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ANALYSIS OF THE HYPERSPHERICAL PATH-TRACKING METHODOLOGY FOR THE SOLUTION OF NONLINEAR ALGEBRAIC SYSTEMS

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Abstract
The hyperspherical path tracking methodology was analyzed as homotopy continuation method, the general strategy is known as predictor-corrector approach with arc-length parameterization, which consists in the applying of a mapping function on a nonlinear system of algebraic equations and transforming this system to an ordinary differential equations system, which is solved like an initial value problem, thence a solution curve is calculated and taken as a connection pathway between the solution of a simpler algebraic system and presumptively the all solutions of the original system. The homotopy pathway is constructed calculating consecutive discrete points along the curve, employing each point as reference for predict the next point; the prediction calculated is then corrected with a local method. A combined strategy of generation of hyperspheres with adaptive radius control was employed as predictor method and the Newton-Raphson method applied over the intersection between the hypersphere and the homotopy pathway as a corrector method. The strategy described above was implemented in a computer code in FORTRAN 90 ®named SEHPE, some classical multisolution problems were analyzed, which showed that the hyperspheres generation is a suitable alternative for the homotopy pathway elucidation.

INTRODUCTION
The determination of the solution vectors of nonlinear sets of algebraic equations is one of the oldest problems in mathematics and engineering; these systems are the main resource often used by mathematicians, engineers and virtually any scientist interested in the approaching and solution of a wide variety of real problems. However, there is not any analytical method to work out these issues, the more sophisticated tools to achieve this purpose are based on iterative computer algorithms (Garcia and Zangwill, 1981; Christiansen, et al., 1996; Jiménez-Islas, 1996; Allgower and Georg, 2003) which can be classified in two groups; Local methods, which only achieve convergence from initial guesses located very close to one of the solutions, and global methods, which converge to one of the solutions at least, regardless if the initial guess is far from this. However, in Engineering there are a lot of examples of problems in which this advantage is not enough, when an equation or a non-linear system of equations have multiple solutions, calculating all the solution vectors becomes necessary in order to choose the more adequately option, for example, Chemical and Biochemical Engineering have some problems in which can exist more than one feasible solution, such as, separation phase problems, real gases modeling, chemical equilibrium, heat and mass transfer, parameter estimation (Jimenez-Islas, 1988), control of microbiologic processes (Mulas et al., 2007), prediction of tridimensional structure of macromolecules (White, 2008), among many others.
This work was particularly focused in one global method known as "Hyperspherical path tracking" which can be included within a wide range of methods originated in the application of topological tools to solve equations and systems of algebraic equations known like "Homotopy methods", these methods not only guarantee the convergence from any initial guess, also allows the location of virtually all the solution vectors of any system of algebraic equations regardless of its topology (Allgower and Georg, 2003).
METHODOLOGY
The development of homotopy methods is very large, many authors have contributed to its study and implementation, among the most important one can cite: Henri Poincaré (1854-1912), famous French mathematician who devised Homotopy, L.J.E. Brower, Jules Jean Leray, Schauder and Lahaye (Rheinboldt, 2000), who provide the basis for the use of pure mathematics Homotopy Theory for solving systems of algebraic equations. Brevity, the continuation homotopy process consists in applying a mapping function (Equation 1) in a system of algebraic equations \( F(x) \); this mapping function contains an additional variable known as homotopy parameter whose value is often taken from zero to one, causing an increment \( R^{n+1} \) in the dimension of the original problem.

\[
H(x,t) = tF(x) + (1-t)E(x)
\]  
(1)

One can note that if the homotopy parameter takes the value \( t = 0 \), it will expected that \( H(x, t) = E(x) \) and at the value \( t = 1 \), the homotopy function \( H(x, t) = F(x) \). The choice of the simpler system \( E(x) \), and the method that will help us to lead \( t \) from 0 to 1 are not trivial issues, these aspects are determinant for the number of solutions that can be found and the sensitivity of the method to initial guesses. This work is based on a simple system \( E(x) \) known as Newton homotopy (Equation 2).

