Solving Polynomial Systems in the Cloud with Polynomial Homotopy Continuation*

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Abstract

Polynomial systems occur in many fields of science and engineering. Polynomial homotopy continuation methods apply symbolic-numeric algorithms to solve polynomial systems. We describe the design and implementation of our web interface and reflect on the application of polynomial homotopy continuation methods to solve polynomial systems in the cloud. Via the graph isomorphism problem we organize and classify the polynomial systems we solved. The classification with the canonical form of a graph identifies newly submitted systems with systems that have already been solved.

Key words and phrases. Blackbox solver, classifying polynomial systems, cloud computing, graph isomorphism, internet accessible symbolic and numeric computation, homotopy continuation, mathematical software, polynomial system, web interface.

1 Introduction

The widespread availability and use of high speed internet connections combined with relatively inexpensive hardware enabled cloud computing. In cloud computing, users of software no longer download and install software, but connect via a browser to a web site, and interact with the software through a web interface. Computations happen at some remote server and the data (input as well as output) are stored and maintained remotely. Quoting [27], "Large, virtualized pools of computational resources raise the possibility of a new, advantageous computing paradigm for scientific research."

This model of computing offers several advantages to the user; we briefly mention three benefits. First, installing software can be complicated and a waste of time, especially if one wants to perform only one single experiment to check whether the software will do what is desired — the first author of [28] has an account on our web server. In cloud computing, the software installation is replaced with a simple sign up, as common as logging into a web store interface. One should not have to worry about upgrading installed software to newer versions. The second

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advantage is that for computationally intensive tasks, the web server can be aided by a farm of compute servers. Thirdly, the input and output files are managed at the server. The user should not worry about storage, as the web server could be aided by file servers. A good web interface helps to formulate the input problems and manage the computed results.

In this paper, we describe a prototype of a first web interface to the blackbox solver of PHC-pack [31]. This solver applies homotopy continuation methods to polynomial systems. Its blackbox solver, available as phc -b at the command line, seems the most widely used and popular feature of the software. Our web interface is currently running at https://kepler.math.uic.edu.

In addition to the technical aspects of designing a web interface, we investigate what it means to run a blackbox solver in the cloud. Because the computations happen remotely, the blackbox solver not only hides the complexity of the algorithms, but also the actual cost of the computations. In principle, the solver could use just one single core of a traditional processor, or a distributed cluster of computers, accelerated with graphics processing units [34], [35]. One should consider classifying the hardness of an input problem and allocating the proper resources to solve the problem. This classification problem could be aided by mining a database of solved problems.

To solve the classification problem we show that the problem of deciding whether two sets of support sets are isomorphic can be reduced to the graph isomorphism problem [21], [22]. Our classification problem is related to the isomorphism of polynomials problem [24] in multivariate cryptology [5], [10]. Support sets of polynomials span Newton polytopes and a related problems is the polytope isomorphism problem, see [18] for its complexity, which is as hard as the graph isomorphism problem.

2 Related Work and Alternative Approaches

The Sage notebook interface and the newer SageMathCloud can be alternative solutions to setting up a standalone cloud service. PHCpack is an optional package in Sage [30], available through the phc.py interface, developed by Marshall Hampton and Alex Jokela, based on the earlier efforts of Kathy Piret [26] and William Stein. We plan to upgrade the existing phc.py in Sage with phcpy [32].

The computational algebraic geometry software Macaulay2 [13] distributes PHCpack.m2 [14], which is a package that interfaces to PHCpack. Macaulay2 runs in the cloud as well. Below are the input commands to the version of Macaulay2 that runs online. The output is omitted.

Macaulay2, version 1.6

```
i1 : loadPackage "PHCpack";
i2 : help(PHCpack);
i3 : help solveSystem;
i4 : R = CC[x,y,z];
i5 : S = {x+y+z-1, x^2+y^2, x+y-z-3};
i6 : solveSystem(S)
```

3 Design and Implementation

All software in this project is free and open source, as an application of the LAMP stack, where LAMP stands for Linux, Apache, MySQL, and Python. Our web server runs Red Hat Linux, Apache [6] as the web server, MySQL [9] as the database, and Python as the scripting language. Our interest in Python originates in its growing ecosystem for scientific computing [25]. In our current implementation we do not take advantage of any web framework. Our web interface consists mainly of a collection of Python CGI scripts.

