

Numerical Optimization for Large Scale Problems

Assignment Report

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Abstract

AP: [TODO]

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1 Introduction

In this section we will describe the implementation details of the algorithms used to solve the optimization problems, namely modified Newton method and truncated Newton method, focusing on the differences with respect to the standard Newton method. These methods will be tested against the Rosenbrock function and three test problems from [1]. The chosen test problems are the extended Rosenbrock function (problem 25), the generalized Broyden tridiagonal function (problem 32) and the banded trigonometric function (problem 16) and results are contained in sections 3, 4 and 5 respectively. AP: [Discuss how experiments are carried out, starting from 11 points, average metrics are reported.] AP: [Discuss convergence rate definition].

1.1 Modified Newton Method

The modified Newton method aims to enhance robustness of the standard Newton method by ensuring positive-definiteness of the Hessian matrix. At iteration k , it is necessary to check whether the Hessian matrix H_k is positive definite: in case it is not, the matrix is modified by adding a matrix B_k in order to ensure positive definiteness. A common choice for B_k is a multiple of the identity matrix, i.e. $B_k = \tau_k I$ so that the whole spectrum of H_k is shifted by τ_k . Then we want to find the smallest τ_k such that $H_k + \tau_k I$ is positive definite, which is $-\lambda_{k, min} + \beta$ where $\lambda_{k, min}$ is the negative eigenvalue with the largest module.

To avoid to have to compute $\lambda_{k, \min}$, we adopted the *Cholesky with Added Multiple of the Identity* algorithm outlined in [2] that consists in building a sequence of τ_k until the modified matrix is positive definite. The sequence is built starting from $\tau_k = \min_i h_{ii} + \beta$ where $\min_i h_{ii}$ is the smallest diagonal element of H_k . Then, at each iteration:

1. positive-definiteness is assessed trying to perform a Cholesky factorization of $H_k + \tau_k I$;
2. if the factorization is not successful, τ_k is increased by a factor c and the process is repeated for a limited number of times $k_{chol, max}$.

In all the experiments we choose $\beta = 10^{-3}$, $k_{chol, max} = 100$. A good value for the constant factor is $c = 2$, but as we will discuss in section 3 for the extended Rosenbrock function a larger value $c = 5$ is beneficial. The method is endowed with a line search strategy with backtracking. We carry on experiments both with and without preconditioning, using the incomplete Cholesky factorization as preconditioner.

1.2 Truncated Newton method

The truncated Newton method aims to reduce the computational cost of the Newton method by adopting the following strategies:

- the newton system $H_k p_k = -\nabla f(x_k)$ is solved approximately by means of an iterative method (i.e. conjugate gradient method), with a tolerance that depends on $\|\nabla f(x_k)\|$;
- whenever a direction of negative curvature is found in the execution of the iterative method, the method is stopped and the direction is used as the search direction to prevent a non-negative curvature direction to be chosen in case of a non-positive definite H_k .

In all the experiments, we choose the relative tolerance for the iterative method at iteration k to be

$$\eta_k = \min\{0.5, \sqrt{\|\nabla f(x_k)\|}\}$$

that is a forcing term that is proven to yield a superlinear convergence rate. The method is endowed with a line search strategy with backtracking. We carry on experiments both with and without preconditioning, using the incomplete Cholesky factorization as preconditioner for the Newton system whenever the Hessian matrix is positive definite.

1.3 Finite differences

Experiments in subsequent sections will adopt both exact and finite differences gradient and Hessian to perform the optimization. When finite differences are adopted, the gradient will be estimated using centered finite differences

$$\frac{\partial f}{\partial x_k} \approx \frac{f(x + he_k) - f(x - he_k)}{2h} \quad (1)$$

while the Hessian will be estimated using forward finite differences, using the following formula

$$\frac{\partial^2 f}{\partial x_k \partial x_j} \approx \frac{f(x + he_k + he_j) - f(x + he_k) - f(x + he_j) + f(x)}{h^2} \quad (2)$$

where e_k and e_j are the k -th and the j -th canonical basis vectors respectively. Moreover, two different approaches will be adopted to choose the step size h : the first one will use a fixed step size while the second one will use a step size that depends on the current point x and that is different for each component, defined as follows

$$h_{k, i} = h |x_{k, i}|$$

where $h_{k, i}$ is the increment for component i at step k , h is a relative step size and $x_{k, i}$ is the i -th component of the point at step k . Due to the large scale nature of the problems, the finite differences method is expected to be slower than the exact method, so ad-hoc implementations that will exploit the sparsity of the Hessian matrix and the separability of the specific functions will be used.

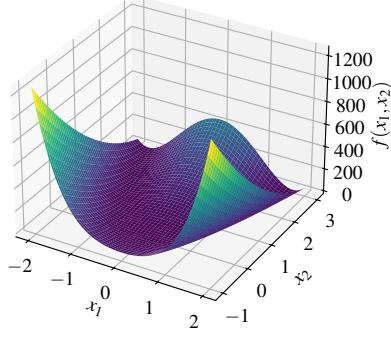


Figure 1: Surface plot of the 2-dimensional extended Rosenbrock function

2 Rosenbrock function

2.1 Exact gradient and Hessian

2.2 Finite differences gradient and Hessian

3 Extended Rosenbrock function

The extended Rosenbrock function is a generalization of the Rosenbrock function to n dimensions, defined as follows. Figure 1 shows the surface plot of the 2-dimensional extended Rosenbrock function: notice that for $n = 2$ it is identical to the standard Rosenbrock function, except for the $\frac{1}{2}$ term.

$$F(x) = \frac{1}{2} \sum_{k=1}^n f_k^2(x), \quad f_k(x) = \begin{cases} 10(x_k^2 - x_{k+1}), & k \bmod 2 = 1 \\ x_{k-1} - 1, & k \bmod 2 = 0 \end{cases} \quad (3)$$

The minimum of the function is in a very flat valley which is easy to reach, but in practice it's harder to converge to a minimum, which makes the extended Rosenbrock function a challenging optimization problem. AP: [Add something to justify the choice of the constant for modified newton method].

