

- When started too far away from the solution, components of the unknowns \$\overline{x}\_k\$, or function vector \$\overline{r}(\$\overline{x}\_k\$)\$, or the Jacobian \$J(\$\overline{x}\_k\$)\$ may blow up; this sort of breakdown is easy to **identify**. (But not necessarily easy to fix...)

The function  $r(x) = -x^5 + x^3 + 4x$  has three non-degenerate real roots. Since the roots are non-degenerate, we expect the fixed point iteration defined by the Newton iteration

$$x \leftarrow x - \frac{f(x)}{f'(x)} = x - \frac{-x^5 + x^3 + 4x}{-5x^4 + 3x^2 + 4}$$

to converge quadratically.

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Nonlinear Equations: Practical Methods

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**Figure:** The Juila set (in white) for Newton's method applied to f(z) =

 $z^3 - 2z + 2$ . Start values in the cyan, pink, yellow shaded regions converge to one of the three zeros of f(z). Values

from the red/black regions do not converge, they are attracted by a cycle of

period 2. Credit: Wikimedia commons.

Peter Blomgren, {blomgren.peter@gmail.com} Nonlinear Equations: Practical Methods

 $f(\mathbf{\bar{x}}) = \frac{1}{2} \|\mathbf{\bar{r}}(\mathbf{\bar{x}})\|^2 = \frac{1}{2} \sum_{i=1}^n r_i^2(\mathbf{\bar{x}}).$ 

Root of  $\bar{\mathbf{r}}(\bar{\mathbf{x}}) = 0 \Rightarrow$  Local minimizer of  $f(\bar{\mathbf{x}})$ .

Local minimizer of  $f(\bar{\mathbf{x}}) \neq \text{Root of } \bar{\mathbf{r}}(\bar{\mathbf{x}}) = 0$ .

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Then we use a line search procedure to identify a step  $\alpha_k$ , satisfying *e.g.* the **Wolfe conditions**.

 $||J_k^T \overline{\mathbf{r}}(\overline{\mathbf{x}}_k)|| \to 0.$ 

As long as we can bound  $\cos \theta_k \geq \delta > 0$ , this guarantees that

Further, if  $||J(\bar{\mathbf{x}})^{-1}||$  is bounded on  $\mathcal{D}$ , then  $\bar{\mathbf{r}}(\bar{\mathbf{x}}_k) \to 0$ .

Nonlinear Equations: Practical Methods

SAN DIEGO STA UNIVERSITY — (12/29) Nonlinear Equations... Practical Line Search Methods Practical Trust-Region Methods

Convergence Algorithm Convergence Rate

We take a look at the search directions generated by Newton and inexact Newton line-search methods — is the condition  $\cos \theta_k \ge \delta > 0$  satisfied???

When the Newton-step is well defined, it is a descent direction for  $f(\cdot)$  whenever  $\mathbf{\bar{r}}(\mathbf{\bar{x}}_k) \neq 0$ , since

$$\mathbf{\bar{p}}_{k}^{T}\nabla f(\mathbf{\bar{x}}_{k}) = -\mathbf{\bar{p}}_{k}^{T}J(\mathbf{\bar{x}}_{k})^{T}\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k}) = -\|\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k})\|^{2} < 0,$$

and we have

Practical Line Search Methods

$$\begin{aligned} \cos \theta_k &= -\frac{\bar{\mathbf{p}}_k^T \nabla f(\bar{\mathbf{x}}_k)}{\|\bar{\mathbf{p}}_k^T\| \|\nabla f(\bar{\mathbf{x}}_k)\|} &= \frac{\|\bar{\mathbf{r}}(\bar{\mathbf{x}}_k)\|^2}{\|J(\bar{\mathbf{x}}_k)^{-1}\bar{\mathbf{r}}(\bar{\mathbf{x}}_k)\| \|J(\bar{\mathbf{x}}_k)^T \bar{\mathbf{r}}(\bar{\mathbf{x}}_k)\|} \\ &\geq \frac{1}{\|J(\bar{\mathbf{x}}_k)^{-1}\| \|J(\bar{\mathbf{x}}_k)^T\|} &= \frac{1}{\kappa(J(\bar{\mathbf{x}}_k))} = \frac{|\lambda|_{\min}}{|\lambda|_{\max}}. \end{aligned}$$

If the condition number  $\kappa(J(\bar{\mathbf{x}}_k))$  is uniformly bounded, we have  $\cos \theta_k \ge \delta > 0$ . When  $\kappa(J(\bar{\mathbf{x}}_k))$  is large, the Newton direction may cause poor performance, since  $\cos \theta_k \rightsquigarrow 0$ .

