

Algorithms for Optimizing Systems with Multiple Extremum Functionals

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Abstract—The problem of minimizing (maximizing) multiple extremum functionals (infinite-dimensional optimization) is considered. This problem cannot be solved by conventional gradient methods. New gradient methods with adaptive relaxation of steps in the vicinity of local extrema are proposed. The efficiency of the proposed methods is demonstrated by the example of optimizing the shape of a hydraulic gun nozzle with respect to the objective functional, which is the average force of the hydraulic pulse jet momentum acting on an obstacle. Two local maxima are found, the second of which is global; in the second maximum, the average force of the jet momentum is three times higher than in the first maximum. The corresponding nozzle shape is optimal. Conventional gradient methods have not found any maximum; i.e., they were unable to solve the problem.

Keywords: infinite-dimensional optimization, optimization methods, gradient, pulse jets

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1. INTRODUCTION

To numerically solve optimization problems for complex systems described by partial derivative equations, it seems appropriate to use the direct optimization approach [1–3]. The essence of this approach is the direct minimization (maximization) of the objective functional by optimization algorithms; the objective functional is

$$J(u) = \int_{\omega} I(v, u) d\omega \rightarrow \min, \quad \omega \subset \bar{\Omega}, \quad (1)$$

$$\text{subject to } \mathbb{D}(\tau, v, u)v = 0, \quad \tau \in \bar{\Omega},$$

where $u(\tau) \in U(S)$ is a control function, $S \subset \bar{\Omega}$, τ is a space-time variable, U is a set of feasible controls, $\bar{\Omega}$ is a closed domain in which the system with the state $v(\tau) \in V(\bar{\Omega})$ operates, and V is the space (admissible set) of system states. The operator \mathbb{D} , which acts on v , includes not only a concrete form of differential equations on Ω but also boundary condition on a part of the boundary $\partial\Omega$. The integrand $I(v(\tau), u(\tau))$ is defined on the set ω , and its value depends on the parameter v and, maybe, on u .

The direct approach does not use any intermediate, e.g., necessary optimality conditions but rather directly solves the problem

$$u_* = \arg \min J(u), \quad (2)$$

where $u_*(\tau)$ is the optimal control providing the global minimum for the functional $J(u)$. Problem (2) is an infinite-dimensional optimization problem because the control u is a function. To solve it, gradient descent methods or conjugate gradient methods generalized to infinite-dimensional spaces are usually used. The convergence of these methods in a finite number of iterations is justified only for finite-dimensional control spaces, when u is a vector and $J(u)$ is a function. Proofs of convergence in such problems are based on the quadratic nature of $J(u)$ or, at least, on its convexity. There are a large number of algorithms for minimizing nonconvex multimodal functions (with varying degrees of justification for convergence), but they cannot be generalized to infinite-dimensional problems.

The conventional gradient methods used in infinite-dimensional spaces have the form

$$u^{k+1}(\tau) = u^k(\tau) - b^k \nabla J^k(u; \tau), \quad \tau \in S, \quad k = 0, 1, \dots, \quad (3)$$

where k is the iteration index and b^k is the step-size factor, which controls the descent depth along the antigradient $-\nabla J^k$. The gradient is calculated using the equations $\mathbb{D}(\tau, v, u)v = 0$. The variety of methods (3) is determined by how the step-size factor b^k for accelerating the convergence to the minimum of $J(u)$ is chosen (see [4–6]).

The generally accepted strategy for choosing the step-size factor b^k is to select it in advance for all iterations:

$$b^k = b > 0 \quad \text{or} \quad b^k = \beta_1(k)b, \quad k = 0, 1, \dots, \quad (4)$$

where $\beta_1(k)$ is a positive function, which is known a priori. This strategy is often used for minimizing convex $J(u)$ [5]. For such optimization problems, this is a relaxation strategy, i.e., it relaxes (decreases) steps such that $\|b^k \nabla J^k\| \xrightarrow{k \rightarrow \infty} 0$ as we get closer to u_* . If we knew the analytical dependence $J(u)$, we could find the optimal b [6]. For this purpose, the knowledge of convexity properties of $J(u)$, such as Lipschitz constant of the gradients or eigenvalues of the Hessian are used. It is clear that such knowledge of the behavior of $J(u)$ can hardly be obtained in the case of infinite-dimensional optimization.

