ZS 8

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8. Iterative Methods for Nonlinear Systems of Equations (N-LSE)

Can't solve these exactly nor directly. Therefore we want to find iterative methods to approximate the real solution.

Note: The methods are based on finding the roots. So you want to formulate your problem in a way, that the root will be solution to the problem.

Existance: A root exists if you find x_1 and x_2 such that $f(x_1) < 0 < f(x_2)$.

Goal: Find x^* such that $f(x^*) = 0$

8.1. 1 Dimensional N-LSE

Bisection algorithm

Always half Intervall $[t_l, t_r]$ to $[t_l, mid], [mid, t_r]$ then choose the subintervall, that fullfills the existance property with x_1 and x_2 being the Interval boundaries.

We stop when $f(mid)$ is close enough to 0, or when the Interval is very small.

⊕ Global convergence and robust
⊖ Linear convergence, no extention to higher dimensions

Note: We require f to be continious

Fixed Point Iteration (FPI)

Fixed Point: x^* is a Fixed Point for $f(x)$ $\iff$ $f(x^*) = x^*$

We introduce a new function $\Phi(x)$ such that:

$$f(x^*) = 0 \iff \Phi(x^*) = x^*$$

We require that $\Phi(x)$ is Lipschitz continious with $L < 1$
(Lipschitz continious: $\exists L > 0\ \forall x, y \in [a,b]: |\Phi(x) - \Phi(y)| \leq L \cdot |x - y|$)

Iteration: $x^{(k)} = \Phi(x^{(k-1)})$ with $x^{(0)}$ being an initial Guess. ($=$ FPI)

Note: $\Phi \in C^1([a,b])$ and $|\Phi'(x^*)| < 1 \implies \Phi$ Lipschitz continious with $L = 1 - \varepsilon$

Convergence: At least linear. (The $L < 1$ guarantees convergence).

Now we have different methods that choose $\Phi(x)$ differently:

Newton Iteration

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})} \qquad \Phi(x) := x - \frac{f(x)}{f'(x)}$$

Convergence: Newton Iterations converge quadratically we need:

- $f(x) \in C^2$
- $f'(x^*) \neq 0$

⊖ Need to compute $f'(x)$ at each iteration. Can slow down.

Secant Method

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)}) \cdot (x^{(k)} - x^{(k-1)})}{f(x^{(k)}) - f(x^{(k-1)})}$$

⊕ Faster to compute, Same Convergence Criterias as Newton
⊖ Only superlinear convergence.

8.2. n-Dimensional N-LSE

$F: D \subset \mathbb{R}^n \to \mathbb{R}^n$ n equations, n unknowns

The 'root' you now want to find is now a vector. z.B. $(0,1,2,3)$ for $\mathbb{R}^4$.

Note: Now we need Norms to measure the distance: $\|x^{(k)} - x^*\|_2 \to 0$
And it turns out all norms are equivalent for $\mathbb{R}^n$

Convergence: At least linear if $\|D\Phi(x^*)\| < 1$

Existance: If $\Phi(x)$ is Lipschitz-continious with $L < 1$ then a unique FP exists.

Stopping Criteria: $\frac{L}{1-L} \|x^{(k+1)} - x^{(k)}\| \leq \tau$ (This guarantees $\|x^{(k)} - x^*\| < \tau$)

Newton Iteration in $\mathbb{R}^n$

$$x^{(k+1)} = x^{(k)} - DF(x^{(k)})^{-1} F(x^{(k)}) \qquad DF(x^{(k)}) = \text{Jacobi}$$

Convergence: For Quadratic convergence we need:

- $F(x^*) = 0$
- $DF(x^*)$ regular

Note: If $DF(x^*)$ is singular we no longer have quadratic convergence.

Note: In practise we often use $\|DF(x^{(k-1)})^{-1} F(x^{(k)})\| \leq \tau \|x^{(k)}\|$ as a stopping criteria

⊕ Quadratic convergence
⊖ Fails in 3 cases:

- Starts near a local minimum and finds this and not the root of f (not Φ!)
- Functions with bad asymptotes to infinity
- Functions that are prone to overshooting.

$\implies$ We can fight overshooting with Damped-Newton.

Damped Newton in $\mathbb{R}^n$

$$x^{(k+1)} = x^{(k)} - \lambda^{(k)} DF(x^{(k)})^{-1} F(x^{(k)})$$

In each iteration $\|x^{(k+1)} - x^{(k+1)}\| \leq \frac{1}{2} \|x^{(k+1)} - x^{(k)}\|$ needs to be satisfied.
In each iteration first choose $\lambda^{(k)} = 1$ and if the condition from above is not satisfied we half $\lambda^{(k)}$. Hence $\lambda^{(k)} = \lambda^{(k)}/2$

Secant Method in $\mathbb{R}^n$ (Broyden's quasi-Newton method)

$$x^{(k+1)} = x^{(k)} - J_k^{-1} F(x^{(k)}) \qquad J_0 = DF(x^{(0)})$$

We can easely calculate J_k^{-1} from J_{k-1}^{-1} with Shermann-Morrison-Woodbury

8.3. Unconstrained Optimization

We have an Optimization Problem. We first model the problem as a Function F such that the Minimum of F will be the solution to our Problem. ($F: \mathbb{R}^n \to \mathbb{R}$)
Number

$\implies$ Instead of Minding roots we want to find the minimum.

Optimization with differentiable objective function

ΔF is the direction of the greates increase/decrease

If $\Delta F(x) = 0$ we found either Minima/Maxima/Saddel
To find out (if $F(x)$ is in C^2) we take the Hessian matrix $H_F(x)$

$H_F(x)$ pos. def. $\to$ Minima
$H_F(x)$ neg. def. $\to$ Maxima
$H_F(x)$ Indefinit $\to$ Saddle point.

Note: We will look a optimizing for convex functions, which makes things much easier. Because local minima is also a global minima.

Gradient Descent

$$x^{(k+1)} = x^{(k)} - t^{(k)} \nabla F(x^{(k)})$$

Stepsize:
- Exact line search
  ↳ $t = \operatorname{argmin}(F(x^{(k)} - t \Delta F(x^{(k)})))$
- Backtracking line search
  ↳ For a fixed $\alpha \in (0, 0.5)$ decrease $t \to \frac{t}{2}$ until:

$$F(x - t\Delta F(x)) < F(x) - \alpha t \|\Delta F(x)\|^2 \quad \text{(start with } t=1\text{)}$$

⊕ Converges on a larger scale than "Newtons method for optimization"
⊖ Line search in every step.
⊖ If not convex: Can get stuck at local Minimum

Newton's method for optimization

$$x^{(k+1)} = x^{(k)} - (H_F(x^{(k)}))^{-1} \nabla F(x^{(k)})$$

⊕ Quadratic Convergence near minimum
⊕ Needs Fewer Iteration
⊖ Compute the and solve LSE in every step

BFGS method (Quasi-Newton method)

Don't compute $H_F^{(k)}$ but approximate it with B_k and compute $(B_{k+1})^{-1}$ with Shermann-Madisson-Woodbury from $(B_k)^{-1}$