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# A globalization strategy for the multigrid solution of elliptic optimal control problems

A. BORZÌ* and K. KUNISCH

Institut für Mathematik und Wissenschaftliches Rechnen, Karl-Franzens-Universität Graz, Heinrich str. 36, A-8010 Graz, Austria

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A globalization strategy for multigrid schemes solving optimal control problems is presented. This approach searches for possible negative eigenvalues of the reduced Hessian considered at the coarsest grid of the multigrid process. If negative eigenvalues are detected, a globalization step in the direction of negative curvature is performed to escape undesired maxima or saddle points. It is shown that the multigrid solution step provides a descent update. Examples are given to illustrate and validate the present approach.

*Keywords*: Optimal control problems; Globalization strategy; Multigrid methods

*AMS*: 49K20; 65N55; 90C30

## 1. Introduction

Recent results [1,2,3,6] give evidence that multigrid methods solve optimality systems with optimal computational complexity. Optimality systems represent first-order necessary conditions for minimization problems subject to differential equations as equality constraints. In a convex setting where the optimal control solution is unique, solving the optimality system is equivalent to solving the optimal control problem. However, in general, these solutions represent only extremal points and additional conditions must be satisfied to guarantee that they are the minima sought. Q1

Our purpose is to formulate fast solvers for optimal control problems that possibly have multiple extremal points. Our approach combines fast multigrid schemes for solving optimality systems [1,2,3,6] with a negative-curvature update introduced to solve global unconstrained minimization problems [see for example refs. 7,12,14].

In the following section optimal control problems are formulated that allow for multiple extremal points satisfying the first-order necessary optimality conditions. In section 3, second-order sufficient conditions for a minimum are discussed in terms of the reduced Hessian and the related eigenvalue problem. The presence of nonpositive eigenvalues indicates possible

*Corresponding author. Email: alfio.borzi@uni-graz.at

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maxima or saddle points. We use the eigenvector corresponding to the negative eigenvalue with largest absolute value to define a globalization step along the direction of negative curvature to escape undesired maxima or saddle points. This step is performed at the coarsest grid of a multigrid scheme for solving the optimality system. The resulting globalized multigrid algorithm is defined in section 4. Further optimization properties of the multigrid scheme are discussed in section 5.

To determine the negative eigenvalue of the reduced Hessian we propose a power method approach in section 6. An example is worked out to further illustrate and validate the approach proposed in this paper. Implementation details are given in the Appendix A. A section of conclusion completes the exposition of the work.

## 2. Optimal control problems

We consider the optimal control problem

$$\begin{cases} \min\limits_{u \in U} J(y, u), \\ e(y, u) = 0 \text{ in } \Omega, \end{cases} \tag{1}$$

where $y$ and $u$ denote the state- and control variables of a controlled partial differential equation expressed as $e(y, u) = 0$, with $e$: $Y \times U \to Z$ for appropriate Hilbert spaces $Y$, $U$, and $Z$. $\Omega$ is an open bounded set in $\mathbb{R}^d$. The cost functional $J$ is formally given by

$$J(y, u) = h(y) + \nu g(u), \tag{2}$$

where $\nu > 0$ is the weight of the cost of the control. Here, $g$ and $h$ are required to be continuously differentiable, bounded from below, and such that $g(u) \to \infty$ as $||u|| \to \infty$. Allowing $g$ and $h$ to be locally nonconvex and $e$ to be possibly nonlinear, problem (1) may have multiple extremals including minima, maxima, and saddle points.

Local minima satisfy the first-order necessary conditions. To define these conditions consider the Lagrangian

$$L(y, u, p) = J(y, u) + \langle e(y, u), p \rangle_{Z,Z^*},$$

where $p$ is the Lagrange multiplier, in the following referred to as the adjoint variable. By equating to zero the Frechét derivatives of $L$ with respect to the triple $(y, u, p)$, we obtain the following optimality system

$$\begin{aligned} e(y, u) &= 0, \\ e_y(y, u)^* p &= -h'(y), \\ \nu g'(u) + e_u^* p &= 0. \end{aligned} \tag{3}$$

Numerical approximations to solutions of system (3) can be obtained, after discretization, using multigrid or other iterative methods starting from any initial guess. The particular choice of the starting approximation determines towards which solution the iterative scheme will converge. Solutions to system (3) are not necessarily local minima, rather they are extremal points.

Our purpose is to introduce in the multigrid scheme a mechanism allowing to distinguish among different types of extremal points and providing the direction for escaping undesired maxima and saddle points.

## 3. Second-order conditions for a minimum

If $J$ and $e$ are twice continuously differentiable, the second-order sufficient conditions for a minimum are given by the optimality system (3) and the following

$$L_{xx}(y, u, p)(v, v) \geq c_1 \|v\|^2, \quad c_1 > 0, \text{ for all } v \in \mathcal{N}(e'(y, u)), \tag{4}$$

where $x = (y, u)$ and $e'$ represents the linearized equality constraint [see for example ref. 6]. We assume that the null space $\mathcal{N}(e'(y, u))$ can be represented by $\mathcal{N}(e'(y, u)) = T(y, u)\, U$, where

$$T(y, u) = \begin{bmatrix} -e_y^{-1} e_u \\ I_u \end{bmatrix},$$

and $e_y$, $e_u$ are evaluated at $(y, u)$. Therefore, condition (4) becomes

$$H(y, u, p)(w, w) \geq c_2 \|w\|^2, \quad c_2 > 0, \tag{5}$$

for all $w \in U$. The operator $H$ is the reduced Hessian defined by

$$H(y, u, p) = T(y, u)^* L_{xx}(y, u, p)\, T(y, u).$$

That is, $H$ is given by

$$H(y, u, p) = L_{uu}(y, u, p) + C(y, u)^* L_{yy}(y, u, p) C(y, u), \tag{6}$$

where $C(y, u) = e_y(y, u)^{-1} e_u(y, u)$, assuming $e_{yu}(y, u) = 0$.

