Visualization of Homotopy's and Their Properties

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Homotopy Continuation

Homotopy continuation, like Newton's method, is an iterative approach for finding the (approximate) isolated complex roots of a polynomial (or solutions to a system of polynomials). But unlike Newton's method this process guarantees every isolated root will be found if seeded by a finite number of appropriately chosen starting points.

One of the nicest (in my opinion) mathematical algorithms is:

n-dimensional Newtons Method

Let $\mathbf{F} \in \mathbb{Q}[x_1, \ldots, x_n]^n$ and $\mathbf{x}_0 \in \mathbb{C}^n$. If we iterate as

$$\mathbf{x}_i = \mathbf{x}_{i-1} - \left[\mathrm{Jac}(\mathbf{F})|_{\mathbf{x}_{i-1}}\right]^{-1} F(\mathbf{x}_{i-1})$$

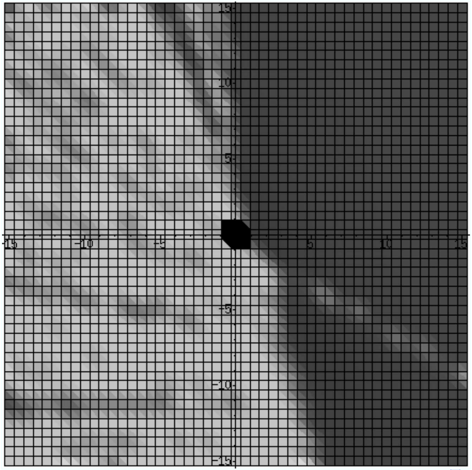
then we will eventually produce $\mathbf{x}_N$, $N \neq \infty$, such that

$$|\mathbf{F}(\mathbf{x}_N) - \mathbf{F}(\mathrm{RootOf}(F))| < \varepsilon$$

for $\varepsilon > 0$.

(This assumes a bunch of things, like infinite precision and non-singular Jacobian, but let's not get bogged down by details).

However, the selection of the starting point $\mathbf{x}_0$ is (too) crucial. Below is a density plot measuring speed of convergence for the system $\mathbf{F} = \left\langle x^2 - \frac{1}{2}y^2 - 2, 2x^2 + xy - 3x - 1 \right\rangle$.



Question.

Can we devise a method to generate better $\mathbf{x}_0$'s (initial guesses)?

Sure we can! Let $\mathbf{p}(z), \mathbf{q}(z) \in \mathbb{Q}[x_1, \ldots, x_n]^n$ (now $z = \mathbf{x}$, to stay consistent with textbook) and $t \in \mathbb{R}$, consider

$$H(z, t) = t\mathbf{q}(z) + (1 - t)\mathbf{p}(z).$$

Suppose that $H(z, 1) = \mathbf{q}(z)$ is exactly solvable and $H(z, 0) = \mathbf{p}(z) = \langle f_1, \ldots, f_n \rangle$ is the system of polynomials we would like to solve. Then $H(z, t)$ is a homotopy relating connecting roots of $\mathbf{q}$ with $\mathbf{p}$.

Now we would like to follow the homotopy paths from $t = 1$ to $t = 0$ using:

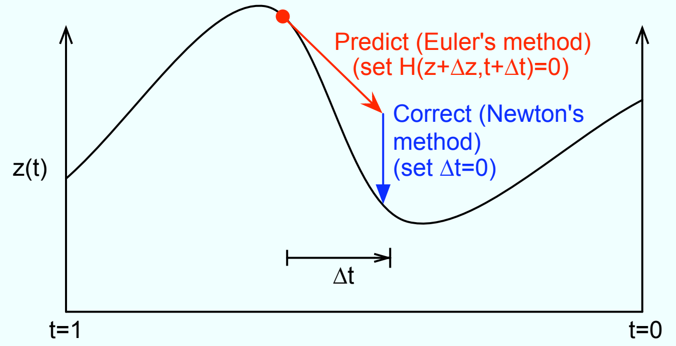
The first order taylor expansion of $H(z, t)$

$$H(z + \Delta z, t + \Delta t) = H(z, t) + H_z(z, t)\Delta z + H_t(z, t)\Delta t.$$