3.1 Exact gradient and Hessian

The gradient of the extended Rosenbrock function is given by the following expression,

$$\frac{\partial F}{\partial x_k} = \begin{cases} 200(x_k^3 - x_k x_{k+1}) + (x_k - 1), & k \bmod 2 = 1 \\ -100(x_{k-1}^2 - x_k), & k \bmod 2 = 0 \end{cases} \quad (4)$$

computation can be eased considering that component k depends only on f_k and f_{k+1} when k is odd, and only on f_{k-1} when k is even. The Hessian of the extended Rosenbrock function is given by the following expression.

$$\frac{\partial^2 F}{\partial x_k \partial x_j} = \begin{cases} 200(3x_k^2 - x_{k+1}) + 1, & j = k, k \bmod 2 = 1 \\ 100, & j = k, k \bmod 2 = 0 \\ -200x_k, & |k - j| = 1, k \bmod 2 = 1 \\ 0, & \text{otherwise} \end{cases} \quad (5)$$

Notice that the Hessian is a sparse matrix, with only n non-zero elements on the diagonal and $n/2$ non-zero elements on the first co-diagonal.

Table 1 shows the results for the *Modified Newton method* applied to the extended Rosenbrock function with exact gradient and Hessian. All attempts were successful, and the method converged in a small number of iterations, with a convergence rate that is close to 2 for all dimensions but 10^5 , where the convergence rate is smaller and close to 1. However, the time required to converge is significantly higher for the 10^5 -dimensional problem, which is expected due to the increased number of function evaluations required to compute the gradient and Hessian. We observe that being the number of iterations necessary to converge to the minimum of the

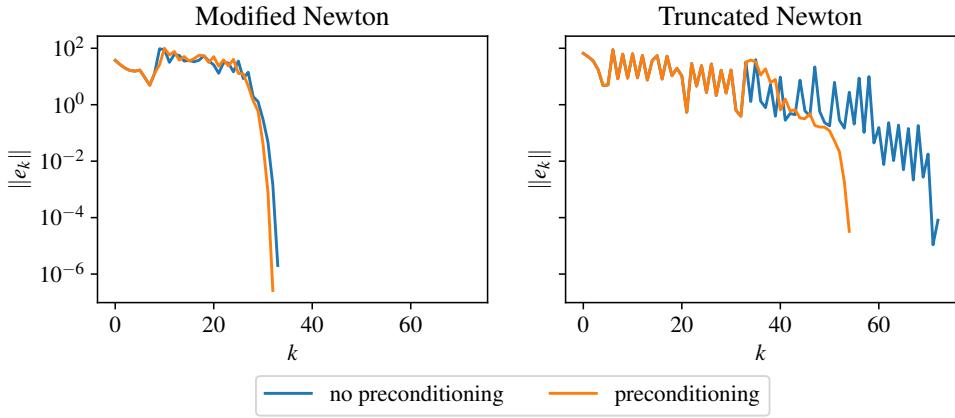


Figure 2: Estimate of the error for Modified Newton method and for the Truncated Newton method applied to the Extended Rosenbrock function with exact gradient and Hessian for $n = 10^5$, random point 1.

Table 1: Results for Modified Newton method applied to Extended Rosenbrock with exact gradient and hessian, metrics are average metrics for successful attempts.

preconditioning dimension	iterations		convergence rate		time		success rate	
	False	True	False	True	False	True	False	True
3	31.91	28.91	1.99	1.51	0.05	0.02	1.00	1.00
4	32.36	29.18	2.10	2.04	0.11	0.08	1.00	1.00
5	26.50	26.00	1.10	1.00	0.68	0.53	1.00	1.00

function very low, the experimental convergence rate is not very reliable, as it is computed as the ratio between the number of iterations and the logarithm of the relative error.

Table 2 shows the results for the *Truncated Newton method* applied to the extended Rosenbrock function with exact gradient and Hessian. All attempts were successful, and the method converged in a small number of iterations. The computed experimental convergence rate is not reliable at all, presumably due to the small number of iterations and truncations of the iterative solver used to solve the Newton system. Moreover, when preconditioning is not adopted we get a negative convergence rate since $\log\|e_k\|$ where e_k is the error at iteration k is not monotonic with respect to k , as shown in figure 2. However, when preconditioning is adopted and k is larger, i.e. for $n = 10^5$, the convergence rate is superlinear as expected from the truncated Newton method with a superlinear forcing term.

Figure 2 shows the estimate of the error for the Modified Newton method and for the Truncated Newton method applied to the Extended Rosenbrock function with exact gradient and Hessian for $n = 10^5$ when starting from random point 1:

- for the *Modified Newton method*, in early iterates the estimated error is not monotonic, but it becomes monotonic after a few iterations regardless of preconditioning;
- for the *Truncated Newton method*, in early iterates the estimated error is not monotonic, but it becomes monotonic after a few iterations, but only if preconditioning is adopted.

Both in the case of the Modified Newton method and the Truncated Newton method, preconditioning improves performance of the optimization algorithms both in terms of number of iterations and time required to converge.

3.2 Finite differences gradient and Hessian

When applying 1, one can notice that the terms $F(x + he_k)$ and $F(x - he_k)$ only differ by terms f_k and f_{k+1} for k odd, by terms f_{k-1} for k even. Then to make function evaluations less expensive, we can define the following function $F_{fd,k}$, which can be plugged in 1 in place of F yielding the same result.

$$F_{fd,k}(x) = \begin{cases} \frac{1}{2}f_k^2(x) + \frac{1}{2}f_{k+1}^2(x), & k \bmod 2 = 1 \\ \frac{1}{2}f_{k-1}^2(x), & k \bmod 2 = 0 \end{cases}$$

The same procedure can be applied for the Hessian, considering that:

Table 2: Results for Truncated Newton method applied to Extended Rosenbrock with exact gradient and hessian, metrics are average metrics for successful attempts.

preconditioning dimension	iterations		convergence rate		time		success rate	
	False	True	False	True	False	True	False	True
3	50.09	31.00	-2.66	11.55	0.01	0.01	1.00	1.00
4	57.27	34.73	-3.06	4.33	0.04	0.03	1.00	1.00
5	64.00	28.50	-5.58	1.62	0.45	0.23	1.00	1.00

- function evaluations to compute entry $h_{k,k}$ differ only by f_k and f_{k+1} for k odd, and only on f_{k-1} for k even;
- function evaluations to compute entry $h_{k,k+1}$ differ only by f_k and f_{k+1} for k odd.

