Numerical Optimization
Lecture Notes #26
Nonlinear Equations: Practical Methods

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Outline

1. Nonlinear Equations...
   - Breakdown of Global Convergence: Blowup / Cycling
   - Toward Increased Robustness

2. Practical Line Search Methods
   - Convergence
   - Algorithm
   - Convergence Rate

3. Practical Trust-Region Methods
   - Fundamentals
   - Algorithm
   - Convergence
As we have seen, both Newton’s and Broyden’s method with unit step $\alpha_k \equiv 1$, must be started “close enough” to the solution $\bar{r}(\bar{x}^*) = 0$ in order to converge.

Broyden’s method also requires the more restrictive $\|B_0 - J(\bar{x}^*)\| \leq \epsilon$.

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

- A type of breakdown that is not as easy to detect is cycling, where the sequence of iterates $\{\bar{x}_k\}$ repeat, i.e. $\bar{x}_{k+m} = \bar{x}_k$, for some $m \geq 1$. Clearly, the larger $m$ is, the harder it is to detect cycling (especially in finite precision, where we have $\bar{x}_{k+m} \approx \bar{x}_k$).
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.
Example: Cycling

Figure: If we start the iteration in $x_0 = 1$, then the Newton iteration cycles $\{1, -1, 1, -1, \ldots \}$ (left figure). On the right we see the rapid convergence to the root $x^* = 0$, for the iteration started at $x_0 = 0.999$. 
If we start the iteration in $x_0 = 1.001$, then the Newton iteration escapes out to the root $1.6004$. . . .

Cycling is quite an exotic occurrence.
**Sidenote:** Convergence of Newton’s Method can be Surprisingly Complex

**Figure:** A Newton 4th power fractal. **Credit:** fractalfoundation.org, Annamarie M.

**Figure:** The Julia 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.
Increased Robustness

We can make both Newton’s and Broyden’s method more robust by using them in a line-search or trust-region framework. However, in order to use these frameworks, we must define a scalar-valued **merit function** with which we measure progress toward the solution.

The most widely used merit function is the sum-of-squares,

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

**Root of \( \bar{r}(\bar{x}) = 0 \) ⇒ Local minimizer of \( f(\bar{x}) \).**

**Local minimizer of \( f(\bar{x}) \) \( \nRightarrow \) Root of \( \bar{r}(\bar{x}) = 0 \).**
Consider the non-linear function $r(x) = \sin(5x) - x$ (pictured to the left) and the associated sum-of-squares objective $f(x) = \frac{1}{2}(\sin(5x) - x)^2$ (pictured to the right). In this range we have gone from three roots, to seven local minima.
Other Merit Functions

The $l_1$-norm

Figure: The $l_1$-norm (sum-of-absolute-values) gives us an alternative objective, with its own problems — the derivative does not exist in the optimal points...
We can build algorithms with global convergence properties by applying the line search approach to the sum-of-squares merit function $f(\bar{x}) = \frac{1}{2} \| \bar{r}(\bar{x}) \|^2$.

**Note:** Convergence is global in the sense that we guarantee convergence to a stationary point for $f(\bar{x})$, i.e. a point $\bar{x}^*$ such that $\nabla f(\bar{x}^*) = 0$.

From a point $\bar{x}_k$, the search direction $\bar{p}_k$ must be a descent direction for $f(\bar{x})$, i.e.

$$
\cos \theta_k = \frac{-\bar{p}_k^T \nabla f(\bar{x}_k)}{\| \bar{p}_k \| \| \nabla f(\bar{x}_k) \|} > 0.
$$

Then we use a line search procedure to identify a step $\alpha_k$, satisfying e.g. the *Wolfe conditions*.
Suppose that $J(\bar{x})$ is Lipschitz continuous in a neighborhood $\mathcal{D}$ of the level set $\mathcal{L}(\bar{x}_0) = \{\bar{x} \in \mathbb{R}^n : f(\bar{x}) \leq f(\bar{x}_0)\}$. Suppose that a line search algorithm is applied and that the search directions $\bar{p}_k$ satisfy $\cos \theta_k > 0$, and the step lengths $\alpha_k$ satisfy the Wolfe conditions. Then the Zoutendijk condition holds, i.e.

$$\sum_{k=0}^{\infty} \cos^2 \theta_k \| J_k^T \bar{r}(\bar{x}_k) \|^2 < \infty$$

As long as we can bound $\cos \theta_k \geq \delta > 0$, this guarantees that $\| J_k^T \bar{r}(\bar{x}_k) \| \to 0$.