Given (z_i, t_i) such that $H(z_i, t_i) \approx 0$ one can predict a new approximate solution $(z_{i+1}, t_{i+1}) = (z_i + \Delta z, t_i + \Delta t)$ by substituting into the taylor expansion:

$$H(z_i + \Delta z, t_i + \Delta t) = H(z_i, t_i) + H_z(z_i, t_i)\Delta z + H_t(z_i, t_i)\Delta t$$

and solving for Δz (remember, we know the value Δt and want $H(z_{i+1}, t_{i+1}) = 0$).



$\Delta z = -H_z^{-1}(z_1, t_1)H_t(z_1, t_1)\Delta t \Rightarrow z_{i+1} = z_i + \Delta z.$

But remember Euler's method is bad so $H(z_{i+1}, t_{i+1})$ could be farther from zero than we would prefer. So we can refine the solution ("correct") by Newton's method. Fortunately we have a good starting point, (z_{i+1}, t_{i+1})! We update:

$z'_{i+1} = -H_z^{-1}(z_1 + \Delta z, t_1)H(z_1, t_1)$

Some thoughts on implementation

Step length (Δt) Double on three to five success (of corrector), half on a fail (of corrector).

Testing for explosions Monitor that Δt isn't too small. Divergent paths may actually fix themselves. When to cut a path off is a important question.

Refine Use Newton's method to refine the solution at the $t \approx 0$.

The bad news:

Start systems Choosing one is non-trivial because we can not tell exactly how many roots the target system has. This results in wasted computation.

Multiple roots Newton's method converges slowly to such roots.

Intersecting paths* A tracker may actually *jump paths* and converge to the wrong root.

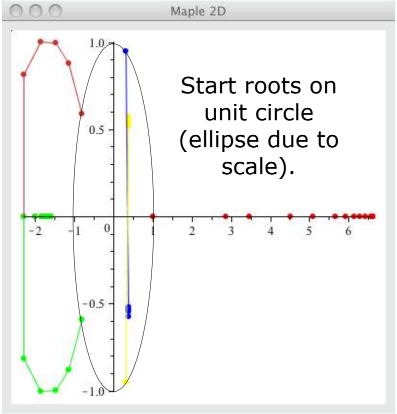
Unlucky corrections* Newton's method is not guaranteed to converge to the root you want.

path jumping

An example where path tracking fails:

$$-7x^5 + 22x^4 - 55x^3 - 94x^2 + 87x - 56$$

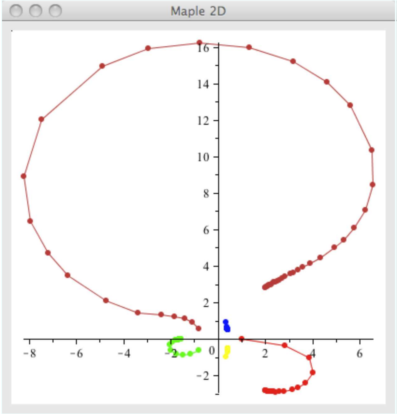
The brown and green paths converge to the real root -1.6 whereas the blue and yellow paths converge to the complex root 0.4-0.5i. The red root is escaping to infinity and is (quickly) flagged as a failed path. We do not find all roots.

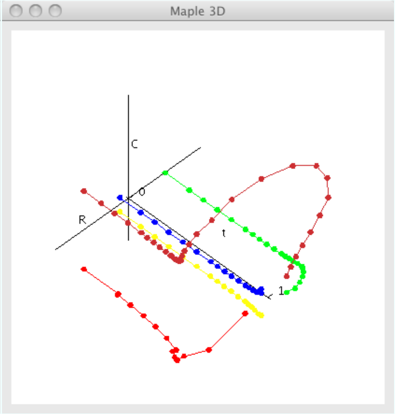


One can guarantee (with probability 1) that we find *all* roots. Let's introduce the random components, $\theta, \phi \in [-\pi, \pi]$ and modify our original homotopy to $q(z) = te^{i\theta}(z^d - e^{i\phi})$.