We distinguish three components in the development of our web interface: the definition of the database, the sign up process, and the collection of Python scripts that are invoked as the user presses buttons. In the next three paragraphs we briefly describe these three components.

MySQL is called in Python through the module MySQLdb. The database manages two tables. One table stores data about the users, which includes their encrypted passwords and generated random names that define the locations of the folders with their data on the server. In the other table, each row holds the information about a polynomial system that is solved. In this original setup, mathematical data are not stored in the database. Every user has a folder which is a generated random 40-character string. With every system there is another generated 40-character string. The Python scripts do queries to the database to locate the data that is needed.

When connecting to the server, the index.html leads directly to the Python script that prints the first login screen. The registration script sends an email to the first time user and an activation script runs when that first time user clicks on the link received in the registration email.

The third component of the web interface consists of the Python scripts that interact with the main executable program, the phc built with the code in PHCpack. Small systems are solved directly. Larger systems are placed in a queue that is served by compute servers.

4 Solving by Polynomial Homotopy Continuation

When applying polynomial homotopy continuation methods to solve polynomial systems, we distinguish two different approaches. The first is the application of a blackbox solver, and the second is a scripting interface.

4.1 Running a Blackbox Solver

For the blackbox solver, the polynomials are the *only* input. The parameters that control the execution options are set to work well on a large class of benchmark examples; and/or tuned automatically during the solving. While the input is purposely minimal, the output should contain various diagnostics and checks. In particular, the user must be warned in case of ill conditioning and nearby singularities. The form of the output should enable the user to verify (or falsify) the computed results.

The current blackbox solver phc -b was designed in [31] for square problems, that is, systems with as many equations as unknowns. Polyhedral homotopies [15] [33] are optimal for sparse polynomial systems. This means that the mixed volume is a sharp root count for generic problems (phc -b calls MixedVol [12] for a fast mixed volume computation). Every path in a polyhedral

homotopy ends at an isolated root, except for systems that have special initial forms [16]. For a survey, see e.g. [20].

Special cases are polynomials in one variable, linear systems, and binomial systems. A binomial system has exactly two monomials in every polynomial. Its isolated solutions are determined by a Hermite normal form of the exponent vectors. Its positive dimensional solution sets are monomial maps [1].

A more general blackbox solver should operate without any assumptions on the dimension of the solution sets. Inspired by tropical algebraic geometry, and in particular its fundamental theorem [17], we can generalize polyhedral homotopies for positive dimensional solution sets, as was done for the cyclic n-roots problems in [2], [3]. This general polyhedral method computes tropisms based on the initial forms and then develops Puiseux series starting at the solutions of the initial forms.

4.2 The Scripting Interface phopy

The Python package phcpy replaces the input and output files by persistent objects. Instead of the command line interface of phc with its interactive menus, the user of phcpy runs Python scripts, or calls functions from the phcpy modules in an interactive Python shell. Version 0.1.4 of phcpy is described in [32].

The current version 0.2.5 exports most of the tools needed to compute a numerical irreducible decomposition [29]. With a numerical irreducible decomposition one gets all solutions, the isolated solutions as well as the positive dimensional sets. The latter come in the form of as many generic points as the degree of each irreducible component, satisfying as many random hyperplanes as the dimension of the component.

5 Pattern Matching with a Database

Solving a system of polynomial equations for the first time with polynomial homotopy continuation happens in two stages. In the first stage, we construct and solve a simpler system than the original problem. This simpler system serves as a start system to solve the original system in the second stage. Polynomial homotopy continuation methods deform systems with known solutions into systems that need to be solved. Numerical predictor-corrector methods track solution paths from one system to another.

In many applications polynomial systems have natural parameters and often users will present systems with the same input patterns.

