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Parallel Homotopy Continuation in Julia

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1 Introduction

Homotopy Continuation is a numerical method for solving systems of polynomial equations. It is based on the idea of "deforming" a given system of equations into a simpler one whose solutions are known, and then tracking the solutions of the original system as the deformation is undone.

In this project, the method will be implemented in the Julia programming language, which is particularly suited for scientific computing. The primary source for this report is [1], where the method is explained in much more detail.

2 Homotopy Continuation

We will only consider square systems of polynomial equations, i.e. systems of n polynomial equations in n variables, although or over- or under-determined systems can often be solved by reducing them to square systems, by respectively choosing a suitable square subsystem or squaring it by adding equations. Morever, we will restrict ourselves to systems which have isolated solutions, i.e. zero-dimensional varieties.

There are many ways to choose the "simpler" system, from now on called a *start system*, but in general we can observe that, by Bezout's theorem, a system $F = (f_1, \ldots, f_n)$ has at most $D := d_1 \ldots d_n$ solutions, where d_i is the degre of $f_i(x_1, \ldots, x_n)$.

Therefore, we can build a start system of the same size and whose polynomials have the same degrees, but whose solutions are easy to find, and thus can be used as starting points for the method.

For instance, the system $G = (g_1, \dots g_n)$, where

$$g_i(x_1, \dots x_n) = x_i^{d_i} - 1,$$

is such a system, since its zero locus is obtained by combining the d_i -th roots of unity in each variable, which are exactly D points:

$$\left\{ \left(e^{\frac{k_1}{d_1}2\pi i}, \dots, e^{\frac{k_n}{d_n}2\pi i}\right), \text{ for } 0 \le k_i \le d_i - 1 \text{ and } i = 1, \dots, n \right\}.$$

2.1 Choosing the homotopy

The deformation between the original system and the start system is a homotopy, for instance the convex combination of F and G

$$H(x,t) = (1-t)F(x) + tG(x), (1)$$

where $x := (x_1, \ldots, x_n)$ and $t \in [0, 1]$. This is such that the roots of H(x, 0) = G(x) are known, and the roots of H(x, 1) = F(x) are the solutions of the original system (the reason why we place the start system at t = 0 and the original system at t = 1 is that we need higher numerical precision for the solutions of the original system, and there are more floating point numbers near to t = 0; see [1], p. 33). Therefore, we can implicitly define a curve z(t) in \mathbb{C}^n by the equation

$$H(z(t),t) = 0, (2)$$

so that in order to approximate the roots of F it is enough to numerically track z(t).

To do so, we derive the expression (2) with respect to t, and get the *Davidenko Differential Equation*

$$\frac{\partial H}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t} + \frac{\partial H}{\partial t} = 0,$$

where $\frac{\partial H}{\partial z}$ is the Jacobian matrix of H with respect to z:

$$\frac{\partial H}{\partial z} = \begin{pmatrix} \frac{\partial H_1}{\partial z_1} & \dots & \frac{\partial H_1}{\partial z_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial H_n}{\partial z_1} & \dots & \frac{\partial H_n}{\partial z_n} \end{pmatrix}.$$

This can be rewritten as

$$\dot{z} = -\frac{\partial H}{\partial z}^{-1} \frac{\partial H}{\partial t}.$$
 (3)

This is a system of n first-order differential equations, which can be solved numerically for z(t) as an initial value problem, which is called *path tracking*.

2.1.1 Gamma trick

While (1) is a fine choice of a homotopy, it's not what it's called a *good homotopy*: in order to ensure that the solution paths z(t) for different roots

- have no singularities, i.e. never cross each other for t > 0 (at t = 0 F could have singular solutions), and
- don't go to infinity for $t \to 0$ (as F could have a solution at infinity),

we can employ the *Gamma trick*: this consists in modifying the linear homotopy (1) by susbtituting the parameter $t \in [0, 1]$ with a complex curve q(t) connecting 0 and 1, such as

$$q(t) = \frac{\gamma t}{\gamma t + (1 - t)},$$

where $\gamma \in (0,1)$ is a random complex parameter.

