Deterministic Global Optimization Algorithm and Nonlinear Dynamics

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Outline

- Motivation
- Dynamic Optimization: Problem and Methods
- Convex Relaxation of the Dynamic Information
- Deterministic Global Optimization Algorithm
- Convergence of the Algorithm
- Case Studies
- Conclusions and Perspectives

Applications of Dynamic Optimization

- Chemical systems
  - Determination of Kinetic Constants from Time Series Data (Parameter Estimation)
  - Optimal Control of Batch and semi-Batch Chemical Reactors
  - Safety Analysis of Industrial Processes
- Biological and ecological systems
- Economic and other dynamic systems

Dynamic Optimization Problem

$$\min_{p} J(x(t_i, p), p\,;\; i = 0, 1, ..., NP)$$

subject to:

$$g_i(x(t_i, p), p) \leq 0\;,\; i = 0, 1, ..., NP$$

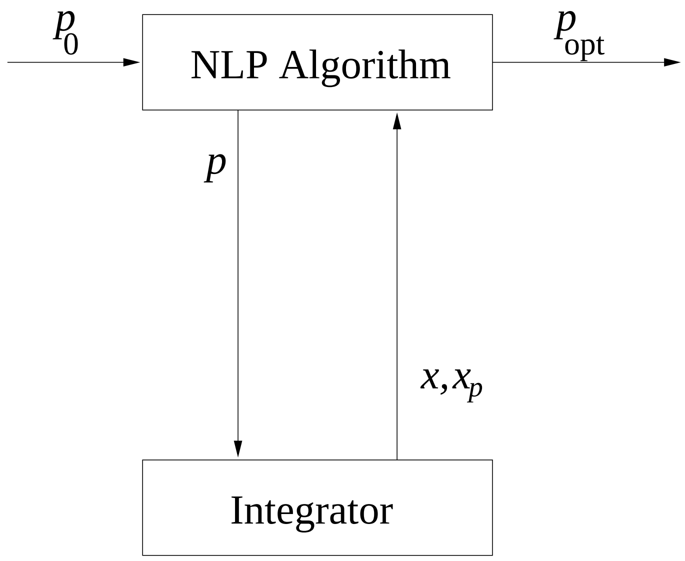
$$p^L \leq p \leq p^U$$

$$\dot{x} = f(t, x, p)\;,\; \forall t \in [t_0, t_{NP}]$$

$$x(t_0, p) = x_0(p)$$

Solution approaches

- Simultaneous approach: full discretization
- Sequential approach:



Usually *nonconvex* NLP Problems

- Multiple optimum solutions exist
- Commercially available numerical solvers guarantee *local optimum* solutions
- Poor economic performance

Algorithm classes (combined with simultaneous or sequential approach)

Stochastic algorithms

Deterministic algorithms

Global optimization methods
Simultaneous approaches

- Application of global optimization algorithms for NLPs

- Issues: problem size; quality of discretization.

- Smith and Pantelides (1996): spatial BB + reformulation

- Esposito and Floudas (2000): αBB algorithm

Global optimization methods: Sequential approaches

- Stochastic algorithms
  - Luus et al. (1990): direct search procedure.
  - Banga and Seider (1996), Banga et al. (1997): randomly directed search.
- Deterministic algorithms
  - New techniques for convex relaxation of time-dependent parts of problem
  - Lack of analytical forms for the constraints / objective function
  - Esposito and Floudas (2000): extension of αBB to handle nonlinear dynamics.
  - Singer and Barton (2002): convex relaxation of integral objective function with linear dynamics
  - Papamichail and Adjiman (2002): convex relaxations of nonlinear dynamics.

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Reformulated NLP Problem

$$\min_{\widehat{x},p} J(\widehat{x}_i, p\,;\; i = 0, 1, ..., NP)$$

subject to:

$$g_i(\widehat{x}_i, p) \leq 0\;,\; i = 0, 1, ..., NP$$

$$\widehat{x}_i = x(t_i, p)\;,\; i = 0, 1, ..., NP$$

$$p \in [p^L, p^U]$$

$$\dot{x} = f(t, x, p)\;,\; \forall t \in [t_0, t_{NP}]$$

$$x(t_0, p) = x_0(p)$$

Convex Relaxation of J and g_i (1)

$$f(z) = f_{CT}(z) + \sum_{i=1}^{bt} b_i z_{B_i,1} z_{B_i,2} + \sum_{i=1}^{ut} f_{UT,i}(z_i) + \sum_{i=1}^{nt} f_{NT,i}(z)$$

