Lecture 6: Line search
A (more) global Newton's Method

COMP5930M Scientific Computation

Today

Line search

Line search algorithms

Implementation

Efficiency

Summary

A modified Newton algorithm with damping

We can view the Newton step as an n-d search for the solution $\mathbf{x}^*$

$$
\begin{aligned}
\mathbf{J}(\mathbf{x}_k)\delta &= -\mathbf{F}(\mathbf{x}_k) \\
\mathbf{x}_{k+1} &= \mathbf{x}_k + \lambda\delta
\end{aligned}
$$

- The vector δ is the current search direction
- We can then seek the optimal distance $\lambda > 0$ to move in that direction (avoiding long steps that cause divergence)
- **Note:** Not guaranteed that $\mathbf{F}(\mathbf{x}_k + \lambda\delta) = \mathbf{0}$ for any $\lambda > 0$.

A modified Newton algorithm with damping

$$\begin{aligned}
\mathbf{J}(\mathbf{x}_k)\delta &= -\mathbf{F}(\mathbf{x}_k) \\
\mathbf{x}_{k+1} &= \mathbf{x}_k + \lambda\delta
\end{aligned}$$

Criteria for choosing $\lambda > 0$:

- Should guarantee a reduction in $|\mathbf{F}(\mathbf{x}_{k+1})|^2 < |\mathbf{F}(\mathbf{x}_k)|^2$ (can't diverge, but not enough to guarantee convergence either)

- Should approximately minimise $|\mathbf{F}(\mathbf{x})|^2$ along the line segment $\mathbf{x}_k + \lambda\delta$

Computing λ

Two possible methods:

- A simple algorithm will begin with $\lambda = 1$
  but reject any step that increases $|\mathbf{F}(\mathbf{x})|^2$

- A more complex algorithm computes the step length λ
  that minimises $|\mathbf{F}(\mathbf{x})|^2$ along the direction δ

1. Line-search by step-halving (Armijo rule)

- ▶ Find Newton search direction $\delta = - \left[\frac{\partial \mathbf{F}}{\partial \mathbf{x}} \right]^{-1} \mathbf{F}(\mathbf{x}_k)$
- ▶ Set $\lambda = 1$
- ▶ Test $|\mathbf{F}(\mathbf{x_k} + \lambda \delta)|^2 < |\mathbf{F}(\mathbf{x_k})|^2$
- ▶ Reject an increase, and repeat with $\lambda \to \frac{\lambda}{2}$

- ▶ Limit the number of rejects to guarantee completion

2. Line-search minimisation (quadratic interpolation)

▸ Using 3 points, construct a quadratic in λ to minimise the one-dimensional function:

$$\phi(\lambda) := |\mathbf{F}(\mathbf{x}_k + \lambda\delta_k)|^2.$$

▸ Find an initial bracket $[\lambda_1, \lambda_2, \lambda_3]$ such that $\min\{\phi(\lambda_1), \phi(\lambda_3)\} > \phi(\lambda_2)$ and compute $\phi_i = \phi(\lambda_i)$.

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▶ Define the quadratic polynomial $q_k(\lambda) := a\lambda^2 + b\lambda + c$ such that $q_k(\lambda_i) = \phi_i$ for $i = 1, 2, 3$

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  - Find the minimiser of q_k, $\lambda^* \in [\lambda_1, \lambda_3]$. The condition on the bracket guarantees that such a minimiser exists.

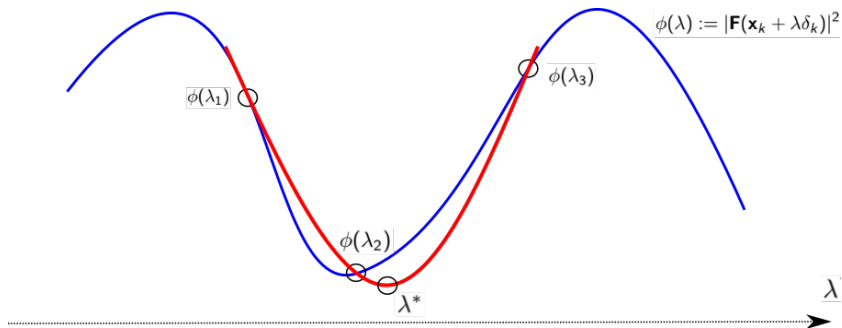 - Set $x_{k+1} = x_k + \lambda^* \delta$ and go to next Newton step.