The addition of ϕ allows us to place our roots along separate great circles of the sphere S^2 given by the co-ordinates (θ, ϕ). The paths now travel through the interior of the sphere and can only collide within a set of measure 0 (i.e. with probability one).

Now we see that the paths are (more or less) well behaved. Note, in the diagrams the paths start from the unit circle.



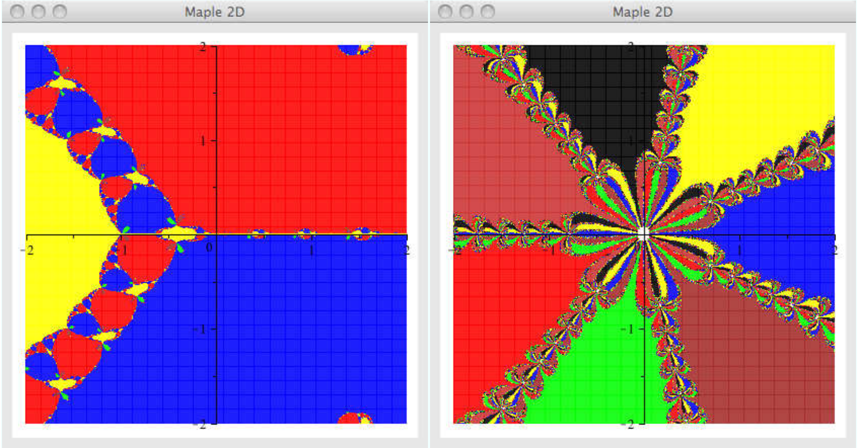


unlucky corrections

Newton's method will converge to different roots depending on what initial value it is seeded. We say **Basin of attraction of a root** = { initial points yielding the root }.

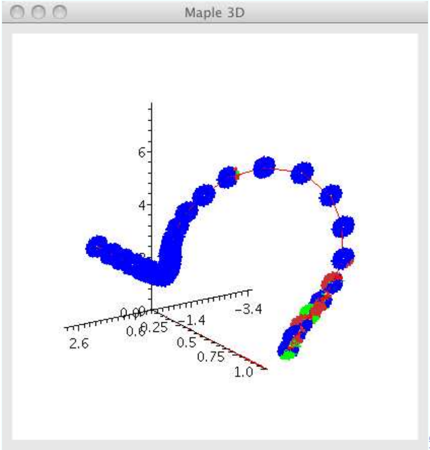
Thereby, Newton's method can throw the path of course by converging to the wrong root. Unfortunately it is hard to predict if this is going to happen.

Why? Because...

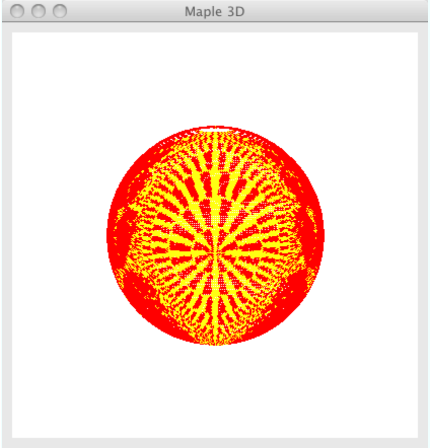


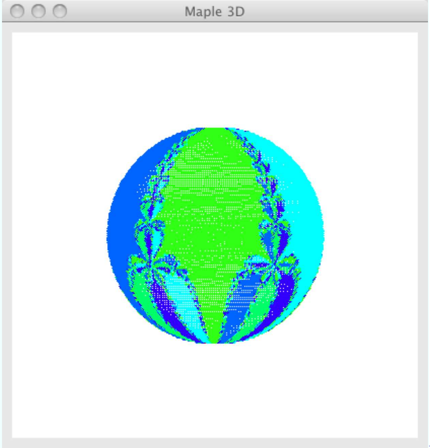
The basin of attraction for $-7x^5 + 22x^4 - 55x^3 - 94x^2 + 87x - 56$ and $x^7 - 1$. In both cases we see that the boundaries are fractal in nature, and therefore hard to study.

