A Mixed-Integer Nonlinear Optimization Case Study

GIAN Short Course on Optimization: Applications, Algorithms, and Computation

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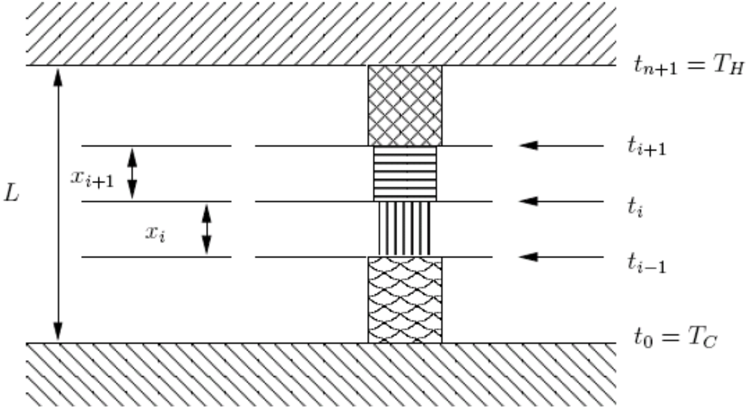
Design of Load-Bearing Thermal Insulation System

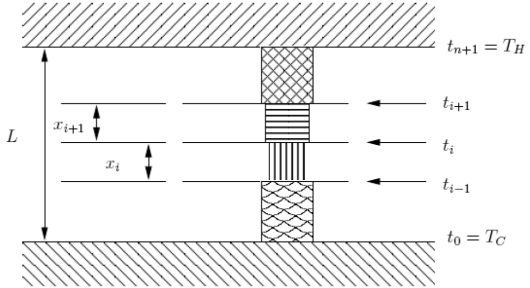


Description of System

Insulation system uses series of heat intercepts
to reduce heat from hot (top) to cold (bottom) surface

Outline

Design of Load-Bearing Thermal Insulation System



Design Goal or Objective

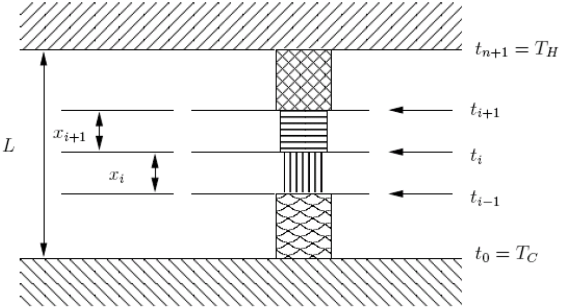
Minimize cooling power needed to run system

- Active cooling at intercepts between layers ⇒ cooling power
- Given hot surface temperature, maintain cold surface temperature below allowable maximum

Discrete Design Variables Overview

Discrete design variables over which we optimize

- Number of intercepts, $n \in \{1, 2, \ldots, N = 10\}$ discrete
- m_i material $m_i \in \mathcal{M}$ of insulator $i = 1, \ldots, n+1$
  where $m_i \in \mathcal{M} = \{$ nylon, teflon, epoxy-normal, epoxy-plane, aluminium, steel, carbon-steel $\}$ ... discrete choice



Continuous Design Variables Overview

Continuous variables over which we optimize

- x_i length of insulator $i = 1, \ldots, n+1$
- a_i area of insulator $i = 1, \ldots, n+1$
- q_i heat flow from intercept i to $i-1$, for $i = 1, \ldots, n+1$
- t_i cooling temperature at intercept $i = 0, \ldots, n+1$
- Δx_i thermal expansion of layer $i = 1, \ldots, n+1$
  can be eliminated later

where layers 0 and $n+1$ are cold and hot surface, respectively

- Cold surface temperature is $t_0 = T_C = 4.3$K (near abs. zero)
- Hot surface temperature is $t_n = T_H = 300$K (27C)

