

Survey of Methods for Solving Systems of Nonlinear Equations, Part I: Root-finding Approaches

Ilias S. Kotsireas
ikotsire@wlu.ca
Wilfrid Laurier University
Canada

Panos M. Pardalos
ppardalos@toxeus.org
Toxeus Systems LLC
Orlando, Florida, USA

Alexander Semenov
asemenov@ufl.edu
University of Florida
Gainesville, Florida, USA

William T. Trevena
wtrevena@ufl.edu
University of Florida
Gainesville, Florida, USA

Michael N. Vrahatis
vrahatis@math.upatras.gr
University of Patras
Patras, Greece

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Abstract

This paper presents a comprehensive survey of methods which can be utilized to search for solutions to systems of nonlinear equations (SNEs). Our objectives with this survey are to synthesize pertinent literature in this field by presenting a thorough description and analysis of the known methods capable of finding one or many solutions to SNEs, and to assist interested readers seeking to identify solution techniques which are well suited for solving the various classes of SNEs which one may encounter in real world applications.

To accomplish these objectives, we present a multi-part survey. In part one, we focus on root-finding approaches which can be used to search for solutions to a SNE without transforming it into an optimization problem. In part two, we will introduce the various transformations which have been utilized to transform a SNE into an optimization problem, and we discuss optimization algorithms which can then be used to search for solutions. In part three, we will present a robust quantitative comparative analysis of methods capable of searching for solutions to SNEs.

Keywords: systems of nonlinear equations, localization of zeros, computation of roots, topological degree, total number of solutions and extrema, interval methods, symbolic computation, tensor methods, homotopy methods

1 Introduction

This paper presents part one of a survey on methods for finding one or many solutions to a *system of nonlinear equations* (SNE):

$$F_m(x) = \Theta_m \equiv (0, 0, \dots, 0)^\top \iff \begin{cases} f_1(x_1, x_2, \dots, x_n) = 0, \\ f_2(x_1, x_2, \dots, x_n) = 0, \\ \vdots \\ f_m(x_1, x_2, \dots, x_n) = 0, \end{cases} \quad (1)$$

where $F_m = (f_1, f_2, \dots, f_m) : \mathcal{D}_n \subset \mathbb{R}^n \rightarrow \mathbb{R}^m$, where f_1, f_2, \dots, f_m are real-valued continuous or continuously differentiable functions on the domain \mathcal{D}_n , and where at least one of f_1, f_2, \dots, f_m is nonlinear. For example, consider the system of transcendental equations

$$F_2(x) = \Theta_2 \equiv (0, 0)^\top \iff \begin{cases} f_1(x_1, x_2) = x_1 - x_1 \sin(x_1 + 5x_2) - x_2 \cos(5x_1 - x_2) = 0, \\ f_2(x_1, x_2) = x_2 - x_2 \sin(5x_1 - 3x_2) + x_1 \cos(3x_1 + 5x_2) = 0, \end{cases} \quad (2)$$

which is comprised of two transcendental equations of two unknowns (See Figure 1).

Finding one or more solutions to a SNE is a challenging and ubiquitous task faced in many fields including chemistry [1, 2, 3], chemical engineering [4], automotive steering [5], power flow [6, 7], large-scale integrated circuit

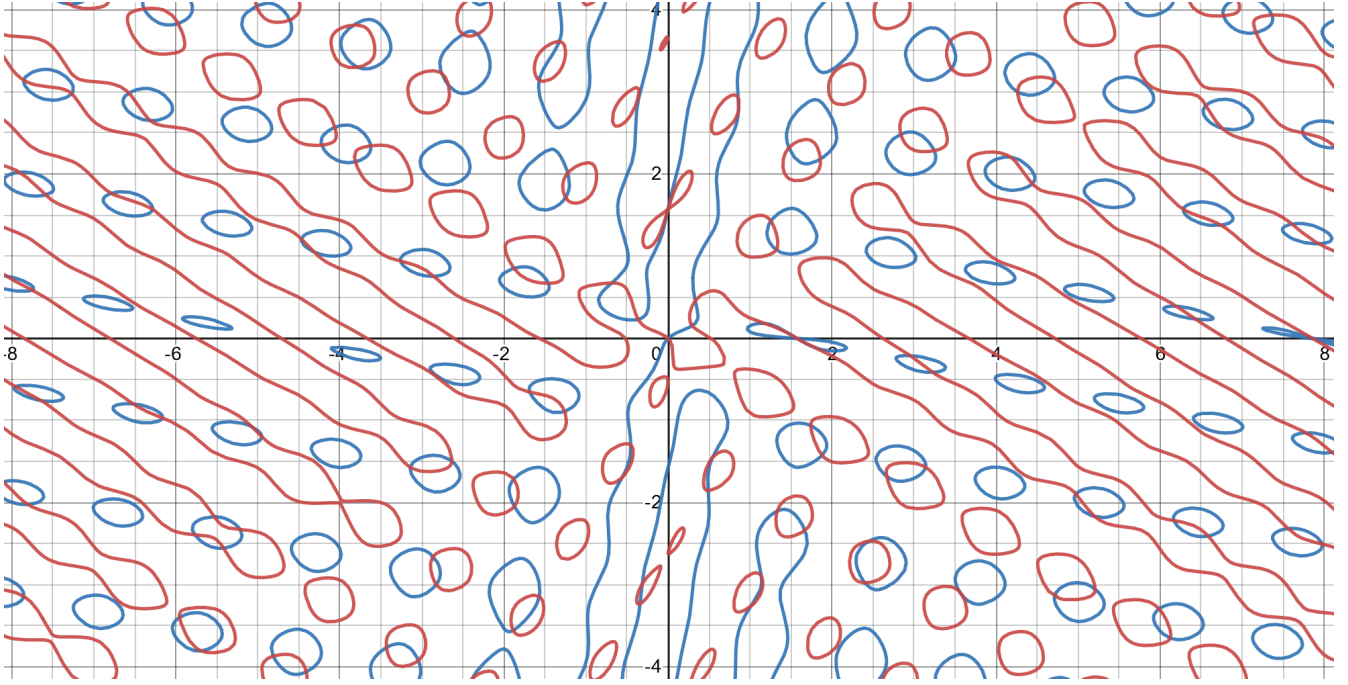


Figure 1: An example of a SNE with two transcendental equations of two unknowns as introduced by Eq. (2): (Blue): $f_1(x_1, x_2) = x_1 - x_1 \sin(x_1 + 5x_2) - x_2 \cos(5x_1 - x_2) = 0$; (Red): $f_2(x_1, x_2) = x_2 - x_2 \sin(5x_1 - 3x_2) + x_1 \cos(3x_1 + 5x_2) = 0$. Solutions to this SNE are defined as the points where the blue and red contours intersect. Finding all of the points within a certain region which satisfy both equations is a challenging task.

designs [8], climate modeling [9], materials engineering [10], robotics [11, 12, 13, 14], nuclear engineering [15], image restoration [16], protein interaction networks [8], neurophysiology [17], economics [18], finance [19], applied mathematics [20], physics [21], finding string vacua [22], machine learning [23, 24], geometric constraint solving (used in computer aided design) [25], and geodesy [26, 27] among others. The problem of solving even a system of polynomial equations has been proven to be NP-hard [28]. Furthermore, it has also been proven [29] that no general algorithm exists for determining whether an integer solution exists for a polynomial equation with a finite number of unknowns and only integer coefficients. The latter has been known as Hilbert’s 10th problem.

1.1 Notation / Scientific Style

Throughout this paper, we utilize $x = (x_1, x_2, \dots, x_n)^\top \in \mathcal{D} \subset \mathbb{R}^n$ to denote a real vector within the bounded domain \mathcal{D} . Furthermore, we utilize $x^* = (x_1^*, x_2^*, \dots, x_n^*)^\top \in \mathcal{D} \subset \mathbb{R}^n$ to denote a real solution to a SNE such that all equations in the SNE are satisfied ($F_m(x^*) = 0$). In an iterative method, we utilize $x^k = (x_1^k, x_2^k, \dots, x_i^k, \dots, x_n^k)^\top \in \mathcal{D} \subset \mathbb{R}^n$ for $k = 0, 1, \dots$ to denote the vector found during the k -th iteration of the iterative method. Here, x_i^k denotes the i -th coordinate of the vector x^k .

1.2 Terminology

Although we refer to Eq. (1) as a *system of nonlinear equations* (SNE), such systems have been referred to in a variety of different ways in literature. For example, articles [30, 31, 32, 33, 34, 35] utilize the abbreviation “SNLE” to refer to a *system of nonlinear equations*, and article [36] uses the abbreviation “SoNE”. Other papers refer to Eq. (1) as a *nonlinear system of equations*, and use the abbreviations “NSE” [37, 38] and “NLS” [39]. Eq. (1) has also been referred to as a *nonlinear equation system* (NES) [40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54]. The survey in article [55] uses the terminology *Nonlinear Equations* (NEs) to refer to a system of one or more nonlinear equations.

