Global and multi-local optimization in the semi-infinite programming context

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Outline

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1. Notation and motivation for global optimization
2. A motivating example
3. The particle swarm algorithm
4. Modification of PSOA for multi-local optimization
5. Numerical results in semi-infinite programming
6. Conclusions and future work

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General formulation - Nonlinear semi-infinite programming

Problem

$$\begin{aligned} \min_{x \in R^n} \ & f(x) \\ s.t. \ & g(x,t) \leq 0 \\ & \forall t \in T \end{aligned} \qquad \text{(NLSIP)}$$

- $f(x)$ is the objective function
- $g(x,t)$ is the *infinite* constraint function
- $T \subset R^p$ is, usually, a cartesian product of intervals ($[\alpha_1, \beta_1] \times [\alpha_2, \beta_2] \times \ldots \times [\alpha_p, \beta_p]$)

Note

A more general problem could be defined, but the extension is straightforward.

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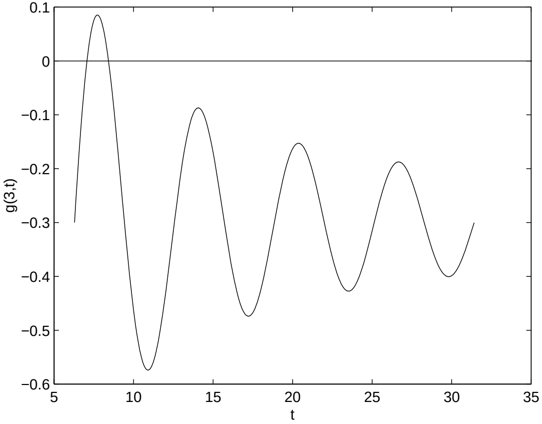
An very simple academic example ($n = 1$ and $p = 1$)

Example

$$\min_{x \in R} \quad x^2, \quad s.t. \ \frac{x}{t}\sin(t) - \frac{x}{10} \leq 0, \quad \forall t \in [2\pi, 10\pi]$$



$$g(3,t) = \tfrac{3}{t}\sin(t) - \tfrac{3}{10}$$

Feasibility

Is $\bar{x} = 3$ feasible?

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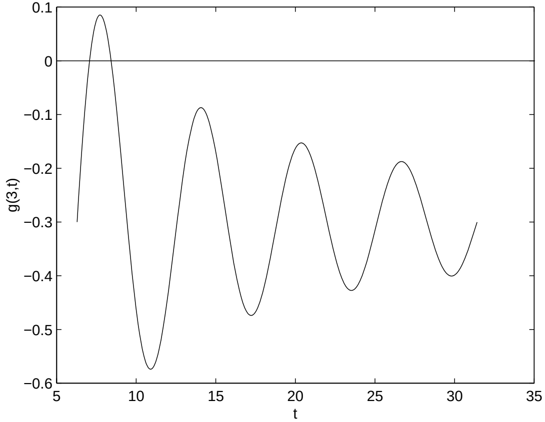

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Feasibility

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Definition of stationary point

Let $x^* \in R^n$ be a point such that

$$g(x^*, t) \leq 0, \ \forall t \in T,$$

and there exists $t^1, t^2, \ldots, t^{m^*}$ $(\in T)$ and non negative numbers $\lambda_*^0, \lambda_*^1, \lambda_*^2, ..., \lambda_*^{m^*}$ such that

$$\lambda_*^0 \nabla_x f(x^*) + \sum_{i=1}^{m^*} \lambda_*^i \nabla_x g(x^*, t^i) = 0.$$

with

$$g(x^*, t^i) = 0, \ \ i = 1, ..., m^*.$$

Then x^* is a stationary point for the (NLSIP).

Where global (multi-local) optimization plays a role?

The t^i, $i = 1, \ldots, m^*$, points are global solutions of the problem

Multi-local problem (also called lower level problem)

$$\max_{t \in T} g(x^*, t)$$

- The simple check for feasibility requests the computation of the global solutions for the lower level problem (not complectly true).
- In order to obtain global convergence for some methods the computation of all the global and local solutions for the lower level problem is necessary.

