# Gradient-based Methods for Optimization. Part I.

**Nathan L. Gibson**

gibsonn@math.oregonstate.edu

**Department of Mathematics**
**Oregon State University**

# Outline

- Unconstrained Optimization
- Newton’s Method
  - Inexact Newton
  - Quasi-Newton
- Nonlinear Least Squares
- Gauss-Newton Method
- Steepest Descent
- Levenberg-Marquardt Method

# Unconstrained Optimization

- Minimize function $f$ of $N$ variables
- I.e., find *local minimizer* $x^*$ such that

$$f(x^*) \leq f(x) \text{ for all } x \text{ near } x^*$$

- Different from *constrained optimization*

$$f(x^*) \leq f(x) \text{ for all } x \in U \text{ near } x^*$$

- Different from *global minimizer*

$$f(x^*) \leq f(x) \text{ for all } x \text{ (possibly in } U\text{)}$$

# Sample Problem

**Parameter Identification**
Consider

$$u'' + cu' + ku = 0; u(0) = u_0; u'(0) = 0 \qquad (1)$$

where $u$ represents the motion of an unforced harmonic oscillator (e.g., spring). We may assume $u_0$ is known, and data $\{u_j\}_{j=1}^{M}$ is given for some times $t_j$ on the interval $[0, T]$.
Now we can state a *parameter identification* problem to be: find $x = [c, k]^T$ such that the solution $u(t)$ to (1) using parameters $x$ is (as close as possible to) $u_j$ when evaluated at times $t_j$.

# Objective Function

Consider the following formulation of the Parameter Identification problem:
Find $x$=$[c, k]^T$ such that the following objective function is minimized:

$$f(x) = \frac{1}{2}\sum_{j=1}^{M} |u(t_j;x) - u_j|^2 \,.$$

This is an example of a *nonlinear least squares problem*.

# Iterative Methods

An iterative method for minimizing a function $f(x)$ usually has the following parts:

- Choose an initial iterate $x_0$
- For $k = 0, 1, \ldots$
  - If $x_k$ optimal, **stop**.
  - Determine a search direction $d$ and a step size $\lambda$
  - Set $x_{k+1} = x_k + \lambda d$

# Convergence Rates

The sequence $\{x_k\}_{k=1}^{\infty}$ is said to converge to $x^*$ with rate $p$ and rate constant $C$ if

$$\lim_{k\to\infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|^p} = C.$$

- **Linear**: $p = 1$ and $0 < C < 1$, such that error decreases.
- **Quadratic**: $p = 2$, doubles correct digits per iteration.
- **Superlinear**: If $p = 1$, $C = 0$. Faster than linear. Includes quadractic convergence, but also intermediate rates.

# Necessary Conditions

**Theorem 1** *Let $f$ be twice continuously differentiable, and let $x^*$ be a local minimizer of $f$. Then*

$$\nabla f(x^*) = 0 \tag{2}$$

*and the* Hessian *of $f$, $\nabla^2 f(x^*)$, is* positive semidefinite.

Recall $A$ *positive semidefinite* means

$$x^T A x \geq 0 \quad \forall x \in \mathbb{R}^N.$$

Equation (2) is called the *first-order necessary condition*.

# Hessian

Let $f : \mathbb{R}^N \to \mathbb{R}$ be twice continuously differentiable ($\mathcal{C}^2$), then

- The **gradient** of $f$ is

$$\nabla f = \left[\frac{\partial f}{\partial x_1}, \cdots, \frac{\partial f}{\partial x_N}\right]^T$$

- The **Hessian** of $f$ is

$$\nabla^2 f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_N \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_N^2} \end{bmatrix}$$

# Sufficient Conditions

**Theorem 2** *Let $f$ be twice continuously differentiable in a neighborhood of $x^*$, and let*

$$\nabla f(x^*) = 0$$

*and the* Hessian *of $f$, $\nabla^2 f(x^*)$, be* positive semidefinite. *Then $x^*$ is a local minimizer of $f$.*

Note: second derivative information is required to be certain, for instance, if $f(x) = x^3$.

# Quadratic Objective Functions

Suppose

$$f(x) = \frac{1}{2}x^T Hx - x^T b$$

then we have that

$$\nabla^2 f(x) = H$$

and if $H$ is symmetric (assume it is)

$$\nabla f(x) = Hx - b.$$

Therefore, if $H$ is positive semidefinite, then the unique minimizer $x^*$ is the solution to

$$Hx^* = b.$$

# Newton's Method

Newton's Method solves for the minimizer of the *local quadratic model* of $f$ about the current iterate $x_k$ given by

$$m_k(x) = f(x_k) + \nabla f(x_k)^T (x - x_k) + \frac{1}{2}(x - x_k)^T \nabla^2 f(x_k)(x - x_k).$$

If $\nabla^2 f(x_k)$ is positive definite, then the minimizer $x_{k+1}$ of $m_k$ is the unique solution to

$$0 = \nabla m_k(x) = \nabla f(x_k) + \nabla^2 f(x_k)(x - x_k). \quad (3)$$

# Newton Step

The solution to (3) is computed by solving

$$\nabla^2 f(x_k) s_k = -\nabla f(x_k)$$

for the Newton Step $s_k^N$. Then the Newton update is defined by

$$x_{k+1} = x_k + s_k^N.$$

Note: the step $s_k^N$ has both direction and length. Variants of Newton's Method modify one or both of these.

# Standard Assumptions

Assume that $f$ and $x^*$ satisfy the following

1. Let $f$ be twice continuously differentiable and
$$\|\nabla^2 f(x) - \nabla^2 f(y)\| \leq \gamma \|x - y\|.$$
2. $\nabla f(x^*) = 0$.
3. $\nabla^2 f(x^*)$ is *positive definite*.

# Convergence Rate

**Theorem 3** *Let the Standard Assumptions hold. Then there exists a* $\delta > 0$ *such that if* $x_0 \in \mathcal{B}_\delta(x^*)$*, the Newton iteration converges quadratically to* $x^*$*.*

- I.e., $\|e_{k+1}\| \leq K\|e_k\|^2$.
- If $x_0$ is not close enough, Hessian may not be positive definite.
- If you start close enough, you stay close enough.