When $m > n$, a SNE can be referred to as an *overdetermined* SNE, and when $n > m$, a SNE can be referred to as an *underdetermined* SNE. When $m = n$, a SNE can be referred to as a *square* SNE [56]. Furthermore, a SNE is considered to be *consistent* if a solution exists which satisfies all equations [25].

For a *square*/ SNE, a *solution* $x^* = (x_1^*, x_2^*, \dots, x_n^*)^\top$ of the SNE $F_n(x) = \Theta_n$ or equivalently a *zero* x^* of

the function $F_n(x)$ or a root x^* of the function $F_n(x)$ is called *simple* if for the determinant of the corresponding Jacobian matrix:

$$J_{F_n}(x) \equiv F'_n(x)_{ij} \equiv \left\{ \frac{\partial f_i(x)}{\partial x_j} \right\}_{ij} \equiv \begin{bmatrix} \frac{\partial f_1(x)}{\partial x_1} & \frac{\partial f_1(x)}{\partial x_2} & \dots & \frac{\partial f_1(x)}{\partial x_n} \\ \frac{\partial f_2(x)}{\partial x_1} & \frac{\partial f_2(x)}{\partial x_2} & \dots & \frac{\partial f_2(x)}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n(x)}{\partial x_1} & \frac{\partial f_n(x)}{\partial x_2} & \dots & \frac{\partial f_n(x)}{\partial x_n} \end{bmatrix}, \quad (3)$$

at x^* it holds that $\det J_{F_n}(x^*) \neq 0$, otherwise it is called *multiple*. The problem of conservation and decomposition of a multiple root into simple roots in the case of systems of homogeneous algebraic equations has been tackled in [57]. This approach can be applied to high dimensional CAD where it is sometimes required to compute the intersection of several hypersurfaces that are a perturbation of a set of original unperturbed hypersurfaces.

When F_n satisfies the *monotonicity condition*:

$$(F_n(x) - F_n(y))^T (x - y) \geq 0, \quad \forall x, y \in \mathbb{R}^n, \quad (4)$$

the corresponding SNE can be referred to as a *system of monotone nonlinear equations* [58]. Furthermore, F_n is considered to be Lipschitz continuous if there exists $L > 0$ such that

$$\|F_n(x) - F_n(y)\|_2 \leq L\|x - y\|_2, \quad \forall x, y \in \mathbb{R}^n. \quad (5)$$

Many of the root finding methods described in Section 3 are guaranteed to converge to a solution when applied to SNEs that satisfy both the monotonicity and Lipschitz continuity conditions (the hybrid spectral methods introduced in [59] for example).

1.3 Comparison to other surveys

Other surveys discussing solution techniques for SNEs include [60] and [55]. We have decided to conduct this comprehensive literature review because many new solution techniques for SNEs have been introduced since the publication of [60] in 1994, and because the recent survey presented in [55] focuses mainly on methods which first convert a SNE into an optimization problem, and then search for multiple solutions to the optimization problem using *Intelligent Optimization Algorithms* (IOAs). The IOAs discussed in article [55] are primarily metaheuristics for global optimization. Although the survey in article [55] provides a very nice discussion of IOAs for solving SNEs reformulated as optimization problems, many of the IOAs they discuss are only introduced at a very high level, only eight IOAs were tested in their computational study, and the IOAs were evaluated on SNEs comprised of 20 equations or less. Also, article [55] only briefly mentions methods which can be used to search for solutions to SNEs without transforming them into optimization problems.

We would like to present a broader survey which covers in detail the large set of methods which can be used to solve a SNE without transforming it into an optimization problem (i.e. homotopy and symbolic computation methods). These methods are our main focus in part one of this survey. In part two, we will expand upon article [55] by introducing additional reformulation techniques and optimization algorithms which have been used to solve SNEs, and by discussing in much more detail many optimization algorithms which were only briefly introduced in article [55]. This will allow us to appropriately set the stage for the comprehensive empirical study we will present in part three of this survey. Furthermore, we believe it is imperative to introduce the reader to a technique for determining the number of solutions to a SNE that exist within a bounded domain. Such techniques are of critical practical importance for those interested in finding all solutions to a SNE that exist within a domain of interest.

1.4 Organization of this survey

We begin this survey by introducing a method which can be used to determine the total number of solutions to a SNE that exist within a given bounded domain. By determining the number of solutions to a SNE which exist within a bounded domain of interest, in the event that no solutions exist, one can avoid spending time and resources searching for solutions all together. Alternatively, if one knows that a specific number of solutions exist to a SNE within a bounded domain of interest, one can continue to search for solutions until the desired number of solutions are found. Next, we introduce root-finding methods which have been utilized in literature to search for solutions to a SNE without transforming it into an optimization problem. We conclude our paper by introducing additional methods which have been used to attempt to solve SNEs, and by highlighting promising areas for future research.

2 Determining the number of solutions to a SNE in a bounded domain

The knowledge of all the solutions of a system of nonlinear equations and/or all the extrema of a function is of major importance in various fields. The total number of the solutions of a system of nonlinear equations can be obtained by computing the topological degree. Suppose that the function $F_n = (f_1, f_2, \dots, f_n): \mathcal{D}_n \subset \mathbb{R}^n \rightarrow \mathbb{R}^n$ is defined and is two times continuously differentiable in a bounded domain \mathcal{D}_n of \mathbb{R}^n with boundary $b(\mathcal{D}_n)$. Suppose further that the solutions of $F_n(x) = \Theta_n$ are not located on $b(\mathcal{D}_n)$, and that they are simple (that the determinant of the Jacobian of F_n at these solutions is non-zero). Then the *topological degree of F_n at Θ_n relative to \mathcal{D}_n* is denoted by $\deg[F_n, \mathcal{D}_n, \Theta_n]$ and can be defined by the following relation:

$$\deg[F_n, \mathcal{D}_n, \Theta_n] = \sum_{x \in F_n^{-1}(\Theta_n)} \text{sgn det } J_{F_n}(x),$$

where $\det J_{F_n}(x)$ denotes the determinant of the Jacobian matrix and sgn defines the three-valued sign function. The above definition can be generalized when F_n is only continuous [61].

It is evident that, since $\deg[F_n, \mathcal{D}_n, \Theta_n]$ is equal to the number of simple solutions of $F_n(x) = \Theta_n$ which give positive determinant of the Jacobian matrix, minus the number of simple solutions which give negative determinant of the Jacobian matrix, then the total number N^s of simple solutions of $F_n(x) = \Theta_n$ can be obtained by the value of $\deg[F_n, \mathcal{D}_n, \Theta_n]$ if all these solutions have the same sign of the determinant of the Jacobian matrix. Thus, Picard considered the following extensions of the function F_n and the domain \mathcal{D}_n [62, 63]:

$$F_{n+1} = (f_1, f_2, \dots, f_n, f_{n+1}): \mathcal{D}_{n+1} \subset \mathbb{R}^{n+1} \rightarrow \mathbb{R}^{n+1}, \quad (6)$$

where $f_{n+1} = y \det J_{F_n}$, $\mathbb{R}^{n+1} : x_1, x_2, \dots, x_n, y$, and \mathcal{D}_{n+1} is the direct product of the domain \mathcal{D}_n with an arbitrary interval of the real y -axis containing the point $y = 0$. Then the solutions of the following system of equations:

$$\begin{aligned} f_i(x_1, x_2, \dots, x_n) &= 0, \quad i = 1, 2, \dots, n, \\ y \det J_{F_n}(x_1, x_2, \dots, x_n) &= 0, \end{aligned}$$

are the same simple solutions of $F_n(x) = \Theta_n$ provided that $y = 0$. Obviously, the determinant of the Jacobian matrix obtained for the function (6) is equal to $(\det J_{F_n}(x))^2$ which is always positive. Thus, the total number N^s of the solutions of the system $F_n(x) = \Theta_n$ can be obtained by the following value of the topological degree:

$$N^s = \deg[F_{n+1}, \mathcal{D}_{n+1}, \Theta_{n+1}].$$

For example, in the one dimensional case, using the above Picard's extensions it is proved that the total number of simple solutions N^s of the equation $f(x) = 0$, where $f: (a, b) \subset \mathbb{R} \rightarrow \mathbb{R}$ is twice continuously differentiable in a predetermined interval (a, b) , is given by the following relation [62, 63]:

$$N^s = -\frac{1}{\pi} \left[\varepsilon \int_a^b \frac{f(x) f''(x) - f'^2(x)}{f^2(x) + \varepsilon^2 f'^2(x)} dx + \arctan \left(\frac{\varepsilon f'(b)}{f(b)} \right) - \arctan \left(\frac{\varepsilon f'(a)}{f(a)} \right) \right], \quad (7)$$

where ε is a small positive constant. Note that N^s was shown to be independent of the value of ε . Also, the above approach can be applied for computing the number of multiple solutions. Obviously, the total number N^e of the extrema of $f \in C^3$ i.e. $x \in (a, b)$ such that $f'(x) = 0$ can be obtained using the above formula (7). For details of the topological degree we refer the interested reader to the books [64, 65, 66, 67, 61, 68]. Details of the computation of the value of the topological degree and its usefulness as well as some applications and issues related to the number of zeros can be found for example in [69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83].