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

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

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

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

and we have

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

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

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

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

$$\bar{p}_k = -\left[J(\bar{x}_k)^T J(\bar{x}_k) + \tau_k I\right]^{-1} J(\bar{x}_k)^T \bar{r}(\bar{x}_k)$$

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

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

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.
The inexactness does not compromise the global convergence behavior:
For an inexact Newton step, $\bar{p}_k$, we have,

$$\|\bar{r}(\bar{x}_k) + J(\bar{x}_k)\bar{p}_k\| \leq \eta_k \|\bar{r}(\bar{x}_k)\|.$$ 

Squaring this inequality gives

$$2\bar{p}_k^T J(\bar{x}_k)^T \bar{r}(\bar{x}_k) + \|\bar{r}(\bar{x}_k)\|^2 + \|J(\bar{x}_k)\bar{p}_k\|^2 \leq \eta_k^2 \|\bar{r}(\bar{x}_k)\|^2$$

$$\Rightarrow \bar{p}_k^T \nabla \bar{r}(\bar{x}_k) = \bar{p}_k^T J(\bar{x}_k)^T \bar{r}(\bar{x}_k) \leq \left[\frac{\eta_k^2 - 1}{2}\right] \|\bar{r}(\bar{x}_k)\|^2.$$ 

We also have,

$$\|\bar{p}_k\| \leq \|J(\bar{x}_k)^{-1}\| \left[\|\bar{r}(\bar{x}_k) + J(\bar{x}_k)\bar{p}_k\| + \|\bar{r}(\bar{x}_k)\|\right] \leq (\eta_k + 1) \|J(\bar{x}_k)^{-1}\| \|\bar{r}(\bar{x}_k)\|,$$

$$\|\nabla \bar{r}(\bar{x}_k)\| = \|J(\bar{x}_k)^T \bar{r}(\bar{x}_k)\| \leq \|J(\bar{x}_k)\| \|\bar{r}(\bar{x}_k)\|.$$ 

Putting it all together...
We can now write down an estimate for $\cos \theta_k$ for the inexact Newton directions

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

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.
Given $\delta \in (0, 1)$ and $c_1, c_2$ with $0 < c_1 < c_2 < \frac{1}{2}$, and $\bar{x}_0 \in \mathbb{R}^n$:

Algorithm: Line Search Newton for Nonlinear Equations

while( $\|\bar{r}(\bar{x}_k)\| > \epsilon$ )
    if $\bar{p} = -J(\bar{x}_k)^{-1}\bar{r}(\bar{x}_k)$ satisfies $\cos \theta_k \geq \delta$
        Accept $\bar{p}_k = \bar{p}$
    else
        Search for $\bar{p}_k(\tau_k)$ satisfying $\cos \theta_k(\tau_k) \geq \delta$
        $\bar{p}_k(\tau_k) = -[J(\bar{x}_k)^T J(\bar{x}_k) + \tau_k I]^{-1} J(\bar{x}_k)^T \bar{r}(\bar{x}_k)$
    endif
    if $\alpha = 1$ satisfies the Wolfe conditions
        $\alpha_k = 1$
    else
        Perform a line-search to find $\alpha_k > 0$ satisfying the Wolfe conditions.
    endif
    $\bar{x}_{k+1} = \bar{x}_k + \alpha_k \bar{p}_k$
endwhile( $k = k + 1$ )
Theorem

