MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Department of Civil and Environmental Engineering

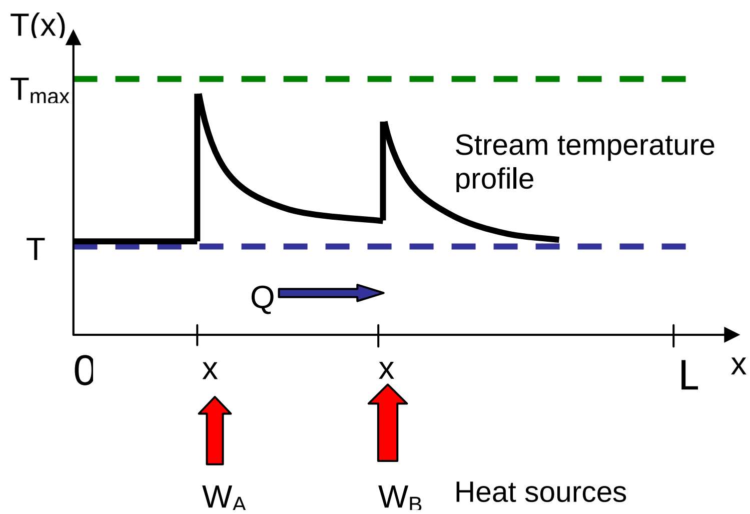
1.731 Water Resource Systems

Lecture 11, Differential Constraints and Response Matrices, Oct. 5, 2006

Standard formulation of optimization problem relies on **algebraic constraints**. In many environmental applications constraints arise most naturally as **differential equations**. How should these differential constraints be handled?

Example – Allocation of waste heat discharges along a stream

Problem is to select heat discharges W_A and W_B at 2 locations x_A and x_B along stream in order to maximize total heat discharged $W_A + W_B$, subject to upper limit (T_{max}) on water temperature T.



Incorporate model based on **stream energy balance** (relates heat discharges and stream temperature):

$$\frac{dE}{dt} = 0 = \rho\gamma Q \frac{dT}{dx} + k_e A \rho\gamma (T - T_0) + W_A \delta(x - x_A) + W_B \delta(x - x_B) \quad ; \quad T(0) = T_0$$

E = Energy per unit length [Joules/m]

ρ = Density of water [kg/m^3]

γ = Specific heat of water [Joules/(kg ° C)]

Q = Stream flow [m^3/day]

T = Water temperature [° C]

T_0 = Air temperature [° C]

A = Stream cross-section [m^2]

k_e = Exchange rate [1/day]

W_A, W_B Source heat flux [Joules/ day]

$\delta(x - x_A)$, $\delta(x - x_B)$ = Dirac delta function at x_A or x_B [1/m], defined by:

$$\int_{x_L}^{x_U} f(x)\delta(x-x')dx = f(x') \quad x_L < x' \le x_U$$
$$= 0 \qquad \text{otherwise}$$

Assume steady state ($dE/dt = 0$) and simplify to:

$$\frac{dT}{dx} = -\alpha(T - T_0) + W_A\delta(x - x_A) + W_B\delta(x - x_B) \quad ; \quad T(0) = T_0$$

$$\alpha = \frac{k_e A}{Q} \qquad \beta = \frac{1}{\rho\gamma Q}$$

Suppose solution to this equation at any x is $T(x, W_A, W_B)$. Then optimization problem is:

$$\underset{W_A, W_B}{Maximize}\; W_A + W_B$$

such that :

$$T(x, W_A, W_B) \le T_{max} \quad ; \quad \forall x$$

Note that the temperature constraint as given here is evaluated at **every *x*** (infinite number of algebraic constraints).

There are three ways to write the constraint $T(x, W_A, W_B) \le T_{max}$ in a practical (finite) form:

1. **Analytical solution** - $T(x, W_A, W_B)$ is written as an **explicit** function of W_A and W_B.
2. **Imbedding** - $T(x, W_A, W_B)$ is defined **implicitly**, by a set of discretized model equations.
3. **Response matrix** - $T(x, W_A, W_B)$ is approximated by a Taylor series expressed in terms of model sensitivity derivatives.

Analytical solution

Solution to stream equation with upstream boundary condition imposed:

$$T(x, W_A, W_B) = T_0 + \beta W_A \int_0^x e^{-\alpha(x-\xi)}\delta(\xi - x_A)\, d\xi + \beta W_B \int_0^x e^{-\alpha(x-\xi)}\delta(\xi - x_B)\, d\xi$$

Apply definition of δ function to get:

$$T(x, W_A, W_B) = T_0 \qquad x \le x_A$$
$$T(x, W_A, W_B) = T_0 + \beta W_A e^{-\alpha(x - x_A)} \qquad x_A < x \le x_B$$
$$T(x, W_A, W_B) = T_0 + \beta W_A e^{-\alpha(x - x_A)} + \beta W_B e^{-\alpha(x - x_B)} \qquad x > x_B$$

Note that temperature is highest at the discharge points x_A and x_B. Therefore, we can apply temperature constraint only at x_A and x_B rather than at all points x:

$$\underset{W_A, W_B}{Maximize}\ W_A + W_B$$

such that :

$$T_0 + \beta W_A - T_{max} \leq 0 \qquad \text{at } x_A$$

$$T_0 + \beta W_A e^{-\alpha(x_B - x_A)} + \beta W_B - T_{max} \leq 0 \qquad \text{at } x_B$$

This is in standard form, with algebraic rather than differential constraints. This approach is best when analytical solution is available, but that is not usually the case.

Imbedding

When an analytical solution is not available an approximate numerical solution can be obtained by discretizing the differential equation over a computational grid of equally spaced points x_1, x_2, …, x_N.