5.1 The Classification Problem

If we solve polynomial systems by homotopy continuation, we first solve a similar system, a system with the same monomial structure, but with generic coefficients. If we could recognize the structure of a new polynomial system we have to solve, then we could save on the total solving time of the new polynomial system, because we skip the first stage of solving the start system.

Furthermore, we could give a prediction of the time it will take to solve the new system with the specific coefficients.

Giving a name such as cyclic n-roots as a query to a search engine is likely to come up with useful results because this problem has been widely used to benchmark polynomial system solvers. But if one has only a particular formulation of a polynomial system, then one would like to relate the particular polynomials to the collection of polynomial systems that have already been solved. Instead of named polynomial systems, we work with anonymous mathematical data where even the naming of the variables is not canonical.

For example, the systems

$$\begin{cases} x^2 + xy^2 - 3 = 0 \\ 2x^2y + 5 = 0 \end{cases} \text{ and } \begin{cases} 3 + 2ab^2 = 0 \\ b^2 - 5 + 2a^2b = 0 \end{cases}$$
 (1)

must be considered isomorphic to each other

The support set of a polynomial is the set of all exponent tuples of the monomials that appear in the polynomial with nonzero coefficient. For the systems in the specific example above, the sets of support sets are

$$\{\{(2,0),(1,2),(0,0)\},\{(2,1),(0,0)\}\}\tag{2}$$

and
$$\{\{(0,0),(1,2)\},\{(0,2),(0,0),(2,1)\}\}.$$
 (3)

Definition 5.1. We say that two sets of support sets are *isomorphic* if there exists a permutation of their equations and variables so that the sets of support sets are identical.

The problem is then to determine whether the sets of support sets of two polynomial systems are isomorphic to each other. This problem is related to the isomorphism of polynomials problem [24]. Algorithms in multivariate cryptology apply Gröbner basis algorithms [10] and graph-theoretic algorithms [5].

5.2 The Graph Isomorphism Problem

If we encode the sets of support sets of a polynomial system into a graph, then our problem reduces to the graph isomorphism problem, for which practical solutions are available [22] and accessible in software [21]. The problem of determining whether two sets of support sets are isomorphic is surprisingly nontrivial. We begin with some theoretical considerations before moving on to implementation.

Definition 5.2. The graph isomorphism problem asks whether for two undirected graphs F, G there is a bijection ϕ between their vertices that preserves incidence—i.e. if a and b are vertices connected by an edge in F, then $\phi(a)$ and $\phi(b)$ are connected by an edge in G.

Proposition 5.3. The problem of determining whether two sets of support sets are isomorphic is equivalent to the graph isomorphism problem.

Proof. We will give a constructive embedding in both directions.

 (\supseteq) We start by showing that graph isomorphism can be embedded in checking isomorphism of sets of support sets. Recall that the incidence matrix of a graph G = (V, E) is a matrix with

#V rows and #E columns where the $(i,j)^{th}$ entry is 1 if the i^{th} vertex and j^{th} edge are incident and 0 otherwise. It is straightforward to show that two graphs are isomorphic if and only if their incidence matrices can be made equal by rearranging their rows and columns.

Now suppose we have a graph with incidence matrix $A = (a_{ij})$. Construct a polynomial by considering the rows as variables and the columns as monomials. To be precise, set

$$p_A = \sum_j \prod_i x_i^{a_{ij}}.$$
 (4)

For example, if a graph has incidence matrix

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \text{then} \quad p_A = x_1 x_2 + x_1 x_3. \tag{5}$$

Switching two columns of the matrix corresponds to reordering the monomials in the sum; switching two rows corresponds to a permutation of variables. Therefore, to determine if two graphs are isomorphic, one may find their incidence matrices, form polynomials from them, and check if the polynomials (thought of as single-polynomial systems) are the same up to permutation of variables. Finally, it is important to note that this is a polynomial time reduction. To create the polynomial, start at the first column and iterate through all of the columns. When done with the first column, we have created the first monomial. Repeat this process for every column, touching every entry in the matrix exactly once. Given an incidence matrix of a graph G = (V, E) with #V = n, #E = m, converting to a polynomial requires $\mathcal{O}(nm)$ operations.

