A Sequential Method for Mathematical Programming

Kazufumi Ito* Karl Kunisch †

September 5, 2014

Abstract

A sequential programming method for constrained optimization, which is referred to as SP method, is presented. It is based on a sequence of linearized constrained problems. Convergence and convergence rate of the method are analyzed based on solutions of the first order optimality conditions and on Lagrange multiplier theory. Unlike the SQP method, the SP method does not rely on an approximation of the Hessian of the Lagrange functional and consequently avoids instabilities due to possible indefiniteness of its Hessian.

The method can be used for non-smooth problems and it can efficiently be implemented by the use of saddle point solvers. The implementation of the algorithms is less involved when compared to the SQP method. The cost of performing each sequential step is very similar to the one for the gradient method with doubling number of unknowns and the method is stable when using damped updates. We also develop a second order convergent version which again be based only on sequential linearization of the equality constraints. The proposed methods are numerically tested for control in the coefficient problems or equivalently of bilinear optimal control problems.

Key words: Sequential linearization, mathematical programming, non-smooth optimization, optimal control.

1 Introduction

In this paper we develop a sequential programming method (SP method) for constraint minimization in Hilbert spaces. The method uses a linearization of the constraints. It is a distinctive feature that it does not rely on second order derivatives. It can be used for non-smooth problems and in many problems of practical interest it avoids instabilities due to possible indefiniteness of the Hessian of the Lagrange functional. The established methods to solve the class of problems that we aim for include the gradient- and conjugate gradient methods, the SQP (Sequential Quadratic Programming) method, and variants thereof.

*Department of Mathematics and Center for Research in Scientific Computation, North Carolina State University, Raleigh, North Carolina (kito@math.ncsu.edu).

†Institute of Mathematics and Scientific Computing, University of Graz, Austria (karl.kunisch@uni-graz.at) and Radon Institute, Austrian Academy of Sciences.

The SQP (Sequential Quadratic Programming) method solves a sequence of optimization subproblems, each of which optimizes a quadratic model for the Lagrangian functional subject to a linearization of the constraints. If the problem has only equality constraints, then the method is equivalent to applying Newton's method to the first-order optimality conditions, or the Karush-Kuhn-Tucker conditions. Like for the Newton method the objective function and the constraints are assumed to be twice continuously differentiable for the SQP method. SQP is quadratically convergent but requires evaluations of the second order derivatives and globalization methods for a stable implementation.

On the other hand gradient based methods (for optimal control problems) use an equation and an adjoint solver to compute the gradient in each step. The cost per step for the gradient method is much less than for the SQP-method but it requires a large number of iterations, in general. These facts motivate us to develop the middle ground between SQP and gradient methods.

The proposed method involves solving a sequence of first-order optimality conditions utilizing linearized equality constraints. We also develop a variant which, under appropriate conditions, can be shown to have second order convergence. The efficiency of the methods depends on the availability of a good saddle point solver. The saddle point systems which need to be solved for the SP and the SQP methods differ by the appearance of off-diagonal terms which involve the current Lagrange multiplier associated to the equality constraints. The SP method is therefor more stable than the SQP method for the class of control problems that is our main motivation. The approach is also applicable for a general class of non-smooth PDE constrained optimization problems. In summary the method offers an alternative to existing methods when the performance should be improved over the gradient method and difficulties involving second order realization should be avoided.

The paper is written in the Hilbert space setup but all discussions are applied to the finite dimensional nonlinear programming. Examples are presented to demonstrate the applicability of the SP method for optimal control problems and an inverse medium problem. Our tests show that the proposed SP method is more stable than the SQP method, and still rapidly convergent.

The literature on iterative solutions to optimization problems in infinite dimensions is by now very rich. We therefore quote only very selectively. In particular we mention the following monographs which mainly focus on mathematical programming problems which arise from PDE-constrained optimization problems, [AN, BGHKW, G, HPUU, IK, T]. We believe that a systematic investigation of the approach that we present has not been carried out before.

In Section 2 we introduce the (basic) SP method for constrained optimization and analyze its convergence and convergence rate. Also, we discuss most relevant saddle point solvers for the SP method. In Section 3 we propose and analyze a second order SP method. A predictor-corrector method is developed based on the saddle point problem. The application of the SP method to non-smooth problems is discussed in Section 4. Numerical examples are given in Section 5.

2 Sequential programming

In this section we introduce a sequential method for mathematical programming. Throughout X and Y denote real Hilbert spaces. We consider the constrained optimization problem for $x \in X$:

$$\min\ F(x) \text{ subject to } E(x) = 0, \quad x \in \mathcal{C}, \tag{P}$$

where $\mathcal{C}$ is a closed convex set in X and $F : X \to \mathbb{R}$ and $E : X \to Y$ are continuously differentiable with locally Lipschitz continuous derivatives. Let x^* denote a solution to (P). The analysis will be given in a neighborhood $U_\epsilon(x^*)$ of x^* with radius $\epsilon \in (0,1)$ to be determined below. Throughout it is assumed that

$$E'(x) \in \mathcal{L}(X,Y) \text{ is surjective for all } x \in U_\epsilon(x^*). \tag{H1}$$

Proceeding iteratively the equality constraint E is linearized at $x_n \in U_\epsilon(x^*)$ and a constrained optimization problem is solved in the subsequent iteration. This is followed by a damped updating step resulting in the following algorithm.

Algorithm 1: Sequential Programming I

1. Choose $x_0 \in U_\epsilon(x^*)$
2. Given $x_n \in \mathcal{C}$, solve for $\bar{x}$

$$\min_{x \in \mathcal{C}} F(x) \text{ subject to } E'(x_n)(x - x_n) + E(x_n) = 0, \tag{2.1}$$

   and associated multiplier $\bar{\lambda}$.

3. Update $x_{n+1} = (1-\alpha)\, x_n + \alpha\, \bar{x},\ \ \alpha \in (0,1)$. Iterate until convergence.

It is assumed that (2.1) admit solutions $\bar{x}$, which depends on n, of course. Assumption (H1) implies that there exist Lagrange multipliers $\lambda^* \in Y$ and $\bar{\lambda} \in Y$ such that the first order necessary optimality conditions for (P) and (2.1) are given by

$$\begin{cases} (F'(x^*) + E'(x^*)^*\lambda^*, \tilde{x} - x^*) \geq 0 \text{ for all } \tilde{x} \in \mathcal{C} \\ \\ E(x^*) = 0. \end{cases} \tag{2.2}$$

and

$$\begin{cases} (F'(\bar{x}) + E'(x_n)^*\bar{\lambda}, \tilde{x} - \bar{x}) \geq 0 \text{ for all } \tilde{x} \in \mathcal{C} \\ \\ E'(x_n)(\bar{x} - x_n) + E(x_n) = 0 \end{cases} \tag{2.3}$$

respectively. Note that the necessary condition to (P) can be written alternatively as

$$\begin{cases} (F'(x^*) + E'(x_n)^*\lambda^* - (E'(x_n)^* - E'(x^*)^*)\lambda^*, \tilde{x} - x^*) \geq 0 \text{ for all } \tilde{x} \in \mathcal{C} \\ \\ E'(x_n)(x^* - x_n) + E(x_n) = E'(x_n)(x^* - x_n) + E(x_n) - E(x^*). \end{cases} \tag{2.4}$$

Consequently (2.2), and hence (2.4), are a perturbed form of problem (2.3) with perturbations $(\Delta_1, \Delta_2) \in X \times Y$ given by

$$\Delta_1 = (E'(x_n)^* - E'(x^*)^*)\lambda^* \quad \text{and} \quad \Delta_2 = E'(x_n)(x^* - x_n) + E(x_n) - E(x^*). \tag{2.5}$$

To describe the main assumption let (x_ξ, λ_ξ) for $\xi \in U_\epsilon(x^*)$, denote the solution to

$$\begin{cases} (F'(x_\xi) + E'(\xi)^*\lambda_\xi, \tilde{x} - x_\xi) \geq 0 \text{ for all } \tilde{x} \in \mathcal{C} \\ \\ E'(\xi)(x_\xi - \xi) + E(\xi) = 0, \end{cases} \tag{2.6}$$

and let $(x_{\tilde{\Delta}}, \lambda_{\tilde{\Delta}})$ be the solution of the perturbed problem

$$\begin{cases} (F'(x_{\tilde{\Delta}}) + E'(\xi)^*\lambda_{\tilde{\Delta}} - \tilde{\Delta}_1, \tilde{x} - x_{\tilde{\Delta}}) \geq 0 \text{ for all } \tilde{x} \in \mathcal{C} \\ \\ E'(\xi)(x_{\tilde{\Delta}} - \xi) + E(\xi) = \tilde{\Delta}_2, \end{cases} \tag{2.7}$$

where $\tilde{\Delta} = (\tilde{\Delta}_1, \tilde{\Delta}_2) \in X \times Y$. We assume Lipschitz continuity of the solution (2.6) with respect to additive perturbations, i.e.

$$|x_\xi - x_{\tilde{\Delta}}|_X \leq c\,|(\tilde{\Delta}_1, \tilde{\Delta}_2)|_{X\times Y}, \tag{H2}$$

for a constant c independent of $\xi \in U_\epsilon(x^*)$ and $(\tilde{\Delta}_1, \tilde{\Delta}_2) \in X \times Y$. Assumption (H2) is well-investigated in the literature, see e.g. [IK] Chapter 2.4, and the references given there. We shall also address a special case below, to highlight the dependence of c on the problem data.

