Homework 4

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1 Exercise 1

1.1 Introduction

In this exercise, we will calibrate a linear spring by minimizing the difference of numerical prediction to measured data. Given a spring who is set into motion by a displacement u_0 at time $t = 0$, the data provided are measurements of the distance from the equilibrium at the time points

$$t_j = (j-1)T/(M-1) \quad \text{for } j = 1, 2, \ldots, M.$$

We know from physics that the function describing the displacement satisfies the IVP

$$u'' + cu' + ku = 0 \text{ where } u(0) = u_0, u'(0) = 0. \tag{1}$$

Here, c and k are two constants named the damping and spring constant respectively. Given the data, we will try to approximate the best choice for c and k such that the norm between the data provided and the solution of the IVP is minimal.

This optimization problem can be stated as

$$\min_x f(x)$$

where $x = (c, k)$ and

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

Here, u_j denotes the data point measured at time t_j. We can see that this problem is a least squares problem.

1.2 The Objective Function and its Gradient

In this section, we will use the notation used in class for least squares problems. Hence, we can write

$$f(x) = \frac{1}{2} \sum_{j=1}^{M} r_j(x)^2$$

where

$$r_j(x) = u(t_j; x) - u_j.$$

In order to determine the gradient of f, we need $\frac{\partial u}{\partial c}$ as well as $\frac{\partial u}{\partial k}$. In view of (1), one can compute that $\frac{\partial u}{\partial c}$ is the unique solution of the IVP

$$y'' + cy' + ky + u' = 0 \text{ where } y(0) = 0, y'(0) = 0, \tag{2}$$

whereas $\frac{\partial u}{\partial k}$ is the solution of

$$y'' + cy' + ky + u = 0 \text{ where } y(0) = 0, y'(0) = 0. \tag{3}$$

The derivation of these two formulas was discussed in class by use of an ad-hoc method. One can also argue by means of the definition of the derivative to show that the partial derivatives satisfy the given ODEs. Interpreting u as a function of t, c and k and using the symmetry of mixed partial derivatives, one readily sees that

$$\begin{aligned}&\left(\frac{\partial u}{\partial c}\right)'' + \left(c\left(\frac{\partial u}{\partial c}\right)' + u'\right) + k\frac{\partial u}{\partial c}\\ =&\frac{\partial}{\partial c}\left(u'' + cu' + ku\right) = \frac{\partial}{\partial c}0 = 0\end{aligned}$$

The boundary conditions can be derived using Lagrangians or the definition of the derivative. Note that the derivation for k is analogous.

In practice, we will have to solve these ODEs for various values of c and k. These ODEs could potentially be stiff and we will therefore solve them with the solver *ode23s*.

For fixed (c, k) we need to be able to evaluate the functions u, $\frac{\partial u}{\partial c}$ and $\frac{\partial u}{\partial k}$ at the points t_j. As our solver uses a dynamic grid dependent on the given equation, we will specify that these points are among the ones computed. However, to solve the IVPs 2 and 3, we need to be able to evaluate u at any point $t \in [0, T]$. To overcome this issue, we will interpolate the return of ode23s linearly. The error of this interpolation is quadratic in terms of the step size, as is well known by the theory of Lagrange-interpolation.

Once we have obtained the partial derivatives of u, we can compute the gradient of f via

$$\begin{aligned}J(x)_{i,j} &= \frac{\partial r_i}{\partial x_j}\\ \nabla f(x) &= J(x)^T r(x)\\ \nabla^2 f(x) &= J(x)J(x)^T + \sum_{j=1}^{M} r_j(x)\nabla^2 r_j(x).\end{aligned}$$

Note that that the computation of the first summand of the Hessian is relatively cheap when one needs to compute the gradient anyway. Subsequently, we will use the term

$$H = J(x)J(x)^T$$

as an approximation of our Hessian. When we speak of the approximated Hessian, we will always address this specific term throughout this document.

