Overview of aBB-based Approaches In Deterministic Global Optimization

Christodoulos A. Floudas

Princeton University

- Department of Chemical Engineering
- Program of Applied and Computational Mathematics
- Department of Operations Research and Financial Engineering
- Center for Quantitative Biology

(Adjiman, Androulakis, Akrotirianakis, Birgin, Caratzoulas, Gounaris, Kreinovich, Meyer, Maranas, Martinez, Neumaier)

Outline

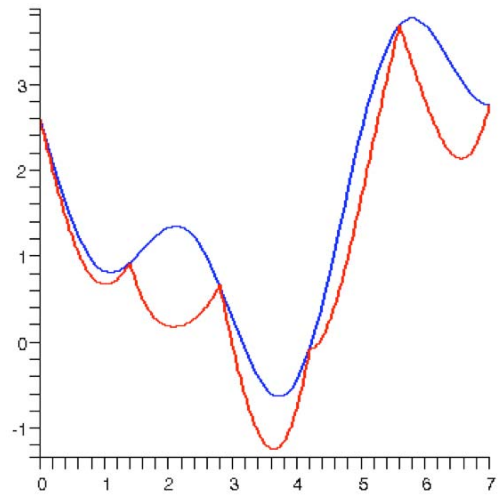
- Deterministic Global Optimization: Objectives & Motivation
- Convex Envelopes:
    - Trilinear Monomials
    - Univariate Monomials
    - Fractional Terms
    - Edge Concave functions
- Checking Convexity: Products of Univariate Functions
- Convex Underestimators for Trigonometric Functions
- PαBB: Piecewise Quadratic Perturbations
- GαBB: Generalized αBB
- Functional Forms of Convex Underestimators
- Augmented Lagrangian Approach for Global Optimization
- **New Class of Convex Underestimators**
- Pooling Problems & Generalized Pooling Problems
- Conclusions

Novel Univariate Underestimator

(Gounaris and Floudas, 2008a)

Use piecewise αBB underestimators and augment them with tangent lines !

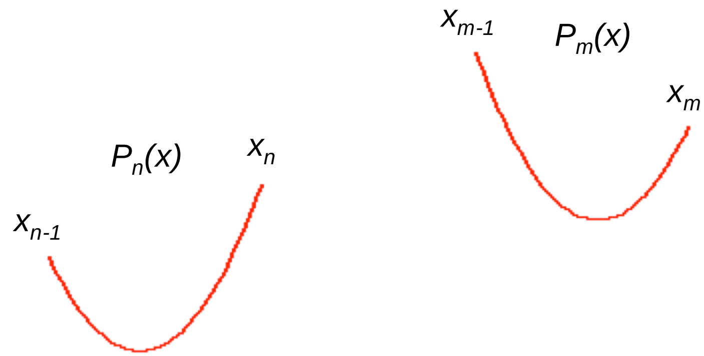
- ***Step 1:*** ***Partition domain $[x^L, x^U]$ in N= subdomains***
- ***Step 2:*** ***Construct αBB underestimators $P_i(x)$, i=1..N***
- ***Step 3:*** ***Identify tangential linear segments T_k, k=1..N^L required for an overall underestimator U(x)***
  - ***→ Use slope comparisons***
  - ***→ Local solver suffices !***
  - ***→ U(x) is smooth (C^1-continuous)***



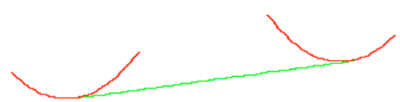
Novel Univariate Underestimator

Step 3 : *Utilize* INNER *and* OUTER *algorithms*

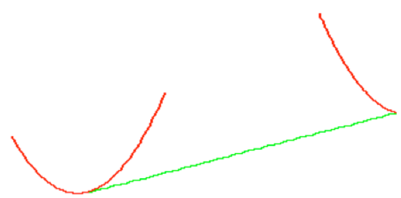
INNER : *Given two convex pieces, identify supporting line segment that underestimates both pieces in their respective subdomains*



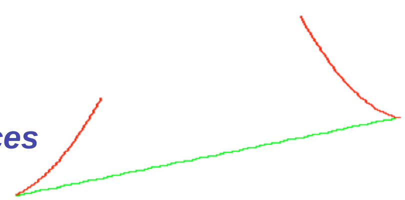
Case 1 : Tangential to both pieces



Case 2 : Tangential only to one piece



Case 3 : Not tangential to any of the two pieces



Applicable case can be identified just by comparing slopes !

Due to convexity of pieces, local techniques (e.g. Newton-Raphson) suffice for calculation of tangential points !

Novel Univariate Underestimator

***Step 3* : Utilize INNER and OUTER algorithms**

OUTER : *Given a set of sequential convex pieces (not necessarily connected), identify those supporting line segments that participate in the overall underestimator*

N : # of pieces
N_L : # of lines in list
n_i : piece from which i^{th} line begins
L_i : i^{th} line in the list (i=1,2,…N_L)
c : candidate line
m : candidate piece

$$N_L = 0,\ n_1 = 1,\ m = 2$$

$$(R):$$

$$\text{while}\ \ (n_{NL+1} \neq N)$$

$$\{$$

$$(r):$$

$$c = INNER(n_{NL+1}, m)$$

$$if\,(NL = 0).or.\left(\frac{dc}{dx} > \frac{dL_{N_L}}{dx}\right)$$

$$\{$$

$$N_L = N_L + 1,\ L_{N_L} = c,\ n_{NL+1} = m,\ m = m+1,\ goto(R)$$

$$\}$$

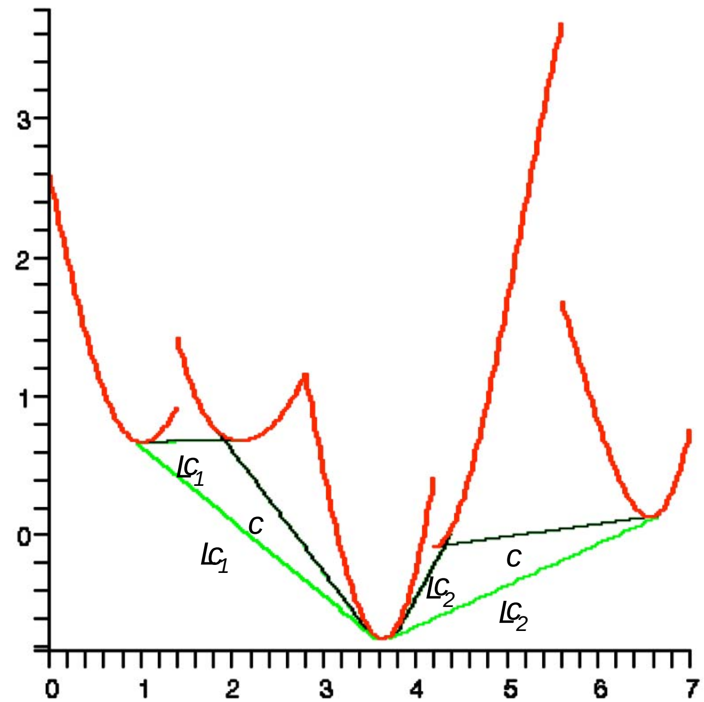
$$else$$

$$\{$$

$$N_L = N_L - 1,\ L_{N_L+1} = void,\ goto(r)$$

$$\}$$

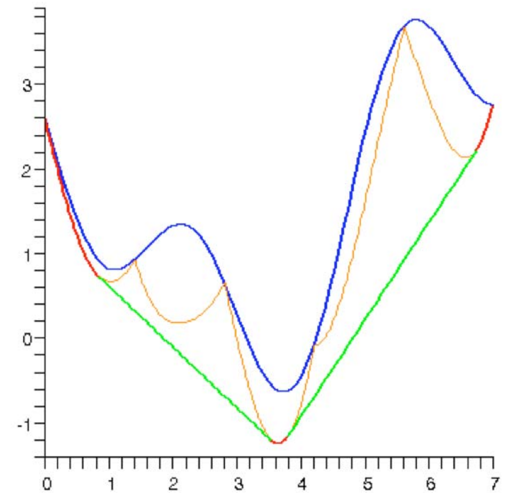
$$\}$$



Novel Univariate Underestimator

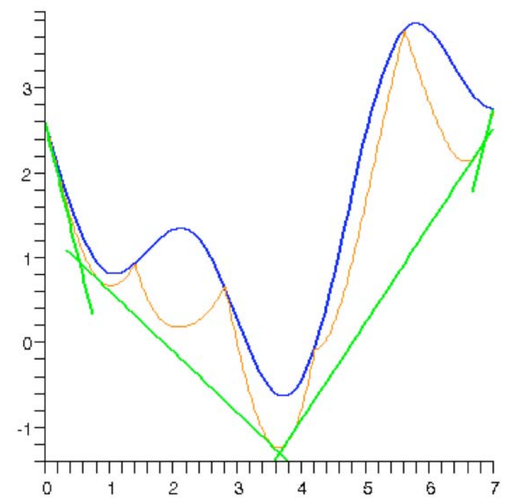
Use piecewise αBB underestimators and augment them with tangent lines !

- ***Step 1:*** *Partition domain $[x^L, x^U]$ in N subdomains*
- ***Step 2:*** *Construct αBB underestimators $P_i(x)$, $i=1..N$*
- ***Step 3:*** *Identify tangential linear segments T_k, $k=1..N^L$ required for an overall underestimator $U(x)$*
  - → *Use slope comparisons*
  - → *Local solver suffices !*
  - → *$U(x)$ is smooth (C^1-continuous)*



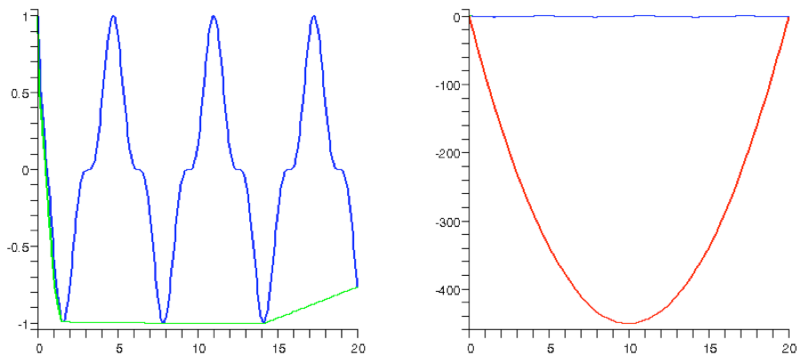
Furthermore, why not take only the tangents into account ?

- ***Step 1:*** *Construct underestimator $U(x)$*
- ***Step 2:*** *Consider linear segments as lines $T_k(x)$*
- ***Step 3:*** *If applicable, augment set T_k with tangent lines at domain edges*
- ***Step 4:*** *New underestimator is $V(x) = \max_k \{T_k(x)\}$*
  - → *Lower bounding problem can now be formulated as an LP !*
  - → *Relaxed constraints are linear !*

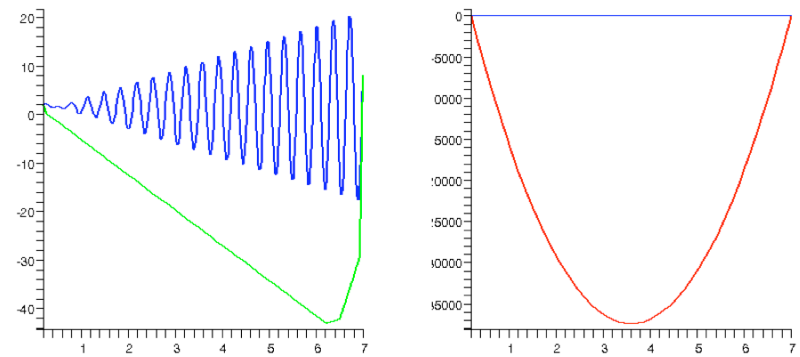


Examples – Univariate Functions

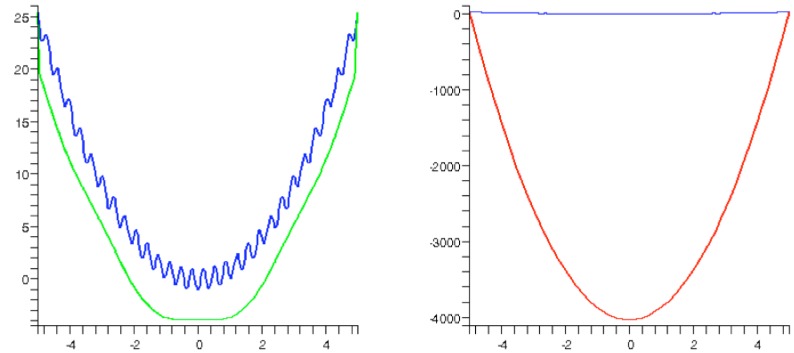
$$f(x) = e^{-3x} - \sin^3 x$$



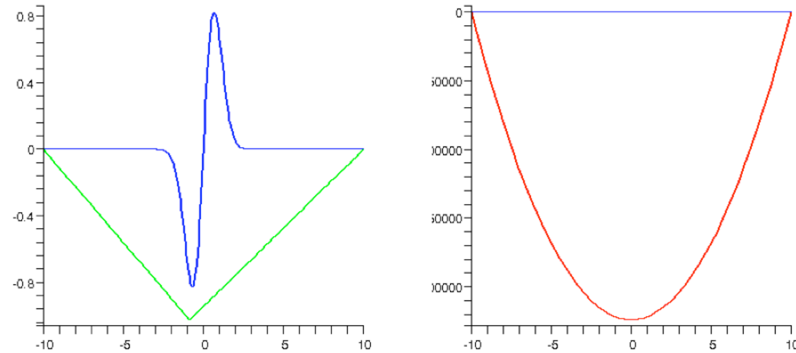
$$f(x) = (3x - 1.4)\sin(18x) + 1.7$$



$$f(x) = x^2 - \cos(18x)$$



$$f(x) = (x + \sin x)e^{-x^2}$$



Note: N = 32
(in all examples)

Examples – Univariate Functions

#	Function $f(x)$	$[x^L, x^U]$	LM	GM	αBB	N = 2	4	8	16	32	64	128	256	512	1024	GO f^*
1	$e^{-3x} - sin^3 x$	$[0, 20]$	4	1	-450	-113	-28.4	-6.46	-1.549	*	*	*	*	*	*	-1
2	$\sum_{k=1}^{5} -cos[(k+1)x] + 4$	$[0.2, 7.0]$	7	1	-516	-126	-32.2	-6.52	*	*	*	*	*	*	*	-1
3	$(x - x^2)^2 + (x-1)^2$	$[-10, 10]$	1	1	*	*	*	*	*	*	*	*	*	*	*	0
4	$(3x - 1.4)sin(18x) + 1.7$	$[0.2, 7.0]$	21	1	-37320	-9320	-2345	-598	-146	-43.0	-18.392	*	*	*	*	-17.58287
5	$2x^2 - \frac{3}{100}e^{-(200(x-0.0675))^2}$	$[-10, 10]$	1	1	-1E+12	-8E+10	-8E+9	-6E+8	-5E+7	-3E+6	-1E+5	-4608	-665	-29.2	-0.94	-0.020903
6	$cosx - sin(5x) + 1$	$[0.2, 7.0]$	6	1	-150	-37.1	-9.82	-2.45	-1.004	*	*	*	*	*	*	-0.952897
7	$-x - sin(3x) + 1.6$	$[0.2, 7.0]$	4	1	-53.2	-16.7	-8.21	-6.430	*	*	*	*	*	*	*	-6.262872
8	$x + sin(5x)$	$[0.2, 7.0]$	7	1	-142	-34.6	-8.97	-1.88	-0.0861	*	*	*	*	*	*	-0.077590
9	$-e^{-x}sin(2\pi x) + 1$	$[0.2, 7.0]$	7	1	-241	-59.3	-14.2	-2.48	-0.25	*	*	*	*	*	*	0.211315
10	$e^{-x}sin(2\pi x)$	$[0.2, 7.0]$	7	1	-242	-60.5	-15.1	-4.19	-0.73	*	*	*	*	*	*	-0.478362
11	$-x + sin(3x) + 1$	$[0.2, 7.0]$	5	1	-55.7	-18.1	-8.91	*	*	*	*	*	*	*	*	-5.815675
12	$xsinx + sin(\frac{10x}{3}) + lnx - 0.84x + 1.3$	$[0.2, 7.0]$	4	1	-263	-58.2	-13.0	-7.398	*	*	*	*	*	*	*	-7.047444
13	$sinx + sin(\frac{10x}{3}) + lnx - 0.84x$	$[2.7, 7.5]$	3	1	-39.7	-11.5	-6.05	-4.632	*	*	*	*	*	*	*	-4.601308
14	$ln(3x)ln(2x) - 0.1$	$[0.2, 7.0]$	1	1	-528	-82.8	-9.02	*	*	*	*	*	*	*	*	-0.141100
15	$\sum_{k=0}^{5} kcos[(k+1)x + k] + 12$	$[0.2, 7.0]$	8	1	-2013	-496	-123	-25.7	-2.86	*	*	*	*	*	*	-0.870885
16	$-\sum_{k=1}^{5} ksin[(k+1)x + k] + 3$	$[0.2, 7.0]$	7	1	-2023	-501	-132	-35.1	-11.19	*	*	*	*	*	*	-9.031249
17	$sin^2(1 + \frac{x-1}{4}) + (\frac{x-1}{4})^2$	$[-10, 10]$	1	1	*	*	*	*	*	*	*	*	*	*	*	0.475689
18	$\sqrt{x}sin^2x$	$[0.2, 7.0]$	3	2	-75.5	-15.6	-1.93	-0.122	*	*	*	*	*	*	*	0
19	$x^2 - cos(18x)$	$[-5, 5]$	29	1	-4026	-1001	-249	-63.0	-16.5	-3.84	-1.459	*	*	*	*	-1
20	e^{x^2}	$[-10, 10]$	1	1	*	*	*	*	*	*	*	*	*	*	*	1

Asterisk = Global Optimum reached (6 decimal digits)

(Test functions from Casado et al., 2003)

Examples – Univariate Functions

#	Function $f(x)$	$[x^L, x^U]$	LM	GM	αBB	N = 2	4	8	16	32	64	128	256	512	1024	GO f^*
21	$\frac{x^2}{20} - cosx + 2$	$[-20, 20]$	7	1	-199	-42.7	-9.60	-0.59	0.733	*	*	*	*	*	*	1
22	$cosx + 2cos(2x)e^{-x^2}$	$[0.2, 7.0]$	2	1	-72.9	-18.6	-3.41	*	*	*	*	*	*	*	*	-0.918397
23	$(x + sinx)e^{-x}$	$[-10, 10]$	1	1	-2E+5	-55163	-1900	-70.4	-3.50	-1.022	-0.8255	*	*	*	*	-0.824239
24	$2sinxe^{-x}$	$[0.2, 7.0]$	2	1	-19.0	-4.38	-0.57	*	*	*	*	*	*	*	*	-0.027864
25	$2cosx + cos(2x) + 5$	$[0.2, 7.0]$	3	2	-30.9	-5.07	2.28	3.335	*	*	*	*	*	*	*	3.5
26	$e^{sin(3x)}$	$[0.2, 7.0]$	5	3	-141	-34.8	-8.22	-1.03	*	*	*	*	*	*	*	0.367879
27	$sinxcosx - 1.5sin^2x + 1.2$	$[0.2, 7.0]$	3	2	-39.2	-9.87	-2.08	-0.4528	*	*	*	*	*	*	*	-0.451388
28	$sinx$	$[0, 20]$	4	3	-50.8	-13.5	-3.84	-1.301	*	*	*	*	*	*	*	-1
29	$2(x-3)^2 - e^{\frac{x}{2}} + 5$	$[0.2, 7.0]$	1	1	-25.1	-5.21	*	*	*	*	*	*	*	*	*	-0.410315
30	$-e^{sin(3x)} + 2$	$[0.2, 7.0]$	4	4	-281	-69.6	-18.1	-3.55	-0.767	*	*	*	*	*	*	-0.718282
31	$-\sum_{i=1}^{10} \frac{1}{k_i(x-a_i)^2+c_i}$	$[0, 10]$	8	1	-5E+8	-2E+7	-6E+5	-37943	-3838	-211	-25.4	-14.689	*	*	*	-14.59265
32	$sin(\frac{1}{x})$	$[0.02, 1]$	6	6	-30312	-7579	-1894	-474	-118	-28.0	-5.83	-1.220	-1.119	-1.094	-1.024	-1
33	$-\sum_{k=1}^{5} ksin[(k+1)x + k]$	$[-10, 10]$	20	3	-17496	-4374	-1096	-276	-79.5	-22.0	*	*	*	*	*	-12.03125
34	$\frac{x^2-5x+6}{x^2+1} - 0.5$	$[0.2, 7.0]$	1	1	-24139	-406	-1.34	*	*	*	*	*	*	*	*	-0.535534
35	$-\sum_{i=1}^{10} \frac{1}{k_i(x-a_i)^2+c_i}$	$[0, 10]$	7	1	-8E+8	-5E+7	-2E+6	-72451	-3154	-439	-39.2	-15.41	-13.993	-13.923	*	-13.92245
36	$\frac{(x+1)^3}{x^2} - 1.7$	$[0.2, 7.0]$	1	1	*	*	*	*	*	*	*	*	*	*	*	-0.35
37	$x^4 - 12x^3 + 47x^2 - 60x - 20e^{-x}$	$[-1, 7]$	1	1	-3716	-606	-79.9	*	*	*	*	*	*	*	*	-32.78126
38	$x^6 - 15x^4 + 27x^2 + 250$	$[-4, 4]$	2	2	-1478	-342	-86.0	2.60	*	*	*	*	*	*	*	7
39	$x^4 - 10x^3 + 35x^2 - 50x + 24$	$[-10, 20]$	2	2	-560	-112	-36.1	-9.41	-2.25	-1.268	*	*	*	*	*	-1
40	$24x^4 - 142x^3 + 303x^2 - 276x + 3$	$[0, 3]$	2	1	-114	-95.2	-90.6	*	*	*	*	*	*	*	*	-89

CPU(sec) = 0.05 avg / 0.07 max (N= 512)
0.09 avg / 0.12 max (N=1024)

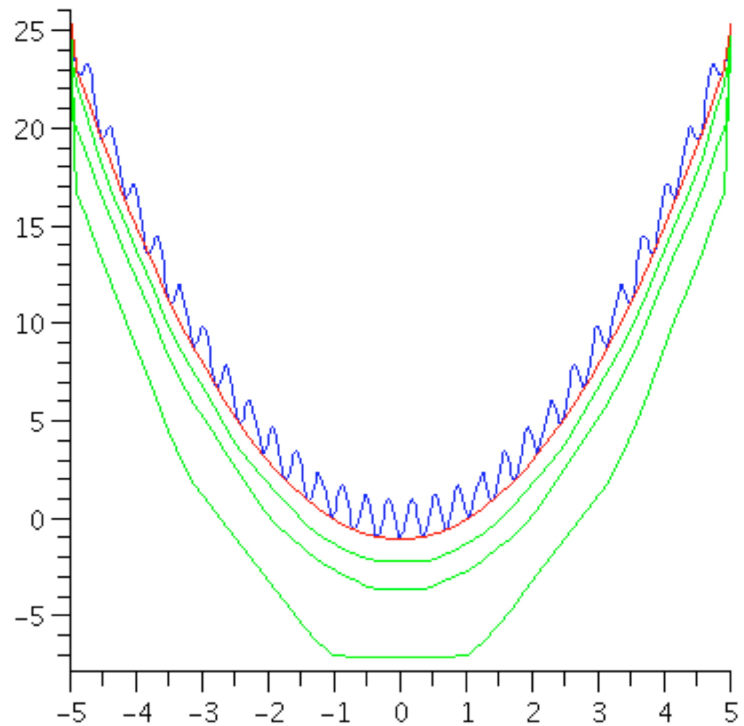
(Test functions from Casado et al., 2003)

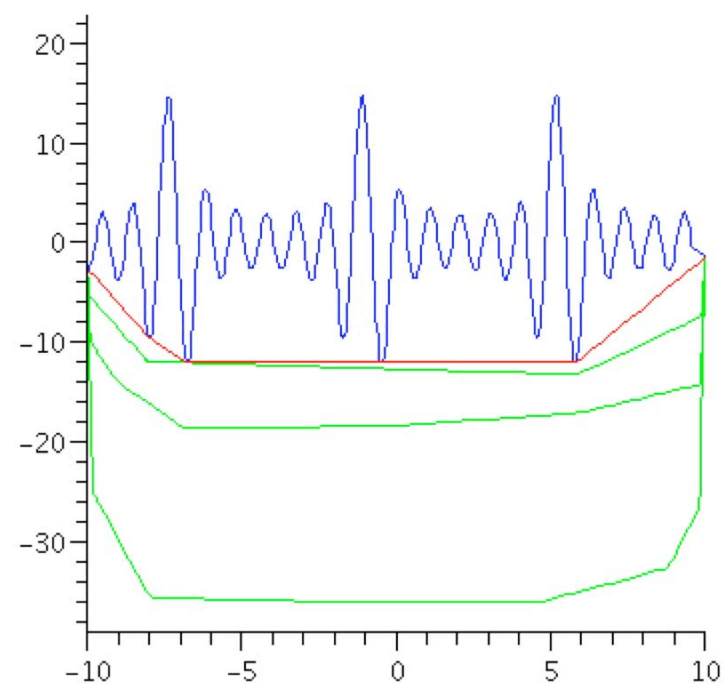
Tightness of U(x), V(x)

Property 1: ***Underestimators become tighter as level of partitioning increases (| →sN , s ∈Í *)***

Property 2: ***There is some <u>finite</u> level of partitioning, for which U(x) is the <u>convex envelope</u> of f(x)***

Property 3: ***There is some <u>finite</u> level of partitioning, for which V(x) is ε-close to U(x)***





Sufficiently large N will CLOSE the GAP at the ROOT NODE of the bb-tree !

