NUMERICAL ANALYSIS AND MATHEMATICAL MODELLING
BANACH CENTER PUBLICATIONS, VOLUME 24
PWN POLISH SCIENTIFIC PUBLISHERS
WARSAW 1990

NUMERICAL SOLUTION OF SOME CLASSES OF COMPLEMENTARITY AND VARIATIONAL PROBLEMS VIA DUALIZATION

JOCHEN W. SCHMIDT

Department of Mathematics, Technical University of Dresden, Dresden, German Democratic Republic

1. Introduction

In this lecture a new numerical approach for solving some classes of linear complementarity problems and of discretized variational problems with side conditions is described. These problems have the common property that they can be formulated as optimization problems which, in the simplest case, are of the special structure

$$F(u) = \sum_{i=1}^{n} F_i(u_{i-1}, u_i) \to \text{Min!} \quad \text{s.t.}\,(u_{i-1}, u_i) \in W_i, \quad i = 1(1)n; \tag{1.1}$$

the functions $F_1, \ldots, F_n$: $R^2 \to R$ are supposed to be strictly convex and the sets $W_1 \subset R^2, \ldots, W_n \subset R^2$ to be closed and convex.

Problem (1.1) can be dualized so that the result is the unconstrained concave program

$$H(u^*) = -\sum_{i=1}^{n} H_i^*(u_{i-1}^*, -u_i^*) \to \text{Max!} \quad \text{with } u_0^* = u_n^* = 0; \tag{1.2}$$

here H_i^* denotes the Fenchel conjugate to F_i with the domain W_i,

$$H_i^*(\xi, \eta) = \sup\{\xi x + \eta y - F_i(x, y) \colon (x, y) \in W_i\}. \tag{1.3}$$

In several cases the two-dimensional programs (1.3) can be solved explicitly. Moreover, under additional assumptions the following return-formulas are valid:

$$u_{i-1} = \partial_1 H_i^*(u_{i-1}^*, -u_i^*), \quad u_i = \partial_2 H_i^*(u_{i-1}^*, -u_i^*), \quad i = 1(1)n. \tag{1.4}$$

Thus, the general strategy is to solve the unconstrained program (1.2) numerically, and then to determine the solution of the constrained program (1.1) by means of (1.4).

This new technique was developed by Burmeister, Heß and Schmidt [1], and Dietze and Schmidt [3] for solving shape preserving spline problems and then extended by Schmidt [8], [9] and Krätzschmar [6] to complementarity and variational problems. Now, the main results of these papers are outlined. In addition, some further extensions are presented; see especially Sections 6, 8.2 and 9. Of course, there are several other methods for solving variational problems computionally, e.g. relaxation methods, methods of gradient type, penalty methods. The reader is referred to the books of Glowinski, Lions and Trémolières [5], and Glowinski [4]. There are also given numerous examples from mechanics, elasticity, hydrodynamics and other areas which adequately can be modeled as constrained variational problems.

2. First examples for complementarity and variational problems

2.1. Tridiagonal linear complementarity problems. Let $A \in R^{(n+1)\times(n+1)}$ be a given symmetric positive definite and tridiagonal matrix and $b, c \in R^{n+1}$ be given vectors. The complementarity problem is that of finding a vector $u = (u_0, u_1, \ldots, u_n) \in R^{n+1}$ such that

$$Au+b \geqslant 0, \quad u \geqslant c, \quad (u-c)^T(Au+b) = 0. \tag{2.1}$$

In view of the Kuhn–Tucker theory this problem is seen to be equivalent to the constrained optimization problem

$$F(u) = u^T Au + 2b^T u \to \text{Min!} \quad \text{s.t. } u \geqslant c. \tag{2.2}$$

Now, it is always possible to pass from (2.2) to a problem (1.1). One way is as follows; see [8]. Let $\varepsilon > 0$ be such that $A - \varepsilon I$ is positive definite; here I denotes the unit matrix. E.g., take $\varepsilon \in (0, \lambda_{\min})$ where $\lambda_{\min}$ is the smallest eigenvalue of A.

Computationally such an ε can be determined by searching using Cholesky's algorithm. For a fixed ε having the desired property let

$$L = \begin{bmatrix} l_0 & & & \\ m_1 & l_1 & & \\ & \cdot & \cdot & \\ & & m_n & l_n \end{bmatrix}$$

be the Cholesky factor to $A - \varepsilon I$, i.e. $LL^T = A - \varepsilon I$. Then

$$\begin{aligned} F(u) &= u^T LL^T u + \varepsilon u^T u + 2b^T u \\ &= (l_0 u_0 + m_1 u_1)^2 + \varepsilon u_0^2 + \tfrac{1}{2}\varepsilon u_1^2 + 2b_0 u_0 \\ &\quad + \sum_{i=2}^{n-1} [(l_{i-1} u_{i-1} + m_i u_i)^2 + \tfrac{1}{2}\varepsilon(u_{i-1}^2 + u_i^2) + 2b_{i-1} u_{i-1}] \\ &\quad + (l_{n-1} u_{n-1} + m_n u_n)^2 + \tfrac{1}{2}\varepsilon u_{n-1}^2 + (\varepsilon + l_n^2) u_n^2 + 2b_{n-1} u_{n-1} + 2b_n u_n, \end{aligned} \tag{2.3}$$

and an objective function (1.1) is obtained by setting

$$F_1(x, y) = (l_0 x + m_1 y)^2 + \varepsilon x^2 + \tfrac{1}{2}\varepsilon y^2 + 2b_0 x,$$