Article [84] also discusses utilizing the topological degree to determine the existence of robust solutions to a SNE.

3 Root finding methods

This section discusses root finding methods which have been utilized to search for solutions to SNEs. Specifically, Section 3.1 - Section 3.10 discuss methods which have been utilized to search for a single solution to a SNE, and Section 3.11 discusses *deflation techniques* which can be used to compute further solutions. Some of the root finding methods introduced in this section are discussed in more detail than others, and after we introduce fundamental root finding methods, we place a particular emphasis on promising methods which do not appear to be widely

discussed in recent literature. We also briefly introduce some of the more well known root finding methods such as *Quasi-Newton methods*, and we cite relevant literature for the interested reader to refer to.

Although many of the root finding methods described in this section are guaranteed to converge to a solution when applied to SNEs that satisfy certain conditions such as monotonicity (Eq. (4)) and Lipschitz continuity (Eq. (5)), none of the methods described in this section are guaranteed to converge to a solution on all classes of SNEs. For example, the root finding method proposed in article [58] was proven to converge on systems of monotone nonlinear equations which satisfy additional regularity conditions, but the proposed method is not guaranteed to converge on all SNEs.

Many of the root finding methods discussed in this section are specialized at solving particular classes of SNEs. For example, Section 3.5 discusses a *tensor-free Chebyshev-Halley method* designed to solve SNEs that are large, sparse, and which may have ill-conditioned or singular Jacobian matrices at a solution [85].

3.1 Classical Newton's and Broyden's methods for finding a single solution

Newton's method [86, 87, 61, 88] for finding roots is a well known approach which can be utilized to find a single solution to a SNE. Starting at a "good" initial guess or approximate solution $x^0 = (x_1^0, x_2^0, \dots, x_n^0)^\top$ of a system of n nonlinear real equations in n real unknowns, when $F_n(x)$ is Lipschitz continuous and the Jacobian matrix $J_{F_n}(x)$ of $F_n(x)$ is available, Newton's method can be used to iteratively find elements of a sequence converging towards a true solution $x^* = (x_1^*, x_2^*, \dots, x_n^*)^\top$ with a quadratic rate of convergence. Newton's method attempts to calculate a new approximate solution x^{k+1} from x^k via

$$x^{k+1} = x^k - J_{F_n}(x^k)^{-1} F_n(x^k), \quad k = 0, 1, 2, \dots$$

Alternatively, instead of calculating the inverse of the Jacobian matrix, one often can solve the system of linear equations:

$$J_{F_n}(x^k) s^k = -F_n(x^k), \quad k = 0, 1, 2, \dots \quad (8)$$

to find the *Newton step* $s^k = x^{k+1} - x^k$. Thus, Newton's method using a initial guess x^0 for each iteration $k = 0, 1, 2, \dots$ performs the following steps:

- (a) **Solve:** the system of linear equation $J_{F_n}(x^k) s^k = -F_n(x^k)$ for s^k .
- (b) **Set:** $x^{k+1} = x^k + s^k$.

In many cases, Step (b) is given by $x^{k+1} = x^k + \lambda s^k$ where λ is selected to guarantee decrease in $\|F_n\|$ (see [87]).

Many expansions upon Newton's method for finding roots have been introduced in literature, and most of these expansions are focused on accelerating the rate of convergence. For example, articles [89, 90, 91, 92, 93, 94] present new techniques based upon Newton's method for finding roots and quadrature rules to accelerate convergence. Newton's method can also be augmented with higher order information to accelerate convergence towards an approximation of a true solution x^* . Overall, Newton's method for finding roots seeks to approximate the solution of a nonlinear system of equations by solving iteratively a sequence of systems of linear equations. In cases where the Jacobian matrix is singular, we refer the interested reader to articles [95, 96]. Convergence results for SNEs which have a Jacobian with a constant rank in the vicinity of a solution are presented in articles [97, 98]. Dimension-reducing modifications of Newton's method that are able to tackle efficiently and effectively, among others, almost linear systems can be found in [99, 100, 101, 102, 103].

In a similar approach, *Broyden's method* [104, 86, 87, 61, 88] using an initial guess x^0 and an initial matrix B_0 such that $\det B_0 \neq 0$, for each iteration $k = 0, 1, 2, \dots$ performs the following steps:

- (a) **Solve:** the system of linear equations $B_k s^k = -F_n(x^k)$ for s^k .
- (b) **Set:** $x^{k+1} = x^k + s^k$.
- (c) **Set:** $y^k = F_n(x^{k+1}) - F_n(x^k)$.
- (d) **Set:** $B_{k+1} = B_k + \frac{1}{(s^k)^\top s^k} (y^k - B_k s^k)(s^k)^\top$.

A good "choice" of B_0 is $B_0 = J_{F_n}(x^0)$. Obviously, by avoiding this choice Broyden's method does not require the computation of the Jacobian matrix. The effectiveness of Broyden's method and Newton's method on different

classes of SNEs has been studied, for example, article [105] compares the effectiveness of Newton’s method, Broyden’s method, and other methods at solving sparse SNEs.

There are many techniques that can be utilized to solve the system of linear equations produced by each iteration of Newton’s or Broyden’s method for finding roots. Two widely used methods for solving a system of linear equations are described in the following sections, and we refer the interested reader to [61] for more methods and details regarding these methods. For a visualization of the basins of convergence for Newton’s and Broyden’s methods, we refer the interested reader to article [106].

3.1.1 Generalized Minimum Residual method (GMRES)

Consider a system of linear equations of the form $Ax = b$. The GMRES method [107] is an iterative method which at the k -th iteration uses the Arnoldi iteration [108] to find an approximate solution x^k in the k -th Krylov subspace \mathcal{K}_k which minimizes the residual $\|b - Ax^k\|_2$. The k -th Krylov subspace of the GMRES method is

$$\mathcal{K}_k = \mathcal{K}_k(A, r^0) = \text{span}\{r^0, Ar^0, A^2r^0, \dots, A^{k-1}r^0\},$$

where $r^0 = b - Ax^0$ is the residual at the initial point x^0 .

GMRES assumes that the matrix A is invertible (and hence square) and that b is normalized such that $\|b\|_2 = 1$. It is worth mentioning that because A is assumed to be invertible, that this technique in its original form can not be utilized with Newton’s method to find an approximate solution to a SNE that has more equations than unknowns ($m > n$).

3.1.2 Successive Overrelaxation method (SOR)

The SOR method is another iterative method for solving a system of linear equations of the form $Ax = b$. If we assume that the diagonal elements a_{ii} of A are all non-zero, at the k -th iteration we can utilize the SOR iteration to find a new approximate solution x^{k+1} to $Ax = b$ by the following update:

$$x^{k+1} = x^k - \omega(D - \omega L)^{-1}(Ax^k - b),$$

where $\omega > 1$ is a relaxation parameter, and $A = D - L - U$ where D , L , and U are diagonal, strictly lower triangular, and strictly upper triangular matrices respectively. Here, L and U have zero diagonal elements, and the assumption that the diagonal elements of A are nonzero ensures that $(D - L)^{-1}$ exists [61]. The Gauss-Seidel iteration is a special case of the SOR where $\omega = 1$.

Though the SOR method and the corresponding Jacobi method [61] can be utilized to solve the series of linear systems produced by Newton’s method, the SOR and Jacobi methods can also be extended to find a single solution to a SNE.

