Gradient-based Methods for Optimization. Part I.

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Outline

- Unconstrained Optimization
- Newton's Method
    - Inexact Newton
    - Quasi-Newton
- Nonlinear Least Squares
- Gauss-Newton Method
- Steepest Descent Method
- 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

$$u'' + cu' + ku = 0; u(0) = u_0; u'(0) = 0 \tag{1}$$

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 $k = 0, 1, \dots$
  - If x_k optimal, **stop**.
  - Determine a search direction d and a step size λ
  - 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

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 $f : \mathbb{R}^N \rightarrow \mathbb{R}$ 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

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 definite, 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

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

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 Lipschitz continuous with constant γ

$$\|\nabla^2 f(x) - \nabla^2 f(y)\| \leq \gamma \|x - y\|.$$

2. $\nabla f(x^*) = 0.$
3. $\nabla^2 f(x^*)$ is *positive definite*.

Convergence Rate

Theorem

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 solve/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,

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

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* and $R'_{ij}(x) = \frac{\partial R_i(x)}{\partial x_j}$.

Approximate Hessian

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

$$\nabla^2 f(x) = R'(x)^T R'(x) + R''(x)R(x)$$

where $R''(x)R(x) = \sum_{j=1}^{M} r_j(x)\nabla^2 r_j(x)$ and $r_j(x)$ is the jth element of the vector $R(x)$.

The second order 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

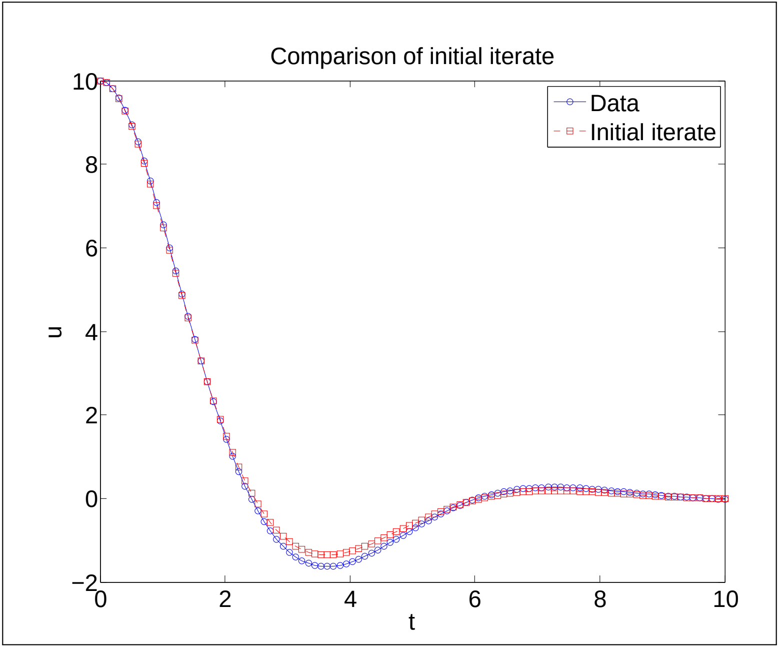
$$\begin{aligned} R'(x_k)^T R'(x_k) s_k &= -\nabla f(x_k) \\ &= -R'(x_k)^T R(x_k). \end{aligned}$$