Underestimating Bilinear Terms (McCormick, 1976)

$$w = z_1 z_2 \quad \text{over} \quad [z_1^L, z_1^U] \times [z_2^L, z_2^U]$$

$$\begin{aligned} w &\geq z_1^L z_2 + z_2^L z_1 - z_1^L z_2^L \\ w &\geq z_1^U z_2 + z_2^U z_1 - z_1^U z_2^U \\ w &\leq z_1^L z_2 + z_2^U z_1 - z_1^L z_2^U \\ w &\leq z_1^U z_2 + z_2^L z_1 - z_1^U z_2^L \end{aligned}$$

Underestimating Univariate Concave Terms

$$\breve{f}_{UT}(z) = f_{UT}(z^L) + \frac{f_{UT}(z^U) - f_{UT}(z^L)}{z^U - z^L}(z - z^L) \quad \text{over} \quad [z^L, z^U] \subset \Re$$

Convex Relaxation of J and g_i (2)

Underestimating General Nonconvex Terms in $\mathcal{C}^2$
(Maranas and Floudas, 1994; Androulakis *et al.*, 1995)

$$\bar{f}_{NT}(z) = f_{NT}(z) + \sum_{i=1}^{m} \alpha_i (z_i^L - z_i)(z_i^U - z_i) \quad \text{over} \quad [z^L, z^U] \subset \Re^m$$

- $\bar{f}_{NT}(z)$ is always less than f_{NT}
- $\bar{f}_{NT}(z)$ is convex if α_i is big enough

$$H_{\bar{f}_{NT}}(z) = H_{f_{NT}}(z) + 2\,\mathrm{diag}(\alpha_i)$$

Rigorous α calculations using the scaled Gerschgorin method
(Adjiman *et al.*, 1998)

$$\forall z \in [z^L, z^U] \; H_{f_{NT}}(z) \in [H_{f_{NT}}] = H_{f_{NT}}([z^L, z^U])$$

Convex Relaxation of $\widehat{x}_i = x(t_i, p)$

$$\widehat{x}_i - x(t_i, p) \leq 0$$
$$x(t_i, p) - \widehat{x}_i \leq 0$$

Constant bounds: $\underline{x}(t_i) \leq \widehat{x}_i \leq \overline{x}(t_i)$

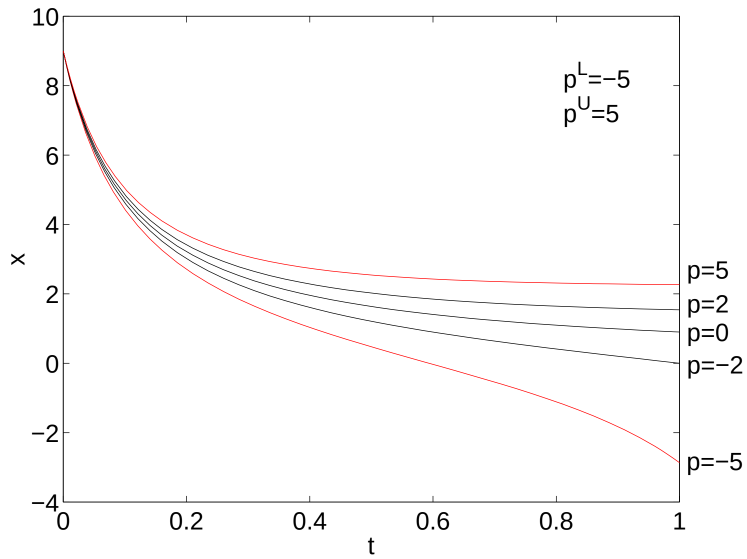
Affine bounds: $\underline{M}(t_i)p + \underline{N}(t_i) \leq \widehat{x}_i \leq \overline{M}(t_i)p + \overline{N}(t_i)$

α-*based bounds* (Esposito and Floudas, 2000):

$$\widehat{x}_{ik} - x_k(t_i, p) + \sum_{j=1}^{r} \alpha_{kij}^{-}(p_j^L - p_j)(p_j^U - p_j) \leq 0$$
$$x_k(t_i, p) + \sum_{j=1}^{r} \alpha_{kij}^{+}(p_j^L - p_j)(p_j^U - p_j) - \widehat{x}_{ik} \leq 0$$

Illustrative example

$$\dot{x}(t) = -x(t)^2 + p\,,\ \forall t \in [0,1]$$
$$x(0) = 9$$
$$p \in [-5,5]$$



How do we find bounding trajectories?

Differential Inequalities (1)

Consider the following parameter dependent ODE:

$$\dot{x} = f(t, x, p), \ \forall t \in [t_0, t_{NP}]$$

$$x(t_0, p) = x_0(p)$$

$$p \in [p^L, p^U] \subset \Re^r$$

where x and $\dot{x} \in \Re^n$, $f: (t_0, t_{NP}] \times \Re^n \times [p^L, p^U] \mapsto \Re^n$ and $x_0: [p^L, p^U] \mapsto \Re^n$.