3.2 Solving a SNE using generalizations of iterative methods for linear systems

The well known and widely used *Gauss-Seidel* iterative method for solving a linear system of equations of the form $Ax = b$ can be generalized for solving SNEs. Thus, if $F_n = (f_1, f_2, \dots, f_n) : \mathcal{D} \subset \mathbb{R}^n \rightarrow \mathbb{R}^n$, then the basic step of the *nonlinear Gauss-Seidel (NGS)* iteration is to solve (in analogy to linear case), the i -th nonlinear one-dimensional equation:

$$f_i(x_1^{k+1}, \dots, x_{i-1}^{k+1}, x_i, x_{i+1}^k, \dots, x_n^k) = 0, \quad k = 0, 1, \dots, \quad i = 1, 2, \dots, n. \quad (9)$$

for x_i , and to set $x_i^{k+1} = x_i$. To obtain x^{k+1} from x^k , we solve successively the n one-dimensional nonlinear equations (9) for $i = 1, 2, \dots, n$. If relaxation parameters ω_k are used, we may set $x_i^{k+1} = x_i^k + \omega_k(x_i - x_i^k)$ and the corresponding method is called *Nonlinear Successive Overrelaxation (NSOR)* method. In an analogous way, the k -th step of the *Nonlinear Jacobi (NJ)* iterative scheme consists of solving the i -th nonlinear one-dimensional equation:

$$f_i(x_1^k, \dots, x_{i-1}^k, x_i, x_{i+1}^k, \dots, x_n^k) = 0, \quad k = 0, 1, \dots, \quad i = 1, 2, \dots, n. \quad (10)$$

for x_i and setting $x_i^{k+1} = x_i$, for $i = 1, 2, \dots, n$. The main characteristic of the nonlinear Jacobi approach is that it can be easily parallelized.

In contrast to the linear case, in general, the analytic solutions of Eqs. (9) and (10) are not available and an one-dimensional rootfinding method must be applied that terminates after a suitable number of steps. Any type

of one-dimensional methods can be used leading to a large variety of combined methods. On the other hand if many steps of these one-dimensional methods are applied the whole procedure becomes cumbersome and thus in practice, in many cases, a few steps or at least one step of these methods is applied. In this case, for example, if we apply the *one-dimensional Newton's method*, the derivative-free *one-dimensional secant method* or the derivative-free *one-dimensional Steffensen method* to Eqs. (9) and (10), we obtain respectively the following methods for solving SNEs [61]:

(a) the *one-step SOR-Newton method*:

$$x_i^{k+1} = x_i^k - \omega_k \frac{f_i(x^{k,i})}{\partial_i f_i(x^{k,i})}, \quad k = 0, 1, \dots, \quad i = 1, 2, \dots, n.$$

where $x^{k,i} = (x_1^{k+1}, x_2^{k+1}, \dots, x_{i-1}^{k+1}, x_i^k, x_{i+1}^k, \dots, x_n^k)^\top$ and where $\partial_i f_i(x)$ denotes the partial derivative of the function $f_i(x)$ with respect to the variable x_i .

(b) the *one-step Jacobi Newton method*:

$$x_i^{k+1} = x_i^k - \omega_k \frac{f_i(x^k)}{\partial_i f_i(x^k)}, \quad k = 0, 1, \dots, \quad i = 1, 2, \dots, n.$$

(c) the derivative-free *one-step SOR secant method*:

$$x_i^{k+1} = x_i^k - \omega_k \frac{x_i^k - x_i^{k-1}}{f_i(x^{k,i}) - f_i(x^{k,i} + (x_i^{k-1} - x_i^k)e^i)} f_i(x^{k,i}), \quad k = 0, 1, \dots, \quad i = 1, 2, \dots, n,$$

where e^i indicates the i -th column of the identity matrix I_n .

(d) the derivative-free *one-step Jacobi secant method*:

$$x_i^{k+1} = x_i^k - \omega_k \frac{x_i^k - x_i^{k-1}}{f_i(x^k) - f_i(x^k + (x_i^{k-1} - x_i^k)e^i)} f_i(x^k), \quad k = 0, 1, \dots, \quad i = 1, 2, \dots, n.$$

(e) the derivative-free *one-step SOR Steffensen method*:

$$x_i^{k+1} = x_i^k - \omega_k \frac{f_i(x^{k,i})^2}{f_i(x^{k,i}) - f_i(x^{k,i} - f_i(x^{k,i})e^i)}, \quad k = 0, 1, \dots, \quad i = 1, 2, \dots, n.$$

(f) the derivative-free *one-step Jacobi Steffensen method*:

$$x_i^{k+1} = x_i^k - \omega_k \frac{f_i(x^k)^2}{f_i(x^k) - f_i(x^k - f_i(x^k)e^i)}, \quad k = 0, 1, \dots, \quad i = 1, 2, \dots, n. \quad (11)$$

Furthermore, since in many problems of practical interest the functions values are known only imprecisely, the traditional and widely applied *one-dimensional bisection method* can be used for a suitable number of steps for computing solutions of Eqs. (9) and (10). Specifically, for the computation of a zero of a continuous function $f: [a, b] \subset \mathbb{R} \rightarrow \mathbb{R}$ the one-dimensional bisection method has been given in [80] by the following sequence:

$$x^{k+1} = x^k + \operatorname{sgn}f(x^0) \operatorname{sgn}f(x^k) (b - a)/2^{k+1}, \quad x^0 = a, \quad k = 0, 1, \dots \quad (12)$$

Similarly, instead of the above sequence we can also use the following one:

$$x^{k+1} = x^k - \operatorname{sgn}f(x^0) \operatorname{sgn}f(x^k) (b - a)/2^{k+1}, \quad x^0 = b, \quad k = 0, 1, \dots \quad (13)$$

Obviously, the sequences (12) and (13) converge to a root $r \in (a, b)$ if for some x^k , $k = 1, 2, \dots$ it holds that $\operatorname{sgn}f(x^0) \operatorname{sgn}f(x^k) = -1$. Also, the number of iterations ν , that are required in obtaining an approximate root r^* such that $|r - r^*| \leq \varepsilon$ for some $\varepsilon \in (0, 1)$ is given by:

$$\nu = \lceil \log_2((b - a)\varepsilon^{-1}) \rceil. \quad (14)$$

The one-dimensional bisection method always converges within the given interval (a, b) and is a globally convergent method. Furthermore, it has a great advantage since it is worst-case optimal; i.e., it possesses asymptotically the best possible rate of convergence in the worst case [109, 68]. Thus, it is guaranteed to converge to an approximate root with a predetermined accuracy using the predefined number of iterations given by Eq. (14). Notice that no other method has this characteristic. This method actually requires only the signs of function values (and the gradient values for the optimization case) to be correct. Thus, it requires only one bit of information, namely the sign of a function value and consequently it can be applied to problems with imprecise function values. Also, this method can be generalized to tackle SNEs and optimization problems. In [80] a straightforward generalization of the bisection method, named *characteristic bisection method* has been presented. For a few details of the bisection and the generalized bisection methods and for some applications we refer the interested reader to [110, 111, 71, 74, 112, 79, 113, 80, 114, 82, 115, 116].

The main characteristic of all the above briefly described methods in this section is that they can tackle n -dimensional SNEs using only one-dimensional rootfinding methods. This issue is very important in cases where the dimension n is large. Also, the corresponding algorithms are very simple to implement with a few lines of code. Notice that, the convergence properties of all the above methods are well studied and analyzed (see for example [61]). On the other hand, although the nonlinear iterative rootfinding methods have been extensively studied, the optimization case has not been thoroughly studied and analyzed. Details and some applications of the above described methods can be found for example in [117, 118, 119, 114, 120].

3.3 Chebyshev-Halley methods

Although Newton's method only has a quadratic rate of convergence, *Halley's method* possesses a cubic rate of convergence. Halley's method, also known as *the method of tangent hyperbolas*, utilizes information from the tensor of second derivatives of $F_n(x)$ to accelerate convergence towards a local minimizer x^* of $F_n(x)$ from an initial guess x^0 . Halley's method attempts to calculate a new approximate solution x^{k+1} to a SNE from x^k using the following scheme:

$$x^{k+1} = x^k - \left\{ I + \frac{1}{2} L_{F_n}(x^k) [I - \alpha L_{F_n}(x^k)]^{-1} \right\} F'_n(x^k)^{-1} F_n(x^k),$$

where α is a real parameter, and $L_{F_n}(x) = F'_n(x)^{-1} F''_n(x) F'_n(x)^{-1} F_n(x)$ is the degree of logarithmic convexity [121, 122, 123]. Therefore, Halley's method is applicable to cases where $F''_n(x)$ can be computed.

Chebyshev's method refers to the case where $\alpha = 0$, the *classical Halley's method* refers to the case where $\alpha = \frac{1}{2}$, and the *super-Halley method* refers to the case where $\alpha = 1$. Details about *Chebyshev-like methods* for solving SNEs can be found in [124].

