

Accelerated derivative-free nonlinear least-squares applied to the estimation of Manning coefficients*

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Abstract

A general framework for solving nonlinear least squares problems without the employment of derivatives is proposed in the present paper together with a new general global convergence theory. With the aim to cope with the case in which the number of variables is big (for the standards of derivative-free optimization), two dimension-reduction procedures are introduced. One of them is based on iterative subspace minimization and the other one is based on spline interpolation with variable nodes. Each iteration based on those procedures is followed by an acceleration step inspired in the Sequential Secant Method. The practical motivation for this work is the estimation of parameters in Hydraulic models applied to dam breaking problems. Numerical examples of the application of the new method to those problems are given.

Key words: Nonlinear least-squares, derivative-free methods, acceleration, Manning coefficients.

1 Introduction

Many statistical learning problems require fitting models to large data sets. Frequently, the number of unknown parameters is not small. Moreover, for different reasons, derivatives of the functions that define the model may not be available, and the sum of squares of residuals is a natural function to be minimized. These considerations lead to the problem

$$\text{Minimize } \|F(x)\|_2^2 \text{ subject to } x \in \Omega \subseteq \mathbb{R}^n, \quad (1)$$

where $F : \Omega \rightarrow \mathbb{R}^m$.

Let us define $f(x) = \frac{1}{2}\|F(x)\|_2^2$. For obtaining a quadratic approximation of $f(x)$ with the property of being exact if $f(x)$ is quadratic, $1 + n + n(n + 1)/2$ evaluations of $f(x)$ are needed. However, if the structure $\frac{1}{2}\|F(x)\|_2^2$ of $f(x)$ is used, the same property can be obtained using only $n + 1$ evaluations of $F(x)$. Considering that evaluating $f(x)$ and $F(x)$ has the same cost, this seems to be a strong argument to take advantage of the sum-of-squares structure of $f(x)$, especially if derivatives are not available.

Ralston and Jennrich [33] introduced a purely local method that, at each iteration, minimizes the norm of the linear model that interpolates $n + 1$ consecutive residuals, providing the first generalization

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of the Sequential Secant Method [2, 42] to nonlinear least squares. Zhang, Conn, and Scheinberg [46] employed different quadratic models for each component of the residual function in order to define conveniently structured trust-region subproblems. Therefore, as in [30, 31, 32], at least $2n + 1$ residual evaluations are computed per iteration. The use of quadratic models allow these authors to prove not only global convergence, but also local quadratic convergence under suitable assumptions [45]. The idea of interpolating a different quadratic for each component of the residual has also been exploited in the POINDERS software [41] with trust-region strategies for obtaining global convergence. Cartis and Roberts [9] introduced a derivative-free Gauss-Newton method for solving nonlinear least squares problems. At each iteration of their method, $n + 1$ residuals are used to interpolate a linear model of $F(x)$. The norm of the linear model is approximately minimized over successive trust regions until sufficient decrease of the sum of squares is obtained. The points used for interpolation are updated in order to preserve well-conditioning. With this framework global convergence and complexity results are proved. All mentioned methods suffer from a high linear algebra cost per iteration related to construct the model and find a model's solution; so a natural idea, explored in the present work, is to apply dimensionality-reduction techniques. While developing this work, we became aware of a work of Cartis and Roberts [10] in which this idea is explored. In [10], a method that performs successive minimizations within random subspaces, employing the model-based framework based on the Gauss-Newton method introduced in [9], is introduced.

Having in mind the estimation of parameters in one-dimensional models that simulate water or mud flow in natural channels, a derivative-free method for large-scale least-squares problems is introduced in the present work. Mathematical models for this type of phenomena consist of partial differential equations with boundary conditions that simulate flood intensity. The initial conditions for this type of models are, in general, well known, but the parameters reflecting density, friction, obstacles, or terrain features must be estimated from data. We are particularly interested in Manning coefficients. Manning's coefficients play a crucial role in the correct modeling of mud or water flow in a natural channel influenced by a flood. In principle, in perfectly straight channels with constant cross-sectional area, these coefficients account for velocity reductions due to friction with the walls or viscosity of the fluid. In real situations, in which the channel is not straight and the cross-sectional area is not constant, Manning's coefficients absorb the information due to these "irregularities", which, in fact, detract the theoretical model from the real situation. The realistic simulation of a natural channel cannot rely on theoretical estimates of Manning's coefficients based on physical considerations linked to ideal situations. Necessarily, such coefficients must be estimated on the basis of (much or little) available data. This is the exercise we propose in the present work, for which we use an ideal situation that allows us to infer the usefulness of the introduced methods in more realistic situations. Incidentally, data collection in real cases was dramatically interrupted in 2020 by the outbreak of the pandemic we are still suffering from. The use of programs whose source code is not available is frequent in this type of research. For this reason, we are interested in investigating the behavior of derivative-free methods to estimate parameters of the models used. The introduced method combines dimensionality-reduction techniques [40, 43] and acceleration steps based on the sequential secant approach [2, 42].

Acceleration schemes, by means of which, given an iterate x^k and its predecessors, one obtains a possible (accelerated) better approximation to the solution may be applied to any of the algorithms mentioned in the previous paragraph. Let us provide a rough description of the sequential secant idea applied to nonlinear least squares problems. Assume that $p \in \{1, 2, \dots, n\}$ is given and $x^0, x^{-1}, \dots, x^{-p} \in \mathbb{R}^n$ are arbitrary. Given $k = 0, 1, 2, \dots$, we define

$$s^{k-1} = x^k - x^{k-1}, \dots, s^{k-p} = x^{k-p+1} - x^{k-p},$$

$$y^{k-1} = F(x^k) - F(x^{k-1}), \dots, y^{k-p} = F(x^{k-p+1}) - F(x^{k-p}),$$

and

$$S_k = (s^{k-1}, \dots, s^{k-p}) \text{ and } Y_k = (y^{k-1}, \dots, y^{k-p}).$$

The Sequential Secant Method for nonlinear least-squares is defined by

$$x^{k+1} = x^k - S_k Y_k^\dagger F(x^k), \tag{2}$$

where Y_k^\dagger denotes the Moore-Penrose pseudo-inverse of Y_k . Its main drawback is that, according to (2), $x^{k+1} - x^k$ always lies in the subspace generated by $\{s^{k-1}, \dots, s^{k-p}\}$. Therefore, all the iterates lie in the affine subspace that passes through x^0 and is spanned by $\{s^{-1}, \dots, s^{-p}\}$. This is not a serious inconvenient if $p = n$ and the increments s^{k-1}, \dots, s^{k-p} remain linearly independent. However, even when $p = n$, the vectors s^{k-1}, \dots, s^{k-p} may become linearly dependent and, consequently, all the iterates x^{k+j} would be condemned to lie in a fixed affine subspace of dimension strictly smaller than n . For these reasons, the pure Sequential Secant Method is not appropriate for solving nonlinear least-squares problems when n is large and, thus, it is required to maintain p reasonable small.

Note, however, that, when $m = n$, under suitable assumptions, the method defined by (2) has Q-superlinearly local converge to a solution of $F(x) = 0$, and its R-rate of convergence is the positive root of $t^{n+1} - t^n - 1 = 0$ [28]. When $m = n$, the problem consists of solving the nonlinear system $F(x) = 0$. This case has been extensively considered in [3]. The drawback pointed out above was overcome in [3] taking auxiliary residual-related directions. The idea of using residuals as search directions for solving nonlinear systems of equations have been introduced and exploited in [22, 23, 26, 38] and analyzed from the point of view of complexity in [11]. Unfortunately, in general nonlinear least-squares problems, it is not possible to use residuals as search directions. Therefore, in the present paper, we suggest different alternatives for choosing the first trial point without residual information at each iteration. This is the place where the dimensionality-reduction techniques place their role – trial points are computed by minimizing the least-squares function in a reduced space. Two alternatives are considered. In one of them, minimizations within small random affine-subspaces are performed. On the other one, the reduced problem has as variables nodes and values of a linear spline from which the values of the original variables are obtained. After the computation of a suitable trial point, we try an acceleration step using sequential secant ideas.

It is worth mentioning that sequential secant acceleration is closely connected with Anderson acceleration [1, 6, 7, 8, 20, 27, 34, 39] and quasi-Newton acceleration [6, 15, 19, 25]. Moreover, the sequential secant algorithm is a particular case of a family of secant methods described in [28] and [21], whereas related multipoint secant methods for solving nonlinear systems and minimization have been introduced in [4, 5, 17, 18, 36, 37] and others.

This paper is organized as follows. In Section 2, we introduce a general scheme that applies to derivative-free optimization (not only nonlinear least-squares) and has the proposed algorithm for nonlinear least squares as particular case. Global convergence results for the general scheme are included in this section. In Section 3, we define the specific algorithm that we use for derivative-free nonlinear least-problems. In Section 4, we present the problem of estimating Manning coefficients and report numerical experiments. Conclusions and lines for future research are stated in Section 5.

Notation. The symbol $\|\cdot\|$ will denote an arbitrary norm.

2 General optimization framework

In this section, we consider the problem

$$\text{Minimize } f(x) \text{ subject to } x \in \Omega, \tag{3}$$

where $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is arbitrary and $\Omega \subset \mathbb{R}^n$ is closed and convex.

The following algorithm applies to the solution of (3). This algorithm resembles the classical Frank-Wolfe algorithm [16] as, at each iteration, minimizes a linear function subject to the true constraints of the problem and an additional constraints that guarantees that the problem is solvable.