(2.4) $$F_i(x, y) = (l_{i-1} x + m_i y)^2 + \tfrac{1}{2}\varepsilon(x^2+y^2) + 2b_{i-1} x, \qquad i = 2(1)n-1,$$

$$F_n(x, y) = (l_{n-1} x + m_n y)^2 + \tfrac{1}{2}\varepsilon x^2 + (\varepsilon + l_n^2) y^2 + 2b_{n-1} x + 2b_n y.$$

Because of $\varepsilon > 0$ the Hessians $F_1'', \ldots, F_n''$ are positive definite. Thus, the functions $F_1, \ldots, F_n$ are strictly convex. The sets $W_1, \ldots, W_n$ describing the constraints may be now, e.g.,

(2.5) $$W_i = \{(x, y) \in R^2 \colon\ x \geqslant c_{i-1},\ y \geqslant c_i\}, \qquad i = 1(1)n.$$

2.2. Discretized ordinary variational problems. Let be $\Omega = [0, 1]$, and $g \geqslant 0$ on Ω. A model problem is to find a function $u \in H^1(\Omega)$ such that

(2.6) $$\int_\Omega \{u' u' + guu - 2fu\}\, d\Omega \to \text{Min!}.$$

The side condition may be

(2.7) $$c \leqslant u \leqslant d \quad \text{on } \Omega,$$

or

(2.8) $$|u'| \leqslant 1 \text{ a.e.} \quad \text{on } \Omega.$$

Let $h > 0$ be the step size, $x_i = ih$ the nodes ($i = 0(1)n$, $nh = 1$), and u_i an approximation to $u(x_i)$ while $g_i = g(x_i)$, $f_i = f(x_i)$ and so on. Then a well-known finite difference approximation reads

(2.9) $$F(u) = \sum_{i=1}^{n} \left\{ \frac{(u_i - u_{i-1})^2}{h} + \frac{h}{2}(g_{i-1} u_{i-1}^2 + g_i u_i^2) - h(f_{i-1} u_{i-1} + f_i u_i) \right\} \to \text{Min!}$$

subject to

(2.10) $$c_i \leqslant u_i \leqslant d_i, \qquad i = 0(1)n,$$

or to

(2.11) $$|u_i - u_{i-1}| \leqslant h, \qquad i = 1(1)n.$$

Here, e.g. in the case of pointwise obstacles, some of the bounds c_i, d_i may be infinite.

For $g_{i-1} + g_i > 0$, $i = 1(1)n$, the functions

(2.12) $$F_i(x, y) = \frac{(y-x)^2}{h} + \frac{h}{2}(g_{i-1} x^2 + g_i y^2) - h(f_{i-1} x + f_i y)$$

are strictly convex. However, if $g_{i-1} = g_i = 0$ for at least one i some of these functions may be only convex. In this case one can proceed as follows; see [8]. If, in addition, the boundary $u_n = \beta$ is prescribed, set

$$(2.13)\quad F_i(x, y) = \frac{(y-x)^2}{h}+\frac{h}{2}(g_{i-1}x^2+g_i y^2)-\varepsilon_{i-1}x^2+\varepsilon_i y^2-h(f_{i-1}x+f_i y)$$

with $\varepsilon_0 = \varepsilon_{n-1} = \varepsilon_n = 0$. Now, choose $\varepsilon_{n-2}, \ldots, \varepsilon_2, \varepsilon_1$ according to

$$(2.14)\qquad \varepsilon_{i-1}\in(0,\ \varepsilon_i/(1+h\varepsilon_i)),\qquad i = n-1(-1)2,$$

starting with the value $\varepsilon_{n-1} = 1/h$. Then, by this ε-procedure the functions $F_1, \ldots, F_{n-2}, F_{n-1}+F_n$ defined by (2.13) become strictly convex.

For making the functions (2.12) strictly convex also the approach of 2.1 using Cholesky factorization applies.

In the case (2.10) the sets W_i may be, e.g.,

$$(2.15)\qquad W_i = \{(x, y)\in R^2:\ c_{i-1} \leqslant x \leqslant d_{i-1},\ c_i \leqslant y \leqslant d_i\}$$

while in the case (2.11) they are

$$(2.16)\qquad W_i = \{(x, y)\in R^2:\ |y-x| \leqslant h\}.$$

3. Description of the dualization technique for a model problem

3.1. Results from Fenchel's theory. In Fenchel's theory to the primal convex program

$$(3.1)\qquad \inf\{f(u)+g(u):\ u\in R^m\}$$

corresponds the dual concave program

$$(3.2)\qquad \sup\{-f^*(u^*)-g^*(-u^*):\ u^*\in R^m\};$$

here f, g: $R^m \to \bar{R} = R\cup\{+\infty, -\infty\}$ are assumed to be proper convex and closed while f^*, g^* are the conjugate functions defined by

$$(3.3)\qquad f^*(u^*) = \sup\{u^T u^*-f(u):\ u\in R^m\},$$

and analogously for g^*. The following essential duality statements are valid, see [13] and [7].