3.4 Tensor methods utilizing higher order derivatives

There exists a class of *tensor methods* which utilizes information from higher order derivatives to accelerate convergence to a single solution of a SNE. In [125], Steihaug and Suleiman utilize the model:

$$\|M^k(d)\|_2 = \left\| F_n(x^k) + J_{F_n}(x^k)d + \frac{1}{2} T^k dd \right\|_2 \leq \eta^k \|F_n(x^k)\|_2. \quad (15)$$

which seeks to determine a step d^k at each iteration. In this model, $T^k = F''_n(x^k)$ is the tensor of second derivatives of $F_n(x^k)$, and $\eta^k \in [0, 1)$. Steihaug and Suleiman proved that any method that can be used to find d^k in Eq. (15) while satisfying $\|d^k\|_2 = O(\|F_n(x^k)\|_2)$ is locally convergent. Furthermore, Steihaug and Suleiman showed that the rate of convergence is at least:

- (a) Q-super-linear when $\eta^k \rightarrow 0$.
- (b) Q-quadratic when $\eta^k = O(\|F_n(x^k)\|_2)$.
- (c) Q-cubic when $\eta^k = O(\|F_n(x^k)\|_2^2)$.
- (d) Q-order $\min\{\hat{p}, 3\}$ when $\eta^k = O(\|F_n(x^k)\|_2^{\hat{p}-1})$, $1 < \hat{p}$.

Furthermore, in order to solve Eq. (15), Steihaug and Suleiman in [125] introduce a class of *inexact Chebyshev-Halley methods* which under some assumptions are locally convergent satisfying Eq. (15) and $\|d^k\|_2 = O(\|F_n(x^k)\|_2)$.

3.5 Tensor-free Chebyshev-Halley method

Instead of calculating the tensor term $T^k d d$ as performed in Eq. (15), Eustaquio *et al.* in [85] avoid calculating the tensor term altogether by introducing a general *tensor-free Chebyshev-Halley method* for solving SNEs. Therefore, though Eq. (15) requires calculating $F_n''(x)$, the method of Eustaquio *et al.* can be utilized in cases where $F_n''(x)$ does not exist. Also, this method does not require the inequality in Eq. (15) to be satisfied. The general framework for the *inexact tensor-free Chebyshev-Halley class* is the following:

1. Given the SNE $F_n(x) = \Theta_n$, the machine precision ε_M , and $k = 0$, select $\alpha \in \mathbb{R}$, a step length $h > 0$, an initial point $x^0 \in \mathbb{R}^n$, a forcing term limit $\tilde{\eta} \in (0, 1)$, and a mapping $C : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n}$.
2. **while** $F_n(x^k) \neq \Theta_n$ **do**
 - (a) Select forcing term tolerances $\eta_1^k \in [0, \tilde{\eta})$ and $\eta_2^k \in [0, \tilde{\eta})$.
 - (b) Compute d_1 such that $\|J_{F_n}(x^k)d_1 + F_n(x^k)\|_2 \leq \eta_1^k \|F_n(x^k)\|_2$.
 - (c) Compute d_2 such that $\|(J_{F_n}(x^k) + \alpha C(x^k))d_2 + \frac{1}{2}C(x^k)d_1\|_2 \leq \eta_2^k \|\frac{1}{2}C(x^k)d_1\|_2$.
 - (d) Set $x^{k+1} = x^k + d_1 + d_2$.
 - (e) Set $k = k + 1$.
3. **end while**

where the authors utilized the mapping $C(x^k) = \frac{1}{h}(J_{F_n}(x^k + h d_1) - J_{F_n}(x^k))$ with step length $h = \sqrt{\varepsilon_M} \|x^k\|_2 / \|d_1\|_2 \in (\varepsilon_M, 0.5)$ and the forcing terms $\eta_1^k = \min\{10^{-8}, \|F_n(x^k)\|_2^2\} \in (2\varepsilon_M, 10^{-8})$ and $\eta_2^k = \min\{10^{-8}, \|F_n(x^k)\|_2\} \in (2\varepsilon_M, 10^{-8})$ to control the level of accuracy of the approximate solution to the SNE. In comparison to Eq. (15), the mapping $C(x^k)$ replaces the tensor term $T^k d$ while still preserving a third-order rate of convergence. As shown in the algorithm above, each iteration only requires approximately solving two linear systems. Eustaquio *et al.* utilized Saad and Schultz's Generalized Minimum Residual method (GMRES) [107] to solve the two linear systems and obtain the inexact Newton steps d_1^k and d_2^k .

The authors proved that any method belonging to their class of inexact tensor-free Chebyshev-Halley methods is locally convergent. Note that the system solved in step 2(b) is analogous to system (8) solved in Newton's method where $d_1 = x^{k+1} - x^k$.

Eustaquio *et al.* conducted a rigorous quantitative comparative analysis of their method against the *Inexact Newton method* and the tensor methods utilizing higher order derivatives presented by Steihaug and Suleiman [125]. Eustaquio *et al.* illustrated that the class of tensor-free Chebyshev-Halley methods are capable of efficiently handling problems that have ill-conditioned or singular Jacobian matrices at the solution.

Furthermore, *Jarrat's method* [126] is defined as a specific case of the tensor-free Chebyshev-Halley method where $\alpha = 1$, $\eta_1^k = 0$, $\eta_2^k = 0$, $h = 2/3$, and the mapping $C(x^k) = h^{-1}(J_{F_n}(x^k + h d_1) - J_{F_n}(x^k))$. Jarrat's method has a convergence rate of four. Articles using Jarrat-like methods to solve SNEs can be found for example in [30, 127, 128].

3.6 Tensor methods not utilizing higher order derivatives

In addition to the class of tensor methods which utilize a tensor of higher order derivatives, other tensor methods exist and have demonstrated effectiveness at solving large, sparse, and ill-formed SNEs with singular Jacobian matrices [129, 130, 131, 132, 133, 134, 135, 136, 137]. In [129] Frank and Schnabel introduced tensor strategies for solving SNEs based around solving the quadratic model:

$$\min_{d \in \mathbb{R}^n} \|M^k(d)\|_2 = \min_{d \in \mathbb{R}^n} \left\| F_n(x^k) + J_{F_n}(x^k)d + \frac{1}{2}T^k d d \right\|_2, \quad (16)$$

where $J_{F_n}(x)$ is the Jacobian matrix of $F_n(x)$, d is the step size, and $T^k \in \mathbb{R}^{n \times n \times n}$ is a carefully chosen tensor.

Expanding upon this formulation, in [137], Bader presents three Krylov-based methods for iteratively solving Eq. (16) to a specified tolerance. Bader's method selects T^k such that the model interpolates $p \leq \sqrt{n}$ function values from its most recent history of iterates. By selecting $p = 1$, Bader reduces the tensor model about x^k to

$$\min_{d \in \mathcal{K}_m} \|M^k(d)\|_2 = \min_{d \in \mathcal{K}_m} \left\| F_n(x^k) + J_{F_n}(x^k)d + \frac{1}{2}a^k ((s^k)^\top d)^2 \right\|_2, \quad (17)$$

where \mathcal{K}_m is a m -dimensional Krylov subspace, and where $a^k, s^k \in \mathbb{R}^n$ are given as follows:

$$a^k = \frac{2(F_n(x^{k-1}) - F_n(x^k) - J_{F_n}(x^k)s^k)}{((s^k)^\top s^k)^2},$$

$$s^k = x^{k-1} - x^k.$$

The *linear Krylov subspace method* finds an approximate solution x_m to the linear system $Ax = b$ from an m -dimensional affine subspace $x^0 + \mathcal{K}_m$ where

$$\mathcal{K}_m(A, r^0) = \text{span}\{r^0, Ar^0, A^2r^0, \dots, A^{m-1}r^0\},$$

$$r^0 = b - Ax^0,$$

and r^0 is the residual at the initial point x^0 .

The three techniques presented by Bader in [137] select \mathcal{K}_m in different ways as a subroutine within the following algorithm:

1. Given the SNE $F_n(x)$, select an initial point x_0 and a maximum number of iterations k_{max} .
2. For $k = 0, 1, 2, \dots, k_{max}$, do:
 - (a) Select a forcing term tolerance $\eta^k \in [0, 1)$.
 - (b) If $k = 0$:
 - i. Calculate the Newton-GMRES [107] step d_N based on the tolerance η^k .
 - ii. Proceed to step 2e.
 - (c) Form the local tensor model (16).
 - (d) Calculate the approximate tensor step d_T according to η^k by solving one of the three methods presented for selecting \mathcal{K}_m .
 - (e) Set $x^{k+1} = x^k + \alpha d$ where a linesearch strategy using the directions d_T and / or d_N is used to select d and α .
 - (f) If x^{k+1} is an acceptable approximate root of $F_n(x)$:
 - i. Stop.