Notice that $H$ is symmetric. Therefore condition (5) requires that, in order to have a minimum, all eigenvalues of the reduced Hessian be positive. Otherwise, the occurrence of nonpositive eigenvalues indicates the presence of possible maxima or saddle points. Thus, in principle, once a solution to system (3) is found, one should solve the eigenvalue problem associated to $H$. If all eigenvalues are positive, we have a minimum and therefore a solution to problem (1). If some eigenvalues are negative, the solution of the optimality system is not a solution to the optimal control problem.

Clearly, in an infinite dimensional setting, the analysis of the spectrum of $H$ may be an overwhelming task. Even after discretization, solving the eigenvalue problem may be computationally more expensive than solving the optimality system.

The multigrid strategy provides a way to overcome this difficulty. A successful multigrid procedure is based on a hierarchy of discrete equations able to represent, at different scales, the underlying continuous problem. In the present work, we make the assumption that spectral properties of the reduced Hessian are well represented on the hierarchy of grids. Subsequently, the globalization strategy is based on the spectral properties of the Hessian $H$ on the coarsest grid. In case negative eigenvalues of the reduced Hessian are detected, we use the eigenvector corresponding to the smallest eigenvalue to determine an escape direction. This direction of negative curvature [12,14] is given by the eigenvector corresponding to the negative eigenvalue with largest absolute value. The implementation of this globalization step within a multigrid framework is subject of the next section.

In the earlier discussion, we tacitly assumed that the spectrum of the Hessian before discretization also consists of pure point-spectrum. This is the case, for example, if $e_y^{-1}$ is a compact operator corresponding to the case of elliptic- or parabolic-type partial differential equations and $g(u) = \frac{1}{2}\|u\|^2$. A similar remark applies, for example, for the choice $g(u) = \frac{1}{2}\|\nabla u\|^2$. In either of these two cases, the resulting reduced Hessian is such that its spectrum can be well represented in a hierarchy of grids.

## 4. Globalization and the full approximation storage multigrid scheme

We formulate a globalization procedure within the multigrid full approximation storage (FAS) scheme [5]. The present approach remains valid for the class of nonlinear multigrid (NMGM) methods discussed in ref. [8]. The choice of FAS or NMGM schemes is motivated by the general applicability of these schemes to linear and nonlinear problems and by the fact that the optimal control variables and not the corresponding errors are represented at all levels of the multigrid process. This is needed in order to define (6) on coarser levels.

Our globalized multigrid approach relies on two features. First, we define the FAS multigrid procedure such that it provides a descent step for the optimal control constrained minimization problem. Secondly, on the coarsest grid we analyze the possible encounter of extremal points that are not minima and define an escape direction, if necessary, on the basis of negative-curvature eigenvectors.

To guarantee a multigrid step which is minimizing, we define the smoothing process based on the gradient of the reduced cost functional and show that the FAS coarse-grid correction step provides a descent update. We postpone the discussion on the optimization properties of the proposed FAS approach to the following section.

In order to define our multigrid solution process consider a sequence of grids $\{\Omega_h\}_{h>0}$ and denote the operators and variables defined on the grid with mesh size $h = h_k = h_0/2^k$, $k = 1, \ldots, M$, with index $k$. On the grid $\Omega_h, h = h_k$, the optimality system (3) is represented by

$$\begin{aligned} e(y_h, u_h)_h &= 0, \\ e_y(y_h, u_h)_h^* p_h &= -h'(y_h), \\ \nu g'(u_h) + e_u^* p_h &= 0. \end{aligned} \tag{7}$$

In general, an initial approximation to the solution of this problem will differ from the exact solution because of errors involving high-frequency as well as low-frequency components. In order to reduce all frequency components of the error, the multigrid strategy combines two complementary schemes. The high-frequency components of the error are reduced by smoothing iterations, whereas the low-frequency error components are effectively reduced by a coarse-grid correction method.

The smoothing iteration $S$ used is a Gauss–Seidel scheme which belongs to the class of collective relaxations [see refs. 2, 3]. A Gauss–Seidel step at $\mathbf{x} \in \Omega_h$ consists in updating the values $y$, $u$, and $p$ such that the resulting residual of the optimality system at that point is zero. The neighboring variables related to the stencils of the operators involved are considered constant during this process. That is, the state equation in system (7) provides $y_h(\mathbf{x})$ as function of $u_h(\mathbf{x})$ at the grid point. Replacing $y_h$ in the adjoint equation by this function, we obtain $p(\mathbf{x})$ as function of $u(\mathbf{x})$. From these considerations, the optimality condition becomes

$$\nu g'(u_h) + e_u^* p_h(u_h) = 0. \tag{8}$$

This equation corresponds to requiring that the gradient of the reduced cost functional $J(y(u), u)$ with respect to the control variable $u$ is zero. Therefore in order to update the control function in the smoothing process, we use condition (8) to perform a few steps of the following descent scheme (compare with ref. [1])

$$u_h^{\text{new}} = u_h - \beta(\nu g'(u_h) + e_u^* p_h(u_h)). \tag{9}$$

An optimal choice of the scaling factor $\beta > 0$ may be done using line search methods. However, for our purpose we choose $\beta = 10^{-2}/\sqrt{\nu}$ and apply (9) at most 10 times. After each step we

check whether $J(y(u_h^{\text{new}}), u_h^{\text{new}})_h \leq J(y(u_h), u_h)_h$ is satisfied; if not, we keep the previous update of $u_h$ and stop iterating. With the new value of $u$ given, new values for $y$ and $p$ are obtained. This completes the Gauss–Seidel step. For more details we refer to the Appendix A where a formal algorithm of the smoothing process is given.

