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Fast interior point solvers for $H^1$-regularized PDE-constrained optimization problems

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We consider Newton systems arising from the interior point solution of PDE-constrained optimization problems. In particular, we examine problems where the control variable is regularized by an $H^1$-norm within the cost functional. We present preconditioned iterative methods for the resulting matrix systems, and justify the potency of our approach through numerical experiments.

1 Problem statement

We consider linear, time-independent PDE-constrained optimization problems with additional bound constraints, of the form:

$$\min_{y,u} \frac{1}{2} \|y - \hat{y}\|_{L_2(\Omega)}^2 + \frac{\beta}{2} \|u\|_{H^1(\Omega)}^2$$

s.t. \hspace{1cm} \mathcal{D}y = u, \quad \text{in } \Omega,
\hspace{1cm} y = f, \quad \text{on } \partial\Omega,
\hspace{1cm} y_a \leq y \leq y_b, \quad \text{a.e. in } \Omega,
\hspace{1cm} u_a \leq u \leq u_b, \quad \text{a.e. in } \Omega,

where $y$ and $u$ denote state and control variables which we wish to determine, $\hat{y}$ is a given desired state, $\beta > 0$ a regularization parameter, $\mathcal{D}$ some differential operator, and $y_a$, $y_b$, $u_a$, $u_b$ prescribed bound constraints on the state and control variables. The problem is solved in a domain $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, with boundary $\partial\Omega$. We highlight that the regularization term corresponding to the control is $\|u\|_{H^1(\Omega)}^2 = \|u\|_{L_2(\Omega)}^2 + \|\nabla u\|_{L_2(\Omega)}^2$ – problems with an $L_2$-norm regularization term for the control are considered in [2], as are time-dependent variants of such problems.

Applying an interior point method and a discretize-then-optimize approach, as in [2], leads to a discrete Lagrangian of the following form:

$$\mathcal{L}(\vec{y}, \vec{u}, \vec{p}) = \frac{1}{2} \vec{y}^T M \vec{y} - \vec{y}^T \vec{y}^\dagger + \frac{\beta}{2} \vec{u}^T (M + K) \vec{u} + \vec{p}^T (A \vec{y} - M \vec{u} - \vec{f})$$

$$- \mu \sum_j \log (y_j - y_{a,j}) - \mu \sum_j \log (y_{b,j} - y_j) - \mu \sum_j \log (u_j - u_{a,j}) - \mu \sum_j \log (u_{b,j} - u_j),$$

of which we wish to find the stationary point. Here $\vec{y}$ and $\vec{u}$ correspond to the discretized adjoint variable and desired state, $y_j$, $y_{a,j}$, $y_{b,j}$, $u_j$, $u_{a,j}$ and $u_{b,j}$ represent the values of $y$, $y_a$, $y_b$, $u$, $u_a$ and $u_b$ at the $j$-th finite element node, $K$ and $M$ are finite element stiffness and mass matrices, $A$ is the finite element matrix related to the PDE operator $\mathcal{D}$, and $\mu$ is the chosen barrier parameter within the interior point method.

Applying Newton iteration (with Newton steps $\vec{s}_y$, $\vec{s}_u$, $\vec{s}_p$, and previous iterates $\vec{y}^*$, $\vec{u}^*$, $\vec{p}^*$) to the resulting first-order optimality conditions leads to matrix systems of the form

$$\begin{bmatrix}
M + D_y & 0 & A^T \\
0 & \beta(M + K) + D_u & -M \\
A & -M & 0
\end{bmatrix}
\begin{bmatrix}
\vec{s}_y \\
\vec{s}_u \\
\vec{s}_p
\end{bmatrix}
= \begin{bmatrix}
(\mu(Y - Y_a)^{-1} \vec{e} - \mu(Y_b - Y)^{-1} \vec{e} + \vec{y}^\dagger - M \vec{y}^* - A^T \vec{p}^*) \\
(\mu(U - U_a)^{-1} \vec{e} - \mu(U_b - U)^{-1} \vec{e} - (M + K) \vec{u}^* + M \vec{p}^*) \\
\vec{f} - A \vec{y}^* + M \vec{u}^*
\end{bmatrix},$$

where

$$D_y = (Y - Y_a)^{-1} Z_{y,a} + (Y_b - Y)^{-1} Z_{y,b}, \quad D_u = (U - U_a)^{-1} Z_{u,a} + (U_b - U)^{-1} Z_{u,b}.$$

Here, $Y, U, Y_a, Y_b, U_a, U_b$ are diagonal matrices containing the entries of $y, u$ (from the previous Newton iteration), $\vec{y}^\dagger$, $\vec{y}^*$, $\vec{u}^*$, $\vec{u}_a$, $\vec{u}_b$ at each finite element node, and $Z_{y,a}, Z_{y,b}, Z_{u,a}, Z_{u,b}$ contain entries of the form $\frac{\mu}{y - y_a}, \frac{\mu}{y_b - y}, \frac{\mu}{u - u_a}, \frac{\mu}{u_b - u}$, respectively.