Complete Mixed Variable Model

$$\text{minimize} \quad \sum_{i=1}^{n} C_i(t_i)\left(\frac{T_H}{t_i} - 1\right) \cdot (q_{i+1} - q_i) \qquad \text{cooling power}$$

$$\text{subject to} \quad q_i = \frac{a_i}{x_i} \int_{t_{i-1}}^{t_i} k(t, m_i)dt \qquad \text{heat transfer}$$

$$\sum_{i=1}^{n} \rho(m_i) a_i x_i \leq M \qquad \text{total mass}$$

$$F \leq a_i \sigma(t, m_i) \; \forall t : \; t_{i-1} \leq t \leq t_i \qquad \text{stress limit}$$

$$\sum_{i=1}^{n} u_i x_i \leq L \frac{\delta}{100} \qquad \text{thermal expansion}$$

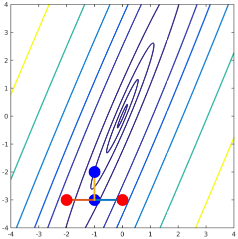
Plus linear constraints: $t_{i-1} \leq t_i \leq t_{i+1}, \quad x_i \geq 0, \quad a_i \geq 0$

$$\sum_{i=1}^{n} x_i = L, \quad t_0 = T_C, \; t_{n+1} = T_H, \quad n \in \{1, \dots, N\}, \quad m_i \in \mathcal{M}$$

Solving Mixed Variable Model with NOMADm

NOMADm pattern-search method

- Matlab code from Mark Abramson ... also C code
- User provides routines for
  - Function & constraints
  - Initial point, ranges
- Launch by typing >> nomadm
- See example heatshield



Challenges of Mixed Variable Model

Mixed Variable Problem not Standard MINLP

- Categorical: n number of intercepts; m_i material type
- Discontinuous objective term: $C(t_i)\left(\frac{T_H}{t_i} - 1\right) \ldots$ where

$$C(t_i) = \begin{cases} 5 & \text{if } t_i \leq 4.2, \\ 4 & \text{if } 4.2 < t_i < 71, \\ 2.5 & \text{if } t_i \geq 71. \end{cases} \quad i = 1, \ldots, n$$

where $C(t_i)$ thermodynamic cycle efficiency of intercept i

- Constraints involve integrals, e.g. heat transfer (Fourier's law)

$$q_i = \frac{a_i}{x_i} \int_{t_{i-1}}^{t_i} k(t, m_i) dt$$

where a_i area, x_i thickness of intercept i

Outline

Modeling Categorical with Binary Variables

Let N upper bound on number of layers

Binary indicator y_i indicates existence of layer i

$$\sum_{i=1}^{N+1} y_i = n + 1$$

$$\begin{aligned} y_{i+1} &\leq y_i, \quad i = 1, \ldots, N \\ x_i &\leq L y_i \quad i = 1, \ldots, N+1 \\ x_i &\geq \epsilon L y_i \quad i = 1, \ldots, N+1 \\ y_i &\in \{0, 1\} \quad i = 1, \ldots, N+1. \end{aligned}$$

- Layer $i+1$ does not exist, if layer i does not
  $\Rightarrow$ layers numbered consecutively from 1
- If layer i does not exist, then $y_i = 0$, hence length, $x_i = 0$
- Eliminate spurious layers ($x_i = 0$) with lower bound, ϵ
  ... interpret as manufacturing tolerance

Modeling Categorical with Binary Variables

Can replace $x_i \leq Ly_i \; i = 1, \ldots, N+1$ by stronger inequalities ...

Theorem (Convex Hull Representation of Number of Layers)

Let $P = \text{conv}\left(\{(x, y) \in \mathbb{R}_+^{N+1} \times \mathbb{B}^{N+1} \mid \sum_{j=1}^{N+1} x_j = L, \right.$

$$y_{i+1} \leq y_i, \quad i = 1, \ldots, N,$$

$$\left. x_i \leq Ly_i, \quad i = 1, \ldots, N+1\} \right).$$

Then inequality

$$\sum_{j=i}^{N+1} x_j \leq Ly_i$$

defines facet of P for $i = 1, 2, \ldots, N+1$.