Novel Multivariate Underestimator

Gounaris, Floudas, JOGO, 2008b

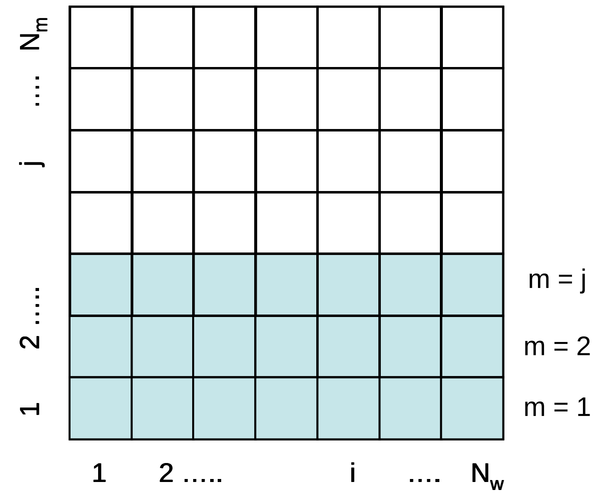
Univariate underestimators are very tight !

Can we make use of them ?

- ***Step 1:*** ***Partition domain into*** $N = \prod_{i=1}^{n} N_i$ ***subdomains***
- ***Step 2:*** ***Select variable 'w' and enumerate all*** $M = N/N_w$ ***permutations of the other domain partitions***
- ***Step 3:*** ***For every permutation 'm', define univariate function*** $G_{wm}(x_w) = \min_{x_i, i \neq w} P(x)$

→ This function is piecewise convex, thus suitable for the univariate methodology

1 2



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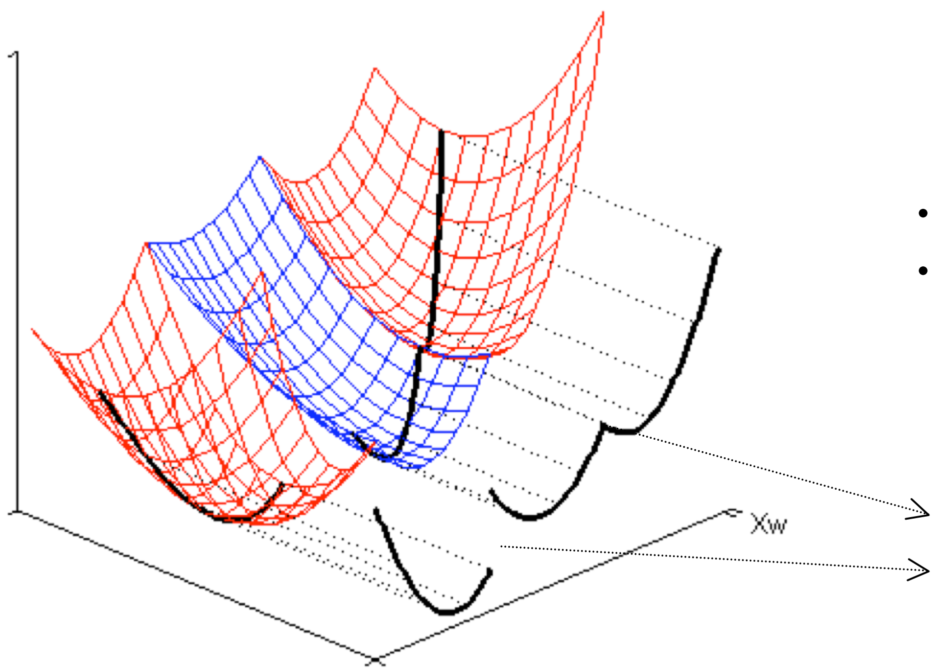


Some pieces are connected

Some others are not

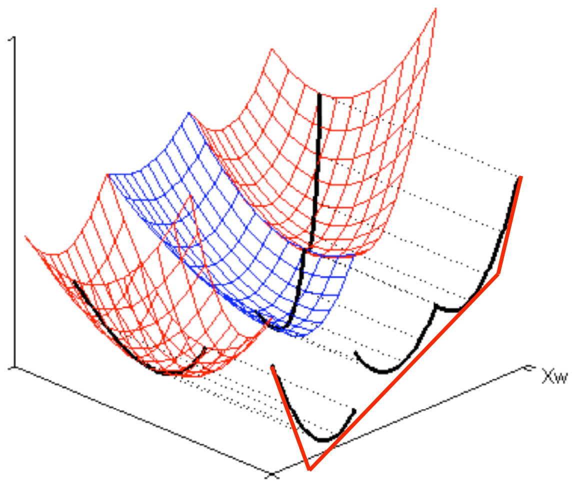
Function $G_{wm}(x_w)$:

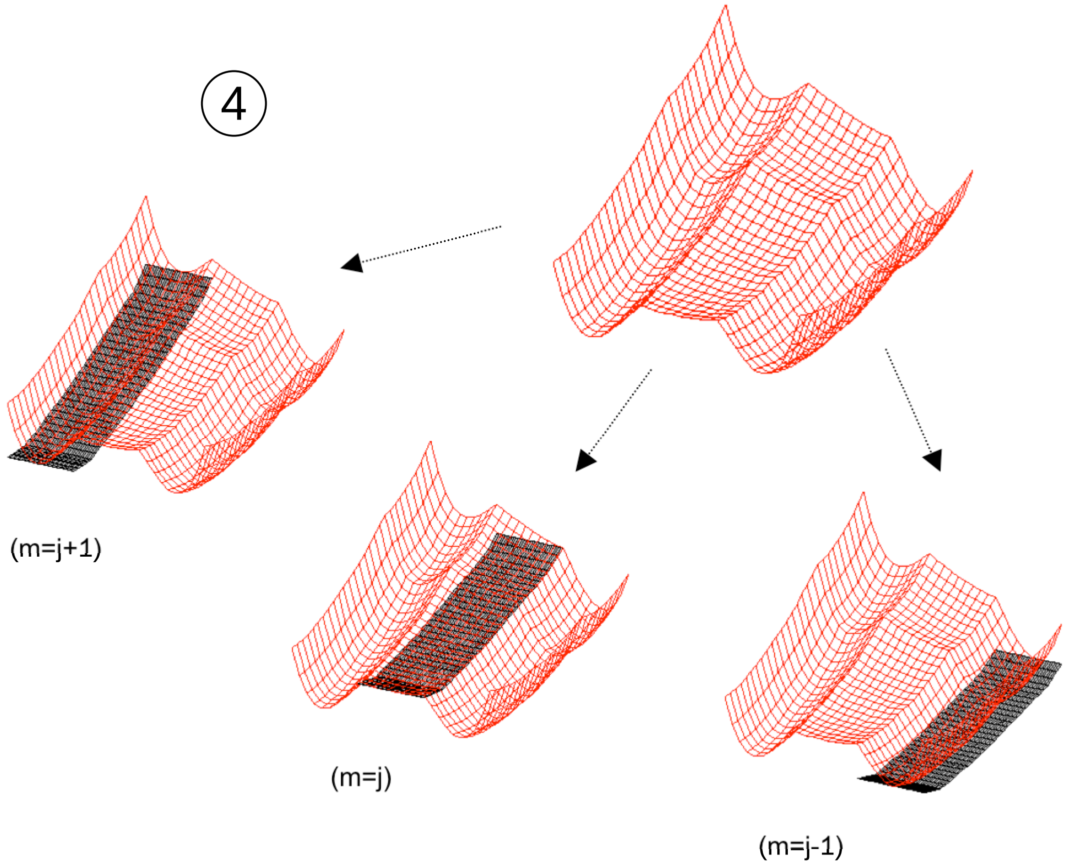
- **Usually not known explicitly**
- **However, evaluations can be done reliably through convex minimization**

Novel Multivariate Underestimator

➢ ***Step 4**: Calculate underestimator $V_{wm}(x_w)$ of $G_{wm}(x_w)$*

→ ***Underestimator $V_{wm}(x_w)$, considered as $V_{wm}(x)$, is valid for the whole subdomain***





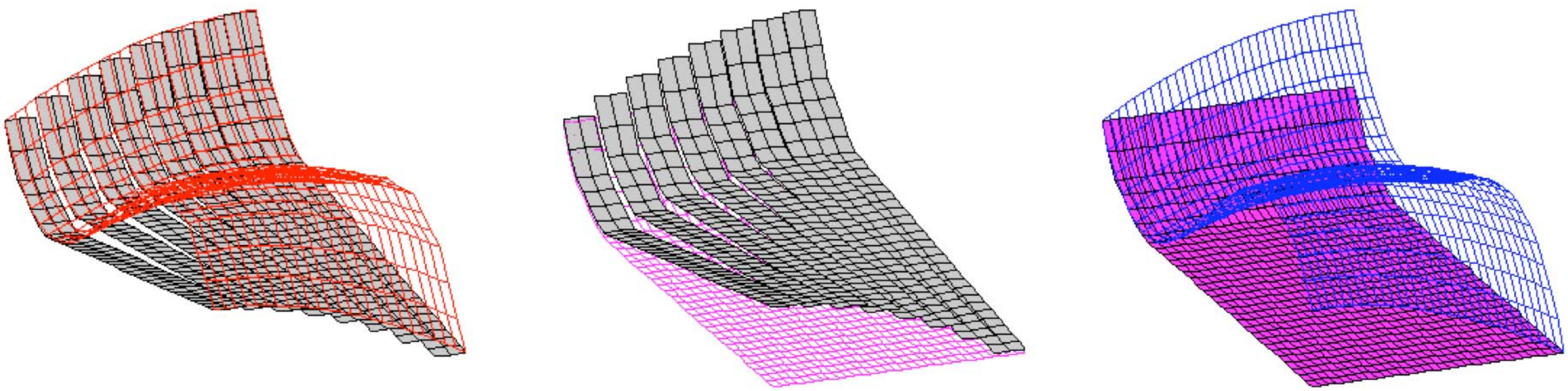
Each of these underestimators is :

- **parallel to all basis vectors, except e_w**
- **piecewise affine**
- **valid for a different subdomain**

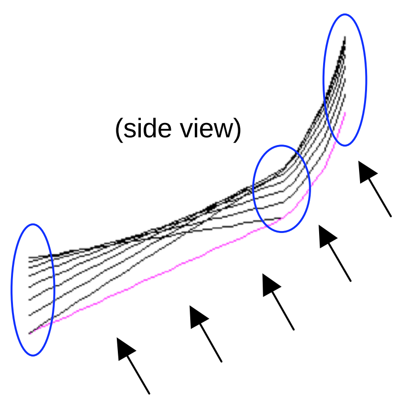
Novel Multivariate Underestimator

➢ ***Step 5**: Repeat for all permutations 'm' and combine into an overall underestimator $V_w(x_w)$ that would be valid for the whole domain*

5



How can we combine all segments into an overall underestimator ?



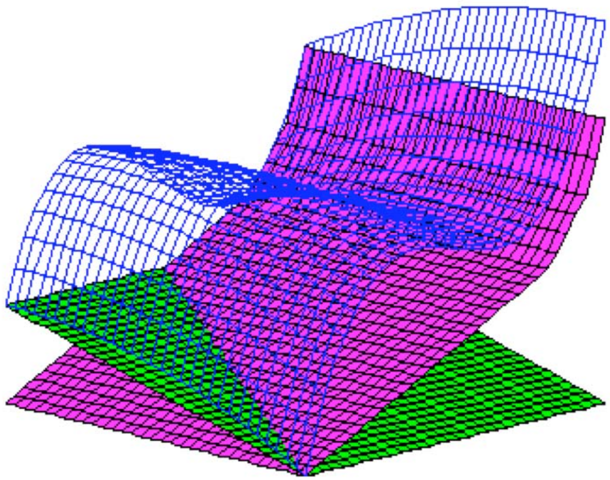
- ***Work on projected plane***
- ***Take into account connection / end points of line segments***
- ***Compute 2D convex hull of these points***

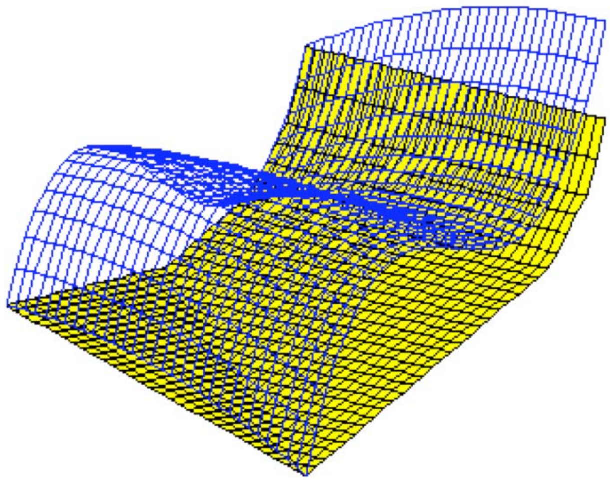
Novel Multivariate Underestimator

- ***Step 6*: Repeat, optionally, for all variables 'w' and construct a more tight underestimator that would be the pointwise maximum of all V_w**

$$V(x) = \max_{w}\{V_w(x)\}$$

6



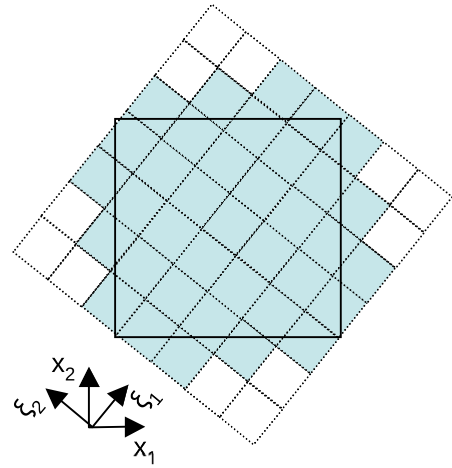


Underestimators are piecewise affine $\Longrightarrow$ Relaxation can be formulated as an LP

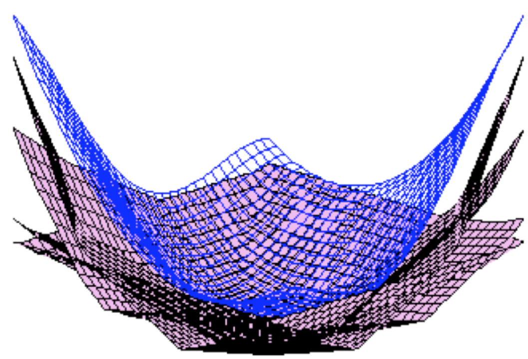
Domain Rotation

Could the lost information due to the projections be recovered ?

- ***Step 1*: Apply orthonormal transformation $\xi = R\,x$**
  - *→ $R \in SO(n)$ (i.e. $R^T = R^{-1}$ and $\det(R) = +1$)*
- ***Step 2*: Specify orthogonal domain that completely includes the original one. Identify subdomains worth considering**
- ***Step 3*: Calculate underestimator $V(\xi)$ and transform back to the original variables x**
  - *→ $V(\xi)$ is still linear, but not necessarily perpendicular to some x_i*
- ***Step 4*: Optionally, repeat with other matrices R and accumulate valid linear cuts**



- **Overall underestimator is the pointwise maximum of all those linear cuts !**



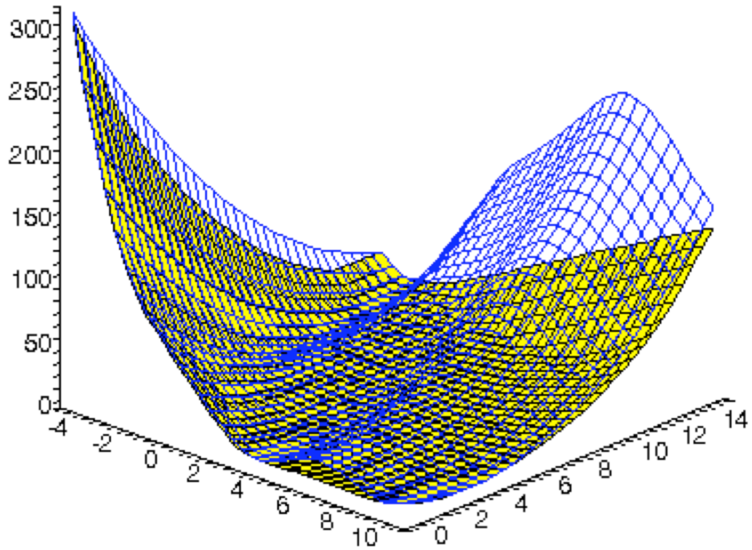
- **Lower bounding problem is just an LP !**

$$\min_{LB,\underline{x}} \quad LB$$
$$s.t. \quad LB \geq V_r(R\underline{x}) \quad \forall r$$

Examples – Bivariate Functions

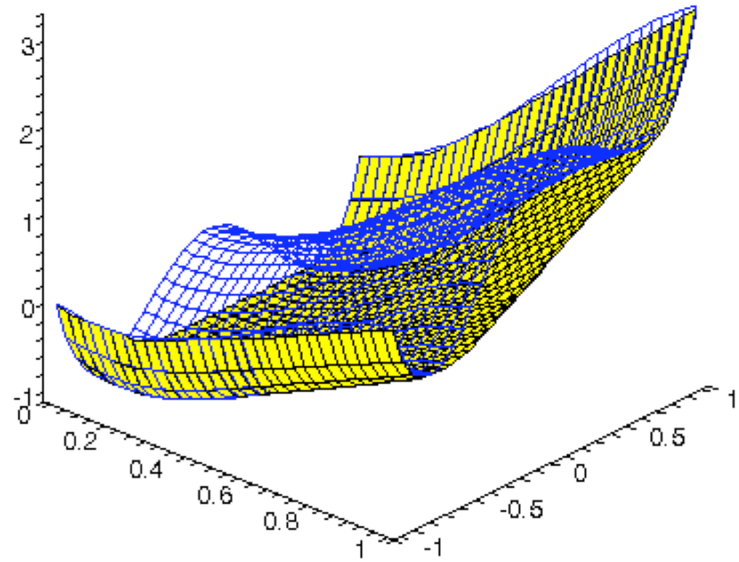
$$f(x_1,x_2)=\left(x_2-\frac{5.1x_1^2}{4\pi^2}+\frac{5x_1}{\pi}-6\right)^2+10\left(1-\frac{1}{8\pi}\right)\cos x_1+10$$

$$f(x_1,x_2)=4x_1^2-2.1x_1^4+\frac{x_1^6}{3}+x_1x_2-4x_2^2+4x_2^4$$



N = (32 x 32)   Δφ = π / 8

Total Linear Cuts   = 162
Global minimum   = 0.398
Lower Bound   = 0.316
αBB Lower Bound = - 884



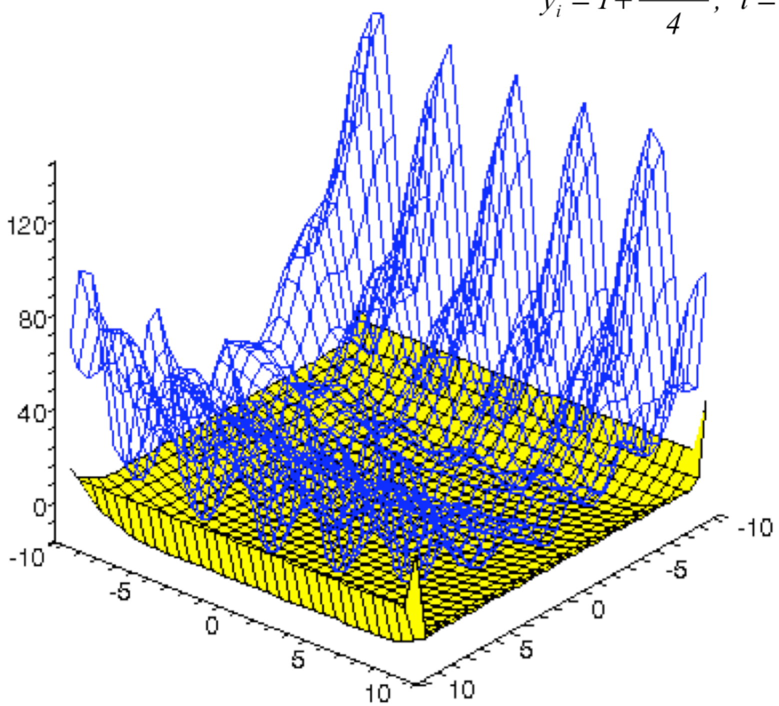
N = (32 x 32)   Δφ = π / 16

Total Linear Cuts   =   309
Global minimum   = -
1.03163
Lower Bound   = -1.03164
αBB Lower Bound = - 6.04

Examples – Bivariate Functions

$$f(x_1,x_2) = \frac{\pi}{2}\left\{10\sin^2(\pi y_1) + (y_1-1)^2\left[1+10\sin^2(\pi y_2)\right] + (y_2-1)^2\right\}$$

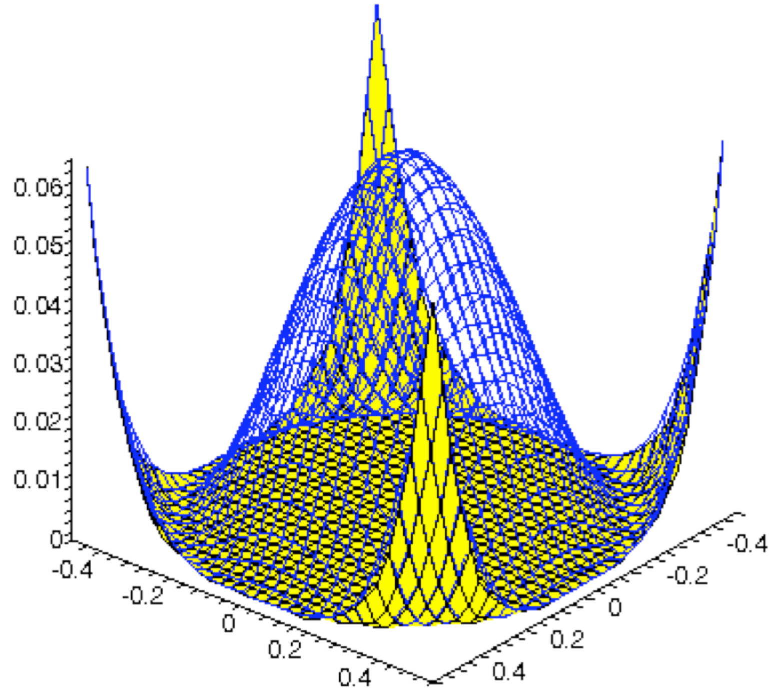
$$y_i = 1 + \frac{x_i - 1}{4}, \quad i = 1,2$$



$N = (8 \times 24)$ $\Delta\varphi = \pi / 8$

Total Linear Cuts = 49
Global minimum = 0
Lower Bound = - 14
αBB Lower Bound = - 8441

$$f(x_1,x_2) = 10^{-5}(x_1-1)^2 + 10^{-5}(x_2-1)^2 + \left(x_1^2 - x_2^2 - \frac{1}{4}\right)^2$$



$N = (32 \times 32)$ $\Delta\varphi = \pi / 8$

Total Linear Cuts = 191
Global minimum = 8×10^{-6}
Lower Bound = -7×10^{-6}
αBB Lower Bound = - 0.69

Examples – Bivariate Functions

#	Function $f(x)$	$[x_1^L, x_1^U] \times [x_2^L, x_2^U]$	αBB	$N_1 = N_2$ *(No Rotation)*						GO f^*
				2	4	8	16	32	64	
1	$\left(x_2 - \frac{5.1}{4\pi^2}x_1^2 + \frac{5}{\pi}x_1 - 6\right)^2 + 10\left(1 - \frac{1}{8\pi}\right) cos(x_1) + 10$	$[-5, 10] \times [0, 15]$	-884	-165	-23.1	-1.39	0.073	0.316	0.359	0.398
2	$x_1^4 + 4x_1^3 + 4x_1^2 + x_2^2$	$[-3, 3] \times [-3, 3]$	-127	-26	-3.16	-0.27	-0.008	0	0	0
3	$100\left(x_1^2 - x_2\right)^2 + (x_1 - 1)^2$	$[-2, 2] \times [-2, 2]$	-4399	-1101	-122.2	-20.7	-3.05	-0.754	-0.115	0
4	$4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$	$[-3, 3] \times [-1.5, 1.5]$	-998	-250	-42.9	-4.98	-1.032	-1.032	-1.032	-1.032
5	$\prod_{i=1}^{2}\left\{\sum_{i=1}^{5} icos\left[(i+1)x_i + 1\right]\right\}$	$[-1, 1] \times [-1, 1]$	-1 E+4	-2550	-501	-159	-126.4	-123.7	-123.6	-123.6
6	$\frac{1}{4}x_1^4 - \frac{1}{2}x_1^2 + \frac{1}{10}x_1 + \frac{1}{2}x_2^2$	$[-1, 1] \times [-1, 1]$	-0.53	-0.38	-0.35	-0.35	-0.35	-0.35	-0.35	-0.35
7	$10^6x_1^2 + x_2^2 - \left(x_1^2 + x_2^2\right)^2 + 10^{-6}\left(x_1^2 + x_2^2\right)^4$	$[-0.01, 0.01] \times [-2, 2]$	-92	-23	-12	-12	-12	-12	-12	-12
8	$(-13 + x_1 + ((5 - x_2)x_2 - 2)x_2)^2$ $+ (-29 + x_1 + ((x_2 + 1)x_2 - 14)x_2)^2$	$[0, 20] \times [-5, 10]$	-5 E+6	-1 E+6	-7 E+4	-5448	-750	-24.9	-2.83	0
9	$\sum_{i=1}^{10}\left\{2 + 2i - \left[exp(ix_1) + exp(ix_2)\right]\right\}^2$	$[0.1, 0.4] \times [0.1, 0.4]$	-3 E+4	-4944	-58.8	103.6	121.5	124.0	124.3	124.4
10	$x_1^2 + \left(x_2 - x_1^2 - 1\right)^2 + \sum_{i=1}^{29}\left(x_2 - \left(x_1 + \frac{i}{29}x_2\right)^2 - 1\right)^2$	$[-1, 1] \times [-1, 1]$	-784	-99.3	-6.89	0.35	0.634	0.663	0.663	0.663
11	$(x_1 - 0.2)^2 + \left(2x_1^2 + x_2^2 - 1\right)^2$ $+10^{-5}\left(exp(\frac{x_2}{10}) - exp(0.2) + exp(\frac{x_1}{10}) - exp(0.1)\right)^2$ $+10^{-5}\left(exp(\frac{x_2}{10}) - exp(0.1)\right)^2$	$[0, 0.5] \times [0, 0.5]$	-0.06	0.13	0.153	0.153	0.153	0.153	0.153	0.153
12	$(x_1 - 1)^2 + (x_2 - 1)^2 + (x_1 + 2x_2 - 3)^2 + (x_1 + 2x_2 - 3)^4$	$[0, 2] \times [0, 2]$	-213	-54.4	-2.53	-0.097	-0.004	-1 E-4	-1 E-5	0