Then to make function evaluations less expensive, we can define the functions $F_{fd,k,k}$ and $F_{fd,k,k+1}$, which can be plugged in 2 in place of F yielding the same result to compute entries $h_{k,k}$ and $h_{k,k+1}$ respectively.

$$F_{fd,k,k}(x) = \begin{cases} \frac{1}{2}f_k^2(x) + \frac{1}{2}f_{k+1}^2(x), & k \bmod 2 = 1 \\ \frac{1}{2}f_{k-1}^2(x), & k \bmod 2 = 0 \end{cases}$$

$$F_{fd,k,k+1}(x) = \begin{cases} \frac{1}{2}f_k^2(x) + \frac{1}{2}f_{k+1}^2(x), & k \bmod 2 = 1 \\ 0, & k \bmod 2 = 0 \end{cases}$$

When plugging the functions $F_{fd,k}$, $F_{fd,k,k}$ and $F_{fd,k,k+1}$ into 1 and 2 it's convenient to expand them so that the computation of the gradient and Hessian is not subject to numerical cancellation. After expanding the functions, the gradient and Hessian can be approximated as follows.

$$\frac{\partial F}{\partial x_k} \approx \begin{cases} 600h^2x_k - 100hx_{k+1} + \frac{1}{2}h + 350h^3 + 300hx_k^2, & k \bmod 2 = 1 \\ -100x_{k-1}^2 + 100x_k, & k \bmod 2 = 0 \end{cases}$$

$$\frac{\partial^2 F}{\partial x_k \partial x_j} \approx \begin{cases} 1200h_kx_k - 200x_{k+1} + 1 + 700h_k^2 + 600x_k^2, & j = k, k \bmod 2 = 1 \\ 100, & j = k, k \bmod 2 = 0 \\ -100h_kh_{k+1} - 200x_k, & |k - j| = 1, k \bmod 2 = 1 \\ 0, & \text{otherwise} \end{cases}$$

Tables 3 and 4 show the results for the *Modified Newton method* applied to the extended Rosenbrock function with absolute and specific finite differences respectively. All attempts were successful, and the method converged in a small number of iterations, with a convergence rate that is close to 2 for all dimensions, when a suitable choice of h is made. On the contrary, when a poor choice of h is made, the convergence rate is close to 1, which is expected since the convergence rate of the Newton method is 2: this happens when $h = 10^{-2}$ or $h = 10^{-4}$, both for the constant increment and the specific increment methodologies. We notice that for a fixed dimension, performance improves as the stepsize h (be it constant or specific) decreases, as expected, up to a certain point where reducing the stepsize does not result in any improvement (i.e. time and iterations do not significantly decrease). This plateau is reached sooner when preconditioning is adopted and when the dimension is lower.

Tables 5 and 6 show the results for the *Truncated Newton method* applied to the extended Rosenbrock function with absolute and specific finite differences respectively. All attempts were successful, and the method converged in a small number of iterations, when a suitable choice of h is made. A larger number of iterations is required when a poor choice of h is made, namely when $h = 10^{-2}$ or $h = 10^{-4}$, both for the constant increment and the specific increment methodologies, yielding a convergence rate of 1. For smaller values of h , the estimate of the convergence rate is not reliable at all and considerations made in subsection 3.1 for the Truncated Newton method applied to the extended Rosenbrock function with exact gradient and Hessian apply here as well. The plateau in performance as the stepsize h decreases is reached slower than in the case of the Modified Newton method, hinting that the Truncated Newton method highly benefits from a finer approximation of the derivatives.

AP: [Consider adding a plot of the plateau in performance as the stepsize h decreases for the Truncated Newton method and for the Modified Newton method.]

Table 3: Results for Modified Newton method applied to Extended Rosenbrock with absolute finite differences, metrics are average metrics for successful attempts.

dimension	preconditioning h	iterations		convergence rate		time		success rate	
		False	True	False	True	False	True	False	True
3	1e-02	149.91	150.82	1.00	1.00	0.07	0.07	1.00	1.00
	1e-04	33.18	32.09	1.01	1.00	0.02	0.02	1.00	1.00
	1e-06	32.09	30.18	1.96	2.09	0.03	0.02	1.00	1.00
	1e-08	32.00	30.18	2.04	2.23	0.02	0.02	1.00	1.00
	1e-10	32.00	30.18	2.00	2.23	0.02	0.02	1.00	1.00
	1e-12	32.00	30.18	2.00	2.23	0.02	0.02	1.00	1.00
4	1e-02	160.09	160.55	1.00	1.00	0.34	0.36	1.00	1.00
	1e-04	34.18	32.55	1.00	1.00	0.12	0.09	1.00	1.00
	1e-06	32.55	30.27	1.89	1.96	0.12	0.08	1.00	1.00
	1e-08	32.55	30.27	1.95	1.98	0.12	0.08	1.00	1.00
	1e-10	32.55	30.27	1.95	1.98	0.11	0.08	1.00	1.00
	1e-12	32.55	30.27	1.95	1.98	0.11	0.08	1.00	1.00
5	1e-02	169.36	169.82	1.00	1.00	3.26	3.36	1.00	1.00
	1e-04	34.82	33.73	1.00	1.00	1.08	0.79	1.00	1.00
	1e-06	34.00	31.73	2.13	2.00	1.17	0.75	1.00	1.00
	1e-08	33.27	31.73	2.60	2.10	1.17	0.73	1.00	1.00
	1e-10	33.45	31.73	1.93	2.10	1.13	0.73	1.00	1.00
	1e-12	33.45	31.73	1.90	2.10	1.15	0.73	1.00	1.00

Table 4: Results for Modified Newton method applied to Extended Rosenbrock with specific finite differences, metrics are average metrics for successful attempts.