Once the smoothing iteration has reduced the rough components of the error, a coarse-grid correction is performed to correct for the components of the error which are smooth. First, a coarse-grid problem is constructed on the grid with mesh size $H = h_{k-1}$. That is,

$$\begin{aligned} e(y_H, u_H)_H &= \tau(y)_h^H, \\ e_y(y_H, u_H)_H^* p_H + h'(y_H) &= \tau(p)_h^H, \\ \nu g'(u_H) + e_u^* p_H &= 0, \end{aligned} \tag{10}$$

where $\tau(y)_h^H$ and $\tau(y)_h^H$ are fine-to-coarse defect corrections defined by

$$\tau(y)_h^H = e(\hat{I}_h^H y_h, \hat{I}_h^H u_h)_H - I_h^H(e(y_h, u_h)_h), \tag{11}$$

$$\tau(p)_h^H = e_y(\hat{I}_h^H y_h, \hat{I}_h^H u_h)_H^* \hat{I}_h^H p_h + h'(\hat{I}_h^H y_h) - I_h^H(e_y(y_h, u_h)_h^* p_h + h'(y_h)). \tag{12}$$

Here $I_h^H\colon L_h^2 \to L_H^2$ denotes a restriction operator and $\hat{I}_h^H\colon L_h^2 \to L_H^2$ another restriction operator not necessarily equal to $I_h^H$. We choose $I_h^H$ to be full-weighting [16] and $\hat{I}_h^H$ to be straight injection. Once the coarse-grid problem is solved, the coarse-grid correction follows

$$y_h^{\text{new}} = y_h + I_H^h(y_H - \hat{I}_h^H y_h), \tag{13}$$

$$u_h^{\text{new}} = u_h + I_H^h(u_H - \hat{I}_h^H u_h), \tag{14}$$

$$p_h^{\text{new}} = p_h + I_H^h(p_H - \hat{I}_h^H p_h), \tag{15}$$

where $I_H^h\colon L_H^2 \to L_h^2$ represents an interpolation operator. Assuming the high-frequency components of the error on the finer grid are well damped by applying $m_1$ pre-smoothing iteration, then the grid $\Omega_H$ should provide enough resolution for the pre-smoothed error. On the coarse grid this error is approximated by $(w_H - \hat{I}_h^H w_h)$ with $w = (y, u, p)$ in corrections (13), (14), and (15). This idea of transferring the problem to be solved to a coarser grid can be applied along a set of nested meshes. Once the coarsest grid is reached, one solves the coarsest problem to convergence by applying, as we do, a few steps of the smoothing iteration. The solution obtained on each grid is then used to correct the approximation on the next finer grid. The coarse-grid correction followed by $m_2$ post-smoothing steps is applied from one grid to the next, up to the finest grid with level $M$. This entire process represents one $V(m_1, m_2)$ cycle of the FAS multigrid process.

In the process described earlier we apply the globalization step at the coarsest grid. At the coarsest level, a convergence check is performed after each smoothing step. Only after this check is passed globalization sets in. In this case an algorithm is called that determines the negative eigenvalue with largest modulus. If such an eigenvalue exists, the normalized eigenvector $\phi_h$ corresponding to the negative eigenvalue with largest absolute value is used to perform the following globalization step

$$u_h^{\text{new}} = u_h - \sigma\phi_h. \tag{16}$$

We choose $|\sigma| = \sqrt{\beta}$ (with $\beta$ as in scheme (9); see ref. [14]) and the sign of $\sigma$ is such that $\sigma\phi_h \cdot (\nu g'(u_h) + e_u^* p_h(u_h)) \geq 0$. Then, the multigrid procedure continues as described.

To summarize the procedure outlined earlier let us express the optimality system by $A_k(w_k) = f_k$, where $w_k = (y_k, u_k, p_k)$. Recall that the multigrid scheme can be interpreted

as an iteration of the type $w^l = w^{l-1} + B_M\,(f_M - A_M(w^{l-1}))$, where $B_k$ is the multigrid iteration operator at level $k$.

The recursive form of the $V(m_1, m_2)$-cycle FAS multigrid algorithm is given as follows:

**FAS multigrid $V(m_1, m_2)$-cycle with globalization step**
Set $B_1 \approx A_1^{-1}$ by iterating with $S_1$ and if $||\text{res}|| < \text{tol}$ perform the globalization step (16).
For $k = 2, \ldots, M$, define $B_k g$ in terms of $B_{k-1}$ as follows.

(i) Set $w_k^{(0)} = \tilde{w}_k$ (starting approximation).
(ii) Smoothing. Define $w_k^{(l)}$ for $l = 1, \ldots, m_1$, by

$$w_k^{(l)} = S_k(w_k^{(l-1)}, f_k).$$

(iii) Coarse grid correction. Set $w_k^{\text{new}} = w_k^{(m_1)} + I_{k-1}^k(q_{k-1} - \hat{I}_k^{k-1} w_k^{(m_1)})$ where $q_{k-1}$ is defined by

$$q_{k-1} = B_{k-1}\left[I_k^{k-1}(f_k - A_k(w_k^{(m_1)})) + A_{k-1}(\hat{I}_k^{k-1} w_k^{(m_1)})\right].$$

(iv) Set $B_k f_k = w_k^{(m_1+m_2+1)}$ where $w_k^{(\ell)}$ for $\ell = m_1 + 2, \ldots, m_1 + m_2 + 1$, is given by step (ii) with $w_k^{(m_1+1)} = w_k^{\text{new}}$.

In the following section, we discuss the optimization properties of the FAS multigrid scheme described earlier.

## 5. Optimization properties of the FAS scheme

Although the focus in this paper lies on the globalization of the multigrid approach, we digress in this section to give an interpretation of the FAS multigrid step as a descent step. Instead of describing the multigrid process as a method that efficiently reduces all frequency components of the error of an initial approximation to the required solution, we consider the multigrid solution step from an optimization point of view. Earlier contribution in this direction can be found in refs. [10,13]. These investigations consider nonlinear multigrid methods as minimization procedures for unconstrained optimization problems only.

