



Solving Nonlinear Equations

Carlos Hurtado

Department of Economics
University of Illinois at Urbana-Champaign
hrtdmrt2@illinois.edu

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On the Agenda

- 1 System of Nonlinear Equations
- 2 Nonlinear Solvers
- 3 In Practice

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1 System of Nonlinear Equations

2 Nonlinear Solvers

3 In Practice

System of Nonlinear Equations

- ▶ A function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is defined as being nonlinear when it does not satisfy the superposition principle:

$$f(x_1 + \cdots + x_n) \neq f(x_1) + \cdots + f(x_n)$$

- ▶ Now that we know what the term nonlinear refers to we can define a system of nonlinear equations.
- ▶ A system of nonlinear equations is a set of equations as the following:

$$f_1(x_1, x_2, \cdots, x_n) = 0,$$

$$f_2(x_1, x_2, \cdots, x_n) = 0,$$

$$\vdots$$

$$f_n(x_1, x_2, \cdots, x_n) = 0$$

where $(x_1, x_2, \cdots, x_n) \in \mathbb{R}^n$ and each f_i is a nonlinear function, for $i = 1, 2, \cdots, n$.

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System of Nonlinear Equations

- ▶ Example of a nonlinear system:

$$3x_1 - \cos(x_2 x_3) - \frac{1}{2} = 0$$

$$x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1 = 0$$

$$e^{-x_1 x_2} + 20x_3 + \frac{10\pi}{3} = 0$$

- ▶ The terms root or solution are frequently used to describe the final result of solving the systems of equations.
- ▶ The root or solution is a point $a = (a_1, a_2, \dots, a_n) \in \mathbb{R}^n$ such that $f_1(a) = f_2(a) = \dots = f_n(a) = 0$

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Fundamentals

- ▶ Simplest problem: Root finding in one dimension.

$$f(x) = 0 \text{ with } x \in [a, b]$$

- ▶ More generally, solving a square system of nonlinear equations.

$$\mathbf{f}(\mathbf{x}) = \mathbf{0} \implies f_i(x_1, x_2, \dots, x_n) = 0 \text{ for } i = 1, \dots, n$$

- ▶ There can be no closed-form answer, we need iterative methods.
- ▶ Iterative methods: initial guess x_0 and update function ϕ

$$x_{k+1} = \phi(x_k)$$

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- ▶ A sequence of iterates x_k that converges to α has order of convergence $p > 0$ if

$$\lim_{k \rightarrow \infty} \frac{|x_{k+1} - \alpha|}{|x_k - \alpha|^p} = C$$

where the constant $0 < C < 1$ is the convergence factor.

- ▶ A method should at least converge linearly, that is, the error should at least be reduced by a constant factor every iteration, for example, the number of accurate digits increases by 1 every iteration.
- ▶ A good iterative method converges quadratically, that is, the number of accurate digits doubles every iteration!

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Nonlinear Solvers

- ▶ A good initial guess is extremely important in nonlinear solvers!
- ▶ Assume we are looking for a unique root $a \leq \alpha \leq b$ starting with an initial guess $a \leq x_0 \leq b$.
- ▶ A method has local convergence if it converges to a given root α for any initial guess that is sufficiently close to α (in the neighborhood of a root).
- ▶ A method has global convergence if it converges to the root for any initial guess.
- ▶ General rule: Global convergence requires a slower method but is safer.
- ▶ It is best to combine a global method to first find a good initial guess close to α and then use a faster local method.

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Nonlinear Solvers

- ▶ Let us start with $f : \mathbb{R} \rightarrow \mathbb{R}$, and the interval $[a,b]$, such that $f(a)$ and $f(b)$ have opposite sign. (How?)
- ▶ We want to find $f(x) = 0$ (The roots).
- ▶ We know how to solve this using Newton's method (At this point you should!)
- ▶ Consider the point $m = \frac{a+b}{2}$
- ▶ Check the intervals $[a, m]$ and $[m,b]$ to see if those have opposite sign.
- ▶ Repeat the algorithm with interval that has opposite signs
- ▶ This is called the bisection method: Global Convergence but Slow.

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Nonlinear Solvers

- ▶ In practice, a robust but fast algorithm for root finding would combine bisection with Newton's method.
- ▶ Specifically, a method like Newton's that can easily take huge steps in the wrong direction and lead far from the current point must be safeguarded by a method that ensures one does not leave the search interval and that the zero is not missed.
- ▶ Once x_k is close to α , the safeguard will not be used and quadratic or faster convergence will be achieved.
- ▶ Newton's method requires first-order derivatives so often other methods are preferred that require function evaluation only (or approximations of the derivatives).

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Nonlinear Solvers

- ▶ What happens if we want to solve a square system of nonlinear equations?

$$\mathbf{f}(\mathbf{x}) = \mathbf{0} \implies f_i(x_1, x_2, \dots, x_n) = 0 \text{ for } i = 1, \dots, n$$

- ▶ We can use Newton's method where $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$.
- ▶ This requires solving many linear systems, which can become complicated when there are many variables.
- ▶ It also requires computing a whole matrix of derivatives, which can be expensive or hard to do (differentiation by hand?)
- ▶ Newton's method converges fast if the Jacobian is well-conditioned, otherwise it can "blow up"
- ▶ Normally use quasi-Newton methods to approximate the Jacobian.

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In Practice

- ▶ It is much harder to construct general robust solvers in higher dimensions and some problem-specific knowledge is required.
- ▶ In python we can use `fsolve` function from `scipy.optimize`
- ▶ In many practical situations there is some continuity of the problem so that a previous solution can be used as an initial guess.
- ▶ For large problems specialized sparse-matrix solvers need to be used.
- ▶ We can think of this as an optimization problem! (How?)

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