THEOREM. *Assume that the optimal value of program* (3.1) *is finite and that there exists a vector*

$$(3.4)\qquad z\in \operatorname{dom} f\cap \operatorname{dom} g,$$

such that f and g are z-stable. Then, program (3.2) *has an optimal solution, and the optimal values are equal,*

$$(3.5)\qquad \inf\{f(u)+g(u):\ u\in R^m\} = \max\{-f^*(u^*)-g^*(-u^*):\ u^*\in R^m\}.$$

In addition, if u^* denotes an optimal solution of (3.2) *then u is optimal for* (3.1) *if and only if u belongs to both subgradients $\partial f^*(u^*)$ and $\partial g^*(-u^*)$,*

$$u \in \partial f^*(u^*) \cap \partial g^*(-u^*). \tag{3.6}$$

For the definitions of proper convexity, z-stability and so on the reader is referred to [13].

3.2. Application to problem (1.1). An application of Fenchel's theory to program (1.1), which turned out to be numerically very interesting, has been elaborated in paper [3]. This work, in turn, was stimulated by the concrete example of a pair of dual programs given in [1].

Introducing the new variables $U_1, \ldots, U_{n-1}$, program (1.1) can be reformulated as a separable one,

$$\begin{gathered} \sum_{i=1}^{n} F_i(u_{i-1}, U_i) \to \text{Min!} \\ \text{s.t.}(u_{i-1}, U_i) \in W_i,\ i = 1(1)n,\ U_i = u_i,\ i = 1(1)n-1. \end{gathered} \tag{3.7}$$

Next define H_i: $R^2 \to \bar{R}$ by

$$H_i(x, y) = \begin{cases} F_i(x, y) & \text{for } (x, y) \in W_i, \\ +\infty & \text{otherwise.} \end{cases} \tag{3.8}$$

Then for $u = (u_0, U_1, u_1, \ldots, U_{n-1}, u_{n-1}, U_n) \in R^{2n}$ set

$$f(u) = \sum_{i=1}^{n} H_i(u_{i-1}, U_i), \tag{3.9}$$

$$g(u) = \begin{cases} 0 & \text{for } U_i = u_i,\ i = 1(1)n-1, \\ +\infty & \text{otherwise.} \end{cases} \tag{3.10}$$

By these definitions program (1.1) becomes a program (3.1). The occurring functions f and g are proper convex and closed.

For stating the corresponding dual program (3.2) the conjugate functions f^* and g^* have to be determined. Using the vector $u^* = (u_0^*, U_1^*, u_1^*, \ldots, U_{n-1}^*, u_{n-1}^*, U_n^*) \in R^{2n}$, in view of the separability of f one gets immediately

$$f^*(u^*) = \sum_{i=1}^{n} H_i^*(u_{i-1}^*, U_i^*), \tag{3.11}$$

where H_i^* is the Fenchel conjugate (1.3). Note that $H_1^*, \ldots, H_n^*$ are defined by programs which are only of the dimension 2. Further, it follows that

$$\begin{aligned} g^* u^* &= \sup\{u^T u^*:\ U_i = u_i,\ i = 1(1)n-1\} \\ &= \begin{cases} 0 & \text{for } u_0^* = 0,\ U_i^* + u_i^* = 0,\ i = 1(1)n-1,\ U_n^* = 0, \\ +\infty & \text{otherwise,} \end{cases} \\ &= g^*(-u^*). \end{aligned} \tag{3.12}$$

Thus, the dual program (3.2) reduces to (1.2).

If, e.g., $H_i^*(\xi, \eta) < +\infty$ for all $(\xi, \eta) \in R^2$ program (1.2) is unconstrained.

Further, let (1.1) be, e.g., a quadratic program with nonempty feasible domain. Then, a vector z having property (3.4) exists such that f and g are z-stable; see [3]. Hence, if (1.1) is solvable in addition, the mentioned duality theorem applies.

3.3. Return-formula (1.4). In addition, it is assumed that the auxiliary programs (1.3) are solvable for all $(\xi, \eta) \in R^2$. In the above examples this assumption holds since there (1.3) are quadratic programs and the Hessians of the objective functions are positive definite. Because of the strict convexity of F_i the maximizer $(\bar{x}_i(\xi, \eta), \bar{y}_i(\xi, \eta)) \in R^2$ in (1.3) is unique for fixed $(\xi, \eta) \in R^2$. Hence, since $(x, y) \in \partial H_i^*(\xi, \eta)$ holds if and only if (x, y) is a maximizer of (1.3), the differentiability of H_i^* follows, and

$$\bar{x}_i(\xi, \eta) = \partial_1 H_i^*(\xi, \eta), \quad \bar{y}_i(\xi, \eta) = \partial_2 H_i^*(\xi, \eta), \quad i = 1(1)n. \tag{3.13}$$

In addition, the partial derivatives are continuous.

Further, let u^* be optimal for (3.2). Then $g^*(-u^*) = 0$ follows, and the Kuhn–Tucker conditions for (3.2), i.e. for

$$\inf\{f^*(u^*)\colon\ u_0^* = 0,\ U_i^* + u_i^* = 0,\ i = 1(1)n-1,\ U_n^* = 0\}$$

yield

$$\partial_1 H_{i+1}^*(u_i^*, U_{i+1}^*) = \partial_2 H_i^*(u_{i-1}^*, U_i^*), \quad i = 1(1)n-1.$$

Now, define the vector u by

$$u_{i-1} = \partial_1 H_i^*(u_{i-1}^*, U_i^*), \quad U_i = \partial_2 H_i^*(u_{i-1}^*, U_i^*), \quad i = 1(1)n.$$

Then one gets $g(u) = 0$, $u^T u^* = 0$, and thus $g^*(-u^*) + g(u) = -u^T u^*$. Hence $u \in \partial g^*(-u^*)$ follows. Further, because of $u = \partial f^*(u^*)$, relation (3.6) is valid, and u solves (3.1). Thus, the present assumptions imply the

PROPOSITION. *Let $(u_0^*, u_1^*, \ldots, u_n^*)$ be a solution of the dual program* (1.2). *Then the vector $(u_0, u_1, \ldots, u_n)$ determined by return-formula* (1.4) *is the unique solution of the primal program* (1.1).