Let us consider the case where $e(y_h, u_h)_h = -\Delta_h y_h - u_h$ and $h(y) = ||y - z||^2_{L^2(\Omega)}/2$, and assume that $g'$ is Lipschitz continuous with Lipschitz constant $\gamma > 0$, and satisfies the following monotonicity requirement

$$(g'(u) - g'(v), u - v) \geq \delta \|u - v\|^2_{L^2(\Omega)},$$

for some $\delta > 0$.

We start our discussion with some comments on the proposed smoothing iteration. Consider a given initial approximation for the control function. In correspondence, assume to solve the state and the adjoint equations exactly. Then, step (9) provides an update for the control which provides a decay. In our case, this process is actually performed at each grid point where solving exactly for the state and adjoint variables reduces to a simple algebraic manipulation. The result is a minimization of the cost functional with respect to the variables defined on the grid point. This smoothing step belongs to the class of successive subspace correction (SSC) methods discussed in ref. [15].

Uniform convergence rates for the SSC iteration applied to a convex functional $F(u)$ are proven in ref. [15] assuming that $F$ is Gateaux differentiable and that there exist constants $K, L > 0$, $p \geq q > 1$, such that

$$\langle F'(u) - F'(v), w - v\rangle \geq K\|u - v\|_V^p, \tag{17}$$

$$\|F'(u) - F'(v)\|_{V'} \leq L\|u - v\|_V^{q-1}, \tag{18}$$

for all $u, v \in V$, and $\langle \cdot, \cdot \rangle$ is the duality pairing between $V$ and its dual space $V'$.

We show that equations (17) and (18) are satisfied by the reduced functional $\hat{J}(u_h)_h = J(y_h(u_h), u_h)_h$ considered here with $\hat{J}'(u_h)_h$ given by

$$\hat{J}'(u_h)_h = \nu g'(u_h) - p_h(u_h) \quad \text{and} \quad p_h(u_h) = -\Delta_h^{-1}(\Delta_h^{-1}u_h + z_h).$$

Here $u_h \in L_h^2(\Omega_h)$, where $L_h^2$ denotes the discrete $L^2$ space of grid functions defined on $\Omega_h$. For grid functions $u_h$ and $v_h$ defined on $\Omega_h$ we use the discrete $L^2$-scalar product

$$(u_h, v_h)_h = h^2 \sum_{\mathbf{x}\in\Omega_h} u_h(\mathbf{x})\, v_h(\mathbf{x}),$$

with associated norm $\|u_h\|_h = (u_h, u_h)_{L_h^2}^{1/2}$.

Now consider equation (17). We have

$$\begin{aligned}
(\hat{J}'(u_h)_h - \hat{J}'(v_h)_h, u_h - v_h)_h &= (\nu g'(u_h) - p_h(u_h) - \nu g'(v_h) + p_h(v_h), u_h - v_h)_h \\
&= \nu(g'(u_h) - g'(v_h), u_h - v_h)_h - (p_h(u_h) - p_h(v_h), u_h - v_h)_h \\
&= \nu(g'(u_h) - g'(v_h), u_h - v_h)_h + (\Delta_h^{-2}(u_h - v_h), u_h - v_h)_h \\
&\geq \nu\delta\, \|u_h - v_h\|_h^2.
\end{aligned}$$

The next step is to show equation (18), as follows

$$\begin{aligned}
\|\hat{J}'(u_h)_h - \hat{J}'(v_h)_h\|_h &= \|\nu g'(u_h) - p_h(u_h) - \nu g'(v_h) + p_h(v_h)\|_h \\
&= \|\nu(g'(u_h) - g'(v_h)) - (p_h(u_h) - p_h(v_h))\|_h \\
&\leq \nu\|g'(u_h) - g'(v_h)\|_h + \|\Delta_h^{-2}(u_h - v_h)\|_h \\
&\leq (\nu\gamma + c)\, \|u_h - v_h\|_h,
\end{aligned}$$

where $c > 0$ is defined by the inequality $\|\Delta_h^{-2}u_h\|_h \leq c\|u_h\|_h$ [see ref. 9]. Therefore, the smoothing iteration (9) provides a minimizing sequence.

Next, we show that the FAS coarse-grid correction provides a descent direction in the sense that

$$(\nu g'(u_h) - p_h, I_H^h(u_H - \hat{I}_h^H u_h))_h < 0,$$

unless $u_H = \hat{I}_h^H u_h$, occurring at convergence.

Starting from an initial approximation and after a few pre-smoothing steps the resulting triple $(y_h, u_h, p_h)$ satisfies the optimality system up to residuals $(d_h^1, d_h^2, d_h^3)$, i.e.,

$$\begin{aligned}
-\Delta_h y_h - u_h &= d_h^1, \\
-\Delta_h p_h + y_h - z_h &= d_h^2, \\
\nu g'(u_h) - p_h &= d_h^3.
\end{aligned} \tag{19}$$

For the coarse-grid process, we take $\hat{I}_h^h = I_h^H$ where $I_h^H$ is the full-weighting restriction operator. For $I_H^h$ we choose bilinear interpolation which is the adjoint of the restriction operator just defined in ref. [8], i.e., $(I_h^H u_h, v_H)_H = (u_h, I_H^h v_H)_h$. We define $z_H = I_h^H z_h$. With this setting, we obtain the following coarse-grid FAS equations

$$\begin{aligned} -\Delta_H y_H - u_H &= I_h^H \Delta_h y_h - \Delta_H I_h^H y_h, \\ -\Delta_H p_H + y_H - z_H &= I_h^H \Delta_h p_h - \Delta_H I_h^H p_h, \\ \nu g'(u_H) - p_H &= 0. \end{aligned} \tag{20}$$

As usual in two-grid convergence analysis, we assume that this coarse system of equations is solved exactly. From the first equation of (20), and using the corresponding equation in (19) we obtain

$$u_H - I_h^H u_h = -\Delta_H (y_H - I_h^H y_h) + I_h^H d_h^1. \tag{21}$$

Combining the fine and coarse adjoint equations, we have

$$p_H - I_h^H p_h = \Delta_H^{-1}(y_H - I_h^H y_h) + \Delta_H^{-1} I_h^H d_h^2. \tag{22}$$

Let us assume that

$$(g'(v_H) - I_h^H g'(v_h), v_H - I_h^H v_h)_H \geq \delta' \|v_H - I_h^H v_h\|_H^2, \tag{23}$$

for some $\delta' > 0$ independent of $v_h$ and $v_H$. Note that equation (23) is satisfied, for example, if $g'$ is linear or if $I_h^H$ is strict injection and $g$ is strictly convex.