Advantages of this strategy are the minimal effort needed for its implementation and the absence of additional evaluations of J or ∇J at each iteration k . Therefore, this strategy can be efficient only in some particular cases and special initial data.

An open question is how to study and solve optimization problems for nonconvex multiple extremum objective functionals? This paper proposes gradient algorithms based on a specific choice of the step-size factor b^k for studying and solving optimization problems off-line (rather than continuous on-line control) of complex partial derivative systems.

2. ALGORITHMS

Consider the following (second) strategy for choosing b^k that uses the adaptive step relaxation

$$b^k = \beta_2(k)b^{k-1}, \quad k = 1, 2, \dots,$$

where $\beta_2(k)$ is a positive not known a priori function the value of which at each iteration is determined (adapted) on the basis of information about the behavior of $J(u)$ acquired earlier. For example, in the case of minimizing convex $J(u)$, this can be the gradient method (see [1]) of the form

$$\begin{aligned} \text{If } J^k < J^{k-1}, \text{ then: } & b^k = b_1 b^{k-1}, \quad u^{k+1} = u^k - b^k \nabla J^k. \\ \text{Otherwise, repeat until } J^k < J^{k-1}: & \\ & b^{k-1} \leftarrow b_2 b^{k-1}, \quad u^{k+1} = u^{k-1} - b^{k-1} \nabla J^{k-1}, \\ & \text{if } b^{k-1} \approx 0 \text{ then stop on iteration } k. \end{aligned} \quad (5)$$

Here $k = 1, 2, \dots, b_1 \geq 1, b_2 < 1$. The initial value b^0 is specified on the basis of the condition $J^1 < J^0$.

Using the parameter b_1 , algorithm (5) can increase steps and thereby accelerate the convergence to the minimum, and the parameter b_2 can be used to control and prevent the method from diverging due to excessively large steps. The termination condition in the loop of repetitions of the previous step controls looping and an excessive number of too small steps when b^{k-1} decreases. If $b^{k-1} \approx 0$, then we should assume that the process of $J(u)$ minimization has reached its limit. The iterations on k then stop. Obviously, algorithm (5) is, in the general case, more efficient for minimizing functionals than the algorithms described earlier in the first strategy, although it requires additional storage of arrays for u^{k-1} and ∇J^{k-1} in memory.

If $J(u)$ is not convex but has a unique extremum (minimum), then the minimization algorithm (5) should also provide for the possibility of weakening the convergence rate if an increase in the norm of the

gradient is detected (hereinafter, the norm is calculated in L_2). This can be done using the following gradient method:

$$\begin{aligned}
 & \text{If } J^k < J^{k-1}, \text{ then:} \\
 & \quad \cdot \text{ if } \|\nabla J^k\| < \|\nabla J^{k-1}\|, \text{ then } b^k = b_1 b^{k-1}, \\
 & \quad \text{otherwise, } b^k = \frac{\|\nabla J^{k-1}\|}{b_3 \|\nabla J^k\|} b^{k-1}; \\
 & \quad \cdot u^{k+1} = u^k - b^k \nabla J^k. \tag{6} \\
 & \text{Otherwise, repeat until } J^k < J^{k-1}: \\
 & \quad b^{k-1} \leftarrow b_2 b^{k-1}, \quad u^{k+1} = u^{k-1} - b^{k-1} \nabla J^{k-1}, \\
 & \quad \text{if } b^{k-1} \approx 0, \text{ then stop on iteration } k.
 \end{aligned}$$

Here, $b_3 \geq 1$. If $J(u)$ decreases and the gradient norm does not decrease (increases), then this indicates that the current step either fell on the concave part of $J(u)$ or jumped over the local minimum and ended up in the area of increased convexity of $J(u)$. In any case, the next step $b^k \nabla J^k$ should not be greater than the previous one. The size of this step is controlled by the parameter b_3 . You must be careful when choosing $b_3 > 1$, since you can significantly slow down the convergence of the algorithm.