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Illustration of quadratic interpolation

$$\phi(\lambda) := |\mathbf{F}(\mathbf{x}_k + \lambda \delta_k)|^2$$

$\phi(\lambda_1)$

$\phi(\lambda_3)$

$\phi(\lambda_2)$

λ^*

λ

2. Line-search minimisation

▶ **Note:** It is not guaranteed the approximate line search with a quadratic results in a descent step $\phi(\mathbf{x}_{k+1}) < \phi(\mathbf{x}_k)$.

▶ We need to require a bit more to ensure convergence

▶ **Armijo condition:** Step length λ should satisfy

$$\phi(\mathbf{x}_k + \lambda \delta) \leq (1 - C\lambda)\phi(\mathbf{x}_k)$$

for some $0 < C < 1$ fixed (e.g. $C = 0.001$). This condition guarantees convergence to a **local minimum**.

2. Line-search minimisation (robust implementation)

- Using 3 points, construct a quadratic in λ and $|\mathbf{F}(\mathbf{x})|^2$ to minimise the one-dimensional function:

$$\phi(\lambda) := |\mathbf{F}(\mathbf{x}_k + \lambda \delta_k)|^2.$$

  - Find an initial bracket $[\lambda_1, \lambda_2, \lambda_3]$ such that $\min\{\phi(\lambda_1), \phi(\lambda_3)\} > \phi(\lambda_2)$ and compute $\phi_i = \phi(\lambda_i)$.

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  - Find the minimiser of q_k, $\lambda^* \in [\lambda_1, \lambda_3]$. The condition on the bracket guarantees that such a minimiser exists.

2. Line-search minimisation (robust implementation)

Using λ^*, a new bracket is chosen:

- If $\lambda^* > \lambda_2$ and $\phi(\lambda^*) > \phi(\lambda_2)$ then the new bracket is $[\lambda_1, \lambda_2, \lambda^*]$.

- If $\lambda^* > \lambda_2$ and $\phi(\lambda^*) < \phi(\lambda_2)$ then the new bracket is $[\lambda_2, \lambda^*, \lambda_3]$.

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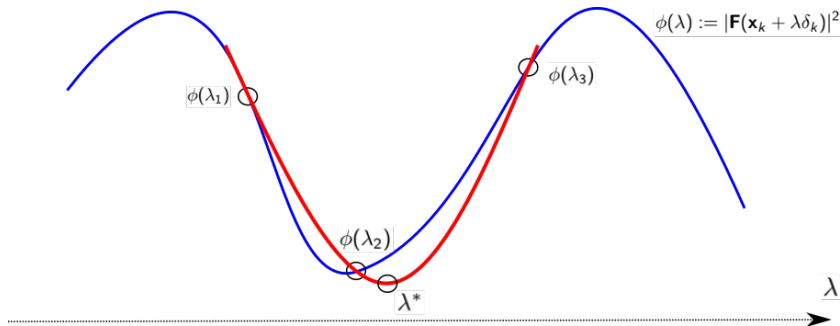- If $\lambda^* > \lambda_2$ and $\phi(\lambda^*) > \phi(\lambda_2)$ then the new bracket is $[\lambda_1, \lambda_2, \lambda^*]$.

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- If $\lambda^* = \lambda_2$ the quadratic step has failed (no new point generated). We return to this case later.