Assuming that $x_n \in U_\epsilon(x^*)$ we obtain for the damped update:

$$x_{n+1} = (1-\alpha)x_n + \alpha\,\bar{x}, \quad \alpha \in (0,1], \tag{2.8}$$

by applying (H2), with $\xi = x_n$, $(x_\xi, \lambda_\xi) = (\bar{x}, \bar{\lambda})$, $(x_{\tilde{\Delta}}, \lambda_{\tilde{\Delta}}) = (x^*, \lambda^*)$ and for the perturbation given in (2.5), that

$$|x_{n+1} - x^*| \leq (1 - \alpha + c\,\alpha\,L|\lambda^*|_Y)|x_n - x^*| + c\,\alpha\,\frac{L}{2}\,|x_n - x^*|^2, \tag{2.9}$$

where L is the Lipschitz constant of E' on $U_\epsilon(x^*)$. In fact, we can estimate

$$\begin{aligned} |x_{n+1} - x^*| &\leq (1-\alpha)|x_n - x^*| + \alpha|\bar{x} - x^*| \leq (1-\alpha)|x_n - x^*| + \alpha c(|\Delta_1|_X + |\Delta_2|_Y) \\ &\leq (1-\alpha)|x_n - x^*| + \alpha c(L|\lambda^*|_Y|x_x - x^*| + |\Delta_2|_Y) \end{aligned}$$

Moreover

$$\begin{aligned} |\Delta_2| &= |E'(x_n)(x^* - x_n) + E(x_n) - E(x^*)| \\ &= |\textstyle\int_0^1 \big(E'(x_n) - E'(x_n + s(x^* - x_n))\big)(x^* - x_n)\,ds| \leq \frac{L}{2}|x_n - x^*|^2. \end{aligned}$$

Combining these estimates, (2.9) follows. If $x_n \in U_\epsilon(x^*)$ we have

$$|x_{n+1} - x^*| \leq (1 - \alpha + c\,\alpha\,L|\lambda^*|_Y + \epsilon\,c\,\alpha\,\frac{L}{2}\,)|x_n - x^*|. \tag{2.10}$$

Thus, if $cL(|\lambda^*|_{Y^*} + \frac{\epsilon}{2}) < 1$, then $x_{n+1} \in U_\epsilon(x^*)$ and the iteration can proceed. We summarize the discussion so far in the following proposition.

Proposition 2.1. *Assume that* (H1) *and* (H2) *hold, and that* $\rho_1 := cL(|\lambda^*|_Y + \frac{\epsilon}{2}) < 1$. *Then Algorithm 1 is well-defined and it converges linearly with rate* $(1 - \alpha(1 - \rho_1))$.

Remark 2.1. Let us consider (H2) for the case $\mathcal{C} = X$ and assume that F is uniformly convex and Lipschitz continuous, i.e. there exist constants $\gamma > 0$ and $L_F > 0$ such that

$$\gamma|x - x^*|^2 \leq (F'(x) - F'(x^*), x - x^*), \quad |F'(x) - F'(x^*)| \leq L_F|x - x^*| \text{ for all } x \in X. \tag{2.11}$$

The error equations are:

$$\begin{cases} F'(x) - F'(x^*) + E'(x_n)^*(\lambda - \lambda^*) = -\Delta_1 \\ E'(x_n)(x - x^*) = -\Delta_2. \end{cases} \tag{2.12}$$

Setting $E_n^\dagger = (E'(x_n)E'(x_n)^*)^{-1}E'(x_n)$ we obtain from the first equation

$$|\lambda - \lambda^*| \leq |E_n^\dagger \Delta_1| + L_F\|E_n^\dagger\|\,|x - x^*|.$$

Moreover (2.12) implies that

$$\gamma|x - x^*|^2 \leq |\Delta_1|\,|x - x^*| + |\Delta_2|(|E_n^\dagger\Delta_1| + L_F\|E_n^\dagger\|\,|x - x^*|).$$

This further implies that

$$\frac{\gamma}{2}|x - x^*|^2 \leq \frac{1}{2\gamma}(|\Delta_1| + L_F|\Delta_2|\,\|E_n^\dagger\|)^2 + |\Delta_2|\,|E_n^\dagger\Delta_1|$$

and hence

$$|x - x^*|^2 \leq \frac{1}{\gamma^2}(|\Delta_1| + L_F|\Delta_2|\,\|E_n^\dagger\|)^2 + \frac{2}{\gamma}|\Delta_2|\,|E_n^\dagger\Delta_1|.$$

Thus we obtain

$$|x - x^*| \leq \frac{1}{\gamma}(|\Delta_1| + L_F|\Delta_2|\,\|E_n^\dagger\|) + \frac{1}{\gamma}|\Delta_2| + \frac{1}{2}\,|E_n^\dagger\Delta_1|,$$

and

$$|x - x^*| \leq \frac{1}{\gamma}|\Delta_1| + \frac{1}{2}\,|E_n^\dagger\Delta_1| + (\frac{L_F}{\gamma}\|E_n^\dagger\| + \frac{1}{\gamma}|)|\Delta_2|,$$

as desired.

Next we consider case where E and F are more regular, and $\mathcal{C} = X$. In particular E and F are assumed to be once respectively twice continuously differentiable, with first, respectively second derivative Lipschitz continuous on $U_\epsilon(x^*)$ with Lipschitz constant $\tilde{L}$. We define the saddle point operators

$$G(x) = \begin{pmatrix} F''(x) & E'(x)^* \\ E'(x) & 0 \end{pmatrix}. \tag{2.13}$$

and assume that for some $\kappa > 0$

$$(x, G(x^*)x) \geq \kappa|x|^2, \text{ for all } x \in \ker E'(x^*). \tag{H3}$$

This implies that for ϵ sufficiently small we have

$$(x, G(\tilde{x})x) \geq \frac{\kappa}{2}|x|^2, \text{ for all } x \in \ker E'(\tilde{x}).$$

for all $\tilde{x} \in U(x^*)$.

Proceeding iteratively we set $z_n = (x_n, \lambda_n)$, $z^* = (x^*, \lambda^*)$ and assume that $(x_n, \lambda_n) \in U_\epsilon(x^*) \times U_\epsilon(\lambda^*)$, where $U_\epsilon(\lambda^*)$ is an ϵ neighborhood of λ^*. For convenience we further set $G_n = G(x_n)$. Then for the update

$$z_{n+1} = (1-\alpha) z_n + \alpha\, z_n, \quad \alpha \in (0,1]$$

we find

$$z_{n+1} - z^* = (1-\alpha)\,(z_n - z^*) + \alpha\, G_n^{-1}\Big(\begin{pmatrix} -(E'(x_n)^* - E'(x^*)^*)\lambda^* \\ 0 \end{pmatrix} + \delta_n \Big) \tag{2.14}$$

with

$$\delta_n = \begin{pmatrix} F'(x^*) - F'(\bar{x}) - F''(x_n)(x^* - \bar{x}) \\ E(x^*) - E'(x_n)(x^* - x_n) - E(x_n) \end{pmatrix}.$$

Thus we have

$$\begin{aligned} |z_{n+1} - z^*| &\leq (1 - \alpha + \alpha\gamma)\,|z_n - z^*| + \alpha\tilde{c}\|G_n^{-1}\|\,|z_n - z^*|^2 \\ &\leq (1 - \alpha + \alpha\gamma + \alpha\tilde{c}\|G_n^{-1}\|)\,|z_n - z^*|, \end{aligned} \tag{2.15}$$

where we use that $\epsilon < 1$, and $|\bar{x} - x^*| \leq cL(|\lambda^*| + \frac{\epsilon}{2})|x_n - x^*|$, $\tilde{c}$ depends on L and $\tilde{L}$, and

$$|G_n^{-1} \begin{pmatrix} (E'(x_n)^* - E'(x^*)^*)\lambda^* \\ 0 \end{pmatrix}| \leq \gamma\,|x_n - x^*|. \tag{2.16}$$

The constant γ is small if either $|\lambda^*|$ is small or if the quadratic variation of E is dominated by the linearization E' of E. The latter will be addressed in Remark 2.2 below. Before that we summarize the above discussion as a proposition.

Proposition 2.2. *Assume that F and E are twice, respectively once, continuously differentiable with locally Lipschitz continuous derivatives, that (H1) and (H3) hold, and that $\rho_2 = \gamma + \epsilon\tilde{L}\sup_{x \in \overline{U_\epsilon(x^*)}} \|G(x)\| < 1$. Then Algorithm 1 is well-defined and it converges linearly with rate $(1 - \alpha(1-\rho))$.*

Remark 2.2. (1) To illustrate the dependence of γ on $G(x)$, E' and λ^* we consider a situation which is typical for stationary optimal control problems: Let $x = (y, u) \in X_1 \times X_2$, with X_1 and X_2 Hilbert spaces, and

$$E(y,u) = e(y) + Bu, \quad B \in \mathcal{L}(X_1, X_2), \quad F(y,u) = F_1(y) + F_2(u),$$

where $F_2(u)''$ is a positive multiple of the identity for each $u \in X_2$, and $F_1(y)''$ is positive definite, $e'(y) \in \mathcal{L}(X_1, Y)$ is an isomorphism for each $y \in X_1$, and otherwise E and F satisfy the regularity properties of Proposition 2.2. For these choices the expression

$$G_n \begin{pmatrix} \delta x \\ \delta\lambda \end{pmatrix} = \begin{pmatrix} (E'(x_n)^* - E'(x^*)^*)\lambda^* \\ 0 \end{pmatrix}$$

is found to be

$$\begin{pmatrix} F_1'' & 0 & e_y^* \\ 0 & F_2'' & B^* \\ e_y & B & 0 \end{pmatrix} \begin{pmatrix} \delta y \\ \delta u \\ \delta\lambda \end{pmatrix} = \begin{pmatrix} r \\ 0 \\ 0 \end{pmatrix}, \tag{2.17}$$

where all expressions are evaluated at (y_n, u_n) and $r = (e'(x_n)^* - e'(x^*)^*)\lambda^*$.