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2 Preconditioning

We now note that the Newton system is of saddle point form (see [1] for a survey of such systems). Using the justification provided in [3,4], we consider the block triangular preconditioners

\[ \mathcal{P}_1 = \begin{bmatrix} M + D_u & 0 & 0 \\ 0 & \beta(M + K) + D_u & 0 \\ A & -M & -\tilde{S}_1 \end{bmatrix}, \quad \mathcal{P}_2 = \begin{bmatrix} -\tilde{S}_2 & 0 & A^T \\ 0 & \beta(M + K) + D_u & -M \\ 0 & -M & 0 \end{bmatrix}, \]

where \( \tilde{S}_1 \) and \( \tilde{S}_2 \) are derived using ‘matching strategies’, as follows:

\[ \tilde{S}_1 = (A + \hat{M})(M + D_u)^{-1}(A + \hat{M})^\top, \]
\[ \tilde{S}_2 = -((A + \hat{M})^\top(M^{-1}(\beta(M + K) + D_u)M^{-1}(A + \hat{M})) \]

with \( \hat{M} = M[\text{diag}(\beta(M + K) + D_u)]^{-1/2}[\text{diag}(M + D_u)]^{1/2} \). Eigenvalue analysis concerning similar preconditioners for interior point methods can be found in [2].

In practice it is sensible to use multigrid methods to apply the inverse of the \((1,1)\)-block, and the approximate Schur complement inverses \( \tilde{S}_1^{-1} \) and \( \tilde{S}_2^{-1} \). We apply both preconditioners \( \mathcal{P}_1 \) and \( \mathcal{P}_2 \) within the GMRES algorithm.

3 Numerical results

We now implement an interior point method, coupled with our GMRES solver (with preconditioners \( \mathcal{P}_1 \) and \( \mathcal{P}_2 \)), for a particular test problem. In more detail, we set \( D = -\nabla^2, \tilde{u} = e^{-64(\beta(1-0.5^2 + (x_2-0.5)^2)}, \) with state and control constraints prescribed based on the physical properties of the problem. The iterative solvers are run to a tolerance of \( 10^{-8} \), with the outer (interior point) solver set to a tolerance of \( 10^{-6} \). We solve for a range of step-sizes \( h \) and values of \( \beta \), using MATLAB R2015a, on a quad-core 3.2 GHz processor. We observe that the number of interior point iterations, as well as the GMRES iteration count, behave robustly for a wide range of parameters. We therefore conclude that our preconditioning strategies are highly effective for parameter consideration.

Table 1: Number of interior point (Newton) iterations required to achieve convergence (blue, left), and average number of GMRES steps per interior point iteration before a relative preconditioned residual norm of \( 10^{-8} \) is achieved (black, right), for the test problem considered.

<table>
<thead>
<tr>
<th>( \mathcal{P}_1 )</th>
<th>( \beta = 1 )</th>
<th>( \beta = 10^{-1} )</th>
<th>( \beta = 10^{-2} )</th>
<th>( \beta = 10^{-3} )</th>
<th>( \beta = 10^{-4} )</th>
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<td>( 0 \leq y \leq 1.5 \times 10^{-5} )</td>
<td>( 0 \leq y \leq 1.5 \times 10^{-4} )</td>
<td>( 0 \leq y \leq 1.5 \times 10^{-3} )</td>
<td>( 0 \leq y \leq 1.5 \times 10^{-15} )</td>
<td>( 0 \leq y \leq 1.5 \times 10^{-15} )</td>
<td>( 0 \leq y \leq 1.5 \times 10^{-15} )</td>
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<tr>
<td>( 0 \leq u \leq 3 \times 10^{-4} )</td>
<td>( 0 \leq u \leq 3 \times 10^{-3} )</td>
<td>( 0 \leq u \leq 3 \times 10^{-2} )</td>
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<th>( \mathcal{P}_2 )</th>
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<td>( 0 \leq u \leq 3 \times 10^{-1} )</td>
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References