Bader's methods demonstrated effectiveness at solving large-scale SNEs, especially those which have ill-conditioned or singular Jacobians at the solution.

3.7 Quasi-Newton method for finding roots

Although Newton's method for finding roots requires the Jacobian $J_{F_n}(x)$, if $J_{F_n}(x)$ is not available, *Quasi-Newton methods* can be utilized. A Quasi-Newton method is any method that utilizes an approximation of $J_{F_n}(x)$ instead of the exact $J_{F_n}(x)$. A classification of Quasi-Newton methods for solving SNEs is presented in article [138]. Examples of Quasi-Newton methods include the methods discussed in articles [139, 140].

One of the most popular Quasi-Newton methods is the *Broyden-Fletcher-Goldfarb-Shanno (BFGS) method* [141, 142, 143, 144]. Popular extension of BFGS method is limited memory BFGS (L-BFGS) [145]. Article [58] combines a memoryless variant of the BFGS method with a projection technique for solving SNEs, and the authors demonstrated the efficiency of the method by solving large SNEs with up to 5000 dimensions in the order of milliseconds or seconds, depending on the problem instance. Other Quasi-Newton methods include the *Symmetric Rank 1 (SR1) method* and the *Davidon-Fletcher-Powell (DFP) method* among others. Quasi-Newton methods were utilized to find solutions to SNEs in articles [146, 147, 148, 149, 150, 151, 152, 153, 154].

3.8 Spectral methods

Spectral methods are another class of derivative-free methods which have been used to solve SNEs, and they are particularly well suited for solving large SNEs because they have a relatively low storage requirement [59]. Spectral methods often utilize spectral parameters and coefficients to help determine the search direction d^k in the update step $x^{k+1} = x^k + \alpha^k d^k$. For example, article [59] presents two *derivative-free hybrid spectral methods* for solving SNEs, and proves that the proposed methods will converge to a solution when applied to SNEs that satisfy the conditions of monotonicity (Eq. (4)) and Lipschitz continuity (Eq. (5)). Other articles which propose applying spectral methods for solving SNEs include [155, 156].

3.9 Hermitian and skew-Hermitian splitting (HSS) based methods

First introduced in [157] for solving linear systems of equations, *Hermitian and skew-Hermitian splitting (HSS) based methods* have been shown to be effective at solving sparse SNEs [158] and SNEs which can be decomposed into a linear part Ax and a nonlinear part $\zeta(x)$ such that $F_m(x) = Ax - \zeta(x)$ [159]. When the linear part Ax is dominant over the nonlinear part $\zeta(x)$, $F_m(x)$ can be referred to as a *weakly nonlinear system*. By separating the linear and nonlinear elements of $F_m(x)$, certain specialized techniques can potentially be utilized to find solutions to $F_m(x)$ more quickly than by utilizing traditional root finding methods. Some of these techniques are derivative-free, including the derivative-free HSS based method introduced in [160] which is guaranteed to converge to a solution on SNEs that satisfy certain conditions.

3.10 Levenberg-Marquardt method

The *Levenberg-Marquardt algorithm* [161, 162] was designed to solve a nonlinear least squares problem that can be in general expressed as $\varphi(x) = \frac{1}{2} \sum_{i=1}^m [f_i(x)]^2$ where $\varphi : \mathbb{R}^n \rightarrow \mathbb{R}$. The Levenberg-Marquardt algorithm is an iterative procedure which at each iteration calculates an updated solution using the rule $x^{k+1} = x^k + \lambda d$, where the search direction d is found by solving equations of the form

$$(J_{F_m}^\top J_{F_m} + \mu I_n)d = -J_{F_m}^\top F_m,$$

where $J_{F_m} \in \mathbb{R}^{m \times n}$ is the Jacobian matrix of F_m , $\mu \in \mathbb{R}$, I_n is the identity matrix, and $F_m : \mathbb{R}^n \rightarrow \mathbb{R}^m$. In article [163], Fletcher proposed the following modification to make the solution scale invariant:

$$(J_{F_m}^\top J_{F_m} + \mu \text{diag}\{J_{F_m}^\top J_{F_m}\})d = -J_{F_m}^\top F_m,$$

where the identity matrix I_n is replaced with the diagonal matrix consisting of the diagonal elements of $J_{F_m}^\top J_{F_m}$. Article [164] proposed to use the Levenberg-Marquardt method for solving a SNE modeling a port mooring structure. The Levenberg-Marquardt algorithm is widely used in many applications, including artificial neural network training (for example, see article [165]).

3.11 Deflation techniques for the computation of further solutions

As illustrated above, there is a plethora of methods for obtaining a single solution of a system of n nonlinear real equations in n real unknowns. Brown and Gearhart in [166] proposed *deflation techniques* for the computation of further solutions of a system of nonlinear equations. Specifically, these techniques proceed as follows: ‘‘Once a solution of a system of nonlinear equations has been obtained a modified system is formed in such a way that it retains those solutions of the original system which remain to be computed except the solutions that has been already computed’’. This procedure may be applied sequentially until all solutions of the original system are obtained.

For example, assume a system of nonlinear equations $F_n(x) = \Theta_n$, where $F_n = (f_1, f_2, \dots, f_n) : \mathcal{D}_n \subset \mathbb{R}^n \rightarrow \mathbb{R}^n$, then to deflate out the p already computed roots r_1, r_2, \dots, r_p in order to compute additional roots, the following *norm deflated function* [166] is applied:

$$\hat{f}_i(x) = \frac{1}{\prod_{j=1}^p \|x - r_j\|} f_i(x), \quad i = 1, 2, \dots, n,$$

or alternatively the following *inner product deflated function* [166] can be used:

$$\tilde{f}_i(x) = \frac{1}{\prod_{j=1}^p \langle \nabla f_i(r_j), (x - r_j) \rangle} f_i(x), \quad i = 1, 2, \dots, n.$$

The above inner product deflated function has proven to be useful in practice when Newton’s method for root finding is used. The deflation techniques can also be extended for the computation of multiple solutions. A study of the deflation techniques for the one dimensional case can be found in article [167]. Also, additional techniques for the optimization case related to the above deflation techniques as well as some applications can be found for example in the papers [168, 169, 170, 171, 172, 173].

4 Symbolic computation methods

Exact algorithmic methods for solving systems of nonlinear polynomial equations have been developed in the realm of *Symbolic Computation*, also called *Computational Algebra*, or *Computer Algebra*. Broadly speaking, this particular subarea of Symbolic Computation can in fact be interpreted as a constructive version of some parts of the well-established mathematical theories of *Commutative Algebra* and *Algebraic Geometry*. We begin this section by a brief presentation (via examples) of the main Symbolic Computation methods for solving systems of nonlinear polynomial equations, namely *resultants* and *Gröbner bases*. We end this section by citing a number of books that discuss extensively all the developments in the area of Symbolic Computation exact methods for solving systems of nonlinear polynomial equations.

4.0.1 Resultants

Historically, the theory of resultants was developed with the aim to provide a systematic means of elimination of variables/unknowns from a system of nonlinear polynomial equations.

The resultant of two univariate polynomials of degrees m, n respectively,

$$p(x) = p_m x^m + \cdots + p_1 + p_0, \quad q(x) = q_n x^n + \cdots + q_1 + q_0,$$

is defined as the determinant of the $(n+m) \times (n+m)$ Sylvester matrix associated to $p(x)$ and $q(x)$, namely:

$$\text{res}_x(p(x), q(x)) = \det \begin{bmatrix} a_m & a_{m-1} & & & \\ 0 & a_m & a_{m-1} & & \\ 0 & 0 & a_m & a_{m-1} & \\ 0 & 0 & 0 & a_m & \\ b_n & b_{n-1} & & & \\ 0 & b_n & b_{n-1} & & \\ 0 & 0 & b_n & b_{n-1} & \\ 0 & 0 & 0 & b_n & \end{bmatrix}.$$

One of the main properties of the resultant is that it is equal to zero, if and only if the two polynomials have a common root.

The resultant of two bivariate polynomials $p = p(x, y), q = q(x, y)$ with respect to the variable x , or with respect to the variable y , is the determinant of their associated Sylvester matrix, when p and q are considered as polynomials in x , or in y respectively.

Let us illustrate the concept of the resultant by a simple but instructive example.