In this example use either of two approximations for the spatial derivative at each computational grid point:

$$\left.\frac{\partial T}{\partial x}\right|_{x_i} \approx \frac{T(x_{i+1}) - T(x_i)}{\Delta x} = \frac{T_{i+1} - T_i}{\Delta x} \qquad \text{Forward difference (explicit)}$$

$$\left.\frac{\partial T}{\partial x}\right|_{x_i} \approx \frac{T(x_i) - T(x_{i-1})}{\Delta x} = \frac{T_i - T_{i-1}}{\Delta x} \qquad \text{Backward difference (implicit)}$$

The Dirac delta function is approximated by $1/\Delta x$.

The **explicit discretization** yields a set of N coupled equations as follows:

$$T_i = T_0 \qquad x_i = x_0$$

$$T_{i+1} = T_i - \alpha \Delta x (T_i - T_0) \qquad x_0 < x_i \leq x_A$$

$$T_{i+1} = T_i - \alpha \Delta x (T_i - T_0) + \beta W_A \qquad x_A < x_i \leq x_B$$

$$T_{i+1} = T_i - \alpha \Delta x (T_i - T_0) + \beta W_B \qquad x_i > x_B$$

These **first-order difference equations** have the same general form as the reservoir storage equation in Problem Set 3.

The system of equations obtained from the **implicit discretization** is most conveniently expressed in matrix form:

$$A_{ki} T_i = b_k (W_A, W_B) \quad i, k = 1, \ldots, N$$

where $A_{ii} = 1$ for $i = 1, \ldots, N$

$A_{i,i\text{-}1} = \alpha \Delta x\text{-}1$ for $i = 2, \ldots, N$

$Ai,k = 0$ otherwise

$b_i = T_0$ for $i = 1$

$b_i = \alpha \Delta x T_0$ for $i > 1$ and $x_i \neq x_A$ or x_B

$b_i = \beta W_A + \alpha \Delta x T_0$ for $x_i = x_A$

$b_i = \beta W_B + \alpha \Delta x T_0$ for $x_i = x_B$

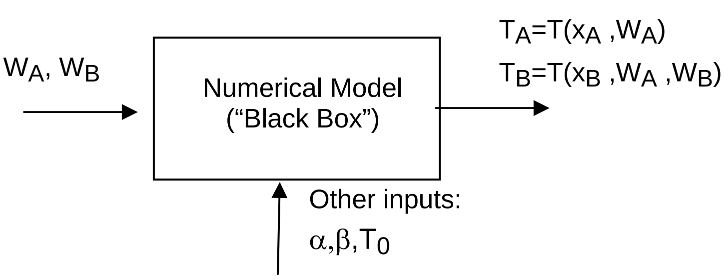
Both the explicit and implicit discretizations are in a form that can be inserted directly into optimization software such as GAMS (note that the implicit matrix equation does need not be solved and the decision variables only appear on the right-hand side – the implicit constraints relating each T_i to W_A and W_B are sufficient).

The disadavantage of imbedding is the **large number of decision variables and constraints** it produces (one for each grid point for each scalar differential equation). This is particularly inefficient in the example problem since we really only care about the temperature solutions at the two points x_A and x_B . Solutions at all the other upstream points need to be computed in order to obtain these two temperatures.

Response Matrix

Response matrix methods represent differential constraints with efficient linear approximations.

Assume we have a numerical model available to evaluate temperatures $T(x_A, W_A)$ and $T(x_B, W_A, W_B)$ at the discrete locations x_A and x_B, for any set of decision variables W_A and W_B.



Expand these temperatures in a Taylor series around nominal decision values (e.g. $W_A = W_B = 0$):

$$T(x_A, W_A) = T(x_A, 0) + \overbrace{\left.\frac{\partial T(x_A, W_A)}{\partial W_A}\right|_{W_A=0}}^{R_{AA}} W_A + \ldots$$

$$T(x_B, W_A, W_B) = T(x_B, 0, 0) + \underbrace{\left.\frac{\partial T(x_B, W_A, 0)}{\partial W_A}\right|_{W_A=0}}_{R_{BA}} W_A + \underbrace{\left.\frac{\partial T(x_B, 0, W_B)}{\partial W_B}\right|_{W_B=0}}_{R_{BB}} W_B + \ldots$$

Associate the sensitivity derivatives with the elements of a response matrix R and rearrange equations:

$$\begin{bmatrix} T_0 \\ T_0 \end{bmatrix} + \begin{bmatrix} R_{AA} & 0 \\ R_{BA} & R_{BB} \end{bmatrix} \begin{bmatrix} W_A \\ W_B \end{bmatrix} = \begin{bmatrix} T_A \\ T_B \end{bmatrix}$$

Resulting constraints for the optimization problem are:

$$\begin{bmatrix} T_0 \\ T_0 \end{bmatrix} + \begin{bmatrix} R_{AA} & 0 \\ R_{BA} & R_{BB} \end{bmatrix} \begin{bmatrix} W_A \\ W_B \end{bmatrix} \le \begin{bmatrix} T_{\max} \\ T_{\max} \end{bmatrix}$$

In this example the response matrix approximation is **exact** because the differential constraints are **linear** in the decision variables. Consequently, the response matrix elements can be identified directly from the analytical solutions above.

More generally, we derive the sensitivity derivatives numerically, from multiple model evaluations. For example:

$$R_{BA} \approx \frac{T(x_B, \varepsilon, 0) - T(x_B, 0, 0)}{\varepsilon}$$

This approach does not require knowledge of the model equations (i.e. the model can be a "black box").

The response matrix approach can also be used to approximate **nonlinear** differential constraints, so long as the Taylor series expansion is sufficiently accurate.