(Test functions from *More et al., 1981; Ge and Qin, 1990*)

Examples – Bivariate Functions

#	Function $f(x)$	$[x_1^L, x_1^U] \times [x_2^L, x_2^U]$	αBB	$N_1 = N_2$ (No Rotation) 2	4	8	16	32	64	GO f^*
13	$(2x_1 + x_2 - 3)^2 + (x_1 x_2 - 1)^2$	$[0,4] \times [0,4]$	-45.8	-4.21	-0.34	-0.05	-0.02	-0.009	-0.005	0
14	$\left(2x_1 - x_2 + \left(x_1 + \frac{4}{3}\right)^3 /18\right)^2 + \left(2x_2 - x_1 + \left(x_2 + \frac{5}{3}\right)^3 /18\right)^2$	$[-1,1] \times [-1,1]$	-6.74	-0.31	-0.13	-0.044	-0.008	-0.002	-2 E-4	0
15	$\left(x_1 + 2\left(x_1 + \frac{4}{3}\right)^3 /54 + \left(x_2 + \frac{5}{3}\right)^3 /54\right)^2 + \left(x_2 + 2\left(x_2 + \frac{5}{3}\right)^3 /54 + \left(x_1 + \frac{4}{3}\right)^3 /54\right)^2$	$[-1,1] \times [-1,1]$	-1.38	-0.14	-0.062	-0.021	-5 E-4	-2 E-4	-1 E-4	0
16	$((3 - 2x_1)x_1 - 2x_2 + 1)^2 + ((3 - 2x_2)x_2 - x_1 + 1)^2$	$[-2,2] \times [-2,2]$	-562	-89.2	-12.0	-1.18	-0.19	-0.04	-0.009	0
17	$\left(x_1\left(2 + 5x_1^2\right) + 1 - x_2(1 + x_2)\right)^2 + \left(x_2\left(2 + 5x_2^2\right) + 1 - x_1(1 + x_1)\right)^2$	$[-2,2] \times [-2,2]$	-3 E+4	-1829	-61.9	-3.66	-0.43	-0.07	-0.01	0
18	$\left(\frac{x_1 + x_2}{2}\right)^2 + \left(x_1^2 + x_2^2 - \frac{2}{3}\right)^2$	$[-2,2] \times [-2,2]$	-138	-33.7	-2.67	-0.35	-0.052	-0.009	-0.001	0
19	$2x_1^2 - 1.05x_1^4 + \frac{x_1^6}{6} + x_1 x_2 + x_2^2$	$[-5,5] \times [-5,5]$	-3900	-967	-58.4	-12.3	-1.043	-2 E-5	-8 E-6	0
20	$\sum_{i=1}^{2} \left\{x_i^2 - 0.1cos(5\pi x_i)\right\}$	$[-1,1] \times [-1,1]$	-22.9	-5.37	-1.182	-0.369	-0.206	-0.2	-0.2	-0.2
21	$-cos(x_1)cos(x_2)exp\left(-(x_1 - \pi)^2 - (x_2 - \pi)^2\right)$	$[-10,10] \times [-10,10]$	-1 E+5	-9861	-533	-53.1	-4.69	-1.20	-1.001	-1
22	$\left(1 - 8x_1 + 7x_1^2 - \frac{7}{3}x_1^3 + \frac{1}{4}x_1^4\right) x_2^2 exp(-x_2)$	$[0,5] \times [0,6]$	-1 E+5	-7041	-374	-29.4	-2.92	-2.375	-2.348	-2.346
23	$sin(x_1 + x_2) + (x_1 - x_2)^2 - 1.5x_1 + 2.5x_2 + 1$	$[-1.5,4] \times [-3,3]$	-15.7	-7.35	-3.24	-1.97	-1.930	-1.921	-1.914	-1.913
24	$1 + sin^2(x_1) + sin^2(x_2) - 0.1exp\left(-x_1^2 - x_2^2\right)$	$[-10,10] \times [-10,10]$	-8179	-2042	-134	-7.90	0.32	0.9	0.9	0.9

CPU(sec) = 0.40 avg / 1.16 max (N=32)
1.86 avg / 6.41 max (N=64)

(Test functions from *More et al., 1981; Ge and Qin, 1990*)

Examples – Multivariate Functions

A. Multilinear

$f(x)$	$[x_i^L, x_i^U], \forall i$	NV	αBB	N=2	N=4	N=8	N=16	G.O.	(rAI)
$x_1x_2 + x_1x_2x_3$	[-1,1]	(3)	-4	-2	-2	-2	-2	**-2**	-2
$x_1x_2 - x_2x_3 - x_3x_4 + x_1x_2x_3 - x_1 + x_4$	[0,1]	(4)	-1.54	-1.062	-1.012	-1.002	-1.001	**-1**	-1
$x_1x_2 + x_2x_3x_4 + x_2x_4 - x_1x_3x_4x_5 + x_2x_3x_5 - x_1x_5$	[-1,1]	(5)	-15	-6.023	-6	-6	-6	**-6**	-6
	[1,3]	(5)	-73.45	-66	-66	-66	-66	**-66**	-66
$\sum_{i=0}^{5}\sum_{j=1}^{6-i}\prod_{k=j}^{k=j+i} x_k$	[-1,1]	(6)	-60.15	-10.21	-4.13	-3.175	-3.072	**-3**	-15

(No Rotation)

- **Method improves over original αBB method, even for N=2**
- **Improvement is consistent with doubling of partitioning**
- **Method will always approach the actual global optimum, thus could potentially improve over existing lower bounding schemes**
- **Note that although lower bounds are presented here, the method is used to compute convex UNDERESTIMATORS that are TIGHT across the COMPLETE DOMAIN**

Examples – Multivariate Functions

B. General Nonconvex

$f(x)$	$[x_i^L, x_i^U], \forall i$	n	αBB	N=2	N=4	N=8	N=16	G.O.
$(4x_1^2 - 2.1x_1^4 + x_1^6/6 + x_1x_2 - 4x_2^2 + 4x_2^4) + (4x_2^2 - 2.1x_2^4 + x_2^6/6 + x_2x_3 - 4x_3^2 + 4x_3^4)$	[-2,2]	(3)	-411.21	-101.6	-14.78	-1.941	-1.291	**-1**
$\sum_{i=1}^{n} \left\{ 0.1\cos(5\pi x_i) + x_i^2 \right\}$	[-1,1]	(3)	-34.31	-8.05	-1.772	-0.554	-0.3095	**-0.3**
		(4)	-45.74	-10.73	-2.363	-0.738	-0.4127	**-0.4**
$-20\exp\left(-0.02\sqrt{n^{-1}\sum_{i=1}^{n} x_i^2}\right) - \exp\left(n^{-1}\sum_{i=1}^{n}\cos(2\pi x_i)\right) + 20 + e$	[1,3]	(3)	-109.9	-24.32	-4.684	-0.019	0.396	**0.396**
		(4)	-109.9	-24.31	-4.679	-0.019	0.396	**0.396**
$\frac{\pi}{n}\left[10\sin^2(\pi x_1) + \sum_{i=1}^{n-1}(x_i - 1)^2\left(1 + 10\sin^2(\pi x_{i+1})\right) + (x_n - 1)^2\right]$	[-10,10]	(3)	-3 E+6	-7 E+5	-2 E+5	-4 E+4	-9 E+3	**0**
		(4)	-3 E+6	-7 E+5	-2 E+5	-5 E+4	-1 E+4	**0**
$\sum_{i=1}^{n-1}\left\{\sum_{k=1}^{5} k\cos[(k+1)x_i + k] \cdot \sum_{k=1}^{5} k\cos[(k+1)x_{i+1} + k]\right\}$	[-10,10]	(3)	-2 E+6	-5 E+5	-1 E+5	-3 E+4	-8 E+3	**-4 E+2** **(approx.)**
$100(x_2 - x_1^2)^2 + (1 - x_1)^2 + 90(x_4 - x_3^2)^2 + (1 - x_3)^2 + 10.1\left[(1 - x_2)^2 + (1 - x_4)^2\right] + 19.8\left[(1 - x_2)(1 - x_4)\right]$	[0,1]	(4)	-217.9	-40.1	-4.405	-0.670	-0.175	**0**
$(x_1 + 10x_2)^2 + 5(x_3 - x_4)^2 + (x_2 - 2x_3)^4 + 10(x_1 - x_4)^4$	[0,1]	(4)	-28.02	-5.027	-0.230	-0.036	-0.007	**0**
$-\frac{1}{2}\sum_{i=1}^{n}\left(x_i^4 - 16x_i^2 + 5x_i\right)$	[-5,2]	(3)	-2409	-526.3	-300	-300	-300	**-300**
		(4)	-3212	-695.9	-400	-400	-400	**-400**
		(5)	-4015	-865.4	-500	-500	-500	**-500**

(No Rotation)

Outline

- Deterministic Global Optimization: Objectives & Motivation
- Convex Envelopes:
    - Trilinear Monomials
    - Univariate Monomials
    - Fractional Terms
    - Edge Concave functions
- Checking Convexity: Products of Univariate Functions
- Convex Underestimators for Trigonometric Functions
- PαBB: Piecewise Quadratic Perturbations
- GαBB: Generalized αBB
- Functional Forms of Convex Underestimators
- Augmented Lagrangian Approach for Global Optimization
- New Class of Convex Underestimators
- **Pooling Problems & Generalized Pooling Problems**
- Conclusions

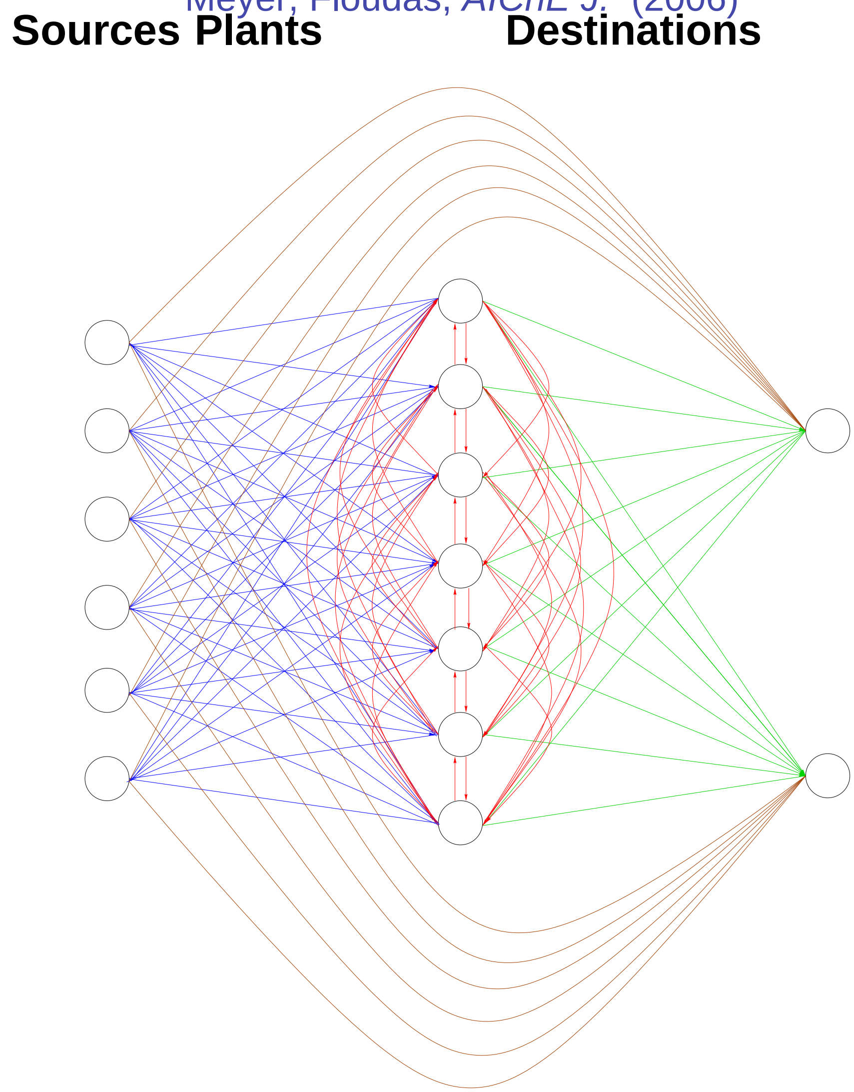
Generalized Pooling Problem

Christodoulos A. Floudas

Princeton University

Generalized Pooling Problem

Meyer, Floudas, *AIChE J.* (2006)



Q1: What is the optimal topology? → Binary Terms

Q2: Which plants exist? → Binary Variables

Global Optimization of the Pooling Problem

- Floudas, Aggrawal, Ciric (1989): global optimum search
- Foulds (1992): convex envelopes for bilinear terms
- Floudas and Visweswaran (1993, 1996): Lagrangian relaxation
- Ben-Tal et al. (1994): “q-formulation” – Lagrangian relaxation
- Quesada and Grossmann (1995): reformulation – linearization
- Adhya et al. (1999): Lagrangian relaxation
- Tawarmalani and Sahinidis (2002): reformulation – linearization of “q-formulation” and analysis
- Audet et al. (2002): branch and cut for nonconvex QP’s

Wastewater Treatment Problem

- intensive water usage in industry:
  - petrochemical
  - pharmaceutical
  - hydrometallurgical
  - paper
- regulation of water pollution:
  - Clean Water Act (EPA, 1977)
- measures on water quality:
  - heavy metals – cadmium, mercury
  - synthetic organics – dioxin, PCB's
  - organic matter – total organic carbon
  - color, odor

Wastewater Treatment Networks

Technologies target contaminants

⬇

Distributed wastewater treatment

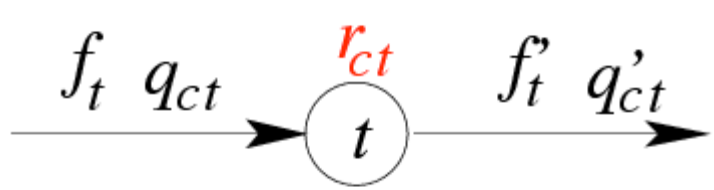
(Eckenfelder *et al.*, 1985)

Mathematical programming formulations:

(Takama *et al.*, 1980, Alva-Argaez, 1998; Galan and Grossmann, 1998; Huang *et al.*, 1999)

- superstructure of alternatives
- nonconvex NLP and MINLP models
- generalized pooling structure
- linear treatment model – removal ratio

$$r_{ct}\, f_t q_{ct} = f_t^{'} q_{ct}^{'}$$



Formulation of Generalized Pooling Problem

Objective: Minimize Overall Cost

- Plant construction and operating costs
- Pipeline construction and operating cost

Binary Variables

- $y^a_{s,e}$: Existence of stream connecting source *s* to exit stream *e*.
- $y^b_{t,e}$: Existence of stream connecting plant *t* to exit stream *e*.
- $y^c_{t,t'}$: Existence of directed stream connecting plant *t* to plant *t'*.
- $y^d_{s,t}$: Existence of stream connecting source *s* to plant *t*.
- y^e_{t}: Existence of plant *t*.

Formulation of Generalized Pooling Problem

Continuous Variables

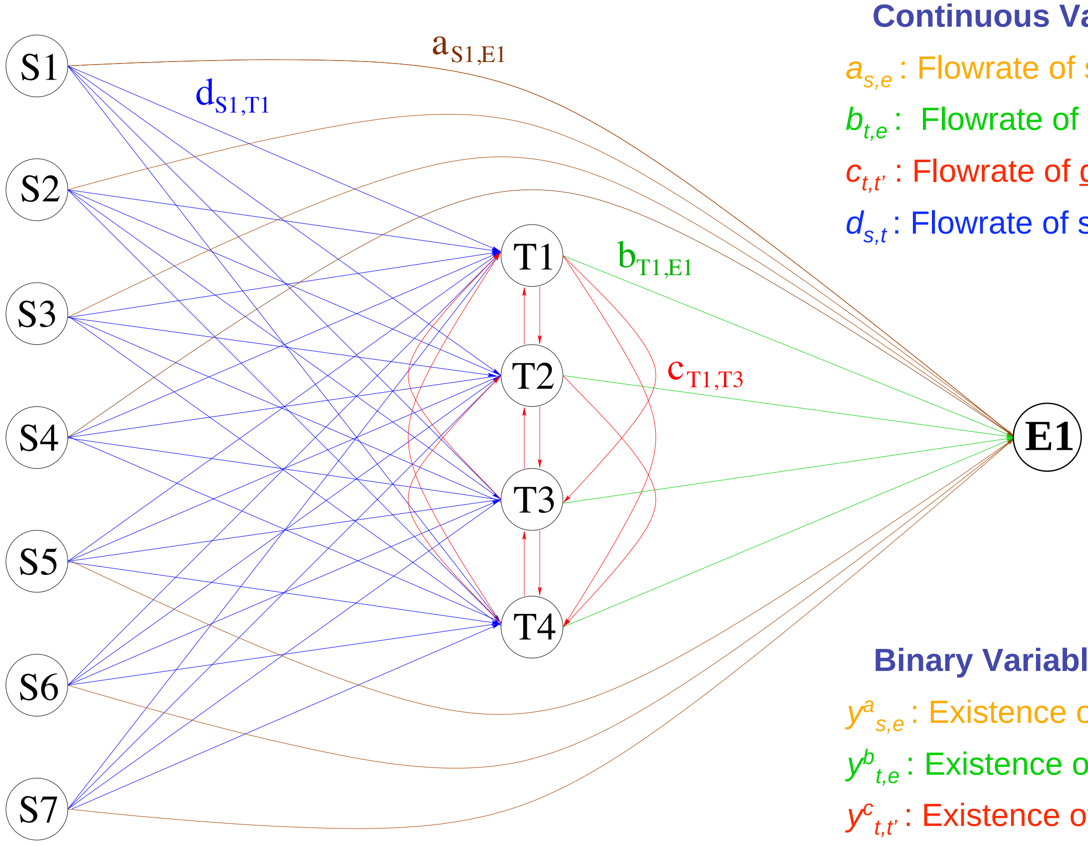
- $a_{s,e}$: Flowrate of stream connecting source s to exit stream e.
- $b_{t,e}$: Flowrate of stream connecting plant t to exit stream e.
- $c_{t,t'}$: Flowrate of directed stream connecting plant t to plant t'.
- $d_{s,t}$: Flowrate of stream connecting source s to plant t.
- e_t: Flowrate of plant t.
- $f_{s,t}$: Concentration of species s in effluent of plant t.

Formulation of Generalized Pooling Problem

Constraints

- Logical constraints on plants, flow through plant is nonzero only if plant exists
- Logical constraints on streams, flow through pipeline is nonzero only if stream exists.
- Logical constraints on streams connecting plant *t* with plant *t'*.
- Mass balance constraints on total flow over plants.
- Mass balance constraints on individual species over plants.
- Bounds on flowrates through pipelines.
- Bounds on flowrates through plants.
- Bounds on overall species concentration in each exit stream.

Superstructure of Plant Existence and Connectivity



Continuous Variables

$a_{s,e}$: Flowrate of stream connecting source s to exit stream e

$b_{t,e}$: Flowrate of stream connecting plant t to exit stream e

$c_{t,t'}$: Flowrate of directed stream connecting plant t to plant t'

$d_{s,t}$: Flowrate of stream connecting source s to plant t

Binary Variables

$y^a_{s,e}$: Existence of stream connecting source s to exit stream e

$y^b_{t,e}$: Existence of stream connecting plant t to exit stream e

$y^c_{t,t'}$: Existence of directed stream connecting plant t to plant t'

$y^d_{s,t}$: Existence of stream connecting source s to plant t

y^e_t : Existence of plant t

Formulation of Generalized Pooling Problem

$$\min_{a,b,c,d,f,y^a,y^b,y^c,y^d,y^e} z^P$$

subject to:

$$
\begin{aligned}
a^L_{s,e} &\le a_{s,e} \le a^U_{s,e} && \text{for all } s \in S, e \in E \\
b^L_{t,e} &\le b_{t,e} \le b^U_{t,e} && \text{for all } t \in T, e \in E \\
c^L_{t,t'} &\le c_{t,t'} \le c^U_{t,t'} && \text{for all } t \in T, t' \in T \\
d^L_{s,t} &\le d_{s,t} \le d^U_{s,t} && \text{for all } s \in S, t \in T \\
f^L_{t} &\le f_{t} \le f^U_{t} && \text{for all } t \in T \\
y^a_{s,e} &\in \{0,1\} && \text{for all } s \in S, e \in E \\
y^b_{t,e} &\in \{0,1\} && \text{for all } t \in T, e \in E \\
y^c_{t,t'} &\in \{0,1\} && \text{for all } t \in T, t' \in T \\
y^d_{s,t} &\in \{0,1\} && \text{for all } s \in S, t \in T \\
y^e_{t} &\in \{0,1\} && \text{for all } t \in T
\end{aligned}
$$

where

$$
\begin{aligned}
z^P = {} & \sum_{s\in S}\sum_{e\in E} c^a_{s,e} a_{s,e} + \sum_{t\in T}\sum_{e\in E} c^b_{t,e} b_{t,e} + \sum_{t\in T}\sum_{t'\in T, t'\neq t} c^b_{t,t'} c_{t,t'} \\
& + \sum_{s\in S}\sum_{t\in T} c^d_{s,t} d_{s,t} + \sum_{s\in S}\sum_{e\in E} c^a y_{s,e} y^a_{s,e} + \sum_{t\in T}\sum_{e\in E} c^b y_{t,e} y^b_{t,e} \\
& + \sum_{t\in T}\sum_{t'\in T, t'\neq t} c^b y_{t,t'} y^c_{t,t'} + \sum_{s\in S}\sum_{t\in T} c^d y_{s,t} y^d_{s,t} + \sum_{t\in T} c^e y_t y^e_t
\end{aligned}
$$

Formulation of Generalized Pooling Problem

$$a_{s,e} - y^a_{s,e} a^U_{s,e} \le 0 \qquad \text{for all } s \in S,\ e \in E$$

$$b_{t,e} - y^b_{t,e} b^U_{t,e} \le 0 \qquad \text{for all } t \in T,\ e \in E$$

$$c_{t,t'} - y^c_{t,t'} c^U_{t,t'} \le 0 \qquad \text{for all } t \in T,\ t' \in T,\ t' \ne t$$

$$d_{s,t} - y^d_{s,t} d^U_{s,t} \le 0 \qquad \text{for all } s \in S,\ t \in T$$

$$a^L_{s,e} y^a_{s,e} - a_{s,e} \le 0 \qquad \text{for all } s \in S,\ e \in E$$

$$b^L_{t,e} y^b_{t,e} - b_{t,e} \le 0 \qquad \text{for all } t \in T,\ e \in E$$

$$c^L_{t,t'} y^c_{t,t'} - c_{t,t'} \le 0 \qquad \text{for all } t \in T,\ t' \in T,\ t' \ne t$$

$$d^L_{d,t} y^d_{s,t} - d_{s,t} \le 0 \qquad \text{for all } s \in S,\ t \in T$$

$$\sum_{s \in S} d_{s,t} + \sum_{t' \in, t' \ne t} c_{t,t'} - e^U_t y^e_t \le 0 \qquad \text{for all } t \in T$$

$$-\sum_{s \in S} d_{s,t} - \sum_{t' \in T, t' \ne t} c_{t,t'} + e^U_t y^e_t \le 0 \qquad \text{for all } t \in T$$

$$\sum_{e \in E} a_{s,e} + \sum_{t \in T} d_{s,t} = f^{feed}_s \qquad \text{for all } s \in S$$

$$\sum_{t' \in T, t' \ne t} c_{t',t} - \sum_{t' \in T, t' \ne t} c_{t,t'} + \sum_{s \in S} d_{s,t} = \sum_{e \in E} b_{t,e} \qquad \text{for all } s \in S$$

$$f_{c,t} \left(\sum_{s \in S} d_{s,t} + \sum_{t' \in T, t' \ne t} c_{t',t} \right) = (1 - r_{c,t}) \left(\sum_{t' \in T, t' \ne t} c_{t',t} f_{c,t'} + \sum_{s \in S} d_{s,t} cs_{c,e} \right) \qquad \text{for all } c \in C,\ t \in T$$

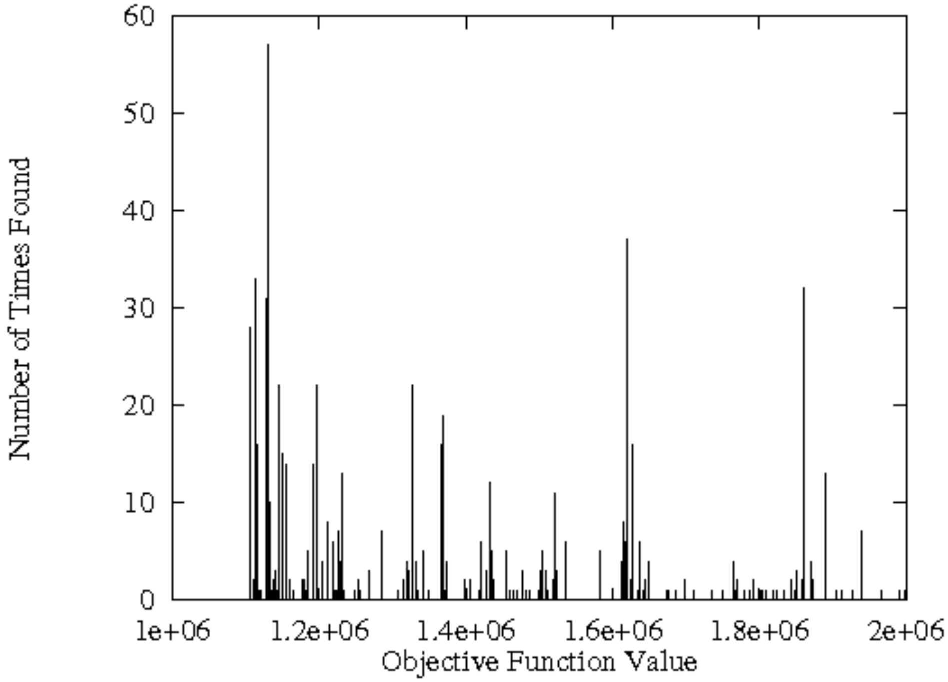
$$\sum_{s \in S} a_{s,e} cs_{c,s} + \sum_{t \in T} b_{t,e} f_{c,t} \le ce_c \left(\sum_{s \in S} a_{s,e} + \sum_{t \in T} b_{t,e} \right) \qquad \text{for all } c \in C,\ e \in E$$

Problem Characteristics

- Mixed integer bilinear programming problem with bilinearities involving pairs of continuous variables, (b,f) and (c,f) and (d,f).
- Nonconvex mass balance constraints on the species include bilinear terms.
- Industrial case study: $|C| = 3$, $|E| = 1$, $|S| = 7$, $|T| = 10$.
- Number of nonconvex equality constraints: $|C| \times (|T| + |E|)$. (33)
- Number of bilinear terms: $|C| \times |T| \times (|E| + |S| + 2|T| - 2)$. (780)
- Complex network structure with numerous feasible yet nonoptimal possibilities.
- Number of binary variables: $|T| \times (|E| + |S| + |T|) + |S| \times |E|$. (187)
- Fixing the y variables, the problem is a nonconvex bilinear NLP.
- Fixing the f variables, the problem is a MILP.
- Fixing the a,b,c,d imposes values on all the other variables.