With these preparations, we are ready to show that the update step of the FAS coarse-grid correction follows a descent direction

$$\begin{aligned} &(\nu g'(u_h) - p_h, I_H^h(u_H - I_h^H u_h))_h \\ &\quad = (I_h^H(\nu g'(u_h) - p_h), u_H - I_h^H u_h)_H \\ &\quad = (\nu I_h^H g'(u_h) - I_h^H p_h, u_H - I_h^H u_h)_H \\ &\quad = (\nu I_h^H g'(u_h) - p_H + \Delta_H^{-1}(y_H - I_h^H y_h) + \Delta_H^{-1} I_h^H d_h^2, u_H - I_h^H u_h)_H \\ &\quad = -\nu(g'(u_H) - I_h^H g'(u_h), u_H - I_h^H u_h)_H + (\Delta_H^{-1}(y_H - I_h^H y_h) + \Delta_H^{-1} I_h^H d_h^2, \\ &\qquad - \Delta_H (y_H - I_h^H y_h) + I_h^H d_h^1)_H \\ &\quad = -\nu(g'(u_H) - I_h^H g'(u_h), u_H - I_h^H u_h)_H - (y_H - I_h^H y_h, y_H - I_h^H y_h)_H \\ &\qquad + (\Delta_H^{-1}(y_H - I_h^H y_h), I_h^H d_h^1)_H - (\Delta_H^{-1} I_h^H d_h^2, \Delta_H (y_H - I_h^H y_h))_H + (\Delta_H^{-1} I_h^H d_h^2, I_h^H d_h^1)_H \\ &\quad \leq -\nu(g'(u_H) - I_h^H g'(u_h), u_H - I_h^H u_h)_H + \frac{1}{2}(\|\Delta_H^{-1} I_h^H d_h^1\|_H^2 + \|\Delta_H^{-1} I_h^H d_h^2\|_H^2 \\ &\qquad + \|I_h^H d_h^1\|_H^2 + \|I_h^H d_h^2\|_H^2) \\ &\quad \leq -\nu\delta' \|u_H - I_h^H u_h\|_H^2 + \frac{1}{2}(\|\Delta_H^{-1} I_h^H d_h^1\|_H^2 + \|\Delta_H^{-1} I_h^H d_h^2\|_H^2 + \|I_h^H d_h^1\|_H^2 + \|I_h^H d_h^2\|_H^2). \end{aligned}$$

Therefore

$$(\nu g'(u_h) - p_h, I_H^h(u_H - I_h^H u_h))_h < 0,$$

if equation (23) holds and the residuals $d_h^1$ and $d_h^2$ are sufficiently small.

Finally, we show that the coarse-grid correction step does not produce over-shooting in the sense that $(\hat{J}'(u_h)_h, \hat{J}'(u_h^{\text{new}})_h)_h \geq 0$. We consider the case where $g'(u) = u$. We have the following

$$\begin{aligned}(\hat{J}'(u_h)_h, \hat{J}'(u_h^{\text{new}})_h)_h &= (\nu u_h - p_h, \nu(u_h + I_H^h(u_H - I_h^H u_h)) - (p_h + I_H^h(p_H - I_h^H p_h))_h \\ &= \|\nu u_h - p_h\|_h^2 + (\nu u_h - p_h, I_H^h[\nu(u_H - I_h^H u_h) - (p_H - I_h^H p_h)])_h \\ &= \|\nu u_h - p_h\|_h^2 - \|I_h^H(\nu u_h - p_h)\|_H^2 \geq 0,\end{aligned}$$

where we use $\|I_h^H\| \leq 1$.

## 6. A power method approach

To establish the existence and to compute the negative eigenvalue of $H$ with largest absolute value, we use a power method-based scheme [see for example ref. 17]. This choice is suggested by the particular structure of the reduced Hessian as given in (6) and by the fact that the power scheme requires only $H$ times vector multiplication as described in the following.

Suppose $A \in \mathbb{R}^{n\times n}$ is diagonalizable (recall that symmetric matrices are diagonalizable) and that $X^{-1}AX = \text{diag}(\gamma_1, \ldots, \gamma_n)$ with $X = [x_1, \ldots, x_n]$ the matrix of eigenvectors of $A$ and $|\gamma_1| > |\gamma_1| \geq \cdots \geq |\gamma_n|$. Given $v^{(0)} \in \mathbb{R}^n$, the power method defines a sequence $v^{(k)}$ as follows

$$\begin{aligned}&\text{for } k = 1, 2, \ldots \\ &\qquad z^{(k)} = Av^{(k-1)} \\ &\qquad \gamma^{(k)} = z_i^{(k)} \text{ where } |z_i^{(k)}| = ||z^{(k)}||_{\max} \\ &\qquad v^{(k)} = \frac{z^{(k)}}{\gamma^{(k)}} \\ &\text{end}\end{aligned} \tag{24}$$

If the starting vector is a linear combination of eigenvectors of $A$, $v^{(0)} = \sum_{i=1}^n a_i x_i$ with $a_1 \neq 0$, then $v^{(k)} \to x_1$ and $\gamma^{(k)} \to \gamma_1$ for $k \to \infty$.

