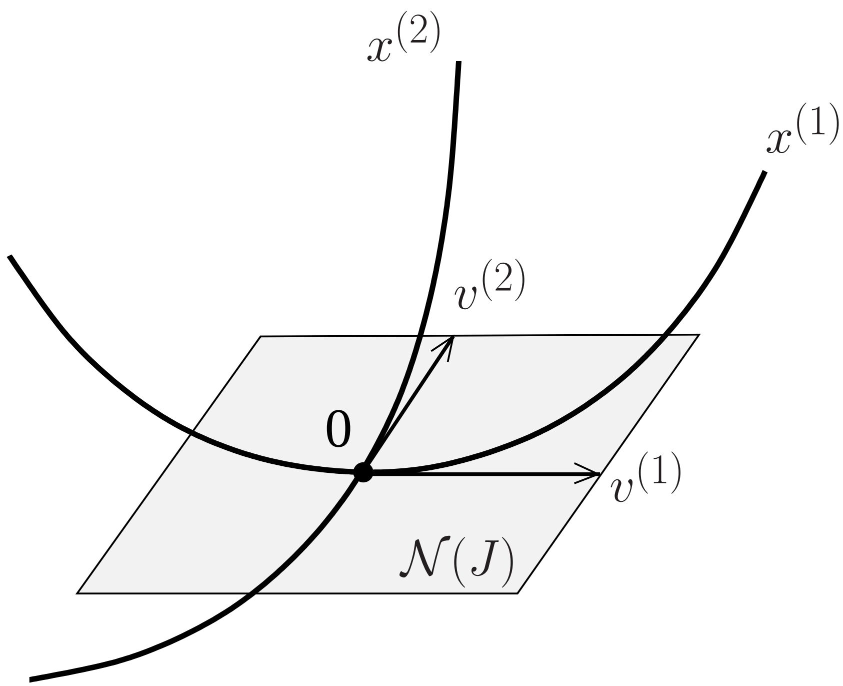
  where $b_{ij} = \langle \varphi, B(q_i, q_j) \rangle,\ i, j = 1, 2.$

- **Def. 5** *A branching point, for which*

  (a) rank $J = N - 1$,

  (b) $b_{12}^2 - b_{11}b_{22} > 0$,

  is called a **simple branching point**.



- Suppose that one solution curve $x = x^{(1)}(s)$ passing through a simple branch point $p = 0$ is known and $v^{(1)} = \dot{x}^{(1)}(0) = q_1$, so that

$$\beta_1^{(1)} = 1,\ \beta_2^{(1)} = 0.$$

Thus, $b_{11} = 0$ and $v^{(2)} = \beta_1^{(2)} q_1 + \beta_2^{(2)} q_2$ tangent to the second solution curve $x = x^{(2)}(s)$ satisfies

$$2b_{12}\beta_1^{(2)} + b_{22}\beta_2^{(2)} = 0$$

or

$$\beta_1^{(2)} = -\frac{b_{22}}{2b_{12}}\beta_2^{(2)}.$$

Lemma 3 *Consider the* $(N+1) \times (N+1)$*-matrix*

$$D(s) = \begin{pmatrix} F_x(x^{(1)}(s)) \\ \left[\dot{x}^{(1)}(s)\right]^{\top} \end{pmatrix}.$$

Its determinant $\psi(s) = \det D(s)$ *has a regular zero at the simple branching point.*

Indeed, let $q_2 \in \mathcal{N}(J)$ be a vector orthogonal to $q_1 = v^{(1)}$. Then

$$D(0)q_2 = 0,$$

so $D(0)$ is singular and has the one-dimensional null-space.

Moreover, one can show that

$$\dot{\psi}(0) = C\langle \varphi, B(q_1, q_2)\rangle = Cb_{12}, \quad C \neq 0,$$

where $D^{\top}(0)p = 0$ with $p = \begin{pmatrix} \varphi \\ 0 \end{pmatrix}$.