This is a "probability one" procedure, i.e. for any particular system we can choose γ outside of a finite amount of rays through the origin to ensure that we get a good homotopy, basically because of the finiteness of the branch locus of the homotopy. After substituting, we have

$$H(x,t) = \frac{(1-t)}{\gamma t + (1-t)} F(x) + \frac{\gamma t}{\gamma t + (1-t)} G(x),$$

and by clearing denominators, we get our final choice of homotopy:

$$H(x,t) = (1-t)F(x) + \gamma tG(x). \tag{4}$$

2.2 Tracking down the roots

We then need to track down individual roots, following the solution paths from a root z_0 of the start system by solving the initial value problem associated to the Davidenko differential equation (3) with starting value z_0 and t ranging from 1 to 0.

This will be done numerically, by using a first-order predictor-corrector tracking method, whose typical iteration goes like this:

- **Predictor:** we first apply Euler's method to get an approximation \tilde{z}_i of the next value of the solution path;
- Corrector: we then use Newton's method to correct \tilde{z}_i using equation (2), so that it becomes a good approximation z_i of the next value of the solution path.

In the following sections, we go into more detail on each of these steps.

2.2.1 Predictor: Euler's method

Recall that Euler's method consists in approximating the solution of the initial value problem associated to a system of first-order ordinary differential equations

$$\begin{cases} \dot{z} = f(z, t) \\ z(t_0) = z_0 \end{cases}$$

by the sequence of points $(z_i)_{i\in\mathbb{N}}$ defined by the recurrence relation

$$z_{i+1} = z_i + h \cdot f(z_i, t_i),$$

where h is the step size. In the case of the Davidenko equation (3), we have

$$f(z,t) = -\left(\frac{\partial H}{\partial z}(z,t)\right)^{-1} \frac{\partial H}{\partial t}(z,t)$$

and $t_0 = 1$, since we are tracking from 1 to 0. For the same reason, we set

$$t_{i+1} = t_i - h$$
.

2.2.2 Corrector: Newton's method

Since we want to solve

$$H(z,t) = 0,$$

we can use Newton's method to improve the approximation $\tilde{z_i}$ obtained by Euler's method. This is done by moving towards the root of the tangent line of H at the current approximation, or in other words through the iteration

$$z_{i+1} = z_i - \left(\frac{\partial H}{\partial z}(z_i, t_{i+1})\right)^{-1} H(z_i, t_{i+1}),$$

where this time $z_0 = \tilde{z}_i$, with \tilde{z}_i and t_{i+1} obtained from the *i*-th Euler step.

Usually, only a few steps of Newton's method are needed; we chose a fixed number of 5 iterations. At which point, we use the final value of the Newton iteration as the starting value for the next Euler step.

2.2.3 Adaptive step size

In order to improve the efficiency of the method, we will use an adaptive step size, which is based on the norm of the residual of Newton's iteration. If the desired accuracy is not reached (say, when the norm of $H(z_i, t_i)$ is bigger than 10^{-8}), then we halve the step size; if instead we have 5 "successful" iterations in a row, we double the step size.

3 Testing the method

To test the method and its scalability, we first launched it on a single-threaded machine, then one a multi-threaded one, and finally parallelized it on a Cluster, whose specifications can be found in the Hardware section. The latter was done by using the Julia package <code>Distributed.jl</code> to parallelize the tracking of the roots on separate nodes, and the <code>SlurmClusterManager</code> package, which allows to run Julia code using the <code>Slurm</code> workload manager.

In order to scale the method to larger systems, we also implemented a random polynomial generator, which can be found in random-poly.jl; this was used to create the systems used to evaluate the performance of the parallel implementation.

For sake of visualization, a set of smaller tests was run, in addition to the parallel ones, on a single-threaded machine and a multi-threaded one (using the <code>@threads</code> macro from the *Threads.jl* package on the root tracking for loop in the file solve.jl); however the multi-threaded runs didn't improve the performance on these smaller systems, as the overhead of the multi-threading was too big compared to the actual computation time.