4. Examples for conjugate functions

Here some examples for Fenchel conjugates (1.3) are given; see [8]. With regard to (2.4), (2.5) let F_i and W_i be

$$F_i(x, y) = (lx + my)^2 + \varepsilon x^2 + \delta y^2 + px + qy, \tag{4.1}$$

$$W_i = \{(x, y) \in R^2\colon\ x \geq \alpha,\ y \geq \beta\}. \tag{4.2}$$

Using the abbreviations

$$\varphi = \xi - p, \quad \psi = \eta - q, \tag{4.3}$$

$$c = \delta l^2 + \varepsilon m^2 + \varepsilon\delta > 0, \quad d = m^2 + \delta > 0, \quad e = l^2 + \varepsilon > 0, \quad b = lm, \tag{4.4}$$

the Fenchel conjugate (1.3) to (4.1), (4.2) reads

(4.5) $$H_i^*(\xi, \eta)$$

$$= \frac{d\varphi^2 - 2b\varphi\psi + e\psi^2}{4c} \quad \text{for } d\varphi - b\psi \geqslant 2\alpha c,\ e\psi - b\varphi \geqslant 2\beta c;$$

$$= \frac{\psi^2 + 4\alpha(d\varphi - b\psi - \alpha c)}{4d} \quad \text{for } d\varphi - b\psi \leqslant 2\alpha c,\ \psi \geqslant 2\beta d + 2\alpha b;$$

$$= \frac{\varphi^2 + 4\beta(e\psi - b\varphi - \beta c)}{4e} \quad \text{for } e\psi - b\varphi \leqslant 2\beta c,\ \varphi \geqslant 2\alpha e + 2\beta b;$$

$$= \alpha\varphi + \beta\psi - \alpha^2 e - 2\alpha\beta b - \beta^2 d \quad \text{for } \varphi \leqslant 2\alpha e + 2\beta b,\ \psi \leqslant 2\beta d + 2\alpha b.$$

This is easily verified. In the discretized variational problem (2.9) with lower bounds only, substitute

(4.6) $$l = -1/\sqrt{h}, \quad m = 1/\sqrt{h}$$

in (4.4), (4.5) in order to get H_i^*. For two-sided obstacles the Fenchel conjugate is computed in [8].

In view of (2.9), (2.11) the conjugate corresponding to

(4.7) $$F_i(x, y) = \frac{(y-x)^2}{h} + \varepsilon x^2 + \delta y^2 + px + qy,$$

(4.8) $$W_i = \{(x, y) \in R^2 \colon |y - x| \leqslant h\}$$

is of interest:

(4.9) $$H_i^*(\xi, \eta)$$

$$= \frac{d\varphi^2 - 2b\varphi\psi + e\psi^2}{4c} \quad \text{for } -2hc \leqslant \delta\varphi - \varepsilon\psi \leqslant 2hc;$$

$$= \frac{(\varphi+\psi)^2 + 4h\delta\varphi - 4h\varepsilon\psi - 4h(\varepsilon+\delta) - 4h^2\varepsilon\delta}{4(\varepsilon+\delta)} \quad \text{for } \delta\varphi - \varepsilon\psi \geqslant 2hc;$$

$$= \frac{(\varphi+\psi)^2 - 4h\delta\varphi + 4h\varepsilon\psi + 4h(\varepsilon+\delta) - 4h^2\varepsilon\delta}{4(\varepsilon+\delta)} \quad \text{for } \delta\varphi - \varepsilon\psi \leqslant -2hc;$$

here choose the quantities l and m in (4.4) according to (4.6).

5. Numerical aspects

For solving problems (1.1) numerically the described results can be used as follows:

Step 0. Transformation of a given problem into a program (1.1). For complementarity problems see 2.1 where this step is performed via Cholesky factorization.

Step 1. Test whether the feasible domain of (1.1) is nonempty or not. This can be done by an algorithm developed in [11] and independently in [2].

Step 2. Computation of a solution of the unconstrained dual program (1.2). In computer tests Newton's method proved here to be very effective.

Step 3. Determination of the solution of (1.1) via return-formula (1.4).

Implementations of this general procedure have been tested on several real problems; see e.g. [1], [6], [8], [12]. In the treated spline problems this approach leads to algorithms for which the arithmetical complexity is $O(n)$. This depends essentially on the facts that Newton's method for (1.2)

$$(5.1)\qquad \begin{aligned} 0 = &-\partial_2 H_i^*(u_{i-1}^*, -u_i^*) + \partial_1 H_{i+1}^*(u_i^*, -u_{i+1}^*) \\ &-\partial_1 \partial_2 H_i^*(u_{i-1}^*, -u_i^*)(\tilde{u}_{i-1}^* - u_{i-1}^*) \\ &+\{\partial_2 \partial_2 H_i^*(u_{i-1}^*, -u_i^*) + \partial_1 \partial_1 H_{i+1}^*(u_i^*, -u_{i+1}^*)\}(\tilde{u}_i^* - u_i^*) \\ &-\partial_1 \partial_2 H_{i+1}^*(u_i^*, -u_{i+1}^*)(\tilde{u}_{i+1}^* - u_{i+1}^*), \qquad i = 1(1)n-1, \end{aligned}$$

is a tridiagonal system for the new iterates $\tilde{u}_1^*, \ldots, \tilde{u}_{n-1}^*$, and that (1.2) is solved really by (5.1) in a very small number of steps. Theoretically, in the case of quadratic programs (1.1), method (5.1) can be shown to terminate after a finite number of steps by entering into a cycle of integer length.