Example 1 Consider the system of two polynomials $f_1(x_1, x_2) = 0, f_2(x_1, x_2) = 0$ in two variables x_1, x_2 , given by:

$$\begin{aligned} f_1(x_1, x_2) &= x_1^2 + x_2^2 - 1, \\ f_2(x_1, x_2) &= x_1 - x_2 - 1. \end{aligned} \tag{18}$$

The resultant of f_1, f_2 , with respect to x_1 is the determinant of their 3×3 Sylvester matrix when considered as polynomials in x_1 , namely, $f_1 = 1 \cdot x_1^2 + 0 \cdot x_1 + (x_2^2 - 1), f_2 = 1 \cdot x_1 + (-x_2 - 1)$,

$$\text{res}_{x_1}(f_1, f_2) = \det \begin{bmatrix} 1 & 0 & x_2^2 - 1 \\ 1 & -x_2 - 1 & 0 \\ 0 & 1 & -x_2 - 1 \end{bmatrix} = 2x_2^2 + 2x_2.$$

By factorizing the resultant and setting it equal to zero, we obtain $x_2 = 0$ and $x_2 = -1$. By substituting each of these two values of x_2 back into (18), we obtain the corresponding values of x_1 as: $x_1 = 1$ and $x_1 = 0$. Therefore, we conclude that the system (18) possesses the two solutions:

$$(x_1 = 1, x_2 = 0), \quad (x_1 = 0, x_2 = -1),$$

which can easily be verified to be correct. In terms of geometric interpretation, the first equation $f_1(x_1, x_2)$ represent the unit circle and the second equation $f_2(x_1, x_2)$ represents a straight line, that intersects the unit circle. The two solutions of the system (18) are the two points of intersection of the (red) unit circle and this (green) straight line in Figure 2 below.

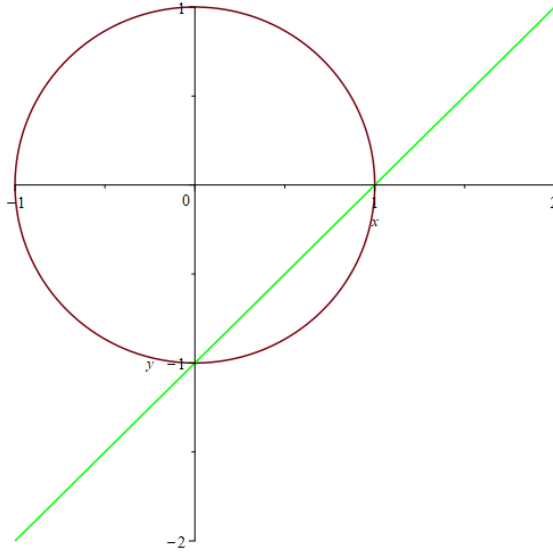


Figure 2: Geometric interpretation of System (18)

4.0.2 Gröbner bases

The theory of Gröbner bases was developed as a multivariate analogue of the classical *Gaussian elimination* for systems of linear equations. Again we illustrate the concept with an example and refer to the aforementioned books for additional details and technicalities.

Example 2 Consider the system of three polynomials $f_1(x_1, x_2, x_3) = 0$, $f_2(x_1, x_2, x_3) = 0$, $f_3(x_1, x_2, x_3) = 0$ in three variables x_1, x_2, x_3 , given by:

$$\begin{aligned} f_1(x_1, x_2, x_3) &= x_1^2 + x_2x_3 - 2, \\ f_2(x_1, x_2, x_3) &= x_1x_3 + x_2^2 - 3, \\ f_3(x_1, x_2, x_3) &= x_1x_2 + x_3^2 - 5. \end{aligned} \tag{19}$$

The lexicographical Gröbner basis of the ideal generated by these three polynomials, with respect to the lexicographical ordering induced by $x_2 > x_1 > x_3$ is given by the three polynomials:

$$\begin{aligned} 8x_2^8 - 60x_2^6 + 142x_2^4 - 172x_2^2 + 1, \\ 88x_2^7 - 680x_2^5 + 1674x_2^3 - 2081x_2 + 117x_1, \\ 152x_2^7 - 1132x_2^5 + 2700x_2^3 - 3403x_2 + 117x_3. \end{aligned} \tag{20}$$

Now we notice that the first polynomial in (20) depends only on x_2 and is of degree 8. In addition, the second polynomial in (20) depends linearly on x_1 and the third polynomial in (20) depends linearly on x_3 . This allows us to express x_1 and x_3 as polynomials in x_2 . Therefore, the solution process starts by finding the 8 roots of the first polynomial in (20) and for each one of those roots, we find the unique values of x_1 and x_3 , given by the last two polynomials in (20). Here are the eight complex roots (four real roots and two pairs of complex conjugate roots) of the first polynomial in (20)

$$\begin{aligned} &-2.16624183202470499 \\ &2.16624183202470499 \\ &-0.07643337499454630 \\ &0.07643337499454630 \\ &-1.329681781358029 - 0.606033421098925 i \\ &-1.329681781358029 + 0.606033421098925 i \\ &1.329681781358029 - 0.606033421098925 i \\ &1.329681781358029 + 0.606033421098925 i \end{aligned}$$

Note that the four real roots and the four complex roots come in pairs of the form $(r, -r)$, a consequence of the fact that the first polynomial in (20) contains only even powers of x_2 . The presence of only even powers of the indeterminate x_2 in the first polynomial in (20) is captured by the fact that the order of the Galois group of this polynomial is smaller than the order of the Galois group of a more “random/generic” polynomial of degree 8.

A very readable, self-contained and pedagogical introduction to Gröbner bases can be found in chapter 10 of [174].

4.0.3 Symbolic computation software systems

One of the major outcomes of the research area of Symbolic Computation (Computer Algebra) in the past few decades, is the advent of the so-called Computer Algebra Systems (CAS). A CAS is defined as a piece of mathematical software that makes advanced functionalities available to the user, in a transparent manner. Such advanced functionalities include univariate and multivariate polynomial factorization, primality testing, integer factorization, root finding, numerical and exact integration, visualization, number theory, linear algebra, commutative algebra, commutative and non-commutative settings, tools for optimization, graph theory, group theory, coding theory, combinatorics, discrete mathematics and so forth. There is a number of commercial and free (open source) CAS available today. Some of the most well-known early CAS (such as Axiom and Macsyma) are largely deprecated today. We focus our attention on those CAS that currently feature a significant user base. We note that CAS are used by millions of research mathematicians, physicists, chemists, astronomers, engineers, practitioners and educators at academic, public, private and government institutions worldwide. In what follows, we provide a brief summary of the main commercial CAS in use today.

- (a) Maple is the flagship Canadian product in the area of mathematical software. It is produced, maintained and distributed by the company Maplesoft, based in Waterloo, Ontario, Canada <https://www.maplesoft.com/>. Maple features an easy-to-learn underlying programming language as well as more than 150 additional packages that significantly expand its core functionalities.
- (b) Magma is the flagship Australian product in the area of mathematical software. It is produced, maintained and distributed by the University of Sydney <http://magma.maths.usyd.edu.au/>. It provides a mathematically rigorous environment for defining and working with structures such as groups, rings, fields, modules, algebras, schemes, curves, graphs, designs, codes and many others. Magma also supports a number of databases designed to aid computational research in those areas of mathematics which are algebraic in nature.
- (c) Mathematica is a flagship American product in the area of mathematical software. It is produced, maintained and distributed by the company Wolfram Research, based in Champaign, Illinois, United States <https://www.wolfram.com/>. Mathematica’s stated purposes include injecting computational intelligence at every level, on every project by unifying algorithms, data, notebooks, linguistics and deployment—enabling powerful workflows across desktop, cloud, server and mobile.
- (d) Matlab is a flagship American product in the area of mathematical software. <https://www.mathworks.com>. It is produced, maintained and distributed by the company MathWorks, based in California, United States. MATLAB’s strong points include matrix manipulations, plotting of functions and data, implementation of algorithms, creation of user interfaces, and interfacing with programs written in other languages.

Some of the most popular non-commercial mathematical software packages include Sage, Singular/Plural, Co-CoA, Macaulay 2 and so forth. Each one has their own strengths and areas of particular focuses. For more information on CAS in general, we refer the interested reader to the comprehensive book [175].

4.0.4 Symbolic computation books

In this section, we present a selection of books in Symbolic computation and related areas. While there is inevitably some overlap among these books, there are also different aspects of polynomial system solving and its applications discussed in each one of them.

1. The classic books [174, 176, 177] are general references for Computer Algebra.
2. The series of books by Teo Mora [178, 179, 180, 181] is an encyclopedic reference to the subject of polynomial system solving.