dimension	preconditioning h	iterations		convergence rate		time		success rate	
		False	True	False	True	False	True	False	True
3	1e-02	139.82	141.45	1.00	1.00	0.06	0.06	1.00	1.00
	1e-04	33.73	32.27	1.00	1.00	0.02	0.02	1.00	1.00
	1e-06	32.09	30.18	1.89	2.06	0.02	0.02	1.00	1.00
	1e-08	32.00	30.18	2.04	2.23	0.02	0.02	1.00	1.00
	1e-10	32.00	30.18	2.00	2.23	0.02	0.02	1.00	1.00
	1e-12	32.00	30.18	2.00	2.23	0.02	0.02	1.00	1.00
4	1e-02	149.55	150.55	1.00	1.00	0.32	0.32	1.00	1.00
	1e-04	34.45	32.45	1.00	1.00	0.12	0.09	1.00	1.00
	1e-06	32.55	30.27	1.81	1.96	0.12	0.09	1.00	1.00
	1e-08	32.55	30.27	1.95	1.98	0.12	0.08	1.00	1.00
	1e-10	32.55	30.27	1.95	1.98	0.12	0.08	1.00	1.00
	1e-12	32.55	30.27	1.95	1.98	0.11	0.08	1.00	1.00
5	1e-02	159.18	160.27	1.00	1.00	3.05	3.17	1.00	1.00
	1e-04	34.64	34.45	1.00	1.00	1.09	0.80	1.00	1.00
	1e-06	33.45	31.73	2.56	2.00	1.16	0.74	1.00	1.00
	1e-08	33.09	31.73	1.84	2.10	1.13	0.73	1.00	1.00
	1e-10	33.45	31.73	1.90	2.10	1.12	0.74	1.00	1.00
	1e-12	33.45	31.73	1.90	2.10	1.14	0.77	1.00	1.00

Table 5: Results for Truncated Newton method applied to Extended Rosenbrock with absolute finite differences, metrics are average metrics for successful attempts.

dimension	preconditioning h	iterations		convergence rate		time		success rate	
		False	True	False	True	False	True	False	True
3	1e-02	182.00	179.27	1.00	1.00	0.02	0.04	1.00	1.00
	1e-04	54.36	37.91	1.00	1.00	0.01	0.01	1.00	1.00
	1e-06	52.82	36.36	-1.48	2.39	0.01	0.01	1.00	1.00
	1e-08	52.91	35.91	-2.12	2.86	0.01	0.01	1.00	1.00
	1e-10	53.36	35.45	-4.10	2.21	0.01	0.01	1.00	1.00
	1e-12	55.64	36.45	-2.49	3.01	0.01	0.01	1.00	1.00
4	1e-02	203.91	192.18	1.00	1.00	0.16	0.17	1.00	1.00
	1e-04	61.64	44.45	1.00	1.00	0.06	0.05	1.00	1.00
	1e-06	59.18	42.55	-1.35	4.36	0.06	0.05	1.00	1.00
	1e-08	61.64	42.09	-1.78	2.34	0.06	0.05	1.00	1.00
	1e-10	62.27	41.91	-2.46	3.14	0.06	0.05	1.00	1.00
	1e-12	61.73	43.00	-2.89	2.65	0.06	0.05	1.00	1.00
5	1e-02	224.55	206.82	1.00	1.00	1.84	1.83	1.00	1.00
	1e-04	74.64	42.91	1.00	1.01	0.73	0.41	1.00	1.00
	1e-06	79.09	49.27	-2.17	2.06	0.81	0.50	1.00	1.00
	1e-08	75.64	49.91	-2.83	7.31	0.75	0.47	1.00	1.00
	1e-10	78.00	51.64	-1.21	3.21	0.75	0.50	1.00	1.00
	1e-12	78.00	53.27	-2.11	2.50	0.77	0.52	1.00	1.00

Table 6: Results for Truncated Newton method applied to Extended Rosenbrock with specific finite differences, metrics are average metrics for successful attempts.

dimension	preconditioning h	iterations		convergence rate		time		success rate	
		False	True	False	True	False	True	False	True
3	1e-02	169.91	169.91	1.00	1.00	0.02	0.03	1.00	1.00
	1e-04	54.45	37.27	1.00	1.02	0.01	0.01	1.00	1.00
	1e-06	51.45	36.27	-2.69	2.35	0.01	0.01	1.00	1.00
	1e-08	53.64	36.27	-3.43	1.91	0.01	0.01	1.00	1.00
	1e-10	54.64	35.27	-2.94	2.01	0.01	0.01	1.00	1.00
	1e-12	53.82	35.91	-4.18	2.56	0.01	0.01	1.00	1.00
4	1e-02	191.09	182.64	1.00	1.00	0.15	0.17	1.00	1.00
	1e-04	64.27	42.55	1.00	1.01	0.06	0.05	1.00	1.00
	1e-06	62.18	43.00	-0.96	2.62	0.06	0.05	1.00	1.00
	1e-08	60.73	40.91	-2.95	2.87	0.06	0.05	1.00	1.00
	1e-10	60.82	42.73	-1.22	3.98	0.06	0.05	1.00	1.00
	1e-12	63.09	42.91	-2.01	2.51	0.06	0.05	1.00	1.00
5	1e-02	213.55	198.64	1.00	1.00	1.68	1.74	1.00	1.00
	1e-04	75.91	40.82	1.00	1.00	0.74	0.42	1.00	1.00
	1e-06	77.91	49.00	-2.96	6.91	0.77	0.49	1.00	1.00
	1e-08	77.64	50.18	-1.96	2.28	0.77	0.48	1.00	1.00
	1e-10	75.00	53.27	-4.07	3.38	0.75	0.52	1.00	1.00
	1e-12	75.09	52.45	-2.09	3.48	0.75	0.52	1.00	1.00

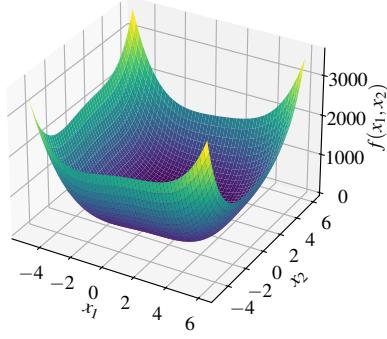


Figure 3: Surface plot of the 2-dimensional generalized Broyden tridiagonal function

4 Generalized Broyden tridiagonal function

The generalized Broyden tridiagonal function is defined as follows.

$$F(x) = \frac{1}{2} \sum_{i=1}^n f_k^2(x) \quad f_k(x) = (3 - 2x_k)x_k + 1 - x_{k-1} - x_{k+1} \quad (6)$$

Figure 3 shows the surface plot of the 2-dimensional generalized Broyden tridiagonal function. Notice that the area where the minimum lies is very flat, which makes it hard to converge to the minimum.