\[
E(x) = F(x) - F(x^0)
\]  
(2)

Then, \( E(x) \) must be deformed in \( F(x) \), not just once. After \( t \) is leading from 0 to 1, whether pathtracking is continued, this value will move away from \( t = 1 \), but eventually it will return to that value, in other words, another solution to the original system is found, and so on, until all real solutions for the problem are found. It should be noted that the homotopy parameter variation is not a trivial task since for each value that it may state, there is only one combination of values for the original problem variables \( x \in R \) that satisfy the equation 1, calculating these values requires a local convergence method like Newton-Raphson, nonlinear relaxation, among many others (Allgower and Georg, 2003). If initial guesses for calculating the discrete points are properly chosen, local methods are not a problem, so that, homotopy pathtracking can be interpreted as the permutation of a very complex problem for a number of simplest problems solved in sequential form. In this work, we used the method of hyperspherical pathtracking, which consists in the computation of tangent vectors to the homotopy path (Wayburn and Seader, 1987) and its intersection with radius controlled hyperspheres whose center is located at the point of the homotopy path that is previous to the point that is being calculated (Jiménez-Islas, 1988; Jiménez-Islas, 1996). The path found is computed and analyzed as a curve composed of ordered pairs \( (P, t) \), where \( P \) is a parameter of arc-length for the homotopy pathway. The method described is summarized in Figure 1.

![Figure 1](image-url)

Figure 1. One-dimensional representation for the hyperspherical path-tracking method
It is important to mention that the method of hyperspherical path-tracking is not the only technique described in the literature used to calculate initial guesses for the Newton corrections, there is a wide variety of methodologies available, but all of them are predictions geometrically open, so they cannot guarantee that the point calculated is really a consecutive point, with the possibility of "skip" segments of the homotopy path, which means the risk of losing solution vectors (Jiménez-Islas, 1996). The hypersphere of tracking is a closed surface, so it has the potential to detect the number of crossings with the homotopy path (see Figure 5). Besides, the using of this predictor/corrector ensures the convergence, no matter how far away it is from the initial guess used, while this falls on the hypersphere surface. The methodology contained in these few lines was implemented in a computer code for solving systems of nonlinear algebraic equations named SEHPE (Jiménez-Islas, 1996) in BASIC language, this code for the hyperspherical path tracking was migrated to FORTRAN 90® to solve some nonlinear systems, which were useful to propose some heuristic criteria to ensure the location of much of the solution vectors of practically any nonlinear systems of algebraic equations.

RESULTS AND DISCUSSION
Convergence properties for hyperspherical predictors

Some highly nonlinear sets of algebraic equations was solved employing SEHPE on FORTRAN 90® in which some code lines were included in order to generate randomly distributed predictions over some of the path tracking hyperspheres surface. All the predictions encouraged convergence for Newton corrections to the nearest homotopy pathway-hypersphere intersection (see Figure 3). Also, it was noted that the proximity of the predictions to the homotopy pathway-hypersphere intersection determines the number of iterations needed to achieve convergence considering a tolerance of $10^{-8}$ (see Figure 4).

Based on previous observations, the maximum limit for iterations in Newton corrections were fixed at 2, if the tolerance is not achieved with any prediction (see Figure 6), the radius of the hypersphere is divided by 2 and the calculation is repeated until achieve convergence. The criterion ensures that even if the hypersphere touch other parts of the homotopic pathway (Figure 5), the corrections produce convergence to the point that truly follows on the curve, minimizing the chances of losing solution vectors, note that although the area has many intersections with the homotopic path the areas that produce convergence to each of these intersections are relatively tiny.
Systems of algebraic equations solved

Example 1 (Kyung *et al.*, 1991)
\[ F_1 = x_1 + 5x_2(x_2 - 1)(x_2 + 1) \]
\[ F_2 = x_2 - 5x_2(x_1 - 1)(x_2 - 1) \]