We apply the power method twice. First, we take $A = H$ and compute an estimate of the eigenvalue of largest absolute value of the reduced Hessian, denoted by $\bar{\mu}$. If $\bar{\mu} < 0$, it is the sought eigenvalue and the corresponding eigenvector is used for the globalization step. Otherwise, we take $A = -H + \bar{\mu} I$ and use the power method to get $-\mu + \bar{\mu}$ where $\mu$ is the smallest eigenvalue of $H$. If $\mu < 0$, it is the negative eigenvalue with largest absolute value, which will be used for the globalization step (16). If $\mu > 0$, no globalization is required.

To illustrate the procedure described earlier and at the same time clarify limitations posed by the discretization, we discuss the following example. Consider problem (1) where $e(y, u) = -\Delta y - u$, with Dirichlet boundary conditions, $u \in L^2(\Omega)$, $\Omega \subset \mathbb{R}^2$, $h(y) = \frac{1}{2}||y||_{L^2(\Omega)}^2$, and $g(u) = -||u||_{L^2(\Omega)}^2 + ||u||_{L^2(\Omega)}^4$. With this setting, the reduced cost can be expressed

as $J(y(u), u) = \frac{1}{2}|| - \Delta^{-1}u||^2_{L^2(\Omega)} + \nu(-||u||^2_{L^2(\Omega)} + ||u||^4_{L^2(\Omega)})$, and the reduced Hessian at $(y(u), u, p(u))$ with $u = 0$ is given by

$$H(y, u, p) = -2\nu I + \Delta^{-1}\,\Delta^{-1}. \tag{25}$$

The eigenvalues $\mu_l$ of $H(y, u, p)$ and $\lambda_l$ of $-\Delta$ with Dirichlet boundary conditions are related by

$$\mu_l = -2\nu + \frac{1}{\lambda_l^2}. \tag{26}$$

It follows that $u = 0$ is a local maximum provided that $\nu > 1/(2\lambda_1^2)$, where $\lambda_1$ is the smallest eigenvalue of $-\Delta$.

Notice that in a discrete setting the largest eigenvalue of the negative Laplacian is finite and of order $\lambda_{\max} \approx c/h^2$. Therefore equation (26) shows that, on a given grid, if $\nu < 1/(2\lambda^2_{h,\max})$ then $\mu_l > 0$ for all $l$, which not only misses to detect the maximum, but in fact characterizes a local minimum at $u = 0$ for the discretized cost. This occurrence has no correspondence in the continuous case where for any small $\nu$ there exists $\bar{l}$ such that $\mu_l < 0$ for $l \geq \bar{l}$.

In a multigrid context, these considerations suggest that a sufficiently fine mesh for the coarsest grid must be chosen in order to properly represent optimal control problems of the type considered here. To further illustrate the problem of estimating correctly the smallest eigenvalue of $H$ on coarse grids, consider the problem related to (25) defined on $\Omega = (0, 1) \times (0, 1)$, discretized by finite differences on a uniform grid with mesh size $h$. We report in table 1 the value of the smallest eigenvalue $\mu$ for different choices of the mesh size $h$ and of the weight $\nu$. Negative values of $\mu$ indicate that $u = 0$ is not a minimum. This expectation can fail if the mesh is too coarse.

From equation (6) we note that each iteration step of the power method requires to solve two problems of the type $e_y(y, u)\, v = f$. For example, with $H$ given by equation (25) we need solve two Poisson problems. Namely, for the first step in (24) we have the following

$$v^{(k-1)} \longrightarrow w^{(k-1)} = (-\Delta)^{-1}\, v^{(k-1)} \longrightarrow s^{(k-1)} = (-\Delta)^{-1} w^{(k-1)}$$
$$\longrightarrow z^{(k)} = -2\nu v^{(k-1)} + s^{(k-1)}.$$

The solution of the intermediate boundary value problems can be obtained using any iterative scheme. Because we solve eigenvalue problems only on coarse grids, it suffice to use simple SOR iteration with optimal relaxation parameter $\omega = 2/(1 + \sin \pi h)$ [see for example ref. 16].

Table 1. The smallest eigenvalue $\mu$ of equation (25).

| $\nu$ | $h = 1/4$ | $h = 1/8$ | $h = 1/16$ | $h = 1/32$ |
|---|---|---|---|---|
| $10^{-2}$ | $-1.99 \times 10^{-2}$ | $-1.99 \times 10^{-2}$ | $-1.99 \times 10^{-2}$ | $-2.00 \times 10^{-2}$ |
| $10^{-4}$ | $-1.16 \times 10^{-4}$ | $-1.95 \times 10^{-4}$ | $-1.99 \times 10^{-4}$ | $-1.99 \times 10^{-4}$ |
| $10^{-6}$ | $8.17 \times 10^{-5}$ | $2.12 \times 10^{-5}$ | $-1.75 \times 10^{-5}$ | $-1.99 \times 10^{-5}$ |
| $10^{-8}$ | $8.37 \times 10^{-5}$ | $4.10 \times 10^{-5}$ | $2.23 \times 10^{-6}$ | $-5.02 \times 10^{-9}$ |

## 7. An example

To illustrate the effectiveness of the globalization strategy presented in the previous sections, consider the following optimal control problem

$$\begin{cases} \min\limits_{u\in\mathbb{R}^2} \dfrac{1}{2}||y-z||^2_{L^2(\Omega)} + \nu g(u), \\ -\Delta y = Du \text{ in } \Omega, \\ y = 0 \text{ on } \partial\Omega, \end{cases} \tag{27}$$

where $z \in L^2(\Omega)$ is a desired target function. Here, the control space consists of a two-component vector $u = (u_1, u_2)$ and the operator $D$ is defined by

$$Du = \begin{cases} u_1 \text{ in } \Omega_1, \\ u_2 \text{ in } \Omega_2, \end{cases}$$

where $\Omega = (0, 1) \times (0, 1)$, $\Omega_1 = \{(x_1, x_2) \in \Omega : x_1 \leq 1/2\}$, and $\Omega_2 = \Omega \setminus \Omega_1$. The optimality system corresponding to problem (27) is as follows

$$\begin{aligned} -\Delta y &= Du, \\ -\Delta p &= -(y - z), \\ \nu g'(u) - D^* p &= 0, \end{aligned} \tag{28}$$

where $g'(u) = (g_{u_1}, g_{u_2})$ and $D^*$ is the adjoint of $D$. The reduced Hessian is

$$H(y, u, p) = \nu g''(u) + D^*(-\Delta)^{-1}(-\Delta)^{-1} D$$

where $g''(u) = (g_{u_i u_j})$.