Thus $\dot{\psi}(0) \neq 0$.

3. Moore-Penrose numerical continuation

- Numerical solution of the ALCP means computing a **sequence of points**

$$x^{(1)}, x^{(2)}, x^{(3)}, \dots$$

approximating the curve M with desired accuracy, given an **initial point** $x^{(0)}$ that is sufficiently close to x_0.

- **Predictor-corrector method:**
  - Tangent prediction: $X^0 = x^{(i)} + h_i v^{(i)}$.
  - Newton-Moore-Penrose corrections towards M:

$$(X^k, V^k),\ k = 1, 2, 3, \dots.$$

  - Adaptive step-size control.

- **Def. 6** *Let* J *be an* $N \times (N+1)$ *matrix with* rank $J = N$. *Its* **Moore-Penrose inverse** *is* $J^{+} = J^{\mathsf{T}}(JJ^{\mathsf{T}})^{-1}$.

- To compute $J^{+}b$ efficiently, set up the system for $x \in \mathbb{R}^{N+1}$:

$$\begin{cases} Jx &= b, \\ v^{\mathsf{T}}x &= 0, \end{cases}$$

where $b \in \mathbb{R}^{N}$ and $v \in \mathbb{R}^{N+1}, Jv = 0, \|v\| = 1$. Then $x = J^{+}b$ is a solution to this system, since

$$JJ^{+}b = b, \quad v^{\mathsf{T}}J^{+}b = (Jv)^{\mathsf{T}}[(JJ^{\mathsf{T}})^{-1}b] = 0.$$

- Let $x^{(i)} \in \mathbb{R}^{N+1}$ be a regular point on the curve

$$F(x) = 0, \; f : \mathbb{R}^{N+1} \to \mathbb{R}^{N},$$

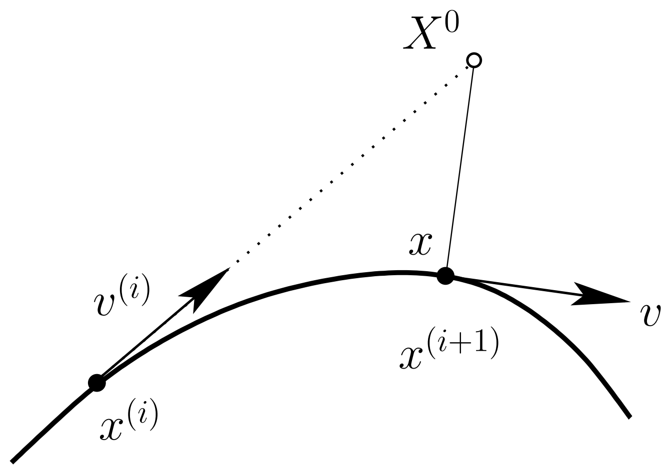
and $v^{(i)} \in \mathbb{R}^{N+1}$ be the tangent vector to this curve at $x^{(i)}$ such that

$$F_x(x^{(i)})v^{(i)} = 0, \quad \|v^{(i)}\| = 1.$$

For the next point $x^{(i+1)} \in \mathbb{R}^N$ on the curve, solve the optimization problem

$$\min_x \{\|x - X^0\| \mid F(x) = 0\},$$

i.e. look for a point $x \in M$ which is nearest to X^0:



This is equivalent to solving the system

$$\begin{cases} F(x) = 0, \\ v^{\mathsf{T}}(x - X^0) = 0, \end{cases}$$

where $v \in \mathbb{R}^N$ satisfies $F_x(x)v = 0$ with $\|v\| = 1$ and X^0 is the prediction.