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Motivation

- A great number of valuable products are produced using fermentation processes and thus optimizing such processes is of great economic importance.
- Fermentation modeling process involves, in general, highly nonlinear and complex differential equations.
- Often optimizing these processes results in control optimization problems for which an analytical solution is not possible.

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The control problem

- The optimal control problem is described by a set of differential equations $\dot{\chi} = h(\chi, u, t),\ \ \chi(t^0) = \chi^0,\ \ t^0 \le t \le t^f$, where χ represent the state variables and u the control variables.
- The performance index J can be generally stated as

$$J(t^f) = \varphi(\chi(t^f), t^f) + \int_{t^0}^{t^f} \phi(\chi, u, t)dt,$$

where φ is the performance index of the state variables at final time t^f and ϕ is the integrated performance index during the operation.

- Additional constraints that often reflet some physical limitation of the system can be imposed.

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The general maximization problem (P) can be posed as

problem (P)

$$\max \quad J(t^f) \tag{1}$$
$$s.t. \quad \dot{\chi} = h(\chi, u, t) \tag{2}$$
$$\underline{\chi} \leq \chi(t) \leq \overline{\chi}, \tag{3}$$
$$\underline{u} \leq u(t) \leq \overline{u}, \tag{4}$$
$$\forall t \in [t^0, t^f] \tag{5}$$

Where the state constraints (3) and control constraints (4) are to be understood as componentwise inequalities.

How we addressed problem (P)?

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Approaches - Fed trajectory $u(t)$ approximated by a Linear spline $w(t)$.

- Penalty function for state constraints
- The multi-local (getting all local optima) problem is easy to solve

Objective function

$$\hat{J}(t^f) = \begin{cases} J(t^f) & \text{if } \underline{\chi} \leq \chi(t) \leq \overline{\chi}, \\ & \forall t \in [t^0, t^f] \\ -\infty & \text{otherwise} \end{cases}$$

State constraints

$$\underline{u} \leq w(t^i) \leq \overline{u}, \quad i = 1, \dots, n$$

Where t^i are the spline knots.

The maximization NLP problem is

$$\max_{w(t^i)} \hat{J}(t^f), \quad s.t. \ \underline{u} \leq w(t^i) \leq \overline{u}, \quad i = 1, \dots, n$$

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Implementation details

- The AMPL modeling language:
  - was used to model five optimal control problems
  - dynamic external library facility was used to solve the ordinary differentiable equations

AMPL - A Modeling Programming Language
www.ampl.com

- The ordinary differentiable equations were solved using the CVODE software package.

http://www.llnl.gov/casc/sundials/

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The problems set

- We obtained numerical results for five case studies.
- Problem
  - `penicillin` refers to a problem of fed-batch fermentation process where the optimal feed trajectory is to be computed while the penicillin production is to be maximized.
  - `ethanol` refers to a similar optimal control problem where the ethanol production is to be maximized.
  - `chemotherapy` is the only optimal control problem that does not refers to a fed-batch fermentation processe. It is a problem of drug administration in chemotherapy. The optimal trajectory to be computed is the quantity of drug that must be present in order to achieve a specified tumor reduction.
  - `hprotein` optimal control problem is to compute a unique trajectory (substrate to be fed) problem `cprotein` includes also a trajectory for an inducer. Both problems refer to a maximization for protein production.

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Characteristics and parameters

- The time displacement (h_i) are fixed while the optimal trajectory values are to be approximated.
- Particle swarm is a population based optimization algorithm and a population size of 60 was used with a maximum of 1000 iterations.
- Since a stochastic algorithm was used we performed 10 runs of the solver and the best solution is reported.

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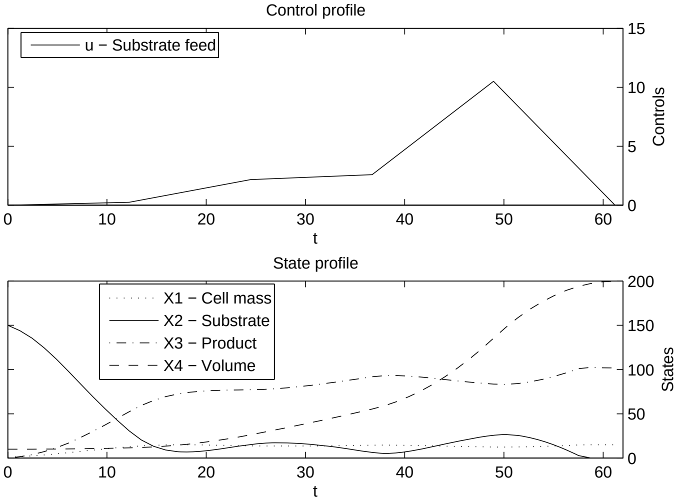
Numerical results