If $J(u)$ is not convex and at the same time has several local extrema, then algorithm (6) should be modified by adapting the parameter b_1 . To ensure that convergence does not end at any physically unsatisfactory local extremum (or you want to check whether other extrema exist), you should approach it with a greater value of b_1 to step over the extremum. And vice versa, in order not to step over the desired extremum, you should approach it carefully, with a reduced b_1 .

The adaptation algorithm of b_1 significantly depends on the specific optimization problem. This procedure requires the painstaking participation of the researcher and is unlikely to be formalized. However, it allows one to study multiple extremum infinite-dimensional optimization problems.

The discussed algorithm for choosing a step-size factor has the form

$$\begin{aligned}
 & \text{If } J^k < J^{k-1}, \text{ then:} \\
 & \quad \cdot \text{ if } \|\nabla J^k\| < \|\nabla J^{k-1}\|, \text{ then} \\
 & \quad \quad \text{(if } u^k \text{ is close to an extremum, then modify } b_1) \quad b^k = b_1 b^{k-1}, \\
 & \quad \text{otherwise, } b^k = \frac{\|\nabla J^{k-1}\|}{b_3 \|\nabla J^k\|} b^{k-1}; \\
 & \quad \cdot u^{k+1} = u^k - b^k \nabla J^k. \\
 & \text{Otherwise, repeat until } J^k < J^{k-1}: \\
 & \quad b^{k-1} \leftarrow b_2 b^{k-1}, \quad u^{k+1} = u^{k-1} - b^{k-1} \nabla J^{k-1}, \\
 & \quad \text{if } b^{k-1} \approx 0, \text{ then stop on iteration } k. \tag{7}
 \end{aligned}$$

There are other strategies for finding b^k involved in the minimization of functionals. For example, there is a linear search strategy at each iteration, which is carried out in two stages. First, an interval is set in the direction $-\nabla J^k$, and then a satisfactory b^k is searched on this interval. Here, the most famous representative is the steepest descent gradient method—this is a complete relaxation strategy, in which at each step along the direction $-\nabla J^k$, the optimal value of the step-size factor is selected on the interval of a given length:

$$b^k = \arg \min_{b>0} J(u^k - b \nabla J^k).$$

This is a remarkable strategy. However, if the control is limited by an admissible set or other specific features of the problem, then selecting an interval containing the minimum of the function $J^k(b)$ can become impossible. Any “endpoint” of an interval that began at the point u^k can go beyond the limits and make solving the equations $\mathbb{D}(\tau, v, u)v = 0$ preposterous.

To elucidate and illustrate the relevance and performance of the proposed algorithms of the second strategy, consider the following example.

3. EXAMPLE

3.1. Statement of the Problem

Let us state the problem of optimal design of a hydraulic gun nozzle the diagram of which is shown in Fig. 1. Piston 2 accelerates under the action of gas in receiver 1 thus pushing water 3 in front of it from a cylindrical barrel into a tapering nozzle 5.

The motion of water in a cylindrical nozzle can be described by the following quasi-one-dimensional quasi-linear hyperbolic system of equations (see [7]):

$$\begin{aligned} \frac{\partial \rho}{\partial t} + w \frac{\partial \rho}{\partial x} + \rho \frac{\partial w}{\partial x} + \frac{\rho w}{\sigma} \frac{d\sigma}{dx} &= 0, \\ \frac{\partial w}{\partial t} + \frac{Bn\rho^{n-2}}{\rho_0^n} \frac{\partial \rho}{\partial x} + w \frac{\partial w}{\partial x} &= 0. \end{aligned} \tag{8}$$

The state of the system is characterized by the vector function $v = \{\rho, w\}$, where ρ is the stream density and w is velocity. This state is determined in the time-spatial domain $\bar{\Omega}$ of water inflow into the nozzle and outflow from it. B and n are constants in the Tait equation of state. The flow control is

$$u(x) = \frac{1}{\sigma(x)} \frac{d\sigma(x)}{dx}, \quad x \in (x_a, x_b), \tag{9}$$

where σ is the nozzle cross section area $\sigma(x) = \sigma_a e^{\int_{x_a}^x u(\zeta) d\zeta}$, $x \in [x_a, x_b]$, and σ_a is the area of the hydraulic gun barrel.