The linearization of the system about X^0 is

$$\begin{cases} F(X^0) + F_x(X^0)(X - X^0) & = & 0, \\ (V^0)^\mathsf{T}(X - X^0) & = & 0, \end{cases}$$

or

$$\begin{cases} F_x(X^0)(X - X^0) & = & -F(X^0), \\ (V^0)^\mathsf{T}(X - X^0) & = & 0, \end{cases}$$

where $F_x(X^0)V^0 = 0$ with $\|V^0\| = 1$. Thus

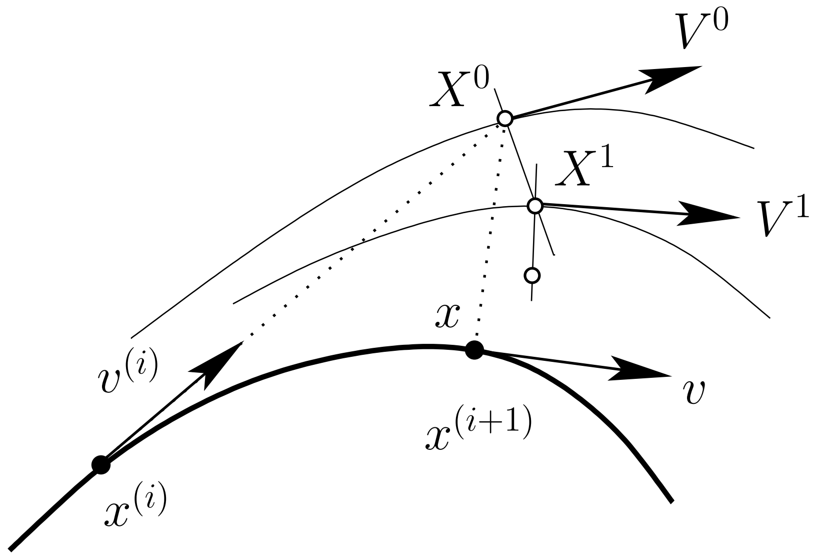
$$X = X^0 - F_x^+(X^0)F(X^0)$$

leading to the **Moore-Penrose corrections**:

$$X^{k+1} = X^k - F_x^+(X^k)F(X^k), \; k = 0, 1, 2, \ldots,$$

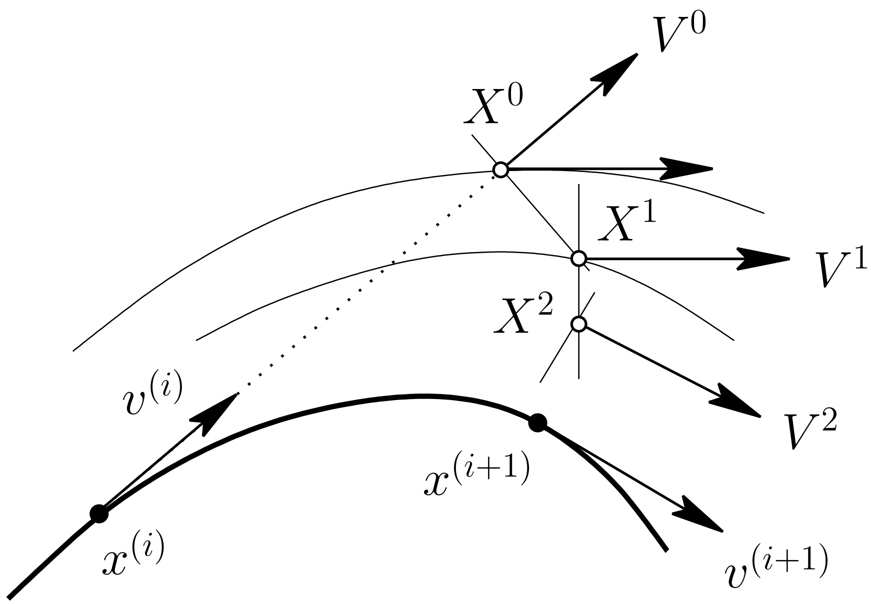
where $V^k \in \mathbb{R}^{N+1}$ such that $F_x(X^k)V^k = 0$ with $\|V^k\| = 1$ should be used to compute $F_x^+(X^k)$.