Problema	NT	n	t^f	Cubic $J(t^f)$	Linear $J(t^f)$	Literature $J(t^f)$
penicillin	1	5	132.00	87.70	88.29	87.99
ethanol	1	5	61.20	20550.70	20379.50	20839.00
chemotherapy	1	4	84.00	15.75	16.83	14.48
hprotein	1	5	15.00	38.86	32.73	32.40
rprotein	2	5	10.00	0.13	0.12	0.16

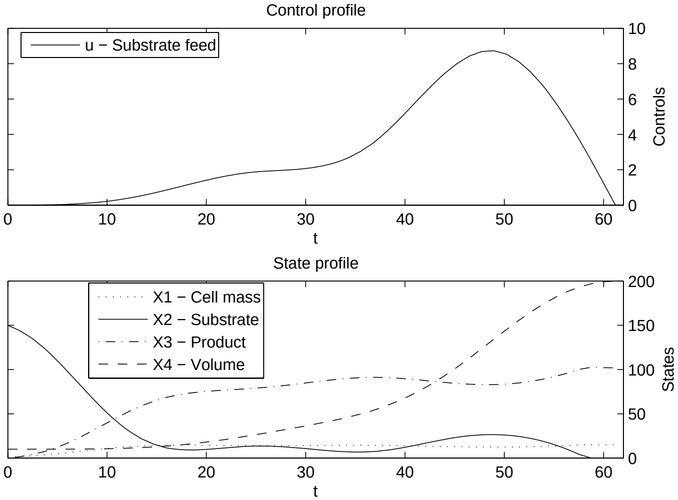
$$J(t^f) = \hat{J}(t^f) = \bar{J}(t^f), \quad \text{for all feasible points - splines}$$

Similar results between approaches. A new solution for the ethanol case.

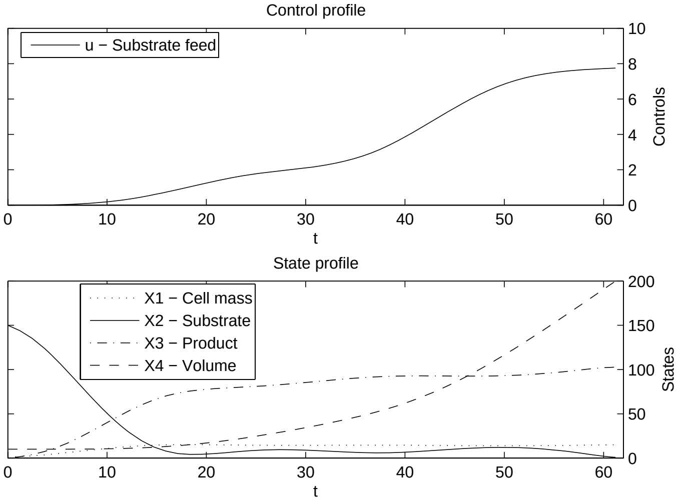
Plots - Linear spline approximation - ethanol case



Plots - Cubic spline approximation - Similar result



Plots - Cubic spline approximation - Best result



Some intermediate conclusions and future work

- Conclusions
  - Viability of the cubic spline approach on fed-batch optimal control.
  - Shown numerical results with particle swarm
  - Similar numerical results with the two approaches
- Future work
  - Numerical experiments with the *E. coli* bacteria
  - Laboratory confirmation of the obtained results (a lab bioreactor will be available)
  - Laboratory confirmation of the two approaches and we expect the cubic approach to obtain a lower gap between simulated and real performance.

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  - Shown numerical results with particle swarm
  - Similar numerical results with the two approaches
- Future work
  - Numerical experiments with the *E. coli* bacteria
  - Laboratory confirmation of the obtained results (a lab bioreactor will be available)
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Outline

We intended to solve the following global optimization problem with a particle swarm algorithm.