Algorithm 2.1. Let $f_{\text{target}} \in \mathbb{R}$, $\Delta > 0$, $\gamma \in (0, 1)$, a sequence $\{\eta_k\}$ of positive numbers such that

$$\sum_{k=0}^{\infty} \eta_k < \infty, \quad (4)$$

and the initial guess $x^0 \in \Omega$ be given. Set $k \leftarrow 0$.

Step 1. If $f(x^k) \leq f_{\text{target}}$, then terminate the execution of the algorithm.

Step 2. Choose $v^k \in \mathbb{R}^n$ such that $\|v^k\| = 1$.

Step 3. Compute d^k as a solution to the supproblem given by

$$\text{Minimize } \langle v^k, d \rangle \text{ subject to } \|d\| \leq \Delta \text{ and } x^k + d \in \Omega. \quad (5)$$

Step 4. Set $\alpha \leftarrow 1$.

Step 5. Set $x^{\text{trial}} \leftarrow x^k + \alpha d^k$.

Step 6. Test the descent condition

$$f(x^{\text{trial}}) \leq f(x^k) + \eta_k - \gamma \alpha^2 \left[f(x^k) - f_{\text{target}} \right]. \quad (6)$$

Step 7. If (6) holds define $\alpha_k = \alpha$, compute $x^{k+1} \in \Omega$ such that

$$f(x^{k+1}) \leq f(x^{\text{trial}}), \quad (7)$$

set $k \leftarrow k + 1$, and go to Step 1. Otherwise, update $\alpha \leftarrow \alpha/2$ and go to Step 5.

Lemma 2.1 *Assume that f is continuous, $x^k \in \mathbb{R}^n$ is an arbitrary iterate of Algorithm 2.1, and $f(x^k) > f_{\text{target}}$. Then, x^{trial} and x^{k+1} satisfying (6) and (7) are well defined.*

Proof: The thesis follows from the continuity of f using that $\eta_k > 0$ and that the successive trials for α tend to zero. \square

Lemma 2.2 *Assume that f is continuous and, for all $k \in \mathbb{N}$, we have that $f(x^k) > f_{\text{target}}$. Then,*

$$\lim_{k \rightarrow \infty} \alpha_k^2 \left[f(x^k) - f_{\text{target}} \right] = 0. \quad (8)$$

Moreover, at least one of the following two possibilities takes place:

$$\lim_{k \rightarrow \infty} \alpha_k = 0; \quad (9)$$

or there exists an infinite subset of indices $K_1 \subset \mathbb{N}$ such that

$$\lim_{k \in K_1} f(x^k) = f_{\text{target}}. \quad (10)$$

Proof: By Lemma 2.1 and the hypothesis, the algorithm generates an infinite sequence $\{x^k\}$ such that $\{f(x^k)\}$ is bounded below. Assume that (8) is not true. Then, there exists $c > 0$ such that

$$\alpha_k^2[f(x^k) - f_{\text{target}}] \geq c \quad (11)$$

for infinitely many indices $k \in K_2$. By the convergence of $\sum_{k=0}^{\infty} \eta_k$, there exists $k_1 \in \mathbb{N}$ such that

$$\eta_k < \gamma c/2$$

for all $k \geq k_1$. Then, by (6), (7), and (11), for all $k \in K_2$ such that $k \geq k_1$,

$$f(x^{k+1}) \leq f(x^k) + \gamma c/2 - \gamma c = f(x^k) - \gamma c/2. \quad (12)$$

Let $k_2 \geq k_1$ such that

$$\sum_{k=k_2}^{\infty} \eta_k < \gamma c/4.$$

Then, by (6) and (7), for all $k \in \mathbb{N}$, $k > k_2$ we have that

$$\begin{aligned} f(x^k) - f(x^{k_2}) &= [f(x^k) - f(x^{k-1})] + [f(x^{k-1}) - f(x^{k-2})] + \dots + [f(x^{k_2+1}) - f(x^{k_2})] \\ &\leq \eta_{k-1} + \eta_{k-2} + \dots + \eta_{k_2} < \gamma c/4. \end{aligned} \quad (13)$$

Thus, between two consecutive terms (not smaller than k_2) of the sequence K_2 , by (13), f increases at most $\gamma c/4$; but, by (12), decreases at least $\gamma c/2$. This implies that $\lim_{k \rightarrow \infty} f(x^k) = -\infty$, which contradicts the fact that $\{f(x^k)\}$ is bounded below. Therefore, (8) is proved.

Now, if (9) does not hold, there exists an infinite set of indices K_1 such that α_k is bounded away from zero. By (8), we have that (10) must take place. \square

By Lemmas 2.1 and 2.2, there are three possibilities for the sequence generated by Algorithm 2.1:

(i) The sequence terminates at some x^k where $f(x^k) \leq f_{\text{target}}$; (ii) The sequence terminates at some x^k where $f(x^k) \leq f_{\text{target}} + \varepsilon_f$ for a given tolerance $\varepsilon_f > 0$; and (iii) The sequence $\{\alpha_k\}$ tends to zero. Possibilities (i) and (ii) are symptoms of success of the algorithm. Possibility (iii) cannot be discarded since, given $\varepsilon_f > 0$, $f(x)$ may be bigger than $f_{\text{target}} + \varepsilon_f$ for every $x \in \Omega$. Therefore, the implications of $\alpha_k \rightarrow 0$ need to be analyzed. With this purpose, in the following lemma we need to assume differentiability of the function f .

Lemma 2.3 *Assume that f admits continuous derivatives for all x in an open set that contains Ω and $\{x^k\}$ is generated by Algorithm 2.1. Assume that $\{f(x^k) - f_{\text{target}}\}$ is bounded away from zero, $x_* \in \mathbb{R}^n$, and $\lim_{k \in K_1} x^k = x_*$. Then, the sequence $\{d^k\}_{k \in K_1}$ admits at least one limit point and, for every limit point d of $\{d^k\}_{k \in K_1}$, we have that*

$$\langle \nabla f(x_*), d \rangle \geq 0. \quad (14)$$

Proof: By Lemma 2.2,

$$\lim_{k \rightarrow \infty} \alpha_k = 0. \quad (15)$$

Since the first trial value for α_k at each iteration is 1, (15) implies that

$$\lim_{k \rightarrow \infty} \alpha_{k,+} = 0,$$

and, for all k large enough,

$$f(x^k + \alpha_{k,+}d^k) > f(x^k) + \eta_k - \gamma\alpha_{k,+}^2 \left[f(x^k) - f_{\text{target}} \right].$$

So, since $\eta_k > 0$,

$$\frac{f(x^k + \alpha_{k,+}d^k) - f(x^k)}{\alpha_{k,+}} > -\gamma\alpha_{k,+} \left[f(x^k) - f_{\text{target}} \right]$$

for all k large enough. Thus, by the Mean Value Theorem, there exists $\xi_{k,+} \in [0, \alpha_{k,+}]$ such that

$$\langle \nabla f(x^k + \xi_{k,+}d^k), d^k \rangle > -\gamma\alpha_{k,+} \left[f(x^k) - f_{\text{target}} \right] \quad (16)$$

for all k large enough.

Since $\|d^k\| \leq \Delta$ for all k , we have that $\{d^k\}_{k \in K_1}$ admits at least one limit point. Let d be an arbitrary limit point of $\{d^k\}_{k \in K_1}$ and let $K_2 \subseteq K_1$ such that

$$\lim_{k \in K_2} d^k = d \quad (17)$$

and $\|d\| \leq \Delta$. By continuity, since $\lim_{k \in K_2} x^k = x_*$ we have that

$$\lim_{k \in K_2} f(x^k) = f(x_*). \quad (18)$$

Then, taking limits for $k \in K_2$ in both sides of (16), by (15), (17), (18), and the fact that (15) implies $\lim_{k \in K_2} \xi_{k,+} = 0$, we get

$$\langle \nabla f(x_*), d \rangle \geq 0$$

as we wanted to prove. □

Lemma 2.4 *Assume that f admits continuous derivatives for all x in an open set that contains Ω and $\{x^k\}$ is generated by Algorithm 2.1. Assume that $\{f(x^k) - f_{\text{target}}\}$ is bounded away from zero, $x_* \in \mathbb{R}^n$, and there exists $K_1 \subset \mathbb{N}$ such that $\lim_{k \in K_1} x^k = x_*$ and*

$$\lim_{k \in K_1} \left\| v^k - \frac{\nabla f(x^k)}{\|\nabla f(x^k)\|} \right\| = 0. \quad (19)$$

Then, for all $d \in \mathbb{R}^n$ such that $\|d\| \leq \Delta$ and $x_ + d \in \Omega$ we have that*

$$\langle \nabla f(x_*), d \rangle \geq 0.$$

Proof: If $\nabla f(x_*) = 0$, we are done; so we assume $\nabla f(x_*) \neq 0$ from now on. By Lemma 2.3, there exists $K_2 \subseteq K_1$ and $\bar{d} \in \mathbb{R}^n$ such that

$$\lim_{k \in K_2} d^k = \bar{d} \quad (20)$$

and

$$\langle \nabla f(x_*), \bar{d} \rangle \geq 0; \quad (21)$$

and, since $\nabla f(x_*) \neq 0$, (21) implies

$$\left\langle \frac{\nabla f(x_*)}{\|\nabla f(x_*)\|}, \bar{d} \right\rangle \geq 0. \quad (22)$$

Given $\varepsilon > 0$, by (19), (20), and the continuity of ∇f , (22) implies that

$$\langle v^k, d^k \rangle \geq -\varepsilon \quad (23)$$

for all $k \in K_2$ large enough. Since, by the definition of Algorithm 2.1, d^k is a solution to (5), (23) implies that

$$\langle v^k, d \rangle \geq -\varepsilon \quad (24)$$

for all $d \in \mathbb{R}^n$ such that $x^k + d \in \Omega$ and $\|d\| \leq \Delta$ and all $k \in K_2$ large enough.