From this system we obtain

$$\delta\lambda = e_y^{-*}(r - F_1''\delta y), \quad \delta u = -(F_2'')^{-1}B^*\delta\lambda, \quad \delta y = -(e_y)^{-1}B\delta u,$$

and consequently

$$\delta u + (F_2'')^{-1}B^* e_y^{-*} F_1'' e_y^{-1} B\,\delta u + (F_2'')^{-1}B^* e_y^{-*}\, r = 0.$$

From these equalities we conclude that

$$|\delta u| \le \|(F_2'')^{-1}B^*\|\,|e_y(y_n)^{-*}r|,\ |\delta y| \le \|Be_y^{-1}(F_2'')^{-1}B^*\|\,|e_y(y_n)^{-*}r|, |\delta\lambda| \le const\,|e_y(y_n)^{-*}r|.$$

Loosely speaking these estimates imply that the constant γ in (2.16) is small if $|\lambda|_\infty$ is small and, in appropriately chosen norms, $|E''|$ is small compared to $|E'|$.

From the expressions for $\delta u, \delta y, \delta\lambda$ it can be seen that the sequences in (2.14)

$$G_n^{-1}(E'(x_n)^* - E'(x^*)^*)\lambda^* \text{ and } G_n^{-1}\delta_n$$

are compact sequences in X in many PDE constrained optimal control problems involving diffusion processes. This implies that the high frequency component of the iterates can be expected to be rapidly convergent.

(2) One can allow an incomplete solution to (2.2). In this case we have

$$\begin{pmatrix} F'(x) + E'(x_n)^*\lambda \\ E'(x_n)(x - x_n) + E(x_n) \end{pmatrix} = \tilde{\delta}_n,$$

and the error term in (2.14) must be replaced by $\delta_n + \tilde{\delta}_n$.

2.1 Comparison to gradient method and SQP

We briefly compare the SP approach with the projected gradient and SQP methods. For this purpose we consider as in Remark 2.2 problems of the form

$$\min \quad F(x) = F_1(y) + F_2(u) \text{ subject to } E(y,u) = 0 \text{ and } u \in \mathcal{C}, \tag{2.18}$$

where $x = (y, u)$ and $E_y(x)$ is bounded invertible. The projected gradient method for this this problem can be expressed as

1. Given u_n, we solve for y_n
$$E(y, u_n) = 0.$$

2. Given $x_n = (y_n, u_n)$ solve for λ_n
$$E_y(x_n)^*\lambda + F_1'(y_n) = 0.$$

3. Update u by

$$u_{n+1} = P_{\mathcal{C}}(u_n - \alpha\,(F_2'(u_n) + E_u(x_n)^*\lambda),$$

where $Proj_{\mathcal{C}}$ denotes the orthogonal projection onto $\mathcal{C}$. Thus, the gradient method requires an equation solver for y_n and an adjoint equation solver for λ.

The SP update can be expressed as: given x_n obtain x_{n+1} by solving the reduced problem

$$\begin{aligned} &\min \quad F_2(u) + (E_u(x_n)^*\lambda, u - u_n)_{X_2} \text{ over } u \in \mathcal{C} \\ &\text{where } (y,\lambda) = (y(u), \lambda(u)) \text{ solve the saddle point problem:} \\ &\begin{cases} E_y(x_n)(y - y_n) + E_u(x_n)(u - u_n) + E(x_n) = 0 \\ E_y(x_n)^*\lambda + F_1'(y) = 0. \end{cases} \end{aligned} \tag{2.19}$$

The solution of the minimization step in (2.19) will depend on the specific problem under consideration. In the case there are no constraints on u, the minimization in (2.19) gives $F_2'(u) + E_u(x_n)^*\lambda = 0$. If F_2 is quadratic in u this allows to expresses u as a function of λ and eliminate u from the saddle point problem.

Thus, the SP method requires to solve saddle point problems for (y, λ) while the gradient method uses a nonlinear solver for y and a linear adjoint solver for λ. That is, there are twice the number of unknowns for the SP method compared to the gradient method.

The SQP update $x = (y, u)$ solves

$$\begin{aligned} \min_{x=(y,u)} \quad & F_1(y_n) + F_2(u_n) + F_1'(y_n)(y - y_n) + F_2'(u_n)(u - u_n) \\ & + \tfrac{1}{2}(x - x_n), \mathcal{L}_{xx}((x_n, \lambda_n)(x - x_n))_X \end{aligned}$$

$$\text{subject to } E_y(x_n)(y - y_n) + E_u(x_n)(u - u_n) + E(x_n) = 0 \text{ and } u \in \mathcal{C},$$

where $\mathcal{L}_{xx}(x_n, \lambda_n)$ is the Hessian of the Lagrangian functional given by

$$\mathcal{L}(x, \lambda) = F_1(y) + F_2(u) + \langle E(x), \lambda \rangle.$$

For large scale problems it is a nontrivial task to evaluate the Hessian of the Lagrangian or to obtain a good approximation to it. Moreover, to benefit from this second order information it is crucial that the Hessian is positive definite on the kernel of $E'(x)$ and that the updates are in the region of attraction. As we shall point out below this can be a mayor difficulty for the SQP method.

2.2 The saddle point problem

Here we consider the case that $\mathcal{C} = X$. Then the necessary condition (2.3) for the SP method is the following the saddle point problem

$$\begin{cases} F'(x) + E'(x_n)^*\lambda = 0 \\ E'(x_n)(x - x_n) + E(x_n) = 0. \end{cases} \tag{2.20}$$

Applying a Newton step to (2.20) we obtain

$$\begin{pmatrix} F''(x_n) & E'(x_n)^* \\ E'(x_n) & 0 \end{pmatrix} \begin{pmatrix} x - x_n \\ \lambda \end{pmatrix} = - \begin{pmatrix} F'(x_n) \\ E(x_n) \end{pmatrix}. \tag{2.21}$$

Alternatively the SQP step described at the end of the previous subsection results in

$$\begin{pmatrix} \mathcal{L}_{xx}(x_n, \lambda_n) & E'(x_n)^* \\ E'(x_n) & 0 \end{pmatrix} \begin{pmatrix} x - x_n \\ \lambda \end{pmatrix} = - \begin{pmatrix} F'(x_n) \\ E(x_n) \end{pmatrix}. \tag{2.22}$$

If $F''(x_n)$ is positive definite on the kernel of $E'(x_n)$ (and in particular if $F''(x_n)$ is positive definite on all of X, compare (2.17)), then system (2.21) is solvable and the direction that is obtained is a decent direction for F, which follow by taking the inner product of the first row in (2.21) with $x - x_n$. Turning to the $1-1$ block in (2.22), it is given by $\mathcal{L}_{xx}(x, \lambda) = F''(x_n) + (E'(x_n)^*\lambda_n)'$. Even if F'' is positive definite on all of X this expression may lack positiveness, unless the iterates are very close to a strict local minimum. As a special case consider the bilinear control problem with $E(y, u) = -\Delta y + uy$ and $F(y, u) = \frac{1}{2}|y - y_d|^2 + \frac{\beta}{2}|u|^2$, in $X = H_0^1 \times L^2$ with given $y_d \in L^2$. Then

$$\mathcal{L}_{xx}(y, u, \lambda) = \begin{pmatrix} I & \lambda \\ \lambda & \beta I \end{pmatrix}.$$

and this expression is not positive definite on the kernel of $E'(y, u)$ for arbitrary (y, u, λ).