Solution Vectors

<table>
<thead>
<tr>
<th>VECTOR(1)</th>
<th>VECTOR(4)</th>
<th>VECTOR(7)</th>
</tr>
</thead>
<tbody>
<tr>
<td>X(1)= 0.552786404493374</td>
<td>X(1)= 0.552786320376311</td>
<td>X(1)= 1.44721361462991</td>
</tr>
<tr>
<td>X(2)= 0.939307831587556</td>
<td>X(2)= 0.111960712536525</td>
<td>X(2)= -1.12163064219482</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>VECTOR(2)</th>
<th>VECTOR(5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>X(1)= 1.44721359496321</td>
<td>X(1)= -1.593262990920477E-008</td>
</tr>
<tr>
<td>X(2)= 0.798425372125783</td>
<td>X(2)= -3.186646863874083E-009</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>VECTOR(3)</th>
<th>VECTOR(6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>X(1)= 1.44721359580060</td>
<td>X(1)= 0.552786391346427</td>
</tr>
<tr>
<td>X(2)= 0.323205275518322</td>
<td>X(2)= -1.05126856910642</td>
</tr>
</tbody>
</table>

Kyung *et al.* (1991), solved this set of equations, they reported only 4 solutions using the same initial guess and the same homotopic form employed in the present study but using differential predictors, note that SEHPE located 7 roots, which shows a clear advantage of the hyperspherical predictors.

Example 2 (Kyung *et al.*, 1991)
\[ F_1 = 0.55 \sin(x_1x_2) - \frac{x_2}{4\pi} - \frac{x_1}{2} \]
\[ F_2 = (1 - 0.25\pi)(e^{x_1} - e) + e^{\frac{x_2}{\pi}} - 2e^{x_1} \]
### Solution Vectors for example 2

<table>
<thead>
<tr>
<th>Vector</th>
<th>Vector 1</th>
<th>Vector 2</th>
<th>Vector 3</th>
<th>Vector 4</th>
<th>Vector 5</th>
<th>Vector 6</th>
<th>Vector 7</th>
<th>Vector 8</th>
<th>Vector 9</th>
<th>Vector 10</th>
<th>Vector 11</th>
<th>Vector 12</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$X(1) = -9.11786508 \times 10^{-1}$</td>
<td>$X(1) = 2.874488000 \times 10^{-1}$</td>
<td>$X(1) = 4.26640133 \times 10^{-1}$</td>
<td>$X(1) = 2.26002925$</td>
<td>$X(1) = 2.260492505855460$</td>
<td>$X(1) = 9.48287491 \times 10^{-1}$</td>
<td>$X(2) = 9.48287491 \times 10^{-1}$</td>
<td>$X(2) = 3.310103184$</td>
<td>$X(1) = 2.874488000 \times 10^{-1}$</td>
<td>$X(2) = 2.261152698279501$</td>
<td>$X(2) = -12.6174951096179$</td>
<td>$X(1) = 2.261152698279501$</td>
</tr>
</tbody>
</table>

**Figure 7.** Homotopy pathway for Example 1 employing $x^0 = [1, 1]^T$

**Figure 8.** Homotopic pathway for Example 2 employing $x^0 = [-0.5, -e]^T$
CONCLUSIONS

The results show that with proper selection of monitoring parameters (maximum number of iterations in Newton corrections, Tolerances, step length increases, numerical algorithms for update the radius of the hyperspheres, among others), the location of all the roots placed on a homotopy path in particular is guaranteed. It should also be noted that the mathematical approach and monitoring of the implementation of the hyperspherical predictors is simpler than the approaches currently used, most authors who have recently published advances in the field (Rheinboldt, 2000; Moon and Linninger, 2009; Khaleghi, et al., 2010) employ public subroutines (Rheinboldt and Burkhardt, 1983; Watson et al., 1997; Dhooge et al., 2006, among others) based on differential tracking with a large number of controls and auxiliary algorithms to ensure “no jumps” and numerical stability during the continuation process. The hyperspherical path tracking represents a robust alternative with verified properties of convergence and simple to implement.

REFERENCIAS


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