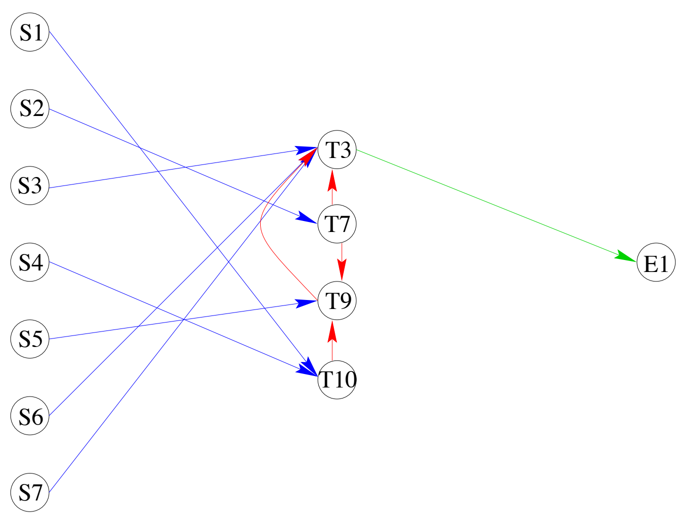
Solutions Using GAMS/DICOPT and Random Starting Points

- Continuous variables initialized with uniformly distributed random numbers.
- Binary variables initialized by rounding the uniformly distributed numbers in [0,1] to the nearest integer.
- DICOPT used to solve problem from 1000 starting points.
- Number of times best known solution was found: 0.

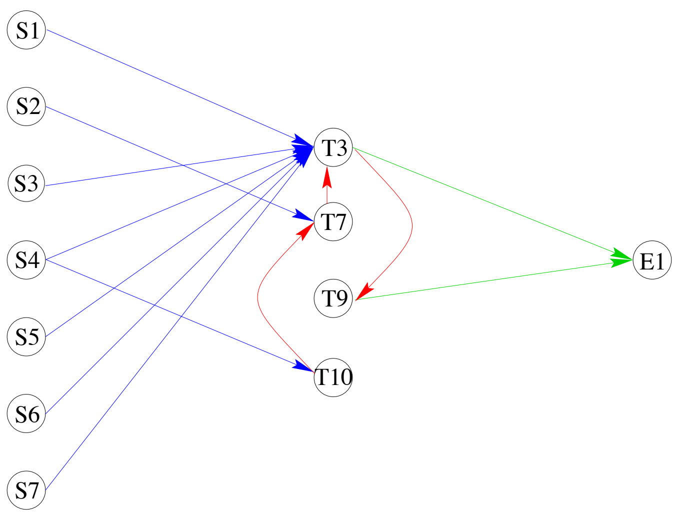


Feasible Solutions

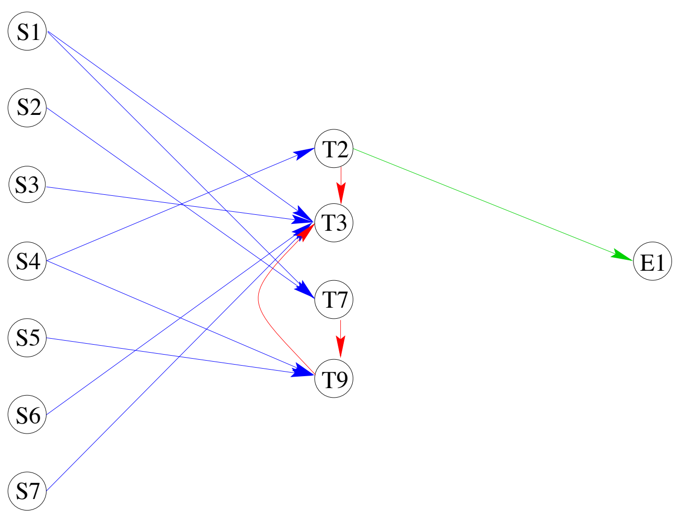
Objective function value: 1.086e6



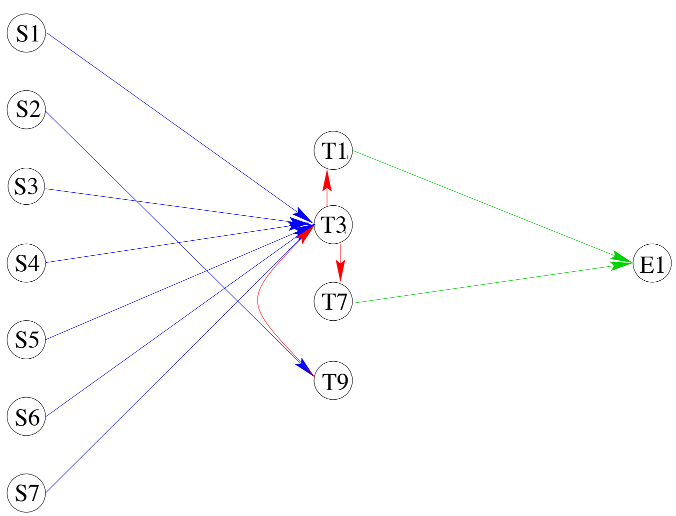
Objective function value: 1.198e6



Objective function value: 1.132e6



Objective function value: 1.620e6



Envelopes of Bilinear Terms

$$x_i y_i \leftarrow w_{i,j}^{x,y}$$

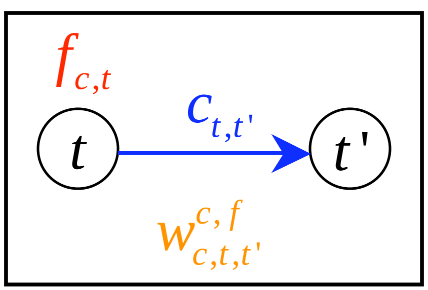
convex envelope: $$\begin{cases} w_{i,j}^{x,y} \ge \underline{y}_j x_i + \underline{x}_i y_j - \underline{x}_i \underline{y}_j \\ w_{i,j}^{x,y} \ge \overline{y}_j x_i + \overline{x}_i y_j - \overline{x}_i \overline{y}_j \end{cases}$$

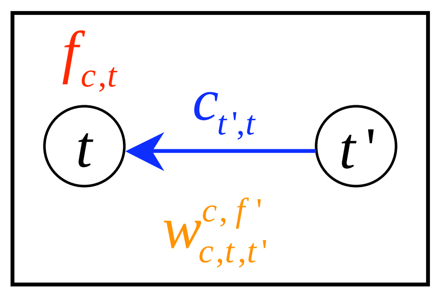
concave envelope: $$\begin{cases} w_{i,j}^{x,y} \le \underline{y}_j x_i + \overline{x}_i y_j - \overline{x}_i \underline{y}_j \\ w_{i,j}^{x,y} \le \overline{y}_j x_i + \underline{x}_i y_j - \underline{x}_i \overline{y}_j \end{cases}$$

$$f_{c,t} c_{t,t'} \leftarrow w_{c,t,t'}^{c,f}$$

$$f_{c,t'} c_{t,t'} \leftarrow w_{c,t,t'}^{c,f'}$$

$$f_{c,t} d_{s,t} \leftarrow w_{c,s,t}^{d,f}$$





Industrial Case Study

Components: 3

Sources: 7

Exit streams: 1

Potential plants: 10

Best known solution: 1.086×10^6

780 Bilinear Terms

Formulation	$\Re$ var.	{0,1} var	Constr.	CPU (s)	Obj (10^6)
Nonconvex	207	187	424	2.5	**1.086**
Bilinear Terms	987	187	3544	58	**0.550**

Lower Bounds using Reformulation Linearization Technique

Original RLT: Sherali and Alamedine (1992)

- MILP Relaxation of the nonconvex MINLP to determine lower bounds on the global optimum.
- Pairs of linear constraints $a_1^T x - b_1 \geq 0$ and $a_2^T x - b_2 \geq 0$ are multiplied together yielding constraints with bilinear terms $[a_1^T x - b_1] \cdot [a_2^T x - b_2] \geq 0$.
- All nonlinear constraints are linearized by replacing each bilinear term with a new variable.
- Linear constraint pairs are chosen such that one constraint contains f variables and the other, a, b, c, or d variables.
- Number of constraints increases.
- Number of continuous variables increases.

Reformulation Linearization Technique Example

Constraints:

$$-c_{t,t'} + y^c_{t,t'} c^U_{t,t'} \geq 0$$

$$f_t - f^U_t \geq 0$$

are multiplied to yield:

$$-c_{t,t'} f_t + y^c_{t,t'} f_t c^U_{t,t'} + c_{t,t'} f^U_t - y^c_{t,t'} f^U_t c^U_{t,t'} \geq 0$$

which is linearized by substituting:

$$c_{t,t'} f_t \leftarrow w^{c,f}_{t,t'}$$

$$y^c_{t,t'} f_t \leftarrow w^{y^c,f}_{t,t'}$$

$$-w^{c,f}_{t,t'} + w^{y^c,f}_{t,t'} c^U_{t,t'} + c_{t,t'} f^U_t - y^c_{t,t'} f^U_t c^U_{t,t'} \geq 0$$

Industrial Case Study

Components: 3

Sources: 7

Exit streams: 1

Potential plants: 10

Best known solution: 1.086×10^6

Formulation	$\Re$ var.	{0,1} var	Constr.	CPU (s)	Obj (10^6)
Nonconvex	207	187	424	2.5	1.086
Bilinear Terms	987	187	3544	58	0.550
RLT	3850	187	19321	3621	0.743

Augmented Binary RLT

(Meyer and Floudas, *AIChE J.* 2006)

- Additional binary variables y^f introduced to facilitate branching on the continuous variables f within a MILP framework.
- Multiple MILP's combined into a single MILP lower bounding problem.
- Takes advantage of the performance of CPLEX 8.0 in solving MILP problems.
- The interval $[f^L, f^U]$ is partitioned into N subintervals.
- Throughout the formulation, f^L and f^U are replaced by parameters f^k and f^{k+1}.
- Variable f is constrained to lie in interval $[f^k, f^{k+1}]$ when binary variable $y^f = 1$ by constraints:

$$\boxed{\begin{array}{ll}
f_{c,t} \geq y^f_{c,t,k}\, f^k_{c,t}, & \forall\, c \in C, t \in T, k \in [1, N] \\
f_{c,t} \leq (1 - y^f_{c,t,k})\, f^U_{c,t} + f^{k+1}_{c,t}, & \forall\, c \in C, t \in T, k \in [1, N] \\
\sum_{k=1}^{N} y^f_{c,t,k} = y^e_t, & \forall\, c \in C, t \in T
\end{array}}$$

- A constraint for interval $[f^k, f^{k+1}]$ is active if $y^k = 1$ and inactive if $y^k = 0$.

RLT to Strengthen MILP Formulation

RLT to improve convergence of MILP

- products of original bound factors

$$\left[\left(-c^{L}_{t,t'} y^{c}_{t,t'} + c_{t,t'}\right)\cdot\left(f_{c,t} - f^{L}_{c,t}\right)\right]_l \geq 0$$

- products of original and discretized constraints

$$\left[\left(-c^{L}_{t,t'} y^{c}_{t,t'} + c_{t,t'}\right)\cdot\left(f_{c,t} - f^{k}_{c,t}\right)\right]_l + M\left(1 - y^{k}_{c,t}\right) \geq 0$$

- new variables (|C|·|T|·(2|T| + |S|))

$$w^{y^b,f}_{c,t} \leftarrow y^{b}_{t} f_{c,t} \qquad w^{y^c,f}_{c,t,t'} \leftarrow y^{c}_{t,t'} f_{c,t}$$

$$w^{y^c,f'}_{c,t,t'} \leftarrow y^{c}_{t,t'} f_{c,t'} \qquad w^{y^d,f}_{c,s,t} \leftarrow y^{d}_{s,t} f_{c,t}$$

$$w^{y^e,f}_{c,t} \leftarrow y^{e}_{t} f_{c,t}$$

Industrial Case Study

Components:	3
Sources:	7
Exit streams:	1
Potential plants:	10

Best known solution:	1.086×10^6
Lower bound on solution:	1.070×10^6
Absolute Gap:	0.016×10^6
Relative Gap:	1.5 %

Formulation	$\Re$ var.	{0,1} var	Constr.	CPU (s)	Obj (10^6)
Nonconvex	207	187	424	2.5	1.086
Bilinear Terms	987	187	3544	58	0.550
RLT	3850	187	19321	3621	0.743
Subnetwork {*t3, t7, t9, t10*}					
Bin RLT N = 2	766	79	4866	519	0.977
Bin RLT N = 3	766	91	6234	816	1.005
Bin RLT N = 4	766	103	7602	3672	1.022
Bin RLT N = 5	766	115	8970	7617	1.031
Bin RLT N = 6	766	127	10338	85800	1.051
Bin RLT N = 7	766	139	11706	59486	1.070

Conclusions

- Motivational Areas & Review of contributions
- Convex Envelopes: Trilinear Monomials; Univariate; Fractional; Edge Concave Functions
- Checking Convexity:Products of Univariate Functions
- Convexification of Trigonometric Functions
- PαBB: Piecewise Quadratic Perturbation Based αBB
- GαBB: Generalized αBB
- Augmented Lagrangian Approach
- Functional Forms of Convex Underestimators
- Novel Convex Underestimators: 1-D, Multivariate Functions
- Generalized Pooling Problems

Exciting theoretical and algorithmic advances with potential impact on several application areas

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Deterministic Global Optimization

Professor C.A. Floudas

Princeton University

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Publications of Floudas' Research Group

10. Protein Folding: Structure & Dynamics

Klepeis J.L., M. Pieja and C.A. Floudas
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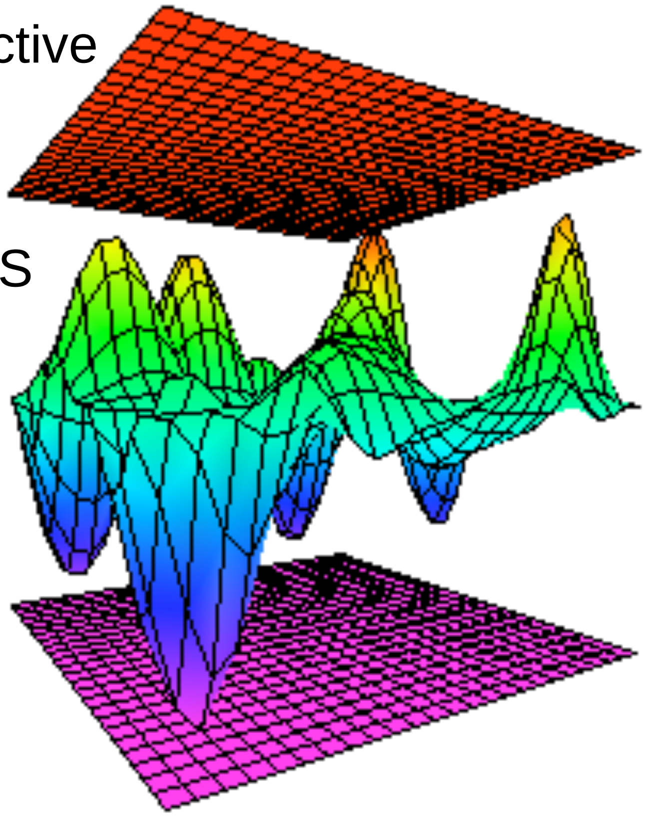
Outline

- **Deterministic Global Optimization**: Objectives & Motivation
- Convex Envelopes:
  - Trilinear Monomials
  - Univariate Monomials
  - Fractional Terms
  - Edge Concave functions
- Checking Convexity: Products of Univariate Functions
- Convex Underestimators for Trigonometric Functions
- PαBB: Piecewise Quadratic Perturbations
- GαBB: Generalized αBB
- Functional Forms of Convex Underestimators
- Augmented Lagrangian Approach for Global Optimization
- New Class of Convex Underestimators
- Pooling Problems & Generalized Pooling Problems
- Conclusions

Deterministic Global Optimization: Objectives

- **Objective 1**
  Determine a global minimum of the objective function subject to the set of constraints
- **Objective 2**
  Determine LOWER and UPPER BOUNDS on the global minimum
- **Objective 3**
  Identify good quality solutions (i.e., local minima close to the global minimum)
- **Objective 4**
  Enclose ALL SOLUTIONS of constrained systems of equations



Objective 2
Objective 3 → **Major Importance in Engineering Applications**

Deterministic Global Optimization: C^2 NLPs

Formulation

$$\begin{aligned}
\min_{\mathbf{x}} \quad & f(\mathbf{x}) \\
\text{s.t.} \quad & \mathbf{h}(\mathbf{x}) = \mathbf{0} \\
& \mathbf{g}(\mathbf{x}) \leq \mathbf{0} \\
& \mathbf{x} \in \mathbf{X} \subseteq R^n
\end{aligned}$$

$$f, \ \mathbf{h}, \ \mathbf{g} \in C^2$$

Application Areas

- **Phase Equilibrium Problems**
  - Minimum Gibbs Free Energy
  - Tangent Plane Stability
- **Pooling/Blending**
- **Parameter Estimation &**
- **Data Reconciliation**
  - Physical Properties
- **Design Under Uncertainty**
- **Robust Stability of Control Systems**
- **Structure Prediction in Clusters**
- **Structure Prediction in Molecules**
- **Protein Folding**
- **Peptide Docking**
- **NMR Structure Refinement**
- **Prediction of Crystal Structure**

Deterministic Global Optimization: MINLPs

Formulation

$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{y}} \quad & f(\mathbf{x},\mathbf{y}) \\
\text{s.t.} \quad & \mathbf{h}(\mathbf{x},\mathbf{y}) = \mathbf{0} \\
& \mathbf{g}(\mathbf{x},\mathbf{y}) \le \mathbf{0} \\
& \mathbf{x} \in \mathbf{X} \subseteq R^n \\
& \mathbf{y} \ \ \text{INTEGER}
\end{aligned}
$$

continuous relaxations

$$f, \ \mathbf{h}, \ \mathbf{g} \in C^2$$

Application Areas

- **Process Synthesis Problems**
  - HENs
  - Separations/Complex Columns
  - Reactor Networks
  - Flowsheets
- **Scheduling, Design, Synthesis of Batch and Continuous Processes**
- **Planning**
- **Synthesis Under Uncertainty**
- **Design, Synthesis of Materials**
- **Metabolic Pathways**
- **Circuit Design**
- **Layout Problems**
- **Nesting of Arbitrary Objects**

Deterministic Global Optimization: Bilevel Nonlinear Optimization, BNLPs

Formulation

$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{y}} \quad & F(\mathbf{x},\mathbf{y}) \\
\text{s.t.} \quad & \mathbf{H}(\mathbf{x},\mathbf{y}) = \mathbf{0} \\
& \mathbf{G}(\mathbf{x},\mathbf{y}) \le \mathbf{0} \\
& \min_{\mathbf{y}} \; f(\mathbf{x},\mathbf{y}) \\
& \quad \text{s.t.} \quad \mathbf{h}(\mathbf{x},\mathbf{y}) = \mathbf{0} \\
& \quad \qquad \mathbf{g}(\mathbf{x},\mathbf{y}) \le \mathbf{0} \\
& \mathbf{x} \in \mathbf{X} \subseteq R^{n1}, \mathbf{y} \in \mathbf{Y} \subseteq R^{n2}
\end{aligned}
$$

Application Areas

- Economics
- Civil Engineering
- Aerospace
- Chemical Engineering
  - Design Under Uncertainty : Flexibility Analysis
  - Chemical Equilibrium Process Design
  - Location/Allocation in Exploration
  - Interaction of Design with Control
  - Optimal Pollution Control
  - Molecular Design
  - Pipe Network Optimization

Deterministic Global Optimization: DAEs - Optimal Control

Formulation

$$
\begin{aligned}
\min \quad & J(\dot{\mathbf{z}}(t), \mathbf{z}(t), \mathbf{x}, \mathbf{u}(t), t) \\
\text{s.t.} \quad & \mathbf{h}_1(\dot{\mathbf{z}}(\mathrm{t}), \mathbf{z}(\mathrm{t}), \mathbf{x}, \mathbf{u}(\mathrm{t}), \mathrm{t}) = \mathbf{0} \\
& \mathbf{h}_2(\mathbf{z}(\mathrm{t}), \mathbf{x}, \mathbf{u}(\mathrm{t}), \mathrm{t}) = \mathbf{0} \\
& \mathbf{z}(\mathrm{t}_0) = \mathbf{z}_0 \\
& \mathrm{t} \in [\mathrm{t}_0, \mathrm{t}_f] \\
& \mathbf{h}_1'(\dot{\mathbf{z}}(\mathrm{t}_\mu), \mathbf{z}(\mathrm{t}_\mu), \mathbf{x}, \mathbf{u}(\mathrm{t}_\mu), \mathrm{t}_\mu) = \mathbf{0} \\
& \mathbf{h}_2'(\mathbf{z}(\mathrm{t}_\mu), \mathbf{x}, \mathbf{u}(\mathrm{t}_\mu), \mathrm{t}_\mu) = \mathbf{0} \\
& \mathbf{g}_1(\dot{\mathbf{z}}(\mathrm{T}), \mathbf{z}(\mathrm{t}), \mathbf{x}, \mathbf{u}(\mathrm{t}), \mathrm{t}) \le \mathbf{0} \\
& \mathbf{g}_2(\mathbf{x}) \le \mathbf{0}
\end{aligned}
$$

DAE at most index one

$$J, \quad \mathbf{h}, \quad \mathbf{g} \;\in\; C^2$$

Application Areas

- Parameter Estimation of Kinetic Models
- Optimal Control
- Interaction of Design and Control
- Dynamic Simulations
- Synthesis of Complex Reactor Networks

Deterministic Global Optimization: Grey-Box Models

Application Areas

- Mechanical Design
- Airplane Design
- Modular Process Simulation

Deterministic Global Optimization: Enclosure of All Solutions

Formulation

$$\mathbf{h}(\mathbf{x}) = \mathbf{0}$$
$$\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$$
$$\mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U$$

$$\mathbf{h},\ \mathbf{g} \in C^2$$

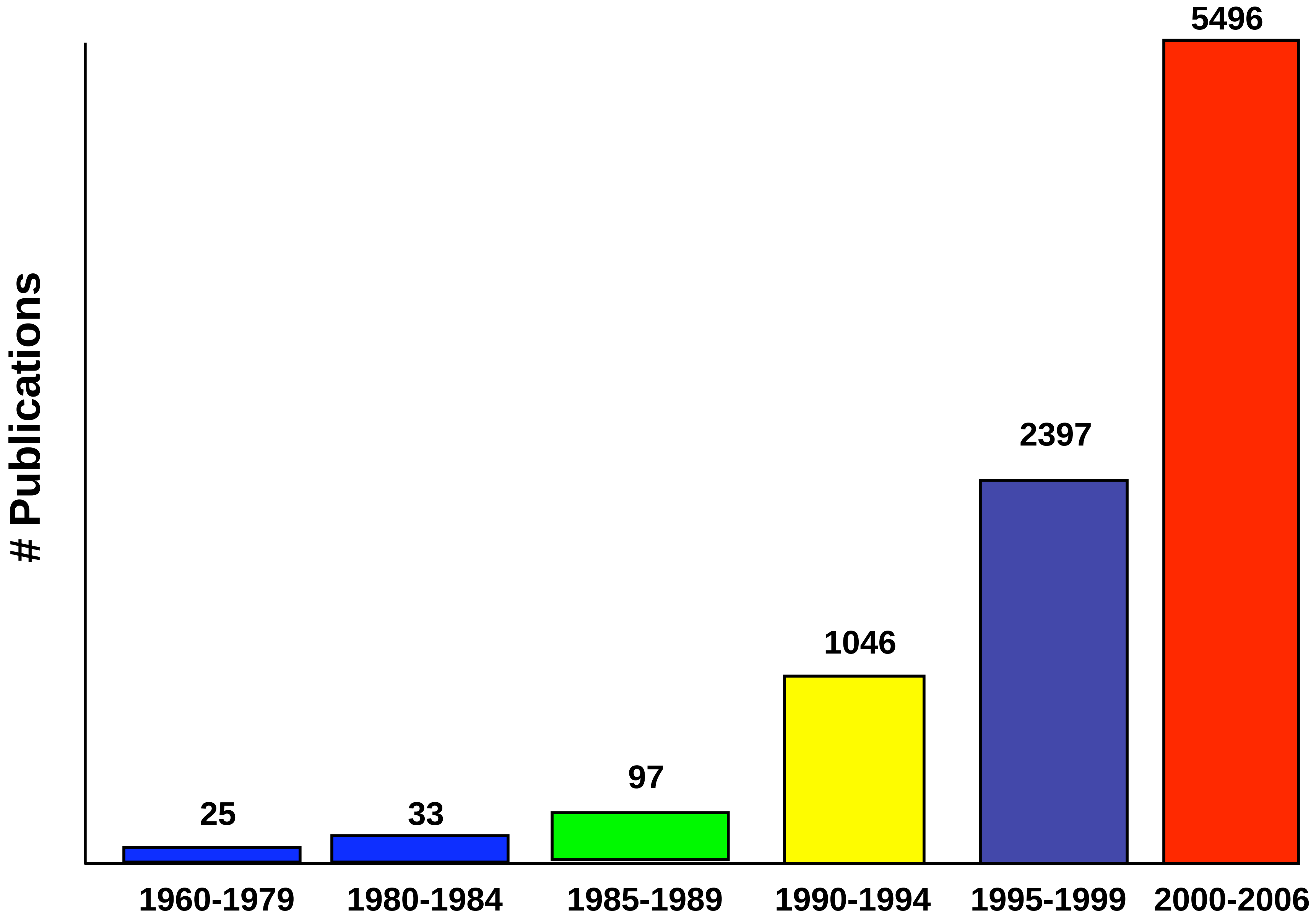
Application Areas

- Process Modeling & Simulation
- of Flowsheets
- Multiple Steady States in
  - CSTRs
  - Reaction Networks
  - Metabolic Networks
  - Homo- & Heterogeneous
  - azeotropic distillation
- Homogeneous
- Heterogeneous
- Reactive