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Inexact Newton, 1 of 2

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# The inexactness does not compromise the global convergence behavior:

For an inexact Newton step,  $\mathbf{\bar{p}}_k$ , we have,

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$$\|\mathbf{ar{r}}(\mathbf{ar{x}}_k) + J(\mathbf{ar{x}}_k)\mathbf{ar{p}}_k\| \leq \eta_k \|\mathbf{ar{r}}(\mathbf{ar{x}}_k)\|$$

Squaring this inequality gives

$$2\mathbf{\bar{p}}_{k}^{T}J(\mathbf{\bar{x}}_{k})^{T}\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k}) + \|\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k})\|^{2} + \|J(\mathbf{\bar{x}}_{k})\mathbf{\bar{p}}_{k}\|^{2} \leq \eta_{k}^{2}\|\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k})\|^{2}$$
  
$$\Rightarrow \quad \mathbf{\bar{p}}_{k}^{T}\nabla\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k}) = \mathbf{\bar{p}}_{k}^{T}J(\mathbf{\bar{x}}_{k})^{T}\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k}) \leq \left[\frac{\eta_{k}^{2}-1}{2}\right]\|\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k})\|^{2}.$$

We also have,

$$\begin{split} \|\mathbf{\bar{p}}_{k}\| &\leq \|J(\mathbf{\bar{x}}_{k})^{-1}\| \left[ \|\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k}) + J(\mathbf{\bar{x}}_{k})\mathbf{\bar{p}}_{k}\| + \|\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k})\| \right] \leq (\eta_{k} + 1)\|J(\mathbf{\bar{x}}_{k})^{-1}\| \|\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k})\|, \\ \|\nabla \mathbf{\bar{r}}(\mathbf{\bar{x}}_{k})\| &= \|J(\mathbf{\bar{x}}_{k})^{T}\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k})\| \leq \|J(\mathbf{\bar{x}}_{k})\| \|\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k})\|. \end{split}$$

Putting it all together...

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### Practical Line Search Methods

Modified Newton Direction

If  $J(\bar{\mathbf{x}})$  is **ill-conditioned** (close to singular), then we must modify the Newton step in order to ensure that  $\cos \theta_k \ge \delta > 0$  holds.

For instance, we can add a  $\tau_k I$  to  $J(\mathbf{\bar{x}}_k)^T J(\mathbf{\bar{x}}_k)$ , and define the modified Newton step to be

$$\mathbf{\bar{p}}_{k} = -\left[J(\mathbf{\bar{x}}_{k})^{T}J(\mathbf{\bar{x}}_{k}) + \tau_{k}I\right]^{-1}J(\mathbf{\bar{x}}_{k})^{T}\mathbf{\bar{r}}(\mathbf{\bar{x}}_{k})$$

Usually, we do not want to do this explicitly. Instead we use the fact that the Cholesky factor of  $J(\bar{\mathbf{x}}_k)^T J(\bar{\mathbf{x}}_k) + \tau_k I$  is identical to  $R^T$ , where R is the upper triangular factor of the **QR-factorization** of the matrix

 $\begin{bmatrix} J(\bar{\mathbf{x}}_k) \\ \sqrt{\tau_k}I \end{bmatrix}.$ 

This factorization can be implemented in such a way that repeating the factorization for an updated value of  $\tau_k^{[\mu+1]} = \tau_k^{[\mu]} + \epsilon$  is cheap.

Practical Line Search Methods Algorithm Practical Trust-Region Methods Convergence Rate

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#### Inexact Newton, 2 of 2

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We can now write down an estimate for  $\cos \theta_k$  for the inexact Newton directions

$$\cos \theta_k = -\frac{\bar{\mathbf{p}}_k^T \nabla \bar{\mathbf{r}}(\bar{\mathbf{x}}_k)}{\|\bar{\mathbf{p}}_k\| \|\nabla \bar{\mathbf{r}}(\bar{\mathbf{x}}_k)\|} \ge \frac{1 - \eta_k^2}{2(1 + \eta_k) \|J(\bar{\mathbf{x}}_k)\| \|J(\bar{\mathbf{x}}_k)^{-1}\|} \ge \frac{1 - \eta_k}{2\kappa(J(\bar{\mathbf{x}}_k))}$$

This is the same bound (with a different constant) as the bound for Newton's method.

- Hence, inexact Newton converges when Newton's method does.