4.1 Exact gradient and Hessian

The gradient of the generalized Broyden tridiagonal function is given by the following expression,

$$\frac{\partial F}{\partial x_k} = \begin{cases} (3 - 4x_1)f_1(x) - f_2(x), & k = 1 \\ (3 - 4x_k)f_k(x) - f_{k+1}(x) - f_{k-1}(x), & 1 < k < n \\ (3 - 4x_n)f_n(x) - f_{n-1}(x), & k = n \end{cases} \quad (7)$$

computation can be eased considering that component k depends only on f_k , f_{k+1} and f_{k-1} . The Hessian of the generalized Broyden tridiagonal function is given by the following expression.

$$\frac{\partial^2 F}{\partial x_k \partial x_j} = \begin{cases} (3 - 4x_1)^2 - 4f_1(x) + 1, & k = j = 1 \\ (3 - 4x_k)^2 - 4f_k(x) + 2, & 1 < k = j < n \\ (3 - 4x_n)^2 - 4f_n(x) + 1, & k = j = n \\ 4x_k + 4x_{k+1} - 6, & |k - j| = 1 \\ 1, & |k - j| = 2 \\ 0, & \text{otherwise} \end{cases} \quad (8)$$

Notice that the Hessian is a banded matrix, with only n non-zero elements on the diagonal, $n - 1$ non-zero elements on the first co-diagonal and $n - 2$ non-zero elements on the second co-diagonal.

Table 7 shows the results for the *Modified Newton method* applied to the generalized Broyden tridiagonal function with exact gradient and Hessian. All attempts are successful, and the method converges in a small number of iterations. Convergence rate is close to 2, which is the expected convergence rate for Newton's method. Preconditioning does not seem to have a significant impact on the performance of the method, compared to its impact on the performance on the extended Rosenbrock function due to the fact that the Hessian matrix for the Newton system is better scaled in the currently considered function.

Table 8 shows the results for the *Truncated Newton method* applied to the generalized Broyden tridiagonal function with exact gradient and Hessian. All attempts are successful, and the method converges in a small number of iterations. When preconditioning is not adopted convergence rate is lower than 2, which is expected since we are solving the Newton system with a relative tolerance that is guaranteed to yield superlinear convergence. Differently from the Modified Newton method, the Truncated Newton method is more sensitive to preconditioning, which can be observed by the fact that the number of iterations is lower when preconditioning is adopted and convergence rate is almost 2.

Table 7: Results for Modified Newton method applied to Generalized Broyden with exact gradient and hessian, metrics are average metrics for successful attempts.

preconditioning dimension	iterations		convergence rate		time		success rate	
	False	True	False	True	False	True	False	True
3	8.636	8.636	1.974	1.978	0.006	0.005	1.00	1.00
4	8.000	8.273	1.829	1.849	0.037	0.034	1.00	1.00
5	7.909	10.545	1.794	1.989	0.291	0.300	1.00	1.00

Table 8: Results for Truncated Newton method applied to Generalized Broyden with exact gradient and hessian, metrics are average metrics for successful attempts.

preconditioning dimension	iterations		convergence rate		time		success rate	
	False	True	False	True	False	True	False	True
3	11.818	9.000	1.774	1.971	0.002	0.003	1.00	1.00
4	12.727	9.727	1.346	1.987	0.014	0.015	1.00	1.00
5	13.727	9.636	1.905	1.923	0.125	0.108	1.00	1.00

Comparing performance of the two methods, the Truncated Newton method is 2 to 3 times faster than the Modified Newton method due to the fact that the Newton system is solved approximately, which is less computationally expensive than solving it exactly. However, the Truncated Newton methods requires more iterations to converge than the Modified Newton method, which is expected since the Modified Newton exactly solves the Newton system at each iteration.

4.2 Finite differences gradient and Hessian

When applying 1, one can notice that the terms $F(x + he_k)$ and $F(x - he_k)$ only differ by terms f_k , f_{k+1} and f_{k-1} . Then to make function evaluations less expensive, we can define the following function $F_{fd,k}$, which can be plugged in 1 in place of F yielding the same result.

$$F_{fd,k}(x) = \frac{1}{2}f_k^2(x) + \frac{1}{2}f_{k+1}^2(x) + \frac{1}{2}f_{k-1}^2(x)$$

The same procedure can be applied for the Hessian, considering that:

- function evaluations to compute entry $h_{k,k}$ differ only by f_k , f_{k+1} and f_{k-1} ;
- function evaluations to compute entry $h_{k,k+1}$ differ only by f_k and f_{k+1} ;
- function evaluations to compute entry $h_{k,k+2}$ differ only by f_{k-1} .

Then to make function evaluations less expensive, we can define the functions $F_{fd,k,k}$, $F_{fd,k,k+1}$, $F_{fd,k,k+2}$, which can be plugged in 2 in place of F yielding the same result to compute entries $h_{k,k}$, $h_{k,k+1}$ and $h_{k,k+2}$ respectively.

$$\begin{aligned} F_{fd,k,k}(x) &= \frac{1}{2}f_k^2(x) + \frac{1}{2}f_{k-1}^2(x) + \frac{1}{2}f_{k+1}^2(x) \\ F_{fd,k,k+1}(x) &= \frac{1}{2}f_k^2(x) + \frac{1}{2}f_{k+1}^2(x) \\ F_{fd,k,k+2}(x) &= \frac{1}{2}f_{k-1}^2(x) \end{aligned}$$

When plugging the functions $F_{fd,k}$, $F_{fd,k,k}$, $F_{fd,k,k+1}$ and $F_{fd,k,k+2}$ into 1 and 2 it's convenient to expand them so that the computation of the gradient and Hessian is not subject to numerical cancellation as previously done for the extended Rosenbrock function in subsection 3.2.