Azeotropes

- Eutectic Points
- Reactive Flash
- Reactive Distillation
- Transition States & Reaction Pathways

Historical Global Optimization Perspective



Outline

- Deterministic Global Optimization
  - Objectives
  - Motivation
- Convexification & Convex Envelopes
- General C^2 NLPs
- MINLPs
- Differential-Algebraic Models
- Grey Box & Nonfactorable Models
- Bilevel Nonlinear Models
- Convex Envelopes
  - Trilinear Monomials
  - Odd Degree Univariate Monomials
  - Fractional Terms
- Convex Underestimators for Trigonometric Functions
- PαBB: Piecewise Quadratic Perturbations
- GαBB: Generalized αBB
- Generalized Pooling Problems
- Conclusions

C^2NLPs

Convexification Techniques

- Björk et al. (2003), Westerlund (2003;2005), Lundell et al. (2007)
  - signomials, quasi-convex convexifications
- Li et al. (2005), Wu et al. (2007)
  - hidden convexity
- Wu et al. (2005)
  - monotone programs
- Zlobec (2005,2006)
  - Liu-Floudas convexification
- Li, Tsai (2005), Tsai, Lin (2007), Tsai et al. (2007), Li et al. (2007)
  - convexity rules for signomial terms
- Gounaris, Floudas (2008)
  - suitable transformations for GGP

Convex & Concave Envelopes

- Tawarmalani, Sahinidis (2001)
  - (x/y) on unit hypercube
  - $f(x)y^2$, $f(x)/y$
- Tawarmalani, Sahinidis (2002)
  - convex extensions for l.s.c
- Liberti, Pantelides (2003)
  - odd degree univariate monomials
- Meyer, Floudas (2003;2005)
  - trilinear monomials
- Meyer, Floudas (2005)
  - edge convex/concave functions
- Tardella (2004, 2008)
  - vertex polyhedral envelopes

C^2NLPs Convex Relaxation

- Adjiman et al. (1998a,b) Hertz et al. (1999) } αBB

$$L(x) = f(x) + \sum_{i=1}^{n} \alpha_i (x_i^U - x_i)(x_i - x_i^L)$$

- Zamora, Grossmann (1998a,b;1999)
  - *(x/y)*
- Ryoo, Sahinidis (2001)
  - multilinear (AI, Recursive, Log, Exp)
- Tawarmalani et al. (2002)
  - tighter LP relaxations: $x \sum y$
- Meyer, Floudas (2005a)
  - PαBB (Piecewise Quadratic Perturbation)
- Caratzoulas, Floudas (2005)
  - Trigonometric functions
- Akrotirianakis, Floudas (2004a,b; 2005)
  - GαBB (Generalized αBB)

$$L(x) = f(x) - \sum_{i=1}^{n} (1 - e^{\gamma_i (x_i - x_i^L)})(1 - e^{\gamma_i (x_i^U - x_i)})$$

- Linderoth (2005)
  - Quadratically constrained
- Sherali (2002,2007), Sherali, Wang (2001), Sherali, Fraticelli (2002), Sherali et al. 2005
  - RLT methodology
- Nie, Demmel, Gu (2006)
  - rational functions
- Gounaris, Floudas (2008a,b)
  - Tight convex underestimators

General C^2NLPs

- **Adjiman et al. (1998a,b)**
  Androulakis, Floudas (1998) } αBB
- **Yamada, Hara (1998)**
  - triangle covering for H_∞
- **Klepeis et al. (1998); Klepeis, Floudas (1999)**
  - solvated peptides
- **Klepeis, Floudas (1999)**
  - free energy calculations
- **Westerberg, Floudas (1999a,b)**
  - dynamics of protein folding
  - transition states
- **Klepeis et al. (1994)**
  - NMR structure refinement
- **Byrne, Bogle (1999)**
  bound constrained interval LP relaxations
- **Gau, Stadtherr (2002a,b)**
  - Interval Newton
  - hybrid preconditioning strategies
  - distributed computing
  - VLE, parameter estimation
- **Lucia, Feng (2002)**
  - differential geometry, global terrain
- **Klepeis et al. (2002): review**
  - DGO, oligopeptides, dynamics, protein-protein interactions
- **Zilinskas, Bogle (2003b)**
  - balanced random IA
- **Klepeis, Floudas (2003b)**
  - αBB + torsional angle dynamics
- **Klepeis, Floudas (2003c)**
  - ASTRO-FOLD: first principles protein structure prediction
- **Klepeis et al. (2003a,b)**
  - hybrid stochastic + deterministic G.O.
- **Lucia, Feng (2003)**
  - terrain approach for multivariable and integral curve bifurcations
- **Schafroth, Floudas (2004)**
  - protein-protein interactions via αBB and Poisson Boltzman
- **Akrotirianakis, Floudas (2004a,b, 2005)**
  - GαBB for box constrained NLPs
  - hybrid G.O. methods

General C^2NLPs (cont'd)

- **Gao (2003;2004;2005;2007)**
  - canonical dual transformation
- **Sun et al. (2005)**
  - saddle points of Augmented Lagrangians
- **Parpas, Rustem, Pistikopoulos (2006)**
  - stochastic DE, linear constraints
- **Marcovecchio et al. (2006)**
  - improve-and-branch algorithm
- **Gattupalli, Lucia (2008)**
  - molecular conformation of alkanes using terrain / funneling methods
- **Parpas, Rustem, Pistikopoulos (2008)**
  - G.O. of robust chance problems
- **Maringer, Parpas (2008)**
  - G.O. of higher order moments in portfolio selection

Concave, Bilinear, Fractional, and Multiplicative Models

- **Zamora, Grossmann (1998b)**
  - B&B approach for bilinear, linear, fractional, univariate, concave
  - contraction operation
- **Shectman, Sahinidis (1998)**
  - finite G.O. for separable concave
- **Zamora, Grossmann (1999)**
  - branch and contract G.O.
  - reduction of nodes in B&B tree
- **Van Antwerp et al. (1999)**
  - bilinear matrix inequality
  - B&B approach
- **Liberti, Pantelides (2006)**
  - reformulation for bilinear programs
- **Nahapetyan, Pardalos (2007)**
  - bilinear relaxation for concave piecewise linear networks
- **Benson (2007)**
  - B&B algorithm for linear sum-of-rations
- **Adhya et al. (1999)**
  - pooling problem
  - Lagrangian relaxation
- **Ryoo, Sahinidis (2003)**
  - linear, generated multiplicative models
  - recursive AI approach for lower bounds
  - greedy heuristics
  - branch and reduce
  - randomly generated problems
- **Goyal, Ierapetritou (2003)**
  - evaluations of infeasible domains via a simplicial OA for concave or quasi-concave constraints
- **Tsai (2005)**
  - nonlinear fractional programming (NFP)
- **Jiao et al. (2006)**
  - generalized linear fractional programming

Phase Equilibrium & Parameter Estimation

- **Maier et al. (1998)**
  - IA for enclosure of homogeneous azeotrope
- **Meyer, Swartz (1998)**
  - test convexity of VLE
- **McKinnon, Mongeau (1998)**
  - IA for phase & chemical reaction equilibrium
- **Hua et al. (1998a,b)**
  - phase stability, EOS
- **Zhu, Xu (1999a,b)**
  - simulated annealing for phase stability
  - Lipschitz G.O. for stability with S.R.V.
- **Harding, Floudas (2000a)**
  - cubic EOS, phase stability, αBB
- **Harding, Floudas (2000b)**
  - enclosure of heterogeneous and reactive azeotropes
- **Tessier et al. (2000)**
  - monotonicity based enhancements of Interval Newton for phase stability
- **Zhu et al. (2000)**
  - simulated annealing for PR, SRK
- **Zhu, Inoue (2001)**
  - B&B with quadratic underestimator for phase stability
- **Xu et al. (2002)**
  - Interval Newton for SAFT
  - stability criterion
- **Cheung et al. (2002)**
  - clusters: solvent-solute interactions, OPLS, tight bounds, binary system
- **Esposito, Floudas (1998)**
  - error-in-variables + αBB for algebraic models
- **Gua, Stadtherr (2000)**
  - IA for error-in-variables
- **Gua et al. (2000)**
  - VLE via IA with Wilson equation for azeotropes
- **Gua et al. (2002)**
  - Interval Newton for parameter estimation catalytic reactor, HEN, VLE

Phase Equilibrium & Parameter Estimation

- **Scurto et al. (2004)**
  - High P solid-fluid equilibrium with cosolvents
- **Nichita et al. (2004)**
  - direct Gibbs minimization using tunneling G.O. method
- **Henderson et al. (2004)**
  - prediction of critical points
- **Freitas et al. (2004)**
  - critical points in binary mixtures
- **Lin, Stadtherr (2004)**
  - interval methods in parameter estimation
- **Lucia et al. (2005)**
  - phase behavior of n-alkane systems
- **Ulas et al. (2005)**
  - uncertainties in parameter estimation and optimal control of batch distillation
- **Nichita et al. (2006)**
  - global phase stability analysis
- **Srinivas, Rangaiah (2006)**
  - random tunneling algorithm in phase equilibrium calculations
- **Singer, Taylor, Barton (2006)**
  -dynamic complex kinetic model
- **Srinivas, Rangaiah (2007)**
  - tabu list in phase equilibrium calculations
- **Mitsos, Barton (2007)**
  - Gibbs tangent plane stability criterion via Lagrangian duality

MINLPs

- **Zamora, Grossmann (1998a)**
  - thermo-based convex underestimators for quadratic/linear fractional
  - hybrid B&B + OA
  - HENs without splitting
- **Westerlund et al. (1998)**
  - extended cutting plane for P-convex MINLPs
  - paper industry application
- **Vecchietti, Grossmann (1999)**
  - disjunctive programming, LOGMIP
  - hybrid modeling framework
  - process synthesis, FTIR
- **Sinha et al. (1999)**
  - solvent design: nonconvex MINLP
  - reduced space B&B approach
  - single component blanked wash design
- **Noureldin, El-Halwagi (1999)**
  - IA for pollution prevention
  - water usage/discharge in tire-to-fuel plant
- **Pörn et al. (1999)**
  - exponential and potential transformation for integer posynomial problems
- **Harjunkoski et al. (1999)**
  - trim loss minimization
- **Adjiman et al. (2000)**
  - SMIN-αBB: heat exchanger network
  - GMIN-αBB: pump networks, trim loss
- **Kesavan, Barton (2000)**
  - generalized Branch & Cut approach
  - decomposition, B&B are special cases
- **Sahinidis, Tawarmalani (2000)**
  - design of just-in-time flowshops
  - design of alternatives to freon
- **Parthasarathy, El-Halwagi (2000)**
  - optimal design of condensation
  - iterative G.O. based on decomposition and physical insights

MINLPs

- **Pörn, Westerlund (2000)**
  - successive linear approximation for objective, line search technique
  - cutting plane approach for P-convex objective and constraints
- **Lee, Grossmann (2001)**
  - nonconvex generalized disjunctive programming
  - convex hull of each nonlinear disjunction
  - two-level B&B approach
  - multicomponent separation, HENs, multistage design of batch plants
- **Björk, Westerlund (2002)**
  - G.O. of HEN synthesis
  - piecewise linear approximation of signomials
- **Wang, Achenie (2002)**
  - solvent design
  - hybrid G.O.: OA + simulated annealing
  - near optimal solutions
- **Ostrovsky et al. (2002)**
  - branch on variables which depend linearly on the search variables
  - tailored B&B approach
  - linear underestimators via a multilevel function representation
  - significant reduction in B&B spacw
- **Dua, Bozinis, Pistikopoulos (2002)**
  - multiparametric mixed-integer quadratic models
  - decomposition approach
  - envelopes of parametric solutions
- **Sahinidis et al. (2003)**
  - alternative refrigerants design
  - integer formulation
  - branch & reduce G.O. approach
- **Vaia, Sahinidis (2003)**
  - parameter estimation + model identification in infrared spectroscopy
  - B&B approach

MINLPs

- **Ostrovsky et al. (2003)**
  - reduced space B&B
  - sweep method for linear underestimators
- **Sinha et al. (2003)**
  - cleaning solvent blends
  - IA based G.O. approach
- **Zhu, Kuno (2003)**
  - hybrid G.O. method
  - revised GBD and convex quadratic underestimation
- **Goyal, Ierapetritou (2003)**
  - MINLPs with concave/Q-concave constraints
  - simplical approximation of convex hull
- **Kallrath (2003)**
  - nonconvex portfolio pf products
  - concave objective, trilinear terms
  - piecewise linear approximation of objective
  - sBB, Baron
  - weak lower bounds
- **Grossmann, Lee (2003)**
  - nonconvex GDP with bilinear equalities
  - use of RLT for convexification
  - convex hull representation of disjunctions
  - two-level approach for pooling, water usage, wastewater networks
- **Lin, Floudas, Kallrath (2004), (2005)**
  - nonconvex product portfolio
  - improved formulation
  - techniques for bound tightening
  - customized B&B
  - large problems solved efficiently
- **Kesavan,Allgor, Gatzke, Barton (2004)**
  - separable MINLPs with nonconvex functions
  - (2) decomposition approaches
  - alternating sequences of relaxed master, (2) NLPs, Outer approximation
  - first approach leads to global solution
  - second approach provides valid lower bounds

MINLPs

- **Yan, Shen, Hu (2004)**
  - line-up competition algorithm
- **Tawarmalani, Sahinidis (2004;2005)**
  - domain reduction strategies
  - polyhedral branch-and-cut
  - BARON framework enhancements
- **Dua, Papalexandri, Pistikopoulos (2004)**
  - multiparametric continuous/integer
- **Munawar, Gudi (2005)**
  - hybrid evolutionary method for MINLPs
  - based on nonlinear transformations
- **Luo, Wang, Liu (2006)**
  - Improved particle swarm optimization algorithm
- **Young, Zheng, Yeh, Jang (2007)**
  - Information-guided genetic algorithm

RECENT APPLICATIONS

- **Lin, Floudas, Kallrath (2005)**
  - product portfolio
- **Ghosh et al. (2005)**
  - flux identification in NMR data
- **Meyer, Floudas (2006)**
  - generalized pooling problem
- **Karuppiah, Grossmann (2006)**
  - integrated water systems
- **Bringas et al. (2007)**
  - groundwater remediation networks
- **Bergamini, Scenna, Aquirre (2007)**
  - heat exchanger networks
  - via piecewise relaxation
- **Exler et al. (2007), Egea et al. (2007)**
  - integrated process and control
- **Karuppiah, Furman, Grossmann (2008)**
  - scheduling refinery crude operations
- **Foteinou, Saharidis, Ierapetritou, Androulakis (2008)**
  - regulatory networks
- **Rebennack, Kallrath, Pardalos (2008)**
  - column enumeration
  - packing of circles & rectangles

Differential-Algebraic Models, DAEs

- **Esposito, Floudas (2000a,b;2001)**
  - parameter estimation with ODEs
  - nonlinear optimal control
  - αBB principles for underestimation
  - alternative was for β calculation
- **Chachuat, Singer, Barton (2005; 2006a,b)**
  - hybrid discrete/continuous dynamic systems
  - emphasis on control parameterization
- **Esposito, Floudas (2002)**
  - isothermal reactor network synthesis
  - αBB framework
- **Lin, Stadtherr (2006;2007)**
  - parameter estimation of dynamic systems
  - constraint propagation scheme for domain reduction
- **Papamichail, Adjiman (2002;2004;2005)**
  - spatial B&B G.O. for DAEs
  - theory of differential inequalities
  - convex relaxations for rigorous bounds for parametric ODEs and their sensitivities
  - parameter estimation of kinetic models
- **Singer, Barton (2003;2004;2006)**
  - G.O. of integral objective with ODEs
  - pointwise integrand scheme for convex relaxations of integral
  - B&B approach
- **Lee, Barton (2003;2004), Barton et al. (2006)**
  - G.O. of linear time varying hybrid systems
  - determination of optimal mode sequence with transition times fixed
  - convex relaxations of Bolza-type functions
  - isothermal PFR
- **Chachuat, Latifi (2003)**
  - spatial B&B G.O. for ODEs
  - first, second order derivatives
  - two point boundary value problem
  - sensitivities vs adjoint approach
- **Banga et al. (2003)**
  - integrated design and operation
  - parameter estimation in bioprocesses
  - stochastic G.O.
  - hybrid approaches for dynamic optimization

Differential-Algebraic Models, DAEs

- **Long, Pollsetty, Gatzke (2006)**
  - Nonlinear Model Predictive Control
  - method for improved convergence rate
  - global NMPC superior to local NMPC
  - alternative was for β calculation
- **Long, Pollsety, Gatzke (2007)**
  - NMPC for hybrid systems
  - mixed-integer dynamic model
  - Stability & uncertainty

Bilevel Nonlinear Optimization

- **Gumus, Floudas (2001)**
  - bilevel NLPs
  - inner level convex relaxation
  - equivalent KKTs
  - αBB principles
- **Floudas, Gumus, Ierapetritou (2001)**
  - G.O. of feasibility test, flexibility index
  - bilevel NLPs
  - αBB framework
- **Pistikopoulos et al. (2003)**
  - linear/linear
  - linear/quadratic
  - quadratic/linear
  - quadratic/quadratic
  - parametric programming
- **Gumus, Floudas (2004, 2005)**
  - bilevel mixed-integer
  - convex envelopes/hull
- **De Saboia, Campelo, Scheimberg (2004); Campelo, Scheimberg (2005)**
  - linear BLP; equilibrium point
- **Ryu, Dua, Pistikopoulos (2004)**
  - transform BLP into single parametric programming problems
- **Babahadda, Gadhi (2006)**
  - convexificator for necessary OCs
- **Solodov (2007)**: bundle method
- **Faisca, Dua, Rustem, Saraiva, and Pistikopoulos (2007)**
  - bilevel quadratic
  - bilevel mixed integer linear
  - w/wo RHS uncertainty
- **Tuy, Migdalas, Hoai-Phuong (2007)**
  - transform into monotonic optimization
  - branch reduce & bound + monotonicity

Semi-Infinite Programming

- **Bhattacharjee, Lemonidis, Green, Barton (2005)**
  - B&B algorithm
  - upper bound = finite inclusion bounds
  - lower bound = convex relaxation of discretized approximation
- **Bhattacharjee, Green, Barton (2005)**
  - use of interval analysis
  - construction of finite nonlinear reformulations
- **Chang and Sahinidis (2005)**
  - study of metabolic networks
  - S-system representation
  - additional constraint to enforce stability of the solution
- **Floudas and Stein (2007)**
  - adaptively construct relaxations
  - use of αBB principles
- **Liu (2007)**
  - homotopy interior point method
  - globally convergent algorithm

Grey-Box and Nonfactorable Models

- **Jones et al. (1998), (2001)**

- kriging model + response surface

- **Byrne, Bogle (2000)**
  - G.O. of modular flowsheets
  - IA approach
  - lower bounds
  - derivatives and their bounds
  - B&B G.O. approach
- **Meyer, Floudas, Neumaier (2002)**
  - G.O. of nonfactorable models
  - new blending functions for
  - sampling
  - linear under/overestimators via IA
  - Branch & Cut G.O. approach
  - oilshale pyrolysis
  - nonlinear CSTR

- **Gutmann (2001)**
  - radial basis function, RBF
- **Zabinsky (2003)**
- **Regis, Shoemaker (2005,2007)**
  - constrained optimization using response surfaces, CORS-RBF
  - controlled Gutmann, CG-RBF
- **Huang, Allen, Notz, Zeng (2006)**
  - kriging meta-model
- **Hu, Fu, Markus (2007)**
  - model reference adaptive search
- **Egea, Vasquez, Banga, Marti (2007)**
  - scatter search metaheuristic
  - kriging-based prediction
- **Davis, Ierapetritou (2008)**
  - Kriging model + response surface
  - B&B for MINLPs under uncertainty
  - small process synthesis problems

Recent Reviews

- Floudas, Akrotirianakis, Caratzoulas, Meyer, Kallrath (2005), "Global Optimization in the 21st Century", *Computers & Chemical Engineering*, 29(6), 1185-1202.
- Floudas (2005), "Systems Engineering Approaches In Computational Biology and Bioinformatics", *AIChE Journal*, 51, 1872-1884.
- Floudas and Gounaris (2009), "Advances in Global Optimization: A Review", J. Global Optimization, in press.

Outline

- Deterministic Global Optimization: Objectives & Motivation
- **Convex Envelopes:**
  - **Trilinear Monomials**
  - **Univariate Monomials**
  - **Fractional Terms**
  - **Edge Concave functions**
- Checking Convexity: Products of Univariate Functions
- Convex Underestimators for Trigonometric Functions
- PαBB: Piecewise Quadratic Perturbations
- GαBB: Generalized αBB
- Functional Forms of Convex Underestimators
- Augmented Lagrangian Approach for Global Optimization
- New Class of Convex Underestimators
- Pooling Problems & Generalized Pooling Problems
- Conclusions

Convex Envelopes for Trilinear Monomials

(Meyer and Floudas, *JOGO*, 2003)

- The convex envelope of a trilinear monomial is polyhedral over a coordinate aligned hyper-rectangular domain.

- A triangulation of the domain defines the convex envelope of the monomial.

- The correct triangulation is determined by a set of conditions related to the minimal affine dependencies of the vertices of the hyper-rectangle.

- An explicit set of formulae for the elements of the convex envelope is defined for each set of conditions.

Convex Envelopes for Trilinear Monomials

(Meyer and Floudas, *JOGO*, 2003)

Positive Bounds

If $\underline{x} \ge 0$, $\underline{y} \ge 0$ and $\underline{z} \ge 0$ and the auxiliary conditions apply:

$$\bar{x}\underline{y}\underline{z} + \underline{x}\bar{y}\bar{z} \le \underline{x}\bar{y}\underline{z} + \bar{x}\underline{y}\bar{z} \qquad \bar{x}\underline{y}\underline{z} + \underline{x}\bar{y}\bar{z} \le \bar{x}\bar{y}\underline{z} + \underline{x}\underline{y}\bar{z}$$

the linear equalities defining the facets of the convex envelope are:

$$w = \underline{y}\underline{z}x + \underline{x}\underline{z}y + \underline{x}\underline{y}z - 2\underline{x}\underline{y}\underline{z}$$

$$w = \bar{y}\bar{z}x + \bar{x}\bar{z}y + \bar{x}\bar{y}z - 2\bar{x}\bar{y}\bar{z}$$

$$w = \underline{y}\bar{z}x + \underline{x}\bar{z}y + \bar{x}\underline{y}z - \underline{x}\underline{y}\bar{z} - \bar{x}\underline{y}\bar{z}$$

$$w = \bar{y}\underline{z}x + \bar{x}\underline{z}y + \underline{x}\bar{y}z - \bar{x}\bar{y}\underline{z} - \underline{x}\bar{y}\underline{z}$$

$$w = \frac{\theta}{\bar{x}-\underline{x}}x + \bar{x}\underline{z}y + \bar{x}\underline{y}z + \left(-\frac{\theta\underline{x}}{\bar{x}-\underline{x}} - \bar{x}\bar{y}\underline{z} - \bar{x}\underline{y}\bar{z} + \underline{x}\bar{y}\bar{z}\right)$$

$$w = \frac{\theta}{\underline{x}-\bar{x}}x + \underline{x}\bar{z}y + \underline{x}\bar{y}z + \left(-\frac{\theta\bar{x}}{\underline{x}-\bar{x}} - \underline{x}\underline{y}\bar{z} - \underline{x}\bar{y}\underline{z} + \bar{x}\underline{y}\underline{z}\right)$$

$$\text{where } \theta = \underline{x}\underline{y}\bar{z} - \bar{x}\underline{y}\underline{z} - \underline{x}\bar{y}\bar{z} + \underline{x}\bar{y}\underline{z}$$

Convex Envelopes for Trilinear Monomials

(Meyer and Floudas, *JOGO*, 2003)

Illustration

To construct the concave envelope of $x_1 x_2 x_3$ for $(x_1, x_2, x_3) \in [1,2]\times[1,2]\times[2,4]$. We substitute $y \leftarrow x_1$, $x \leftarrow x_2$, and $z \leftarrow x_3$ and check conditions:

$$\bar{x}\underline{y}\underline{z} + \underline{x}\bar{y}\bar{z} \le \underline{x}\bar{y}\underline{z} + \bar{x}\underline{y}\bar{z} \qquad \bar{x}\underline{y}\underline{z} + \underline{x}\bar{y}\bar{z} \le \bar{x}\bar{y}\underline{z} + \underline{x}\underline{y}\bar{z}$$

which translate into,

$$\bar{x}_2\underline{x}_1\underline{x}_3 + \underline{x}_2\bar{x}_1\bar{x}_3 \le \underline{x}_2\bar{x}_1\underline{x}_3 + \bar{x}_2\underline{x}_1\bar{x}_3$$

$$(3)(1)(2)+(1)(2)(4)\le(1)(2)(2)+(3)(1)(4)$$

$$14 \le 16$$

and,

$$\bar{x}_2\underline{x}_1\underline{x}_3 + \underline{x}_2\bar{x}_1\bar{x}_3 \le \underline{x}_2\underline{x}_1\bar{x}_3 + \bar{x}_2\bar{x}_1\underline{x}_3$$

$$(3)(1)(2)+(1)(2)(4)\le(1)(1)(4)+(3)(2)(2)$$

$$14 \le 16$$

Both conditions hold, so we can use the substitutions in the facet defining equations.