Consider the problem

$$\text{Minimize } \left\langle \frac{\nabla f(x_*)}{\|\nabla f(x_*)\|}, d \right\rangle \text{ subject to } \|d\| \leq \Delta \text{ and } x_* + d \in \Omega \quad (25)$$

that, by compactity, admits a solution d_* ; and suppose, by contradiction, that

$$\left\langle \frac{\nabla f(x_*)}{\|\nabla f(x_*)\|}, d_* \right\rangle = -c < 0. \quad (26)$$

Therefore,

$$\left\langle \frac{\nabla f(x_*)}{\|\nabla f(x_*)\|}, x_* + d_* - x_* \right\rangle = -c < 0.$$

This implies, by (19), that

$$\langle v^k, x_* + d_* - x^k \rangle \leq -c/2 < 0 \quad (27)$$

for $k \in K_2$ large enough. Let us write $\tilde{d}^k = x_* + d_* - x^k$. Since $x_* + d_* \in \Omega$, we have that $x^k + \tilde{d}^k \in \Omega$. If, for some $k \in K_2$ large enough, we have that $\|\tilde{d}^k\| \leq \Delta$, taking $\varepsilon < -c/2$, we get a contradiction between (27) and (24). This contradiction comes from the assumption (26), which, as a consequence, is false, completing the proof.

We now consider the case in which $\|\tilde{d}^k\| > \Delta$ for all $k \in K_2$ large enough. Since

$$\|\tilde{d}^k\| = \|x_* + d_* - x^k\| \leq \|d_*\| + \|x_* - x^k\| \leq \Delta + \|x_* - x^k\|,$$

defining

$$\hat{d}^k = \frac{\tilde{d}^k}{1 + \|x^k - x_*\|/\Delta}, \quad (28)$$

we have that $\|\hat{d}^k\| \leq \Delta$ and, by the convexity of Ω , $x^k + \hat{d}^k \in \Omega$. Moreover, by (27), since $\lim_{k \in K_2} x^k = x_*$,

$$\langle v^k, \hat{d}^k \rangle \leq -c/4 < 0 \quad (29)$$

for $k \in K_2$ large enough. Taking $\varepsilon < -c/4$, we get the contradiction between (29) and (24) and the proof is complete. \square

Theorem 2.1 *Assume that f admits continuous derivatives for all x in an open set that contains Ω and $\{x^k\}$ is generated by Algorithm 2.1. Assume that the level set defined by $f(x^0) + \eta$ is bounded, where $\eta = \sum_{k=0}^{\infty} \eta_k$, and there exists an infinite sequence of indices K_1 such that (19) holds. Then, given $\varepsilon > 0$, either exists an iterate x^k such that $f(x^k) \leq f_{\text{target}} + \varepsilon$ or there exists a limit point x_* of $\{x^k\}$ such that $\langle \nabla f(x_*), d \rangle \geq 0$ for all d such that $x_* + d \in \Omega$.*

Proof: Since the level set defined by $f(x^0) + \eta$ is bounded, the sequence $\{x^k\}_{k \in K_1}$ admits a limit point. Therefore, the thesis follows from Lemma 2.4. \square

Remark. Let us show that Assumption (19) is plausible. With this purpose, assume that it does not hold. Then, there exists $\varepsilon > 0$ such that for all $k \in \mathbb{N}$,

$$\left\| v^k - \frac{\nabla f(x^k)}{\|\nabla f(x^k)\|} \right\| > \varepsilon.$$

Clearly, if we choose randomly the vectors v^k in the unitary sphere, the probability of this event is zero. Therefore, assumption (19) holds with probability 1.

3 Practical algorithm for nonlinear least-squares

In this section, we are interested in the application of Algorithm 2.1 to large scale nonlinear least squares problems of the form

$$\text{Minimize } \frac{1}{2} \|F(x)\|_2^2, \quad (30)$$

where $F : \mathbb{R}^n \rightarrow \mathbb{R}^m$ and $\|\cdot\|_2$ is the Euclidean norm. Consequently, we define

$$f(x) = \frac{1}{2} \|F(x)\|_2^2. \quad (31)$$

The proposed algorithm for solving (30) is a particular case of Algorithm 2.1 for the case $\Omega = \mathbb{R}^n$, but it includes two additional features: minimizations in reduced spaces and acceleration steps.

Algorithm 3.1. Let $f_{\text{target}} \in \mathbb{R}$, $\Delta > 0$, $\gamma \in (0, 1)$, a sequence $\{\eta_k\}$ of positive numbers such that

$$\sum_{k=0}^{\infty} \eta_k < \infty,$$

and the initial guess $x^0 \in \mathbb{R}^n$ be given. Set $k \leftarrow 0$.

Step 1. If $f(x^k) \leq f_{\text{target}}$, then terminate the execution of the algorithm.

Step 2. Compute $x^{\text{trial}} \in \mathbb{R}^n$ by means of a Reduction Algorithm.

Step 3. Test the descent condition

$$f(x^{\text{trial}}) \leq f(x^k) + \eta_k - \gamma \left[f(x^k) - f_{\text{target}} \right]. \quad (32)$$

If $x^{\text{trial}} \neq x^k$ and (32) holds, set $d^k = x^{\text{trial}} - x^k$, $\alpha_k = 1$, $v^k = d^k / \|d^k\|$, and go to Step 9.

Step 4. Choose $v^k \in \mathbb{R}^n$ such that $\|v^k\| = 1$.

Step 5. Compute d^k as a solution to the subproblem given by

$$\text{Minimize } \langle v^k, d \rangle \text{ subject to } \|d\| \leq \Delta.$$

Step 6. Set $\alpha \leftarrow 1$.

Step 7. Set $x^{\text{trial}} \leftarrow x^k + \alpha d^k$.

Step 8. Test the descent condition

$$f(x^{\text{trial}}) \leq f(x^k) + \eta_k - \gamma \alpha^2 \left[f(x^k) - f_{\text{target}} \right]. \quad (33)$$

If (33) does not hold, update $\alpha \leftarrow \alpha/2$ and go to Step 7. Otherwise, set $\alpha_k = \alpha$.

Step 9. Compute, by means of the Acceleration Algorithm, $x^{k+1} \in \mathbb{R}^n$ such that

$$f(x^{k+1}) \leq f(x^{\text{trial}}).$$

Set $k \leftarrow k + 1$ and go to Step 1.

Lemmas 2.1, 2.2, 2.3, 2.4, and Theorem 2.1 hold for Algorithm 3.1 exactly in the same way as they do for Algorithm 2.1. In order to complete the definition of Algorithm 3.1, we now introduce two possible Reduction Algorithm and an Acceleration Algorithm. Both Reduction algorithms employ BOBYQA [32] for minimizing $f(x)$ over manifolds of moderate dimension.

3.1 Affine-subspaces-based Reduction Algorithm

In this Reduction Algorithm the manifold over which we minimize $f(x)$ at each iteration is an affine subspace. At iteration k , we consider an affine transformation $\mathcal{T}_k : \mathbb{R}^{n_{\text{red}}} \rightarrow \mathbb{R}^n$, with $n_{\text{red}} \leq n$, given by $\mathcal{T}_k(d) := x^k + M_k d$, where $M_k \in \mathbb{R}^{n \times n_{\text{red}}}$ is a matrix with random (with uniform distribution) elements $m_{ij} \in [-1, 1]$. So the problem to be solved at iteration k is given by

$$\text{Minimize}_{d \in \mathbb{R}^{n_{\text{red}}}} \|F(\mathcal{T}_k(d))\|_2^2. \quad (34)$$

The natural initial guess for this problem is given by $d = 0$. The minimization on small-dimensional subspaces has been used in [40, 43]. Moreover, in the context of derivative-free optimization, it has been recently employed in [10].

3.2 Linear-interpolation-based Reduction Algorithm

At iteration k , we consider a linear-spline-based transformation $\mathcal{S}_k : \mathbb{R}^{n_{\text{red}}} \rightarrow \mathbb{R}^n$, with $n_{\text{red}} \leq n$, where $n_{\text{red}} = 2\kappa + 2$ for some $\kappa \geq 0$. Variables of the reduced model are p_1, \dots, p_κ , and $v_0, v_1, \dots, v_\kappa, v_{\kappa+1}$, with $0 \leq p_j \leq 1$ for $j = 1, \dots, \kappa$. Define $p_0 = 0$ and $p_{\kappa+1} = 1$. If $p_{j_1} = p_{j_2} = \dots$ for $j_1 \neq j_2 \neq \dots$, then redefine v_{j_1}, v_{j_2}, \dots as their average. Let $\bar{p}_0 < \dots < \bar{p}_{\bar{\kappa}+1}$ (with $\bar{\kappa} \leq \kappa$) be a permutation of $p_0, \dots, p_{\kappa+1}$ in which repeated values were eliminated and let $\bar{v}_0, \dots, \bar{v}_{\bar{\kappa}+1}$ be the corresponding (reordered) values. We define a piecewise linear function $L : [0, 1] \rightarrow \mathbb{R}$ such that $L(\bar{p}_j) = \bar{v}_j$ for $j = 0, \dots, \bar{\kappa} + 1$. The transformation \mathcal{S}_k is given by $\mathcal{S}_k(v_0, \dots, v_{\kappa+1}, p_1, \dots, p_\kappa) := x^k + d(v, p)$, where $[d(v, p)]_i = L((i-1)/(n-1))$ for $i = 1, \dots, n$. So the *bound constrained* problem to be solved at iteration k is given by

$$\text{Minimize}_{(v,p) \in \mathbb{R}^{n_{\text{red}}}} \|F(\mathcal{S}_k(v, p))\|_2^2 \text{ subject to } 0 \leq p_j \leq 1 \text{ for } j = 1, \dots, \kappa. \quad (35)$$

As initial guess, we consider $v = 0$ and p with random (with uniform distribution) components $p_j \in [0, 1]$ for $j = 1, \dots, \kappa$.