In figure 1, we can see that our gradient gives us quadratic convergence up to a distance of roughly 10^{-4}, then the error is linear. This can be explained by the

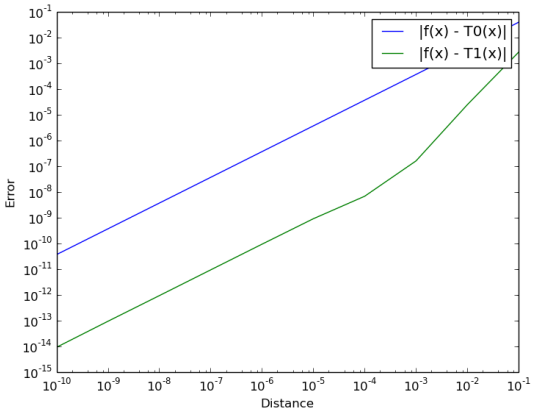


Figure 1: Error of Taylor Polynomials of degree 0 and 1

fact that we introduce more sources of errors by use of linear interpolation and ODE solvers. These errors become dominant for small distances and therefore overshadow the usual quadratic convergence of the first order Taylor polynomial.

1.3 Convergence on $[0.1, 5]^2$

In this section, we will analyze the convergence of the Gauss-Newton method applied to our objective function f on an equidistant 20×20 grid of $\Omega = [0.1, 5]^2$.

1.3.1 The Setup

We will use the Gauss-Newton method for our approximation. In our code, this was realized by replacing the Hessian by our approximation in the method NewtonCG of the OptimTools package. By taking a closer look at the code, this is equivalent to using damped Newton with this approximation.

We also use standard armijo-line search with a starting step length of 1. We iterate until the maximum number of iterations (=100) is reached or our current iterate is accurate within a tolerance of 10^{-2}. On this grid, the maximum number of iterations was never reached. Figure 2 displays a contour plot of $\log(f)$ to give us an idea of what we should expect when applying Gauss-Newton and BFGS. As the logarithm is monotonically increasing, $\log(f)$ attains its minimum at the same point and has the same contour lines as f. As we can see from this plot, the minimum of the objective function is approximately attained at $(0.8, 4.5)$. Based on the contour lines and the curvature, Gauss-Newton should perform much better for $k > c$ than for $k < c$ as the much higher residuals for $k < c$ suggest.

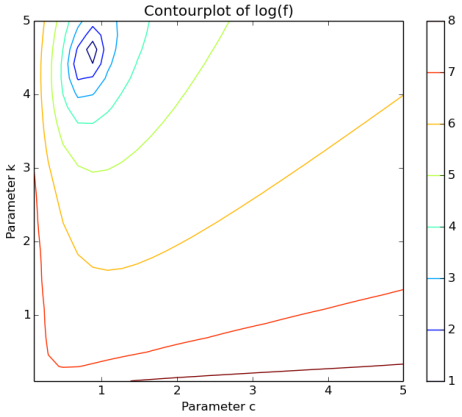


Figure 2: Contour plot of $\log(f)$

1.3.2 Interpretation

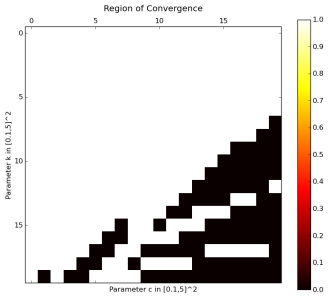
We will display the run time, the number of iterations and the convergence at every point of the grid in figure 3. Note that this matrix plot corresponds to the region Ω and the x and y-axis correspond to c and k respectively. Let us first look at plot (a), which displays whether we reached a tolerance of 10^{-2}. Here, white represents convergence and black represents failure of the method. As the contour plot suggested, we get convergence at every point where $c > k$. However, for $c < k$ there are many points where our method fails. The cause for failure at **all** of these points was that the ODE solver could not solve the IVP within the given accuracy, which was 10^{-8}. This problem could not be resolved by modifying the accuracy. It seems to be the case that the differential equations become too stiff for large residuals.

When we look at the run time, it is interesting to see that the contour plot did not mislead us. The convergence is much faster for values $c < k$, which is on par with our expectation. Apart from that the run time decreases as we get close to our estimation of the parameters, which reaffirms our guess.

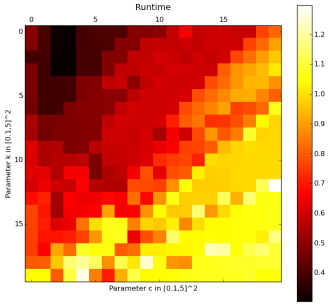
Lastly, the number of iterations looks at first glance a little chaotic. However, note that for $c > k$, the area where the number of iterations is low corresponds to the points where the method failed. I guess it is desirable for a method to fail quickly if it fails, this should however not distract from the fact that for converging starting points the number of iterations is lower when $c < k$, which agrees with the run time results. Hence, we can again conclude that the best guess for the parameter is $(0.8, 4.5)$.