System (8) is an expression for calculating the value of the operator $\mathbb{D}v$ complemented by boundary conditions. The left boundary condition is the equation of the piston motion of mass m_p :

$$\frac{dw}{dt} + \frac{\sigma_a B}{m_p} \left(\left(\frac{\rho}{\rho_0} \right)^n - 1 \right) = 0.$$

On the right boundary, which interacts with the atmosphere, the water density is $\rho = \rho_0 = 10^3 \text{ kg/m}^3$. The initial conditions are $w_0 = 76 \text{ m/s}$, $\rho = \rho_0$. The barrel radius is $R_a = 33 \times 10^{-3} \text{ m}$, the nozzle length is 0.253 m , and the initial length of the water column is 0.28 m .

Let us define the objective functional. We will maximize the mean force of action of the hydraulic pulse jet momentum on the obstacle

$$J = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} \rho \sigma w^2 dt \Big|_{x_b},$$

where t_1 is the beginning of the jet outflow from the nozzle and t_2 is the finite time of jet formation. In particular, $t_1 \approx 2.7 \times 10^{-3} \text{ s}$, and the outflow time is $t_2 - t_1 = 3 \times 10^{-4} \text{ s}$.

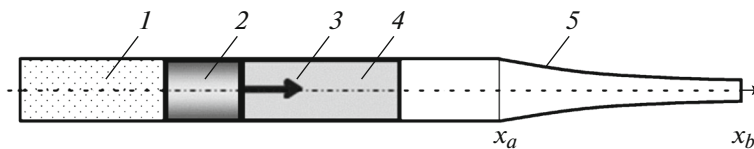


Fig. 1. Scheme of the piston hydraulic gun.

A similar problem was earlier considered in [8, 9] in the framework of the classical variational calculus approach. Various optimality conditions were proposed; however, no optimal nozzle shape was found. Only the use of the optimization approach and the development of adaptive gradient algorithms made it possible to solve this difficult optimization problem.

In what follows, we use the functional J in the form

$$J(u) = \int_{\omega} I(w, u) dt \rightarrow \max, \quad \omega = x_b \times (t_1, t_2), \tag{10}$$

where the integrand is

$$I(w, u)|_{\omega} = \frac{\rho_0 \sigma_b w_b^2}{t_2 - t_1} = \frac{\rho_0 \sigma_a e^{\int_{x_a}^{x_b} u(x) dx} w_b^2}{t_2 - t_1}.$$

Let us determine the domain of control $u(x)$ in more detail—this is the set $S = (x_a, x_b)$, and the nozzle shape $\sigma(x)$ is defined on $[x_a, x_b]$. The range of control is the half-space of admissible values

$$U(S) = \{u : u(x) \leq 0 \quad \forall x \in (x_a, x_b)\} \tag{11}$$

This U corresponds to $\sigma(x) \leq \sigma_a$, which is physically reasonable. We must also take into account one more constraint. In the case of supersonic outflow when $w \geq c_0 = 1475$ m/s, the jet disintegrates. This constraint is not part of the optimization problem statement, but is an indicator of possible unsuccessful optimization.