Let us now return to (2.20) and comment on possible numerical approaches. First consider the case that F' is strictly monotone, i.e.,

$$\langle F'(x) - F'(z), x - z \rangle_{X^* \times X} \geq \omega \, |x - z|^2, \quad x, \ z \in X.$$

for some $\omega > 0$. The preconditioned Uzawa algorithm (explicit method) [G] is given by

$$\begin{cases} \dfrac{x^{k+1} - x^k}{\alpha_k} = P(F'(x^k) + E'(x_n)^*\lambda^k) \\[2ex] \dfrac{\lambda^{k+1} - \lambda^k}{\beta_k} = E'(x_n)(x^{k+1} - x_n) + E(x_n) \end{cases} \tag{2.23}$$

for step-sizes $\alpha_k, \ \beta_k$, where P is a pre-conditioner. For PDE optimization $F'(x^k) + E'(x^k)^*\lambda^k \in X^*$, where X^* is the dual space of a Hilbert space X and $P : X^* \to X$ can be chosen as the Riesz map of X^*. Alternatively the augmented Lagrangian method (implicit method) can be chosen, see eg. [IK]. For sufficiently large $c > 0$ the iteration step is given by

$$\begin{cases} F'(x^{k+1}) + E'(x_n)^*\lambda^{k+1} = 0, \\ \lambda^{k+1} = \lambda^k + c\,(E'(x_n)(x^{k+1} - x_n) + E(x_n)) \end{cases} \tag{2.24}$$

The second case we consider is that of a control problem with $x = (y, u) \in X_1 \times X_2$, $E(y, u) = e(y) + Bu = 0$ with $B \in \mathcal{L}(X_2, Y)$, and $F(x) = \frac{1}{2}((y - z, Q(y - z)) + |u|^2)$, with Q positive definite on X_1 and $z \in X_1$. That is, we consider

$$\min \quad \frac{1}{2}((y - z, Q(y - z)) + |u|^2) \text{ subject to } e(y) + Bu = 0.$$

The saddle point problem for obtaining the update (y,u,λ) reduces to solving

$$\begin{pmatrix} Q & e'(y_n)^* \\ e'(y_n) & -BB^* \end{pmatrix} \begin{pmatrix} y \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix},$$

where $(f,g)=(Qz,-e(y_n)+e'(y_n)y_n)$, and and setting $u=-B^*\lambda$. If $e'(y_n)$ is bounded invertible, then from the second equation $y=e'(y_n)^{-1}(g-\frac{1}{\alpha}Bu)$, and from the first equation

$$\lambda = e'(y_n)^{-*}(f-Qe'(y_n)^{-1}(g-\frac{1}{\alpha}Bu)).$$

Thus, we obtain the following equation for the update u:

$$(I+\frac{1}{\alpha}B^*e'(y_n)^{-*}Qe'(y_n)^{-1}B)u = \frac{1}{\alpha}B^*e'(y_n)^{-*}(Qe'(y_n)^{-1}g-f), \tag{2.25}$$

which can efficiently be solved by the conjugate gradient method. Equation (2.25) is well-posed with moderate condition number if $e'(y)^{-1}$ is compact. A forward and an adjoint solver involving $e'(y_n)^{-1}$ and its adjoint are necessary per evaluation of the left hand side.

2.3 Inequality constraints and primal-dual active set method

We consider a nonlinear programming problem with functional description of the inequality constraint:

$$\min \quad F(x) \text{ subject to } E(x)=0,\ \ G(x)\le 0,$$

where the range space of G is either $L^2(\Omega)$ or $\mathbb{R}^m$. The SP method involves the linearization of the constraints and is given by

$$\min \quad F(x) \text{ subject to } E'(x_n)(x-x_n)+E(x_n)=0,\ \ G'(x_n)(x-x_n)+G(x_n)\le 0.$$

The necessary optimality is

$$\begin{cases} F'(x)+E'(x_n)^*\lambda+G'(x_n)^*\mu=0 \\ E'(x_n)(x-x_n)+E(x_n)=0 \\ \mu=\max(0,\mu+c\,(G'(x_n)(x-x_n)+G(x_n))). \end{cases}$$

where $\mu\ge 0$ is the Lagrange multiplier for the inequality constraint $G(x)\le 0$ and the last equality is the complementarity condition. The max $-$ operation must be interpreted either point-wise for a.e. $x\in\Omega$ if the image of G is $L^2(\Omega)$ or coordinate-wise, if the image of G is $\mathbb{R}^m$.

This problem can efficiently be solved by the primal-dual active method [IK] which iteratively solves the following system for (x^k,λ^k,μ^k)

$$\begin{cases} F'(x^k)+E'(x_n)^*\lambda^k+G'(x_n)^*\mu^k=0 \\ E'(x_n)(x^k-x_n)+E(x_n)=0 \\ G'(x_n)(x^k-x_n)+G(x_n)=0 \text{ on the active set } \{x:(\mu^{k-1}+c(G'(x_n)(x^{k-1}-x_n)+G(x_n)))(x)>0\} \\ \mu^k=0 \text{ on the inactive set } \{x:(\mu^{k-1}+c\,(G'(x_n)(x^{k-1}-x_n)+G(x_n)))(x)0=0\}. \end{cases}$$

If the image space of G is a coordinate space, then the active and inactive sets have to be defined coordinate-wise rather than pointwise-wise.

3 Second order sequential programming

In this section we discuss a second order sequential programming method. As in Section 2 let x^* denote a local minimum to (P) and assume that (H1) holds. Moreover let $U_\epsilon(x^*, \lambda^*) = U_\epsilon(x^*) \times U_\epsilon(\lambda^*)$ denote a neighborhood of radius $\epsilon \in (0,1)$ in $X \times Y^*$.

In order to obtain a second order method it is necessary to incorporate the term $(E'(x_n)^* - E'(x^*)^*)\lambda^*$ to the update. Thus we consider

$$\begin{aligned} \min \quad & F(x) + \langle \lambda_n, E(x) - (E'(x_n)(x - x_n) + E(x_n))\rangle \\ & \text{subject to } E'(x_n)(x - x_n) + E(x_n) = 0 \text{ and } x \in \mathcal{C}. \end{aligned} \tag{3.1}$$

We observe that the term $\langle \lambda_n, E(x) - (E'(x_n)(x - x_n) + E(x_n))\rangle$ can be understood as approximation to $\frac{1}{2}\langle \lambda_n, E''(x_n)(x - x_n, x - x_n)\rangle$ which appears as second summand of $\frac{1}{2}(x - x_n), \mathcal{L}_{xx}((x_n, \lambda_n)(x - x_n))_X$ in the SQP method.

The update according to (3.1) results in the following algorithm.

Algorithm 2: Sequential Programming II

1. Choose $(x_0, \lambda_0) \in U_\epsilon(x^*, \lambda^*)$.
2. Given (x_n, λ_n), solve (3.1) for (x, λ).
3. Update $(x_{n+1}, \lambda_{n+1}) = (x, \lambda)$. Iterate until convergence.

Condition (H4) below will guarantee that the iterates of Algorithm 2 lie in $U_\epsilon(x^*, \lambda^*)$. The necessary optimality condition for (3.1) is given by

$$\begin{cases} (F'(x) + (E'(x)^* - E'(x_n)^*)\lambda_n + E'(x_n)^*\lambda, \tilde{x} - x) \geq 0 \text{ for all } \tilde{x} \in \mathcal{C} \\ \\ E'(x_n)(x - x_n) + E(x_n) = 0. \end{cases} \tag{3.2}$$

When compared to (2.3) this is the saddle problem involving the linearized equation where $F'(x)$ is replaced by $F'(x) + E'(x)^*\lambda_n$. The necessary optimality condition to (P) can be expressed to follow the structure of (3.2) as

$$\begin{cases} (F'(x^*) + (E'(x^*)^* - E'(x_n)^*)\lambda_n + E'(x_n)^*\lambda^* - \Delta_1, \tilde{x} - x^*) \geq 0 \text{ for all } \tilde{x} \in \mathcal{C} \\ \\ E'(x_n)(x^* - x_n) + E(x_n) = \Delta_2, \end{cases} \tag{3.3}$$

where

$$\Delta_1 = (E'(x^*)^* - E'(x_n)^*)(\lambda_n - \lambda^*) \text{ and } \Delta_2 = E'(x_n)(x^* - x_n) + E(x_n) - E(x^*). \tag{3.4}$$

As in Section 2 we consider a perturbed system which for the second order case is given by

$$\begin{cases} (F'(x_{\tilde\Delta}) + E'(x_{\tilde\Delta})^*\mu + E'(\xi)^*(\lambda_{\tilde\Delta} - \mu) - \tilde\Delta_1, \tilde x - x_{\tilde\Delta}) \geq 0 \text{ for all } \tilde x \in \mathcal{C} \\ \\ E'(\xi)(x_{\tilde\Delta} - \xi) + E(\xi) = \tilde\Delta_2, \end{cases} \tag{3.5}$$

for $(\xi, \mu) \in U_\epsilon(x^*, \lambda^*)$, and $\tilde\Delta = (\tilde\Delta_1, \tilde\Delta_2) \in X \times Y$. We assume Lipschitz continuity of the solutions to (3.5) with respect perturbations $\tilde\Delta = (\tilde\Delta_1, \tilde\Delta_2) \in X \times Y$. i.e. that there exists c such that

$$|x_{(\xi,\mu)} - x_{\tilde\Delta}|_X + |\lambda_{(\xi,\mu)} - \lambda_{\tilde\Delta}|_{Y^*} \leq c\,|(\tilde\Delta_1, \tilde\Delta_2)|_{X\times Y}, \tag{H4}$$

where $(x_{(\xi,\mu)}, \lambda_{(\xi,\mu)})$ denotes the solution to (3.5) with $(\tilde\Delta_1, \tilde\Delta_2) = 0$.

Proposition 3.1. *Assume that* (H1) *and* (H4) *hold. Then Algorithm 2 is locally quadratically convergent.*

This follows by applying (H4) with $(\xi, \mu) = (x_n, \lambda_n))$ to (3.2) and (3.3), and using local Lipschitz continuity of $x \to E'(x)$ to estimate Δ_1 and Δ_2.