Convex Envelopes for Trilinear Monomials

(Meyer and Floudas, *JOGO*, 2003)

Facet Defining Equations

$$w = 2x_2 + 2x_1 + 1x_3 - 4,$$

$$w = 8x_2 + 12x_1 + 6x_3 - 48,$$

$$w = 4x_2 + 4x_1 + 3x_3 - 16,$$

$$w = 4x_2 + 6x_1 + 2x_3 - 16,$$

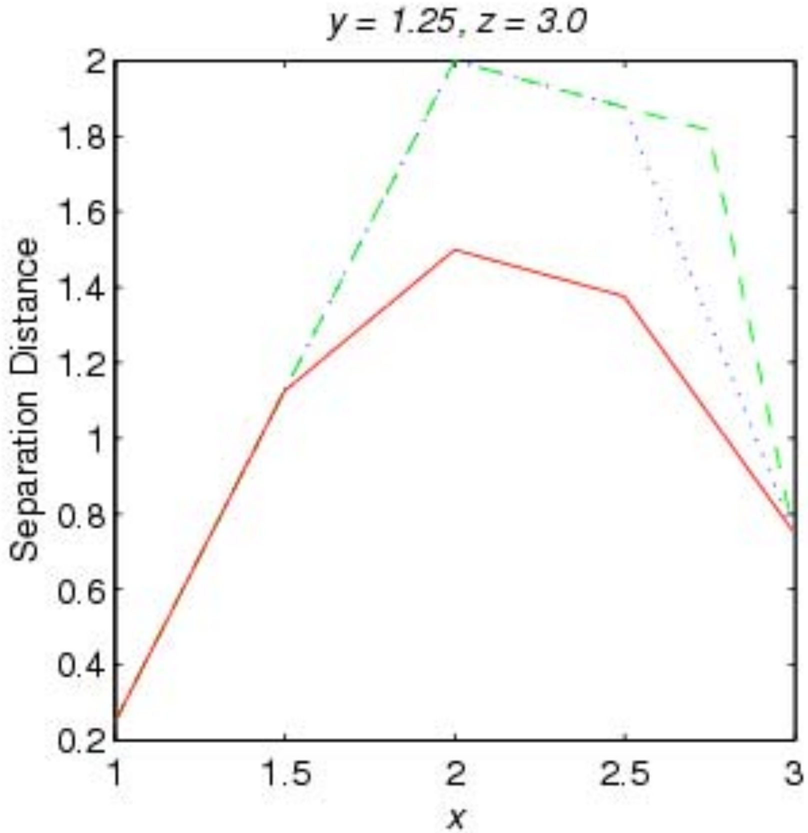
$$w = 5x_2 + 6x_1 + 3x_3 - 21,$$

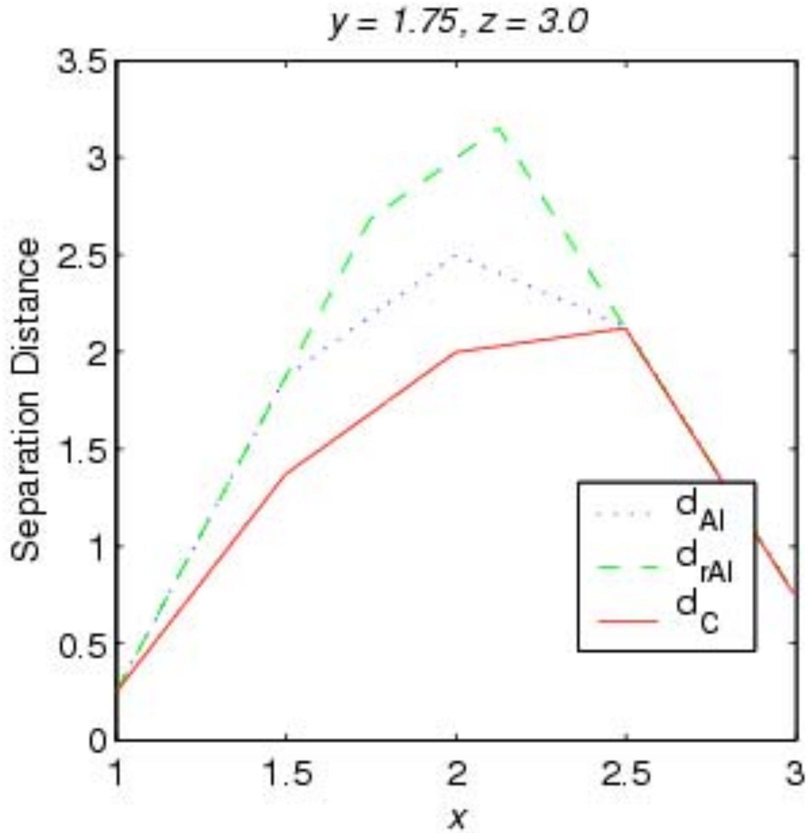
$$w = 3x_2 + 4x_1 + 2x_3 - 11.$$

Comparison with Lower Bounding Approximations

The separation distance between the function *xyz* and the convex envelope (d_C) is compared with the separation distance between *xyz* and:

- the Arithmetic Interval lower bounding approximation (d_{AI}) and,
- the Recursive Arithmetic Interval lower bounding approximation (d_{rAI}).





Convex Envelopes for Odd Degree Univariate Monomials

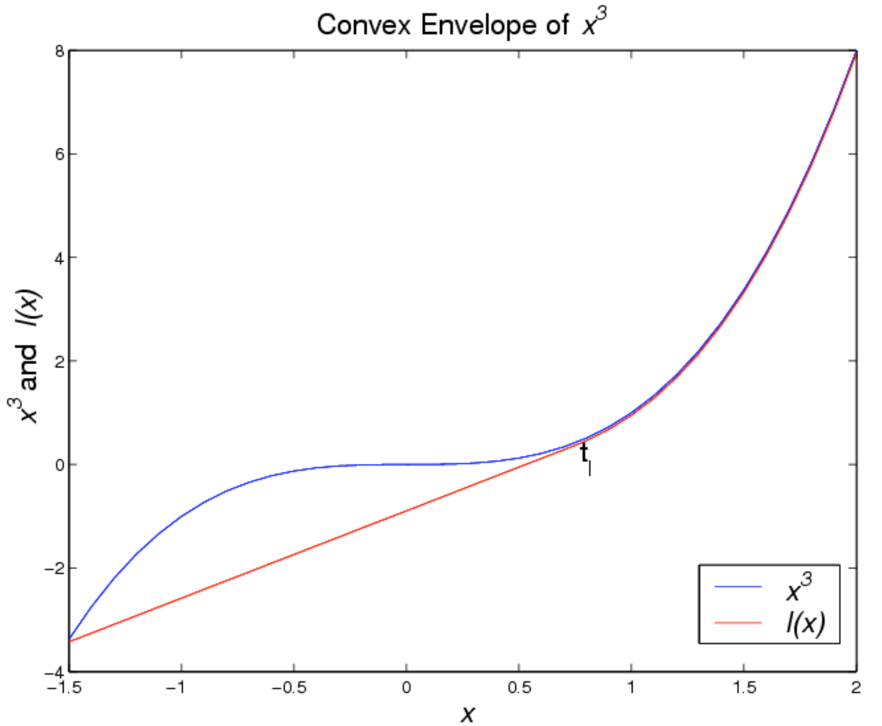
(Liberti and Pantelides, *JOGO*, 2002)

Univariate monomial of degree 2*k*+1 in interval $x \in [\underline{x}, \overline{x}]$ where $0 \in [\underline{x}, \overline{x}]$:

$$f(x) := x^{2k+1}$$

Convex envelope $l(x)$ separates from $f(x)$ at t_l.

$$t_l := r_k \underline{x}$$



Convex Envelopes for Odd Degree Univariate Monomials

(Liberti and Pantelides, *JOGO*, 2002)

if $t_l < \overline{x}$:

$$l_k(x) := \begin{cases} \underline{x}^{2k+1}\left(1 + R_k\left(\dfrac{x - \underline{x}}{lx}\right)\right) & \text{if } x < t_l \\ x^{2k+1} & \text{if } x \geq t_u \end{cases}$$

otherwise:

$$l_k(x) := \underline{x}^{2k+1} + \frac{\overline{x}^{2k+1} - \underline{x}^{2k+1}}{\overline{x} - \underline{x}}(x - \underline{x})$$

where $R_k := \dfrac{r_x^{2k+1} - 1}{r_k - 1}$ and r_k are constants:

k	r_k	k	r_k
1	-0.5000000000	6	-0.7721416355
2	-0.6058295862	7	-0.7921778546
3	-0.6703320476	8	-0.8086048979
4	-0.7145377272	9	-0.8223534102
5	-0.7470540749	10	-0.8340533676

Linear Underestimators for Odd Degree Univariate Monomials

(Liberti and Pantelides, *JOGO*, 2002)

- linear underestimators are derived through linearization of the convex envelope at the end points.
- $w_k := x^{2k+1}$.

if $t_l \leq \overline{x}$:

$$\boxed{\begin{array}{l} w_k \geq \underline{x}^{2k+1}\left(1+R_k\left(\dfrac{x}{\underline{x}}-1\right)\right) \\ w_k \geq (2k+1)\underline{x}^{2k}x-2k\overline{x}^{2k+1} \end{array}}$$

otherwise:

$$\boxed{w_k \geq \underline{x}^{2k+1}+\frac{\overline{x}^{2k+1}-\underline{x}^{2k+1}}{\overline{x}-\underline{x}}(x-\underline{x}).}$$

Convex Envelope for Fractional Terms

(Tawarmalani and Sahinidis, *JOGO*, 2001)

- Fractional term $\frac{x}{y}$ in interval $(x, y) \in [\underline{x}, \overline{x}] \times [\underline{y}, \overline{y}]$ where $\underline{x} \geq 0$, $\underline{y} > 0$.

New variables: y_p, z_p, z where z stands in for $\frac{x}{y}$.

$$
\boxed{
\begin{array}{ll}
y_p \geq \dfrac{x}{z_p}\left(\dfrac{\overline{x} - x}{\overline{x} - \underline{x}}\right)^2 & y_p \geq \underline{y}\left(\dfrac{x - \underline{x}}{\overline{x} - \underline{x}}\right) \\
y_p \leq y - \dfrac{\overline{x}}{z - z_p}\left(\dfrac{x - \underline{x}}{\overline{x} - \underline{x}}\right)^2 & y_p \leq \overline{y}\left(\dfrac{\overline{x} - x}{\overline{x} - \underline{x}}\right) \\
y_p \geq \underline{y}\left(\dfrac{\overline{x} - x}{\overline{x} - \underline{x}}\right) & y_p \geq y - \underline{y}\left(\dfrac{x - \underline{x}}{\overline{x} - \underline{x}}\right) \\
z - z_p \geq 0 & z_p \geq 0
\end{array}
}
$$

- Explicit form for domain $(x, y) \in [\underline{x}, \overline{x}] \times (0, \infty)$.

$$
\boxed{z \geq \frac{1}{y}\left(\frac{x + \sqrt{\underline{x}\,\overline{x}}}{\sqrt{\overline{x}} + \sqrt{\underline{x}}}\right)^2}
$$

Convex Envelopes for Edge-Concave Functions

(Meyer and Floudas, *Math. Programming*, 2005)

Definition:

An **Edge-Concave function** is a function that has a **Vertex Polyhedral Convex Envelope**

Several classes of functions are edge-concave on certain domains:

- Concave functions over polytopes
- Multilinear functions over hypercubes

(Rikun, 1997)

Constructive Characterization of the Convex Envelope

(Horst and Tuy, 1993; Floudas, 2000)

Edge-concave function $f : P \to R$

Polytope $P = conv\{x^1, x^2, \ldots, x^m\} \subset R^n$

$$\min_{\lambda_i \geq 0} \sum_{i=1}^{m} \lambda_i f(x^i)$$

$$s.t. \quad \sum_{i=1}^{m} \lambda_i x^i = x$$

$$\sum_{i=1}^{m} \lambda_i = 1$$

Convex Envelopes for Edge-Concave Functions

(Meyer and Floudas, *Math. Programming*, 2005)

Alternative Characterization of the Convex Envelope	=	**Through a system of facet-defining hyperplanes (FDH)**

Examples:a) Bilinear envelopes (McCormick, 1976;Al-Khayyal,Falk,1983)

b) Trilinear envelopes (Meyer and Floudas, 2003; 2004)

c) Special forms of multilinear functions over hypercubes (Sherali, 1997)

Convex Envelopes for Edge-Concave Functions

(Meyer and Floudas, *Math. Programming*, 2005)

Edge-concave function $f : conv(V) \rightarrow R$

Set of vertices of hyperrectangle $V = \left\{ x^1, x^2, \ldots, x^{2^n} \right\} \subseteq R^n$

ALGORITHM

Step1: Dominance Relations

Evaluate function at each vertex point x^i
and determine the dominant subsets $X = \left\{ x^i : i \in P(\lambda) \right\} \subseteq V$

Convex Envelopes for Edge-Concave Functions

(Meyer and Floudas, *Math. Programming*, 2005)

Edge-concave function $f : conv(V) \to R$

Set of vertices of hyperrectangle $V = \{x^1, x^2, \ldots, x^{2^n}\} \subseteq R^n$

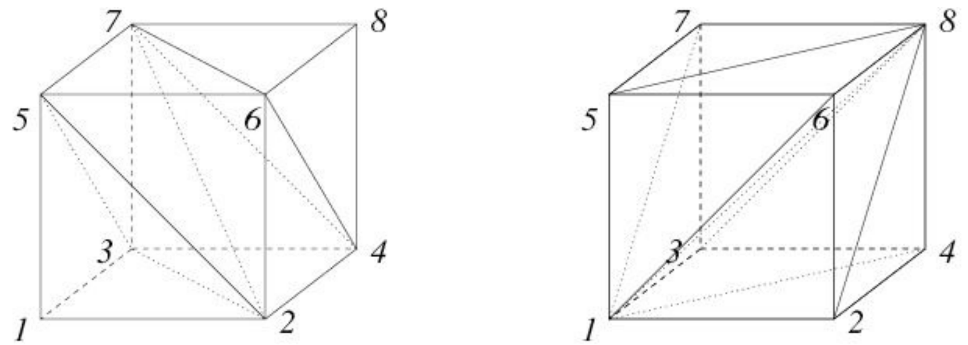
ALGORITHM

Step1: Dominance Relations

Evaluate function at each vertex point x^i and determine the dominant subsets $X = \{x^i : i \in P(\lambda)\} \subseteq V$

Step2: Triangulation Class

Determine the triangulation type
(6 different ways for 3d cube)



(a) Triangulation type **A** (b) Triangulation type **B**

Convex Envelopes for Edge-Concave Functions

(Meyer and Floudas, *Math. Programming*, 2005)

Edge-concave function $f : conv(V) \to R$

Set of vertices of hyperrectangle $V = \left\{ x^1, x^2, \ldots, x^{2^n} \right\} \subseteq R^n$

ALGORITHM

Step1: Dominance Relations	Evaluate function at each vertex point x^i and determine the dominant subsets $X = \left\{ x^i : i \in P(\lambda) \right\} \subseteq V$
Step2: Triangulation Class	Determine the triangulation type (6 different ways for 3d cube)
Step3: Reorientation	Apply Transformation: Representative triangulation → Current triangulation

Convex Envelopes for Edge-Concave Functions

(Meyer and Floudas, *Math. Programming*, 2005)

Edge-concave function $f : conv(V) \to R$

Set of vertices of hyperrectangle $V = \{x^1, x^2, \ldots, x^{2^n}\} \subseteq R^n$

ALGORITHM

Step1: Dominance Relations	Evaluate function at each vertex point x^i and determine the dominant subsets $X = \{x^i : i \in P(\lambda)\} \subseteq V$
Step2: Triangulation Class	Determine the triangulation type (6 different ways for 3d cube)
Step3: Reorientation	Apply Transformation: Representative triangulation → Current triangulation
Step4: Compute Facets	Calculate FDH from the cells of the current triangulation

Solve linear system of equations:

$$\begin{bmatrix} 1 & x_1^{i_1} & x_2^{i_1} & x_3^{i_1} \\ 1 & x_1^{i_2} & x_2^{i_2} & x_3^{i_2} \\ 1 & x_1^{i_3} & x_2^{i_3} & x_3^{i_3} \\ 1 & x_1^{i_4} & x_2^{i_4} & x_3^{i_4} \end{bmatrix} \begin{bmatrix} \pi_0 \\ \pi_1 \\ \pi_2 \\ \pi_3 \end{bmatrix} = \begin{bmatrix} f(x^{i_1}) \\ f(x^{i_2}) \\ f(x^{i_3}) \\ f(x^{i_4}) \end{bmatrix}$$

FDH is: $w = \langle \pi, x \rangle + \pi_0$

Outline

- Deterministic Global Optimization: Objectives & Motivation
- Convex Envelopes:
  - Trilinear Monomials
  - Univariate Monomials
  - Fractional Terms
  - Edge Concave functions
- **Checking Convexity: Products of Univariate Functions**
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Convexity of Products of Univariate Functions

(Gounaris and Floudas, *JOTA*, 2008)

$$f(\underline{x}) = \prod_{i=1}^{N} f_i(x_i) = f_1(x_1)\, f_2(x_2) \ldots.\, f_n(x_n)$$

When is f(x) convex?

Convexity of Products of Univariate Functions

(Gounaris and Floudas, *JOTA,* 2008)

$$f(\underline{x}) = \prod_{i=1}^{N} f_i(x_i) = f_1(x_1)\, f_2(x_2)....f_n(x_n)$$

When is f(x) convex?

Sufficient Conditions

- **Every factor should be strictly positive**
- **Every factor should be strictly convex**
- **For every factor:** $f_i(x_i)\, f_i^{//}(x_i) - \left(f_i^{/}(x_i)\right)^2 \geq 0$

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Sufficient Conditions

- **Every factor should be strictly positive**
- **Every factor should be strictly convex**

$\}$ **An even number of factors are allowed to instead be strictly negative and strictly concave**

- **For every factor:** $f_i(x_i)\, f_i^{//}(x_i) - \left(f_i^{/}(x_i)\right)^2 \geq 0$

Convexity of Products of Univariate Functions

(Gounaris and Floudas, *JOTA*, 2008)

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Sufficient Conditions

- **Every factor should be strictly positive**
- **Every factor should be strictly convex**

An even number of factors are allowed to instead be strictly negative and strictly concave

- **For every factor**: $f_i(x_i)\, f_i^{//}(x_i) - \left(f_i^{/}(x_i)\right)^2 \geq 0$

These conditions are in fact necessary if all factors share the same functional form

Convexity of Products of Univariate Functions

(Gounaris and Floudas, *JOTA*, 2008)

$$f(\underline{x}) = \left\{ \frac{1.8}{x_2} + 1.2x_2 - \frac{3\log(1-x_1)}{x_2} - 2x_2\log(1-x_1) \right\} \frac{e^{x_3 - x_4}}{x_4^{1.2}}$$

Is f(x) convex in $\left[\frac{1}{3}, \frac{2}{3}\right]^4$?

Convexity of Products of Univariate Functions

(Gounaris and Floudas, *JOTA*, 2008)

$$f(\underline{x}) = \left\{ \frac{1.8}{x_2} + 1.2x_2 - \frac{3\log(1-x_1)}{x_2} - 2x_2\log(1-x_1) \right\} \frac{e^{x_3-x_4}}{x_4^{1.2}}$$
$$= f_1(x_1)\, f_2(x_2)\, f_3(x_3)\, f_4(x_4)$$

Is f(x) convex in $\left[\frac{1}{3},\frac{2}{3}\right]^4$?

$$f_1(x_1) = 0.6 - \log(1-x_1)$$

$$f_2(x_2) = \frac{2x_2^2+3}{x_2}$$

$$f_3(x_3) = e^{x_3}$$

$$f_4(x_4) = \frac{e^{-x_4}}{x_4^{1.2}}$$

Yes!
….because all four functions satisfy the sufficient conditions in [1/3,2/3]

Convexity of Products of Univariate Functions

(Gounaris and Floudas, *JOTA*, 2008)

Which functions are suitable for convexification transformations in multilinear and geometric programming?

Exponential	$x \rightarrow e^y$	(Maranas and Floudas, 1995)	(used on every factor)
Reciprocal	$x \rightarrow \dfrac{1}{y}$	(Li, Tsai and Floudas, 2007)	(used only on factors raised to positive powers)

Convexity of Products of Univariate Functions

(Gounaris and Floudas, *JOTA*, 2008)

Which functions are suitable for convexification transformations in multilinear and geometric programming?

Exponential $x \rightarrow e^{y}$ (Maranas and Floudas, *C&ChE*, 1997) (used on every factor)

Reciprocal $x \rightarrow \frac{1}{y}$ (Li, Tsai and Floudas, *Opt. Letters*, 2007) (used only on factors raised to positive powers

WHY?

- They satisfy the conditions
- They satisfy the conditions when they are raised to some power κ>0
- The exponential function satisfies the conditions even when raised to some negative power, thus it can convexify any arbitrary posynomial program

In fact, it is the only functional form with such a capability (Gounaris and Floudas, *JOTA,*2008)

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- Deterministic Global Optimization: Objectives & Motivation
- Convex Envelopes:
  - Trilinear Monomials
  - Univariate Monomials
  - Fractional Terms
  - Edge Concave functions
- Checking Convexity: Products of Univariate Functions
- **Convex Underestimators for Trigonometric Functions**
- PαBB: Piecewise Quadratic Perturbations
- GαBB: Generalized αBB
- Functional Forms of Convex Underestimators
- Augmented Lagrangian Approach for Global Optimization
- New Class of Convex Underestimators
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- Conclusions

Convex Underestimators for Trigonometric Functions

Caratzoulas, Floudas, *JOTA* (2005)

$$f(x) = \alpha \sin(x+s) \qquad x \in \left[x^L, x^U\right] \qquad \alpha > 0$$

$$g(x) = \alpha \sin(x + x_L + s) \qquad x \in \left[0, D = x^U - x^L\right] \qquad \alpha > 0$$

- Key Idea: Construct a 3-parameter (α,b,x_s) trigonometric function

$$\phi(x) = -\alpha \sin\left[k(x - x_s)\right] + b \qquad x \in [0, D] \qquad \alpha \geq 0$$

$$k = \frac{2\pi}{L}$$

L : period of $\phi(x)$

AND

prove properties for the calculation of

(α,b,x_s)

such that $\phi(x)$ is a convex underestimator

Convex Underestimators for Trigonometric Functions

- For $\phi(x)$ to be convex:

$$\begin{aligned} x_s &\le 0 \\ L &\ge 2(D - x_s) \end{aligned} \quad \Rightarrow \quad L = 2(D - x_s) + M$$

- Property 1: matching $g(x)$ and $\phi(x)$ at the bounds results in:

$$\alpha = \frac{\Delta + \delta_{\Delta,0}(f^L - T)}{\sin(kx_s) + \sin\left\{k\left[D - (D-q)\delta_{\Delta,0} - x_s\right]\right\}}$$

$$b = f^L - \alpha \sin(kx_s)$$

$$\Delta = f^L - f^U = g(0) - g(D)$$

$$T = t(q) = g(q_0) + g'(q - q_0)$$

$$\delta_{\Delta,0} = \begin{cases} 1 & \text{if } \Delta = 0 \\ 0 & \text{otherwise} \end{cases}$$

Convex Underestimators for Trigonometric Functions

- **Property 2:** The phase shift x_s is:

$$x_s = -\frac{M}{2} > 0 \qquad \text{if } \Delta = 0 \qquad (1)$$

$$\tan(kx_s) = -\frac{\Delta \sin(kq) + (T - f^L)\sin(kD)}{\Delta(1-\cos(kq)) + (T - f^L)(1-\cos(kD))} \qquad \text{if } \Delta \neq 0 \qquad (2)$$

- Note: (a) Equation (2) needs to be solved numerically since k depends on x_s
  (b) a few Newton iterations suffice
  (c) Equation (2) always has a solution

Convex Underestimators for Trigonometric Functions

- **Property 3:** $g(x) \geq \phi(x)$ (i.e., $\phi(x)$ underestimates $g(x)$)
- **Property 4:** $\phi(x)$ is convex
- **Property 5:** Maximum Separation Distance, U_{max}

$$U_{max} = \max(\bar{g}(x) - \phi(x)) \cong \bar{g}(x) - f^{L} + \frac{\Delta}{4rD(1-rD)} \qquad \text{for } \Delta \neq 0$$

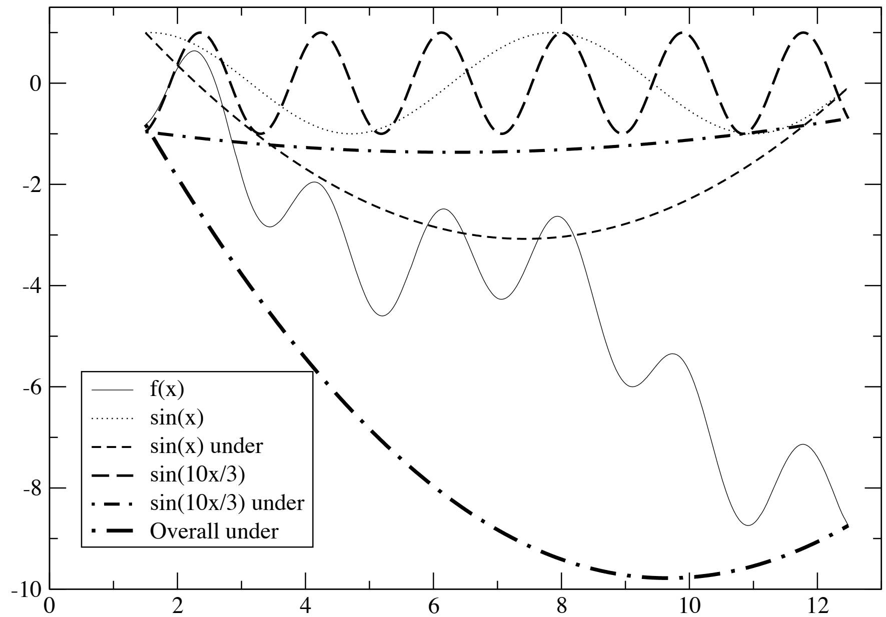
$$U_{max} = \max(\bar{g}(x) - \phi(x)) \cong \bar{g}(x) - f^{L} + \frac{(f^{L} - T)D^{2}}{4q(D-q)} \qquad \text{for } \Delta = 0$$

- Note: (a) As D grows, r → 0, rD(1-rD) → D^{-1}, U_{max} grows **linearly** with D for $\Delta \neq 0$.