3.3 Acceleration Algorithm

We adopt a Sequential Secant approach for defining the acceleration. The scheme, that generalizes the one adopted in [3] for solving nonlinear systems of equations, is as follows.

1. If $k = 0$, then define $x^{k+1} = x^{\text{trial}}$.
2. If $k > 0$, then choose $k_{\text{old}} \in \{0, 1, \dots, k - 1\}$,

$$\begin{aligned}
 s^j &= x^{j+1} - x^j \text{ for all } j = k_{\text{old}}, \dots, k - 1, \\
 s^k &= x^{\text{trial}} - x^k, \\
 y^j &= F(x^j + s^j) - F(x^j) \text{ for all } j = k_{\text{old}}, \dots, k. \\
 S_k &= (s^{k_{\text{old}}}, \dots, s^k), \\
 Y_k &= (y^{k_{\text{old}}}, \dots, y^k), \\
 x_{\text{accel}}^k &= x^k - S_k Y_k^\dagger F(x^k).
 \end{aligned}$$

3. If $f(x_{\text{accel}}^k) \leq f(x^{\text{trial}})$, then define $x^{k+1} = x_{\text{accel}}^k$. Otherwise, define $x^{k+1} = x^{\text{trial}}$.

This algorithm differs from the plain acceleration scheme defined in (2) in a very substantial way. In (2), the definition of x^{k+1} depends only on the previous iterates and lies in the affine subspace determined by them. Therefore, in (2), the successive iterates do not escape from a fixed p -dimensional affine subspace, where p is the number of previous iterates that contribute to the acceleration process. On the contrary, here, we define x^{k+1} as the possible result of an acceleration that includes the trial point x^{trial} which, in principle, does not belong to any pre-determined affine subspace. As a consequence, the accelerated point has the chance of exploring the whole domain in a more efficient way.

4 Estimation of Manning coefficients in the Saint-Venant equation

In the present work, we are interested in the estimation of parameters in one-dimensional models that simulate water or mud flow in natural channels. The presence of extreme boundary conditions can be a consequence of upstream levee breakage, a subject that is studied in the context of the interdisciplinary research and action group CRIAB (acronym for ‘‘Dams Conflicts, Risks and Impacts’’ in Portuguese) at the University of Campinas. The initial conditions for this type of models are, in general, well known, but the parameters reflecting density, friction, obstacles, or terrain features must be estimated from data. Mathematical models for this type of phenomena consist of partial differential equations with boundary conditions that simulate flood intensity. The use of programs whose source code is not available is frequent in this type of research. For this reason we are interested in investigating the behavior of derivative-free methods to estimate parameters of the models used.

For simplicity, in this study we assume that the phenomenon we are interested in is well represented by the Saint-Venant equations [35]. More sophisticated tools are beyond the scope of the present work. The Saint-Venant equations

$$A_t + Q_x = 0 \tag{36}$$

and

$$Q_t + (QV)_x + gA\hat{z} + \frac{\xi PV|V|}{8} = 0. \tag{37}$$

simulate the evolution of mean velocity, wetted cross-sectional area, depth, and flow in a one-dimensional channel. In (36) and (37), $A = A(x, t)$ is the wetted cross sectional area at position x and time t ; $V = V(x, t)$ is the mean velocity; $Q = Q(x, t) = A(x, t) V(x, t)$ is the flow rate; $P = P(x, t)$ is the wetted perimeter, that is, the perimeter enclosing the wetted area taking away the air contact surface; g is the acceleration of gravity, approximately $9.8m/s^2$; $\hat{z} = \hat{z}(x, t) = z_x/(1 + (z_x)^2)$, where $z = z(x, t) = h(x, t) + z_b(x)$, $h(x, t)$ is the maximum channel depth at point x and time t , and $z_b(x)$ is the vertical coordinate of the channel bottom at point x (therefore, $z_x = h_x + (z_b)_x$); and $\xi = \xi(x)$ is the adimensional Manning coefficient whose estimation using data is the subject of the present study. The estimation of Manning coefficients is a very hard problem related with the simulation of floods in natural channels [13]. In the present work, we adopt that (a) Manning coefficients vary at different points of the channel but are invariant in time and (b) the best estimation of Manning coefficients is the one that provides the best predictions of streams in a period of time.

We assume that the channel under consideration extends one-dimensionally from $x = x_{\min}$ to $x = x_{\max}$. The boundary condition on the left (x_{\min}) simulates a flow rate that grows linearly from $8.245 m^3/s$ to $200 m^3/s$ in 1,200 seconds and decreases to the initial flow rate between 1,200 seconds and 3,600 seconds, remaining stationary thereafter. The initial depth is 1.2 meters. The second derivatives of other state variables are assumed to be zero both in $x = x_{\min}$ and in $x = x_{\max}$. We consider that wetted cross-sectional areas and velocities are measured between times $t = t_{\min}$ and $t = t_{\max}^{\text{obs}}$, at equally spaced points in the interval $[x_{\min}, x_{\max}]$. The physical characteristics of this channel were taken from [29] and [14]. Synthetic data were created with $x_{\min} = 0$ meters, $\Delta x = 6$ meters, $x_{\max} \in \{3,000, 3,600, \dots, 9,000\}$ meters, $t_{\min} = 0$ seconds, and $\Delta t = 0.1$ seconds. The value of t_{\max}^{obs} , maximum observation time, was subject to experimentation; while t_{\max}^{pred} , maximum time for prediction, was set to $t_{\max}^{\text{pred}} = 3,600$ seconds. The transversal area was considered to be rectangular with a width of 5 meters. We assumed that the true value for the adimensional Manning coefficients at the discretized space points is 0.0366 plus a random uniform perturbation of up to 1%. We set $(z_b)_x = 0.001$. For the purposes of this research, we found it satisfactory to solve the Saint-Venant equations by finite differences using a Lax-Friedrichs type scheme [24] with artificial diffusion coefficient equal to 0.9.

The considerations above lead to a problem of the form

$$\text{Minimize}_{\xi \in \mathbb{R}^{n_x}} \sum_{i=1}^{n_t} \sum_{j=0}^{n_x} \sum_{k=1}^2 \left(y(\xi, t_i, x_j, k) - y_{ijk}^{\text{obs}} \right)^2, \quad (38)$$

where $x_j = x_{\min} + j\Delta x$ for $j = 0, \dots, n_x$, $t_i = t_{\min} + i\Delta t$ for $i = 1, \dots, n_t$ and $n_x, x_{\min}, \Delta x, n_t, t_{\min}$, and Δt are given. When $k = 1$, y_{ijk}^{obs} ($i = 1, \dots, n_t, j = 0, \dots, n_x$) corresponds to a given observation of transversal area; while, when $k = 2$, it corresponds to a given observed velocity. The problem has n_x unknowns and $2n_t(n_x + 1)$ terms in the summation. $y(\xi, t_{\min}, x_j, k)$ does not depend on ξ and it is assumed to be known for $k = 1, 2$ and $j = 0, \dots, n_x$; while the given values of Δx and Δt are such that, if ξ and $y(\xi, t_i, x_j, k)$ for $j = 0, \dots, n_x$ are known, then $y(\xi, t_{i+1}, x_j, k)$, for $j = 0, \dots, n_x$, may be computed in finite time. In a generalization to (38), it is assumed that most of the observations are not available and, then, (38) is substituted with

$$\text{Minimize}_{\xi \in \mathbb{R}^{n_x}} \sum_{\{(i,j,k) \in S\}} \left(y(\xi, t_i, x_j, k) - y_{ijk}^{\text{obs}} \right)^2, \quad (39)$$

where $S \subseteq \hat{S}$ is given, $\hat{S} = \{(i, j, k) \mid i = 1, \dots, n_t, j = 0, \dots, n_x, k = 1, 2\}$, and $|S| \ll |\hat{S}|$. For further reference, we denote by $n_o = |S|$ the number of available observations. Note that, if $S = \hat{S}$, then $n_o = 2n_t(n_x + 1)$; while if, for example, only 10% of the observations are available, then we have $n_o = 0.2n_t(n_x + 1)$.

Approximately solving (39) provides a value $\bar{\xi}$; and this value $\bar{\xi}$ is then used to predict that

$$y_{ijk}^{\text{obs}} \approx y(\bar{\xi}, t_i, x_j, k) \text{ for } (i, j, k) \in \widehat{S}^+,$$

where $t_{\max}^{\text{obs}} = t_{\min} + n_t \Delta t$ is the largest time instant at which observations considered in (39) were collected, $t_{\max}^{\text{pred}} > t_{\max}^{\text{obs}}$, and $\widehat{S}^+ = \{(i, j, k) \mid t_{\max}^{\text{obs}} < t_i \leq t_{\max}^{\text{pred}}, j = 0, \dots, n_x, k = 1, 2\}$ represents the set of indices of the y_{ijk}^{obs} , *not yet observed*, whose predicted value is given by $y(\bar{\xi}, t_i, x_j, k)$.