Below is what we call a **tube of attraction**. For the brown path of $-7x^5 + 22x^4 - 55x^3 - 94x^2 + 87x - 56$ we plot a small disc basin for each time step. Notice how the path stabilized when the basin is dominated by one root.



To visualize the basin for the *entire* complex plane (because it looks cool) we use a stereographic projection to plot it on the Riemann sphere. From left to right is the basin of attraction for $x^3 - 1$ and $x^5 + 1$.





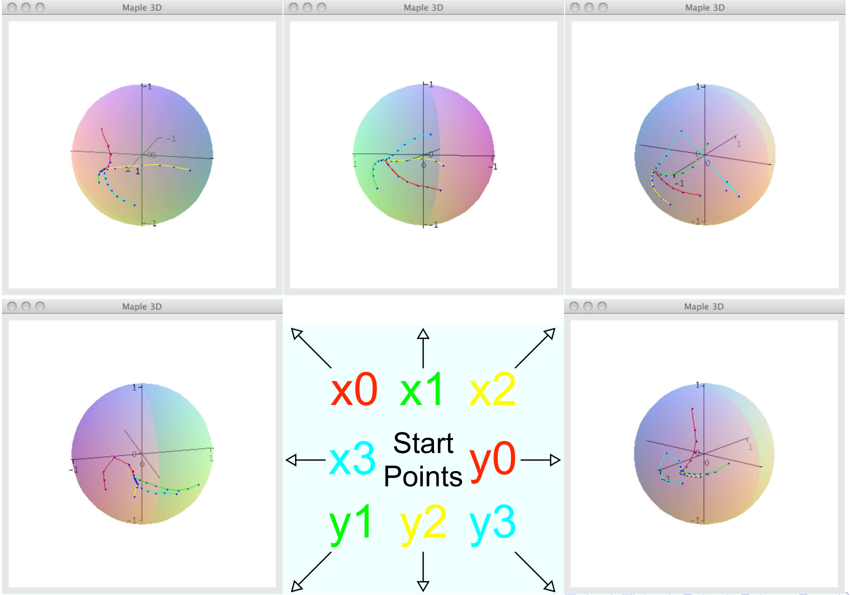
A phenomena we do not observe in the univariate case is diverging paths. Consider the target system

$$p(z) = \left[\begin{array}{c} x^3 y + x y^2 + 1 \\ x^4 + x y^2 + 1 \end{array} \right]$$

Now $\frac{\partial H}{\partial z}$ (the Jacobian) can become singular and our predictor will point to infinity.

To visualize this we again use stereographic projection to plot the paths on a Riemann sphere so we may see paths converge to infinity (the north pole).

The target system $p(z)$ may have up to 16 roots so we must track 16 paths. This is illustrated on the next slide. All possible pairs (x_i, y_j) with $0 \leq i, j \leq 3$ constitute our 16 start points. Each sphere represents a path that a single component of the solution (x or y) takes. We will observe that half the paths diverge.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Maple 3D
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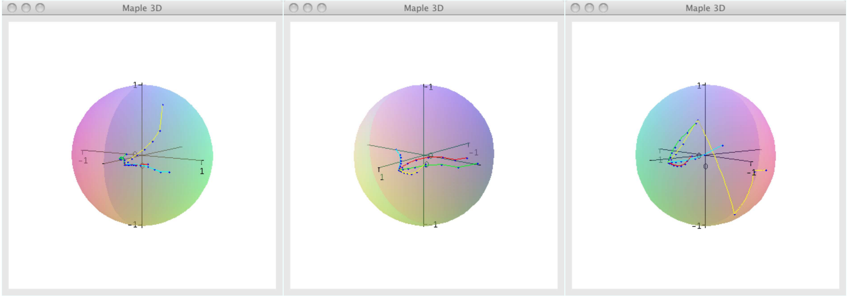
Maple 3D
x0 x1 x2
x3 Start Points y0
y1 y2 y3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The End.