Tables 9 and 10 show the results for the *Modified Newton method* applied to the generalized Broyden tridiagonal function with absolute and specific finite differences respectively. All attempts are successful, but attempts with $h = 10^{-2}$ which don't converge within the fixed maximum number of iterations $k_{max} = 1000$, both for absolute and specific differences, for all dimensions. This is probably due to the fact that $h = 10^{-2}$ is not a suitable increment for the finite differences method to approximate the gradient and Hessian of the generalized

Table 9: Results for Modified Newton method applied to Generalized Broyden with absolute finite differences, metrics are average metrics for successful attempts.

dimension	preconditioning h	iterations		convergence rate		time		success rate	
		False	True	False	True	False	True	False	True
3	1e-04	8.545	8.545	2.016	2.010	0.006	0.006	1.00	1.00
	1e-06	8.545	8.636	1.964	1.979	0.006	0.006	1.00	1.00
	1e-08	8.636	8.636	1.974	1.978	0.006	0.005	1.00	1.00
	1e-10	8.636	8.636	1.974	1.978	0.006	0.006	1.00	1.00
	1e-12	8.636	8.636	1.973	1.978	0.006	0.006	1.00	1.00
4	1e-04	7.909	8.273	1.803	1.829	0.036	0.031	1.00	1.00
	1e-06	8.000	8.273	1.832	1.851	0.036	0.031	1.00	1.00
	1e-08	8.000	8.273	1.829	1.849	0.038	0.031	1.00	1.00
	1e-10	8.000	8.273	1.829	1.849	0.038	0.031	1.00	1.00
	1e-12	8.000	8.273	1.829	1.849	0.038	0.032	1.00	1.00
5	1e-04	7.818	10.455	1.751	2.045	0.321	0.344	1.00	1.00
	1e-06	7.909	10.545	1.796	1.992	0.333	0.332	1.00	1.00
	1e-08	7.909	10.545	1.794	1.989	0.324	0.337	1.00	1.00
	1e-10	7.909	10.545	1.794	1.989	0.314	0.325	1.00	1.00
	1e-12	7.909	10.545	1.794	1.989	0.320	0.328	1.00	1.00

Table 10: Results for Modified Newton method applied to Generalized Broyden with specific finite differences, metrics are average metrics for successful attempts.

dimension	preconditioning h	iterations		convergence rate		time		success rate	
		False	True	False	True	False	True	False	True
3	1e-04	8.545	8.636	1.977	2.000	0.006	0.006	1.00	1.00
	1e-06	8.545	8.636	1.964	1.979	0.006	0.005	1.00	1.00
	1e-08	8.636	8.636	1.974	1.978	0.007	0.007	1.00	1.00
	1e-10	8.636	8.636	1.973	1.978	0.006	0.006	1.00	1.00
	1e-12	8.636	8.636	1.973	1.978	0.007	0.006	1.00	1.00
4	1e-04	7.909	8.273	1.804	1.835	0.037	0.031	1.00	1.00
	1e-06	8.000	8.273	1.830	1.850	0.050	0.031	1.00	1.00
	1e-08	8.000	8.273	1.829	1.849	0.038	0.032	1.00	1.00
	1e-10	8.000	8.273	1.829	1.849	0.038	0.032	1.00	1.00
	1e-12	8.000	8.273	1.829	1.849	0.038	0.031	1.00	1.00
5	1e-04	7.818	10.545	1.752	2.020	0.315	0.325	1.00	1.00
	1e-06	7.909	10.545	1.795	1.990	0.314	0.326	1.00	1.00
	1e-08	7.909	10.545	1.794	1.989	0.329	0.329	1.00	1.00
	1e-10	7.909	10.545	1.794	1.989	0.325	0.327	1.00	1.00
	1e-12	7.909	10.545	1.794	1.989	0.313	0.325	1.00	1.00

Table 11: Results for Truncated Newton method applied to Generalized Broyden with absolute finite differences, metrics are average metrics for successful attempts.

dimension	preconditioning h	iterations		convergence rate		time		success rate	
		False	True	False	True	False	True	False	True
3	1e-02	13.000	NaN	1.051	NaN	0.002	NaN	0.09	NaN
	1e-04	11.818	9.091	1.773	2.009	0.003	0.003	1.00	1.00
	1e-06	11.818	9.000	1.774	1.972	0.003	0.003	1.00	1.00
	1e-08	11.818	9.000	1.774	1.971	0.003	0.003	1.00	1.00
	1e-10	11.818	9.000	1.774	1.971	0.003	0.003	1.00	1.00
	1e-12	11.818	9.000	1.774	1.971	0.003	0.004	1.00	1.00
4	1e-04	12.727	9.545	1.347	1.995	0.019	0.018	1.00	1.00
	1e-06	12.727	9.727	1.346	1.990	0.018	0.017	1.00	1.00
	1e-08	12.727	9.727	1.346	1.987	0.018	0.017	1.00	1.00
	1e-10	12.727	9.727	1.346	1.987	0.018	0.018	1.00	1.00
	1e-12	12.727	9.727	1.346	1.987	0.019	0.018	1.00	1.00
5	1e-04	13.727	9.545	1.905	1.903	0.160	0.132	1.00	1.00
	1e-06	13.727	9.636	1.905	1.926	0.162	0.133	1.00	1.00
	1e-08	13.727	9.636	1.905	1.923	0.159	0.137	1.00	1.00
	1e-10	13.727	9.636	1.905	1.923	0.161	0.132	1.00	1.00
	1e-12	13.727	9.636	1.905	1.923	0.156	0.132	1.00	1.00

Broyden tridiagonal function. When the method converges, it does so in a small number of iterations with a convergence rate close to 2, which is the expected convergence rate for Newton's method.

