APPLICATIONS OF ACCELERATED OPTIMIZATION MODELS IN SOLVING THE WATER POLUTION PROBLEM

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Abstract: Human impacts on the living environment, habitats, land use and natural resource cause many environmental issues (air pollution, biodiversity, climate change, energy, global warming, water pollution, etc.). Among them, in this paper we chose the water resources planning as a general goal problem that we attempt to solve using some chosen optimization models. Taking all needed parameters that define the measure of pollution, we apply efficient accelerated gradient method and its hybrid version as a tool to solve the goal problem. The chosen applicative methods are the transformed accelerated double step-size method (*TADSS*) and the hybrid *TADSS*, (i.e. *HTADSS*) scheme. Good convergence and numerical properties of both models are confirmed in relevant papers. The search directions of chosen methods are of the gradient descent form. With that, the iterative step lengths parameters of the applicative methods are derived using the adequate Backtracking line search algorithms. In both of these models we also use the initial improvement of the inexact line search procedure which additionally upgrades the performance characteristics of the applied model. Finally, the relevant accelerated parameters of chosen models are derived using the features of the second order Taylor's expansions that are taken on the objective iterative rules. The hybrid applicative method, *HTADSS* model, is defined using the Khan's hybridization three-term principle. Several contemporary researches show that from this hybrid rule at least eight efficient minimalization methods are developed. Numerical comparations, taken on a large-scale test functions with application of the Dolan-Moré benchmarking optimization software, confirmed that Khan's hybrid approach is justified to use as a way of improving the objective accelerated gradient minimization method. The both applicative optimization models, are confirmedly efficient regarding usually analyzed performance metrics: the number of iterations, the CPU time and the number of function evaluations. Proven good convergence and performance features, the efficiency, as well as, the robustness of the objective minimization scheme were the guiding criteria in choosing the applicative optimization methods for generating the relevant solver-models for the posed water resources planning problem. Proposed idea of application of the TADSS and the HTADSS optimization models for solving water resources planning problem can be used similarly for solving some other environmental issues mentioned above. Furthermore, this approach is applicative on various methods of different optimization classes. Further researches concerning this theme might consider studying of the appropriately chosen type of optimization method as an adequate application for solving a certain environmental issue.

Keywords: accelerated gradient method, line search, convergence rate, unconstrained optimization.

1. INTRODUCTION

Optimization methods can be easily applied in solving significant number of contemporary problems from various scientific, medical, engineering, ecological and many others fields. Herein, we specially pay attention on accelerated gradient method for solving unconstrained optimization tasks studied by many authors (Powel (1970), Nocadal, J.& Wright S.J. (1999), Jacoby, S.L.S.; Kowalik, J.S.& Pizzo, J.T (1977), Andrei, N. (2020), etc.). We choose two prominent models of such classes and apply them in solving one of the environmental issues: water resources planning.

Unconstrained optimization problem is stated as finding the extreme value of the posed objective function *f*. Due to the duality principle each optimization problem may be viewed as minimization problem

$$\min f(x),\ x \in \mathbb{R}^n, \quad (1)$$

where $f: R^n \to R$ is the goal function. As proposed in Stanimirović, P.S., & Miladinović, M.B. (2010), using the accelerated gradient methods problem (1) can be solved by applying the following iterative rule

$$x_{k+1} = x_k - t_k \gamma_k^{-1} g_k. \quad (2)$$

In relation (2), x_{k+1} presents the current iterative point, x_k the previous one, t_k is iterative step length, g_k is the gradient of the function f and γ_k is an approximation of the function's Hessian or of its inverse. Evidently, the three crucial elements of accelerated gradient descent methods are: the value of the iterative step length, the vector of the search direction, i.e. gradient vector and the value of the accelerated factor.

- ***Iterative step size parameter*** can be calculated by the exact line search procedure, defined by the following minimization problem

  $$f(x_k + t_k d_k) = \min f(x_k + t d_k), \quad t > 0.$$

  The other way to compute this parameter is to apply some of the inexact line search techniques, such as Wolfe's, Goldstein's, Armijo's etc. In both of the chosen applicative methods, the Armijo's Backtracking line search algorithms are used in deriving the iterative step length value, t_k. With that, in both applied algorithms the authors use the initial improvement of the inexact line search procedure that additionally upgrades the performance characteristics of the applied model. Backtracking algorithm is given below

  Backtracking algorithm:
  1. Objective function $f(x)$, the direction d_k of the search at the point x_k and numbers $0 < \sigma < 0.5$ and $\beta \in (0,1)$ are required;
  2. $t = 1$;
  3. $f(x_k + td_k) > f(x_k) + \sigma t g_k^T d_k$, take $t := t\beta$;
  4. Return $t_k = t$.

- ***Search direction vector*** in any accelerated gradient descent scheme is surely the direction of the negative gradient, i.e. $-g_k$, since that is the most certain descending direction.
- ***Accelerated parameter*** usually presents a positive scalar approximation of the function's Hessian G_k or of its inverse

  $$\gamma_k I \backsim G_k, \gamma_k > 0,$$

  Among the several constructive approaches in calculating this important element of an accelerated gradient iteration, in this paper we choose the use of second order Taylor's expansion of the posed iteration to develop the iterative accelerated factor value, $0 < \gamma_k \leq 1$.