# Problems (and solutions)

- Need derivatives
  - Use finite difference approximations
- Needs solution of linear system at each iteration
  - Use iterative linear solver like CG (Inexact Newton)
- Hessians are expensive to find (and factor)
  - Use chord (factor once) or Shamanskii
  - Use Quasi-Newton (update $H_k$ to get $H_{k+1}$)
  - Use Gauss-Newton (first order approximate Hessian)

# Nonlinear Least Squares

Recall,

$$f(x) = \frac{1}{2}\sum_{j=1}^{M} |u(t_j;x) - u_j|^2 .$$

Then for $x = [c, k]^T$

$$\nabla f(x) = \begin{bmatrix} \sum_{j=1}^{M} \frac{\partial u(t_j;x)}{\partial c} \left(u(t_j;x) - u_j\right) \\ \sum_{j=1}^{M} \frac{\partial u(t_j;x)}{\partial k} \left(u(t_j;x) - u_j\right) \end{bmatrix} = R'(x)^T R(x)$$

where $R(x) = [u(t_1;x) - u_1, \ldots, u(t_M;x) - u_M]^T$ is called the *residual*.

# Approximate Hessian

In terms of the residual $R$, the Hessian of $f$ becomes

$$\nabla^2 f(x) = R'(x)^T R'(x) + \sum_{j=1}^{M} r_j(x) \nabla^2 r_j(x)$$

where $r_j(x)$ is the $j$th element of the vector $R(x)$. The second term requires the computation of $M$ Hessians, each size $N \times N$. However, if we happen to be solving a *zero residual problem*, this second order term goes to zero. One can argue that for *small residual problems* (and good initial iterates) the second order term is neglibible.

# Gauss-Newton Method

The equation defining the Newton step

$$\nabla^2 f(x_k) s_k = -\nabla f(x_k)$$

becomes

$$\begin{aligned} R'(x_k)^T R'(x_k) s_k &= -\nabla f(x_k) \\ &= -R'(x_k)^T R(x_k). \end{aligned}$$

We define the Gauss-Newton step as the solution $s_k^{GN}$ to this equation.

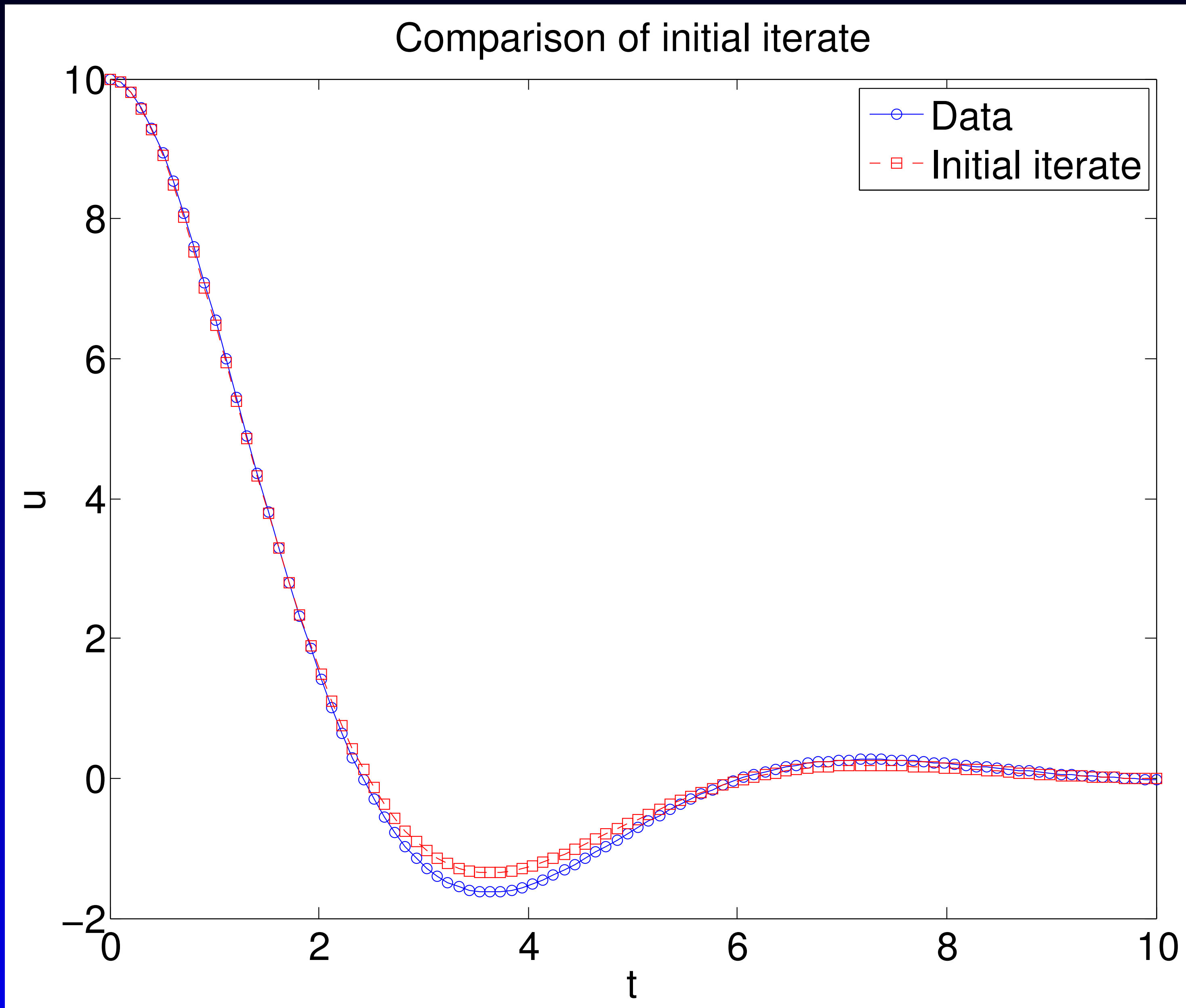
You can expect close to *quadratic* convergence for small residual problems. Otherwise, not even *linear* is guaranteed.