Geometry of the Moore-Penrose iterations



Each correction occurs within the plane orthogonal to the null-vector V^k at X^k.

Approximate $V^k : F_x(X^{k-1})V^k = 0$.



Each correction occurs within the plane orthogonal to the previous null-vector V^{k-1} at X^k.

Implementation

Iterate for $k = 0, 1, 2, \ldots$

$$J = F_x(X^k), \quad B = \begin{pmatrix} J \\ V^{k\top} \end{pmatrix},$$
$$R = \begin{pmatrix} JV^k \\ 0 \end{pmatrix}, \quad Q = \begin{pmatrix} F(X^k) \\ 0 \end{pmatrix},$$
$$W = V^k - B^{-1}R, \quad V^{k+1} = \frac{W}{\|W\|}$$
$$X^{k+1} = X^k - B^{-1}Q.$$

If $\|F(X^k)\| < \varepsilon_0$ and $\|X^{k+1} - X^k\| < \varepsilon_1$ then

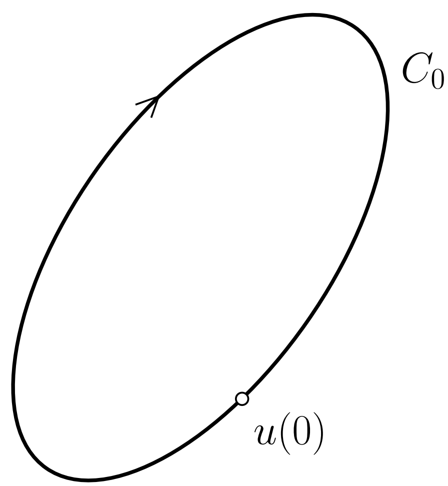
$$x^{(i+1)} = X^{k+1}, \quad v^{(i+1)} = V^{k+1}.$$

4. Limit cycles of autonomous ODEs

- Assume, the ODE system

$$\dot{u} = f(u, \alpha), \quad u \in \mathbb{R}^n, \ \alpha \in \mathbb{R},$$

has at α_0 an isolated periodic orbit (**limit cycle**) C_0.



- Let $u_0(t + T_0) = u_0(t)$ denote the corresponding periodic solution with minimal period T_0.

- Consider a **periodic boundary-value problem** on $[0, 1]$:

$$\begin{cases} \dot{w} - T_0 f(w, \alpha) & = & 0, \\ w(0) - w(1) & = & 0. \end{cases}$$

Clearly, $w(\tau) = u_0(T_0\tau + \sigma_0),\ \alpha = \alpha_0$ is a solution to this BVP for any phase shift σ_0.

- Let $v(\tau)$ be a smooth period-1 function. To fix σ_0, impose the **integral phase condition**:

$$\Psi[w] = \int_0^1 \langle w(\tau), \dot{v}(\tau)\rangle d\tau = 0$$

Lemma 4 *The condition*

$$\int_0^1 \langle w(\tau), \dot{v}(\tau)\rangle d\tau = 0$$

*is a necessary condition for the L_2-***distance**

$$\rho(\sigma) = \int_0^1 \|w(\tau+\sigma) - v(\tau)\|^2 d\tau$$

between 1-periodic smooth functions w and v to achieve a local minimum with respect to possible shifts σ at $\sigma = 0$.

Since $\|w\|^2 = \langle w, w\rangle$,

$$\begin{aligned}
\frac{1}{2}\dot{\rho}(0) &= \int_0^1 \langle w(\tau+\sigma) - v(\tau), \dot{w}(\tau+\sigma)\rangle d\tau \Big|_{\sigma=0} \\
&= \int_0^1 \langle w(\tau) - v(\tau), \dot{w}(\tau)\rangle d\tau \\
&= \int_0^1 \langle w(\tau), \dot{w}(\tau)\rangle d\tau - \int_0^1 \langle v(\tau), \dot{w}(\tau)\rangle d\tau \\
&= \frac{1}{2}\int_0^1 d\|w(\tau)\|^2 - \int_0^1 \langle v(\tau), \dot{w}(\tau)\rangle d\tau \\
&= \int_0^1 \langle w(\tau), \dot{v}(\tau)\rangle d\tau \ .
\end{aligned}$$

