Systems of nonlinear equations

Related topics:

- Scalar root-finding
- Systems of linear equations
- Optimization

Consider m nonlinear functions $f_\alpha(x_1, ..., x_m)$, $\alpha = 1, \cdots, m$.

Here

$$\mathbf{x} = (x_1, \cdots, x_m)^T \in H \subset \mathbb{R}^m \ .$$

Define

$$\mathbf{F}(\mathbf{x}) = (f_1(\mathbf{x}), \cdots, f_m(\mathbf{x}))^T$$

Then $\mathbf{F}(\mathbf{x})$ defines a non-linear mapping

$$\mathbf{F} : H \longrightarrow H^* \subset \mathbb{R}^m$$

Systems of nonlinear equations

The task is to find roots of

$$\begin{cases} f_1(x_1, ..., x_m) = 0 \\ f_2(x_1, ..., x_m) = 0 \\ \cdots \\ f_m(x_1, ..., x_m) = 0 \end{cases} \tag{1}$$

Need to specify the problem:

Does it have a root? How many? Which ones do we look for?

A (formally) equivalent minimization problem

Consider

$$\chi(\mathbf{x}) = \sum_{\alpha=1}^{m} f_\alpha^2(\mathbf{x})$$

Note that the solution of $\mathbf{F}(\mathbf{x}) = 0$ is a global minimum of $\chi(\mathbf{x})$ with $\chi_{\min} = 0$.

However, $\chi(\mathbf{x})$ may have spurious local minima $\mathbf{x}_{\mathrm{loc}}$ with $\chi(\mathbf{x}_{\mathrm{loc}}) > 0$.

Iterative methods

Iterative methods:

$$\mathbf{x}^{(0)} \to \mathbf{x}^{(1)} \to \cdots \to \mathbf{x}^{(k)} \to \cdots$$

Here

$$\mathbf{x}^{(k)} = \left(x_1^{(k)}, x_2^{(k)}, \cdots, x_m^{(k)}\right)^T$$

Linear iterative methods

A general form of a single-step linear iterative method

$$\mathbf{B}_k \frac{\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}}{\tau_k} + \mathbf{F}(\mathbf{x}^{(k)}) = 0\,, \qquad k = 0, 1, \ldots$$

If it converges at all, the limit is the solution of $\mathbf{F}(\mathbf{x}) = 0$.

- if $\tau_k = \mathrm{const}$, the method is *stationary*, else *non-stationary*.
- if $\mathbf{B}_k = \mathbf{1}$, the method is *explicit*, else *implicit*

Linear iterative methods

Consider a single step $\mathbf{x}^{(k)} \longrightarrow \mathbf{x}^{(k+1)}$:

$$\mathbf{B}_k\,\mathbf{x}^{(k+1)} = \mathbf{g}_k$$

i.e. a system of linear equations with

$$\mathbf{g}_k = \mathbf{B}_k\,\mathbf{x}^{(k)} - \tau\,\mathbf{F}(\mathbf{x}^{(k)})$$

Can solve the linear system with either direct or iterative methods.

Inner and outer iterations

Inner iterations (внутренние итерации): solving

$$\mathbf{B}_k\,\mathbf{x}^{(k+1)} = \mathbf{g}_k\,,$$

at fixed k.

Outer iterations (внешние итерации): iterations over k.

Inner iterations need not be done until convergence!

Convergence

Convergence of (outer iterations)

Let $\mathbf{B} = \mathrm{const}$ and $\tau = \mathrm{const}$ for simplicity.

Rewrite the outer iterations

$$\begin{aligned} \mathbf{x}^{(k+1)} &= \mathbf{S}(\mathbf{x}^{(k)})\,, \\ \mathbf{S}(\mathbf{x}) &= \mathbf{x} - \tau\,\mathbf{B}^{-1}\mathbf{F}(\mathbf{x}) \end{aligned} \tag{2}$$

$\mathbf{x}_*$ is called a *fixed point* of $\mathbf{S}$ if

$$\mathbf{x}_* = \mathbf{S}(\mathbf{x}_*)$$

Root-finding problem $\mathbf{F}(\mathbf{x}) = 0$ is equivalent to the fixed-point problem of the operator $\mathbf{S}$.

Squeezing operators

Let $\mathbf{S}(\mathbf{x})$ is an operator defined on some $H \subset \mathbb{R}^m$.

$\mathbf{S}(\mathbf{x})$ is *squeezing* on H if, for all $\mathbf{x}' \in H$ and $\mathbf{x}'' \in H$,

$$\|\mathbf{S}(\mathbf{x}') - \mathbf{S}(\mathbf{x}'')\| \leqslant q\|\mathbf{x}' - \mathbf{x}''\|$$

Here $0 < q < 1$ is a *squeezing coefficient*.

Convergence: the fixed-point theorem

Theorem

Let $\mathbf{S}(\mathbf{x})$ is defined on $U_{r,\mathbf{a}} = \{\mathbf{x} \in \mathbb{R}^m \ : \ \|\mathbf{x} - \mathbf{a}\| \leqslant r\}$ and is squeezing on $U_{r,\mathbf{a}}$.
Suppose, further, that $\|\mathbf{S}(\mathbf{a}) - \mathbf{a}\| \leqslant (1-q)r \quad 0 < q < 1$

Then,

1. $\mathbf{S}$ has a unique stationary point $\mathbf{x}_* \in U_{r,\mathbf{a}}$.
2. iterations (2) converge to $\mathbf{x}_*$ for any $\mathbf{x}^{(0)} \in U_{r,\mathbf{a}}$
   Moreover,

$$\|\mathbf{x}^{(n)} - \mathbf{x}_*\| \leqslant q^n \|\mathbf{x}^{(0)} - \mathbf{x}_*\| \,,$$

$$\|\mathbf{x}^{(n)} - \mathbf{x}_*\| \leqslant \frac{q^n}{1-q} \|\mathbf{S}(\mathbf{x}^{(0)}) - \mathbf{x}^{(0)}\|$$

Examples

Relaxation method

An explicit stationary method with $\mathbf{B}_k = \widehat{\mathbf{1}}$, $\tau_k = \tau$:

$$\mathbf{S}(\mathbf{x}) = \mathbf{x} - \tau\,\mathbf{F}(\mathbf{x})$$

Converges if $\|\mathbf{S}'(\mathbf{x})\| < 1$, where $\mathbf{S}' = \widehat{\mathbf{1}} - \tau\,\mathbf{J}$.