Let $x = (x_1, x_2, ..., x_n)^T$ and $x_{k^-} = (x_1, x_2, ..., x_{k-1}, x_{k+1}, ..., x_n)^T$. The notation $f(t, x, p) = f(t, x_k, x_{k^-}, p)$ is used.

Theory on diff. inequalities (Walter, 1970) has been extended.

Differential Inequalities (2)

Bounds on the solutions of the parameter dependent ODE:

$$\dot{\underline{x}}_k = \inf f_k(t, \underline{x}_k, [\underline{x}_{k-}, \overline{x}_{k-}], [p^L, p^U])$$

$$\dot{\overline{x}}_k = \sup f_k(t, \overline{x}_k, [\underline{x}_{k-}, \overline{x}_{k-}], [p^L, p^U])$$

$$\forall t \in [t_0, t_{NP}] \text{ and } k = 1, ..., n$$

$$\underline{x}(t_0) = \inf x_0([p^L, p^U])$$

$$\overline{x}(t_0) = \sup x_0([p^L, p^U])$$

$\underline{x}(t)$ is a subfunction and $\overline{x}(t)$ is a superfunction for the solution of the ODE, i.e.,

$$\underline{x}(t) \le x(t, p) \le \overline{x}(t) \ , \ \forall p \in [p^L, p^U] \ , \ \forall t \in [t_0, t_{NP}]$$

Quasi-monotonicity

Definition 1: Let g(x) be a mapping $g : \mathcal{D} \mapsto \Re$ with $\mathcal{D} \subseteq \Re^n$. Again the notation $g(x) = g(x_k, x_{k-})$ is used. The function g is called unconditionally partially isotone (antitone) on $\mathcal{D}$ with respect to the variable x_k if

$$g(x_k, x_{k-}) \leq g(\tilde{x}_k, x_{k-}) \text{ for } x_k \leq \tilde{x}_k \ \ (x_k \geq \tilde{x}_k)$$

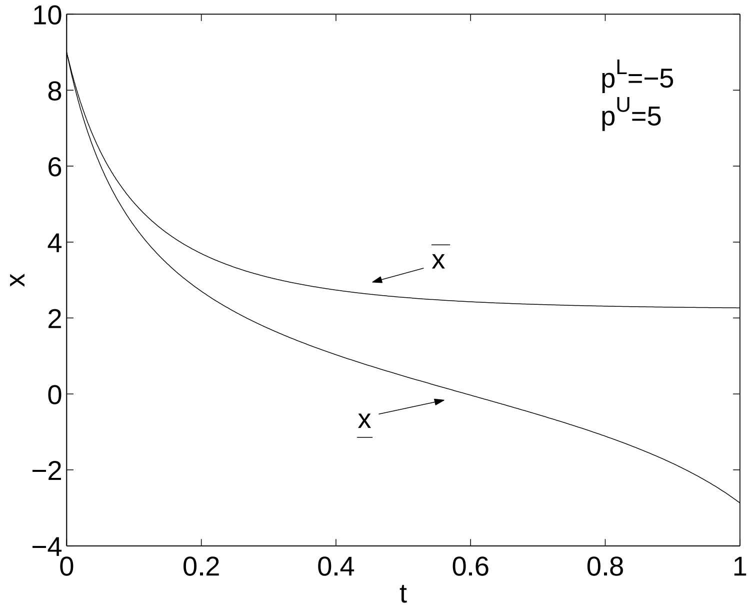
and for all $(x_k, x_{k-}), (\tilde{x}_k, x_{k-}) \in \mathcal{D}$.

Definition 2: Let $f(t,x) = (f_1(t,x), ..., f_2(t,x))^T$ and each $f_k(t, x_k, x_{k-})$ be unconditionally partially isotone on $\mathcal{I}_0 \times \Re \times \Re^{n-1}$ with respect to any component of x_{k-}, but not necessarily with respect to x_k. Then f is quasi-monotone increasing on $\mathcal{I}_0 \times \Re^n$ with respect to x (Walter, 1970)

Example: Constant bounds

$$\dot{\underline{x}}(t) = -\underline{x}(t)^2 - 5 \qquad \dot{\overline{x}}(t) = -\overline{x}(t)^2 + 5$$

$$\underline{x}(0) = 9 \qquad \overline{x}(0) = 9$$



Parameter Dependent Bounds

Let $\underline{f}(t, x, p) \le f(t, x, p)\ \forall x \in [\underline{x}(t), \overline{x}(t)],\ \forall p \in [p^L, p^U],\ \forall t \in [t_0, t_{NP}]$ and $\underline{\underline{x}}_0(p) \le x_0(p)\ \forall p \in [p^L, p^U]$, where $\underline{f} :\ [t_0, t_{NP}] \times \Re^n \times [p^L, p^U] \mapsto \Re^n$ and $\underline{\underline{x}}_0 :\ [p^L, p^U] \mapsto \Re^n$.

