Pseudo arc ontinuation method

Our goal is to continue *numerically* a curve $\mathcal{C} \subset \mathbb{R}^{n+1}$, defined implicitely by the equation $F(z) = 0$, being $F : \mathbb{R}^{n+1} \longrightarrow \mathbb{R}^n$ a smooth function. Let us assume that $z^j \in \mathbb{R}^{n+1}$, is a *regular* point of $\mathcal{C}$, so $F\left(z^j\right) = 0$, and $\operatorname{Rank} DF\left(z^j\right) = n$. Moreover, let $v^j \in \mathbb{R}^{n+1}$ be an unitary vector tangent to the curve $\mathcal{C}$ at the point z^j, $v^j \in T_{z^j}\mathcal{C}$, so $\|v^j\| = 1$, and $DF\left(z^j\right) v^j = 0$.

Then, it is possible to find a new point on the curve, $z^{j+1} \in \mathcal{C}$, and a new unitary tangent vector, to $\mathcal{C}$ at z^{j+1}, $v^{j+1} \in T_{z^{j+1}}\mathcal{C}$, $\|v^{j+1}\| = 1$. If, on its turn, z^{j+1} is a regular point of $\mathcal{C}$, then one can look for yet another point on $\mathcal{C}$, $z^{j+2} \in \mathcal{C}$, and a new unitary tangent vector to $\mathcal{C}$ at z^{j+2}, $v^{j+2} \in T_{z^{j+2}}\mathcal{C}$, $\|v^{j+2}\| = 1$, and so on.

Of course, there are several numerical methods to do this *step-by-step* continuation of $\mathcal{C}$ from an inital point on the curve, $z^j \in \mathcal{C}$, and a (normalizsed) tangent direction at that point, $v^j \in T_{z^j}\mathcal{C}$. The one we outline here is the so called *pseudo arc continuation method* (see [1], Chap. 10, Sect. 2, for a complete description). In a nutshell, it consists in the three stages discussed below.

The continuation algorithm

Stage 1: Prediction. Take $\hat{z}^{j+1} = z^j + h_j v^j \in z^j + \langle v^j \rangle$ as an approximation for another new point $z^{j+1} \in \mathcal{C}$. Here $h_j > 0$ is the pseudo arc length, and can be conveniently adapted at each step.

Stage 2: Correcton. Refine the approximation $\hat{z}^{j+1}$ to find $z^{j+1} \in \mathbb{R}^{n+1}$ such that $F\left(z^{j+1}\right) = 0$. However, as the system $F(z) = 0$ has n equations and $n+1$ unknowns $z_1, z_2, \ldots, z_n, z_{n+1}$, we need to ask for an additional condition: in particular, we shall require that $z^{j+1} \in \hat{z}^{j+1} + \langle v^j \rangle^{\perp}$, i.e., that z^{j+1} belongs to the hyperplane orthogonal to the vector v^j that holds $\hat{z}^{j+1}$ (see Figure 1). The corresponding equation con be formulated as

$$\begin{aligned}
\left\langle v^j, z^{j+1} - \hat{z}^{j+1} \right\rangle &= \left\langle v^j, z^{j+1} - z^j - h_j v^j \right\rangle \\
&= \left\langle v^j, z^{j+1} \right\rangle - \left\langle v^j, z^j \right\rangle - h_j \left\langle v^j, v^j \right\rangle \\
&= \left\langle v^j, z^{j+1} \right\rangle - \left\langle v^j, z^j \right\rangle - h_j = 0,
\end{aligned}$$

where $\langle \cdot, \cdot \rangle$ stands for the *inner* (or dot) product $\langle \xi, \eta \rangle := \xi_1\eta_1 + \cdots + \xi_m\eta_m$, $\xi, \eta \in \mathbb{R}^m$. Hence z^{j+1} will be given by the solution of the nonlinear system,

$$\begin{aligned}
F(z) &= 0, \\
\left\langle v^j, z \right\rangle &= \left\langle v^j, z^j \right\rangle - h_j
\end{aligned} \tag{1}$$

that can be solved by some iterative method (for example, that Newton method) taking as initial approximation. $z^{(0)} = \hat{z}^{j+1}$.

Stage 3: Tangent vector. To find the tangent vector to the curve at the new point $z^{j+1} \in \mathcal{C}$ found at Stage 2, $v^{j+1} \in T_{z^{j+1}}\mathcal{C}$, first we solve the $(n+1)$-dimensional linear system

$$\begin{aligned}
DF\left(z^{j+1}\right) v &= 0, \\
\left\langle v^j, v \right\rangle &= 1.
\end{aligned} \tag{2}$$

As it is pointed out in [1]:

(i) If $\mathcal{C}$ is a regular curve and z^j, z^{j+1} are close enough, the system (2) is nonsingular.

(ii) The solution, $v^* \in \mathbb{R}^{n+1}$, of (2) satisfies $\langle v^j, v^* \rangle = 1$, so the direction along the curve is preserved.

Next, we normalize. If $v^* \in \mathbb{R}^{n+1}$ denotes the solution of (2), we divide by its norm, so $v^{j+1} = v^* / \|v^*\|$. This is the tangent vector we look for. ◊

Now, the process can be iterated using the output of Stage 3, the tangent vector $v^{j+1} \in T_{z^{j+1}}\mathcal{C}$, to feed Stage 1 and find a another point close to the curve $\mathcal{C}$, and so on. If at Stage 2, $\operatorname{Rank} DF\left(z^k\right) < n$, for the new computed point, $z^k \in \mathcal{C}$, then the curve $\mathcal{C}$ is not regular at that point, so one has to stop the process and analyse for the possible appearing of branches (bifurcations).