In [8] the following variational problem with side conditions is used for computational tests:

$$(5.2)\qquad \begin{aligned} &\int_0^1 \{u'(t)^2 - 2u(t)\sin 4\pi t\}\, dt \to \text{Min!} \\ &\text{s.t. } u(0) = u(1) = 0,\ u(t) \geqslant 0 \text{ for } 0 \leqslant t \leqslant 1. \end{aligned}$$

The discretization (2.9) is, after applying an ε-procedure, dualized in the sense of (1.2). The behaviour of Newton's method (5.1) applied to (1.2) depends on the starting vector, of course, and even divergence may occur. In this case a combination with the gradient method is recommended. In the present example using the starting values $u_1^* = \ldots = u_{n-1}^* = 0$ Newton's method always worked.

For some dimensions $n = 1/h$ the numbers of Newton steps are given in the following table:

n	8	16	32	64	128	256
Newton steps	2	4	9	13	25	61

Indeed, the number of steps now increases rather rapidly with n. Notice for this that the matrix A_n which describes the present program (2.9) becomes singular as n tends to infinity.

6. Linear complementarity problems with band matrices

6.1. 5-Diagonal matrices. Here, once more the complementarity problem (2.1) is considered, but the matrix A should be now 5-diagonal. Again, A is supposed to be symmetric and positive definite. Let $\varepsilon > 0$ be such that $A-\varepsilon I$ is also positive definite, and let

$$L = \begin{bmatrix} l_0 & & & & \\ m_1 & l_1 & & & \\ n_2 & m_2 & l_2 & & \\ \ddots & \ddots & \ddots & & \\ & n_n & m_n & l_n \end{bmatrix}$$

be the Cholesky factor to $A-\varepsilon I$. Then one gets

(6.1)

$$\begin{aligned} F(u) &= u^T Au+2b^T u = u^T LL^T u+\varepsilon u^T u+2b^T u \\ &= (l_0 u_0+m_1 u_1+n_2 u_2)^2+\varepsilon u_0^2+\tfrac{1}{2}\varepsilon u_1^2+\tfrac{1}{3}\varepsilon u_2^2+2b_0 u_0 \\ &\quad +(l_1 u_1+m_2 u_2+n_3 u_3)^2+\tfrac{1}{2}\varepsilon u_1^2+\tfrac{1}{3}\varepsilon u_2^2+\tfrac{1}{3}\varepsilon u_3^2+2b_1 u_1 \\ &\quad +\sum_{i=3}^{n-3} (l_{i-1} u_{i-1}+m_i u_i+n_{i+1} u_{i+1})^2+\tfrac{1}{3}\varepsilon(u_{i-1}^2+u_i^2+u_{i+1}^2) \\ &\quad +2b_{i-1} u_{i-1}+(l_{n-3} u_{n-3}+m_{n-2} u_{n-2}+n_{n-1} u_{n-1})^2+\tfrac{1}{3}\varepsilon u_{n-3}^2+\tfrac{1}{3}\varepsilon u_{n-2}^2 \\ &\quad +\tfrac{1}{2}\varepsilon u_{n-1}^2+2b_{n-3} u_{n-3}+(l_{n-2} u_{n-2}+m_{n-1} u_{n-1}+n_n u_n)^2 \\ &\quad +\tfrac{1}{3}\varepsilon u_{n-2}^2+(l_{n-1} u_{n-1}+m_n u_n)^2+\tfrac{1}{2}\varepsilon u_{n-1}^2+(\varepsilon+l_n^2)u_n^2 \\ &\quad +2(b_{n-2} u_{n-2}+b_{n-1} u_{n-1}+b_n u_n). \end{aligned}$$

By means of this procedure the 5-diagonal complementarity problem (2.1) is reformulated as a program of the special structure

$$\begin{aligned} &F(u) = \sum_{i=1}^{n-1} F_i(u_{i-1}, u_i, u_{i+1}) \to \text{Min!} \\ &\text{s.t.} (u_{i-1}, u_i, u_{i+1}) \in W_i,\ i = 1(1)n-1. \end{aligned} \tag{6.2}$$

The functions $F_1, \ldots, F_{n-1}$: $R^3 \to R^1$ are strictly convex while the sets $W_1 \subset R^3, \ldots, W_{n-1} \subset R^3$ are closed and convex.