Global optimization problem

$$\max_{t \in T} \bar{g}(t) \equiv g(\bar{x}, t)$$

with $T \in R^p$.

The Particle Swarm Paradigm (PSP)

The PSP is a population (swarm) based algorithm that mimics the social behavior of a set of individuals (particles).

An individual behavior is a combination of its past experience (cognition influence) and the society experience (social influence).

In the optimization context a particle $\wp$, at time instant k, is represented by its current position ($t^{\wp}(k)$), its best ever position ($y^{\wp}(k)$) and its traveling velocity ($v^{\wp}(k)$).

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The new travel position and velocity

The new particle position is updated by

Update position

$$t^{\wp}(k+1) = t^{\wp}(k) + v^{\wp}(k+1),$$

where $v^{\wp}(k+1)$ is the new velocity given by

Update velocity

$$v_j^{\wp}(k+1) = \iota(k) v_j^{\wp}(k) + \mu\omega_{1j}(k)\left(y_j^{\wp}(k) - t_j^{\wp}(k)\right) + \nu\omega_{2j}(k)\left(\hat{y}_j(k) - t_j^{\wp}(k)\right),$$

for $j = 1, \ldots, p$.

- $\iota(k)$ is a weighting factor (inertial)
- μ is the cognition parameter and ν is the social parameter
- $\omega_{1j}(k)$ and $\omega_{2j}(k)$ are random numbers drawn from the uniform $(0,1)$ distribution

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The best ever particle

$\hat{y}(k)$ is a particle position with global best function value so far, *i.e.*,

Best position

$$\hat{y}(k) \in \arg\min_{a \in \mathcal{A}} \bar{g}(a)$$
$$\mathcal{A} = \left\{ y^1(k), \ldots, y^s(k) \right\} .$$

where s is the number of particles in the swarm.

Note

In an algorithmic point of view we just have to keep track of the particle with the best ever function value.

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Features

Population based algorithm.

- Good
  - Easy to implement.
  - Easy to parallelize.
  - Easy to handle discrete variables.
  - Only uses objective function evaluations.
- Not so good
  - Slow rate of convergence near an optimum.
  - Quite large number of function evaluations.
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- With a proper selection of the algorithm parameters finite termination of the algorithm can be established, in a probabilistic sense.
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Multi-local revisited

Given $\bar{x}$ the multi-local optimization problem is defined as

Multi-local optimization problem

$$\max_{t \in T} g(\bar{x}, t) \equiv \bar{g}(t)$$

with $T \in R^n$.

The multi-local concept

All the global and local optima are to be computed.

Some characteristics

These problems are mostly differentiable and the objective function computation is costless.

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PSP with the steepest ascent direction

The new particle position update equation is kept while the new velocity equation is given by

Steepest ascent velocity

$$v_j^{\wp}(k+1) = \iota(k) v_j^{\wp}(k) + \mu\omega_{1j}(k)\left(y_j^{\wp}(k) - t_j^{\wp}(k)\right) + \nu\omega_{2j}(t)\left(\nabla_j \bar{g}(y_j^{\wp}(k))\right),$$

for $j = 1, \ldots, p$, where $\nabla \bar{g}(t)$ is the gradient of the objective function.

Each particle uses the steepest ascent direction computed at each particle best position ($y^{\wp}(k)$).

The inclusion of the steepest ascent direction in the velocity equation aims to drive each particle to a neighbor local maximum and since we have a population of particles, each one will be driven to a local maximum.

PSP with an ascent direction

Other approach is to use

Ascent velocity formula

$$w^{\wp} = \frac{1}{\sum_{j=1}^{m} |\bar{g}(z_j^{\wp}) - \bar{g}(y^{\wp})|} \sum_{j=1}^{m} (\bar{g}(z_j^{\wp}) - \bar{g}(y^{\wp})) \frac{(z_j^{\wp} - y^{\wp})}{\|z_j^{\wp} - y^{\wp}\|}$$

as an ascent direction at $y^{\wp}$, in the velocity equation, to overcome the need to compute the gradient.