5. Boundary-value continuation problems

- **Def. 7 BVCP**: *Find a* **branch** *of solutions* $(u(\tau), \beta)$ *to the following boundary-value problem with integral constraints*

$$\begin{cases} \dot{u}(\tau) - H(u(\tau), \beta) & = & 0, \quad \tau \in [0, 1], \\ B(u(0), u(1), \beta) & = & 0, \\ \int_0^1 C(u(\tau), \beta)\, d\tau & = & 0, \end{cases}$$

starting from a given solution $(u_0(\tau), \beta_0)$*. Here* $u \in \mathbb{R}^{n_u}, \beta \in \mathbb{R}^{n_\beta}$ *and*

$$H : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\beta} \to \mathbb{R}^{n_u},$$
$$B : \mathbb{R}^{n_u} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_\beta} \to \mathbb{R}^{n_b},$$
$$C : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\beta} \to \mathbb{R}^{n_c}$$

are smooth functions.

- The BVCP is (formally) **well posed** if

$$n_\beta = n_b + n_c - n_u + 1.$$

6. Discretization via orthogonal collocation

- **Mesh points:** $0 = \tau_0 < \tau_1 < \cdots < \tau_N = 1$.

- **Basis points:**

$$\tau_{i,j} = \tau_i + \frac{j}{m}(\tau_{i+1} - \tau_i),$$

where $i = 0, 1, \ldots, N-1,\ \ j = 0, 1, \ldots, m$.

- **Approximation:**

$$u^{(i)}(\tau) = \sum_{j=0}^{m} u^{i,j} l_{i,j}(\tau), \quad \tau \in [\tau_i, \tau_{i+1}],$$

where $l_{i,j}(\tau)$ are the **Lagrange basis polynomials**

$$l_{i,j}(\tau) = \prod_{k=0, k\neq j}^{m} \frac{\tau - \tau_{i,k}}{\tau_{i,j} - \tau_{i,k}}$$

and $u^{i,m} = u^{i+1,0}$.

- **Orthogonal collocation:**

$$F : \begin{cases} \left(\sum_{j=0}^{m} u^{i,j} l'_{i,j}(\zeta_{i,k})\right) - H(\sum_{j=0}^{m} u^{i,j} l_{i,j}(\zeta_{i,k}), \beta) = 0, \\ B(u^{0,0}, u^{N-1,m}, \beta) = 0, \\ \sum_{i=0}^{N-1} \sum_{j=0}^{m} \omega_{i,j} C(u^{i,j}, \beta) = 0, \end{cases}$$

  where $\zeta_{i,k},\ k = 1, 2, \ldots, m$, are the **Gauss points** (roots of the Legendre polynomials relative to the interval $[\tau_i, \tau_{i+1}]$), and $\omega_{i,j}$ are the **Lagrange quadrature coefficients**.

- **Approximation error:** Introduce

$$h = \max_{i=1,2,\ldots,N} |\tau_i - \tau_{i-1}|$$

  – in the basis points:

$$\|u(\tau_{i,j}) - u^{i,j}\| = O(h^m)$$

  – in the mesh points:

$$\|u(\tau_i) - u^{i,0}\| = O(h^{2m})$$

- BVCP for the **limit cycle branch** with $\alpha \in \mathbb{R}$:

$$\begin{cases} \dot{w}(\tau) - Tf(w(\tau),\alpha) & = & 0, \ \ \tau \in [0,1], \\ w(0) - w(1) & = & 0, \\ \int_0^1 \langle w(\tau), \dot{v}(\tau) \rangle \ d\tau & = & 0. \end{cases}$$