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 2×2 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
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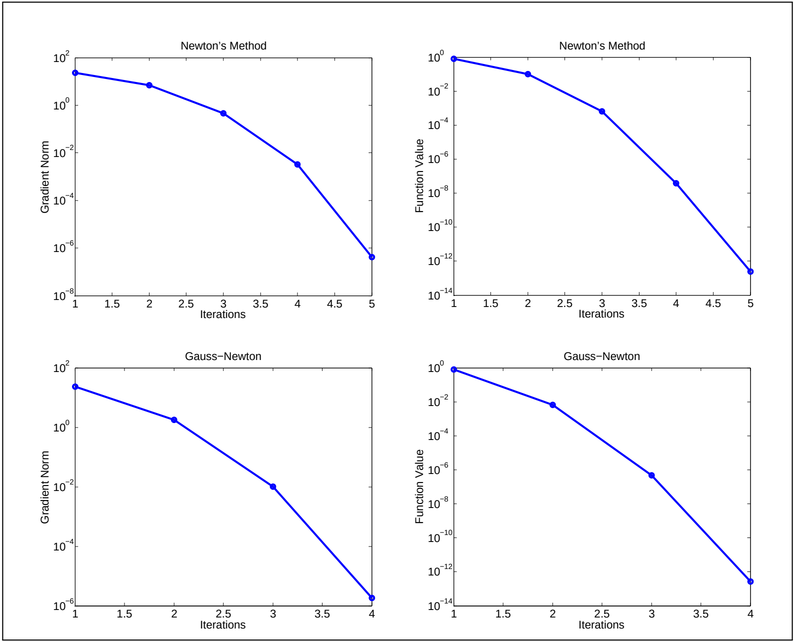
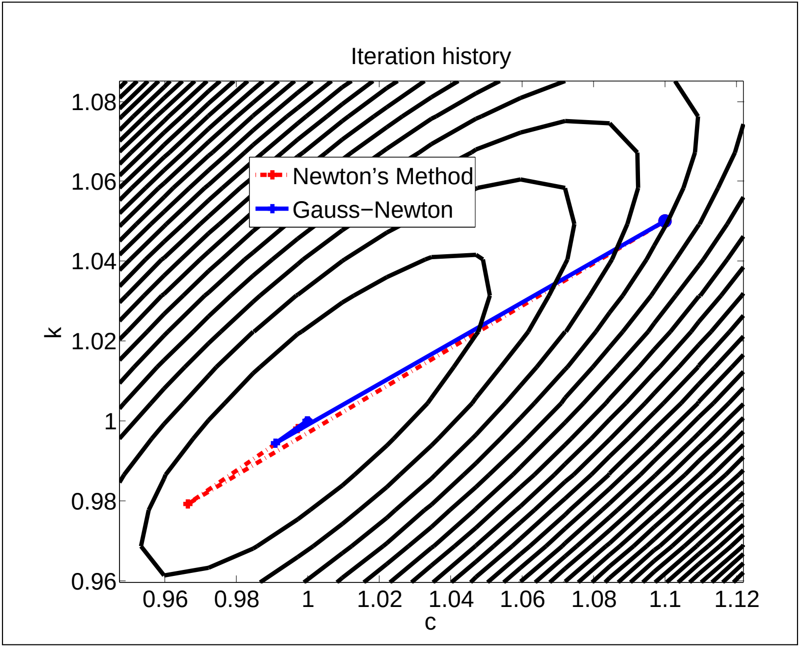
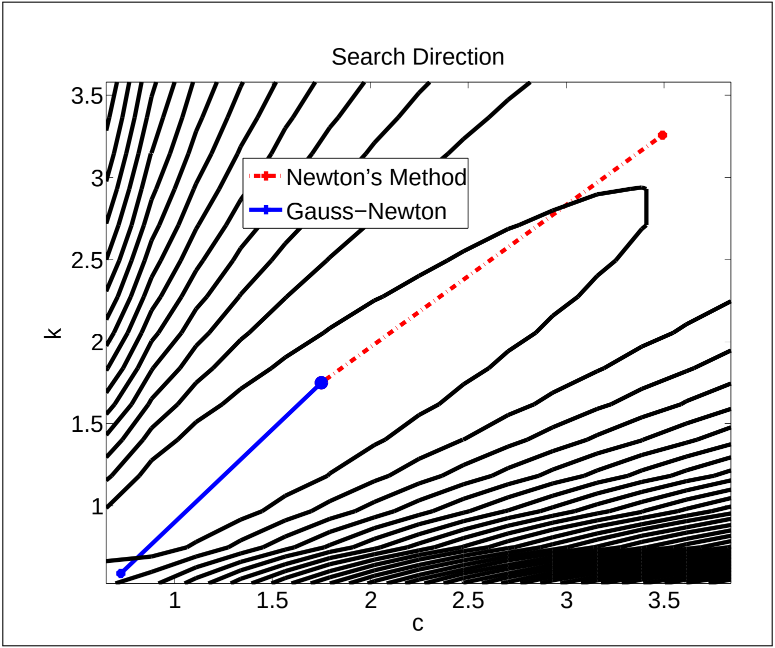
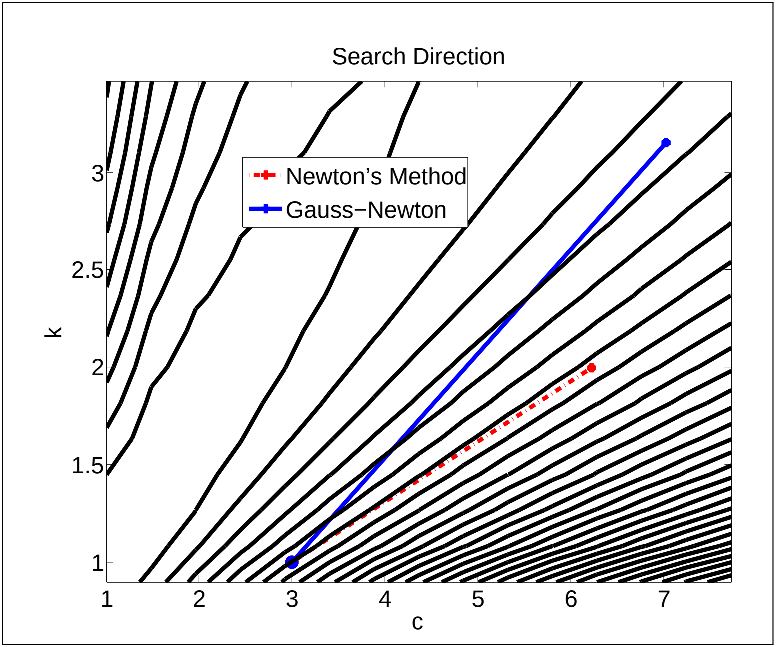