4.1 Numerical results

We implemented Algorithm 3.1, together with the two Reduction Algorithms (Sections 3.1 and 3.2) and the Acceleration Algorithm (Section 3.3) in Fortran 90. All tests were conducted on a computer with a 3.4 GHz Intel Core i5 processor and 8GB 1600 MHz DDR3 RAM memory, running macOS Mojave (version 10.14.6). Code was compiled by the GFortran compiler of GCC (version 8.2.0) with the -O3 optimization directive enabled. In the rest of this section, mainly in figures and tables, Algorithm 3.1 is sometimes referred to as SESEM, that stands for ‘‘Sequential Secant Method’’. Based on [3] and on preliminar numerical experiments, we set $\gamma = 10^{-4}$, $\eta_k =$ for $k = 0, 1, \dots$, and $\Delta = 10$ in Algorithm 3.1, and $p = 1000$, i.e. $k_{\text{old}} = \max\{0, k - p\}$, in the Acceleration Algorithm.

In section 4.1.1, we aim to determine (i) the amount of observations (starting at $t_{\min} = 0$ and at intervals $\Delta t = 0.1$ seconds), determined by the maximum observation time t_{\max}^{obs} , and (b) the precision of the optimization process that are required to recover Manning coefficients ξ suitable for making predictions up to $t_{\max}^{\text{pred}} = 3,600$ seconds. Sections 4.1.2 and 4.1.3 are related to the calibration and analysis of the proposed method. In Section 4.1.2, the dimension of the subproblem solved at each iteration is determined; while in Section 4.1.3 the influence of the Acceleration Algorithm in the overall process is observed. In Section 4.1.4, a set of instances of increasing size, mimic the the size of real-life instances, is solved. Section 4.1.5 presents the behavior of the solvers BOBYQA [32] and DFBOLS [46] in the set of considered instances.

4.1.1 Choice of a tolerance that leads to acceptable solutions

Given data coming from observations, we seek to estimate the Manning coefficients by means of which the Saint-Venant equations produce the best reproduction of data. In real cases, we are tempted to believe that an accuracy of around 10% in the prediction of depths and velocity is sufficiently good and that more accurate reproduction is not justified since observation and modeling errors may be, many times, of that order. However, we have no guarantees about the quality of predictions for data that are not available yet; and it can be argued that, although an excessive precision in the available data has no effect in the reproduction of these data, it may have a significant effect in the reproduction of observations that are not available yet. Therefore, it is sensible to test our inversion procedure not only up to the precision compatible with observation and modeling errors but also with moderate higher precisions.

Assume that an iterative optimization process is applied to (39) to compute $\bar{\xi}$; and that this process stops when it finds $\bar{\xi}$ satisfying

$$\left[\sum_{\{(i,j,k) \in S\}} \left(y(\bar{\xi}, t_i, x_j, k) - y_{ijk}^{\text{obs}} \right)^2 \right] \leq \epsilon \left[\sum_{\{(i,j,k) \in S\}} \left(y_{ijk}^{\text{obs}} \right)^2 \right], \quad (40)$$

where $\epsilon > 0$ is a given tolerance. Of course, $\bar{\xi}$ depends on ϵ and on the problem data. In particular, $\bar{\xi}$ depends on the set of available observations S , that depends on t_{\max}^{obs} . Assume that, after computing $\bar{\xi}$,

$t_{\max}^{\text{pred}} > t_{\max}^{\text{obs}}$ is chosen and observations y_{ijk}^{obs} with $(i, j, k) \in S^+ \subseteq \widehat{S}^+$ become available. We define that, for the given S^+ and t_{\max}^{pred} , $\bar{\xi}$ is *acceptable* if we have that

$$\eta(\bar{\xi}) := \frac{\sum_{\{(i,j,k) \in S^{US+}\}} \left(y(\bar{c}, t_i, x_j, k) - y_{ijk}^{\text{obs}} \right)^2}{\sum_{\{(i,j,k) \in S^{US+}\}} \left(y_{ijk}^{\text{obs}} \right)^2} \leq 10^{-4}. \quad (41)$$

Let the problem data n_x , x_{\min} , Δx , t_{\min} , and Δt (note that n_t is missing here) be given and assume that an instant t_{\max}^{pred} is chosen. The question is: Which are the number of observations n_o and the optimization tolerance ϵ that make the computed $\bar{\xi}$ to be acceptable? We aim to answer this question empirically considering a typical instance of (39) with $n_x = 500$, $x_{\min} = 0$, $\Delta x = 6$, $t_{\min} = 0$, $\Delta t = 0.1$, and S randomly chosen in such a way that $n_o = |S| \approx 0.1(2n_t(n_x + 1))$, i.e. assuming that approximately 90% of the observations are not available. (Units of measure are meters for space and seconds for time.) Setting $t_{\max}^{\text{pred}} = 3,600$ and varying a constant $\nu \in \{10^{-4}, 2 \times 10^{-4}, \dots, 40 \times 10^{-4}\}$, used to define $n_t(\nu)$ such that $t_{\max}^{\text{obs}} \approx \nu t_{\max}^{\text{pred}}$, we defined 40 instances of problem (39). (The number of observations is $n_o \approx 0.2n_t(\nu)(n_x + 1)$; $\nu = 10^{-4}$ corresponds to $n_o = 427$, while $\nu = 4 \times 10^{-3}$ corresponds to $n_o = 14,460$.) For each instance, a solution satisfying (40) was computed considering 36 different tolerances $\epsilon \in \{7.5 \times 10^{-13}, 5 \times 10^{-13}, 2.5 \times 10^{-13}, \dots, 10^{-4}\}$. For each combination (ν, ϵ) , we obtained a solution $\bar{\xi}(\nu, \epsilon)$, that is said to be acceptable if (41) holds. Figure 1 displays, as a function of ν and ϵ , the value of the prediction error $\eta(\bar{\xi}(\nu, \epsilon))$ defined in (41). In the figure, cold colors (blue, cyan, and green) correspond to solutions that are not acceptable; while hot colors (yellow, orange, red, and dark red) correspond to acceptable solutions. The figure shows (on the left) that acceptable solutions were not found when the number of observations $n_o(\nu)$ was smaller than the number of unknowns $n_x = 500$. When the number of observations is larger than the number of unknowns, acceptable solutions are only found when $\epsilon \leq 10^{-9}$.

4.1.2 Choice of the subproblems' dimension

We now consider an instance of problem (39) with $n_x = 500$, $x_{\min} = 0$, $\Delta x = 6$, $n_t = 10$, $t_{\min} = 0$, $\Delta t = 0.1$, and S randomly chosen in such a way that $n_o = |S| \approx 0.1(2n_t(n_x + 1))$, i.e. assuming that approximately 90% of the observations are not available. The choice $n_t = 10$ combined with $\Delta t = 0.1$ means that observations are collected at intervals of 0.1 seconds during 1 second; and since we are assuming that 90% of the observations will not be available, this means that there will be $n_o \approx 0.1 \times 2 \times 10 \times (n_x + 1) = 2(n_x + 1) > n_x$ observations available. We aim to find solutions to this instance satisfying (40) with $\epsilon = 10^{-9}$ that, for this instance, corresponds to $f_{\text{target}} \approx 1.9633 \times 10^{-5}$. Due to analysis in the previous paragraph, it is expected the computed solution to be acceptable according to (41); so the solution can be used to make predictions for the next 3,559 seconds.

The instance in the previous paragraph will be used to observe the behavior of two variants of Algorithm 3.1, with affine-subspaces-based and with linear-interpolation-based subproblems, under variations of the subproblems' dimension n_{red} . Each variation of Algorithm 3.1 uses, at every iteration, the same reduction strategy and the same subproblem's dimension. As mentioned in the previous paragraph, $f_{\text{target}} \approx 1.9633 \times 10^{-5}$; while the initial guess is always $x^0 = 0$. Figures 2 and 3 show the results. Since both reduction strategies have a random component, the instance was solved ten times for each considered value of n_{red} . Figure 2 shows boxplots of two performance measures (CPU time and number of functional evaluations) of Algorithm 3.1 with affine-subspace-based subproblems and $n_{\text{red}} \in \{4, 5, \dots, 9\} \cup \{10, 15, \dots, 50\}$. The boxplots show that the efficiency of the method is inversely proportional to the size of the subproblems. Thus, it is worth noticing that with $n_{\text{red}} \in \{2, 3\}$ the performance measures present a large standard deviation and some outliers, while the method fails

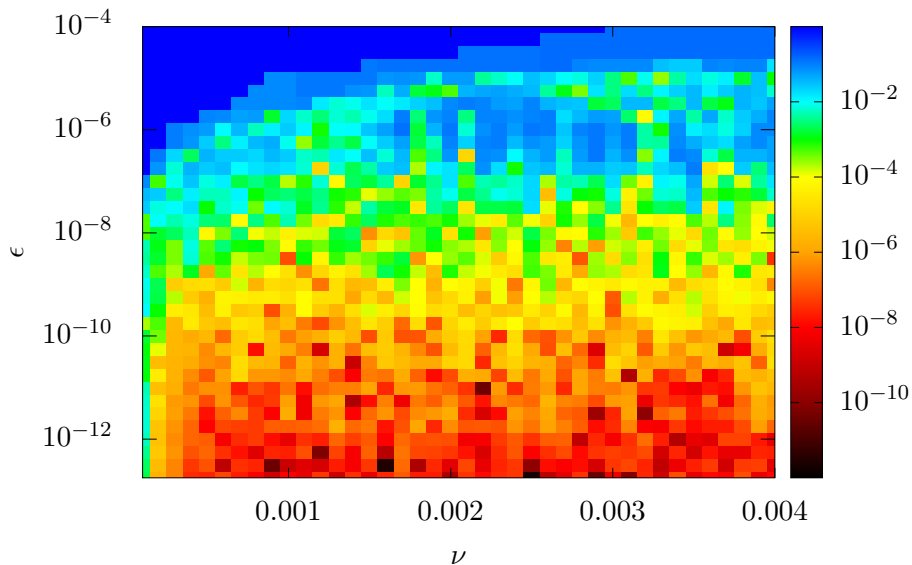


Figure 1: Acceptability of solutions $\bar{\xi}(\nu, \epsilon)$ to instances with varying number of observations $n_t(\nu)$ solved with varying tolerances ϵ . Hot colors show that acceptable solutions can be computed when the number of observations is larger than the number of unknowns and the tolerance to stop the optimization process is tight (smaller than 10^{-9}).

a few times, characterizing a situation in which the method has difficulties in improving the current approximation to a solution by inspecting a very small search space. Figure 3 shows boxplots of two performance measures (CPU time and number of functional evaluations) of Algorithm 3.1 with linear-interpolation-based subproblems and $n_{\text{red}} \in \{8, 10, 12, 14, 16, 18, 20, 30, 40, 50\}$. The boxplots show a uniform performance of the method for $n_{\text{red}} \leq 20$; while, for $n_{\text{red}} > 20$, the efficiency decreases when n_{red} increases.

