Mixed-Integer PDE-Constrained Optimization

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We consider the solution of mixed-integer partial differential equation (PDE) constrained optimization (MIPDECO) problems. This is a difficult class of problems that combines the combinatorial complexity of integer variables with the computational challenges of PDE constraints. We introduce a trust-region algorithm for MIPDECO and show its effectiveness on two classes of problems motivated by practical applications:

(1) *Determination and location of a set of discrete sources from noisy measurements.* This model is loosely motivated by applications in groundwater flow, where we want to find the location of pollutants in the subsurface; see, for example, [7, 3].
(2) *Design of an electromagnetic cloak.* This model is a mixed-integer formulation of the topology optimization formulation for an electromagnetic cloak design; see, for example, [5].

Both models include a PDE that is defined over a two- or three-dimensional domain and discretized by using quadrilateral finite elements. The source inversion model involves a linear advection-diffusion PDE, while the cloak-design is modeled by using a 2D Helmholtz equation. In both cases, the integer variables are binary indicator variables that model the presence of the source and the presence of cloaking material. Both models can be expressed abstractly as

$$\left\{ \begin{array}{ll} \min\limits_{u,w} & \mathcal{J}(u,w) \\ \text{s.t.} & \mathcal{C}(u,w) = 0 \\ & w \in \{0,1\}^p \end{array} \right\} \quad \Leftrightarrow \quad \left\{ \begin{array}{ll} \min\limits_{w} & \mathcal{J}(u(w),w) \\ \text{s.t.} & w \in \{0,1\}^p \end{array} \right\}, \tag{1}$$

where $\mathcal{F}$ is the objective function, $\mathcal{C}$ represents the PDE and boundary conditions, u are the state variables, and w are the binary control variables. We assume that given w, we can uniquely solve the PDE to obtain $u(w)$, resulting in an equivalent reduced-space formulation on the right. The presence of mesh-dependent integer variables in these models makes the use of commercial branch-and-cut (see, e.g., [1]) prohibitively expensive (and impractical for 3D extensions of our models). Consequently, we develop a trust-region heuristic that is described next.

1. Trust-Region Method for MIPDECO

We present a new improvement heuristic for MIPDECO that is motivated by trust-region methods for nonlinear optimization; see, for example, [2]. Our method is also related to local-branching heuristics for MINLP [4, 6].

The key idea is to work with the reduced-space formulation in (1) and to define a trust-region subproblem around a current iterate, $w^{(k)}$, as

$$\left\{ \begin{array}{ll} \min\limits_{w} & \mathcal{J}^{(k)} + {g^{(k)}}^T (w - w^{(k)}) \\ \text{s.t.} & \|w - w^{(k)}\|_1 \leq \Delta_k, \quad \text{and } w \in \{0,1\}^p \end{array} \right. , \tag{2}$$

where $g^{(k)} := \nabla_w \mathcal{J}(u(w^{(k)}), w^{(k)})$ is the reduced gradient, and $\Delta_k \in \mathbb{Z}_+$ is the ℓ_1 trust-region radius. We note that because $w \in \{0,1\}^p$, the trust-region constraint can be written equivalently as a single affine constraint. Given this subproblem, we define a trust-region algorithm as follows.

Given $w^{(0)} \in \{0,1\}^p$, gradient, $g^{(0)}$, set $\Delta_0 = \bar{\Delta}$ and $k \leftarrow 0$;
while $\Delta_k > 0$ **do**
  Solve trust-region subproblem (2) for $\hat{w}$;
  Evaluate $\mathcal{J}(\hat{w}, u(\hat{w}))$ (PDE) & $\rho_k = \frac{\mathcal{J}(w^{(k)}) - \mathcal{J}(\hat{w})}{-{g^k}^T \left(\hat{w} - w^{(k)}\right)} = \frac{\text{ActRed}}{\text{PredRed}}$;
  if $\rho_k > \bar{\rho}$ **then**
    accept step: $w^{(k+1)} = \hat{w}$, possibly increase Δ_k;
  else
    reject step: $w^{(k+1)} = w^{(k)}$, reduce $\Delta_{k+1} = \left\lfloor \frac{\Delta_k}{2} \right\rfloor$;
  Set $k \leftarrow k + 1$;

The algorithm requires two PDE solves (forward and adjoint) per successful iteration, and we can solve the subproblem (2) efficiently by recasting it as a simple knapsack problem.

2. Computational Results

The results of the trust-region approach to solving the source inversion problem are shown in Figure 1, which shows the location of the original sources, the observations, u, with the measurement locations in red, and the final solution from the trust-region approach, which has an intersection-over-union (IoU) score of 82.3%.

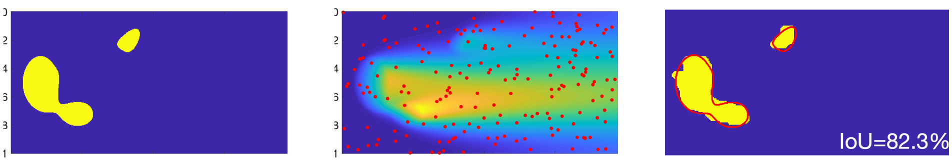

Figure 1. Original sources, the observations with measurement locations in red, and the final trust-region iterate.

We have also applied this method to the design of an electromagnetic scatterer. Figure 2 shows the solution of the continuous relaxation final trust-region problem and the corresponding wave difference, or objective functional, demonstrating the effectiveness of our approach.

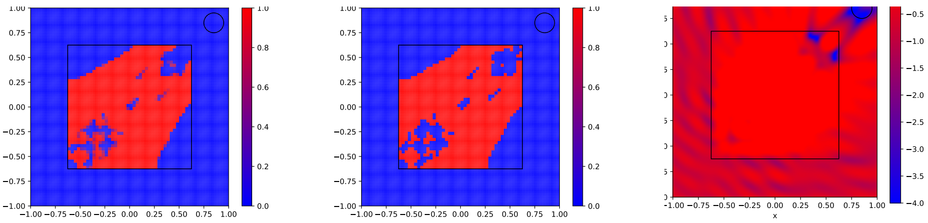

FIGURE 2. Solution of continuous relaxation final trust-region problem, and the logarithm of the wave difference.

3. Conclusions, Outlook, and Open Problems

We have presented a trust-region heuristic for solving MIPDECOs and have shown its effectiveness in solving realistic applications. Our approach leaves open a number of important questions and opportunities for future research.

(1) Currently, the algorithm stops when (2) cannot make any more progress. It would be interesting to see whether this stopping criterion can be replaced by a formal criterion based on the convergence of lower and upper bounds.
(2) Multigrid methods may provide an interesting refinement strategy for obtaining even better solutions.
(3) A formal convergence analysis of the algorithm based on topology optimization is an open problem, as well as the characterization of solutions under mesh refinement.

Despite these gaps in its theoretical justification, the proposed trust-region scheme performs well in practice, and we are working on other applications that could benefit from this approach.

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