...perhaps because of our choice of predictor-corrector which could be unsuitable for larger systems.

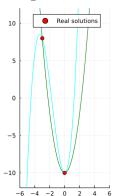
The Julia implementation for the tests described above can be found in Appendix B.

4 Appendix A: Results

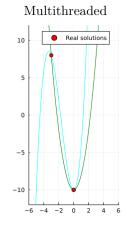
4.1 Single- vs Multi-threaded

Here are the plots for the solutions of four different 2x2 systems for the single-threaded and multi-threaded cases, with the corresponding systems and the real solutions shown in red.

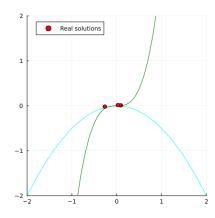
Single-threaded

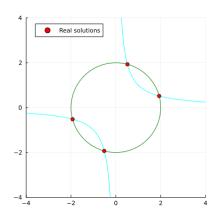


$$\begin{cases} x^3 + 5x^2 - y - 1 \\ 2x^2 - y - 1 \end{cases}$$

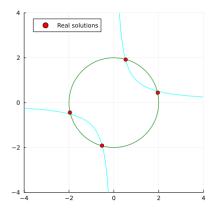


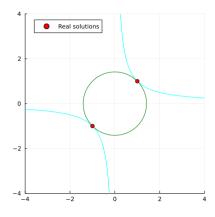
$$\begin{cases} x^2 + 2y \\ y - 3x \end{cases}$$



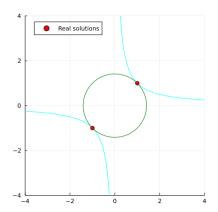


$$\begin{cases} x^2 + y^2 - 4 \\ xy - 1 \end{cases}$$





$$\begin{cases} x^2 + y^2 - 2\\ xy - 1 \end{cases}$$



4.2 Parallelization

Below are the plotted residual norms for the solutions of a randomly generated 3x3 system for the parallelized runs, compared with single-threaded runs for the same systems (the latter were run on a single node of the cluster):

The running times for the parallel runs are the following:

5 Appendix B: Implementation

5.1 Julia code

Listing 1: solve.jl

```
1 # External deps
 2 using LinearAlgebra
 3 using TypedPolynomials
 4 using Distributed, SlurmClusterManager
 5 slurm_manager = SlurmManager()
 6 addprocs(slurm_manager)
8 # Local deps
9 include("random-poly.jl")
10 include("plot.jl")
11 using .RandomPoly
11 using .RandomPoty
12 using .Plot
13 @everywhere begin
14 include("start-system.jl")
15 include("homotopy.jl")
16 include("euler-newton.jl")
17 include("adapt-step.jl")
18 end
     # Macros defined in an @everywhere block aren't available inside it
19
20 @everywhere begin
       using .StartSystem
22
       using .Homotopy
23
24
25
       using .EulerNewton
       using .AdaptStep
    end
26
27
    @everywhere function compute_root(H, r, maxsteps=200)
28
29
       step\_size = 0.001
       x0 = r
m = 0
30
31
32
33
       steps = 0
       while t > 0 && steps < maxsteps
         x0 = en_step(H, x0, t, step_size)
(m, step_size) = adapt_step(H, x0, t, step_size, m)
35
36
37
          t -= step_size
38
          steps += 1
39
       return (x0, steps)
41 end
42
    # Main homotopy continuation loop
function solve(F, G, roots)
43
44
45
       H = homotopy(F, G)
46
47
       result = Array{Future}(undef, length(roots))
48
       for i in eachindex(roots)
49
50
        result[i] = @spawnat :any compute_root(H, roots[i])
51
       sols = Array{ComplexF64,2}(undef, length(roots), length(F))
       steps = Array{Int64}(undef, length(roots))
```

```
for i in eachindex(roots)
            (solution, step_array) = fetch(result[i])
 55
            sols[i, :] = solution
steps[i] = step_array
 56
 57
 58
  59
 60
         return (sols, steps)
 61 end
 62
 63 # @polyvar x y

64 # C = [x^3 - y + 5x^2 - 10, 2x^2 - y - 10]

65 # Q = [x^2 + 2y, y - 3x^3]

66 # F = [x^2 + 1, x^2 + y^2 - 4]
  67 # T = [x*y - 1, x^2 + y^2 - 2]
 68
 69 R = random_system(5, 5)
70 println("System: ", R)
 71 (G, roots)=start_system(R)
72 println("Number of roots: ", length(roots))
 73
 74 # Parallel execution
 75 println("PARALLEL")
 76 @time begin
         (sol, steps) = solve(R, G, roots)
 78 end
 79 println("Number of steps: ", steps)
80 # converting sR to array of arrays instead of a matrix
81 sol = [sol[i, :] for i in 1:length(sol[:, 1])]
 82 sol = filter(u -> imag(u[1)) < 0.1 && imag(u[2]) < 0.1, sol)
83 sol = map(u -> real.(u), sol)
  84 vars = variables(R)
  85 println("Solutions: ", sol)
 86 println("Norms (lower = better): ", [norm([f(vars => s) for f in R]) for s in
              sol])
 87
 88 # Single execution
 89 println("SINGLE")
  90
      wait(rmprocs(workers()))
 91 @time begin
        (sol, steps) = solve(R, G, roots)
 92
 93 end
 94 println("Number of steps: ", steps)
95 # converting sR to array of arrays instead of a matrix
 96 sol = [sol[i, :] for i in 1:length(sol[:, 1])]
 97 sol = filter(u \rightarrow imag(u[1]) < 0.1 && imag(u[2]) < 0.1, sol)
 98 sol = map(u -> real.(u), sol)
99 vars = variables(R)
100 println("Solutions: ", sol)
101 println("Norms (lower = better): ", [norm([f(vars => s) for f in R]) for s in
              sol])
102
103 # See https://github.com/kleinhenz/SlurmClusterManager.jl/issues/11
104 finalize(slurm_manager)
105
106 # Plotting the system and the real solutions
107 # ENV["GKSwstype"] = "nul"
107 # ENV["GKSwstype"] = "nul"

108 # plot_real(sC, C, 6, 12, "1")

109 # plot_real(sQ, Q, 2, 2, "2")

110 # plot_real(sF, F, 4, 4, "3")

111 # plot_real(sT, T, 4, 4, "4")

112 # plot_real(sol, R, 5, 5, "random")
```

Listing 2: start-system.jl

```
1 module StartSystem
2 using TypedPolynomials
3
4 export start_system
5
6 # Define start system based on total degree
```

```
function start_system(F)
degrees = [maxdegree(p) for p in F]
G = [x.i^d - 1 for (d, x.i) in zip(degrees, variables(F))]
T = [[exp(2im*pi/d)^k for k=0:d-1] for d in degrees]
roots = vec([collect(root) for root in collect(Iterators.product(r...))])
return (G, roots)
dend
end
```

Listing 3: homotopy.jl

Listing 4: homogenize.jl

```
1 module Homogenize
      using TypedPolynomials
3
4
      export homogenize, homogenized_start_system
5
      function homogenize(F)
 8
        return [sum([h^(maxdegree(p)-maxdegree(t))*t for t in p.terms]) for p in F
9
10
11
      function homogenized_start_system(F)
12
        degrees = [maxdegree(p) for p in F]
13
        @polyvar h
        r = [[exp(2im*pi/d)^k for k=0:d-1] for d in degrees]
roots = vec([vcat(collect(root), 1) for root in collect(Iterators.product(r ...))])
14
15
16
17
        return (G, roots)
18
      end
19 end
```