To directly maximize the objective functional (10), we should find its gradient ∇J . The technique of analytical calculation of the gradient of an implicitly specified functional is a difficult problem in its own right. For this purpose, the approach described in [1] can be used, which we applied in [10]. This gives the following expression for the gradient:

$$\nabla J(u, x) = \int_{t_1}^{t_2} \rho w f_1 dt + \kappa J, \quad x \in (x_a, x_b),$$

where f_1 is the component of the system state adjoint of v and $\kappa = 0.17$ is the weighting coefficient for leveling out the computational noise of the solution to the original nonlinear problem $\mathbb{D}(\tau, v, u)v = 0$ and of the linear adjoint problem on $[x_a, x_b] \times [t_1, t_2] \subset \bar{\Omega}$:

$$\begin{aligned} -\frac{\partial f_1}{\partial t} - w \frac{\partial f_1}{\partial x} - \frac{B n \rho^{n-2}}{\rho_0^n} \frac{\partial f_2}{\partial x} + w u f_1 &= 0, \\ -\frac{\partial f_2}{\partial t} - \rho \frac{\partial f_1}{\partial x} - w \frac{\partial f_2}{\partial x} + \rho u f_1 &= 0. \end{aligned}$$

On the left boundary, we have $f_1 = 0$. On the right, during outflow from t_1 to t_2 , we have $f_1 + \frac{w}{\rho_0} f_2 + \frac{2\sigma_b w_b}{t_2 - t_1} = 0$. The initial (terminal) condition at t_2 is $f_1 = 0, f_2 = 0$. The problem is solved backward in time starting from the zero terminal state.

3.2. Estimation of Convexity of the Objective Functional

To get an idea of the convexity of functional (10), let us consider control in the class of cone functions.

In this case $J(u) = J(R_b)$; i.e., J is a function of the nozzle exit radius R_b , and $\sigma(x) = \pi \left(\frac{R_b - R_a}{x_b - x_a} x + R_a \right)^2$, $R_a = \sqrt{\sigma_a/\pi}$. The resulting function J is shown in Fig. 2.

The right point in the plot corresponds to the nozzle in the shape of a barrel with $R_b = R_a$. The left point in the plot corresponds to the minimum possible nozzle exit at which the outflow is not yet supersonic. Near this point, there is $\max J$ with a large concavity and a very small vicinity of subsonic flow. In the process of changing the radius of the nozzle from the barrel to the minimum permissible narrowing, the functional changes its initial convexity to concavity. Moreover, the concavity is much stronger than the initial convexity.

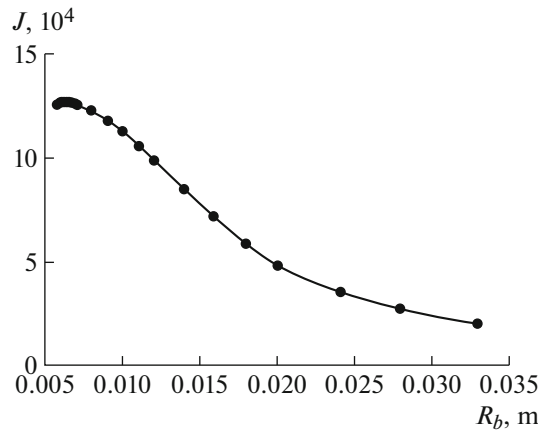


Fig. 2. Dependence of the functional as a function $J(R_b)$.

If we maximize the function $J(R_b)$ starting from $R_b = R_a$ using the classical finite-dimensional gradient method with the first strategy of choosing $b = b^0$, then small initial steps $b\nabla J^k$ are replaced by large steps (due to the growth to the gradient) when moving to the left. Since concavity occurs in a relatively small vicinity of the maximum, large steps can lead to jumping over the extremum until a supersonic outflow appears, which is unacceptable. It may be possible to get to $\max J$ only with a very small b and, naturally, an excessively large number of iteration steps. The use of the steepest descent gradient method, the conjugate gradient method, and other methods using a linear search for the best b^k is impossible here, since such a search, in the general case, will begin with a supersonic outflow.

In this situation, to achieve $\max J$, it is advisable to use method (6) with an adaptive strategy for selecting b^k . We first use this method to practically optimize an arbitrary nozzle shape. The solution to the problem was programmed in Delphi 7, and calculations were carried out on a computer with the Windows performance index 3.5 on a space-time grid 40×500 for less than a minute.