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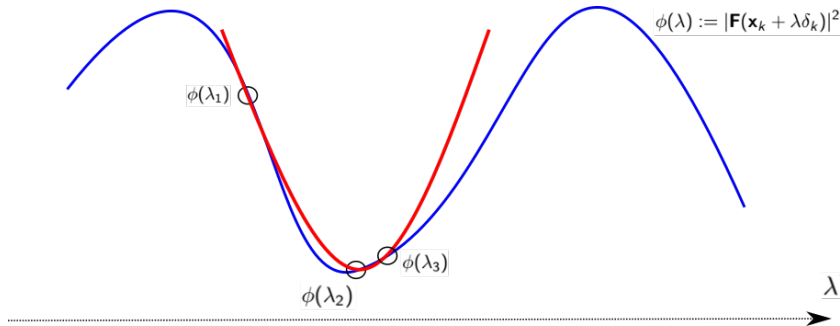
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Selection of new bracket

Here $\lambda^* > \lambda_2$ and $\phi(\lambda^*) > \phi(\lambda_2)$ so the new bracket is $[\lambda_1, \lambda_2, \lambda_*]$

Construction of new parabola

Now we find the next λ^* and iterate

2. Line-search minimisation (robust implementation)

Similar decision tree applies in the case $\lambda^* < \lambda_2$:

- If $\lambda^* < \lambda_2$ and $\phi(\lambda^*) > \phi(\lambda_2)$ then the new bracket is $[\lambda^*, \lambda_2, \lambda_3]$.

- If $\lambda^* < \lambda_2$ and $\phi(\lambda^*) < \phi(\lambda_2)$ then the new bracket is $[\lambda_1, \lambda^*, \lambda_2]$.

- If $\lambda^* < \lambda_2$ and $\phi(\lambda^*) = \phi(\lambda_2)$, we can choose either one.

- If $\lambda^* = \lambda_2$ the quadratic step has failed (no new point generated).

2. Line-search minimisation (robust implementation)

If the quadratic step failed, $\lambda^* = \lambda_2$, check if:

- Bracket is smaller than tolerance, $\lambda_3 - \lambda_1 <$ TOL. If so, stop.

- Otherwise, perturb $\lambda_2 \rightarrow \lambda_2 \pm \varepsilon$ and retry quadratic step.

The quadratic step is iterated in the new bracket until:

$$\lambda_3 - \lambda_1 < TOL$$

or

$$\phi(\lambda_2) < TOL.$$

Newton's method

```
function [ x,f ] = newtonSysL( fnon, fjac, x0, tol, maxIt )

n = length(x0);

x = x0;                % initial point
f = feval(fnon,x);     % initial function values
normf = norm(f);
it = 0;

while (normf>tol) && (it<maxIt)

  J = feval( fjac, n, x, f, fnon ); % build Jacobian
  delta = -J\f;                     % solve linear system


  [ x,f,normf ] = lineSearch( fnon, x, normf, delta, 4 );


  it = it + 1;

end

end
```

Line search

```
function [ x,f,normf ] = lineSearch( fnon, x0, normf0, delta, maxStep )

step = 0;
lambda = 1;
x1 = x0 + delta;          % first update of x
f1 = feval(fnon,x1);      % new function values
normf1 = norm(f1);

while ( normf1 > normf0 )  && ( step < maxStep )
  step = step + 1;
  lambda = lambda/2;
  x1 = x0 + lambda*delta;   % update x
  f1 = feval(fnon,x1);
  normf1 = norm(f1);
end

x = x1;     % accept final value
f = f1;
normf = normf1;

end
```

Computational expense

For a single Newton iteration:

	Function calls	Algorithmic
Evaluate $\mathbf{J}$	n	n^2
Solve $\mathbf{J}\delta = -\mathbf{F}$	1	n^3
Update $\mathbf{x}_{k+1}$	$\approx$ 2-3	n

Line-search failure

- It is possible that the line search will not find a suitable point

- The algorithm extends the convergence of Newton's Method from purely local, but does not guarantee global convergence from any initial point $\mathbf{x}_0$

- A good initial point $\mathbf{x}_0$ is still critical

Comparison of Newton-based approaches

- **Newton**
    - Not robust in general for scalar case
    - Rarely converges in vector case

- **Newton + bisection (scalar case only)**
    - Dekker's method uses secant instead of Newton
    - Completely robust

- **Newton + line-search**
    - Better convergence but not guaranteed to be robust

Summary

- The practical Newton-type algorithm is composed of several <u>non-trivial stages</u> at each iteration
  - Solution of linear system to find Newton direction δ
  - Line-search to find optimal step length λ

- Each stage offers several algorithmic possibilities with performance and efficiency considerations

- The final choice is generally problem dependent