Remark 3.1. Concerning condition (H4) we return to the special case of Remark 2.1. In the present case the error equations turn out to be

$$\begin{cases} F'(x) + E'(x)^*\lambda_n - (F'(x^*) + E'(x^*)^*\lambda_n) + E'(x_n)^*(\lambda - \lambda^*) = -\Delta_1 \\ E'(x_n)(x - x^*) = -\Delta_2. \end{cases} \tag{3.6}$$

Replacing (2.11) by

$$\begin{aligned} &\gamma|x - x^*|^2 \leq (F'(x) + E'(x)^*\mu - (F'(x^*) + E'(x^*)^*\mu), x - x^*), \\ &|F'(x) + E'(x^*)^*\mu - (F'(x^*) + E'(x^*)^*\mu)| \leq L_F|x - x^*| \text{ for all } x \in X, \mu \in U_\epsilon(\lambda^*), \end{aligned} \tag{3.7}$$

we can proceed as in Remark 2.1 to argue that

$$|(x, \lambda) - (x^*, \lambda^*)| \leq C\,|(\Delta_1, \Delta_2)|$$

for a constant C independent of $\lambda_n \in U(\lambda^*)$.

From Remark 2.1 and Remark 3.1 it is apparent that existence and Lipschitz continuous dependence of solutions with respect to perturbations of equations (2.3) and (3.2) involve the behavior of $x \to F'(x)$, respectively $x \to F'(x) + E'(x)^*\mu$ for $\mu \in Y^*$, on $\ker E'(x)$. Monotonicity is more likely to hold for $x \to F'(x)$ than for $x \to F'(x) + E'(x)^*\mu$. This suggests the following predictor-corrector strategy to solve (3.2).

3.1 Predictor-Corrector method

We propose a solution method for (3.2) using the first order update $\hat x_{n+1}$ based on (2.2) as a predictor step, followed by the corrector step

$$\begin{cases} (F'(x) + (E'(\hat x_{n+1})^* - E'(x_n)^*)\lambda_n + E'(x_n)^*\lambda, \tilde x - x) \geq 0 \text{ for all } \tilde x \in \mathcal{C} \\ \\ E'(x_n)(x - x_n) + E(x_n) = 0, \end{cases} \tag{3.8}$$

which arises from replacing the first x in (3.2) by $\hat{x}_{n+1}$. The corrector step involves the same saddle point problem of the linearized problem at x_n as the predictor step, with $(E'(\hat{x}_{n+1})^* - E'(x_n)^*)\lambda_n$ as perturbation. The corrector step avoids evaluating second derivatives and a possible indefiniteness due to the term $F'(x) + E'^*(x)\lambda_n$, which appears in the second order method.

To obtain insight into the convergence properties of this predictor-corrector strategy, we put ourselves into the situation with $F \in C^2(X, \mathbb{R})$, $E \in C^1(X, Y)$, and $\mathcal{C} = X$, as described just above (2.13).

Let us denote

$$z^* = (x^*, \lambda^*), \quad z_n = (x_n, \lambda_n), \quad \hat{z}_n = (\hat{x}_n, \lambda_n), \quad z = (x, \lambda).$$

From (2.15) with $\alpha = 1$ we have that

$$|\hat{z}_{n+1} - z^*| \le \gamma |z_n - z^*| + \tilde{c} \|G_n^{-1}\| \, |z_n - z^*|^2. \tag{3.9}$$

Turning to the corrector step, we first need to obtain a linear bound on $|z - z^*|$. For this purpose we express the necessary optimality condition for (P) as

$$\begin{cases} (F'(x^*) + E'(x_n)^*\lambda^* - \hat{\Delta}_1 + (E'(\hat{x}_{n+1})^* - E'(x_n)^*)\lambda_n, \tilde{x} - x^*) \ge 0 \text{ for all } \tilde{x} \in \mathcal{C} \\ \\ E'(x_n)(x^* - x_n) + E(x_n) = \Delta_2, \end{cases} \tag{3.10}$$

where Δ_2 was defined in (2.5) and $-\hat{\Delta}_1 = (E'(x^*)^* - E'(\hat{x}_{n+1})^*)\lambda_n + (E'(x^*)^* - E'(x_n)^*)(\lambda^* - \lambda_n)$. Now we require a condition which is slightly more general than (H2), namely that c can be chosen such that

$$|z_{\tilde{\Delta}} - z_{\Xi}|_X \le c\,|\tilde{\Delta} - \Xi|_{X \times Y}, \tag{H2'}$$

where $z_{\tilde{\Delta}} = (x_{\tilde{\Delta}}, \lambda_{\tilde{\Delta}})$ is the solution to (2.7) and analogously for z_{Ξ}. Applying (H2') to (3.8) and (3.10) with $\xi = x_n$, $-\tilde{\Delta}_1 = (E'(\hat{x}_{n+1})^* - E'(x_n)^*)\lambda_n$, $\tilde{\Delta}_2 = 0$, $\Xi_1 = -\hat{\Delta}_1 + (E'(\hat{x}_{n+1})^* - E'(x_n)^*)\lambda_n$, $\Xi_2 = \Delta_2$, we obtain

$$|z - z^*| \le c(|\hat{\Delta}_1| + |\Delta_2|),$$

which together with (3.9) implies the existence of a constant c_1 such that

$$|z - z^*| \le c_1 |z_n - z^*|. \tag{3.11}$$

Next we use the error equation

$$G_n(z - z^*) = \tilde{\delta}_n$$

where

$$\tilde{\delta}_n = \begin{pmatrix} -\hat{\Delta}_1 + F'(x^*) - F'(x) - F''(x_n)(x^* - x) \\ -\Delta_2. \end{pmatrix}.$$

We obtain by (3.11) that

$$|z - z^*| = |G_n^{-1} \begin{pmatrix} (E'(x^*)^* - E'(\hat{x}_n)^*)\lambda_n \\ 0 \end{pmatrix} | + \hat{c}\,|z_n - z^*|^2.$$

Assuming that (2.16) holds uniformly in a neighborhood $U_\epsilon(x^*,\lambda^*) = U_\epsilon(x^*)\times U_\epsilon(\lambda^*)$ of (x^*,λ^*), in the sense that

$$|G(\tilde{x})^{-1}\begin{pmatrix} (E'(x)^* - E'(x^*)^*)\lambda \\ 0 \end{pmatrix}| \le \gamma\,|x - x^*|, \tag{3.12}$$

for all $\tilde{x}\in U_\epsilon(x^*)$, $(x,\lambda)\in U_\epsilon(x^*,\lambda^*)$, we have for some constant $\hat{c}$

$$|z - z^*| \le \gamma|\hat{x}_{n+1} - x^*| + \hat{c}\,|z_n - z^*|^2.$$

Combining this estimate with (3.9) we find for yet another constant $\tilde{c}$ that

$$|z - z^*| \le \gamma^2|z_n - z^*| + \tilde{c}|z_n - z^*|^2,$$

if (H1), (H2'), (H3), and (3.12) hold. Thus, while we cannot obtain quadratic convergence anymore, the constant γ from the first order update is improved to γ^2 by the predictor-corrector method. Note that for the predictor corrector method the system matrix need not be updated.

3.2 Non-smooth optimization

We return to the optimization problem in separable form

$$\min \quad F_1(y) + F_2(u) \quad \text{subject to } E(y,u) = 0 \text{ and } u\in\mathcal{C}, \tag{3.13}$$

where $F_1\in C^1(X_1,\mathbb{R})$, $E\in C^1(X,Y)$, with locally Lipschitz continuous derivatives, and F_2 is locally Lipschitz continuous and convex, but not necessarily C^1 on X_2. As in the previous section we consider an iterative second order SP method which on each iteration level solves, for given $x_n = (y_n,u_n)$, the following problem:

$$\begin{cases} \min_{u\in\mathcal{C}} \quad F_1(y) + F_2(u) + \langle \lambda_n, E(y,u) - (E'(y_n,u_n)(y-y_n,u-u_n) + E(y_n,u_n)\rangle \\[2ex] \quad \text{subject to } E'(y_n,u_n)(y-y_n,u-u_n) + E(y_n,u_n) = 0. \end{cases} \tag{3.14}$$

Note that if (y^*,u^*) is an optimizer of (3.13), then it is a solution to a perturbation of problem (3.14):

$$\begin{cases} \min\ F_1(y) + F_2(u) + \langle \lambda_n, E(y,u) - (E'(x_n)(y-y_n,u-u_n)) + E(x_n)\rangle_{X^*,X} - (\Delta_1, x)_X \\[2ex] \quad \text{subject to } E'(x_n)(y-y_n,u-u_n) + E(x_n) = \Delta_2, \end{cases} \tag{3.15}$$

where $x = (y,u)$, and $\Delta = (\Delta_1,\Delta_2)\in X\times Y$ was defined in (3.4).

Let (y_{n+1},u_{n+1}) be the solution of (3.14), with associated multiplier λ_{n+1}, and let λ^* be a multiplier for the equality constraint in (3.13). We assume Lipschitz continuity of solutions to (3.15), i.e. we assume the existence of a constant C such that:

$$|y_{n+1} - y^*| + |u_{n+1} - u^*| + |\lambda_{n+1} - \lambda^*| \le C\,|\Delta| \tag{3.16}$$

for all n. An example, illustrating the feasibility of this assumption is given at the end of the section. From the definition of Δ and assumption (3.16) we have local quadratic convergence of the sequential programming method (3.14):

$$|y_{n+1} - y^*| + |u_{n+1} - u^*| + |\lambda_{n+1} - \lambda^*| \leq M\,(|y_n - y^*|^2 + |u_n - u^*|^2 + |\lambda_n - \lambda^*|). \tag{3.17}$$

Utilizing the convexity assumption on F_2, the necessary optimality for (3.14) is given by

$$\begin{cases} F_1'(y) + (E_y(y,u)^* - E_y(y_n,u_n)^*)\lambda_n + E_y(y_n,u_n)^*\lambda = 0 \\ E_y(y_n,u_n)(y - y_n) + E_u(y_n,u_n)(u - u_n) + E(y_n,u_n) = 0. \\ F_2(v) - F_2(u) + ((E_u(y,u)^* - E_u(y_n,u_n)^*)\lambda_n + E_u(y_n,u_n)^*\lambda, v - u) \geq 0 \text{ for all } v \in \mathcal{C} \end{cases} \tag{3.18}$$

One can eliminate (y, λ) as a function of u by solving the first two equation for (y, λ), given u. This results in the following algorithm, for which a concrete special case is given in Example 4.5.