$\mathbf{J}$ is the Jacobian of $\mathbf{F}(\mathbf{x})$:

$$\mathbf{J} = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} & \dfrac{\partial f_1}{\partial x_2} & \cdots & \dfrac{\partial f_1}{\partial x_m} \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ \dfrac{\partial f_m}{\partial x_1} & \dfrac{\partial f_m}{\partial x_2} & \cdots & \dfrac{\partial f_m}{\partial x_m} \end{bmatrix}$$

Newton's method

Linearize $f_\alpha(\mathbf{x})$ around $\mathbf{x} = \mathbf{x}^{(k)}$:

$$
\begin{aligned}
f_\alpha(\mathbf{x}) = f_\alpha(\mathbf{x}^{(k)}) &+ \left(x_1 - x_1^{(k)}\right) \left.\frac{\partial f_\alpha}{\partial x_1}\right|_{\mathbf{x}=\mathbf{x}^{(k)}} + \cdots \\
&+ \left(x_m - x_m^{(k)}\right) \left.\frac{\partial f_\alpha}{\partial x_m}\right|_{\mathbf{x}=\mathbf{x}^{(k)}} \\
&+ \quad \text{higher-order terms}
\end{aligned}
$$

$\alpha = 1, \ldots, m$

Newton's method

Then, the original system becomes

$$\sum_{j=1}^{m} \left(x_j - x_j^{(k)} \right) \left. \frac{\partial f_\alpha}{\partial x_j} \right|_{\mathbf{x}=\mathbf{x}^{(k)}} + f_\alpha(\mathbf{x}^{(k)}) = 0 \,, \qquad \alpha = 1, \cdots, m$$

And the iterations are

$$\mathbf{J}(\mathbf{x}^{(k)}) \cdot \left(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)} \right) + \mathbf{F}(\mathbf{x}^{(k)}) = 0$$

i.e. it's a stationary method with $\mathbf{B}_k = \mathbf{J}(\mathbf{x}^{(k)})$ and $\tau = 1$.

Convergence is quadratic.

Modified Newton's method

Compute/factorize the Jacobian once.

The iterations are

$$\mathbf{J}(\mathbf{x}^{(0)}) \cdot \left(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\right) + \mathbf{F}(\mathbf{x}^{(k)}) = 0$$

Can cycle several iterations, then recompute the Jacobian etc.

Convergence is linear.

Non-linear iterations

Nonlinear Jacobi, Seidel

The main idea: each outer iteration is a sequence of 1D root-finding operations.

Non-linear Jacobi method

Solve w.r.t. $x_j^{(k+1)}$ for each $j = 1, \ldots, m$

$$f_j(x_1^{(k)}, x_2^{(k)}, \ldots, x_{j-1}^{(k)}, x_j^{(k+1)}, x_{j+1}^{(k)} \ldots, x_m^{(k)}) = 0$$

Non-linear Seidel method

Solve w.r.t. $x_j^{(k+1)}$ for each $j = 1, \ldots, m$

$$f_j(x_1^{(k+1)}, x_2^{(k+1)}, \ldots, x_{j-1}^{(k+1)}, x_j^{(k+1)}, x_{j+1}^{(k)} \ldots, x_m^{(k)}) = 0$$

Hybrid methods

The main idea:

- Use different methods for inner and outer iterations.
- Can use a (small) fixed number of inner iterations.

I.e. do not need to require convergence of inner iterations.

Hybrid methods: a Newton/Seidel example

Use non-linear Seidel method for outer iterations. For inner iterations use p Newton's steps.

Define $y_j \equiv x_j^{(k)}$.

$$\frac{\partial f_j}{\partial x_j}\left(x_1^{(k+1)},\dots,x_{j-1}^{(k+1)},y_j^{(s)},x_{j+1}^{(k)},\dots\right)\left(y_j^{(s+1)}-y_j^{(s)}\right)$$
$$+f_j\left(x_1^{(k+1)},\dots,x_{j-1}^{(k+1)},y_j^{(s)},x_{j+1}^{(k)},\dots\right)=0$$

for $j = 1, \dots, m$.

Here s idexes the inner iterations: $s = 0, \dots, p$,

$$y_j^{(0)} = x_j^k\,, \qquad y_j^{(p+1)} = x_j^{(k+1)}$$

Hybrid methods: a Newton/Seidel example with $m = 2$

Take $p = 0$, i.e. make only one inner iteration.

The iteration becomes

$$\frac{\partial f_1(x_1^{(k)}, x_2^{(k)})}{\partial x_1}\left(x_1^{(k+1)} - x_1^{(k)}\right) + f_1(x_1^{(k)}, x_2^{(k)}) = 0$$

$$\frac{\partial f_2(x_1^{(k+1)}, x_2^{(k)})}{\partial x_2}\left(x_2^{(k+1)} - x_2^{(k)}\right) + f_2(x_1^{(k+1)}, x_2^{(k)}) = 0$$

with $k = 0, 1, \ldots$