Newton's Method
Gradient Norm
10^{2}
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
1
1.5
2
2.5
3
3.5
4
4.5
5
Iterations
Newton's Method
Function Value
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
1
1.5
2
2.5
3
3.5
4
4.5
5
Iterations
Gauss−Newton
Gradient Norm
10^{2}
10^{0}
10^{-2}
10^{-4}
10^{-6}
1
1.5
2
2.5
3
3.5
4
Iterations
Gauss−Newton
Function Value
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
1
1.5
2
2.5
3
3.5
4
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: Parameter identification problem, locally convergent iterations. CPU time Newton: 3.4s, Gauss-Newton: 1s.


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


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

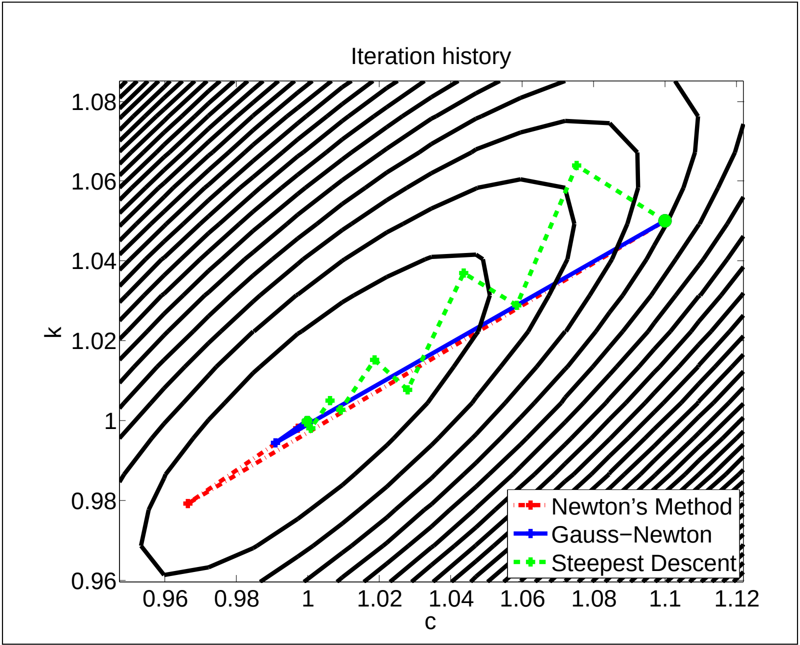

Search Direction
Newton's Method
Gauss−Newton
k
3
2.5
2
1.5
1
c
1
2
3
4
5
6
7

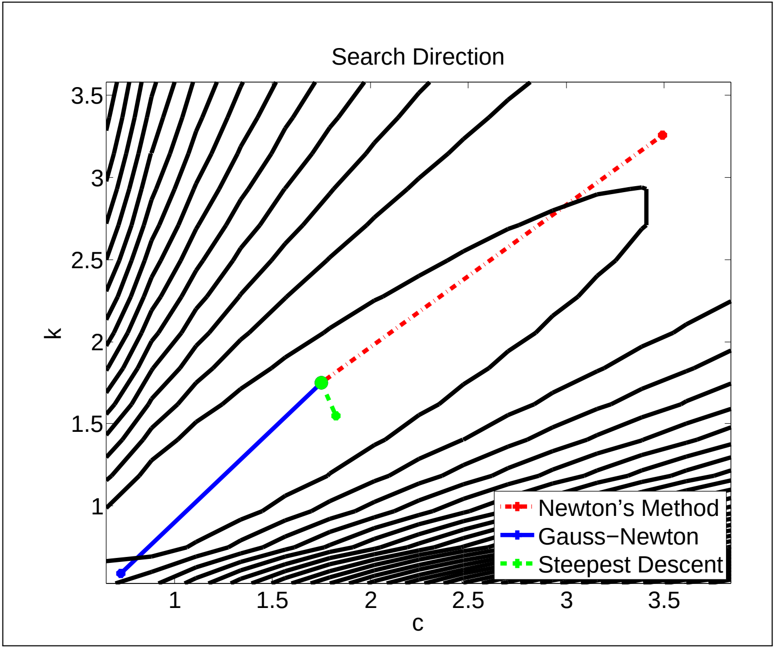
Global Convergence

- 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 λ.


Iteration history
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
Newton's Method
Gauss−Newton
Steepest Descent


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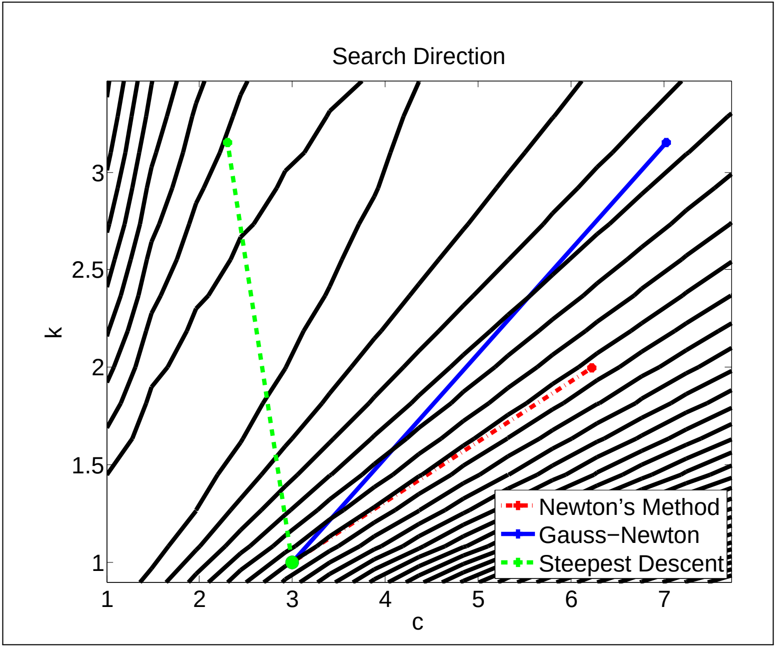
3.5
c
Newton's Method
Gauss−Newton
Steepest Descent


Search Direction
k
3
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2
1.5
1
c
1
2
3
4
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6
7
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