# Numerical Example

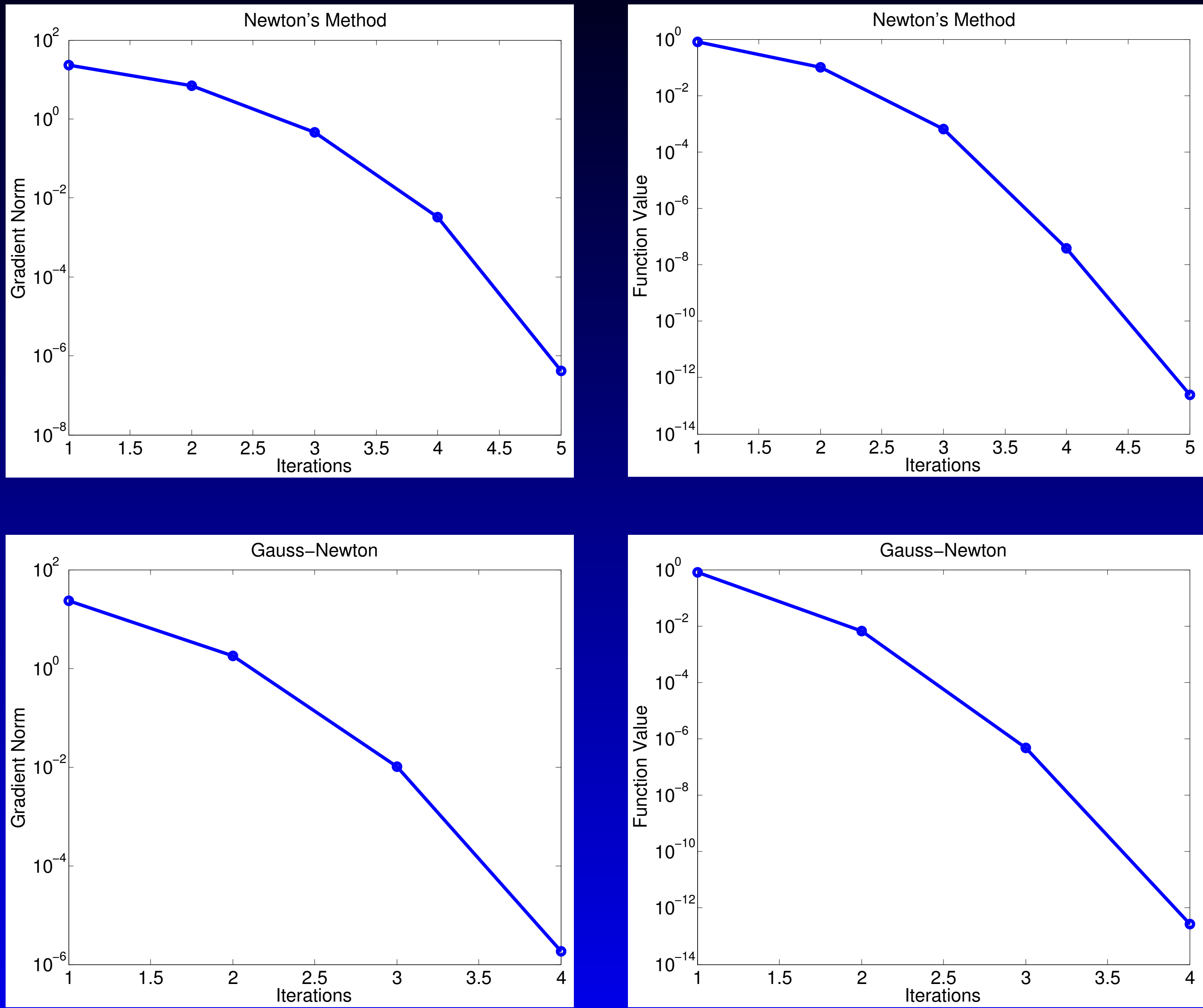
- Recall

$$u'' + cu' + ku = 0; u(0) = u_0; u'(0) = 0.$$

- Let the true parameters be $x^* = [c, k]^T = [1, 1]^T$. Assume we have $M = 100$ data $u_j$ from equally spaced time points on $[0, 10]$.
- We will use the initial iterate $x_0 = [1.1, 1.05]^T$ with Newton's Method and Gauss-Newton.
- We compute gradients with forward differences, analytical $2 \times 2$ matrix inverse, and use `ode15s` for time stepping the ODE.



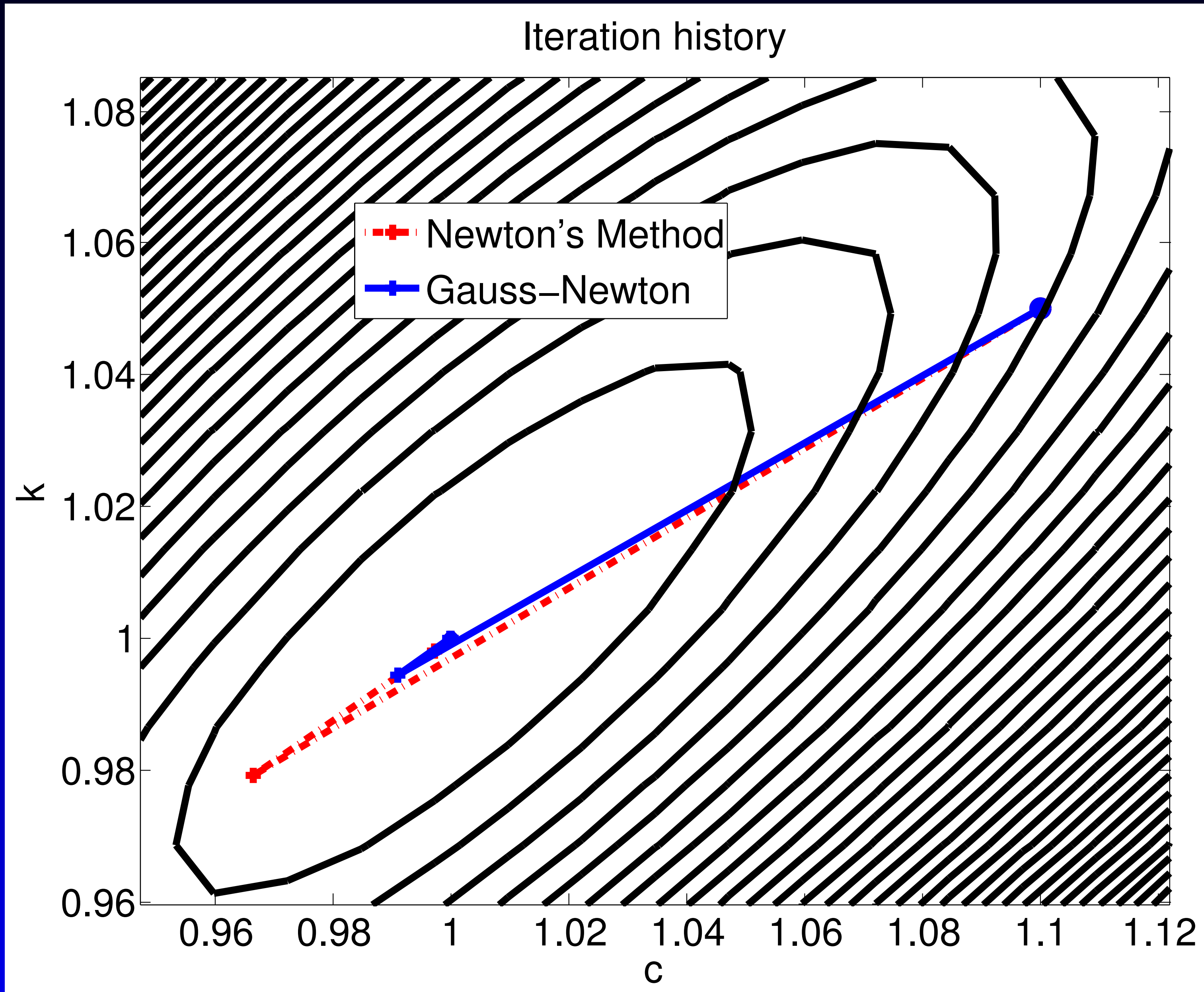
Comparison of initial iterate
Data
Initial iterate
u
t
10
8
6
4
2
0
−2
0
2
4
6
8
10