Where

- $y^{\wp}$ is the best position of particle $\wp$
- $\{z_j^{\wp}\}_{j=1}^{m}$ is a set of m (random) points close to y^p,

Under certain conditions $w^{\wp}$ simulates the steepest ascent direction.

Stopping criterion

We propose the stopping criterion

Minimum velocity attained

$$\max_{\wp}[v^{\wp}(k)]_{opt} \leq \epsilon_{\wp}$$

where

Constrained velocity

$$[v^{\wp}(k)]_{opt} = \left(\sum_{j=1}^{p} \begin{cases} 0 & \text{if } t_j^{\wp}(k) = \beta_j \text{ and } v_j^{\wp}(k) \geq 0 \\ 0 & \text{if } t_j^{\wp}(k) = \alpha_j \text{ and } v_j^{\wp}(k) \leq 0 \\ \left(v_j^{\wp}(k)\right)^2 & \text{otherwise} \end{cases} \right)^{1/2}$$

The stopping criterion is based on the optimality conditions for the multi-local optimization problem.

Environment

- We have coined the solver as MLOCPSOA (Multi-Local Optimization Particle Swarm Algorithm)
- Implemented in the C programming language
- Interfaced with AMPL (`www.ampl.com`)

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Test problems set

	Problems	p	N_{t^*}	$\bar{g}^*$
1	b2	2	1	0.000E+00
2	bohachevsky	2	1	0.000E+00
3	branin	2	3	3.979E-01
4	dejoung	3	1	0.000E+00
5	easom	2	1	-1.000E+00
6	f1	30	1	-1.257E+04
7	goldprice	2	1	3.000E+00
8	griewank	6	1	0.000E+00
9	hartmann3	3	1	-3.863E+00
10	hartmann6	6	1	-3.322E+00
11	hump	2	2	0.000E+00
12	hump_camel	2	2	-1.032E+00
13	levy3	2	18	-1.765E+02
14	parsopoulos	2	12	0.000E+00
15	rosenbrock10	10	1	0.000E+00
16	rosenbrock2	2	1	0.000E+00

Test problems

	Problems	p	N_{t^*}	$\bar{g}^*$
17	rosenbrock5	5	1	0.000E+00
18	shekel10	4	1	-1.054E+01
19	shekel5	4	1	-1.015E+01
20	shekel7	4	1	-1.040E+01
21	shubert	2	18	-1.867E+02
22	storn1	2	2	-4.075E-01
23	storn2	2	2	-1.806E+01
24	storn3	2	2	-2.278E+02
25	storn4	2	2	-2.429E+03
26	storn5	2	2	-2.478E+04
27	storn6	2	2	-2.493E+05
28	zakharov10	10	1	0.000E+00
29	zakharov2	2	1	0.000E+00
30	zakharov20	20	1	0.000E+00
31	zakharov4	4	1	0.000E+00
32	zakharov5	5	1	0.000E+00

Parameters

- For each problem, the optimizer was run 5 times with different initial particle positions and velocities (randomly chosen from the search domain)
- The algorithm terminates if the stopping criterion is met with $\epsilon_p = 0.01$ or the number of iterations exceeds $K^{max} = 100000$
- Coefficients μ and ν were both set to 1.2
- The inertial parameter $\iota(t)$ was linearly scaled from 0.7 to 0.2 over a maximum of K^{max} iterations
- The swarm size is given by $\min(6^p, 100)$, where p is the problem dimension.