4.1.3 Influence of the acceleration scheme

Still considering the same instance, we now analyze the influence of the acceleration in the performance of Algorithm 3.1 with affine-subspaces-based subproblems ($n_{\text{red}} = 4$) and with linear-interpolation-based subproblems ($n_{\text{red}} = 20$). Figure 4 shows the results. The figure shows that, when the affine-subspaces reduction strategy is considered, the acceleration improves the efficiency of the method in approximately two orders of magnitude; while it appears to have no relevant effect in combination with the linear-interpolation-based reduction strategy; although it appears to speed up the convergence of the method in its final iterations.

4.1.4 Solving larger instances

We now consider a set of instances exactly as the one already described but with $n_x \in \{500, 600, \dots, 1,500\}$. (These values correspond to $x_{\text{max}} = 3,000, 3,600, 4,200, \dots, 9,000$, respectively.) Table 1 presents the performance of Algorithm 3.1 with affine-subspaces-based subproblems ($n_{\text{red}} = 4$) and with linear-interpolation-based subproblems ($n_{\text{red}} = 20$). As before, the initial guess x^0 is always the

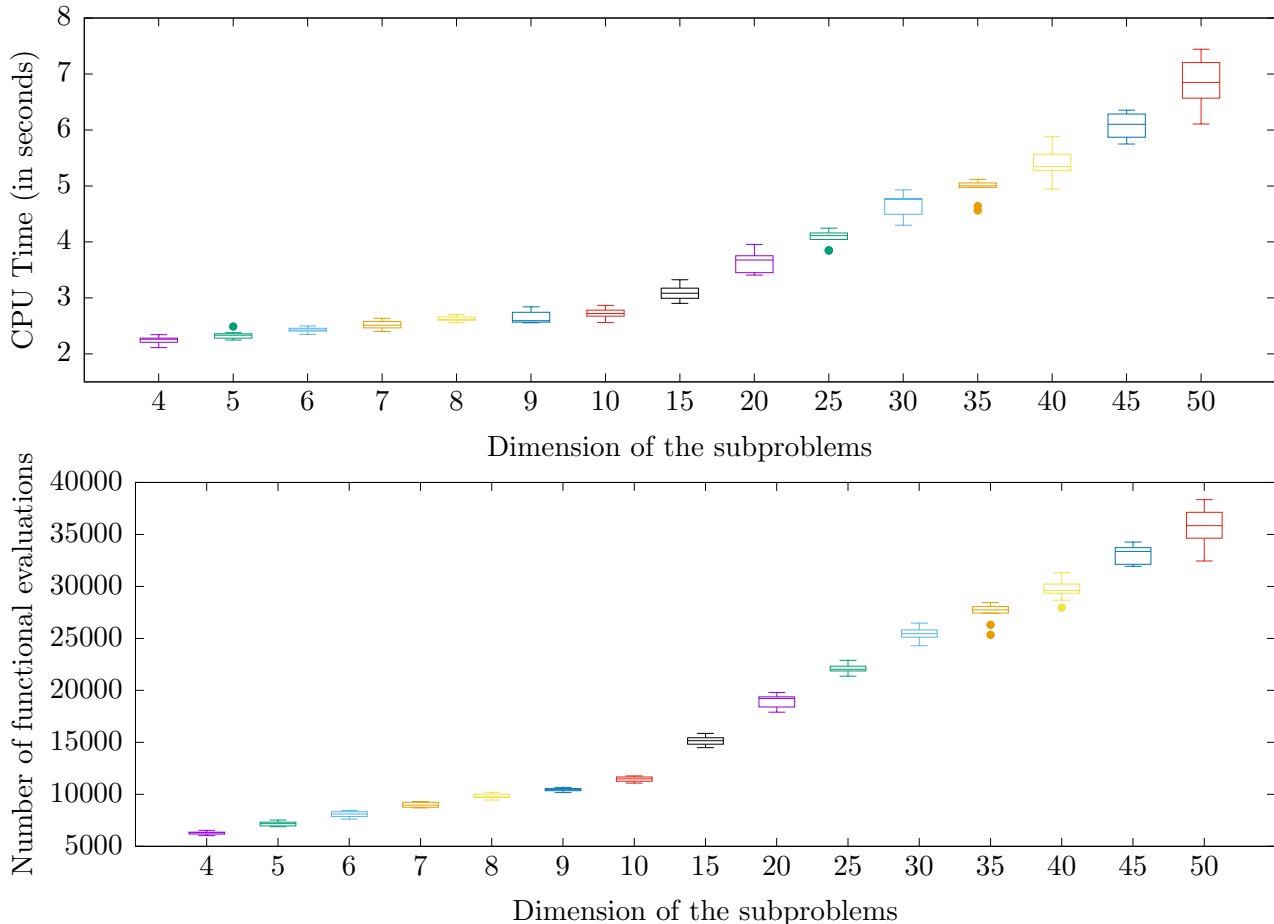


Figure 2: Boxplots of performance metrics of Algorithm 3.1 with the affine-subspaces-based reduction strategy applied to the instance with $n_x = 500$ varying the subproblems' dimension n_{red} .

origin, f_{target} corresponds to the value of the right-hand-side in (40) with $\epsilon = 10^{-9}$. In the table, $\|F(\bar{\xi})\|_2^2$ corresponds to the left-hand-side in (40), i.e.,

$$\|F(\bar{\xi})\|^2 = \sum_{\{(i,j,k) \in S\}} \left(y(\bar{\xi}, t_i, x_j, k) - y_{ijk}^{\text{obs}} \right)^2,$$

#it stands for the number of iterations, #fent stands for the number of functional evaluations, and Time stands for the CPU time in seconds. Since the method is run ten times per instance, values in the table correspond to averages. In addition, for the CPU time, the standard deviation is also presented in the table; and boxplots are given in Figures 5 and 6. A comparison between Figures 5 and 6 makes it clear that the cost of the affine-subspaces strategy grows together with the size of the instances; while the linear-interpolation strategy appears to absorb the cost of increasing sizes by incorporation some knowledge of the problem's solution.