  (b) As D grows, U_{max} grows linearly with D for $\Delta = 0$.

Convex Underestimators for Trigonometric Functions

$$f(x) = \sin(x) + \sin(10x/3) + \ln(x) - 0.84x, \qquad 1.5 \le x \le 12.485$$



$$\sin(x) \rightarrow \phi(x) = 24.91\left[\sin\left(2\pi x / L\ \right) + 10.11\right] + 21.83$$

$$\sin(10x/3) \rightarrow \phi(x) = 4.28\left[\sin\left(2\pi x / L_2\right) + 41.22\right] + 2.92$$

Initial lower bound = -9.7818 at x = 9.656

αBB with α = 6.0007 → Initial lower bound = -185.23

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PαBB:
Piecewise Quadratic Perturbations

Christodoulos A. Floudas

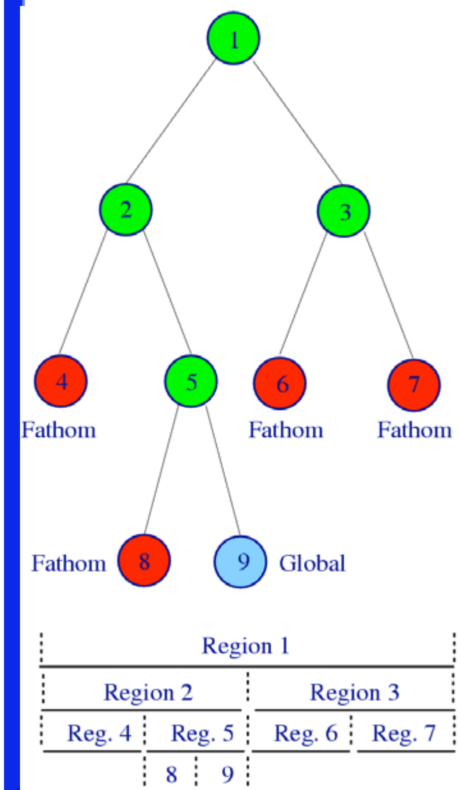
Princeton University

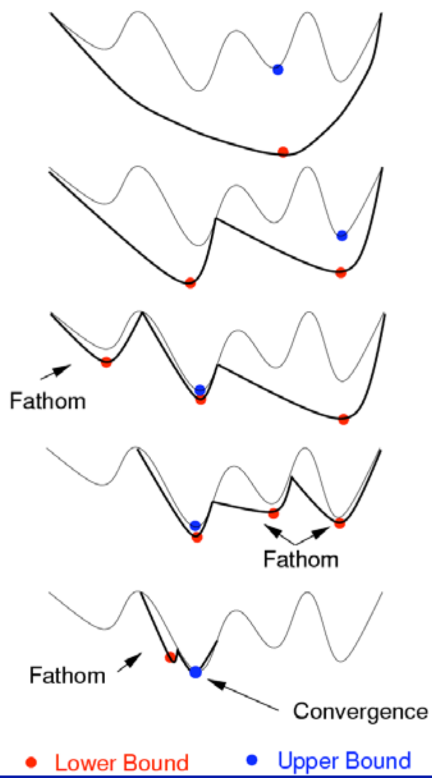
C^2 NLPs - The αBB Framework

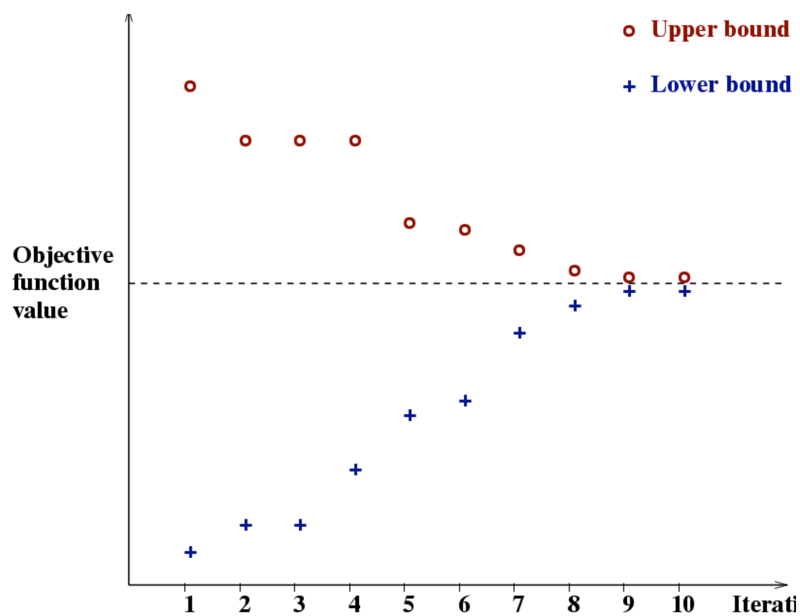
$$
\begin{array}{lrcl}
\min_{\mathbf{x}} & f(\mathbf{x}) & & \\
\text{s.t.} & \mathbf{h}(\mathbf{x}) & = & \mathbf{0} \\
 & \mathbf{g}(\mathbf{x}) & \leq & \mathbf{0} \\
 & \mathbf{x} \in \mathbf{X} \subseteq \mathcal{R}^n & &
\end{array}
$$

f , $\mathbf{h}$, $\mathbf{g}$ twice continuously differentiable

- Based on a branch-and-bound framework
- Upper bound on the global solution is obtained by solving the full nonconvex problem to local optimality
- Lower bound is determined by solving a valid convex underestimation of the original problem
- Convergence is obtained by successive subdivision of the region at each level in the brand & bound tree
- Guaranteed ε-convergence for C^2 NLPs







Convex Lower Bounding: The αBB Framework

(Androulakis et al., *JOGO*,1995; Adjiman et al.,*Comp.&Chem.Eng*. 1998)

- Decompose each constraint into a sum of terms

$$f(x) = f_L(x) + f_C(x) + \sum_{i \in B} a_i x_1^i x_2^i + \sum_{i \in T} b_i x_1^i x_2^i x_3^i$$

LINEAR CONVEX BILINEAR TRILINEAR

$$+ \sum_{i \in F} c_i \frac{x_1^i}{x_2^i} + \sum_{i \in FT} d_i \frac{x_1^i x_2^i}{x_3^i} + \sum_{i \in S} f_S^i(x)$$

FRACTIONAL FRACTIONAL TRILINEAR SIGNOMIAL

$$+ \sum_{i \in UC} f_{UC}^i(x^i) + f_{GNC}(x)$$

UNIVARIATE CONCAVE GENERAL NONCONVEX

- Develop valid convex underestimators for each term

Convex Lower Bounding: The αBB Framework

Linear Terms

Convex Terms

} → unchanged

Bilinear Terms (McCormick, 1976; Al Kayyal, Falk, 1983)

Define $w_B = x_1 x_2$ and introduce: Convex Envelope

$$
\boxed{
\begin{aligned}
w_B &\geq x_1^L x_2 + x_2^L x_1 - x_1^L x_2^L \\
w_B &\geq x_1^U x_2 + x_2^U x_1 - x_1^U x_2^U \\
w_B &\leq -x_1^U x_2 - x_2^L x_1 + x_1^U x_2^L \\
w_B &\leq -x_1^L x_2 - x_2^U x_1 + x_1^L x_2^U
\end{aligned}
}
$$

Key Property (Androulakis et al., 1995)

$$
\boxed{\max_{x_1, x_2} (x_1 x_2 - w_B) = \frac{(x_1^U - x_1^L)(x_2^U - x_2^L)}{4}}
$$

Convex Lower Bounding: The αBB Framework

General C^2 Nonconvex Terms

(Maranas, Floudas, 1994; Androulakis et. al, 1995)

$$L(x) = f_{GNC}(x) - \sum_{i=1}^{n} \alpha_i (x_i^U - x_i)(x_i - x_i^L)$$

$$\alpha \geq \max\left\{0, -\frac{1}{2} \min_{i, x^L \leq x \leq x^U} \lambda_{i,H}(x)\right\}$$

P1: $f_{GNC}(x) \geq L(x)$

P2: $f_{GNC}(x) = L(x)$ at corner points

P3: $L(x)$ is convex in $\left[x^L, x^U\right]$

P4: $L^{D_1}(x) \geq L^{D_2}(x)$ where $D_1 \subseteq D_2$

P5: Maximum Separation Distance

$$\max\left(f_{GNC}(x) - L(x)\right) = \frac{1}{4}\sum_{i=1}^{n} \alpha_i (x_i^U - x_i^L)^2$$

P6: Convexity of *L(x)*

$$L(x) \text{ is convex if } H_{GNC}(x) + 2Diag(\alpha_i)$$
$$\text{is positive semidefinite } \quad \forall\, \alpha \in \left[x^L, x^U\right]$$

Rigorous Calculations of α: The αBB Framework

(Adjiman, Floudas, 1996; Adjiman et al., 1998a,b)

Key Ideas

- Derive Hessian matrix, $H(x)$, of $f_{GNC}(x)$
- Compute INTERVAL Hessian in $[x^L, x^U]$

$$[H(x)]_{ij} = [h_{ij}^L(x), h_{ij}^U(x)]$$

- $H \subseteq [H]$
- Compute α : $[H] + 2Diag(\alpha)$ is P.S.D.

Uniform Diagonal Shift Matrix

O(*n*²) Methods

- Gerschgorin Theorem

O(*n*³) Methods

- Hertz
- Lower Bounding Hessian
- Mori-Kokane
- E-Matrix Approach

Non-Uniform Diagonal Shift Matrix

- Scaled Gerschgorin Theorem
- H-Matrix
- Semi-definite Programming

Scaled Gerschgorin Theorem: The αBB Framework

Gerschgorin Theorem for real matrices:

$$\lambda_{\min} \geq \min_i \left(h_{ii} - \sum_{j \neq i} |h_{ii}| \right)$$

Theorem for Interval Matrices (Adjiman et al., 1998a,b)

$$\alpha_i = \max\left[0, -\frac{1}{2}\left[h_{ii}^L - \sum_{j \neq i} \max\left(\left|h_{ii}^L\right|, \left|h_{ii}^U\right|\right)\frac{d_j}{d_i}\right]\right]$$

$$\Downarrow$$

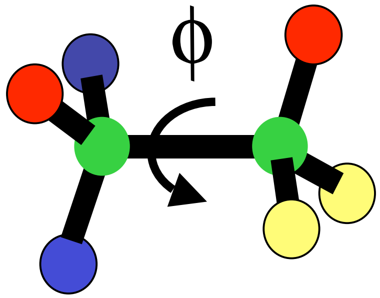
$$[H_{NT}] + 2Diag(\alpha_i) \text{ is positive semidefinite}$$

- d is a positive vector
  Use $d_i = 1$ or $d_i = x_i^U - x_i^L$

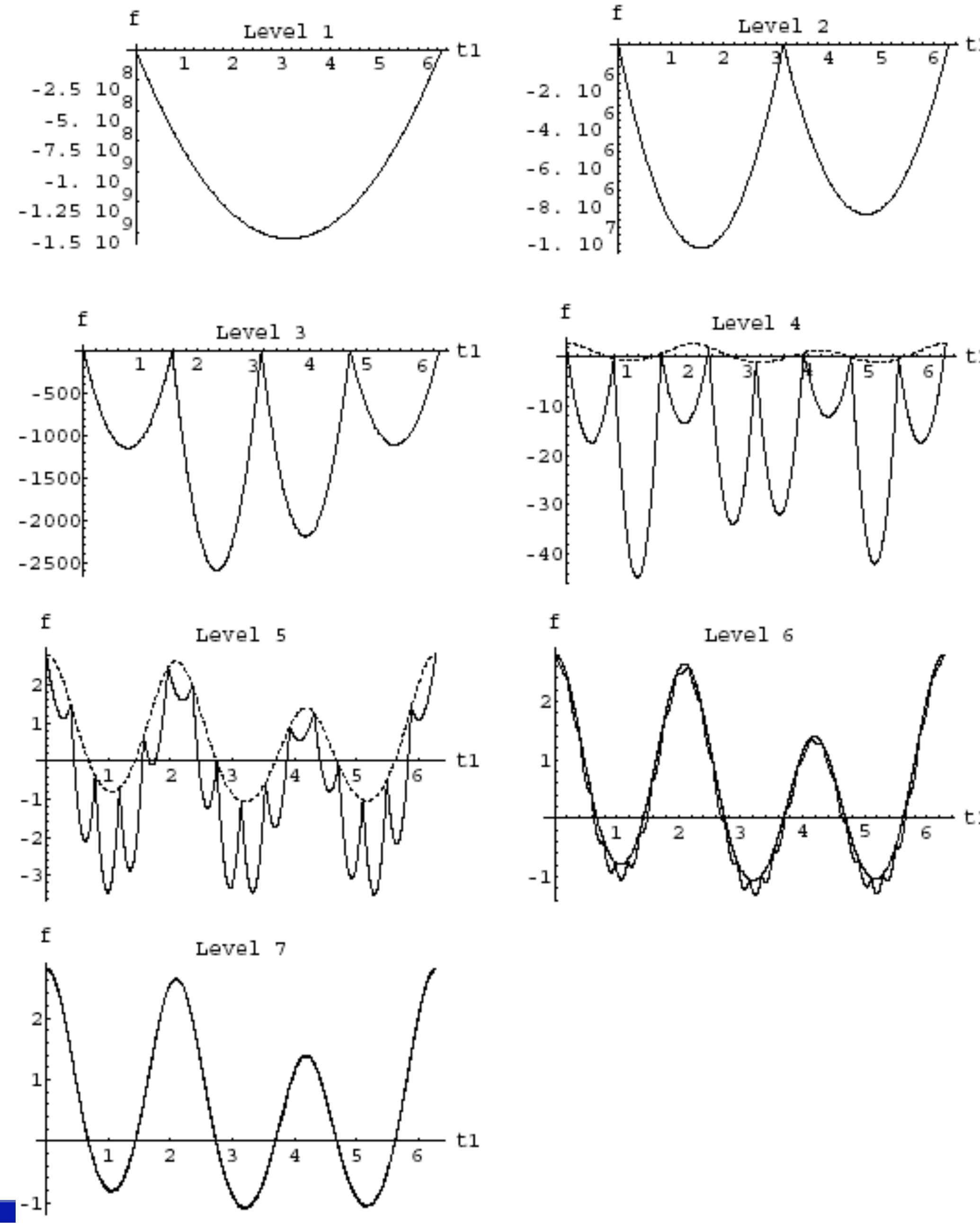
Inexpensive and simple technique

C2 NLPs - Illustrative Example

Pseudoethane



$$f(\phi)=\frac{588600}{\left(3r^2-4\cos\theta\, r^2-2\left(\sin^2\theta\cos\left(\phi-\frac{2\pi}{3}\right)-\cos^2\theta\right)r^2\right)^6}-\frac{1079.1}{\left(3r^2-4\cos\theta\, r^2-2\left(\sin^2\theta\cos\left(\phi-\frac{2\pi}{3}\right)-\cos^2\theta\right)r^2\right)^3}+\frac{600800}{\left(3r^2-4\cos\theta\, r^2-2\left(\sin^2\theta\cos\phi-\cos^2\theta\right)r^2\right)^6}-\frac{1071.5}{\left(3r^2-4\cos\theta\, r^2-2\left(\sin^2\theta\cos\phi-\cos^2\theta\right)r^2\right)^3}+\frac{481300}{\left(3r^2-4\cos\theta\, r^2-2\left(\sin^2\theta\cos\left(\phi+\frac{2\pi}{3}\right)-\cos^2\theta\right)r^2\right)^6}-\frac{1064.6}{\left(3r^2-4\cos\theta\, r^2-2\left(\sin^2\theta\cos\left(\phi+\frac{2\pi}{3}\right)-\cos^2\theta\right)r^2\right)^3}$$



αBB Underestimator: Room for Improvement?

$$q(x) = \sum_{i=1}^{n} \alpha_i \left(x_i - \underline{x}_i\right) \cdot \left(\overline{x}_i - x_i\right)$$

- Curvature of the perturbation function is constant.
- The eigenvectors of the Hessian matrix of the perturbation function are aligned with the coordinate axes.

A Refinement of the αBB Underestimator

Meyer, Floudas, *JOGO,* (2005)

Central Idea

- Partition the domain into subregions.
- Calculate the α parameters in each subregion.
- Construct an underestimator for the whole domain using these α's.

Properties of the Underestimator Function

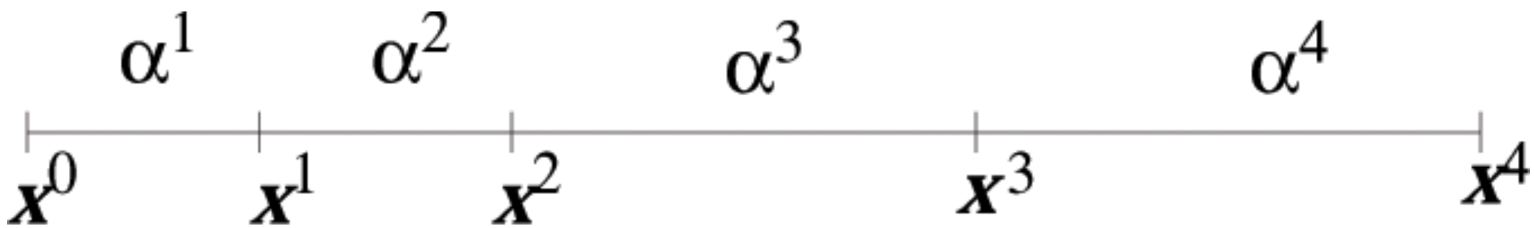
- smoothness
- convexity
- underestimation

Structure of the Underestimator Function

- sum of piecewise quadratic univariate functions
- underestimator matches function at vertices

Piecewise C²-Continuous Underestimator

- Partition interval $[\underline{x}_i, \overline{x}_i]$ into N_i subintervals.
- Endpoints of the subintervals: $x_i^0, x_i^1, \cdots, x_i^{N_i}$.



A smooth convex underestimator $f(x)$ in an interval $x \in [\underline{x}, \overline{x}]$:

$$\phi(x) := f(x) - q(x)$$

$$q(x) := \sum_{i=1}^{n} q_i^k(x_i) \qquad \text{for } x_i \in \left[x_i^{k-1}, x_i^k\right]$$

$$q_i^k(x_i) := \alpha_i^k \left(x_i - x_i^{k-1}\right) \cdot \left(x_i^k - x_i\right) + \beta_i^k x_i + \gamma_i^k$$

Joining the Pieces

- Smoothness: function q_i^k and their gradients must match at the internal endpoints x_i^k.
- Tight at extrema: $q_i(x) = 0$ at $\{\underline{x}_i, \overline{x}_i\}$.

$$q_i^k(x_i^k) = q_i^{k+1}(x_i^k) \quad \text{for all } k = 1, \cdots, N_i - 1$$

$$\frac{dq_i^k(x_i^k)}{dx_i} = \frac{dq_i^{k+1}(x_i^k)}{dx_i} \quad \text{for all } k = 1, \cdots, N_i - 1$$

$$q_i^1(x_i^0) = 0$$

$$q_i^{N_i}(x_i^{N_i}) = 0$$

Expands to a linear system in β and γ.

Formulae for β and γ

Linear System

$$\beta_i^k x_i^k + \gamma_i^k = \beta_i^{k+1} x_i^{k+1} + \gamma_i^{k+1} \qquad \text{for all } k = 1, \ldots, N_i$$

$$-\alpha_i^k \left(x_i^k - x_i^{k-1}\right) + \beta_i^k = \alpha_i^{k+1}\left(x_i^{k+1} - x_i^k\right) + \beta_i^{k+1} \qquad \text{for all } k = 1, \ldots, N_i$$

$$\beta_i^1 x_i^0 + \gamma_i^0 = 0$$

$$\beta_i^{N_i} x_i^{N_i} + \gamma_i^{N_i} = 0$$

Solution

$$\beta_i^1 = \left(\sum_{k=1}^{N_i - 1} s_i^k \left(x_i^k - x_i^{N_i}\right)\right) \Big/ \left(x_i^{N_i} - x_i^0\right)$$

$$\beta_i^k = \beta_i^1 + \sum_{j=1}^{k-1} s_i^j \qquad \text{for all } k = 2, \ldots, N_i$$

$$\gamma_i^k = -\gamma_i^1 x_i^0 - \sum_{j=1}^{k-1} s_i^j x_i^j \qquad \text{for all } k = 1, \ldots, N_i$$

where $s_i^k = -\alpha_i^k \left(x_i^k - x_i^{k-1}\right) - \alpha_i^{k+1}\left(x_i^{k+1} - x_i^k\right)$.

Illustration: Lennard-Jones Potential Energy Function

$f(x) = \frac{1}{x^{12}} - \frac{2}{x^6}$ in the interval $[\underline{x}, \overline{x}] = [0.85, 2.00]$.

- First term: convex, dominates when x is small
- Second term: concave, dominates when x is large

Minimum eigenvalues:

$$\min f'' = \begin{cases} \frac{156}{\overline{x}^{14}} - \frac{84}{\overline{x}^{8}} & \text{if} \quad \overline{x} \leq 1.21707 \\ -7.47810 & \text{if} \quad [\underline{x}, \overline{x}] \ni 1.21707 \\ \frac{156}{\underline{x}^{14}} - \frac{84}{\underline{x}^{8}} & \text{if} \quad \underline{x} \geq 1.21707 \end{cases}$$

Illustration: Lennard-Jones

Standard αBB underestimator:

$$f(x) - \frac{7.47810}{2}(\overline{x} - x)\cdot(x - \underline{x})$$

2 subinterval underestimator:

k	x^k	min f''	α^k	β^k	γ^k
0	0.850				
1	1.425	-7.47810	3.73905	1.62764	-1.38349
2	2.000	-3.84462	1.92231	-1.62764	3.25528

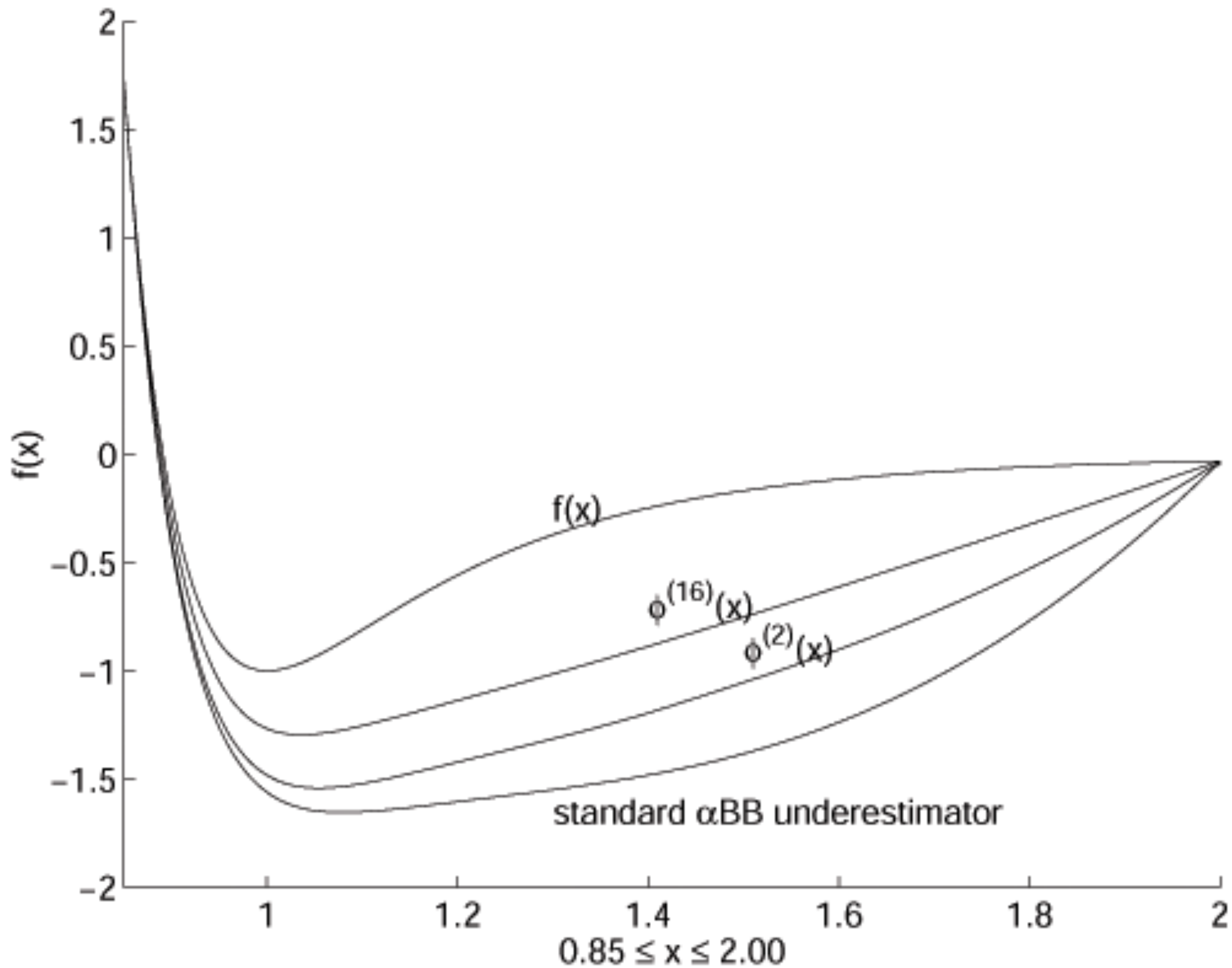
Underestimator when $0.850 \le x \le 1.425$:

$$f(x) - \left(3.73905(1.425 - x)\cdot(x - 0.850) + 1.62764x - 1.38349\right)$$

Underestimator when $1.425 \le x \le 2.00$:

$$f(x) - \left(1.92231(2.000 - x)\cdot(x - 1.425) - 1.62764x + 3.25528\right)$$

Illustration: Lennard-Jones



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Generalized αBB

Christodoulos A. Floudas

Princeton University

Requirements of Convex Underestimators for Nonconvex Functions

- Definition of a relaxation function $\Phi(x;\gamma)$ that is convex and negative for every $x \in X$.
- By adding $\Phi(x;\gamma)$ to the original nonconvex function $f(x)$ we obtain an underestimating function of $f(x)$, i.e.,

$$L(x;\gamma) = f(x) + \Phi(x;\gamma)$$
$$\Phi(x;\gamma) \le 0, \forall x \in X, \gamma \ge 0$$

- $L(x;\gamma)$ is an underestimator of $f(x)$.