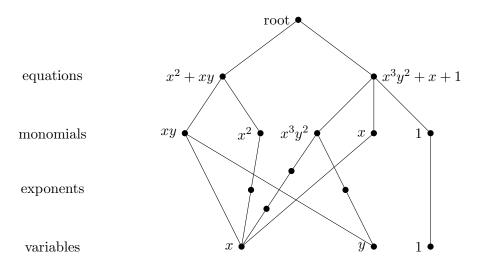


Figure 1: Basic graph from system

(\subseteq) We now show the other direction: checking isomorphism of sets of support sets can be embedded in graph isomorphism. To do so, we give a way of setting up a graph from a set of support sets, which is most easily seen via an example. The graph for the system $\{x^2 + xy, x^3y^2 + x + 1\}$ is shown in Figure 1. As can be seen from the diagram, we build a graph beginning with a root node to ensure the graph is connected. We attach one node for each equation, then attach

nodes to each equation for its monomials. Finally we put a row of variable nodes at the bottom and connect each monomial to the variables it contains via as many segments as the degree of the variable in the monomial.

At this point our graph setup is inadequate, as two different systems could have isomorphic graphs. Consider the graphs for $\{x,y\}$ and $\{x^4\}$, seen in Figure 2. Even though the systems are different, the graphs are clearly isomorphic. To remedy this, self-loops are added in order to partition the graph into root, equations, monomials, and variables by putting one self-loop at the root node, two on each equation node, etc. This graph will uniquely represent our system since any automorphism will be a permutation of nodes within their partitions. Partitioning by self-loops is possible because there are no self-loops in the initial setup. The graph in Figure 1 is drawn without the self-loops for the sake of readability.

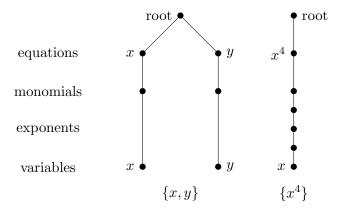


Figure 2: Isomorphic graphs

The time to complete this process is easily seen to be polynomial in the number of monomials and the sum of their total degrees.

Because we have shown that two sets of support sets are isomorphic if and only if two uniquely dependent graphs are isomorphic, and had previously shown that two graphs are isomorphic if and only if two uniquely dependent polynomials are equal up to rearranging variables, we are done. Note that this puts our problem in GI, the set of problems with polynomial time reduction to the graph isomorphism problem.

5.3 Computing Canonical Graph Labelings With Nauty

The graph isomorphism problem is one of the few problems which is not known to be P or NP-complete [22]. Although there is no known worst-case polynomial time algorithm, solutions which are fast in practice exist. One such solution is nauty [21], a program which is able to compute both graph isomorphism and canonical labelings. More information on nauty and other software for solving graph isomorphism can be found in [22].

Because nauty can incorporate the added information of ordered partitions, we chose to revise our setup to take advantage of this and minimize the number of nodes. Instead of using self-loops to partition the graph, we specify equations, monomials, and variables to be three of the partitions. We then check for which exponents occur in the system, and attach nodes representing

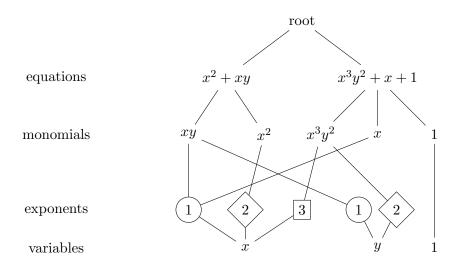


Figure 3: Nauty graph setup

these exponents to the variables where appropriate. Instead of using a sequence of nodes and edges to record the degree as we did in the proof, we instead attach monomials to these exponent nodes. We group these exponent nodes so that all the nodes representing the lowest exponent are in the first partition, all representing the second lowest are in the second partition, etc. The setup is shown in Figure 3, where the different shapes of the exponent nodes represent the distinct partitions.