3.3. The First Local Maximum

Let the initial approximation be

$$u^0(x) = 0,$$

which corresponds to the barrel with $\sigma^0(x) = \pi R_a^2$. The initial value of the step-size factor is

$$b^0 = \frac{0.5}{\|\nabla J^0\|},$$

which corresponds to the first step $\|u^1 - u^0\| = 0.5$. First, consider the optimization problem without condition (11) of the nozzle expansion control.

For maximizing $J(u)$, we apply the gradient method (6)

If $J^k > J^{k-1}$, then:

$$\cdot \text{ if } \|\nabla J^k\| < \|\nabla J^{k-1}\|, \text{ then } b^k = b_1 b^{k-1},$$

$$\cdot \text{ otherwise, } b^k = \frac{\|\nabla J^{k-1}\|}{b_3 \|\nabla J^k\|} b^{k-1};$$

$$\cdot u^{k+1} = u^k + b^k \nabla J^k.$$

(12)

Otherwise, repeat until $J^k > J^{k-1}$:

$$b^{k-1} \leftarrow b_2 b^{k-1}, \quad u^{k+1} = u^{k-1} + b^{k-1} \nabla J^{k-1},$$

if $b^{k-1} \approx 0$, then stop on iteration k .

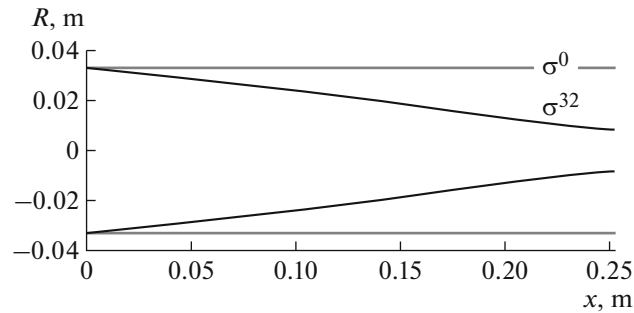


Fig. 3. Optimal nozzle shape in the first extremum.

We fitted the following values of the parameters: $b_1 = 1.05$, $b_2 = 0.3$, $b_3 = 1.05$. Fitting was carried out based on the following considerations: b_1 should be small for a “cautious” approach to the nearest strongly concave extremum; in all calculations, b_2 satisfactorily fulfilled its task with its value 0.3; b_3 is a little greater than unity; otherwise, at greater values, the convergence significantly slowed down, and at $b_3 = 1$, there was too large jump over the first extremum (due to a sharp change in convexity). The iterations were stopped when $\|u^k - u^{k-1}\|/\|u^{k-1}\| \leq 10^{-6}$.

The optimization results are presented in Fig. 3 in the form of the nozzle radius for different areas σ . The optimal nozzle shape turned out to be a cone with the value of the objective functional $J = 1.26 \times 10^5$.

The conventional infinite-dimensional gradient method (3) with a constant step-size factor failed to get into the considered local max J . For $b \gtrsim 10b^0$, the jump over the extremum was accompanied by a supersonic outflow. As b decreased to $10^{-2}b^0$, the convergence was not achieved even after several thousand iterations; uncontrolled expansion of the nozzle was observed after the jump over the local max J .

3.4. The Second Local Maximum

Let us find out whether the first maximum of the objective functional is global. To do this, it is necessary to use method (12), to crudely jump over both the maximum and the minimum nearby behind it to again satisfy the functional growth condition $J^k > J^{k-1}$. Let us increase the steps in the vicinity of the maximum using the parameter b_1 from 1.05 to $b_1 = 1.16$. In this case, we jumped over the local maximum and minimum into the growth region of J ; however, if constraint (11) is not applied, then an unnatural expansion of the nozzle beyond the limits of the hydraulic gun barrel occurs, which leads to the abnormal termination of the calculation of the flow state. Below in Fig. 4, the dotted lines show the intermediate expansion of the nozzle for iteration $k = 41$.