Requirements of Convex Underestimators for Nonconvex Functions

- $L(x;\gamma)$ has to match $f(x)$ at the corner points of X, that is, $\Phi(x^c;\gamma)=0,$ where x^c is a corner point of X.
- Convexity of the underestimating function:

$$\boxed{H_L(x;\gamma)=H_f(x)+H_\Phi(x;\gamma)}$$

If the Hessian of the relaxation function, $H_\Phi(x;\gamma)$, is positive definite enough, then the Hessian of the underestimator, $H_L(x;\gamma)$, can be positive definite.

The New Relaxation Function

Akrotirianakis, Floudas, *JOGO*, 2004, 2005

$$\Phi(x;\gamma) = -\sum_{i=1}^{n} (1 - e^{\gamma_i (x_i - x_i^L)})(1 - e^{\gamma_i (x_i^U - x_i)})$$

Properties:

- $\Phi(x;\gamma)$ is a separable function
- $\Phi(x;\gamma) \leq 0$ for all $x \in X$ and $\gamma_i \geq 0, i = 1,\ldots n$
- $\Phi(x^c;\gamma) = 0$ for every corner point of X
- $H_\Phi(x;\gamma)$ is a diagonal and positive definite matrix
- $\Phi(x;\gamma)$ is a convex function
- $\Phi(x;\gamma)$ achieves its minimum at the middle point of X and its maximum at the corner points of X

The New Underestimating Function

$$L_1(x;\gamma) = f(x) - \sum_{i=1}^{n} (1 - e^{\gamma_i (x_i - x_i^L)})(1 - e^{\gamma_i (x_i^U - x_i)})$$

Properties:

- $L_1(x;\gamma)$ underestimates $f(x)$
- $L_1(x;\gamma)$ matches $f(x)$ at the corner points of X
- Underestimators constructed over a subset of a set are always tighter than the underestimator of the original set.

The New Underestimating Function

Properties (cont.):

- The maximum separation distance is achieved at the middle point of X:

$$\boxed{d_{\max} = \max_{x \in X} \{ f(x) - L_1(x;\gamma) \} = \sum_{i=1}^{n} (1 - e^{0.5\gamma(x_i^U - x_i^L)})^2}$$

- Existence Theorem: The positive semidefiniteness of $H_\Phi(x;\gamma)$ guarantees the existence of a vector γ, such that the Hessian of $L_1(x;\gamma)$ is positive semi-definite. Hence, $L_1(x;\gamma)$ is a convex underestimator.

Comparison of Underestimators

$$L_1(x;\gamma) = f(x) + \Phi(x;\gamma)$$
$$= \quad f(x) - \sum_{i=1}^{n} (1 - e^{\gamma_i (x_i - x_i^L)})(1 - e^{\gamma_i (x_i^U - x_i)})$$

$$L_{\alpha BB}(x;\gamma) = f(x) + \varphi(x;\gamma)$$
$$= \quad f(x) - \sum_{i=1}^{n} (x_i - x_i^L)(x_i^U - x_i)$$

- Lemma: $|\Phi(x;\gamma)| \le |\varphi(x;\alpha)|$, for some α and γ
- Tightness Theorem: The convex underestimator $L_1(x;\gamma)$ is tighter than the convex underestimator $L_{\alpha BB}(x;\alpha)$, that is,

$$\boxed{L_{\alpha BB}(x;\alpha) \le L_1(x;\gamma), \forall x \in X}$$

Maximum Separation Distance

Theorem 2: Let $\gamma^U = (\gamma_1^U, \ldots, \gamma_n^U)$ be the solution of the system of nonlinear equations

$$\boxed{\sigma_i + \gamma_i^2 + \gamma_i^2 e^{\gamma_i (x_i^U - x_i^L)} = 0, i = 1, \ldots, n}$$

Then the underestimator $L_{\alpha BB}(x; \alpha^U)$ with

$$\boxed{\alpha^L = \left(\frac{4(1 - e^{\gamma_1^L (x_1^U - x_1^L)})^2}{(x_1^U - x_1^L)^2}, \ldots, \frac{4(1 - e^{\gamma_n^L (x_n^U - x_n^L)})^2}{(x_n^U - x_n^L)^2}\right)}$$

has the same maximum separation distance as the underestimator $L_1(x; \gamma^U)$.

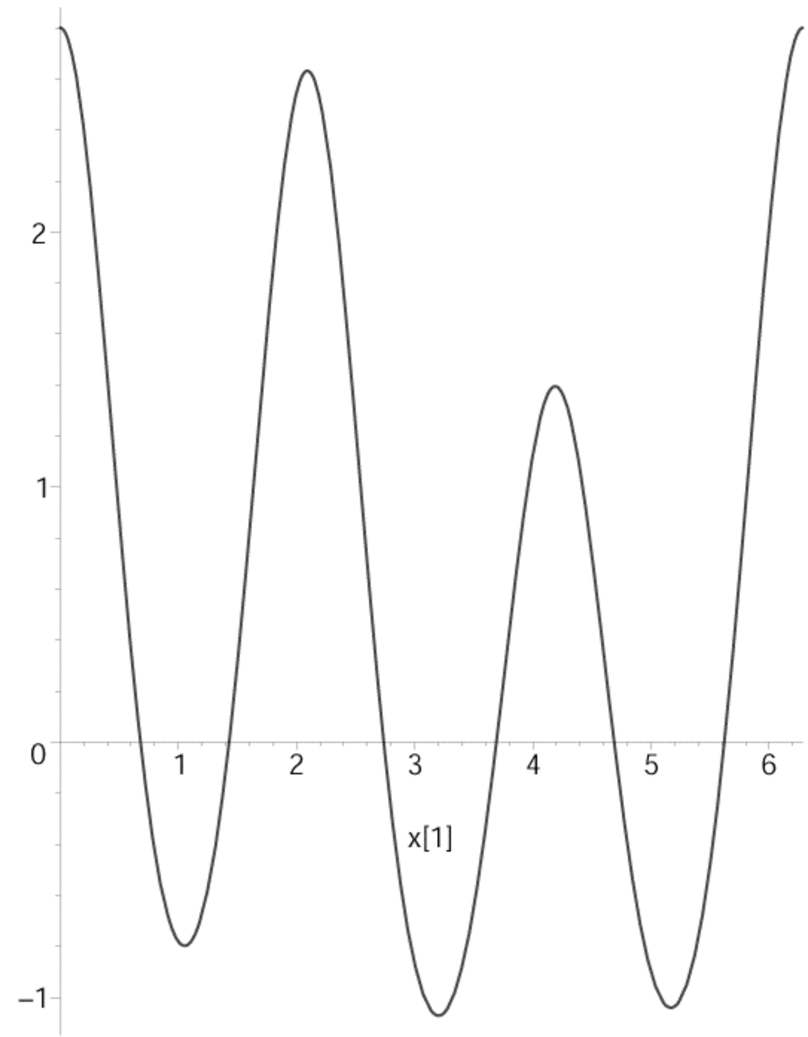
Maximum Separation Distance

Remarks:

- Every interval $[\gamma_i^L, \gamma_i^U]$ corresponds to another interval $[\alpha_i^L, \alpha_i^U]$.
- Every underestimator $L_1(x;\gamma)$ with $\gamma_i > \gamma_i^U, \forall i$ is looser than the underestimator $L_{\alpha BB}(x;\alpha^U)$.
- $L_{\alpha BB}(x;\alpha^L)$ and $L_1(x;\gamma^L)$ are tighter than $L_{\alpha BB}(x;\alpha^U)$ and $L_1(x;\gamma^U)$ respectively.
- Only the underestimator $L_{\alpha BB}(x;\alpha^U)$ is known to be convex *a priori*.

Illustrative Example

$$
\begin{aligned}
f(\phi) = {} & \frac{588600}{\left(3r^2 - 4\cos\theta\, r^2 - 2\left(\sin^2\theta\cos\left(\phi - \frac{2\pi}{3}\right) - \cos^2\theta\right) r^2\right)^6} \\
& - \frac{1079.1}{\left(3r^2 - 4\cos\theta\, r^2 - 2\left(\sin^2\theta\cos\left(\phi - \frac{2\pi}{3}\right) - \cos^2\theta\right) r^2\right)^3} \\
& + \frac{600800}{\left(3r^2 - 4\cos\theta\, r^2 - 2\left(\sin^2\theta\cos\phi - \cos^2\theta\right) r^2\right)^6} \\
& - \frac{1071.5}{\left(3r^2 - 4\cos\theta\, r^2 - 2\left(\sin^2\theta\cos\phi - \cos^2\theta\right) r^2\right)^3} \\
& + \frac{481300}{\left(3r^2 - 4\cos\theta\, r^2 - 2\left(\sin^2\theta\cos\left(\phi + \frac{2\pi}{3}\right) - \cos^2\theta\right) r^2\right)^6} \\
& - \frac{1064.6}{\left(3r^2 - 4\cos\theta\, r^2 - 2\left(\sin^2\theta\cos\left(\phi + \frac{2\pi}{3}\right) - \cos^2\theta\right) r^2\right)^3}
\end{aligned}
$$



Illustrative Example

- αBB value: α^U =77.12 (corresponding γ value is γ^U=1.07).
- GαBB value: γ^L=0.85 (corresponding α value is α^L=1.07).
- The method checks if there exist $\gamma \in [\gamma^L, \gamma^U]$ or $\alpha \in [\alpha^L, \alpha^U]$ such that $L_1(x;\gamma^U)$ or $L_{\alpha BB}(x;\alpha^L)$ are convex underestimators of $f(x)$ in X.
- After 21 partitions of the initial domain the algorithm concludes that $L_1(x;\gamma^U)$ is convex.

Illustrative Example

- The minimum obtained by the αBB is

$$\boxed{\min L_{\alpha BB}(x;\alpha^U) = -762.24}$$

- The minimum obtained by GαBB is

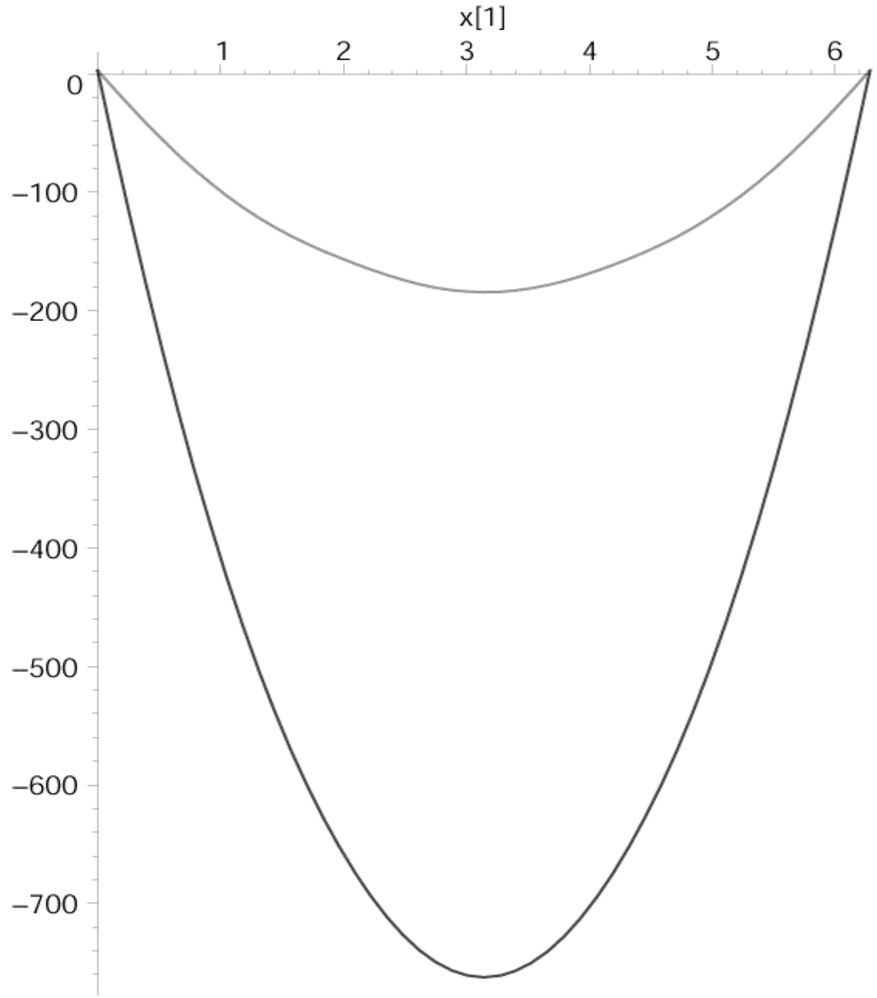
$$\boxed{\min L_1(x;\gamma^L) = -184.42}$$

- Improvement ratio:

$$\boxed{\frac{\min L_{\alpha BB}(x;\alpha^U)}{\min L_1(x;\gamma^L)} = 0.242}$$

Illustrative Example

- Comparison of $L_{\alpha BB}(x;\alpha^{L})$ and $L_1(x;\gamma^{U})$:



Outline

- Deterministic Global Optimization: Objectives & Motivation
- Convex Envelopes:
  - Trilinear Monomials
  - Univariate Monomials
  - Fractional Terms
  - Edge Concave functions
- Checking Convexity: Products of Univariate Functions
- Convex Underestimators for Trigonometric Functions
- PαBB: Piecewise Quadratic Perturbations
- GαBB: Generalized αBB
- **Functional Forms of Convex Underestimators**
- Augmented Lagrangian Approach for Global Optimization
- New Class of Convex Underestimators
- Pooling Problems & Generalized Pooling Problems
- Conclusions

Functional Forms of Convex Underestimators

(Floudas and Kreinovich, 2006, *Opt.Letters* 2008)

Given an optimization problem, we need to:

- Select appropriate technique/method to solve it, e.g., Gradient methods
  Usually depends on problem type and formulation
- Select appropriate values for adjustable parameters, e.g., Step size
  Usually select empirically – identify "optimal" values
- **Select appropriate auxiliary functions**,
  e.g., Convex underestimators
  Impractical to try all possible functions

QUESTION:

Is there an "optimal" auxiliary function to use ?

(SHORT) ANSWER:

YES, in many cases !

Functional Forms of Convex Underestimators

(Floudas and Kreinovich, 2006,2008)

αBB Convex Underestimator

(Maranas and Floudas, 1994; Androulakis et al., 1995; Adjiman et al., 1998a,b)

$$L(x) = f(x) - \Phi(x)$$

$$\Phi(x) = \sum_{i=1}^{n} \alpha_i \cdot (x_i - x_i^L) \cdot (x_i^U - x_i)$$

What if we perform a linear rescaling ? (i.e., change units in our model)

$$\left.\begin{array}{l} x_i \rightarrow g_i(x_i) = \lambda_i \cdot x_i \\ x_i \rightarrow h_i(x_i) = \mu_i \cdot x_i \end{array}\right\} \Rightarrow \Phi(x) = \sum_{i=1}^{n} \alpha_i \cdot \Big(g(x_i) - g(x_i^L)\Big) \cdot \Big(h(x_i^U) - h(x_i)\Big)$$

$$\Rightarrow \Phi(x) = \sum_{i=1}^{n} (\alpha_i \cdot \lambda_i \cdot \mu_i) \cdot (x_i - x_i^L) \cdot (x_i^U - x_i)$$

Functional Forms of Convex Underestimators

(Floudas and Kreinovich, 2006,2008)

What if we generalize to a non-linear rescaling ?

$$\left.\begin{array}{l} x_i \to g_i(x_i) = e^{+\gamma_i \cdot x_i} \\ x_i \to h_i(x_i) = e^{-\gamma_i \cdot x_i} \end{array}\right\} \Rightarrow \Phi(x) = \sum_{i=1}^{n} \alpha_i \cdot \left(g(x_i) - g(x_i^L)\right) \cdot \left(h(x_i^U) - h(x_i)\right)$$

$$\Rightarrow \Phi(x) = \sum_{i=1}^{n} (\alpha_i \cdot e^{\gamma_i \cdot (x_i^U - x_i^L)}) \cdot (1 - e^{\gamma_i \cdot (x_i - x_i^L)}) \cdot (1 - e^{\gamma_i \cdot (x_i^U - x_i)})$$

Generalized αBB Convex Underestimator

(Akrotirianakis and Floudas, *JOGO*, 2004a,b)

$$\boxed{\begin{array}{c} L(x) = f(x) - \Phi(x) \\ \Phi(x) = \sum_{i=1}^{n} (1 - e^{\gamma_i \cdot (x_i - x_i^L)}) \cdot (1 - e^{\gamma_i \cdot (x_i^U - x_i)}) \end{array}}$$

Functional Forms of Convex Underestimators

(Floudas and Kreinovich, 2006,2008)

- Why do linear and exponential functions perform well in αBB methods ?

- Are there better functional forms to do the job ?

"Optimal" has to be "Invariant"

- SHIFT

$$\left(g(x+s)-g(x^L+s)\right)\cdot\left(h(x^U+s)-h(x+s)\right)=\eta\cdot\left(g(x)-g(x^L)\right)\cdot\left(h(x^U)-h(x)\right)$$

- SIGN

$$\left(g(-x)-g(-x^U)\right)\cdot\left(h(-x^L)-h(-x)\right)=\eta\cdot\left(g(x)-g(x^L)\right)\cdot\left(h(x^U)-h(x)\right)$$

- SCALE

$$\lambda>0\quad\left(g(\lambda\cdot x)-g(\lambda\cdot x^L)\right)\cdot\left(h(\lambda\cdot x^U)-h(\lambda\cdot x)\right)=\eta\cdot\left(g(x)-g(x^L)\right)\cdot\left(h(x^U)-h(x)\right)$$

$$\lambda<0\quad\left(g(\lambda\cdot x)-g(\lambda\cdot x^U)\right)\cdot\left(h(\lambda\cdot x^L)-h(\lambda\cdot x)\right)=\eta\cdot\left(g(x)-g(x^L)\right)\cdot\left(h(x^U)-h(x)\right)$$

Functional Forms of Convex Underestimators

(Floudas and Kreinovich, 2006,2008)

Which pairs of functional forms exhibit "Invariance" ?

- SHIFT

$$g(x) = h(x) = A + k \cdot x$$

$$g(x) = h(x) = A + C \cdot e^{\gamma \cdot x}$$

- SIGN

$$h(x) = -g(-x)$$

- SCALE

$$g(x) = h(x) = A \cdot x^{\gamma}$$

$$g(x) = h(x) = A + k \cdot \ln(x)$$

- SHIFT + SIGN

$$g(x) = h(x) = x \longrightarrow \alpha\text{BB}$$

$$g(x) = e^{\gamma \cdot x}, h(x) = -e^{-\gamma \cdot x} \longrightarrow \text{g-}\alpha\text{BB}$$

Both convex underestimation schemes are "optimal" !

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Augmented Lagrangian Method with variable lower-level constraints

(Birgin, Floudas and Martinez, 2007)

$$\begin{aligned} &\min f(x) \\ s.t.\quad & h(x) = 0 \\ & g(x) \le 0 \\ & x \in \Omega \end{aligned}$$

(Ω is a set of "simple" constraints)

Define Augmented Lagrangian function:

$$L_\rho(x,\lambda,\mu) = f(x) + \frac{\rho}{2}\left\{\sum_{i=1}^{m}\left[h_i(x) + \frac{\lambda_i}{\rho}\right]^2 + \sum_{j=1}^{p}\left[\max\left(0, g_j(x) + \frac{\mu_j}{\rho}\right)\right]^2\right\}$$

Global optimization algorithm:

- At each outer Iteration, perform ε-global minimization of Augmented Lagrangian under "simple" constraints
- Solve subproblems using αBB method
- Proven convergence to an ε- global minimizer

Augmented Lagrangian Method with variable lower-level constraints

(Birgin, Floudas and Martinez, 2007)

ALGORITHM

Step 0: Let $\{\varepsilon_k\}$ be a sequence such that $\lim_{k\to\infty} \varepsilon_k = \varepsilon \geq 0$

Initialize $\lambda_{\min} < \lambda_{\max}$ $\mu_{\max} > 0$ $\gamma > 1$ $0 < \tau < 1$ $k = 1$

Select $\lambda_i^1 \in [\lambda_{\min}, \lambda_{\max}]$ $\mu_j^1 \in [0, \mu_{\max}]$ $\rho_1 > 0$

Augmented Lagrangian Method with variable lower-level constraints

(Birgin, Floudas and Martinez, 2007)

ALGORITHM

Step 1: Find an ε_k-global minimizer $x^k \in \Omega \cap P_k$ of $L_{\rho k}(x, \lambda^k, \mu^k)$; that is,

$$L_{\rho k}(x^k, \lambda^k, \mu^k) \leq L_{\rho k}(x, \lambda^k, \mu^k) + \varepsilon_k \quad \forall x \in \Omega \cap P_k$$

- **Use αBB global optimization method**

- P_k is an auxiliary constraint set that incorporates information obtain during the solution iterations (optional)

Augmented Lagrangian Method with variable lower-level constraints

(Birgin, Floudas and Martinez, 2007)

ALGORITHM

Step 2: Define: $$V_j^k = \max\left\{ g_j(x^k), -\frac{\mu_j^k}{\rho_k} \right\}$$

If $\max\left\{ \left\| h(x^k) \right\|_\infty, \left\| V^k \right\|_\infty \right\} \leq \tau \max\left\{ \left\| h(x^{k-1}) \right\|_\infty, \left\| V^{k-1} \right\|_\infty \right\}$ (or if $k = 1$)

$$\rho_{k+1} = \rho_k$$

else

$$\rho_{k+1} = \gamma \rho_k \quad \text{(increase } \rho \text{)}$$

Augmented Lagrangian Method with variable lower-level constraints

(Birgin, Floudas and Martinez, 2007)

ALGORITHM

Step 3: Compute: $$\lambda_i^{k+1} = \max\left\{\lambda_{\min}, \min\left\{\lambda_i^k + \rho h_i(x^k), \lambda_{\max}\right\}\right\}$$

$$\mu_j^{k+1} = \max\left\{0, \min\left\{\mu_j^k + \rho g_j(x^k), \mu_{\max}\right\}\right\}$$

Increment: $k = k + 1$

Augmented Lagrangian Method with variable lower-level constraints

(Birgin, Floudas and Martinez, 2007)

CONVERGENCE

Theorem 1: Point $x^* = \lim_{k \to \infty} x^k$ is feasible

Theorem 2: Point $x^* = \lim_{k \to \infty} x^k$ is an ε-global minimizer

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CONVERGENCE

Theorem 1: Point $x^* = \lim_{k\to\infty} x^k$ is feasible

Theorem 2: Point $x^* = \lim_{k\to\infty} x^k$ is an ε-global minimizer

EXAMPLE *(Haverly's Pooling Problem – 3 cases)*

$$\begin{aligned}
\min \quad & -9x_1 - 15x_2 + 6x_3 + c_1 x_4 + 10(x_5 + x_6) \\
s.t. \quad & x_7 x_8 + 2x_5 - 2.5x_1 \le 0 \\
& x_7 x_9 + 2x_6 - 1.5x_2 \le 0 \\
& 3x_3 + x_4 - x_7(x_8 + x_9) = 0 \\
& x_8 + x_9 - x_3 - x_4 = 0 \\
& x_1 - x_8 - x_5 = 0 \\
& x_2 - x_9 - x_6 = 0 \\
& (0,\ldots,0) \le x \le (c_2, 200, 500, \ldots, 500)
\end{aligned}$$

case	c1	c2
(a)	16	100
(b)	16	600
(c)	13	100

Augmented Lagrangian Method with variable lower-level constraints

(Birgin, Floudas and Martinez, 2007)

EXAMPLE *(Haverly's Pooling Problem – 3 cases)*

Problem Stats			
case	n	m	f(x*)
(a)	11	8(6)	-400
(b)	11	8(6)	-600
(c)	11	8(6)	-750

Augmented Lagrangian Method with variable lower-level constraints

(Birgin, Floudas and Martinez, 2007)

EXAMPLE *(Haverly's Pooling Problem – 3 cases)*

Problem Stats

case	n	m	f(x*)
(a)	11	8(6)	-400
(b)	11	8(6)	-600
(c)	11	8(6)	-750

Time

case	variable $\varepsilon_k=\max\{\varepsilon,10^{-k}\}$			
	$\varepsilon=10^{-1}$	$\varepsilon=10^{-2}$	$\varepsilon=10^{-3}$	$\varepsilon=10^{-4}$
(a)	0.09	0.11	0.13	0.13
(b)	0.64	0.70	0.73	0.76
(c)	0.07	0.09	0.17	0.16

Iterations

case	variable $\varepsilon_k=\max\{\varepsilon,10^{-k}\}$			
	$\varepsilon=10^{-1}$	$\varepsilon=10^{-2}$	$\varepsilon=10^{-3}$	$\varepsilon=10^{-4}$
(a)	8	8	8	8
(b)	13	13	13	13
(c)	8	8	8	8

 # Nodes

case	variable $\varepsilon_k=\max\{\varepsilon,10^{-k}\}$			
	$\varepsilon=10^{-1}$	$\varepsilon=10^{-2}$	$\varepsilon=10^{-3}$	$\varepsilon=10^{-4}$
(a)	78	88	100	104
(b)	563	613	651	671
(c)	60	72	84	88