Algorithm 3: Sequential Programming III

1. Given $u \in \mathcal{C}$, solve the first two equations of (3.18) for $(y(u), \lambda(u))$.
2. Solve the variational inequality for $u \in \mathcal{C}$:

   $$F_2(v) - F_2(u) + ((E_u(y(u),u)^* - E_u(y_n,u_n)^*)\lambda_n + E_u(y_n,u_n)^*\lambda(u), v - u) \geq 0, \tag{3.19}$$

   for all $v \in \mathcal{C}$.
3. Set $u_{n+1} = u$. Iterate until convergence.

Example 3.1. Here we give a simple example illustrating assumption (3.16) and consider

$$\begin{cases} \min \frac{1}{2}|y - z|^2_{L^2} + \frac{\beta_1}{2}|u|^2_{L^2} + \beta_2|u|_{L^1} \\ \text{subject to} \\ -\Delta y = u \;\text{ on } \Omega,\; y = 0 \text{ on } \partial\Omega, \end{cases} \tag{3.20}$$

where $\beta_1 > 0, \beta_2 > 0$, and Ω is bounded domain with Lipschitz continuous boundary condition. We set $X = H^1_0(\Omega) \times L^2(\Omega)$ and $Y = H^{-1}(\Omega)$. Setting $\Delta_1 = (\Delta_1^1, \Delta_1^2) \in H^1_0(\Omega) \times L^2(\Omega)$ problem (3.15) can be expressed as

$$\begin{cases} \min \frac{1}{2}|y - z|^2_{L^2} + \frac{\beta_1}{2}|u|^2_{L^2} + \beta_2|u|_{L^1} + (\Delta_1^1, \Delta y)_{L^2} - (\Delta_1^2, u)_{L^2} \\ \text{subject to} \\ -\Delta y - u = \Delta_2 \;\text{ on } \Omega,\; y = 0 \text{ on } \partial\Omega, \end{cases}$$

and further, setting $\Delta_1^s = \Delta_1^1 + \Delta_1^2$, and $\zeta = \Delta^{-1}\Delta_2 + z$, where Δ denotes the Laplacian with Dirichlet boundary conditions,

$$\min \frac{1}{2}|(-\Delta)^{-1}u - \zeta|_{L^2}^2 + \frac{\beta_1}{2}|u|_{L^2}^2 + \beta_2|u|_{L^1} - (\Delta_1^s, u)_{L^2} - (\Delta_1^1, \Delta_2)_{L^2}.$$

The first order optimality condition for this problem is given by

$$((\beta_1 + \Delta^{-2})u + (-\Delta_1 + \Delta^{-1}\zeta), v - u)_{L^2} + \beta_2|v|_{L^1} - \beta_2|u|_{L^1} \geq 0 \text{ for all } v \in L^2(\Omega). \quad (3.21)$$

Let $(\bar{\Delta}_1, \bar{\Delta}_2) \in X \times Y$ denote another perturbation and let $\bar{u}$ be the associated solution to (3.21) with (Δ_1, Δ_2) replaced by $(\bar{\Delta}_1, \bar{\Delta}_2)$. From (3.21) used for u and $\bar{u}$ it follows that

$$\beta_1|u - \bar{u}|_{L^2}^2 \leq (|\Delta_1^s - \bar{\Delta}_1^s|_{L^2} + |(-\Delta)^{-1}(\zeta - \bar{\zeta})|_{L^2})|u - \bar{u}|_{L^2}.$$

Consequently there exists a constant C, independent of the perturbations, such that

$$\beta_1\,|u - \bar{u}|_{L^2} \leq C|\Delta - \bar{\Delta}|_{X \times Y}.$$

Using the primal equations, and the adjoint equations, which are given by

$$-\Delta\lambda = -(y - z), \text{ in } \Omega, \ \lambda = 0 \text{ on } \partial\Omega, \quad -\Delta\bar{\lambda} = -(\bar{y} - z), \text{ in } \Omega, \ \bar{\lambda} = 0 \text{ on } \partial\Omega,$$

we obtain

$$\beta_1\,|(y, u, \lambda) - (\bar{y}, \bar{u}, \bar{\lambda})|_{X \times Y^*} \leq C|\Delta - \bar{\Delta}|_{X \times Y},$$

for another constant C, independent of the perturbations. This is the desired Lipschitz continuous dependence.

4 Applications and numerical examples

In this section we first briefly describe the SP methods for two specific applications. Subsequently numerical results are presented.

Application 4.1. *(ODE Optimal Control Problem)* Let $x = (y, u) \in X = H^1(0, T; \mathbb{R}^n) \times L^2(0, T; \mathbb{R}^m)$ and consider the optimal control problem:

$$\begin{cases} \min \quad \int_0^T (\ell(y(t)) + h(u(t)))\,dt, \\ \text{subject to the dynamical constraint} \\ E(y, u) = -\frac{d}{dt}y(t) + f(y(t)) + Bu(t) = 0, \quad y(0) = y_0, \\ \text{and the control constraint } u \in \mathcal{C} = \{u(t) \in U, \ a.e.\}, \end{cases} \quad (4.1)$$

where U is a closed convex set in $\mathbb{R}^m$. Then, the necessary optimality condition for the linearized problem is given by

$$\begin{cases} E'(y_n, u_n)(y - y_n, u - u_n) + E(y_n, u_n) = -\dfrac{d}{dt}y + f'(y_n)(y - y_n) + f(y_n) + Bu = 0, y(0) = y_0, \\ F'(y) + E_y(y_n, u_n)\lambda = \dfrac{d}{dt}\lambda + f'(y_n)^t\lambda + \ell'(y) = 0, \lambda(T) = 0, \\ u(t) = \text{argmin}_{v \in U}\{h(v) + (B^t\lambda(t), v)\}. \end{cases}$$

If $h(u) = \frac{\alpha}{2}|u|^2$ and $U = \mathbb{R}^m$, then $u(t) = -\frac{B^t\lambda(t)}{\alpha}$. Thus, (2.2) is equivalent to solving the two point boundary value for (y, λ):

$$\begin{cases} \dfrac{d}{dt}y = f'(y_n)(y - y_n) + f(y_n) - \dfrac{1}{\alpha}BB^t\lambda, \quad y(0) = y_0, \\ -\dfrac{d}{dt}\lambda = f'(y_n)^*\lambda + \ell'(y), \quad \lambda(T) = 0. \end{cases}$$

Similarly, the second order update is equivalent to

$$\begin{cases} \dfrac{d}{dt}y = f'(y_n)(y - y_n) + f(y_n) - \dfrac{1}{\alpha}BB^t\lambda, \quad y(0) = y_0, \\ -\dfrac{d}{dt}\lambda = f'(y_n)^*\lambda + (f'(y) - f'(y_n))^*\lambda_n + \ell'(y), \quad \lambda(T) = 0. \end{cases}$$

Application 4.2. *(Nonlinear control in the coefficient problem)* For the state variable y and the control variable u we consider

$$\begin{cases} \min \dfrac{1}{2}\displaystyle\int_\Omega |y - z|^2\,dx + \dfrac{\beta}{2}\int_\Omega |u|^2\,dx + F_2(u), \\ \text{subject to} \\ -\mu\Delta y + g(y) + uy = 0 \text{ in } \Omega,\ y = 0 \text{ on } \partial\Omega, \end{cases}$$

where Ω is a bounded domain with boundary $\partial\Omega, \mu > 0, \beta > 0, z \in L^2(\Omega)$ is given, g is a possibly nonlinear mapping. At first the not necessarily quadratic term F_2 is mainly considered to illustrate how it effects different iterative algorithm. We shall return to it in Example 4.5 below. We next present the formalism for the first and second order SP methods.

The first order SP step solves

$$G_n(y_n, u_n)\begin{pmatrix} y \\ u \\ \lambda \end{pmatrix} = \begin{pmatrix} z \\ 0 \\ g'(y_n)y_n - g(y_n) + y_n u_n \end{pmatrix}, \tag{4.2}$$

for (y, u, λ), where

$$G_n(y_n, u_n) = \begin{pmatrix} I & 0 & -\mu\Delta_D + (g'(y_n) + u_n)I \\ 0 & \beta I + F_2'(\cdot) & y_n I \\ -\mu\Delta_D + (g'(y_n) + u_n)I & y_n I & 0 \end{pmatrix},$$

and Δ_D denotes the Laplace operators with Dirichlet. In the case of the predictor-corrector method the predictor solves (4.2) for $(\hat{y}, \hat{u}, \hat{\lambda})$ and in the corrector step (4.2) is solved with the new right hand side

$$\begin{pmatrix} (g'(y_n) - g'(\hat{y}_n))\lambda_n + (u_n - \hat{u}_n)\lambda_n + z \\ (y_n - \hat{y}_n)\lambda_n \\ g'(y_n)y_n - g(y_n) + y_n u_n \end{pmatrix}.$$

The second order update is given by

$$\hat{G}_n(y_n,u_n,\lambda_n)\begin{pmatrix}y\\u\\\lambda\end{pmatrix}=\begin{pmatrix}(g'(y_n)+u_n)\lambda_n+z\\y_n\lambda_n\\g'(y_n)y_n-g(y_n)+y_nu_n\end{pmatrix},$$

where

$$\hat{G}_n(y_n,u_n,\lambda_n)=\begin{pmatrix}I+\lambda_n g'(\cdot)I & \lambda_n I & -\mu\Delta_D+(g'(y_n)+u_n)I\\ \lambda_n I & \beta I+F_2'(\cdot) & y_n I\\ -\mu\Delta_D+(g'(y_n)+u_n)I & y_n I & 0\end{pmatrix}.$$

It can be checked that for $g=0$, the second order step coincides with the SQP-update.