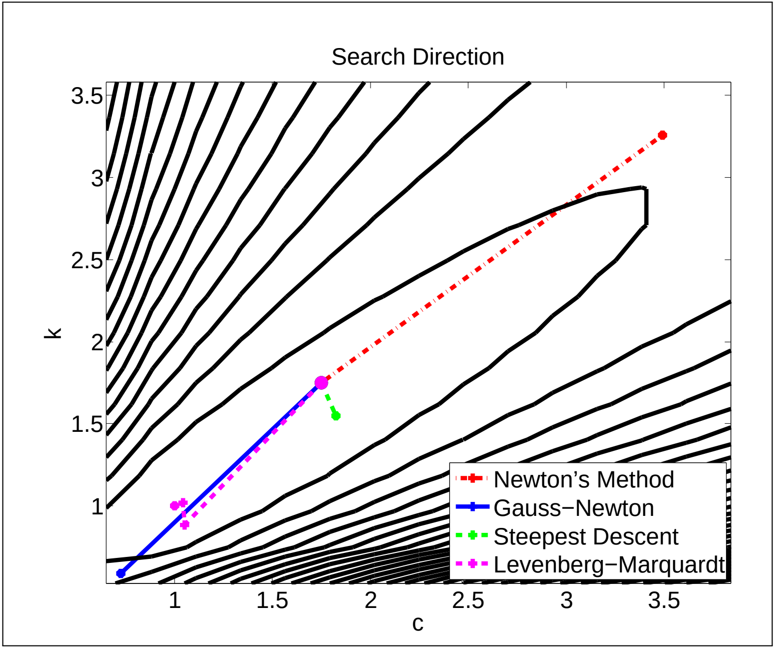
Recall the objective function

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

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* ν_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
k
c
3.5
3
2.5
2
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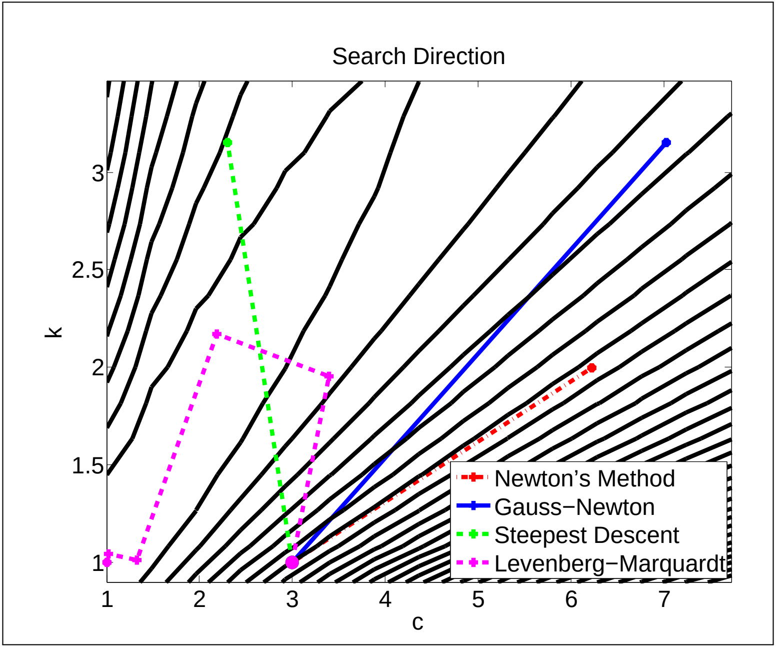
Newton’s Method
Gauss−Newton
Steepest Descent
Levenberg−Marquardt


Search Direction
k
3
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2
1.5
1
c
1
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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 ν involves interpolation between GN direction ($\nu = 0$) and SD direction (large ν).
- See

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doc lsqnonlin
```

for MATLAB instructions for LM and GN.

Levenberg-Marquardt Idea

- If iterate is not close enough to minimizer so that GN does not give a descent direction, increase ν to take more of a SD direction.
- As you get closer to minimizer, decrease ν to take more of a GN step.
  - For zero-residual problems, GN converges quadratically (if at all)
  - SD converges linearly (guaranteed)

LM Alternative Perspective

- Approximate Hessian may not be positive definite (or well-conditioned), increase ν to add regularity.
- As you get closer to minimizer, Hessian will become positive definite (by Standard Assumptions). Decrease ν, as less regularization is necessary.
- Regularized problem is "nearby problem", want to solve actual problem as soon as is feasible.

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

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

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

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

References

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2. Marquardt, D., “An Algorithm for Least-Squares Estimation of Nonlinear Parameters”, SIAM Journal Applied Math., Vol. 11, pp. 431-441, 1963.
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