If $\underline{f}$ is quasi-monotone increasing w.r.t. x and $\underline{\underline{x}}(t, p)$ is the solution of the ODE:

$$\dot{\underline{\underline{x}}} = \underline{f}(t, \underline{\underline{x}}, p),\ \forall t \in [t_0, t_{NP}]$$

$$\underline{\underline{x}}(t_0, p) = \underline{\underline{x}}_0(p)$$

$$p \in [p^L, p^U]$$

then $\quad \underline{\underline{x}}(t, p) \le x(t, p)\ ,\ \forall p \in [p^L, p^U]\ ,\ \forall t \in [t_0, t_{NP}]$.

Affine Bounds

Let $\underline{f}(t,\underline{\underline{x}},p) = A(t)\underline{\underline{x}} + B(t)p + C(t)$ and $\underline{\underline{x}}_0(p) = Dp + E$, where $A(t)$, $B(t)$ and $C(t)$ are continuous on $[t_0, t_{NP}]$. Then the analytical solution is (Zadeh and Desoer, 1963):

$$\begin{aligned}\underline{\underline{x}}(t,p) \;&=\; \left\{\Phi(t,t_0)D + \int_{t_0}^{t} \Phi(t,\tau)B(\tau)d\tau\right\}p \\ &\quad +\Phi(t,t_0)E + \int_{t_0}^{t} \Phi(t,\tau)C(\tau)d\tau,\end{aligned}$$

where $\Phi(t,t_0)$ is the transition matrix:

$$\begin{aligned}&\dot{\Phi}(t,t_0) = \underline{A}(t)\Phi(t,t_0) \;\; \forall t \in [t_0, t_{NP}] \\ &\Phi(t_0,t_0) = I\end{aligned}$$

and I is the identity matrix. $\underline{\underline{x}}(t,p) = \underline{M}(t)p + \underline{N}(t)$.

$\underline{M}(t_i)$, $\underline{N}(t_i)$ calculation

1. Apply $\underline{\underline{x}}(t_i, p) = \underline{M}(t_i)p + \underline{N}(t_i)$ for $r+1$ values of p
2. Calculate $\underline{\underline{x}}(t_i, p)$ for the $r+1$ values of p from the integration of the linear ODE
3. Solve n linear systems to find the $r+1$ unknowns for each one of the n dimensions of x

Example: Affine bounds

Underestimating IVP

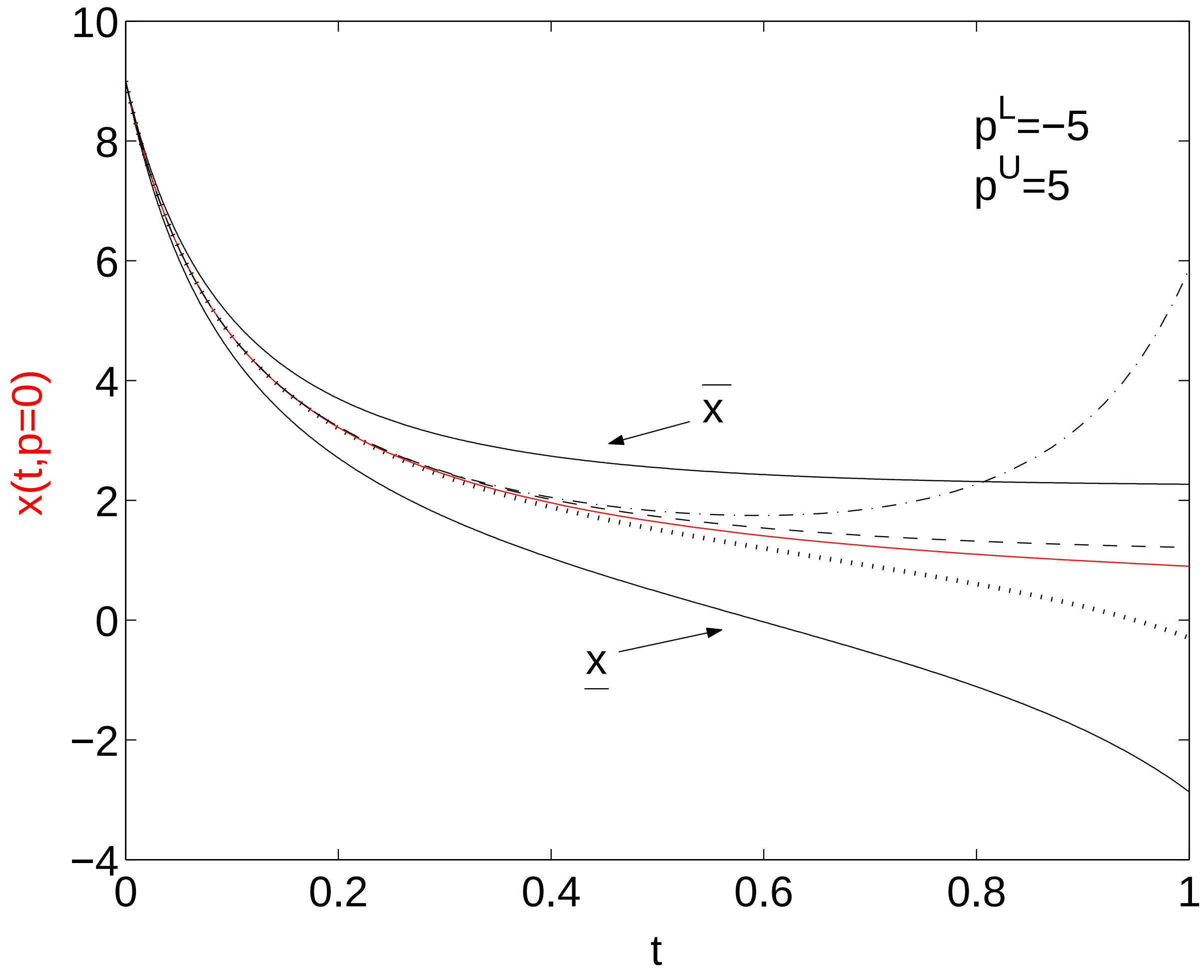
$$\dot{\underline{\underline{x}}} = -(\underline{x} + \overline{x})\underline{\underline{x}} + \underline{x}\overline{x} + v \quad \forall t \in [0, 1]$$
$$\underline{\underline{x}}(0, v) = 9$$