Modeling Material Properties

Indicator y_i represents existence of layer i ... let $z_{ij} \in \{0, 1\}$:

$$z_{ij} = \begin{cases} 1 & \text{if layer } i \text{ has material } j \\ 0 & \text{otherwise} \end{cases}, \quad i = 1, \ldots, n, \quad j = 1, \ldots, |\mathcal{M}|$$

Only existing layers have material type:

$$\sum_{j=1}^{|\mathcal{M}|} z_{ij} = y_i, \quad i = 1, \ldots, N+1.$$

Constraints of data functions (e.g thermal conductivity $k(t, m_i)$):

$$k(t, m_i) = \sum_{j=1}^{|\mathcal{M}|} z_{ij} k(t, M_j),$$

where $\mathcal{M} = \{M_1, \ldots, M_p\}$ set of possible materials.

Modeling Categorical Variables m_i and n

$z_{ij} \in \{0,1\}$ where $z_{ij} = 1 \;\Leftrightarrow\;$ layer i has j^{th} material

$$\sum_{j=1}^{|\mathcal{M}|} z_{ij} = y_i, \quad i = 1, \ldots, N+1.$$

... only existing layers can choose material

Maximum length constraint simplifies

$$\sum_{j=1}^{n} x_i = L \quad \Leftrightarrow \quad \sum_{j=i}^{N+1} x_i = L \qquad \text{... since } \epsilon L y_i \leq x_i \leq L y_i$$

Maximum mass constraint ($\rho_j = \rho(M_j)$ density of material M_j)

$$\sum_{i=1}^{n} \rho(m_i) a_i x_i \leq M \quad \Leftrightarrow \quad \sum_{i=1}^{N+1} \sum_{j=1}^{|\mathcal{M}|} \rho_j z_{ij} a_i x_i \leq M$$

Outline

Propagating Binary Variables into Model/Simulation

Heat transfer equation with categorical $m_i \in \mathcal{M}$

$$q_i = \frac{a_i}{x_i} \int_{t_{i-1}}^{t_i} k(t, m_i) dt \quad \Leftrightarrow \quad x_i q_i = a_i \int_{t_{i-1}}^{t_i} k(t, m_i) dt$$

... becomes equation with binary variables z_{ij} (M_j parameter)

$$x_i q_i = a_i \int_{t_{i-1}}^{t_i} \sum_{j=1}^{\mathcal{M}} z_{ij} k(t, M_j) dt = a_i \sum_{j=1}^{\mathcal{M}} z_{ij} \int_{t_{i-1}}^{t_i} k(t, M_j) dt$$

Same computational cost as categorical model:

- form $\hat{k}(t) := \sum_{j=1}^{\mathcal{M}} z_{ij} k(t, M_j)$ from data look-up
- integrate $\hat{k}(t)$ ... convex combination of materials

$\Rightarrow$ black-box MINLP without categorical variables

Smoothing with Discrete Temperatures

Fine temperature discretization $t_i \in \{T_1 < T_2 < \ldots < T_D\}$

$$\Leftrightarrow t_i = \sum_{r=1}^{D} d_{ir} T_r, \quad 1 = \sum_{r=1}^{D} d_{ir}, \quad d_{ir} \in \{0,1\}$$

... $d_{ir} = 1$ iff $t_i = T_r$ is SOS-1 $\Rightarrow$ at most $\log(D)$ branching levels

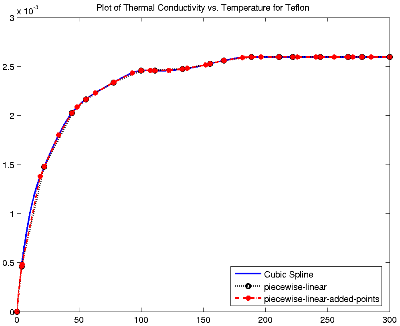
Model simplifications & smoothing

1. smooth objective coefficients
2. integrals are precomputed & smooth
3. bilevel optimization becomes smooth
4. tighter MIP formulation, e.g. $t_i \geq T_H(1 - y_{i+1})$ ...

