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E-man Part 3[#]: Tutorial on gravitational algorithm in Structure activity relationships (SXR)

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(Dedicated with reverence to Prof (Dr.) Antonio Braibanti, Section of Applied Physical Chemistry, Pharmaceutical Department, University of Parma, Italy, on his eighty fifth-birth anniversary)

ABSTRACT

The challenges for the twenty-first century chemist are nano-, molecular- level processes in biology, interfaces of environment and industry. The on-line acquisition of terabytes of multi-dimensional data from hyphenated instruments, knowledge extraction and intelligent planning require interdisciplinary tools. The current research-tutorial on application of gravitational algorithm, Nature's algorithms mimics Evolution (Name), in rational drug design throws light on prospects of multi-disciplinary tools in chemical science. The applications of gravitational algorithm in chemical industry and engineering and recent advances along with its hybridization with PSO, etc. are briefed. The mapping of nature's way into mathematical space and futuristic focus in core methodology are covered. The indispensable rationalization of experiential and computational output with the state-of-the-art optimization and feature selection algorithms is illustrated with QSAR dataset. The tools used are computational quantum chemistry for optimization of 3D-geometry of molecules, molecular descriptors as explanatory feature variables, neural networks in data driven QSAR, gravitational algorithm in selecting optimum number of features from a pool of more than one thousand topological, electrostatic, quantum-chemical, WHIM descriptors of 2D- and 3D- category.

Keywords: Gravitational algorithm, Research-tutorial, E-man, Neural network, QSAR, Feature selection, Name, Chemicalindustry, Hybrid-Gravalg.

[#]Part 2: Journal of Applicable Chemistry, 2012, 1 (1), 109-124

INTRODUCTION

One of the most complex systems ever known to a human being of any intellectual order is his brain. It is a hard nut to break. The goal of probing into natural phenomena, mimicking and synthesis of prototypes requires the investigation/understanding/ integration/feeling of processes at a single cell, molecule and/or atom level. But, the deeper understanding and the march towards artificial brain (rat to a common man and finally Einstein) on a chip/computer will be a light house for navigators in the ocean of knowledge or a (bat) radar to reach destination/destiny of intelligence through intermediate ports/ground truth. The thrust area of this century if not decade is to plan the synthesis of brain, molecule by molecule for future

research. The inner urge is not to show off the alternate creation of the nature or mimicking biological brain on a computer. It is to understand brain on a computer as completely as possible based on yester years mature paradigms. This mega mile stone event paves way to control/eradicate dreaded psychological aberrations and probe into the mind and consciousness states. Measurement is a scale representation of perception quantitatively. Direct observation with human senses and/or using the state-of-the-art-instruments, number crunching, non-numeric/concept computations, information tools, knowledge extraction and intelligence-sparkles are all only tiny steps to understand the micro (nano-) processes in presence of several disturbances.

The sparkles of science are perennial; physics, chemistry and biology are beacons with a focus to understand, rectify, control and mimic macroscopic and microscopic nature (Chart 1). Now, nanomaterials, a single molecule and a cell posed multifaceted challenges for experiments, theory, simulation and computations. The unique intelligent targeted experiments posed a cut throat competition to the yesteryears' unquestionable theoretical foundations of physical sciences. The experimental proof of existence of boson is a consequence of theoretical and experimental approaches with a blend of high end instruments.

Chart 1: OOP representation of physics in nature and corresponding E-man modules

```
Physics_in_nature   : [  Gravity , Charge , Music, River course]

Eman_gravity        : [  Gravitational]

Eman_ charge        : [  Charged system]

Eman_ riverCourse   : [  Water drop,
                         Intelligent water drop]

Eman_music_         : [  Harmony
                         Cuckoo]
```

Gravitation (law of physics) in nature

Newton's law of universal gravitation points out that every point mass (Fig. 1) in the universe attracts every other point mass with a force directly proportional to the product of their masses and inversely proportional to the square of the distance between them (Table 1). Further, spherical objects with symmetrical masses attract as if all their mass were concentrated at their centers. Due to gravitational attraction, objects move globally towards the heavier ones. The generalized gravitational constant (G), elementary charge etc. are physical quantities and are universal in nature. For example, the gravitational force between an electron and proton (imagine) at a distance of one meter is approximately 10^{-67} newtons (SI unit of force needed to accelerate 1 kilogram of mass at the rate of one meter per square of a second : $kg.m/s^2$) while the electromagnetic force between the same two particles is approximately 10^{-28} newtons.