Overestimating IVPs

$$\dot{\overline{\overline{x}}}_1 = -2\underline{x}\overline{\overline{x}}_1 + \underline{x}^2 + v \quad \forall t \in [0, 1]$$
$$\overline{\overline{x}}_1(0, v) = 9$$

$$\dot{\overline{\overline{x}}}_2 = -2\overline{x}\overline{\overline{x}}_2 + \overline{x}^2 + v \quad \forall t \in [0, 1]$$
$$\overline{\overline{x}}_2(0, v) = 9$$

Example: Affine bounds for $p = 0$

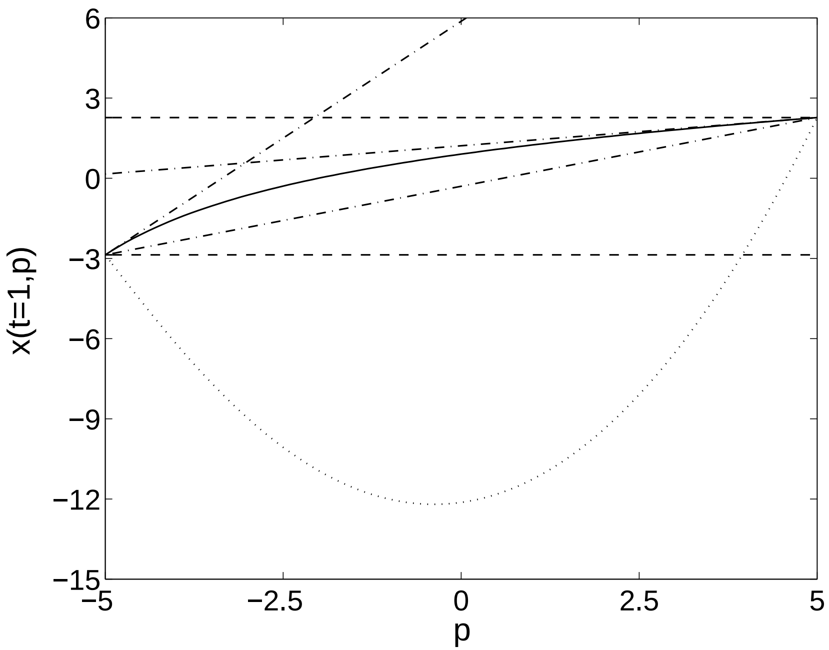


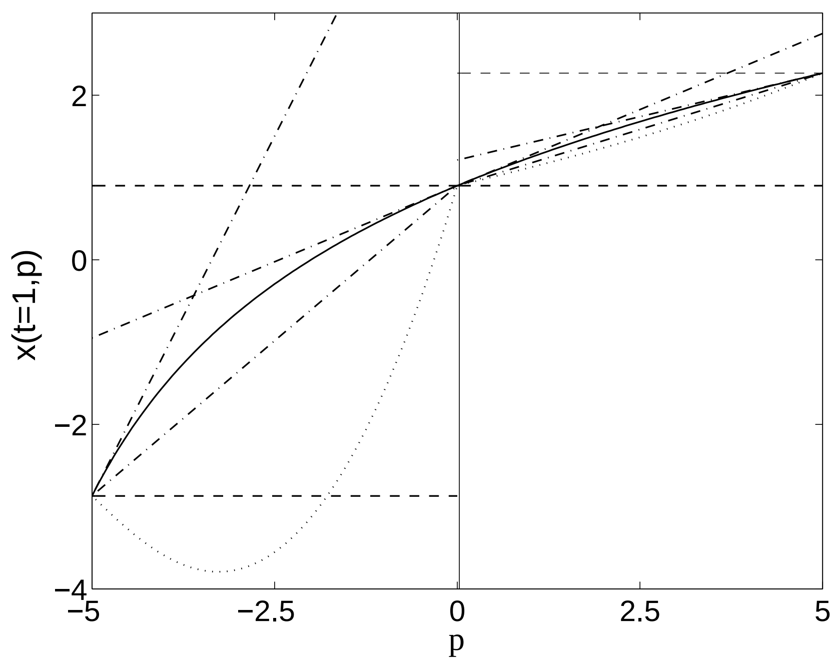
α calculation for $x_k(t_i, p)$

$$[H_{x_k(t_i)}] \ni H_{x_k(t_i)}(p) = \nabla^2 x_k(t_i, p),\ \forall p \in [p^L, p^U] \subset \Re^r$$