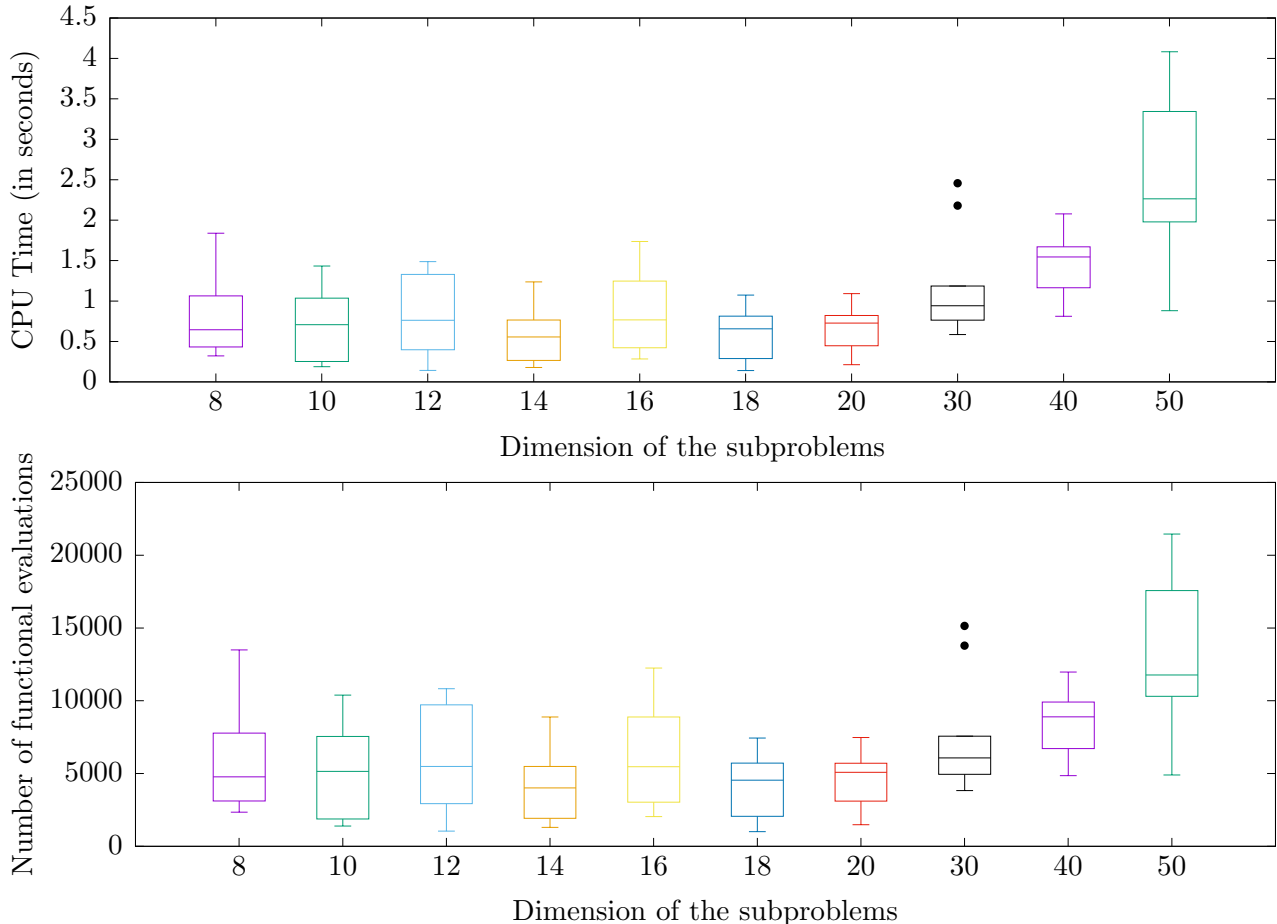


Figure 3: Boxplots of performance metrics of Algorithm 3.1 with the linear-interpolation-based reduction strategy applied to the instance with $n_x = 500$ varying the subproblems' dimension n_{red} .

4.1.5 Comparison with BOBYQA and DFBOLS

This section ends presenting the performance of BOBYQA and DFBOLS¹ applied to the same instances of Table 1. Aiming a fair comparison, both methods were modified to stop as soon as they reach a solution ξ satisfying $\|F(\xi)\|_2^2 \leq f_{\text{target}}$. Table 2 shows the results. Figures in the table show that both variants of Algorithm 3.1 outperforms BOBYQA and DFBOLS by several orders of magnitude when the CPU time is considered as performance measure. While DFBOLS is the most time consuming method, it is the most efficient if the number of functional evaluations is considered. It is worth noticing that the comparison between the behaviors of the considered methods is restricted to their application to the problem under consideration.

5 Final remarks

In this paper, we presented a general scheme under which globally convergent derivative-free algorithms for nonlinear least squares with sequential secant acceleration can be defined. Our main motivation was the estimation of parameters in hydraulic models governed by partial differential equations. The

¹Provided by Hongchao Zhang on January 11th, 2021.

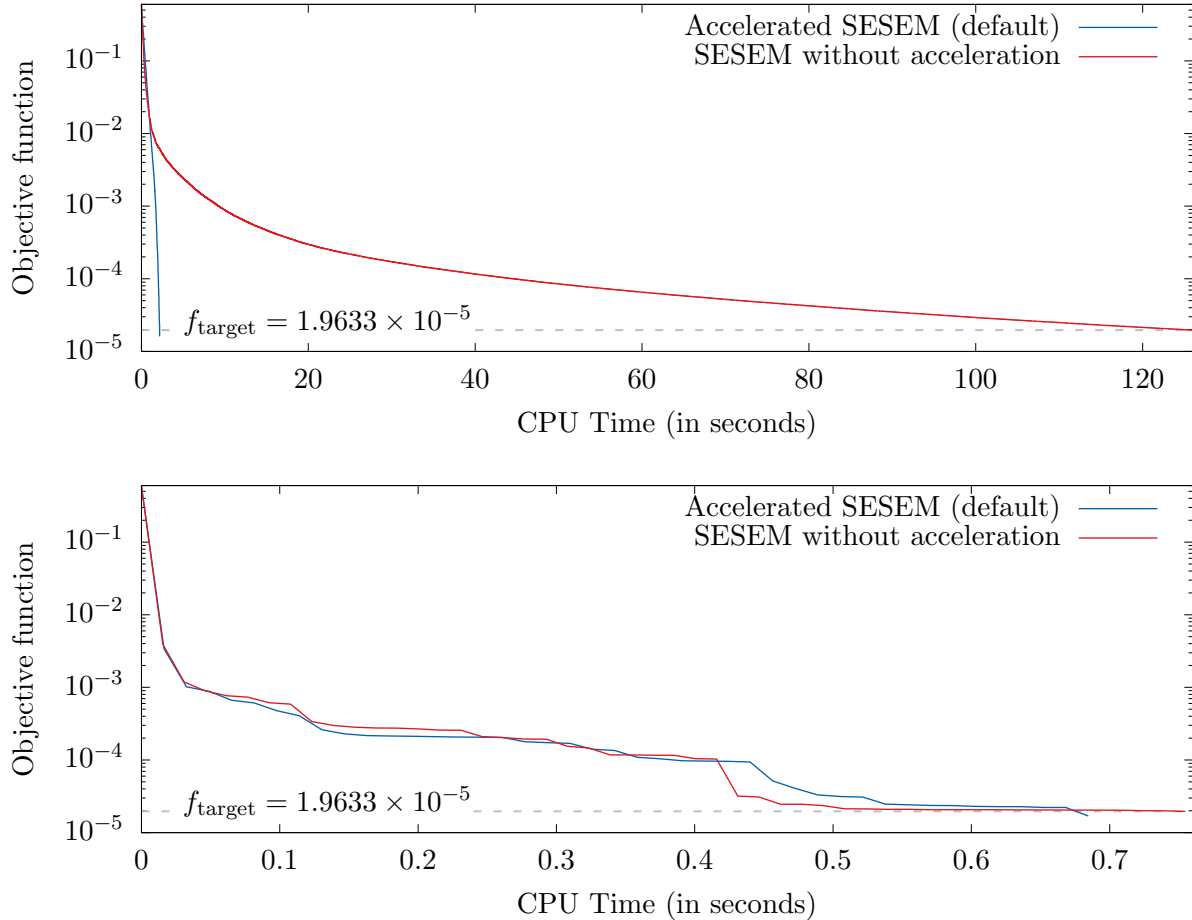


Figure 4: Influence of the acceleration in the performance of Algorithm 3.1 with affine-subspaces-based subproblems (top) and with linear-interpolation-based subproblems (bottom) when applied to the instance with $n_x = 500$.

non-availability of derivatives come from the fact that these models may be computed by “partially black-box” codes and the possible uncertainty of function evaluations motivated by the lack of precise geometrical parameters during the estimation process.

Algorithms based on interpolating quadratic models like BOBYQA [32] (see, also, [12]) use to be effective for this type of optimization problems. However, big costs associated with model building and its minimization make it necessary to employ schemes in which the number of variables is not very large. Partial minimization over random affine subspaces is an adequate dimension-reduction procedure [10, 40, 43]; and we showed that acceleration based on the sequential secant framework is effective to increase the performance of that approach. In addition, we developed a new reduction procedure based on variable linear interpolation in which the variables of subproblems are a set of independent variables with coordinates corresponding to (also) variable nodes. The effectiveness of this new approach is associated with the structure of the variables of the problem. If, in the original underlying problem, the unknown is a continuous function that depends on a single variable, the one-dimensional interpolatory scheme tends to be quite effective. This is the case of our problem of estimating the Manning coefficients, which, as a consequence, does not need acceleration to obtain

n_x	n_o	SESEM with affine subspaces ($n_{\text{red}} = 4$)					SESEM with linear splines ($n_{\text{red}} = 20$)				
		$\ F(\bar{\xi})\ ^2$	#it	#fcnt	Time		$\ F(\bar{\xi})\ ^2$	#it	#fcnt	Time	
				avg stdev						avg stdev	
500	1,058	1.86e-05	464	6,293	2.19	0.07	1.87e-05	38	4,598	0.64	0.29
600	1,257	2.10e-05	568	7,765	4.25	2.14	1.99e-05	39	5,094	0.81	0.46
700	1,471	2.63e-05	669	9,265	5.65	1.11	2.49e-05	42	5,109	0.93	0.54
800	1,669	3.06e-05	740	10,051	7.65	0.21	2.89e-05	43	4,984	1.03	0.48
900	1,908	3.53e-05	829	11,192	10.32	0.23	3.17e-05	45	5,514	1.25	0.51
1,000	2,106	3.83e-05	921	12,538	14.07	0.30	3.72e-05	45	6,021	1.59	0.65
1,100	2,312	4.26e-05	1,024	14,089	19.01	0.86	4.00e-05	41	5,304	1.45	0.75
1,200	2,484	4.66e-05	1,360	19,924	34.46	1.87	4.46e-05	46	5,364	1.58	0.80
1,300	2,677	5.05e-05	1,713	26,404	54.18	3.29	4.88e-05	46	5,802	1.84	1.03
1,400	2,885	5.45e-05	2,124	33,796	78.93	5.04	4.82e-05	43	5,227	1.79	0.91
1,500	3,090	5.83e-05	2,725	44,897	115.64	6.70	5.05e-05	48	5,916	2.34	1.01

Table 1: Performance of Algorithm 3.1 with affine-subspaces-based subproblems ($n_{\text{red}} = 4$) and with linear-interpolation-based subproblems ($n_{\text{red}} = 20$) applied to instances of increasing size with $x_{\text{max}} \in \{3,000, 3,600, \dots, 9,000\}$.

n_x	n_o	BOBYQA			DFBOLS		
		$\ F(\xi)\ ^2$	#fcnt	Time	$\ F(\xi)\ ^2$	#fcnt	Time
500	1,058	1.96e-05	7,593	278.68	2.63e-07	1,006	1,907.91
600	1,257	2.34e-05	8,176	511.07	2.39e-07	1,206	5,679.65
700	1,471	2.73e-05	10,601	1,057.75	5.16e-07	1,406	13,413.81
800	1,669	3.14e-05	15,353	1,948.76	1.16e-07	1,606	31,103.48
900	1,908	3.58e-05	12,901	2,133.89	–	–	>10h
1,000	2,106	3.92e-05	21,674	4,376.88	–	–	–
1,100	2,312	4.32e-05	18,916	5,967.14	–	–	–
1,200	2,484	4.67e-05	22,419	11,584.94	–	–	–
1,300	2,677	5.06e-05	26,074	16,742.44	–	–	–
1,400	2,885	5.46e-05	34,286	26,692.62	–	–	–
1,500	3,090	5.84e-05	29,473	26,325.37	–	–	–

Table 2: Performance of BOBYQA and DFBOLS applied to instances of increasing size with $x_{\text{max}} \in \{3,000, 3,600, \dots, 9,000\}$.

the best possible results. In more complicated cases, the “true” unknown of the problem may be a continuous function of 2, 3, or more variables. In this case, our variable-node interpolation scheme should be conveniently adapted by means of incorporation of multi-dimensional interpolation devices. In the present work, the new dimensionality-reduction scheme, as well as the acceleration process, were applied in connection with the derivative-free general-purpose solver BOBYQA [32]. In exactly the same way, both features can be used in connection with derivative-free least-squares methods such as the ones introduced in [9, 10, 46].