In order to dualize this program it is written as a separable one by introducing new variables,

$$\begin{aligned} &\sum_{i=1}^{n-1} F_i(u_{i-1}, U_i, V_{i+1}) \to \text{Min!} \\ &\text{s.t.} (u_{i-1}, U_i, V_{i+1}) \in W_i,\ i = 1(1)n-1,\ U_1 = u_1,\ V_i = U_i = u_i, \\ &\qquad i = 2(1)n-2,\ V_{n-1} = U_{n-1}. \end{aligned} \tag{6.3}$$

Following the lines described in 3.2 an intermediate dual program is seen to be

$$(6.4)\qquad \begin{aligned} &-\sum_{i=1}^{n-1} H_i^*(u_{i-1}^*, U_i^*, V_{i+1}^*) \to \text{Max!} \\ &\text{with } u_0^* = 0,\ U_1^* + u_1^* = 0,\ V_i^* + U_i^* + u_i^* = 0,\ i = 2(1)n-2, \\ &\qquad\qquad V_{n-1}^* + U_{n-1}^* = 0,\ V_n^* = 0. \end{aligned}$$

Setting $V_i^* = v_i^*$ and $U_i^* = -u_i^* - v_i^*$ a dual program corresponding to (6.2) reads

$$(6.5)\qquad \begin{aligned} &H(u^*, v^*) = -\sum_{i=1}^{n-1} H_i^*(u_{i-1}^*, -u_i^* - v_i^*, v_{i+1}^*) \to \text{Max!} \\ &\text{with } u_0^* = v_1^* = u_{n-1}^* = v_n^* = 0. \end{aligned}$$

Here H_i^* denotes the Fenchel conjugate to F_i and W_i,

$$(6.6)\qquad H_i^*(\xi, \eta, \zeta) = \sup\{\xi x + \eta y + \zeta z - F_i(x, y, z) \colon (x, y, z) \in W_i\}.$$

In the present situation H_i^* is also easily computed explicitly.

Newton's method applied to (6.4) leads to linear systems which are now block-tridiagonal with (2,2)-blocks.

The essential return-formula (1.4) also carries over. Following the lines of 3.3 one gets under the same assumptions

$$(6.7)\qquad \begin{aligned} u_{i-1} &= \partial_1 H_i^*(u_{i-1}^*, -u_i^* - v_i^*, v_{i+1}^*), \\ u_i &= \partial_2 H_i^*(u_{i-1}^*, -u_i^* - v_i^*, v_{i+1}^*), \\ u_{i+1} &= \partial_3 H_i^*(u_{i-1}^*, -u_i^* - v_i^*, v_{i+1}^*), \qquad i = 1(1)n-1. \end{aligned}$$

6.2. 7-Diagonal and general band matrices. As now is obvious, the complementarity problem (2.1) with a 7-diagonal symmetric and positive definite matrix A can be transformed into a program

$$(6.8)\qquad \begin{aligned} &F(u) = \sum_{i=1}^{n-2} F_i(u_{i-1}, u_i, u_{i+1}, u_{i+2}) \to \text{Min!} \\ &\text{s.t.} (u_{i-1}, u_i, u_{i+1}, u_{i+2}) \in W_i, \qquad i = 1(1)n-2, \end{aligned}$$

and the functions $F_1, \ldots, F_{n-2}\colon R^4 \to R^1$ are strictly convex. Along the lines of 3.2 one is led to the dual program

$$(6.9)\qquad \begin{aligned} &H(u^*, v^*, z^*) = -\sum_{i=1}^{n-2} H_i^*(u_{i-1}^*, -u_i^* - v_i^*, v_{i+1}^* + z_{i+1}^*, -z_{i+2}^*) \to \text{Max!} \\ &\text{with } u_0^* = v_1^* = z_2^* = u_{n-2}^* = v_{n-1}^* = z_n^* = 0, \end{aligned}$$

where

(6.10)

$$H_i^*(\xi, \eta, \zeta, \omega) = \sup\{\xi x+\eta y+\zeta z+\omega w-F_i(x, y, z, w): (x, y, z, w)\in W_i\}.$$

The linear Newton systems for (6.9) here are block-tridiagonal with (3,3)-blocks.

Under the usual assumptions the return-formula turns out to be

$$\begin{aligned} u_{i-1} &= \partial_1 H_i^*(u_{i-1}^*, -u_i^*-v_i^*, v_{i+1}^*+z_{i+1}^*, -z_{i+2}^*),\\ u_i &= \partial_2 H_i^*(u_{i-1}^*, -u_i^*-v_i^*, v_{i+1}^*+z_{i+1}^*, -z_{i+2}^*),\\ u_{i+1} &= \partial_3 H_i^*(u_{i-1}^*, -u_i^*-v_i^*, v_{i+1}^*+z_{i+1}^*, -z_{i+2}^*),\\ u_{i+2} &= \partial_4 H_i^*(u_{i-1}^*, -u_i^*-v_i^*, v_{i+1}^*+z_{i+1}^*, -z_{i+2}^*), \qquad i = 1(1)n-2. \end{aligned}$$

This approach likewise applies to complementarity problems with general band matrices. In view of the previous explanations it seems to be not necessary to give details.

7. Higher order finite elements in ordinary variational problems

Finite elements methods of higher order applied to (2.6) require to treat the following generalization of program (1.1):

$$(7.1)\qquad \begin{aligned} &F(u, v) = \sum_{i=1}^{n} F_i(u_{i-1}, u_i, v_i)\to \text{Min!}\\ &\text{s.t.}\,(u_{i-1}, u_i, v_i)\in W_i, \qquad i = 1(1)n. \end{aligned}$$

Under the usual assumptions a dual program to (7.1) reads

$$(7.2)\qquad H(u^*) = -\sum_{i=1}^{n} H_i^*(u_{i-1}^*, -u_i^*, 0)\to \text{Max!} \qquad \text{with } u_0^* = u_n^* = 0,$$

where

$$(7.3)\qquad H_i^*(\xi, \eta, \zeta) = \sup\{\xi x+\eta y+\zeta z-F_i(x, y, z): (x, y, z)\in W_i\},$$

and the return-formula turns out to be now

$$(7.4)\qquad \begin{aligned} u_{i-1} &= \partial_1 H_i^*(u_{i-1}^*, -u_i^*, 0),\\ u_i &= \partial_2 H_i^*(u_{i-1}^*, -u_i^*, 0),\\ v_i &= \partial_3 H_i^*(u_{i-1}^*, -u_i^*, 0), \qquad i = 1(1)n. \end{aligned}$$

For more details concerning also the application the reader is referred to [6].