$$i = 0, 1, ..., NS,\ k = 1, 2, ..., n$$

1. 1st and 2nd order sensitivity equations
2. Create bounds using Differential Inequalities
3. Construct the interval Hessian matrix
4. Calculate α using the scaled Gerschgorin method

Example: All bounds





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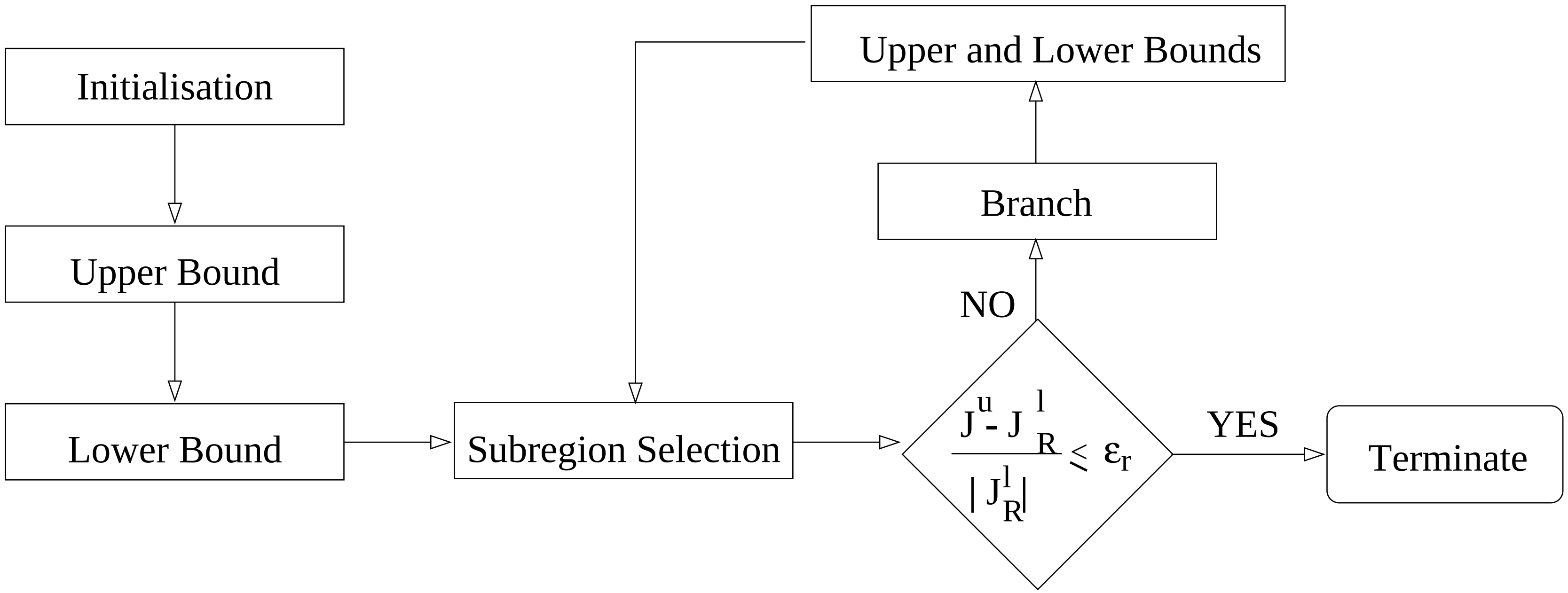
Spatial BB Algorithm (Horst and Tuy, 1996)



Global optimization algorithm

Step 1 Initialization: empty list of subregions, bounds on solution

Step 2 First upper bound calculation (local optimization)

Step 3 First lower bound calculation, including relaxation. Add subregions to list.