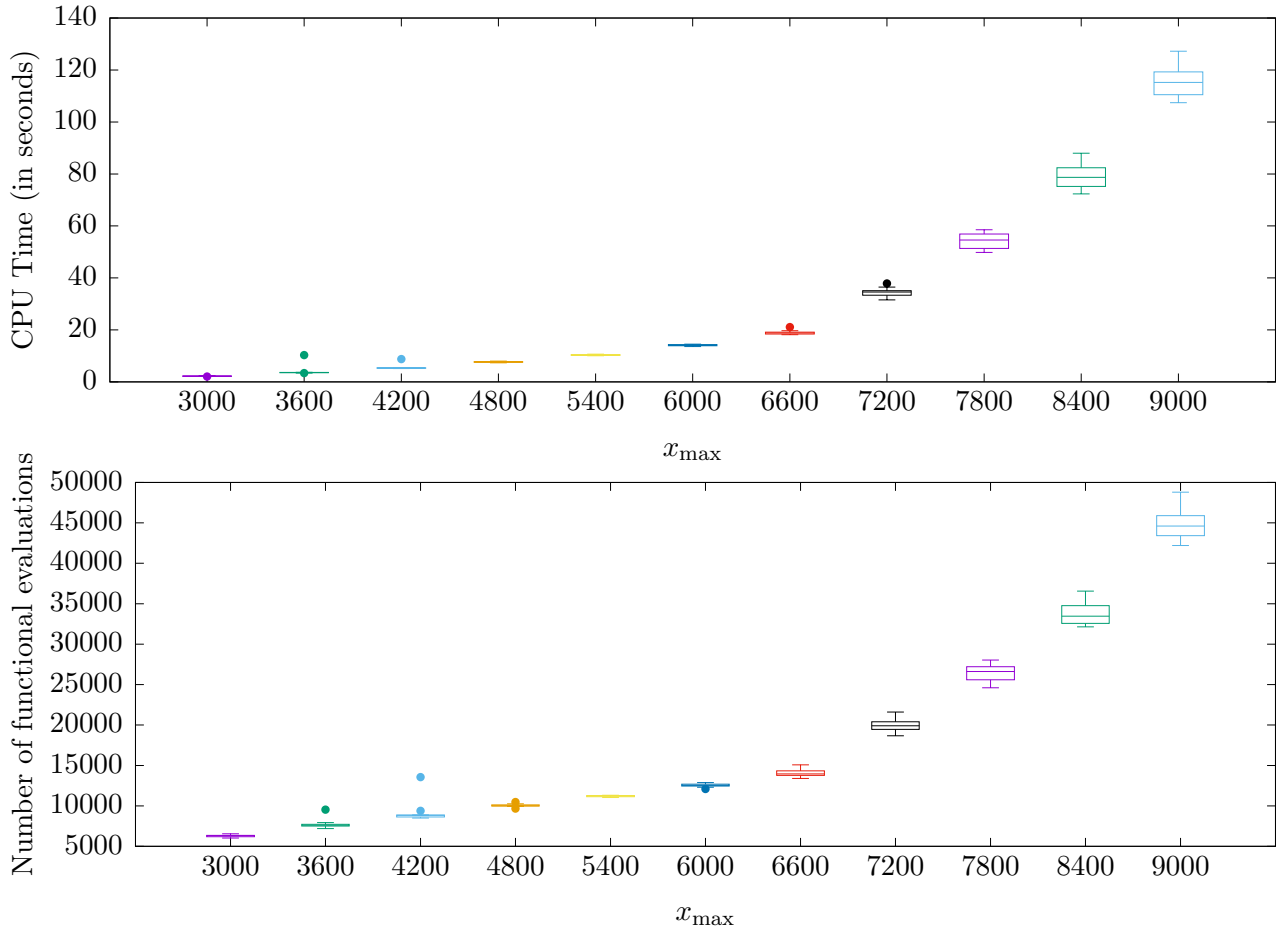


Figure 5: Boxplots of performance metrics of Algorithm 3.1 with affine-subspaces-based subproblems ($n_{\text{red}} = 4$) applied to instances of increasing size with $x_{\max} \in \{3,000, 3,600, \dots, 9,000\}$.

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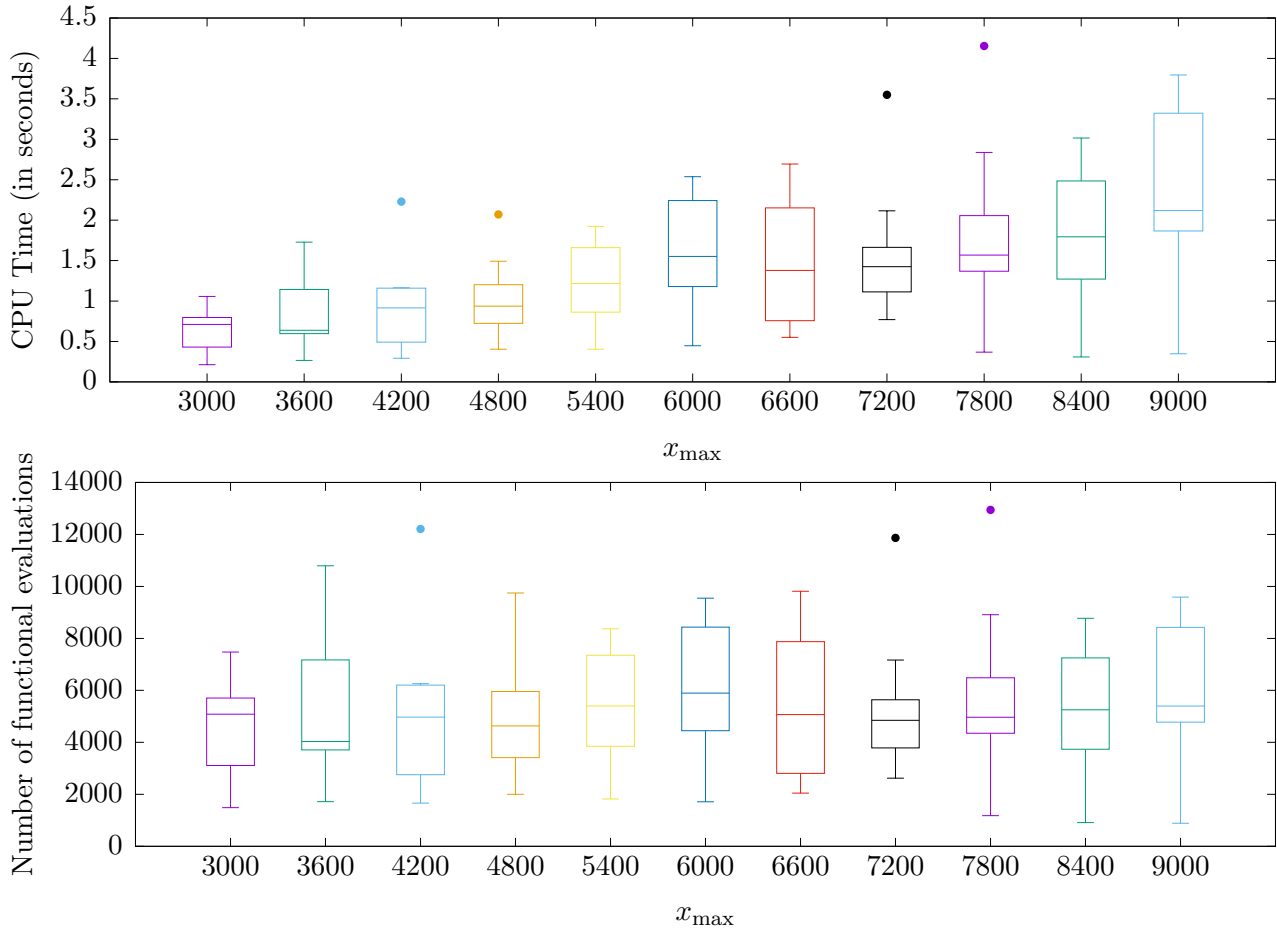


Figure 6: Boxplots of performance metrics of Algorithm 3.1 with linear-interpolation-based subproblems ($n_{\text{red}} = 20$) applied to instances of increasing size with $x_{\max} \in \{3,000, 3,600, \dots, 9,000\}$.

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