1.4 Gauss-Newton vs BFGS

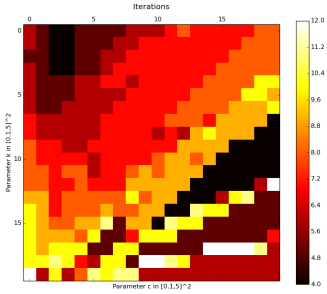
In this section, we will compare the Gauss-Newton method to a standard implementation of BFGS. The setting is the same as last time, but we will restrict



(a) Region of Convergence

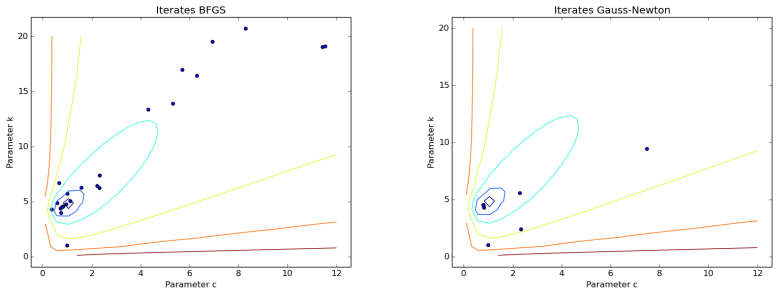


(b) Runtime



(c) Iterations

Figure 3: Global Convergence



(a) BFGS Iterates (b) Gauss-Newton Iterates

Figure 4: Iterates on Contour Plot of $\log(f)$

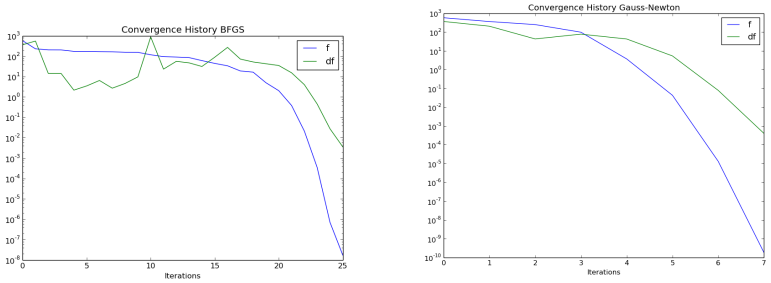
ourselves to the starting point $(1, 1)$. We have measured the run time, the number of iterations and the number of IVPs that had to be solved.

Method	**Iterations**	**Run time**	**Memory**	**Eval. f,df,H**	**IVPs**
BFGS	26	1.628233	14.3Mb	76,27,0	130
Gauss-Newton	8	0.617532	5.6Mb	18,8,8	50

Table 1: Performance Comparison $x_0 = (1, 1)$, Run time in sec

Even though the problem is very different, these results are similar to the ones obtained in the last homework problem. Even though we use a different way to approximate our Hessian, it turns out that the a Newton method with approximated Hessian often performs better than a standard BFGS. Gauss-Newton needs less iterations, has a faster run time and less function and gradient evaluations. Even though BFGS avoids the evaluation of the Hessian, this does not have a huge impact as evaluating our approximation of the Hessian requires the same ODEs to be solvend and replaces a matrix-vector product by a matrix-matrix product. So, while it costs more, the effect in this particular problem is not very strong. Also, the number of IVPs that need to be solved is lower for Gauss-Newton which is probably the main reason for the quicker run time. We can also observe that the memory consumption of BFGS is much higher, although this difference might be greatly reduced by a limited-memory implementation of BFGS.

In figure 4, you can see the iterates of both Gauss-Newton and BFGS. It is interesting to note that the iterates of both methods look almost chaotic. As both of them use approximated curvature information, it is not surprising that one can not predict the next iterate based on the contours and the position of the solution. However, it might surprise that especially some of the iterates of BFGS are far out and are much further away from the solution than our initial guess in the euclidean norm. But, we already observed the big difference in performance between the cases $c < k$ and $c > k$. Here, our initial case satisfies



(a) BFGS (b) Gauss Newton

Figure 5: Convergence History

$c = k$ and is therefore just on the edge. Comparing both methods, we can observe yet again that Gauss-Newton performs superior.