Step 4 Subregion selection

- Terminate if list is empty
- Choose region with lowest lower bound otherwise

Step 5 Check for convergence (relative tolerance, max iter)

Step 6 Branch with standard rule (least reduced axis)

Step 7 Upper bound for new regions (not needed at every iteration)

Step 8 Lower bound calculation for each region. Go to Step 4.

Lower bound calculation for region R (Step 8)

Let J^L be the lower bound on the parent region of R.
Let J^U be the best known upper bound.

- Obtain bounds on the differential variables
- If affine bounds are used, obtain necessary matrices
- Form convex relaxation of problem for region R
- If a feasible solution with objective function J_R^L is obtained, then
  - If affine bounds are used and $J_R^L < J^L$, set $J_R^L = J^L$
  - If $J_R^L \leq J^U$, add R to the list of subregions

Outline of proof of convergence

Three main properties are needed:

- Bound improvement after branching
  - Constant bounds improve after branching
  - α-based bounds improve after branching
  - Affine bounds do not improve after branching.
    Ensure improvement through test in Step 8: if $J_R^L < J^L$, set $J_R^L = J^L$
- Bound improving selection operation
  - Consequence of region selection criterion (Step 6)
- Consistent bounding operation
  - Maximum distance between objective function and its relaxation converges to zero.
  - Maximum distance between any constraint and its relaxation converges to zero.

Key elements of proof

Bounds on the solutions of the ODE are such that:

$$\dot{\underline{x}}_k = \text{inf}\, f_k(t, \underline{x}_k, [\underline{x}_{k-}, \overline{x}_{k-}], [p^L, p^U]) \geq \text{inf}\, f_k(t, [\underline{x}, \overline{x}], [p^L, p^U])$$

$$\dot{\overline{x}}_k = \text{sup}\, f_k(t, \overline{x}_k, [\underline{x}_{k-}, \overline{x}_{k-}], [p^L, p^U]) \leq \text{sup}\, f_k(t, [\underline{x}, \overline{x}], [p^L, p^U])$$

$$\forall t \in [t_0, t_{NP}] \text{ and } k = 1, ..., n$$

Inclusion monotonicity of interval operations ensures consistency of bounding operation with constant bounds.

Similar approach can be taken to show α-based underestimators yield a consistent bounding operation:

- Interval Hessian matrix obtained through differential inequalities has desired properties.
- Hence, α and α-based bounds have desired properties.

Implementation of algorithm

- MATLAB 5.3 implementation
- NLPs: Use fmincon function (Optimization Toolbox)
- IVP solution: ode45 (Runge-Kutta based on Dormand-Prince pair)
- Interval calculations: INTLAB with directed outward rounding.
- Runs performed on an Ultra 60 workstation.

Case Study I: *Parameter estimation for* 1^{st} *order reaction* (Tjoa and Biegler, 1991) $A \xrightarrow{k_1} B \xrightarrow{k_2} C$

$$\min_{k_1,k_2} \sum_{j=1}^{10} \sum_{i=1}^{2} (x_i(t_j) - x_i^{exp}(t_j))^2$$

subject to:

$$\begin{aligned} &\dot{x}_1 = -k_1 x_1 \\ &\dot{x}_2 = k_1 x_1 - k_2 x_2 \end{aligned} \quad \forall t \in [0,1]$$
$$\begin{aligned} &x_1(0) = 1 \\ &x_2(0) = 0 \\ &0 \le k_1 \le 10 \\ &0 \le k_2 \le 10 \end{aligned}$$

- Up to 8 affine underestimators and 8 affine overestimators can be constructed.
- α-values ≤ 0.5. Convexity is identified.

Results for case study I

Obj. fun. = 1.1856e-06; $k_1 = 5.0035$; $k_2 = 1.0000$

Underestimation scheme	Branching strategy	ϵ_r	Iter.	CPU time (sec)
C	1	1.00e-02	3,501	2,828
C	1	1.00e-03	34,508	22,959
C & A	1	1.00e-02	37	767
C & A	1	1.00e-03	39	801
C & α	1	1.00e-02	31	396
C & α	1	1.00e-03	35	420
C & α	2	1.00e-02	27	366
C & α	2	1.00e-03	31	407
C & A & α	1	1.00e-02	31	959
C & A & α	2	1.00e-02	27	875