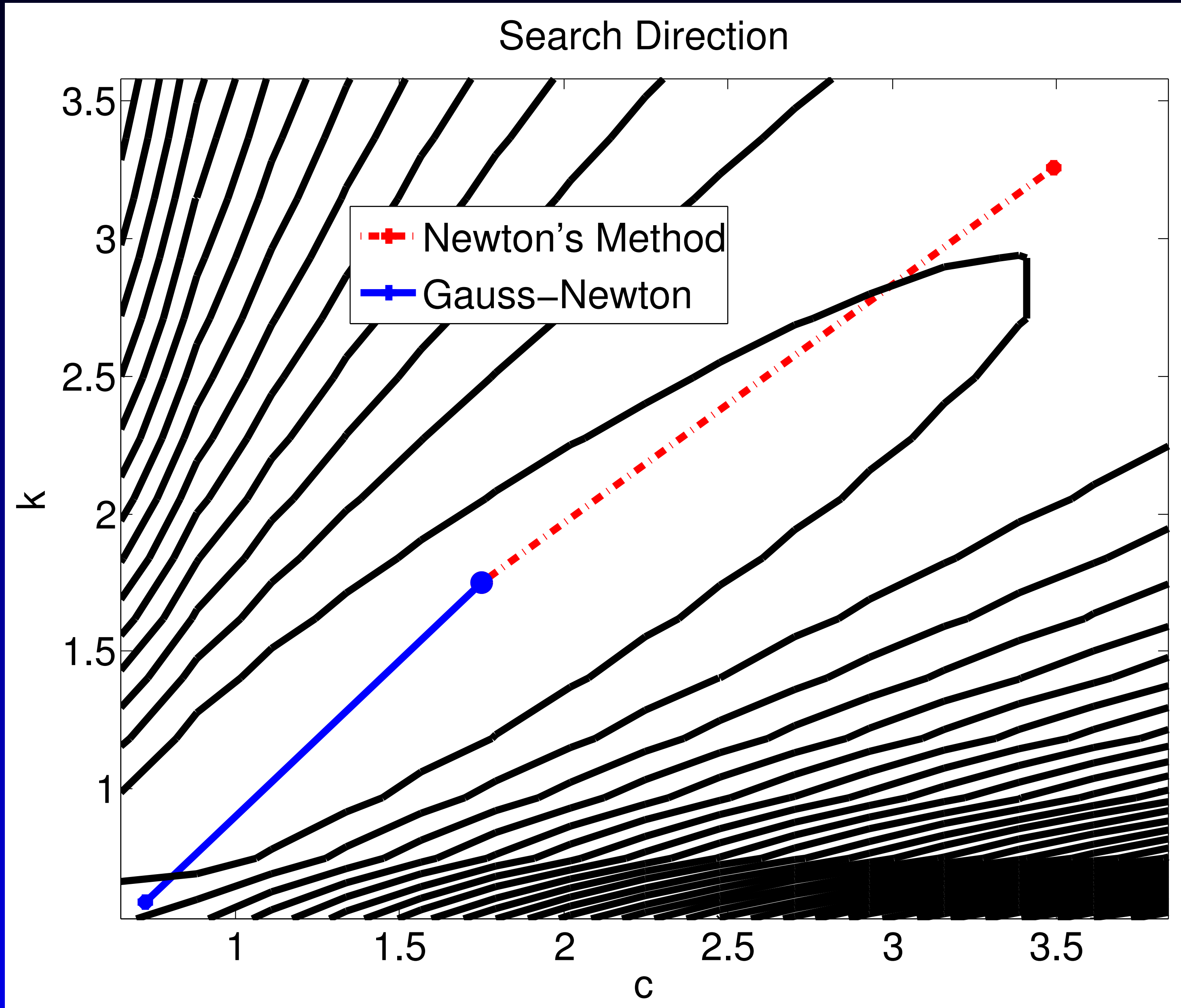


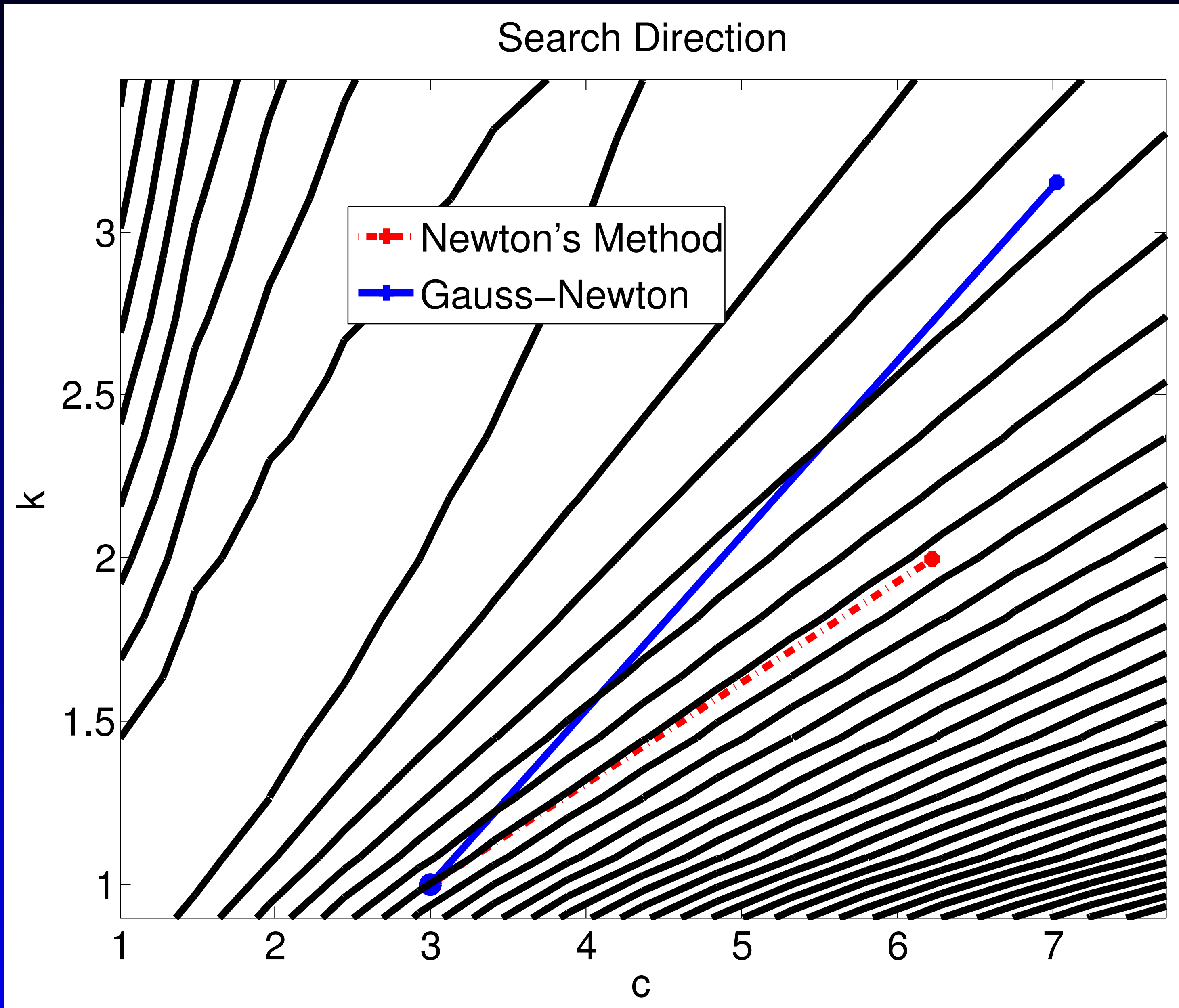
Newton's Method
Gradient Norm
Iterations
Newton's Method
Function Value
Iterations
Gauss–Newton
Gradient Norm
Iterations
Gauss–Newton
Function Value
Iterations