Tables 11 and 12 show the results for the *Truncated Newton method* applied to the generalized Broyden tridiagonal function with absolute and specific finite differences respectively. All attempts are successful, but attempts with $h = 10^{-2}$ which converge within the fixed maximum number of iterations $k_{max} = 1000$ only once for $n = 10^3$, regardless of the type (absolute or specific) of finite differences adopted. When the method converges, it does so in a small number of iterations with a convergence rate that as expected is superlinear, almost quadratic for $n = 10^5$, even if preconditioning is not adopted. When preconditioning is adopted, the number of iterations is lower and the convergence rate is closer to 2, which is the expected convergence rate for Newton's method.

Also for this function, it's evident that the Truncated Newton method is faster than the Modified Newton method, but requires more iterations to converge. Moreover, the Truncated Newton method is more sensitive to preconditioning than the Modified Newton method.

5 Banded trigonometric function

The banded trigonometric function is defined as follows.

$$f(x) = \sum_{i=1}^n i[(1 - \cos x_i) + \sin x_{i-1} - \sin x_{i+1}] \quad (9)$$

Figure 4 shows the surface plot of the 2-dimensional banded trigonometric function. It has a highly oscillatory landscape with multiple peaks and valleys due to its sinusoidal terms. This results in a mix of locally smooth and rapidly changing regions, making optimization sensitive to initialization and prone to multiple local minima.

5.1 Exact gradient and Hessian

The gradient of the banded trigonometric function is given by the following expression.

$$\frac{\partial F}{\partial x_k} = \begin{cases} k \sin x_k + 2 \cos x_k, & 1 \leq k < n \\ n \sin x_n - (n-1) \cos x_n, & k = n \end{cases} \quad (10)$$

The Hessian of the banded trigonometric function is given by the following expression.

$$\frac{\partial^2 F}{\partial x_k \partial x_j} = \begin{cases} k \cos x_k - 2 \sin(x_k), & k = j \\ 0, & \text{otherwise} \end{cases} \quad (11)$$

Table 12: Results for Truncated Newton method applied to Generalized Broyden with specific finite differences, metrics are average metrics for successful attempts.

dimension	preconditioning h	iterations		convergence rate		time		success rate	
		False	True	False	True	False	True	False	True
3	1e-04	11.818	9.091	1.773	1.986	0.003	0.003	1.00	1.00
	1e-06	11.818	9.000	1.774	1.971	0.003	0.003	1.00	1.00
	1e-08	11.818	9.000	1.774	1.971	0.003	0.003	1.00	1.00
	1e-10	11.818	9.000	1.774	1.971	0.003	0.004	1.00	1.00
	1e-12	11.818	9.000	1.774	1.971	0.003	0.003	1.00	1.00
4	1e-04	12.727	9.545	1.347	1.982	0.018	0.017	1.00	1.00
	1e-06	12.727	9.727	1.346	1.989	0.017	0.018	1.00	1.00
	1e-08	12.727	9.727	1.346	1.987	0.018	0.018	1.00	1.00
	1e-10	12.727	9.727	1.346	1.987	0.017	0.017	1.00	1.00
	1e-12	12.727	9.727	1.346	1.987	0.018	0.018	1.00	1.00
5	1e-04	13.727	9.636	1.905	1.930	0.155	0.133	1.00	1.00
	1e-06	13.727	9.636	1.905	1.924	0.159	0.131	1.00	1.00
	1e-08	13.727	9.636	1.905	1.923	0.160	0.134	1.00	1.00
	1e-10	13.727	9.636	1.905	1.923	0.158	0.132	1.00	1.00
	1e-12	13.727	9.636	1.905	1.923	0.156	0.132	1.00	1.00

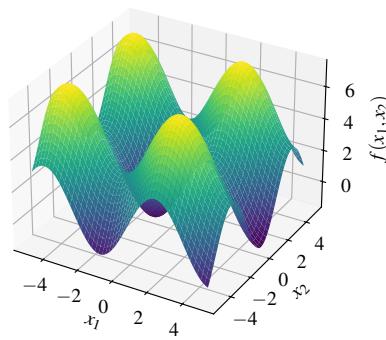


Figure 4: Surface plot of the 2-dimensional banded trigonometric function

Table 13: Results for Modified Newton method applied to Banded Trigonometric with exact gradient and hessian, metrics are average metrics for successful attempts. Results are given only with preconditioning adopted.

dimension	iterations	convergence rate	time	success rate
3	14.273	2.782	0.018	1.00
4	7.000	2.946	0.021	0.09
5	7.000	2.946	0.115	0.09

Table 14: Results for Truncated Newton method applied to Banded Trigonometric with exact gradient and hessian, metrics are average metrics for successful attempts. Results are given only with preconditioning adopted.

dimension	iterations	convergence rate	time	success rate
3	14.273	2.790	0.009	1.00
4	20.818	2.714	0.028	1.00
5	25.273	2.774	0.302	1.00

Notice that the Hessian is a diagonal matrix, which makes the optimization problem easier to solve. AP: [Make some considerations on the conditioning number of the Hessian.]

5.2 Finite differences gradient and Hessian

When applying 1, one can notice that the terms $F(x + he_k)$ and $F(x - he_k)$ only differ by summands with indices $i = k$ and $i = k \pm 1$. Then to make function evaluations less expensive, we can define the following function $F_{fd,k}$, that can be plugged in 1 in place of F yielding the same result.

$$F_{fd,k} = \sum_{i=k-1}^{k+1} i[(1 - \cos x_i) + \sin x_{i-1} - \sin x_{i+1}]$$

Some of the terms in $F_{fd,k}$ are constant and do not depend on x_k , so they will eventually subtract and we can further simplify the expression.

$$F_{fd,k} = \begin{cases} -k \cos x_k + 2 \sin x_k, & 1 \leq k < n \\ n \cos x_n - (n-1) \sin x_n, & k = n \end{cases}$$

The same procedure can be applied to the Hessian, considering that terms in 2 only differ by summands with indices $i = k$ and $i = k \pm 1$. When plugging the function $F_{fd,k}$ into 1 and 2 it's convenient to expand them so that the computation of the gradient and Hessian is not subject to numerical cancellation. After expanding the functions, the gradient and Hessian can be approximated as follows.