It is worthwhile to compare the second order SP update with the SQP method. Assuming C^2 regularity of g and F_2 its update form is given by

$$G_{SQP_n}(y_n,u_n,\lambda_n)\begin{pmatrix}y\\u\\\lambda\end{pmatrix}=\begin{pmatrix}(g''(y_n)y_n+u_n)\lambda_n+z\\y_n\lambda_n-F'(u_n)+F''(u_n)u_n\\g'(y_n)y_n-g(y_n)+y_nu_n\end{pmatrix},$$

where

$$G_{SQP_n}(y_n,u_n,\lambda_n)=\begin{pmatrix}I+\lambda_n g''(y_n)I & \lambda_n I & -\mu\Delta_D+(g'(y_n)+u_n)I\\ \lambda_n I & \beta I+F_2''(u_n) & y_n I\\ -\mu\Delta_D+(g'(y_n)+u_n)I & y_n I & 0\end{pmatrix}.$$

The system matrices $G_n(y_n,u_n)$, $\hat{G}_n(y_n,u_n,\lambda_n)$ and $G_{SQP_n}(y_n,u_n,\lambda_n)$, differ foremost by the fact that λ_n does not appear in $G_n(y_n,u_n)$. The second-order SP method and the SQP method differ in the first equation, where the term $\lambda_n(g'(y_{n+1})-g'(y_n))$ is replaced by $\lambda_n g''(y_n)(y_{n+1}-y_n)$, and in the second equation, where $F_2'(u_{n+1})$ is replaced by $F_2'(u_n)+F''(u_n)(u_{n+1}-u_n)$ in the SQP step. In case that g' and F_2' are affine, these two methods coincide.

Partial second order SP-method Concerning the second order derivatives g'' and F_2'' in G_{SQP_n}, respectively the nonlinear terms g' and F_2' in $\hat{G}_n$, we shall investigate the following procedures in our numerical tests: Delete the $\lambda_n g'$ respectively $\lambda_n g''$ terms, and the corresponding term on the right hand side, if they lead to conditioning problems or are too complex. In the case that F_2 is a pointwise and convex operator, and not necessarily C^2, replace F_2'' by

$$F_2''(u_n)\sim\frac{F'(u_n)-F'(u_{n-1})}{u_n-u_{n-1}}. \tag{4.3}$$

We refer to this procedure as partial second order SP-method.

Next we turn to describing numerical experiments with the SP algorithms that we proposed. Most of the calculations were performed for variants of Application 4.2. In all the cases the we present results which are obtained without line searches. Unless specified otherwise, the step length is fixed to be $\alpha=.9$ and $F_2=0$. We monitored the evolution of the cost during the iteration to ensure that a local minimum rather than a genuine critical point is attained. All computations are initialized with $y_0=z, u_0=0$, and $\lambda_0=0$, if needed.

Example 4.1. Here we consider the bilinear control problem in Application 4.2 with $g = 0$, $\beta = 10^{-4}$, $\mu = 10^{-2}$, and the damping parameter was set to be $\alpha = .9$. The computations were carried out on a uniform 64×64 grid of the unit square, discretizing the control problem by a standard finite difference method and using a five point stencil for the Laplacian. In examples 4.1 - 4.3 we chose Neumann boundary conditions which allow to construct test cases which distinguish between states y which are uniformly bounded away from zero or not. Note that due to the bilinear structure of u and y in the state equation, the set $\mathcal{S} = \{x : y(x) = 0\}$ plays an important role, since on $\mathcal{S}$ the influence of u on the state is only given implicitly through other quantities of the control problem. At first we chose

$$z = \cos \pi x_1 \cdot \cos \pi x_2 + 2 + \delta \sin 4x_1 \cdot \sin 3x_2,\ g = -(1 + \mu\pi^2) \cos \pi x_1 \cos \pi x_2 - 2. \tag{4.4}$$

For this choice of g, and $u \equiv 1$, the solution to the state equals z with $\delta = 0$, and hence the term $\delta \sin 4x_1 \cdot \sin 3x_2$ can be considered as noise in the data. In this case the set $\mathcal{S}$ is empty. We denote by e the maximum of the L^2 error in the system of equations describing optimality, namely primal and adjoint equations and the optimality condition. For this example e was less than 10^{-8} in 8 iterations for the first order SP-method for $\delta = .5$. The first order convergence-rate-constant is less than .1.

For the next test we changed z and g to be

$$z = \cos \pi x_1 \cdot \cos \pi x_2 + \delta \sin 4x_1 \cdot \sin 3x_2,\ g = -(1 + \mu\pi^2) \cos \pi x_1 \cos \pi x_2. \tag{4.5}$$

In this case $\mathcal{S}$ is not empty anymore. The error e was found to be below 10^{-7} in 13 iterations with rate constant bounded by .51. To obtain $e < 10^{-8}$ the algorithm required 16 iterations.

Example 4.2. Here we compare the first and the second order SP-methods. First we computed with the second order method for the same specifications as in Example 4.1 with (4.5). The method converges q-quadratically and reaches a residue error level $\leq 10^{-13}$ in five iterations. If δ is changed from $\delta = .5$ to $\delta = 2$ seven iterations are required for the same stopping criterion. Next we changed β and μ to be $\beta = .01$ and $\mu = 10^{-4}$, expecting that $|\lambda|$ would increase compared to the earlier parameter settings. This is in fact the case, with the norm of the converged λ increasing from .001 to .033 as the pair (β, μ) is changed from $(.0001, .01)$ to $(.01, .0001)$. The second order method did not converge anymore even when reducing the (constant) step size as much as to $\alpha = .2$. The first order method converged with rate approximately .7. If β is further reduced to $\beta = .1$, then $|\lambda| = .1461$. The first order algorithm converges if the step-size parameter is reduced to $\alpha = .5$. Termination with $e < 10^{-8}$ is reached in 41 iterations.

Example 4.3. As before we use the default settings as in Example 4.1 with z as in (4.5), but now we change g to be $g(y) = |y| - (1 + \mu\pi^2) \cos \pi x_1 \cos \pi x_2$, so that the state equation becomes

$$-\mu\Delta y + |y| + uy = (1 + \mu\pi^2) \cos \pi x_1 \cos \pi x_2 \text{ in } \Omega, \quad y = 0 \text{ on } \partial\Omega.$$

Strictly speaking, the theory is not applicable for this nonlinearity but the example serves well the purpose that the proposed first order scheme can handle nonsmooth nonlinearities. In fact, convergence is reached after 17 iterations with rate constant bounded by .48. We also tested the predictor corrector version of the SP algorithm for the same problem and found convergence in 11 iterations with linear rate constant about .27. This improved convergence rate is consistent with the theoretical considerations in Section 3.1.

The second order partial SP-method, as explained at the end of Application 5.2 converges with linearly with rate constant .01 within 6 iterations for the generic choice $\alpha = .9$, and it converges quadratically within 4 iterations. If, however, μ is decreased to .0001 we cannot obtain convergence with the second order partial SP method, whereas the predictor corrector SP method converges within 33 iterations for $\alpha = .5$.

Example 4.4. Here we change from Neumann to Dirichlet boundary conditions and consider the case of the cubic nonlinearity with anti-monotone sign, specifically $g(y) = -y^3 - \sin(\pi(x_1 + x_2))$, and $F_2 = 0$. The equation constraint is therefore given by

$$-\mu\Delta y - y^3 + uy = \sin(\pi(x_1 + x_2)) \text{ in } \Omega,\ y = 0 \text{ on } \partial\Omega.$$

Further z is chosen as the solution to $-\Delta z + (1 + \sin(\pi(x_1 + x_2))z = \sin(\pi(x_1 + x_2))$. Note that on purpose the 'data' z are generated with a different diffusion coefficient, and without the nonlinear term. As above, unless specified otherwise, $\alpha = .9$, $\mu = .01$, and the grid size is 64×64.

We first tested with $\beta = 10^{-4}$. In this case the partial second order SP iteration converges (with the default $\alpha = .9$) in 8 iterations with linear convergence constant $\sim .13$. For this choice also SQP converges using full steps (almost) quadratically within 5 iterates.

We also carried out tests with $\beta = .05$, which leads to larger values of the iterates of the adjoint variables. In this case the partial second order SP method still converges with the default step length. This is not the case for the full SQP method which diverges unless a step size control is utilized or the fixed step length is reduzed to $\leq .4$.