| | Newton | | Gauss-Newton | |
|---|---|---|---|---|
| $k$ | $\|\|\nabla f(x_k)\|\|$ | $f(x_k)$ | $\|\|\nabla f(x_k)\|\|$ | $f(x_k)$ |
| 0 | 2.330e+01 | 7.881e-01 | 2.330e+01 | 7.881e-01 |
| 1 | 6.852e+00 | 9.817e-02 | 1.767e+00 | 6.748e-03 |
| 2 | 4.577e-01 | 6.573e-04 | 1.016e-02 | 4.656e-07 |
| 3 | 3.242e-03 | 3.852e-08 | 1.844e-06 | 2.626e-13 |
| 4 | 4.213e-07 | 2.471e-13 | | |

Table 1: Parameter identification problem, locally convergent iterations. CPU time Newton: 3.4s, Gauss-Newton: 1s.


Iteration history
Newton's Method
Gauss–Newton
1.08
1.06
1.04
1.02
1
0.98
0.96
k
0.96
0.98
1
1.02
1.04
1.06
1.08
1.1
1.12
c


Search Direction
Newton's Method
Gauss–Newton
k
c
3.5
3
2.5
2
1.5
1
1
1.5
2
2.5
3
3.5


Search Direction
Newton's Method
Gauss–Newton
k
c
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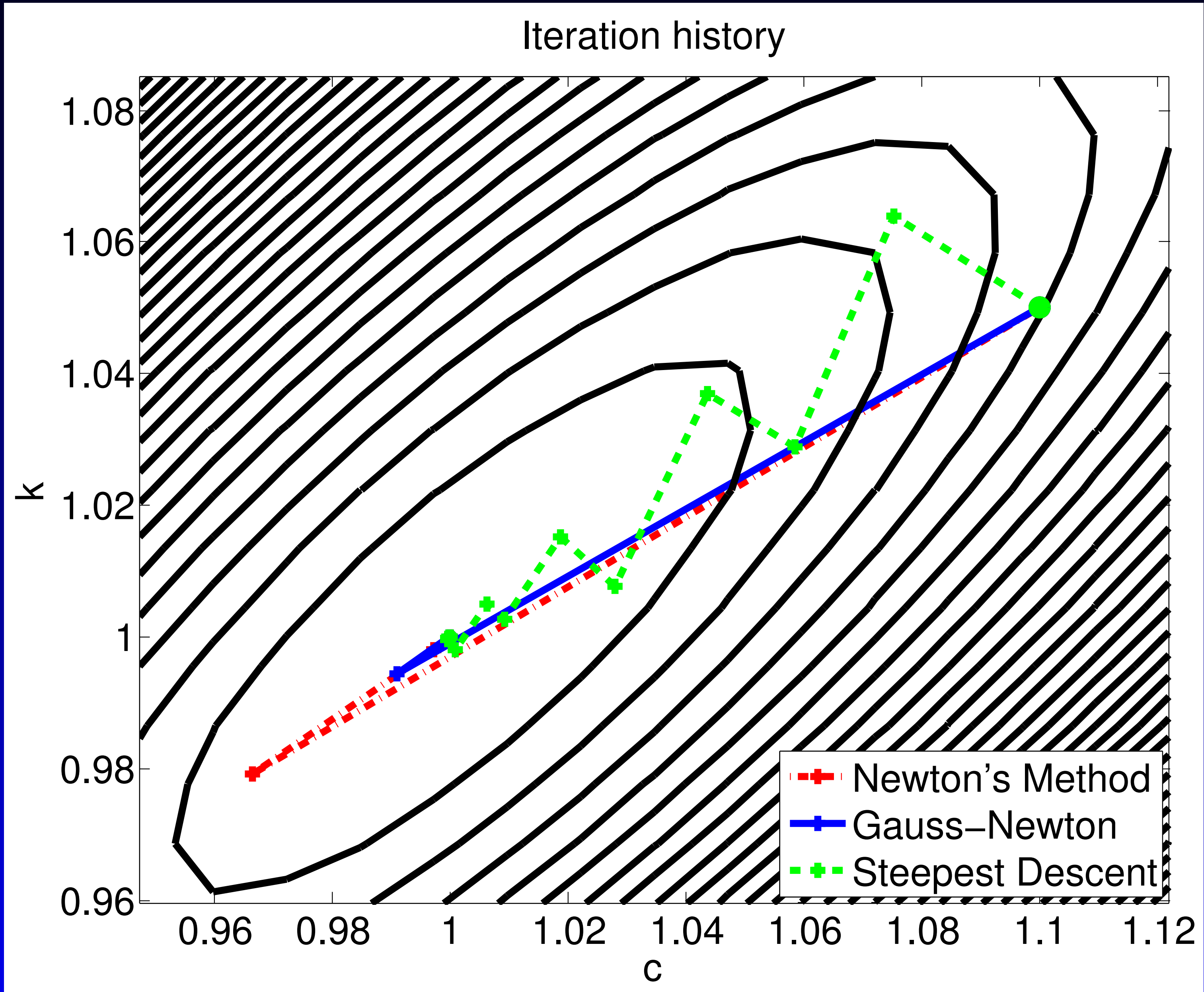
2.5
3

# Global Convergence

- Newton direction may not be a descent direction (if Hessian not positive definite).
- Thus Newton (or any Newton-based method) may increase $f$ if $x_0$ not close enough. Not *globally convergent*.
- Globally convergent methods ensure (sufficient) decrease in $f$.
- The *steepest descent* direction is always a descent direction.