Listing 5: euler-newton.jl

```
1 module EulerNewton
2    using LinearAlgebra
3    using TypedPolynomials
4
5    export en_step
6
7    # Euler-Newton predictor-corrector
8    function en_step(H, x, t, step_size)
9
10    # Predictor step
11    vars = variables(H(t))
12    # Jacobian of H evaluated at (x,t)
13    JH = [jh(vars=>x) for jh in differentiate(H(t), vars)]
```

```
# \partial H/\partial t is the same as \gamma G-F=H(1)-H(0) for our choice of homotopy \Delta x = JH \ -[gg(vars=>x) for gg in H(1)-H(0)]
15
16
17
              xh = x + \Delta x * step\_size
18
              # Corrector step
19
              JHh=differentiate(H(t-step_size), vars)
20
              for _ in 1:5
21
22
                \begin{array}{lll} & \exists H = [jh(vars=>xh) \ \ \mbox{for jh in JHh}] \\ \Delta x = \exists H \ \ -[h(vars=>xh) \ \mbox{for h in H(t-step\_size)}] \\ & xh = xh \ + \Delta x \end{array} 
23
24
25
26
              return xh
27
          end
28 end
```

Listing 6: adapt-step.jl

```
1 module AdaptStep
    using LinearAlgebra
    using TypedPolynomials
    export adapt_step
5
6
    # Adaptive step size
    8
10
      if \Delta > 1e-8
11
12
        step = 0.5 * step
        m = 0
13
      else
14
        m+=1
15
        if (m == 4) \&\& (step < 0.05)
16
        step = 2 * step
17
         m = 0
18
        end
19
      end
20
21
      return (m, step)
22
23 end
```

Listing 7: random-poly.jl

```
1 module RandomPoly
        export random_system
 3
         using TypedPolynomials
 5
         using Random
 6
         using Distributions
        # Random polynomial of degree n in m variables
function random_poly(n, m)
   x = [TypedPolynomials.Variable{Symbol("x[$i]")}() for i in 1:m]
 8
10
11
            \label{local_monomial_powers} $$ monomial_powers=collect(Iterators.product([0:n for \_ in 1:m]...)) $$ monomials = [prod(x.^i) for i in monomial\_powers if sum(i) <= n && sum(i) !
12
13
14
15
            return sum(map(m -> rand(Normal()) * m, monomials))
16
17
        # Generate a system of m random polynomials in m variables
# of degree d_i randomly chosen between 1 and max_degree
function random_system(m, max_degree)
18
19
20
         d = rand(1:max_degree, m)
```

```
22    random_polys = [random_poly(d[i], m) for i in 1:m]
23
24    return random_polys
25    end
26    end
```

Listing 8: plot.jl

```
module Plot
      using Plots, TypedPolynomials
      export plot_real
       function plot_real(solutions, F, h, v, name)
         plot(xlim = (-h, h), ylim = (-v, v), aspect_ratio = :equal)
 8
         contour!(-h:0.1:h, -v:0.1:v, (x,y)->F[1](variables(F)=>[x,y]), \ levels=[0],\\
         cbar=false, color=:cyan)
contour!(-h:0.1:h, -v:0.1:v, (x,y)->F[2](variables(F)=>[x,y]), levels=[0],
cbar=false, color=:green)
 9
         scatter!([real(sol[1]) for sol in solutions], [real(sol[2]) for sol in
    solutions], color = "red", label = "Real solutions")
10
         png(joinpath("./plots", "solutions" * name))
12
13
      end
14 end
```

5.2 Hardware

For the single-threaded runs, the code was executed on a laptop with an Intel Core i7-3520M CPU @ 3.60GHz and 6 GB of RAM.

The multithreaded runs were tested on a desktop with an AMD FX-8350 CPU @ 4.00GHz with 4 cores and 8 threads, and 12 GB of RAM.

Finally, the parallel computations were run on a cluster with 20 nodes, each having a CPU @ 1.008GHz with 4 Performance cores, 2 efficiency cores and 4 GB of RAM.

References

- [1] Bates, Daniel J. Numerically solving polynomial systems with Bertini. SIAM, Society for Industrial Applied Mathematics, 2013.
- [2] https://docs.julialang.org/en/v1/stdlib/Distributed