8. Discretized partial variational problems

Here the following $2D$ model problem is considered: Find $u \in H^1(\Omega)$, $\Omega = [0, 1] \times [0, 1]$ with

$$\int_\Omega \{\operatorname{grad} u \operatorname{grad} u + g u^2 - 2fu\} \, d\Omega \to \text{Min!} \tag{8.1}$$

$$\text{s.t. } c \leqslant u \leqslant d \quad \text{on } \Omega, \tag{8.2}$$

or

$$\text{s.t. } |\operatorname{grad} u| \leqslant 1 \text{ a.e.} \quad \text{on } \Omega, \tag{8.3}$$

where $g \geqslant 0$ on Ω.

8.1. A first discretization. Let $h > 0$ be the step size $x_i = ih$, $nh = 1$, and (x_i, x_j) the nodes. Denote by u_{ij} an approximation to $u(x_i, x_j)$. Then, if approximating problem (8.1), (8.2) by the finite difference method which corresponds to (2.9) a program of the structure

$$\begin{aligned} F(u) = \sum_{i=1}^{n} \sum_{j=0}^{n} F_{ij}(u_{i-1j}, u_{ij}) + \sum_{i=0}^{n} \sum_{j=1}^{n} G_{ij}(u_{ij-1}, u_{ij}) &\to \text{Min!} \\ \text{s.t. } (u_{i-1j}, u_{ij}) \in V_{ij}, \; i = 1(1)n, \; j = 0(1)n, & \\ (u_{ij-1}, u_{ij}) \in W_{ij}, \; i = 0(1)n, \; j = 1(1)n, & \end{aligned} \tag{8.4}$$

arises. The functions F_{ij}, G_{ij}: $R^2 \to R^1$ are supposed to be strictly convex, the sets $V_{ij} \subset R^2$, $W_{ij} \subset R^2$ to be closed and convex. Following the lines of 3.2 the unconstrained dual program

$$\begin{aligned} H(u^*, v^*, w^*) = & -\sum_{i=1}^{n} \sum_{j=0}^{n} H^*_{ij}(u^*_{i-1j}, -u^*_{ij} - w^*_{ij}) \\ & -\sum_{i=0}^{n} \sum_{j=1}^{n} K^*_{ij}(v^*_{ij-1}, -v^*_{ij} + w^*_{ij}) \to \text{Max!} \end{aligned} \tag{8.5}$$

with $u^*_{0j} = -w^*_{0j}$, $u^*_{nj} = 0$, $j = 0(1)n$, $v^*_{i0} = w^*_{i0}$, $v^*_{in} = 0$, $i = 0(1)n$,

is obtained, where

$$\begin{aligned} H^*_{ij}(\xi, \eta) &= \sup\{\xi x + \eta y - F_{ij}(x, y): \; (x, y) \in V_{ij}\}, \\ K^*_{ij}(\xi, \eta) &= \sup\{\xi x + \eta y - G_{ij}(x, y): \; (x, y) \in W_{ij}\}. \end{aligned} \tag{8.6}$$

The return-formula now reads

$$\begin{aligned} u_{i-1j} &= \partial_1 H^*_{ij}(u^*_{i-1j}, -u^*_{ij} - w^*_{ij}), \\ u_{ij} &= \partial_2 H^*_{ij}(u^*_{i-1j}, -u^*_{ij} - w^*_{ij}), \quad i = 1(1)n, \; j = 0(1)n, \\ u_{ij-1} &= \partial_1 K^*_{ij}(v^*_{ij-1}, -v^*_{ij} + w^*_{ij}), \\ u_{ij} &= \partial_2 K^*_{ij}(v^*_{ij-1}, -v^*_{ij} + w^*_{ij}), \quad i = 0(1)n, \; j = 1(1)n. \end{aligned} \tag{8.7}$$

This approach has been developed in [6]. There are also given some numerical results.

8.2. A second discretization. In order to cover finite difference approximations to problem (8.1), (8.3) and also some finite element approximations to (8.1), (8.2) as well as to (8.1), (8.3) one has to treat programs of the type

$$(8.8)\quad \begin{aligned} & F(u) = \sum_{i=1}^{n}\sum_{j=1}^{n} F_{ij}(u_{i-1j-1}, u_{ij-1}, u_{i-1j}, u_{ij}) \to \text{Min!} \\ & \text{s.t.} (u_{i-1j-1}, u_{ij-1}, u_{i-1j}, u_{ij}) \in W_{ij},\ i = 1(1)n,\ j = 1(1)n \end{aligned}$$

with strictly convex functions F_{ij}: $R^4 \to R^1$ and closed convex sets $W_{ij} \subset R^4$. For dualizing (8.8) the Fenchel conjugate to F_{ij} and W_{ij} has to be determined according to

$$(8.9)\quad H_{ij}^*(\xi, \eta, \varrho, \sigma) = \sup\{\xi x + \eta y + \varrho r + \sigma s - F_{ij}(x, y, r, s): (x, y, r, s) \in W_{ij}\}.$$