Snag: much larger relaxation & intercept temperatures discrete

Evaluation of Integrals

Finer grid $T_C = T_1 < T_2 < \ldots < T_D = T_H$ for $k(t, m)$
Approximate curves $k(t, M_j)$ on fine mesh



Values of thermal expansion, $k(t, M_j)$ for $M_j =$ teflon

Introduce variables $v_{ij} \approx \int_{t_{i-1}}^{t_i} k(t, M_j) dt$ ...

Smooth Integral Approximation

Precompute integrals $V_{rj} \approx \int_{T_1}^{T_r} k(t, M_j)dt$ and observe

$$v_{ij} = \int_{t=t_i}^{t_{i+1}} k(t, M_j)dt = \int_{t=T_1}^{t_{i+1}} k(t, M_j)dt - \int_{t=T_1}^{t_i} k(t, M_j)dt,$$

Recall $\sum d_{ir} T_r = t_i$ and $\sum d_{ir} = 1$:

$$\int_{t=T_1}^{t_i} k(t, M_j)dt = \sum_{r=1}^{D} d_{ir} \int_{t=T_1}^{T_r} k(t, M_j)dt = \sum_{r=1}^{D} d_{ir} V_{rj}$$

$$\Rightarrow \quad v_{ij} = \sum_{r=1}^{D} d_{i+1,r} V_{rj} - \sum_{r=1}^{D} d_{ir} V_{rj}$$

... linear set of constraints

Smooth Objective Coefficients

Another standard MIP trick to simplify the objective function:

$$\left(\frac{T_H}{t_i} - 1\right) = \left(\frac{T_H}{\sum_{r=1}^{D} d_{ir} T_r} - 1\right) = \left(\sum_{r=1}^{D} d_{ir} \frac{T_H}{T_r} - 1\right).$$

Replace $C_i(t_i)$ in objective function by parameters $\hat{C}_r$

$$\hat{C}_r := \begin{cases} 5 & \text{if } T_r \leq 4.2 \\ 4 & \text{if } 4.2K < T_r < 71K \\ 2.5 & \text{if } T_r \geq 71K \end{cases}$$

$\Rightarrow$ smooth objective function

$$\sum_{i=1}^{N} \left(\sum_{r=1}^{D} d_{ir} \hat{C}_r \left(\frac{T_H}{T_r} - 1 \right) \right) \cdot (q_{i+1} - q_i)$$

Comparison of Models

Model sizes for $N = 20$: plus 1 integer variable n

	smoothness	0-1 vars	SOS	cont vars	cons
P_0	discont.	168		106	402
P_1	continuous	228		106	502
P_2	smooth	168	21	6934	6792

Solvers:

1. `FilMINT` outer approximation branch-and-cut
2. `MINLP` nonlinear branch-and-bound
3. `MINLP-g` multi-start some BB nodes in `MINLP`

Numerical Results

Different objectives ... can become negative $\Rightarrow$ *power* ≥ 0

Objective Function for $N = 10$: 1.06

- same as Abramson, but $n \leq N + 1$ active ... optimal???
- `MINLP-g` gets modest 1% improvement

Results for $N = 20$

	Objective Function		Solution times [s]	
	FilMINT	MINLP	FilMINT	MINLP
P_0	2.08	integer infeasible	67	192
P_1	2.64	0.98	91	11 hrs
P_2	–	–	–	–

Can solve P_2 if we restrict to two materials & use clever cuts

Conclusions

- Model categorical variables with binary variables & SOS-1
  convey logic inherent in categorical variables to solver
  $\Rightarrow$ continuous relaxation possible ... rigorous MINLP
- Formulate thermal insulation problem in `AMPL`
  - allows use of smooth MINLP solvers
  - `AMPL` model not as easy as we thought
- Discretized temperature model
  - large smooth MINLP model
  - 0-1 variables linearize model (e.g. integration)