In figure 5, the norm of $f(x_k)$ and $\nabla f(x_k)$ are visualized for BFGS and Gauss-Newton. The first noteworthy observation is that the norm of the gradient does not decrease monotonically in both cases. This was not to be expected, as there is no general result on monotonically decreasing gradients for any of the methods. When we look at the norm of the objective function, we can see that the convergence starts off very slowly and then dramatically increases at the end. Thus, our convergence is much better when we are close to the solution. This is not surprising for any Newton or quasi-Newton method. In this case, the fact that the residuals are much smaller close to the solution, is one of the reasons why Gauss-Newton performs so much better close to the solution. We can conclude that for least squares problems where the optimal solution has small residuals, the choice of a good initial guess can be key.

1.5 Noise

In this section we will compare BFGS and Gauss-Newton at the point $(1, 5)$. Additionally, we have added noise to the data and we will analyze how the noise affects our result. The noise is generated by use of *randn* and ϵ will denote the maximum norm of our noise. The following table shows how the noise affects the computational costs.

Method	**Iterations**	**Run time**	**Eval. f,df,H**	**IVPs**
BFGS, $\epsilon = 0$	7	0.61078	28,8,0	44
Gauss-Newton, $\epsilon = 0$	5	0.3541	9,5,5	29
BFGS, $\epsilon = 10^{-8}$	7	0.61121	28,8,0	44
Gauss-Newton, $\epsilon = 10^{-8}$	5	0.3569	9,5,5	29
BFGS, $\epsilon = 1$	7	0.789382	27,8,0	43
Gauss-Newton, $\epsilon = 1$	5	0.547566	9,5,5	29
BFGS, $\epsilon = 10$	9	9.589382	32,10,0	52
Gauss-Newton, $\epsilon = 10$	8	4.547566	16,8,8	48

Table 2: Performance Comparison with Noise $x_0 = (1, 5)$, Runtime in sec

Note that the performance depends on the random numbers, not just their norm. Hence, the results in this table should not be understood absolute, but relative with respect to the random numbers.

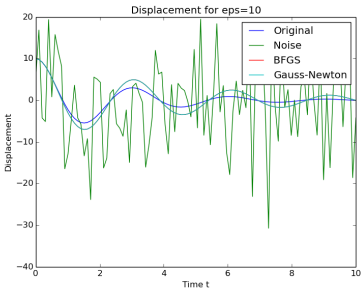
We can see from this table that both methods are relatively robust when it comes to noise. For $\epsilon \leq 1$, the performance is not significantly influenced. When we set $\epsilon = 10$, which is an unreasonable large noise given that the maximum displacement of our spring is also 10, we can see that the methods converge slower but not as much as one might expect.

When I really tried to break things, I found out that BFGS performs much worse than Gauss-Newton for $\epsilon = 100$ and both mehtods failed to converge for $\epsilon = 1000$. But, such a noise makes results worthless anyway, so these results should not be considered when comparing the robustness and efficiency of both algorithms.

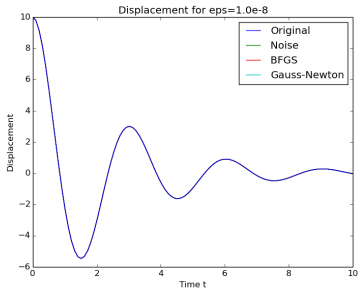
From the data obtained, it is hard to say which method is more robust. Both methods scale similarly with the amount of noise and in this setting one can say that they both handle a reasonable amount of noise very well.

We will now take a closer look at the accuracy of our approximation by plotting our final displacement in figure 6 side-by-side with the actual solution and the noised data. We can see that the approximated solutions are always very close provided that the methods converge. Even when the noise is very strong, the approximated parameters are further off, but the displacement is still surprisingly close. From these pictures, it seems plausible that a noise of 10^{-8} might be negligable in most circumstances. Both methods always converge to the same solution, so the only difference in noise handling lies in computational costs.

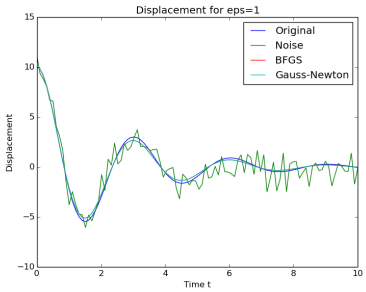
Based on this one could hypothesize that for similar types of problems small noise is negligible both in computational costs and acccuracy of approximation.



(a) $\epsilon = 10$



(b) $\epsilon = 10^{-8}$



(c) $\epsilon = 10^{-2}$

Figure 6: Plots of displacement for various ϵ