3. The theory of Gröbner bases, see [182, 183, 184, 185], was initially developed by Bruno Buchberger and further extended by several other researchers. The *Buchberger algorithm* to compute Gröbner bases of polynomial systems is implemented in every major Symbolic Computation software today. This includes commercial software, such as Maple, Magma and Mathematica and open source software, such as Singular [186], Plural [187], CoCoA [188, 189, 190, 191] and the Macaulay2 software system [192].
4. The book [193] discusses aspects of systems of polynomial equations from the viewpoints of computational commutative algebra, discrete geometry, elimination theory, real geometry, as well as their applications in various domains such as partial differential equations, economics, probability, and statistics.
5. The book [194] and its second edition [195], describe useful algorithmic aspects of systems with symmetries, treated using *Invariant Theory*. The book [196] is concerned with polynomial systems with symmetries, that arise in the context of dynamical systems. The french-language book [197] is devoted exclusively to polynomial system solving methods. The french-language book [198] contains a series of chapters on polynomial system solving.
6. The books [199] and [200] describe the emerging area of *Algebraic Statistics*, while the book [201] focuses on numerical aspects of polynomial system solving. On the other hand, the book [202] focuses on theoretical aspects of polynomial system solving. Furthermore, the books trilogy [203, 204, 205] examine the foundation of polynomial system solving from the algebraic geometry standpoint as well as the applications standpoint. The Galois group of a polynomial is inextricably linked with the more general *Galois Theory*, we mention the three books [206, 207, 208].

5 Homotopy / Continuation methods

Homotopy methods, also referred to as *continuation methods*, may be used for finding solutions to polynomial equations and systems of polynomial equations [209, 210, 211]. Polynomial equations often arise in kinematics and robotics related problems [14, 12]; papers [6, 7] apply homotopy methods to solve systems of power flow equations; large-scale integrated circuit designs and protein-protein interaction equation are solved using homotopy method in [8], [27] applies homotopy methods for solving SNEs arising in geodesy; [22] applies homotopy for finding string vacua, [4] applies homotopy methods in chemical engineering. Homotopy (or deformation) of a system of equations $F_n(x) = \Theta_n \equiv (0, 0, \dots, 0)^\top$ (cf. Eq. (1)) is a function H_n such that $H_n(x, 1) = G_n(x)$, and $H_n(x, 0) = F_n(x)$, where the roots of $G_n(x)$ are known. For example, it is possible to choose a convex homotopy, $H_n(x, \lambda) = \lambda G_n(x) + (1 - \lambda)F_n(x)$, where $\lambda \in [0, 1]$ and trace the curve, called the *homotopy path*, from a starting point $(x, 1)$ to solution point $(x, 0)$. Thus, gradually deforming solutions of a starting system $G_n(x) = \Theta_n$ into the solutions to the target system $F_n(x) = \Theta_n$. At each step of the process, a solution of the current system $H_n(x, \tilde{\lambda}) = \Theta_n$ is used as a starting solution to the next system $H_n(x, \tilde{\lambda} + \Delta\lambda) = \Theta_n$, which is solved using Newton-type methods that require an invertible Jacobian. In the case of polynomial systems it is trivial to find solutions of the starting system $G_n(x) = \Theta_n$. Common approaches for defining $G_n(x)$ include fixed point homotopy, where $G_n(x) = x - x^0$ (where x^0 is a starting solution) and Newton homotopy, where $G_n(x) = F_n(x) - F_n(x^0)$. The latter is also referred to a *global homotopy*, where $H_n(x, \lambda) = F_n(x) - \lambda F_n(x^0)$, where x^0 is a starting solution [209]. An adaptive method for selecting the steps of the homotopy path is presented in [212]. As per [213], advantages of homotopy methods are 1) handling of singular solutions, 2) possibility to obtain multiple solutions using one homotopy path, and 3) preserving Morse indices for gradient systems. Paper [12] introduces a collision-based homotopy continuation technique. Article [214] discusses the problem of divergent homotopy paths and proposes an algorithm which performs projective path tracking.

Article [215] describes the software package PHCpack for solving polynomial systems using the homotopy method. Other software packages implementing homotopy continuation methods include Bertini [216] and Hom-Lab [217]. Paper [218] describes a monodromy-based solver.

6 Interval methods

Interval arithmetic was introduced in article [219]. Books on *interval methods* include [220] and [221]. A real interval X is defined as a set of real numbers between lower and upper bounds

$$X = [a, b] = \{x \in \mathbb{R} \mid a \leq x \leq b\}.$$

Interval arithmetic is a set of operations such as addition, subtraction, multiplication, and division, defined on the intervals. Further, interval functions, domain and range of which are the intervals, have been defined. In addition to that, interval differentiation and integration have also been proposed. The most important benefit of interval analysis is its accountability for rounding errors due to limited machine precision. If a value is represented as a single number, rounding errors occurring during the computations may accumulate, thus leading to a wrong result. In interval arithmetic a value is represented by a lower and upper bound which provide reliable results during the computations. Further, interval arithmetic can be used to model uncertainty, often arising in practical problems; for example, uncertainty due to imprecise measurements [222]. Interval arithmetic was standardized by the IEEE in 2015 [223]. Global optimization problems can be solved using the *interval branch-and-bound method* which iteratively splits the search space, and removes its parts that do not contain a global solution; multiple splitting schemes have been proposed in the literature [224]. In this case, application of interval arithmetic allows to guarantee, if a solution exists within a region of interest. Paper [225] proposes to use interval methods for inclusion and exclusion tests, where inclusion tests check existence of the solution within an interval, and exclusion tests check its non-existence. The *interval Newton method* [226] is a generalization of a Newton method for interval arithmetic; it can be used to find zeros of a function. Interval Newton method attempts to iteratively narrow down the new interval solution $[x^{k+1}]$ from $[x^k]$ via

$$[x^{k+1}] = [x^k] \cap ([x^k] - J_{f_n}([x^k])^{-1} f_n([x^k])), \quad k = 0, 1, 2, \dots$$

Paper [227] presents an *interval branch-and-prune algorithm* that is capable of finding all solutions of a polynomial system, and the article evaluates the proposed method on large systems with up to 320 variables. An interval method was also effectively applied to solve large polynomial systems with up to 2500 variables in [228]. Article [229] provides a modification of the interval branch-and-bound method and applies it to solving systems of equations. A method of solving nonlinear equations by using interval arithmetic was patented [230]. Article [231] presents details of implementation of a parallel interval optimization algorithm and its application for solving systems of nonlinear equations. A software package for solving equations using interval methods is presented in [232] and [233]. Article [234] provides interval extensions to Halley's method (discussed in Section 3.3 of this paper), and applies it to finding roots of a single nonlinear equation. Interval methods are utilized to find all solutions of the kinematics SNEs in [235, 236]. Articles [237, 238] suggests to use linear programming (LP) for finding all solutions of the SNE; the method in the paper is best suited to SNEs consisting of linear equations with relatively few nonlinear terms. The method is based on the surrounding nonlinear equations by rectangles, based on interval arithmetic. Then, LP can be used to remove parts of the solution space that do not contain the solutions. Paper [239] proposes to extend this method and utilize LP narrowing, that is capable to solve large scale ($n = 50\,000$) separable SNEs. Article [240] proposes an extension of the interval method for a SNE based on its transformation to separable form. Paper [241] describes the UniCalc SNE solver software which is based on interval methods. Another software package for interval optimization, that can also be used to solve SNEs is RealPlayer [242].

7 Synopsis and concluding remarks

This article presents part one of a survey on methods for solving a system of nonlinear equations (SNE). In part one we have presented a comprehensive survey of methods which can be utilized to search for solutions to a SNE without transforming a SNE into an optimization problem. Since many of the SNEs that arise in real world applications are considered over a finite bounded domain \mathcal{D} , we first introduced a technique which can be utilized to determine the number of solutions to a SNE that exist within \mathcal{D} . Then, we introduced a diverse set of root-finding methods which can be used to search for solutions to a SNE. Next, we described additional methods which have been used to search for solutions to SNEs including methods from symbolic computation, homotopy / continuation methods, and interval methods.

Analyzing this literature has led us to conclude that although there are a variety of root-finding methods which are guaranteed to converge to a solution when applied to SNEs that satisfy certain conditions (such as monotonicity (Eq. 4) and Lipschitz continuity (Eq. 5)), for general SNEs, there is no guarantee that any of the methods described in this paper will converge to a solution in finite time. However, a new taxonomy of SNEs is needed to facilitate the identification of new classes of tractable problems, and to compare the performance of the methods that are most capable of solving them. We are actively working on the development of such a taxonomy. Additionally, we are actively exploring methods capable of solving systems of nonlinear equations and inequalities.

In part one of this survey, we discussed methods for solving SNEs without transforming them into optimization problems. In part two of this survey, we will describe various transformations which can be utilized to transform a

SNE into an optimization problem, and we will discuss optimization algorithms which can then be used to search for solutions. In part three of this survey, we will present a robust quantitative comparative analysis of methods capable of searching for solutions to SNEs.

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