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Nonlinear Equations... Fundamentals Practical Line Search Methods Algorithm Practical Trust-Region Methods Convergence

Trust Region for Nonlinear Equations

The dogleg method has the **advantage** over methods trying to attain the exact solution to the subproblem in that **only one linear system needs to be solved per iteration**.

Global convergence for the trust-region algorithm is described in the two following theorems (which should look somewhat familiar...): –

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Trust Region for Nonlinear Equations

Convergence, 1 of 2

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# Theorem

Let  $\eta = 0$  in the trust-region algorithm. Suppose that  $J(\bar{\mathbf{x}})$  is continuous in a neighborhood  $\mathcal{D}$  of the level set  $\mathcal{L}(\bar{\mathbf{x}}_0) = \{\bar{\mathbf{x}} \in \mathbb{R}^n : f(\bar{\mathbf{x}}) \leq f(\bar{\mathbf{x}}_0)\}$  and that  $\|J(\bar{\mathbf{x}})\|$  is bounded above on  $\mathcal{L}(\bar{\mathbf{x}}_0)$ . Suppose in addition that all approximate solutions of the trust-region subproblem satisfy  $(c_1 > 0, \gamma \ge 1)$ 

$$m_k(0) - m_k(\mathbf{\bar{p}}_k) \ge c_1 \|J(\mathbf{\bar{x}}_k)^T \mathbf{\bar{r}}(\mathbf{\bar{x}}_k)\| \min\left\{\Delta_k, \frac{J(\mathbf{\bar{x}}_k)^T \mathbf{\bar{r}}(\mathbf{\bar{x}}_k)}{J(\mathbf{\bar{x}}_k)^T J(\mathbf{\bar{x}}_k)}\right\},\$$
$$\|\mathbf{\bar{p}}_k\| \le \gamma \Delta_k.$$

We then have that

Theorem

 $\lim \inf_{k \to \infty} \|J(\mathbf{\bar{x}}_k)^T \mathbf{\bar{r}}(\mathbf{\bar{x}}_k)\| = 0$ 

Finally, we state a result regarding the convergence rate. Note that

Suppose that the sequence  $\{\bar{\mathbf{x}}_k\}$  generated by the trust-region

problem  $\bar{\mathbf{r}}(\bar{\mathbf{x}}) = 0$ . Suppose also that  $J(\bar{\mathbf{x}})$  is Lipschitz continuous

subproblem is solved exactly for all sufficiently large k. Then the

Thus we can design a globally convergent method which converges quadratically! — **Robustness** and **Speed** in the same algorithm!

algorithm converges to a non-degenerate solution  $\bar{\mathbf{x}}^*$  of the

in an open neighborhood  $\mathcal{D}$  of  $\bar{\mathbf{x}}^*$  and that the trust-region

the result requires exact solution of the subproblem.

sequence  $\{\bar{\mathbf{x}}_k\}$  converges quadratically to  $\bar{\mathbf{x}}^*$ .

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Trust Region for Nonlinear Equations	convergenc	ce, 2 of 2	Trust Region for Nonlinear Equations		Local Convergence

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# Theorem

Let  $\eta \in (0, \frac{1}{4})$  in the trust-region algorithm. Suppose that  $J(\bar{\mathbf{x}})$  is Lipschitz continuous in a neighborhood  $\mathcal{D}$  of the level set  $\mathcal{L}(\bar{\mathbf{x}}_0) = \{\bar{\mathbf{x}} \in \mathbb{R}^n : f(\bar{\mathbf{x}}) \le f(\bar{\mathbf{x}}_0)\}$  and that  $\|J(\bar{\mathbf{x}})\|$  is bounded above on  $\mathcal{L}(\bar{\mathbf{x}}_0)$ . Suppose in addition that all approximate solutions of the trust-region subproblem satisfy  $(c_1 > 0, \gamma \ge 1)$ 

$$m_k(0) - m_k(\mathbf{\bar{p}}_k) \ge c_1 \|J(\mathbf{\bar{x}}_k)^T \mathbf{\bar{r}}(\mathbf{\bar{x}}_k)\| \min\left\{\Delta_k, \frac{J(\mathbf{\bar{x}}_k)^T \mathbf{\bar{r}}(\mathbf{\bar{x}}_k)}{J(\mathbf{\bar{x}}_k)^T J(\mathbf{\bar{x}}_k)}\right\},\$$

$$\|\mathbf{\bar{p}}_k\| \leq \gamma \Delta_k.$$

We then have that

$$\lim_{k\to\infty}\|J(\mathbf{\bar{x}}_k)^T\mathbf{\bar{r}}(\mathbf{\bar{x}}_k)\|=0$$