Example 4.5. To illustrate Algorithm 3 we consider

$$\begin{cases} \min \dfrac{1}{2}\displaystyle\int_\Omega |y-z|^2\,dx + \int_\omega \big(\frac{\beta_1}{2}|u|^2 + \beta_2|u|\big)\,dx \\ \text{subject to} \\ -\mu\Delta y + yu = g \text{ in } \Omega, \quad \dfrac{\partial y}{\partial n} = 0 \text{ on } \partial\Omega, \end{cases} \tag{4.6}$$

where $g = g(x)$. Subproblem (3.19) of Algorithm 3 is the necessary optimality condition for

$$\min \frac{\beta_1}{2}|u|^2_{L^2} + \beta_2|u|_{L^1} + (\boldsymbol{f}, u) \tag{4.7}$$

where $\boldsymbol{f} = \boldsymbol{f}(y, \lambda) = \lambda_n(y(u) - y_n) + \lambda(u)y_n$ and $y = y(u), \lambda = \lambda(u)$ are the solutions to

$$\begin{aligned} &-\mu\Delta y + u_n y + y_n u = g + y_n u_n \quad \text{in}\,\Omega, && \frac{\partial y}{\partial n} = 0 \text{ on } \partial\Omega, \\ &-\mu\Delta\lambda + u_n\lambda + u\lambda_n = z - y + u_n\lambda \quad \text{in}\,\Omega, && \frac{\partial \lambda}{\partial n} = 0 \text{ on } \partial\Omega. \end{aligned}$$

We propose to solve (4.7) by a primal dual active set strategy. For this purpose we note that (4.7) is equivalent to

$$\begin{cases} 0 = \beta_1 u + \beta_2 p + \not{f} \\ p \in \partial |u|, \end{cases} \tag{4.8}$$

where the inclusion is equivalent to $u \in \partial I_K(p)$, with I_K to indicator function of the set $K = \{p \in L^2(\Omega) : -1 \le p(x) \le 1\}$. Thus (4.8) can be expressed as

$$\begin{cases} 0 = \beta_1 u + \beta_2 p + \not{f} \\ u = \max(0, u + p - 1) + \min(0, u + p + 1), \end{cases} \tag{4.9}$$

where the max and min operations act pointwise with respect to $x \in \Omega$. Thus u is the Lagrangian multiplier for the bilateral constraint $-1 \le p(x) \le 1$.

Given (y_n, u_n, λ_n) we use an iterative algorithm with variables $(y^k_{n+1}, u^k_{n+1}, \lambda^k_{n+1})$ to obtain $(y_{n+1}, u_{n+1}, \lambda_{n+1})$. For the description of the algorithm the index $n+1$ is not used.

Algorithm 3 (applied)

1. Choose a damping parameter $\alpha \in (0, 1]$, and set $(y^0, u^0, \lambda^0) = (y_n, u_n, \lambda_n)$, and $p^0 = \frac{1}{\beta_2}(\beta_1 u^0 + \not{f}(y_n, \lambda_n)) = -\frac{1}{\beta_2}(\beta_1 u^0 + \lambda_n y_n)$.

2. For $k = 0, \ldots,$ maxit:
   set

$$\mathcal{A}^k_+ = \{u^k + p^k - 1 > 0\},\ \mathcal{A}^k_- = \{u^k + p^k + 1 < 0\},\ \mathcal{A}^h = \mathcal{A}^k_+ \cup \mathcal{A}^k_-,$$
$$\mathcal{I} = \{u^k + p^k - 1 \le 0\} \cup \{u^k + p^k + 1 \ge 0\}.$$

   Set

$$\hat{u} = \begin{cases} 0 & \text{on } \mathcal{I}^k \\ -\dfrac{1}{\beta_1}(\lambda_n y^k + y_n \lambda^k - \lambda_n y_n) - \dfrac{\beta_2}{\beta_1} & \text{on } \mathcal{A}^k_+ \\ -\dfrac{1}{\beta_1}(\lambda_n y^k + y_n \lambda^k - \lambda_n y_n) + \dfrac{\beta_2}{\beta_1} & \text{on } \mathcal{A}^k_- \end{cases}$$

$$\hat{p} = \begin{cases} -\dfrac{1}{\beta_2}(\lambda_n(y^k - y_n) + \lambda^k y_n) & \text{on } \mathcal{I}^k \\ 1 & \text{on } \mathcal{A}^k_+ \\ -1 & \text{on } \mathcal{A}^k_-. \end{cases}$$

   Solve for $(\hat{y}, \hat{\lambda})$

$$\begin{pmatrix} -\mu\Delta + (u_n - \frac{y_n \lambda_n}{\beta_1}\chi_{\mathcal{A}^k})I & \frac{-y_n^2}{\beta_1}\chi_{\mathcal{A}^k} \\ I - \frac{\lambda_n^2}{\beta_1}\chi_{\mathcal{A}^k} I & -\mu\Delta + (u_n - \frac{y_n\lambda_n}{\beta_1})\chi_{\mathcal{A}^k} \end{pmatrix} \begin{pmatrix} y \\ \lambda \end{pmatrix} = \text{RHS},$$

where

$$RHS = \begin{pmatrix} g + y_n u_n - \frac{1}{\beta_1}\lambda_n y_n^2 \chi_{\mathcal{A}^k} + \frac{\beta_2}{\beta_1} y_n \chi_{\mathcal{A}_+^k} - \frac{\beta_2}{\beta_1} y_n \chi_{\mathcal{A}_-^k} \\ z + u_n \lambda_n - \frac{1}{\beta_1}\lambda_n^2 y_n \chi_{\mathcal{A}^k} + \frac{\beta_2}{\beta_1}\lambda_n \chi_{\mathcal{A}_+^k} - \frac{\beta_2}{\beta_1}\lambda_n \chi_{\mathcal{A}_-^k} \end{pmatrix},$$

with $\chi_{\mathcal{A}}$ the characteristic function of the set $\mathcal{A}$.

Set $(y^{k+1}, u^{k+1}, \lambda^{k+1}, p^{k+1}) = \alpha(\hat{y}, \hat{u}, \hat{\lambda}, \hat{p}) + (1-\alpha)(y^k, u^k, \lambda^k, p^k)$.

Set $k = k+1$.

3. Set $(y_{n+1}, u_{n+1}, \lambda_{n+1}) = (y^{\text{maxit}}, u^{\text{maxit}}, \lambda^{\text{maxit}})$.

Above $\mathcal{A}_+^k$ is shorthand for $\mathcal{A}_+^k = \{x : u^k(x) + p^k(x) - 1 > 0\}$. To initialize at level $n = 0$ we use $(y^0, u^0, \lambda^0) = (z, 1, 0)$. For the numerical example to be given below we chose maxit $= 3$. Further we updated the active/inactive sets and (u^k, p^k) 5 times per iteration without updating (y, λ), i.e. without solving (2).

We present a numerical result for the choice

$$z = \cos \pi x_1 \cos \pi x_2 + x_1 x_2 + \delta \sin 4x_1 \sin 3x_2,\ g = (1 + \mu\pi^2) \cos \pi t x_1 \cos \pi x_2 + x_1 x_2,$$

with $\mu = .01$, $\delta = .5$. For $\delta = 0$ we have $-\mu\Delta z + uz = g$ for $u \equiv 1$. Moreover, $\beta_1 = 0.01$, and $\beta_2 = 0.05$. The outer (n-) iteration was terminated after 12 iterations when the numerical error defined as the maximum over the L^2-norms of the primal and adjoint equations, and the two equations in (4.9) representing the complementarity condition, was smaller than 10^{-8}. For the damping parameter $\alpha = .7$ the linear convergence rate constant was $\sim .3$. The numerical solution for the control u is depicted in Figure 1. As expected due to the L^1-cost it has sparsity structure. Similar convergence properties were observed for the choice $(\beta_1, \beta_2) = 10^{-5}, 5 \cdot 10^{-5}$, for example.

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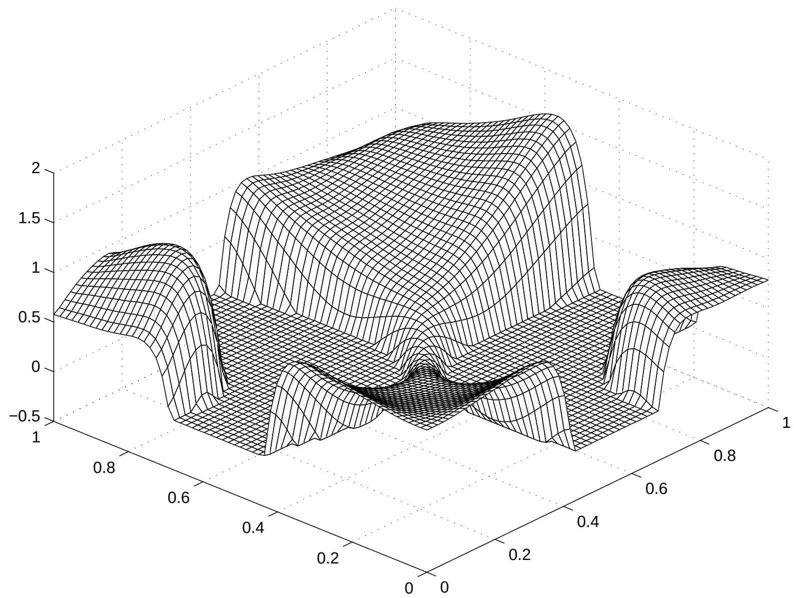

Figure 1: Example 4.5

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