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Numerical results

	Gradient version					Approximate descent direction version			
	F.O.	N_{afe}	N_{age}	g_a^*	g_{best}	F.O.	N_{afe}	g_a^*	g_{best}
1	100	3444343	873	0,000E+00	0,000E+00	100	3602386	0,000E+00	0,000E+00
2	100	2782058	545	0,000E+00	0,000E+00	100	3600983	0,000E+00	0,000E+00
3	100	1740823	1397	3,979E-01	3,979E-01	100	3601171	3,979E-01	3,979E-01
4	100	1647820	4420	2,618E-23	0,000E+00	100	10003223	0,000E+00	0,000E+00
5	100	283500	70615	-1,000E+00	-1,000E+00	100	3601354	-1,000E+00	-1,000E+00
6	Not differentiable					100	10104250	-1,448E+04	-1,468E+04
7	20	3600000	59	2,431E+01	4,583E+00	100	3600967	3,000E+00	3,000E+00
8	20	10000000	7754	1,084E-02	0,000E+00	0	10004487	2,257E-02	1,503E-02
9	100	10000000	483	-3,850E+00	-3,861E+00	100	10002098	-3,862E+00	-3,863E+00
10	40	10000000	525	-2,937E+00	-3,185E+00	100	10002652	-3,202E+00	-3,242E+00
11	100	963259	1082	-1,032E+00	-1,032E+00	100	3600946	-1,032E+00	-1,032E+00
12	100	1171181	1329	4,651E-08	4,651E-08	100	3601098	2,362E-06	6,756E-07
13	0	3600000	439	-1,276E+02	-1,592E+02	49	3601052	-1,765E+02	-1,765E+02
14	85	2952979	2295	4,922E-23	3,749E-33	75	3600819	2,607E-07	9,685E-08
15	0	10000000	154	8,051E+04	3,387E+04	0	10009292	8,726E+00	7,386E+00
16	0	3600000	91	3,046E+00	1,190E+00	100	3601268	1,437E-06	5,698E-07

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18	100	10000000	1850	-9,160E+00	-1,026E+01	100	10004066	-1,052E+01	-1,052E+01
19	100	10000000	2126	-7,801E+00	-8,760E+00	100	10003906	-1,012E+01	-1,014E+01
20	100	10000000	1909	-9,401E+00	-9,997E+00	100	10004069	-1,037E+01	-1,039E+01
21	0	3600000	335	-1,024E+02	-1,648E+02	60	3600999	-1,867E+02	-1,867E+02
22	100	1366222	973	-4,075E-01	-4,075E-01	100	3600804	-4,075E-01	-4,075E-01
23	100	3600000	570	-1,806E+01	-1,806E+01	100	3600902	-1,806E+01	-1,806E+01
24	100	3600000	194	-2,278E+02	-2,278E+02	100	3601003	-2,278E+02	-2,278E+02
25	100	3600000	167	-2,429E+03	-2,429E+03	100	3601160	-2,429E+03	-2,429E+03
26	90	3600000	81	-2,477E+04	-2,478E+04	100	3601278	-2,478E+04	-2,478E+04
27	10	3600000	58	1,607E+05	-2,436E+05	100	3601418	-2,493E+05	-2,493E+05
28	0	10000000	141	4,470E+02	3,102E+01	60	10009759	3,977E-02	2,506E-02
29	0	10000000	135	1,289E+05	7,935E+02	0	10016905	3,633E-01	2,404E-01
30	100	1433664	16314	8,325E-112	0,000E+00	100	3601264	4,987E-07	4,464E-08
31	100	10000000	313	1,997E-13	2,780E-21	100	10005221	2,231E-04	6,612E-05
32	40	10000000	160	8,338E+00	3,031E-04	100	10006065	2,005E-03	1,186E-03

Outline

The test set

- The test problems were obtained from SIP where $\bar{x}$ was replaced by x^*, where x^* is the SIP solution included in the SIPAMPL database. SIPAMPL stands for SIP with AMPL and is a software package that provides, among other features, a database of SIP coded problems.
- All SIP problems considered have only one infinite constraint.

SIP problem	Test problem	p	Obs
watson2	sip_wat2	1	Unidimensional
vaz3	sip_vaz3	2	Air pollution abatement
priceS6	sip_S6	6	Higher dimension in SIPAMPL
priceU	sip_U	6	Higher dimension in SIPAMPL
random	sip_rand	6	Random generated with known solution

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`random`	`sip_rand`	6	Random generated with known solution

Numerical results

- A population of 40 particles and a maximum of 2000 iterations was used, with the steepest ascent direction version.
- sip_wat2 a global and a local maxima were found. 10 particles converged to the local maxima $t = 1$ with $\bar{g}(1) = -0.058594$ and the remaining 30 to the global one ($t = 0$) with $\bar{g}(0) = -2.5156e - 08$
- In sip_vaz3 the objective function is flat (equal to zero) in a region.