Suppose that a line search algorithm that uses Newton search directions yields a sequence \( \{ \bar{x}_k \} \) that converges to \( \bar{x}^* \), where \( \bar{r}(\bar{x}^*) = 0 \) and \( J(\bar{x}^*) \) is non-singular. Suppose also that there is an open neighborhood \( D \) of \( \bar{x}^* \) such that the components \( r_i(\bar{x}) \) are twice differentiable, with \( \| \nabla r_i(\bar{x}) \| \) bounded for \( \bar{x} \in D \). If the unit step length \( \alpha_k \) is accepted whenever it satisfies the Wolfe conditions, with \( c_2 < \frac{1}{2} \), then the convergence is Q-quadratic; that is \( \| \bar{x}_{k+1} - \bar{x}^* \| = O(\| \bar{x}_k - \bar{x}^* \|^2) \).

**Note:** This theorem applies to any algorithm which eventually uses the Newton search direction.
The most commonly used trust-region method for nonlinear equations is simply “standard trust-region” applied to the merit function $f(\bar{x}) = \frac{1}{2} \| \bar{r}(\bar{x}) \|^2$, using $B_k = J(\bar{x}_k)^T J(\bar{x}_k)$ as the approximate Hessian in the model function $m_k(\bar{p})$. (Levenberg-Marquardt style...)

Global convergence follows directly from previously proved theorems for convergence of trust-region methods.

Rapid local convergence can be shown under the assumption that the Jacobian $J(\bar{x})$ is Lipschitz continuous.

In the next few slides we take a closer look at the trust-region method for nonlinear equations.
Our model function is given by

\[
m_k(\bar{p}) = \frac{1}{2} \| \bar{r}(\bar{x}_k) + J(\bar{x}_k)\bar{p} \|^2_2
= f(\bar{x}_k) + \bar{p}^T J(\bar{x}_k)^T \bar{r}(\bar{x}_k) + \frac{1}{2} \bar{p}^T J(\bar{x}_k)^T J(\bar{x}_k)\bar{p}.
\]

As usual we generate the step \( \bar{p}_k \) by solving the sub-problem

\[
\bar{p}_k = \arg \min_{\bar{p} \in \mathbb{R}^n} m_k(\bar{p}), \quad \text{subject to } \| \bar{p} \| \leq \Delta_k.
\]

We can express \( \rho_k \), the ratio of actual to predicted reduction as

\[
\rho_k = \frac{\| \bar{r}(\bar{x}_k) \|^2 - \| \bar{r}(\bar{x}_k + \bar{p}_k) \|^2}{\| \bar{r}(\bar{x}_k) \|^2 - \| \bar{r}(\bar{x}_k) + J(\bar{x}_k)\bar{p}_k \|^2}.
\]
Given $\Delta > 0$, $\Delta_0 \in (0, \Delta)$ and $\eta \in [0, \frac{1}{4})$

**Algorithm: Trust Region for Nonlinear Equations**

```plaintext
while( $\|\bar{r}(\bar{x}_k)\| > \epsilon$ )
    $\bar{p}_k = \arg \min_{\bar{p} \in \mathbb{R}^n} m_k(\bar{p})$, subject to $\|\bar{p}\| \leq \Delta_k$ 
    $\rho_k = \frac{\|\bar{r}(\bar{x}_k)\|^2 - \|\bar{r}(\bar{x}_k + \bar{p}_k)\|^2}{\|\bar{r}(\bar{x}_k)\|^2 - \|\bar{r}(\bar{x}_k + J(\bar{x}_k)\bar{p}_k)\|^2}$
    if( $\rho_k < \frac{1}{4}$ )
        $\Delta_{k+1} = \frac{1}{4}\|\bar{p}_k\|$
    else
        if( $\rho_k > \frac{3}{4}$ and $\|\bar{p}_k\| = \Delta_k$ )
            $\Delta_{k+1} = \min(2\Delta_k, \Delta)$
        else
            $\Delta_{k+1} = \Delta_k$
        endif
    endif
    if( $\rho_k > \eta$ ) { $\bar{x}_{k+1} = \bar{x}_k + \bar{p}_k$ } else { $\bar{x}_{k+1} = \bar{x}_k$ } endif
endwhile( $k = k + 1$ )
```

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We take a closer look at the solution of the subproblem [TR] using the dogleg method.