We choose the cost function $g(u)$ to be the following triple-well potential

$$g(u_1, u_2) = 1 - (u_1^2 + u_2^2) + \frac{(u_1^2 + u_2^2)^2}{10} - \frac{(u_1^3 - 3u_1 u_2^2)}{10},$$

see figure 1. This function possesses one maximum, three minima, and three saddle points reported in table 2.

For the purpose of clear illustration, we formulate the optimal control problem in such a way that its extremal points coincide with those of $g$. This can be achieved by defining $z$ as the (numerical) solution of $-\Delta z = D u$ with $u$ chosen in table 2. Starting at the extremal points, the multigrid scheme without globalization step stagnates on these points which are solutions of the optimality system. When using the globalization step and starting from the maximum or from any of the saddle points, the multigrid algorithm provides a fast iteration converging to a minimum. To show this fact, we report in table 3 information on the convergence history of the multigrid scheme starting from an extremal point which is not a minimum. We denote with $(u_1^0, u_2^0)$ the initial value of the control. Moreover $z$ is defined as the solution to $-\Delta z = D u$ with $u = (u_1^0, u_2^0)$. In table 3, the solution and the values of the tracking functional given in terms of the discrete $L^2(\Omega)$ norm, $||y - z||_{L_h^2}$, are presented. With $\rho_y$, $\rho_p$ we denote the multigrid convergence factors as the 'asymptotic' value of the ratio between the discrete $L^2$-norm of the residuals of the state and adjoint equations resulting from two successive multigrid cycles [see for example ref. 8]. The results of table 3 demonstrate convergence to a minimum with typical multigrid convergence factor. The computational work used for the

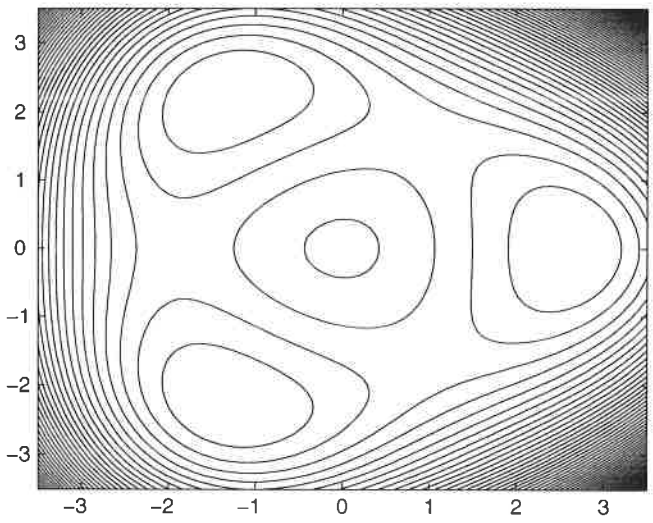


Figure 1. Contour plot of the triple-well potential.

globalization step involves power method iterations which in turn require to solve two Poisson problems on a $8 \times 8$ mesh at each iteration step. This is less work than required by one step of the smoothing iteration at the finest level. We remark that starting away from extremal points, the multigrid scheme converges towards a minimum without need for a globalization step.

The example above has the advantage that we know the character of its extremal points.

We tested the proposed algorithm for optimal control of semilinear elliptic partial differential equations with sever nonlinearities, including Bratu's problem. In all the cases that we tested, the multigrid algorithm found a local minimum without use of the globalization step.

In the smoothing algorithm, the gradient update of $u$ given by descent scheme (9) can be accelerated by a Newton step applied to (8). This is properly done by performing Newton steps followed by the evaluation of $J$. If the value of the cost functional is not reduced the gradient update follows. We remark that close to a maximum the Newton step may provide an update towards the maximum, that is, it does not reduce the value of $J$. On the other hand,

Table 2. Extremal points of $g$.

| | | | |
|---|---|---|---|
| Maxima | (0, 0) | – | – |
| Minima | (−1.32115, −2.28829) | (−1.32115, 2.28829) | (2.64229, 0) |
| Saddle points | (−1.89229, 0) | (0.94614, −1.63878) | (0.94614, 1.63878) |

Table 3. Convergence behavior of multigrid iteration with globalization step, $\nu = 10^{-2}$. Results after 10 $V(2, 2)$-cycles, coarsest mesh $8 \times 8$, finest mesh $256 \times 256$, $M = 6$.

| $(u_1^0, u_2^0)$ | $(u_1, u_2)$ | $\|y - z\|_{L_h^2}$ | $\rho_y, \rho_p$ |
|---|---|---|---|
| (0, 0) | (−1.271, −2.228) | $7.25 \times 10^{-2}$ | 0.14, 0.15 |
| (−1.89229, 0) | (−1.300, −2.249) | $4.12 \times 10^{-2}$ | 0.12, 0.24 |
| (0.94614, −1.63878) | $(2.628, -1.121 \times 10^{-3})$ | $6.85 \times 10^{-2}$ | 0.14, 0.15 |
| (0.94614, 1.63878) | $(2.631, 1.651 \times 10^{-2})$ | $2.74 \times 10^{-2}$ | 0.11, 0.18 |

Table 4. Rosenbrock function. Convergence behavior of multigrid iteration.