Then, the program

$$H(u^*, v^*, z^*) = -\sum_{i=1}^{n}\sum_{j=1}^{n} H_{ij}^*(u_{i-1j-1}^*, v_{ij-1}^*, -u_{i-1j}^* - z_{i-1j}^*, -v_{ij}^* + z_{ij}^*) \to \text{Max!}$$

$$(8.10)\qquad \begin{aligned} \text{with } & u_{i0}^* = -z_{i0}^*,\ v_{i0}^* = z_{i0}^*,\ u_{in}^* = v_{in}^* = 0,\ i = 0(1)n, \\ & v_{0j}^* = z_{0j}^* = 0,\ u_{nj}^* = z_{nj}^* = 0,\ j = 0(1)n, \end{aligned}$$

is dual to (8.8), and the return-formula carries over. If a solution (u^*, v^*, z^*) of (8.10) is known, the solution u of (8.8) is computed directly by

$$(8.11)\quad \begin{aligned} u_{i-1j-1} &= \partial_1 H_{ij}^*(u_{i-1j-1}^*, v_{ij-1}^*, -u_{i-1j}^* - z_{i-1j}^*, -v_{ij}^* + z_{ij}^*), \\ u_{ij-1} &= \partial_2 H_{ij}^*(u_{i-1j-1}^*, v_{ij-1}^*, -u_{i-1j}^* - z_{i-1j}^*, -v_{ij}^* + z_{ij}^*), \\ u_{i-1j} &= \partial_3 H_{ij}^*(u_{i-1j-1}^*, v_{ij-1}^*, -u_{i-1j}^* - z_{i-1j}^*, -v_{ij}^* + z_{ij}^*), \\ u_{ij} &= \partial_4 H_{ij}^*(u_{i-1j-1}^*, v_{ij-1}^*, -u_{i-1j}^* - z_{i-1j}^*, -v_{ij}^* + z_{ij}^*), \\ & \qquad i = 1(1)n,\ j = 1(1)n. \end{aligned}$$

The details of this approach are intended to be discussed in a forthcoming paper.

9. A general program

A more general program covering all programs treated up to now reads as follows,

$$(9.1)\quad \begin{aligned} & \sum_{(i,j,k,l)\in Z} F_{ijkl}(u_i, u_j, u_k, u_l, v_{ijkl}) \to \text{Min!} \\ & \text{s.t.} (u_i, u_j, u_k, u_l, v_{ijkl}) \in W_{ijkl},\ (i, j, k, l) \in Z. \end{aligned}$$

Here Z is a given set of ordered 4-indices,

$$Z \subset \{(i, j, k, l):\ 0 \leqslant i < j < k < l \leqslant n\}.$$

The functions F_{ijkl}: $R^5 \to R^1$ are assumed to be strictly convex, the sets $W_{ijkl} \subset R^5$ to be closed and convex.

For fixed i let Z_i be the following set of 3-indices:

$$Z_i = \{(j, k, l):\ (i, j, k, l) \in Z \text{ or } (l, i, j, k) \in Z \text{ or } (k, l, i, j) \in Z \text{ or } (j, k, l, i) \in Z\}. \tag{9.2}$$

Then, a program dual to (9.1) can be formulated,

$$\begin{aligned} &-\sum_{(i,j,k,l)\in Z} H^*_{ijkl}(u^*_{ijkl}, u^*_{jkli}, u^*_{klij}, u^*_{lijk}, 0) \to \text{Max!} \\ &\text{with } \sum_{(j,k,l)\in Z_i} u^*_{ijkl} = 0,\ i = 0(1)n. \end{aligned} \tag{9.3}$$

Of course, this program is unconstrained since the occurring equality constraints are easily eliminated. The function H^*_{ijkl} is defined by

$$H^*_{ijkl}(\xi, \eta, \varrho, \sigma, \zeta) = \sup\{\xi x + \eta y + \varrho r + \sigma s + \zeta z - F_{ijkl}(x, y, r, s, z):\ (x, y, r, s, z) \in W_{ijkl}\}. \tag{9.4}$$

Finally, the corresponding return-formula is given,

$$\begin{aligned} u_i &= \partial_1 H^*_{ijkl}(u^*_{ijkl}, u^*_{jkli}, u^*_{klij}, u^*_{lijk}, 0), \\ u_j &= \partial_2 H^*_{ijkl}(u^*_{ijkl}, u^*_{jkli}, u^*_{klij}, u^*_{lijk}, 0), \\ u_k &= \partial_3 H^*_{ijkl}(u^*_{ijkl}, u^*_{jkli}, u^*_{klij}, u^*_{lijk}, 0), \\ u_l &= \partial_4 H^*_{ijkl}(u^*_{ijkl}, u^*_{jkli}, u^*_{klij}, u^*_{lijk}, 0), \\ v_{ijkl} &= \partial_5 H^*_{ijkl}(u^*_{ijkl}, u^*_{jkli}, u^*_{klij}, u^*_{lijk}, 0), \quad (i, j, k, l) \in Z. \end{aligned} \tag{9.5}$$

10. A further generalization

In the preceding theory the variables u_i, v_i, u_{ij}, v_{ijkl} are assumed to be real numbers. However, all results are also valid for variables being real vectors. In paper [10], a spline problem is considered which leads to a program (1.1) where the variables $u_0, \ldots, u_n$ are two-dimensional vectors.

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Presented to the Semester
Numerical Analysis and Mathematical Modelling
February 25 – May 29, 1987