# Steepest Descent Method

- We define the *steepest descent direction* to be $d_k = -\nabla f(x_k)$. This defines a direction but not a step size.
- We define the Steepest Descent update step to be $s_k^{SD} = \lambda_k d_k$ for some $\lambda_k > 0$.
- We will talk later about ways of choosing $\lambda$.


Iteration history
1.08
1.06
1.04
1.02
1
0.98
0.96
k
0.96
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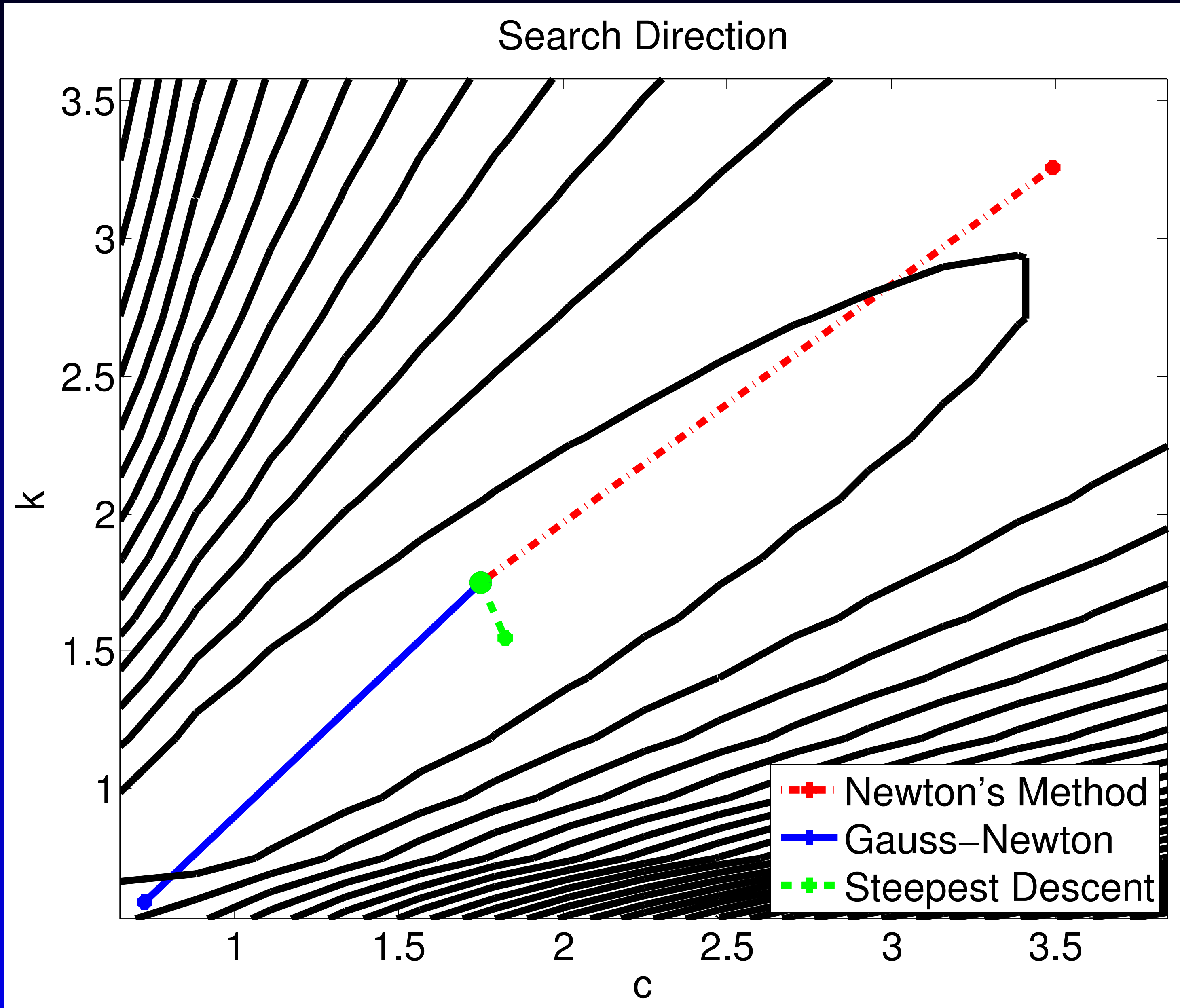
1.02
1.04
1.06
1.08
1.1
1.12
c
Newton's Method
Gauss−Newton
Steepest Descent