| $\nu$ | $10^{-2}$ | $10^{0}$ | $10^{2}$ |
|---|---|---|---|
| $\rho_y, \rho_p$ | 0.19, 0.14 | 0.11, 0.15 | 0.14, 0.15 |

close to minima the Newton step accelerates convergence. This may be advantageous when solving optimal control problems having flat minima. For example, consider the Rosenbrock function

$$g(u_1, u_2) = 100(u_2 - u_1^2)^2 + (1 - u_1)^2,$$

which possesses a minimizer at $u = (1, 1)$. Choosing the desired target function such that $-\Delta z = D(1, 1)$ and $\nu$ sufficiently large, the optimal control problem (27) has a minimum at $u = (1, 1)$. In this case there are no maxima or saddle points and the globalization step is not activated. In fact the smallest eigenvalue of $H$ results always positive in the multigrid process. As starting value for the multigrid iteration we take $u^0 = (u_1^0, u_2^0) = (10, 10)$. In this case, the Newton-based multigrid smoothing requires fewer iterations than the one based on the pure gradient smoother. The resulting convergence factors are similar to that reported for the previous example and the local minimum is attained with high accuracy. This fact is shown in table 4.

## 8. Conclusions

We presented the combination of a globalization step and a multigrid scheme for the solution of optimal control problems having multiple extremal points. The globalization step was applied at the coarsest grid of the multigrid process to detect directions of negative curvature which were used to escape undesired maxima and saddle points.

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## Appendix A: Implementation details of the smoothing procedure

In the following, we give implementation details regarding the smoothing procedure discussed in section 4. For this purpose, we take the problem defined in section 7 discretized by finite differences on a uniform grid $\Omega_h$ with mesh size $h$. The negative Laplacian with homogeneous Dirichlet boundary conditions is approximated by the five-point stencil and is denoted by $-\Delta_h$.

Consider the optimality system (28) at $\mathbf{x} \in \Omega_h$, where $\mathbf{x} = (ih, jh)$ and $i, j = 1, \ldots, N$ index the grid points. We have

$$-(y_{i-1\,j} + y_{i+1\,j} + y_{i\,j-1} + y_{i\,j+1}) + 4y_{ij} = h^2 (D_h u)_{ij}, \tag{A1}$$

$$-(p_{i-1\,j} + p_{i+1\,j} + p_{i\,j-1} + p_{i\,j+1}) + 4p_{ij} + h^2 y_{ij} = h^2 z_{ij}, \tag{A2}$$

$$\nu g'(u_{ij}) - D_h^* p_{ij} = 0. \tag{A3}$$

The neighboring variables are considered constant during the smoothing step at $\mathbf{x}$. Therefore, define the following two functions of $i, j$, treated as constants at this grid point,

$$C_{y\,ij} = (y_{i-1\,j} + y_{i+1\,j} + y_{i\,j-1} + y_{i\,j+1}) \quad \text{and} \quad C_{p\,ij} = (p_{i-1\,j} + p_{i+1\,j} + p_{i\,j-1} + p_{i\,j+1}).$$

Inserting $C_{y\,ij}$ and $C_{p\,ij}$ in (A1) and (A2), respectively, we obtain $y_{ij}$ and $p_{ij}$ as functions of $u_{ij}$ as follows

$$y_{ij}(u_{ij}) = \frac{(C_{y\,ij} + h^2 (D_h u)_{ij})}{4}, \tag{A4}$$

and

$$p_{ij}(u_{ij}) = \frac{(4\, C_{p\,ij} - h^2\, C_{y\,ij} + 4\, h^2\, z_{ij} - h^4\, (D_h u)_{ij})}{16}. \tag{A5}$$

Next, consider (A3) and replace $p_{ij}$ by (A5) to obtain

$$16\nu g_{u_1}(u) + h^4\, u_1 = D_h^* (4\, C_{p\,ij} - h^2\, C_{y\,ij} + 4\, h^2 z_{ij})_1 \tag{A6}$$

and

$$16\nu g_{u_2}(u) + h^4\, u_2 = D_h^* (4\, C_{p\,ij} - h^2\, C_{y\,ij} + 4\, h^2 z_{ij})_2, \tag{A7}$$

where $u = (u_1, u_2)$ and $D_h^*(\cdot)_l$, $l = 1, 2$, represents numerical integration of the quantities in parenthesis on $\Omega_{h_1}$ and $\Omega_{h_2}$, respectively.

Now, we give a formal description of the smoothing algorithm used in the multigrid scheme.

### A.1 *Smoothing algorithm*

(i) Compute $f_l = D_h^* (4\,C_{p\,ij} - h^2\,C_{y\,ij} + 4\,h^2\,z_{ij})_l$, $l = 1, 2$.

(ii) Gradient update of $u$

For $m = 1, \ldots, 10$

$$u_l^m = u_l^{m-1} - \beta(16\nu g_{u_l}(u^{m-1}) + h^4 u_l^{m-1} - f_l), \quad l = 1, 2,$$

if $J(y(u^m), u^m)_h > J(y(u^{m-1}), u^{m-1})_h$ set $u = u^{m-1}$ and goto step (iii); otherwise set $u = u^m$ and continue.

(iii) Gauss–Seidel update of $y$ and $p$

For $i, j = 1, \ldots, N$

$C_{y\,ij} = (y_{i-1\,j} + y_{i+1\,j} + y_{i\,j-1} + y_{i\,j+1})$

$$y_{ij} = \frac{(C_{y\,ij} + h^2 (D_h u)_{ij})}{4}$$

$C_{p\,ij} = (p_{i-1\,j} + p_{i+1\,j} + p_{i\,j-1} + p_{i\,j+1})$

$$p_{ij} = \frac{(4\,C_{p\,ij} - h^2\,C_{y\,ij} + 4\,h^2\,z_{ij} - h^4\,(D_h u)_{ij})}{16}.$$

To evaluate the cost functional during the gradient step of the smoothing algorithm we use

$$J(y(u^m), u^m)_h = \frac{h^2}{2} \sum_{ij} \left( \frac{C_{y\,ij} + h^2 (D_h u^m)_{ij}}{4} - z \right)^2 + \nu g(u^m).$$

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