The Cauchy point is given by

\[
\tilde{p}_k^c = -\tau_k \left( \frac{\Delta_k}{\|J(\bar{x}_k)^T \bar{r}(\bar{x}_k)\|} \right) J(\bar{x}_k)^T \bar{r}(\bar{x}_k),
\]

where

\[
\tau_k = \min \left\{ 1, \frac{\|J(\bar{x}_k)^T \bar{r}(\bar{x}_k)\|^3}{\Delta_k \bar{r}(\bar{x}_k)^T J(\bar{x}_k) (J(\bar{x}_k)^T J(\bar{x}_k)) J(\bar{x}_k)^T \bar{r}(\bar{x}_k)} \right\}.
\]

For the full step, we use the fact that the model Hessian \( B_k = J(\bar{x}_k)^T J(\bar{x}_k) \) is symmetric semi-definite; when \( J(\bar{x}_k) \) has full rank we get

\[
\tilde{p}_k^J = - \left[ J(\bar{x}_k)^T J(\bar{x}_k) \right]^{-1} \left[ J(\bar{x}_k)^T \bar{r}(\bar{x}_k) \right] = -J(\bar{x}_k)^{-1} \bar{r}(\bar{x}_k).
\]
The dogleg selection of $\bar{p}_k$ is given by:

**Algorithm: Dogleg Selection**

1. Calculate $\bar{p}^c_k$
2. if $(\|\bar{p}^c_k\| = \Delta_k)$
   - $\bar{p}_k = \bar{p}^c_k$
3. else
   - Calculate $\bar{p}^j_k$
   - if $(\|\bar{p}^j_k\| < \Delta_k)$
     - $\bar{p}_k = \bar{p}^j_k$
   - else
     - $\bar{p}_k = \bar{p}^c_k + \tau(\bar{p}^j_k - \bar{p}^c_k)$, where $\tau \in [0, 1]: \|\bar{p}_k\| = \Delta_k$
   - endif
4. endif
Trust Region for Nonlinear Equations

From previous results we know that the exact solution of the subproblem [TR] has the form

$$\bar{p}_k = -\left[J(\bar{x}_k)^T J(\bar{x}_k) + \lambda_k I\right]^{-1} \left[J(\bar{x}_k)^T \bar{r}(\bar{x}_k)\right]$$

for some $\lambda_k \geq 0$, and that $\lambda_k = 0$ if $\|\bar{p}_k\| \leq \Delta_k$.

Note that this is the same linear system that gives the Levenberg-Marquardt step $\bar{p}_k^{LM}$ in the discussion on nonlinear least squares.

In a sense the LM-approach for non-linear equations is a special case of the LM-approach for nonlinear least squares problems.

We can identify an approximation of $\lambda_k$ using the Cholesky factorization, e.g. *modelhess* in the project code; alternatively we can base the search on the QR-factorization.
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...): –
Theorem

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

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

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

We then have that

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

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

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

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

We then have that

$$\lim_{k \to \infty} \| J(\bar{x}_k)^T \bar{r}(\bar{x}_k) \| = 0$$
Finally, we state a result regarding the convergence rate. Note that the result requires exact solution of the subproblem.

Theorem

Suppose that the sequence \( \{\bar{x}_k\} \) generated by the trust-region algorithm converges to a non-degenerate solution \( \bar{x}^* \) of the problem \( \bar{r}(\bar{x}) = 0 \). Suppose also that \( J(\bar{x}) \) is Lipschitz continuous in an open neighborhood \( \mathcal{D} \) of \( \bar{x}^* \) and that the trust-region subproblem is solved exactly for all sufficiently large \( k \). Then the sequence \( \{\bar{x}_k\} \) converges quadratically to \( \bar{x}^* \).

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