Search Direction
k
c
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3
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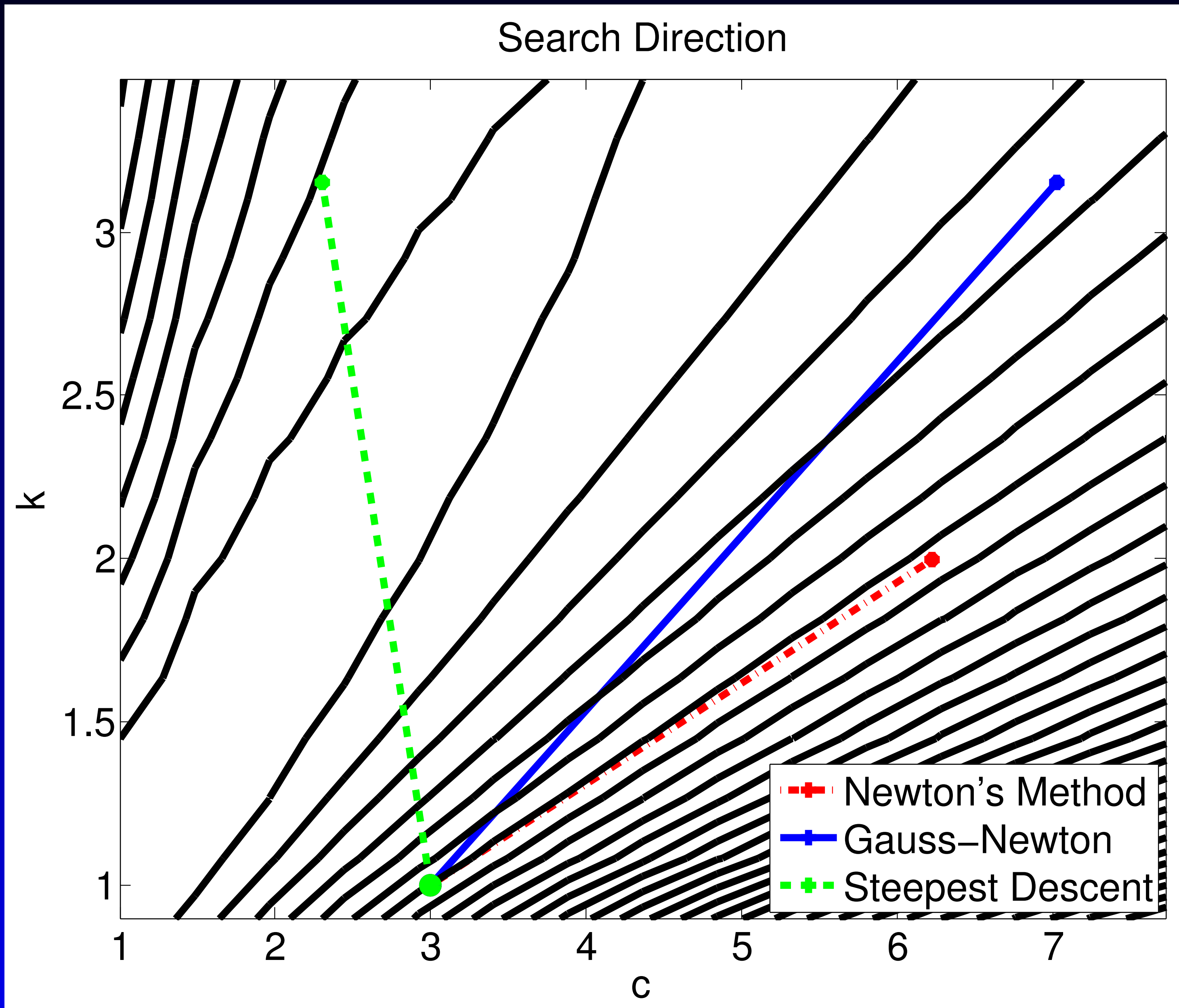
3.5
Newton's Method
Gauss–Newton
Steepest Descent



Search Direction
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3
4
5
6
7
1
1.5
2
2.5
3
Newton's Method
Gauss–Newton
Steepest Descent

# Steepest Descent Comments

- Steepest Descent direction is best direction *locally*.
- The negative gradient is perpendicular to level curves.
- Solving for $s_k^{SD}$ is equivalent to assuming $\nabla^2 f(x_k) = I/\lambda_k$.
- In general you can only expect *linear* convergence.
- Would be good to combine global convergence property of Steepest Descent with *superlinear* convergence rate of Gauss-Newton.