t	$\bar{g}(t)$	$npar$
$(-0.783012, 2.172526)$	0.000000	1
$(-0.112199, -0.686259)$	0.000000	1
$(-0.278460, 0.095245)$	0.000000	1
$(-0.446057, 1.157275)$	0.000000	1
$(0.443709, 3.811052)$	0.000000	1
$(3.684002, -0.629689)$	0.500007	22
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Numerical results

- A population of 40 particles and a maximum of 2000 iterations was used, with the steepest ascent direction version.
- `sip_wat2` a global and a local maxima were found. 10 particles converged to the local maxima $t = 1$ with $\bar{g}(1) = -0.058594$ and the remaining 30 to the global one ($t = 0$) with $\bar{g}(0) = -2.5156e - 08$
- In `sip_vaz3` the objective function is flat (equal to zero) in a region.

t	$\bar{g}(t)$	$npar$
$(-0.783012, 2.172526)$	0.000000	1
$(-0.112199, -0.686259)$	0.000000	1
$(-0.278460, 0.095245)$	0.000000	1
$(-0.446057, 1.157275)$	0.000000	1
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Numerical results

- sip_S6 a reported global maximizer and two local with objective function values of 0.027092, -3.69008 and -1.95425 respectively.

t	$\bar{g}(t)$
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$(1.622134, 1.687810, 2.000000, 0.085439, 2.000000, 0.350174)$	0.024811
...	
$(1.634326, 1.671065, 2.000000, 0.054348, 2.000000, 2.000000)$	-1.954538
...	

- sip_U reported two global maximizers and eleven local maximizers

t	$\bar{g}(t)$	$npar$
(-0.665555,-1.000000,1.00,1.00,1.00,1.00)	-0.002587	1
(-0.689138,-0.933410,1.00,1.00,1.00,1.00)	-0.003319	1
(-0.890160,-1.000000,1.00,1.00,1.00,1.00)	-0.000225	1
(-0.894640,-1.000000,1.00,1.00,1.00,1.00)	-0.000103	1
(-0.897369,-1.000000,1.00,1.00,1.000,1.00)	-0.000648	1
(1.000000,1.000000,1.00,1.00,1.00,1.00)	0.239638e-07	35

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Numerical results

- `sip_rand` are known to be any combination of $x_1 = 0.204475, 0.613425$, $x_2 = 0.286248, 0.858745$, $x_3 = 0.358527$, $x_4 = 0.420428$, $x_5 = 0.112190, 0.336571, 0.560951, 0.785332$ and $x_6 = 1$. When $x_i = 1$, $i = 1, \ldots, 5$ we may be in the presence of a local maximizer.

x	$f(x)$
(1.000000,0.844527,1.000000,0.439280,1.000000,1.000000)	0.099529
(0.605034,0.875442,0.322422,0.464760,1.000000,0.882592)	0.103833
(1.000000,0.290493,0.358070,0.391673,1.000000,1.000000)	0.111176
(1.000000,0.282674,1.000000,0.423782,1.000000,1.000000)	0.100581
(1.000000,0.831978,0.303846,0.384511,1.000000,0.946638)	0.100823
(1.000000,0.832307,0.374898,0.431689,1.000000,1.000000)	0.109419
(1.000000,0.301931,1.000000,0.430023,1.000000,1.000000)	0.099764
(0.213111,0.299029,0.366111,1.000000,1.000000,0.997780)	0.035990
(1.000000,0.882755,0.336751,0.459651,1.000000,1.000000)	0.107248
(1.000000,0.861285,0.380012,0.383345,1.000000,0.977121)	0.108998
(1.000000,0.306139,0.325222,0.398052,1.000000,1.000000)	0.108086
...	

Outline

Conclusions and future work

- We have presented a new multi-local optimization algorithm that evaluates multiple optimal solutions for multi-modal optimization problems
- The MLOCPSO algorithm adapts the unimodal particle swarm optimizer using ascent directions information to maintain diversity and to drive the particles to neighbor local maxima
- Ascent directions are obtained through the gradient vector or an heuristic method to produce an approximate ascent direction.
- Experimental results indicate that the proposed algorithm is able to evaluate multiple optimal solutions with reasonable success rates.
- The use of a properly scaled gradient vector and the optimizer performance analysis on high-dimensional problems are issues under investigation.

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THE END

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