If we couple this graph with an ordered list of the exponents that occur in the system, we once again have an object that uniquely represents the isomorphism class of our system. In addition, nauty works by computing the automorphisms of a graph and determining one of them to be canonical; the automorphisms must respect the partition, hence partitioning reduces the number of possibilities to check. So not only does this use fewer vertices and edges than our previous setup, but the use of partitions speeds up nauty's calculations.

Another advantage to using nauty is that it computes generators of the automorphism group of the graph. Some of these generators permute the equations and monomials. These are unimportant and may be discarded, but the generators that permute the variables are quite useful, as PHCpack has the ability to take advantage of symmetry in polynomial systems. If a system remains the same under certain changes of variables, runtime may be significantly decreased if this symmetry is passed to phc.

It is worth noting that by Frucht's theorem [11] and our Proposition 5.3 we immediately obtain that for any group G there is a polynomial system with G as its symmetry structure. If we want to actually find systems with particular structures this is fairly impractical, however, as the proof of Frucht's theorem uses the Cayley graph which has a node for every group element, meaning that a system built with this method would have a variable for every group element.

We are primarily interested in using nauty in the context of storing tuples of support sets in a database. Because of this, the canonical labeling feature is much more useful than the ability to check graph isomorphism—looking up a system in a database ought not be done by going through a list of systems and querying nauty as to whether they are isomorphic to the one we are looking

up, since this would be highly inefficient. Instead we simply parse the system into its graph form (including partition data), pass this information to nauty and compute the canonical labeling, and attach the exponent data, as a string, to nauty's output. This process gives us a string that uniquely corresponds to the isomorphism class of the system, which we can then store in a database.

5.4 Benchmarking the Canonization

Timings reported in this section were done on a 3.5 GHz Intel Core i5 processor in a iMac Retina 5K running version 10.10.2 of Mac OS X, with 16 GB RAM. Scripts are available at https://github.com/sommars/PolyGraph.

In order to design an intelligent storage system, it is necessary to know an upper bound of the length of the string. As polynomial systems can be arbitrarily large, leading to arbitrarily long strings from nauty, we chose to analyze a number of well known systems to act as benchmarks, giving us an idea of an upper bound. First, consider the cyclic n-root polynomial systems. These systems consist of n equations: $\sum_{i=1}^{n} \prod_{j=i}^{i+k} x_{j \mod n} = 0$ for k from 0 to n-2, and $x_1 \dots x_n-1=0$. For example, the cyclic-3 system is

$$\begin{cases} x_1 + x_2 + x_3 = 0 \\ x_1 x_2 + x_2 x_3 + x_3 x_1 = 0 \\ x_1 x_2 x_3 - 1 = 0. \end{cases}$$
 (6)

These systems have a lot of symmetry, so they are an interesting case for us to benchmark this process. We tested against both small and large values of n to gain a thorough understanding of how this system will be canonized. Experiments in small dimensions are summarized in Table 1. The computation time, an average of three trials, is quite fast, though the length of the string grows quickly. In comparison, note that the calculation of the root counts in the blackbox solver of PHCpack (which includes the mixed volume computation) for the cyclic 10-roots problems takes 48.8 seconds.

n	$_{ m time}$	#nodes	#characters
4	0.006	29	526
6	0.006	53	$1,\!256$
8	0.006	85	$2,\!545$
10	0.007	125	$5{,}121$
12	0.007	173	8,761

Table 1: Cyclic n-root benchmark for small n. For each n, its takes only milliseconds. We list the number of nodes in the graph and the length of the canonical form.

For large instances of cyclic n-roots, the exponential growth of the number of solutions increases so much that we may no longer hope to be capable of computing all solutions. Nevertheless, with GPU acceleration [?], we can manage to track a limited number of paths. Table 2 illustrates the relationship between the dimension n, the time, and the sizes of the data.

n	time	#nodes	#characters
16	0.010	293	20,029
32	0.045	1,093	$168,\!622$
48	0.265	$2,\!405$	601,702
64	1.200	4,229	$1,\!427,\!890$
80	4.316	$6,\!565$	2,778,546
96	15.274	9,413	4,784,390
112	38.747	12,773	8,595,408
128	80.700	16,645	13,094,752

Table 2: For larger values of the dimension of the cyclic n-root problem, times and sizes of the data start to grow exponentially.