2. MATERIALS AND METHODS

In this Section we list two chosen accelerated gradient schemes as applicative methods for solving the posed problem of water resources planning.

First applicative method is *Transformed double step size method*, in short the *TADSS* method, introduced in Stanimirović, P.S.; Milovanović, G.V.; Petrović, M.J. & Kontrec, N. (2015). The *TADSS* iteration and related accelerated parameter expression are given by the following relations

$$x_{k+1} = x_k - [\alpha_k(\gamma_k{}^{-1} - 1) + 1]g_k. \quad (3)$$

$$\gamma_{k+1}^{TADSS} = 2\frac{f(x_{k+1}) - f(x_k) + \psi_k \|g_k\|^2}{\psi_k^2 \|g_k\|^2}, \quad \psi_k = [\alpha_k \gamma_k^{-1} - \alpha_k^2) + 1]. \quad (4)$$

The second chosen accelerated gradient model is constructed by applying the Khan's hybridization rule (Khan, S.H. (2013)) on the *TADSS* iteration. In Petrović, M.J., & Rakočević, V. (2022) the authors confirmed that from Khan's hybrid rule at least eight efficient minimalization methods are developed. Derived scheme is presented in Petrović, M.J.; Rakočević, V., Valjarević, D.,& Ilić, D. (2020) and named *hybrid TADSS*, or *HTADSS*. Expressions of the *HTADSS* iteration and of the accelerated parameter are

$$x_{k+1} = x_k - \alpha(t_k(\gamma_k^{-1} - 1) + 1)g_k, \quad \alpha \in (1,2),$$
$$\gamma_{k+1}^{HTADSS} = 2\frac{f(x_{k+1}) - f(x_k) + \alpha\varphi_k\|g_k\|^2}{\alpha^2\varphi_k^2\|g_k\|^2}, \quad (5)$$

where

$$\varphi_k = t_k(\gamma_k^{-1} - 1) + 1. \quad (6)$$

In relevant papers the authors confirmed good performance profiles and convergence properties of both chosen methods regarding three analyzed metrics: the number of iterations, the CPU time and the number of function evaluations.

3. RESULTS

We now state the goal problem of water resources planning

$$\text{Minimize} \sum_{j=1}^{n} f_j(x_j),$$

subject to:

$$\sum_{j=1}^{n} a_{ij}x_j \geq b_i \quad (i = 1, 2, \ldots, m)$$
$$0 \leq x_j \leq u_j \quad (j = 1, 2, \ldots, n), \quad (7)$$

In problem (6), x_j is the pounds of Biological Oxygen Demand, $f_j(x_j)$ presents the cost of removing x_j pounds of Biological Oxygen Demand at source *j* cost, b_i is the minimum desired improvement in water quality at point *i* in the system, a_{ij} is the quality response, at point *i* in the water system, caused by removing one pound of Biological Oxygen Demand at source *j*, u_j is the maximum pounds of Biological Oxygen Demand that can be removed at source *j*.

Remark 1: *Pounds of Biological Oxygen Demand is an often-used measure of pollution.*

Before we apply the *TADSS* and the *HTADSS* as applicative models for solving problem (6), we first transform this constrained problem into its unconstrained variant

$$\min_{X \in R^n} F^*(x) \equiv F(x) + \lambda P(x) \quad (8)$$

where

$$P(x) = \sum_{i=1}^{n}\left[\max\left(0, b_i - \sum_{j=1}^{n} a_{ij}x_j\right)\right]^2.$$

Remark 2: Obviously, $P(x)=0$ according to conditions from the problem (6)

$$\sum_{j=1}^{n} a_{ij}x_j \geq b_i \Leftrightarrow \sum_{j=1}^{n} a_{ij}x_j - b_i \geq 0, i = \overline{1,n} \Leftrightarrow b_i - \sum_{j=1}^{n} a_{ij}x_j \leq 0, i = \overline{1,n}.$$

We are now able to present merged applicative *TADSS* and *HTADSS* models for removing waste from the water system.

Applicative *TADSS* and *HTADSS* methods

Required: $0 < \rho < 1,\ 0 < \tau < 1, x_0, \gamma_0 = 1.$

1. Set $k=0$, compute $F(x_0), g_0$;
2. If $\|g_k\| < \varepsilon$, go to step 8; else go to step 3;
3. Calculate the step size t_k using the Backtracking algorithm;
4. Compute x_{k+1} using the expression (3) [(5)] and function F^* from (8);
5. Generate the accelerated parameter γ_{k+1} using the expression (4) [(6)] and function F^* from (8);
6. If $\gamma_{k+1} < 0$ or $\gamma_{k+1} > 1$ take $\gamma_{k+1} = 1$;
7. Set $k:=k+1$ and go to step 2;
8. Return x_{k+1} and $F^*(x_{k+1})$.

4. DISCUSSIONS AND CONCLUSIONS

Presented algorithms can be applied for solving the problem of removing waste from the water system. With adequately defined inputs these models can be further numerically tested. With that, a comparative analysis can be conducted between these two algorithms and the efficiency rate can be established. Finally, the research presented in this paper leaves the open space for applying various optimization methods to solve real life problems, especially those that concern environmental issues.

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