$$\frac{\partial F}{\partial x_k} \approx \begin{cases} \frac{2k \sin x_k \sin h + 4 \cos x_k \sin h}{2h}, & 1 \leq k < n \\ \frac{2n \sin x_n \sin h - 2(n-1) \cos x_n \sin h}{2h}, & k = n \end{cases}$$

$$\frac{\partial^2 F}{\partial x_k^2} \approx \begin{cases} (k \cos x_k - 2 \sin x_k) - h(k \sin x_k + 2 \cos x_k), & 1 \leq k < n \\ (n \cos x_n - (n-1) \sin x_n) - h(n \sin x_n - (n-1) \cos x_n), & k = n \end{cases}$$

The approximation for the gradient is obtained applying the trigonometric identities for the sum of angles. The approximation for the Hessian is obtained by applying the aforementioned trigonometric identities in order to isolate the following terms.

$$\cos(2h) - 2 \cos h \approx -1 - h^2 + \mathcal{O}(h^4), \quad \sin(2h) - 2 \sin h \approx -h^3 + \mathcal{O}(h^5)$$

To avoid numerical cancellation, it is necessary to substitute them with their Taylor expansions.

6 Conclusions

References

- [1] Ladislav Luksan and Jan Vlček. *Test Problems for Unconstrained Optimization*. Nov. 2003.
- [2] Jorge Nocedal and Stephen J. Wright. “Numerical optimization”. English (US). In: *Springer Series in Operations Research and Financial Engineering*. Springer Series in Operations Research and Financial Engineering. Springer Nature, 2006, pp. 1–664.

Table 15: Results for Modified Newton method applied to Banded Trigonometric with absolute finite differences, metrics are average metrics for successful attempts. Results are given only with preconditioning adopted.

dimension	h	iterations	convergence rate	time	success rate
3	1e-02	14.818	2.548	0.010	1.00
	1e-04	14.545	2.807	0.007	1.00
	1e-06	14.091	2.842	0.006	1.00
	1e-08	14.182	2.575	0.006	1.00
	1e-10	13.364	2.630	0.006	1.00
	1e-12	13.909	2.695	0.006	1.00
4	1e-02	8.000	2.256	0.018	0.09
	1e-04	13.000	2.605	0.032	0.18
	1e-06	6.000	2.857	0.014	0.09
	1e-08	14.500	2.844	0.033	0.18
	1e-10	7.000	2.948	0.015	0.09
	1e-12	7.000	2.946	0.016	0.09
5	1e-02	8.000	2.256	0.123	0.09
	1e-04	8.000	2.951	0.129	0.09
	1e-06	6.000	2.856	0.100	0.09
	1e-08	6.000	2.749	0.098	0.09
	1e-10	7.000	2.948	0.108	0.09
	1e-12	7.000	2.946	0.117	0.09

Table 16: Results for Modified Newton method applied to Banded Trigonometric with specific finite differences, metrics are average metrics for successful attempts. Results are given only with preconditioning adopted.

dimension	h	iterations	convergence rate	time	success rate
3	1e-04	9.000	1.074	0.018	0.09
	1e-06	16.600	1.104	0.007	0.91
	1e-08	13.636	2.582	0.006	1.00
	1e-10	13.455	2.636	0.006	1.00
	1e-12	13.818	2.377	0.006	1.00
4	1e-04	9.000	1.074	0.021	0.09
	1e-06	6.000	2.895	0.014	0.09
	1e-08	6.000	2.750	0.014	0.09
	1e-10	7.000	2.948	0.015	0.09
	1e-12	7.000	2.946	0.017	0.09
5	1e-04	13.000	1.001	0.201	0.09
	1e-06	6.000	2.894	0.121	0.09
	1e-08	6.000	2.749	0.107	0.09
	1e-10	7.000	2.948	0.111	0.09
	1e-12	7.000	2.946	0.121	0.09

Table 17: Results for Truncated Newton method applied to Banded Trigonometric with absolute finite differences, metrics are average metrics for successful attempts. Results are given only with preconditioning adopted.

dimension	h	iterations	convergence rate	time	success rate
3	1e-02	15.091	2.735	0.007	1.00
	1e-04	14.182	2.476	0.006	1.00
	1e-06	14.182	2.488	0.006	1.00
	1e-08	14.273	2.776	0.007	1.00
	1e-10	14.273	2.756	0.007	1.00
	1e-12	14.182	2.758	0.006	1.00
4	1e-02	19.545	2.709	0.034	1.00
	1e-04	19.818	2.609	0.037	1.00
	1e-06	20.727	2.665	0.034	1.00
	1e-08	21.364	2.740	0.036	1.00
	1e-10	20.636	2.731	0.033	1.00
	1e-12	20.455	2.729	0.034	1.00
5	1e-02	24.455	2.717	0.375	1.00
	1e-04	26.727	2.516	0.379	1.00
	1e-06	25.636	2.754	0.384	1.00
	1e-08	25.636	2.770	0.394	1.00
	1e-10	25.727	2.770	0.396	1.00
	1e-12	25.364	2.727	0.424	1.00

Table 18: Results for Truncated Newton method applied to Banded Trigonometric with specific finite differences, metrics are average metrics for successful attempts. Results are given only with preconditioning adopted.

dimension	h	iterations	convergence rate	time	success rate
3	1e-02	15.182	2.257	0.006	1.00
	1e-04	15.091	2.836	0.007	1.00
	1e-06	14.000	2.710	0.007	1.00
	1e-08	14.273	2.800	0.006	1.00
	1e-10	14.545	2.785	0.007	1.00
	1e-12	14.182	2.781	0.006	1.00
4	1e-02	19.273	2.159	0.033	1.00
	1e-04	20.182	2.668	0.034	1.00
	1e-06	20.636	2.790	0.035	1.00
	1e-08	21.000	2.666	0.035	1.00
	1e-10	20.727	2.647	0.033	1.00
	1e-12	20.182	2.746	0.033	1.00
5	1e-02	24.364	2.263	0.372	1.00
	1e-04	25.455	2.733	0.365	1.00
	1e-06	26.273	2.627	0.418	1.00
	1e-08	25.636	2.785	0.393	1.00
	1e-10	25.455	2.770	0.377	1.00
	1e-12	24.909	2.375	0.395	1.00