Another interesting class of benchmark polynomial systems that we can formulate for any dimension is the computation of Nash equilibria [8]. We use the formulation of this problem as in [23]. The number of isolated solutions also grows exponentially in n. Table 3 summarizes our computational experiments. As before, the times represent an average of three trials.

n	time	#nodes	#characters
4	0.006	47	977
5	0.006	98	2,325
6	0.007	213	7,084
7	0.013	472	18,398
8	0.054	1,051	51,180
9	0.460	2,334	$134,\!568$
10	4.832	$5,\!153$	331,456
11	73.587	11,300	872,893
12	740.846	24,615	$2,\!150,\!512$

Table 3: The cost of the canonization for the Nash equilibria polynomial systems for increasing dimension n, with the running time expressed in seconds, the number of nodes, and the size of the canonical form.

Compared to the cyclic n-roots problem, the dimensions in Table 3 are just as small as in Table 1, but the time and sizes grow much faster for the Nash equilibria than for the cyclic n-roots. We suspect two factors. First, while structured, the Nash equilibria systems are not as sparse as the cyclic n-roots problems. Second, unlike the cyclic n-roots problem every equation in the Nash equilibria system has the same structure, so the full permutation group leaves the sets of support sets invariant.

We end with a system formulated by S. Katsura, see [4] and [19]. Table 4 shows the cost of the canonization of this system. Because there is no symmetry in the support sets, the cost of the canonization increases not as fast in the dimension n as with the other two examples.

The actual cost of the computation of the canonical form may serve as an initial estimate on the cost of solving the system.

n	time	#nodes	#characters
25	0.020	929	24,906
50	0.090	3,411	112,654
75	0.546	$7,\!454$	254,770
100	1.806	13,061	495,612
125	4.641	20,229	793,662
150	10.860	28,961	1,157,498
175	21.194	$39,\!254$	1,587,115
200	52.814	$51,\!111$	$2,\!082,\!562$
225	98.118	$64,\!529$	2,643,891

Table 4: The cost of the canonization of the Katsura system for increasing dimension n. The number of solutions for the n-dimensional version of the system equals 2^n .

5.5 Storing Labelings in a Database

There are many different ways to design a database to store a given set of information. We do not contend that this is necessarily the best way, but it is certainly an effective way of storing our uniquely identifying information that will lead to fast lookup. Consider the explicitly described schema in Figure 4.

Section	Name	Datatype	Description
	$n_node_variable$	INT	Number of variables nodes
Craph Nadas	$n_node_monomial$	INT	Number of monomial nodes
Graph Nodes	$n_node_equation$	INT	Number of equation nodes
	n_node_degree	INT	Number of degree nodes
Degree Set	n_degree	INT	Sum of all degrees
Degree Set	degrees	VARCHAR	Set of all degrees
	$graph_length$	INT	Length of complete graph
Graph	$graph_filename$	VARCHAR	Complete graph in file
Polynomial Info	$poly_filename$	VARCHAR	Information and Reference file for poly-
			nomial system

Figure 4: Database structure for polynomial system graph

Each of the data elements in it are used to partition the database from the previous elements, so it can be seen as a B-tree structure. For identifying whether or not a set of support sets is already in our database, this would lead to a search time of $O(\log n)$ [7].

6 Conclusions

The practical considerations of offering a cloud service to solve polynomial systems with polynomial homotopy continuation led to the classification problem of polynomial systems. To solve this

problem, we linked the isomorphism problem for sets of support sets to the graph isomorphism problem and applied the software nauty.

Although no polynomial time algorithm are known to solve the graph isomorphism problem, we presented empirical results from benchmark polynomial systems that the computation of a canonical form costs much less than solving a polynomial system.

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