Constraint (11) is easily implemented by projecting the control onto the admissible set U . After executing the step using any adaptive relaxation algorithm, the resulting control u^{k+1} is further adjusted:

$$\text{if } u^{k+1}(x) > 0, \text{ then } u^{k+1}(x) = 0, \quad x \in (x_a, x_b).$$

Further optimization of a bounded nozzle using method (12) and the conventional method (3) with any b^0 , led to a supersonic outflow. For (12), this “failure” means that the parameter b_1 controlling the step increase was unacceptably large, and the possible second local max J was rudely jumped over. Here, instead of method (12), it is necessary to use a method like (7) and reduce b_1 in the vicinity of the expected max J .

The vicinity of the expected maximum can be determined by the outflow velocity $w_b = w(x_b, t)$, $t \in (t_1, t_2)$. It should be close to the speed of sound c_0 . In particular, this speed was assumed to be $w_b > 800$ m/s. If it was exceeded, the step-size enhancement was cancelled, i.e., $b_1 = 1$.

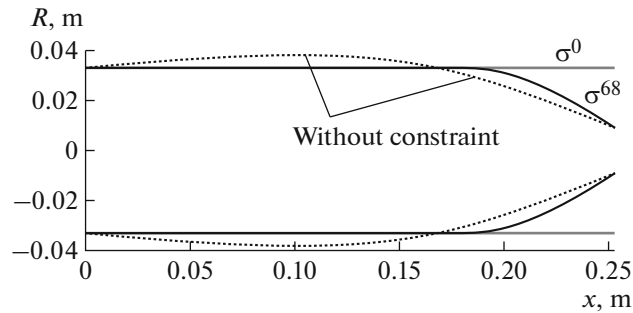


Fig. 4. Optimal nozzle shape in the second extremum.

Method (7) for maximizing the objective functional J is

$$\begin{aligned}
 &\text{If } J^k > J^{k-1}, \text{ then:} \\
 &\cdot \text{ if } \|\nabla J^k\| < \|\nabla J^{k-1}\|, \text{ then} \\
 &\quad (\text{if } w_b > 800, \text{ then } b_1 = 1.0) b^k = b_1 b^{k-1}, \\
 &\quad \text{otherwise, } b^k = \frac{b^{k-1} \|\nabla J^{k-1}\|}{b_3 \|\nabla J^k\|}; \\
 &\cdot u^{k+1} = u^k + b^k \nabla J^k. \\
 &\text{Otherwise, repeat until } J^k > J^{k-1}: \\
 &\quad b^{k-1} \leftarrow b_2 b^{k-1}, \quad u^{k+1} = u^{k-1} + b^{k-1} \nabla J^{k-1}, \\
 &\quad \text{if } b^{k-1} \approx 0, \text{ then stop on iteration } k.
 \end{aligned} \tag{13}$$

The parameters of the method were the same: the initial $b_1 = 1.16, b_2 = 0.3, b_3 = 1.05$.

The solid lines in Fig. 4 show the radius of the nozzle of the obtained optimal area σ^{68} at the last iteration $k = 68$. The “else repeat” block in (13) was triggered only at the end of iterations at $k \geq 66$, which required an additional 12 calculations of J . The value of the objective functional was $J = 3.75 \times 10^5$, i.e. 3 times greater (better) than in the first local maximum.

Therefore, the second local maximum is global, and the corresponding nozzle shape is optimal.

CONCLUSIONS

The proposed gradient methods for minimizing (maximizing) objective functionals, with step-size factors for adaptive relaxation of steps when approaching the extremum made it possible to solve the difficult multiple extremum problem of optimizing the shape of a hydraulic gun nozzle. Two local maxima of the objective functional were identified, which characterizes the mean force of action of the hydraulic pulse jet momentum on the obstacle. The second maximum had a value of the objective functional three times greater (better) than the first one. The resulting nozzle corresponding to the global maximum should be considered optimal. The use of the conventional gradient method did not allow us to find any local extremum of the objective functional. That is, it was not possible to solve the formulated problem by the gradient method with a constant step-size factor, and in all likelihood it is impossible.

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CONFLICT OF INTEREST

The author declares that he has no conflicts of interest.

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