# Levenberg-Marquardt Method

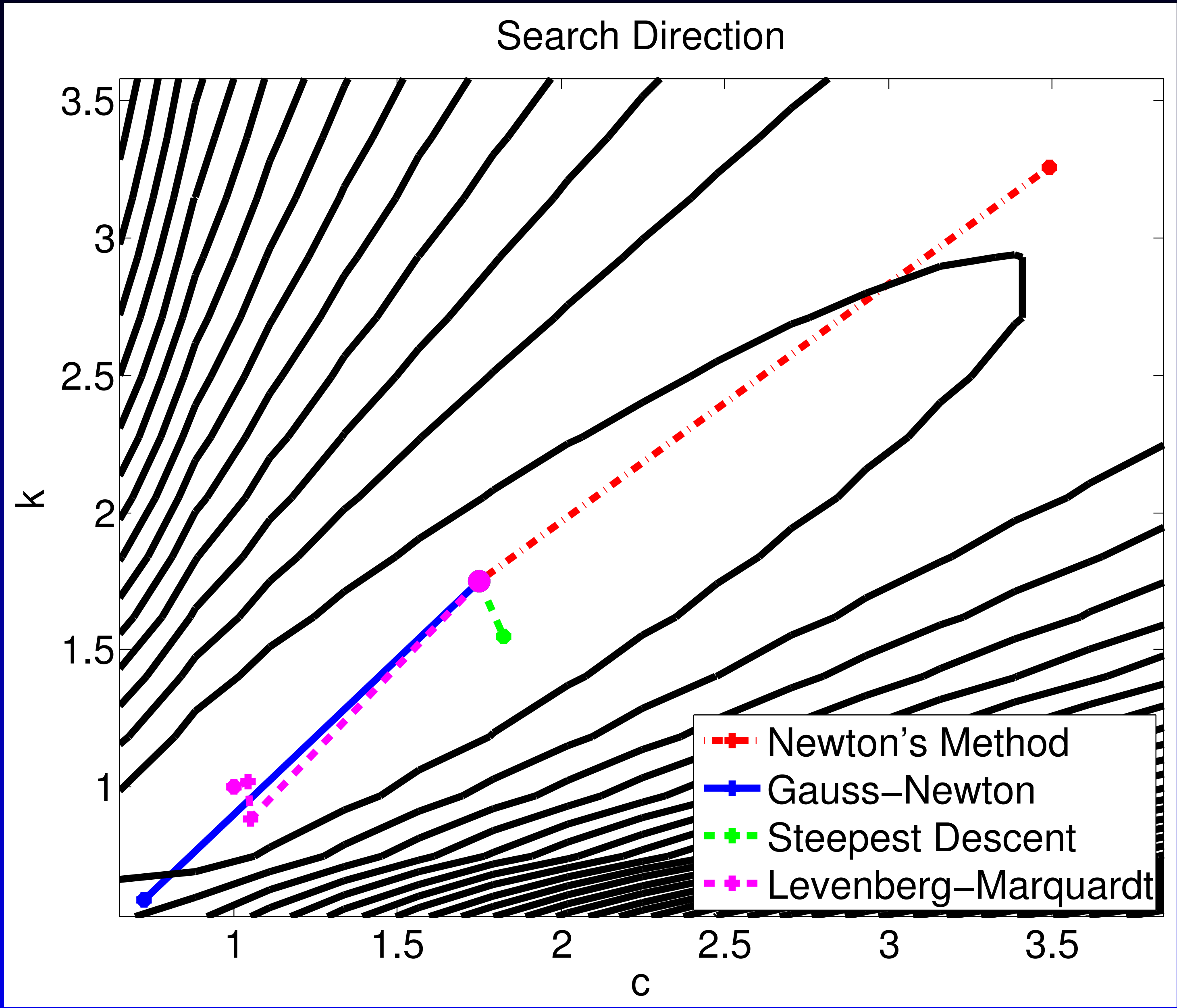
Recall the objective function

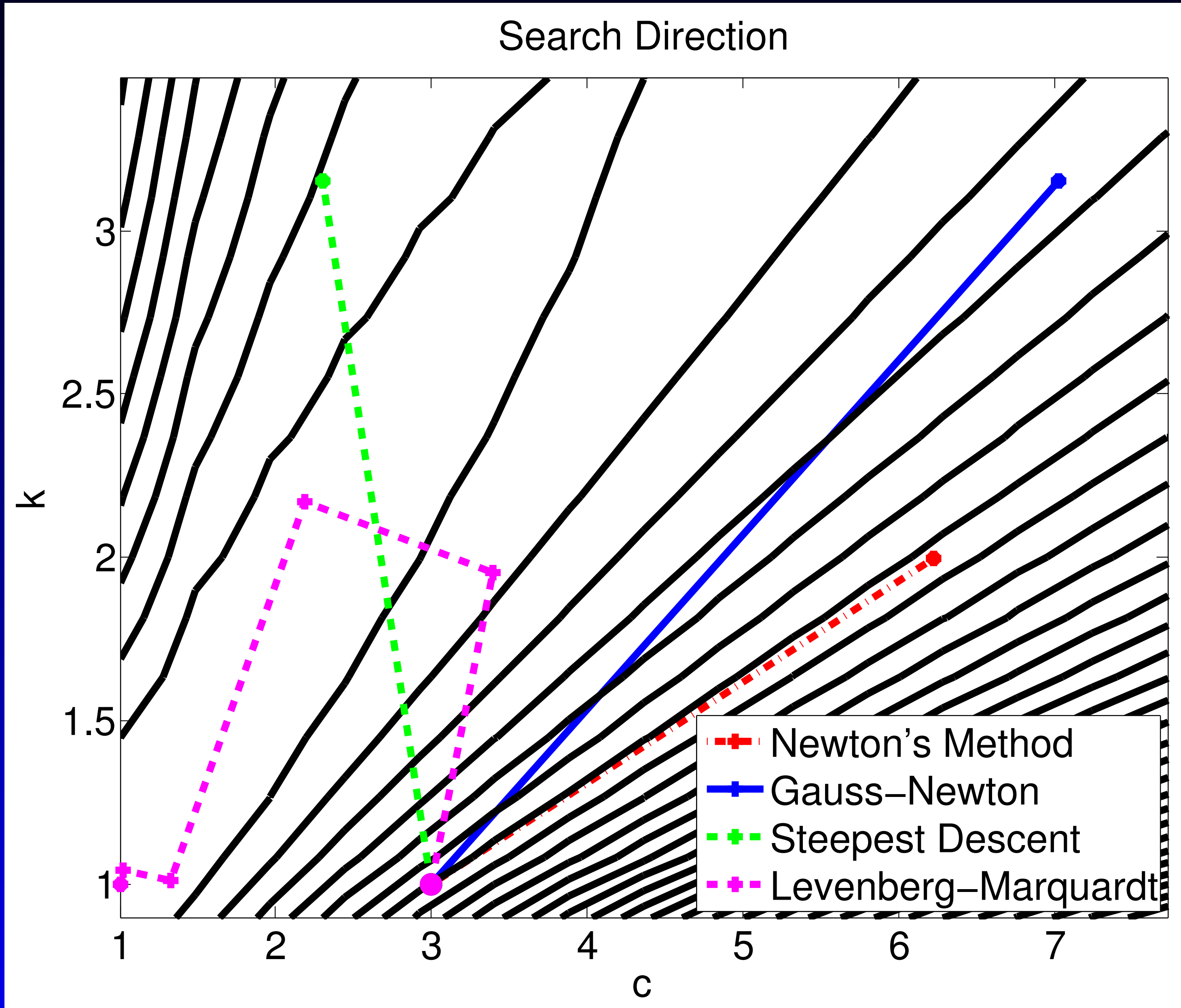
$$f(x) = \frac{1}{2}R(x)^T R(x)$$

where $R$ is the residual. We define the Levenberg-Marquardt update step $s_k^{LM}$ to be the solution of

$$\left(R'(x_k)^T R'(x_k) + \nu_k I\right) s_k = -R'(x_k)^T R(x_k)$$

where the *regularization parameter* $\nu_k$ is called the Levenberg-Marquardt parameter, and it is chosen such that the approximate Hessian $R'(x_k)^T R'(x_k) + \nu_k I$ is positive definite.


Search Direction
3.5
3
2.5
2
1.5
1
k
1
1.5
2
2.5
3
3.5
c
Newton's Method
Gauss−Newton
Steepest Descent
Levenberg−Marquardt


Search Direction
k
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2.5
2
1.5
1
c
1
2
3
4
5
6
7
Newton's Method
Gauss−Newton
Steepest Descent
Levenberg−Marquardt

# Levenberg-Marquardt Notes

- Robust with respect to poor initial conditions and larger residual problems.
- Varying $\nu$ involves interpolation between GN direction ($\nu = 0$) and SD direction (large $\nu$).
- We will talk later on strategies for choosing $\nu$.
- See

  ```
  doc lsqnonlin
  ```

  for MATLAB instructions for LM and GN.

# Summary

- Taylor series with remainder:

$$f(x) = f(x_k) + \nabla f(x_k)^T(x - x_k) + \frac{1}{2}(x - x_k)^T \nabla^2 f(\xi)(x - x_k)$$

- Newton:

$$m_k^N(x) = f(x_k) + \nabla f(x_k)^T(x - x_k) + \frac{1}{2}(x - x_k)^T \nabla^2 f(x_k)(x - x_k)$$

- Steepest Descent:

$$m_k^{SD}(x) = f(x_k) + \nabla f(x_k)^T(x - x_k) + \frac{1}{2}(x - x_k)^T \frac{1}{\lambda_k} I(x - x_k)$$

- Gauss-Newton:

$$m_k^{GN}(x) = f(x_k) + \nabla f(x_k)^T(x - x_k) + \frac{1}{2}(x - x_k)^T R'(x_k)^T R'(x_k)(x - x_k)$$

- Levenberg-Marquardt:

$$m_k^{LM}(x) = f(x_k) + \nabla f(x_k)^T(x - x_k) + \frac{1}{2}(x - x_k)^T \left(R'(x_k)^T R'(x_k) + \nu_k I\right)(x - x_k)$$