Case Study II: *Parameter estimation for catalytic cracking of gas oil* (Tjoa and Biegler, 1991)

$$
\begin{array}{ccc}
A & \xrightarrow{k_1} & Q \\
k_3 \searrow & & \swarrow k_2 \\
& S &
\end{array}
$$

$$\min_{k_1,k_2,k_3} \sum_{j=1}^{20} \sum_{i=1}^{2} (x_i(t_j) - x_i^{exp}(t_j))^2$$

subject to:

$$
\left.\begin{array}{l}
\dot{x}_1 = -(k_1 + k_3)x_1^2 \\
\dot{x}_2 = k_1 x_1^2 - k_2 x_2
\end{array}\right. \forall t \in [0, 0.95]
$$

$$
\begin{array}{l}
x_1(0) = 1 \\
x_2(0) = 0 \\
0 \leq k_1 \leq 20 \\
0 \leq k_2 \leq 20 \\
0 \leq k_3 \leq 20
\end{array}
$$

Results for case study II

Obj. fun. $= 2.6557e-03$; $k = (12.2141, 7.9799, 2.2215)^T$

Underestimation scheme	Branching strategy	ϵ_r	Iter.	CPU time (sec)
C	1	6.41e-02	10,000	16,729
C	1	1.33e-02	100,000	152,816
C & A	1	1.00e-02	67	26,597
C & A	1	1.00e-03	94	35,478
C & α	1	1.00e-02	73	11,415
C & α	1	1.00e-03	88	13,524
C & α	2	1.00e-02	65	10,116
C & α	2	1.00e-03	81	12,300

32 affine underestimators + 64 affine overestimators

Case Study III: *Parameter estimation for reversible gas phase reaction* (Bellman, 1967):

$$2NO + O_2 \rightleftharpoons 2NO_2$$

$$\begin{array}{ll}
\min\limits_{k_1,k_2} & \displaystyle\sum_{j=1}^{14} (x(t=t_j,k_1,k_2) - x^{exp}(t_j))^2 \\
\text{s.t.} & \dot{x} = k_1(126.2 - x)(91.9 - x)^2 - k_2 x^2 \ \ \forall t \in [0, 39] \\
& x(t=0,k_1,k_2) = 0 \\
& 0 \le k_1 \le 0.1 \\
& 0 \le k_2 \le 0.1
\end{array}$$

x is the difference of the pressure of the system from the initial pressure.

k_1 and k_2 are the rate constants of the forward and reverse reactions.

Results for case study III

Obj. fun.=21.86671; $k_1 = 4.5771\text{e-}06$; $k_2 = 2.7962\text{e-}04$

Underestimation scheme	Branching strategy	ϵ_r	Iter.	CPU time (sec)
constant	1	1.00e-02	75,441	58,513

- only constant bounds used
- 32 affine underestimators + 128 affine overestimators
  - stiff systems, expensive to integrate
  - quality of bounds not better than constant bounds
- quality of α-based bounds poor due to wrapping effect

Case Study IV: *Optimal control with end-point constraint* (Goh and Teo, 1988)

Problem formulation using control vector parameterization:

$$
\begin{array}{rll}
\min\limits_{u_1,u_2} & x_2(t=1,u_1,u_2) & \\
\text{s.t.} & \dot{x}_1 = u_1(1-t) + u_2 t & \forall t \in \\
 & \dot{x}_2 = x_1^2 + (u_1(1-t) + u_2 t)^2 & [0,1] \\
 & x_1(t=0,u_1,u_2) = 1 & \\
 & x_2(t=0,u_1,u_2) = 0 & \\
 & x_1(t=1,u_1,u_2) \geq 1 & \\
 & x_1(t=1,u_1,u_2) \leq 1 & \\
 & -1 \leq u_1 \leq 1 & \\
 & -1 \leq u_2 \leq 1 &
\end{array}
$$

16 affine underestimators + 2 affine overestimators

Results for case study IV

Obj. fun.=9.24242e-01; $u_1 = -0.4545$; $u_2 = 0.4545$

Underestimation scheme	Branching strategy	ϵ_r	Iter.	CPU time (sec)
C	1	1.00e-02	302	317
C	1	1.00e-03	1,062	1,106
C & A	1	1.00e-02	150	2787
C & A	1	1.00e-03	527	9922
C & α	1 or 2	1.12e-13	0	8

α-based bounds recognize convexity of problem at root node.

Conclusions

- *Three types of rigorous convex relaxations* have been developed
- Convergence of the algorithm has been proved
- A BB global optimization algorithm has been applied successfully to case studies in parameter estimation and optimal control
- References:
  - Papamichail and Adjiman, J. Glob Opt, 2002.
  - Papamichail and Adjiman, Comp Chem Eng, 2003.

Perspectives

- Basic theoretical developments of recent years make global optimization of problems with nonlinear IVPs in the constraints possible.
- Practical applicability limited by
  - cost of constructing underestimators and overestimators,
  - quality of estimators for highly nonlinear systems (e.g. oscillatory) and long time horizons.
- Further research needed to
  - identify classes of IVPs for which current estimators are effective,
  - develop new estimators for other problem classes,
  - establish basic theory for DAE systems.