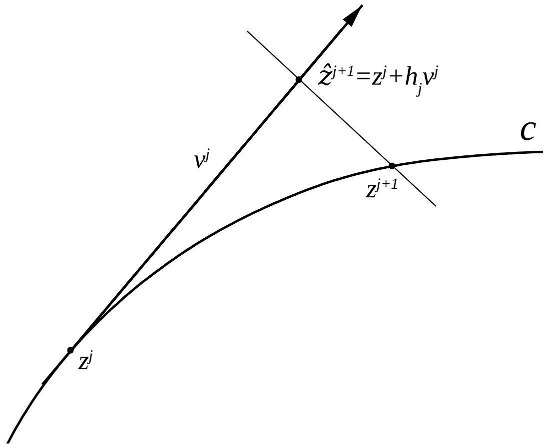

Figure 1: We add an extra condition: $z^{j+1} \in \hat{z}^{ji+1} + \left\langle v^j \right\rangle^{\perp}$. See [1], Figure 10.6(b).

Initial point and tangent vector

Nonetheless, to start the process described above, we need an initial point on he curve, $z^0 \in \mathcal{C}$, as well as its corresponding tangent vector, $z^0 \in \mathcal{C}$ and $v^0 \in T_{z^0}\mathcal{C}$ for, otherwise, we cannot write neither the nonlinear system (1) nor the linear system (2).

To find z^0 we can proceed as follows: let us assume that we have an approximation for the initial solution, $\hat{z}^0 = (\hat{z}_1^0, \ldots, \hat{z}_n^0, \hat{z}_{n+1}^0)$, then we fix one of its components, suppose that we take the last one, $\hat{z}_{n+1}^0$ and solve the n-dimensional system,

$$\begin{aligned} F_1\left(z_1, \ldots, z_n, \hat{z}_{n+1}^0\right) &= 0, \\ F_2\left(z_1, \ldots, z_n, \hat{z}_{n+1}^0\right) &= 0, \\ \ldots\ldots\ldots\ldots\ldots\ldots&\ldots\ldots \\ F_n\left(z_1, \ldots, z_n, \hat{z}_{n+1}^0\right) &= 0, \end{aligned}$$

by the Newton method, starting with $z_1 = \hat{z}_1^0, \ldots, z_n = \hat{z}_n^0$. If the method converges, we have an initial point on the curve, $z^0 = (z_1^0, \ldots, z_n^0, \hat{z}_{n+1}^0)$.

Next, we look for the tangent vector to $z^0 \in \mathcal{C}$, $v_0 \in T_{z^0}\mathcal{C}$. To this end, we select n linearly independent columns of $DF\left(z^0\right)$. If the curve is regular at z^0, $\operatorname{Rank} DF\left(z^0\right) = n$. Hence, for some i, $i \in \{1, 2, \ldots, n, n+1\}$, columns $1, \ldots, i-1, i+1, \ldots, n, n+1$ are; so we fix $v_i = 1$, solve the system

$$\begin{aligned} \frac{\partial F_1}{\partial x_1}\left(z^0\right) v_1 + \cdots + \frac{\partial F_1}{\partial x_{i-1}}\left(z^0\right) v_{i-1} + \frac{\partial F_1}{\partial x_{i+1}}\left(z^0\right) v_{i+1} + \cdots + \frac{\partial F_1}{\partial x_n}\left(z^0\right) v_n + \frac{\partial F_1}{\partial x_{n+1}}\left(z^0\right) v_{n+1} &= -\frac{\partial F_1}{\partial x_i}\left(z^0\right), \\ \frac{\partial F_2}{\partial x_1}\left(z^0\right) v_1 + \cdots + \frac{\partial F_2}{\partial x_{i-1}}\left(z^0\right) v_{i-1} + \frac{\partial F_2}{\partial x_{i+1}}\left(z^0\right) v_{i+1} + \cdots + \frac{\partial F_2}{\partial x_n}\left(z^0\right) v_n + \frac{\partial F_2}{\partial x_{n+1}}\left(z^0\right) v_{n+1} &= -\frac{\partial F_2}{\partial x_i}\left(z^0\right), \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots&\ldots\ldots\ldots \\ \frac{\partial F_n}{\partial x_1}\left(z^0\right) v_1 + \cdots + \frac{\partial F_n}{\partial x_{i-1}}\left(z^0\right) v_{i-1} + \frac{\partial F_n}{\partial x_{i+1}}\left(z^0\right) v_{i+1} + \cdots + \frac{\partial F_n}{\partial x_n}\left(z^0\right) v_n + \frac{\partial F_n}{\partial x_{n+1}}\left(z^0\right) v_{n+1} &= -\frac{\partial F_n}{\partial x_i}\left(z^0\right), \end{aligned}$$

and normalyse the solution, v^*, to get $v^0 = v^* / \|v^*\|$. Now, we use the pair $z^0 \in \mathcal{C}$, $v^0 \in T_{z^0}\mathcal{C}$ as input of Stage 1 to fire up the continuation algorithm.

1 References

[1] Yuri A. Kuznetsov. *Elements of Applied Bifurcation Theory*, volume 112 of *Applied Mathematical Sciences*. Springer-Verlag, New York, third edition, 2004. 1, 2