- Corresponding HUGE ALCP:

$$F(x) = 0, \quad x = (\{w^{j,k}\}, T, \alpha) \in \mathbb{R}^{mnN+n+2}$$

where $j = 0, 1, \ldots, N-1, \ k = 0, 1, \ldots, m.$

- The derivative of BVCP with respect to $x = (w, T, \alpha)$:

$$\begin{bmatrix} D - Tf_w(w,\alpha) & -f(w,\alpha) & -Tf_\alpha(w,\alpha) \\ \delta_0 - \delta_1 & 0 & 0 \\ \mathrm{Int}_{\dot{v}} & 0 & 0 \end{bmatrix}$$

has the one-dimensional null-space at a generic cycle.

- The orthogonal collocation produces a sparse Jacobian matrix F_x:

$$
\left(\begin{array}{cccccccccccccccc}
w_1^{0,0} & & w_1^{0,1} & & w_1^{1,0} & & w_1^{1,1} & & w_1^{2,0} & & w_1^{2,1} & & w_1^{3,0} & & T_1 & \alpha_1 \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & & & & & & & & \bullet & \bullet \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & & & & & & & & \bullet & \bullet \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & & & & & & & & \bullet & \bullet \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & & & & & & & & \bullet & \bullet \\
 & & & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & & & & \bullet & \bullet \\
 & & & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & & & & \bullet & \bullet \\
 & & & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & & & & \bullet & \bullet \\
 & & & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & & & & \bullet & \bullet \\
 & & & & & & & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
 & & & & & & & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
 & & & & & & & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
 & & & & & & & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & \bullet & & & & & & & & & & & \bullet & \bullet & & \\
\bullet & \bullet & & & & & & & & & & & \bullet & \bullet & & \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & &
\end{array}\right)
$$

that has a one-dimensional null-space at generic points satisfying $F(x) = 0$.

Computation of the multipliers

- After Gauss elimination:

$$
\left(\begin{array}{cccccccccccccccc}
w_1^{0,0} & & w_1^{0,1} & & w_1^{1,0} & & w_1^{1,1} & & w_1^{2,0} & & w_1^{2,1} & & w_1^{3,0} & & T_1 & \alpha_1 \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & & & & & & & & \bullet & \bullet \\
\bullet & \bullet & \circ & \bullet & \bullet & \bullet & & & & & & & & & \bullet & \bullet \\
\bullet & \bullet & \circ & \circ & \bullet & \bullet & & & & & & & & & \bullet & \bullet \\
\bullet & \bullet & \circ & \circ & \circ & \bullet & & & & & & & & & \bullet & \bullet \\
 & & & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & & & & \bullet & \bullet \\
 & & & & \bullet & \bullet & \circ & \bullet & \bullet & \bullet & & & & & \bullet & \bullet \\
\bullet & \bullet & & & \circ & \circ & \circ & \circ & \bullet & \bullet & & & & & \bullet & \bullet \\
\bullet & \bullet & & & \circ & \circ & \circ & \circ & \circ & \bullet & & & & & \bullet & \bullet \\
 & & & & & & & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
 & & & & & & & & \bullet & \bullet & \circ & \bullet & \bullet & \bullet & \bullet & \bullet \\
* & * & & & & & & & \circ & \circ & \circ & \circ & \star & \star & \bullet & \bullet \\
* & * & & & & & & & \circ & \circ & \circ & \circ & \star & \star & \bullet & \bullet \\
\bullet & \bullet & & & & & & & & & & & \bullet & \bullet & & \\
\bullet & \bullet & & & & & & & & & & & \bullet & \bullet & & \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet
\end{array}\right)
$$

- Let P_0 be the matrix block marked by $*$'s and P_1 the matrix block marked by $\star$'s. We have $w_1^{0,0} = w_1(0), w^{N,0} = w_1(1)$ implying

$$P_0 w_1(0) + P_1 w_1(1) = P_0 u_1(0) + P_1 u_1(T) = 0 \;\Rightarrow\; M(T) = -P_1^{-1} P_0$$