Table 1: Gravitational law of Newton

For point masses

$$Force(m_i, m_j) = \frac{m_i * m_j}{x_i - x_j}^2 * G$$

If mass m_i is moving under acceleration (acc)

$$Then \quad Force(m_i, acc) = m_i * \left\{ \frac{m_j}{x_i - x_j}^2 * G \right\} = m_i * \text{acc}$$

If mass m_i falls under acceleration due to gravity of earth

$$Then \quad Force(m_i, g) = m_i * \left\{ \frac{m_{earth}}{(x_i - x_{earth})}^2 * G \right\} = m_i * g$$

$$g = \left\{ \frac{m_{earth}}{radius_{earth}}^2 * G \right\}$$

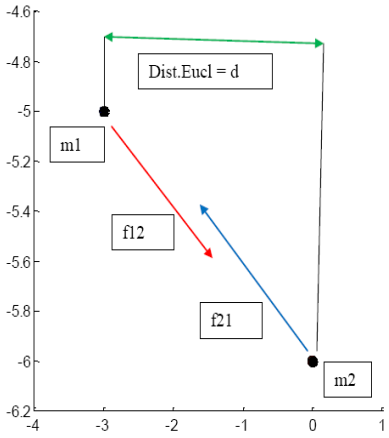
$$= \left\{ \frac{5.97219\, x10^{24}\ \text{kg}}{6.371\, x\ 10^6\, m}^2 * 6.67384\, x10^{-11} m^3 kg^{-1} \sec^{-2} \right\}$$

$$= 9.8196\, \text{m}\sec^{-2}$$

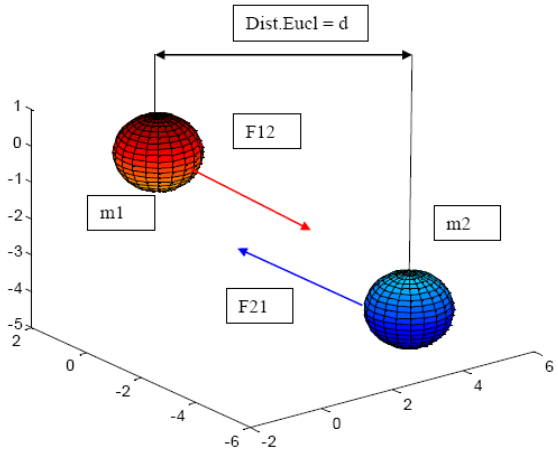
The ratio of electromagnetic force to gravitational pull (10^{39}) is incidentally equal akin to how heavier the planet Sun is to a microgram quantity.

$$\left\{ \frac{mass_{Sun}}{microgram} \right\} = \left[\frac{1.98855 \pm \ 0.00025 \ \times 10^{30}\ kg}{10^{-6}\ \times\ 10^{-3}\ kg} \right] = 1.9\ \times\ 10^{39}$$

But, both these forces are weaker when compared to even weakest of weaker chemical interactions.

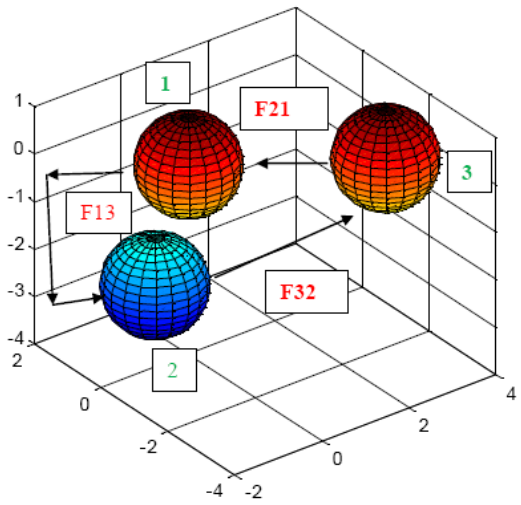


(a) Point masses Nsol = 2

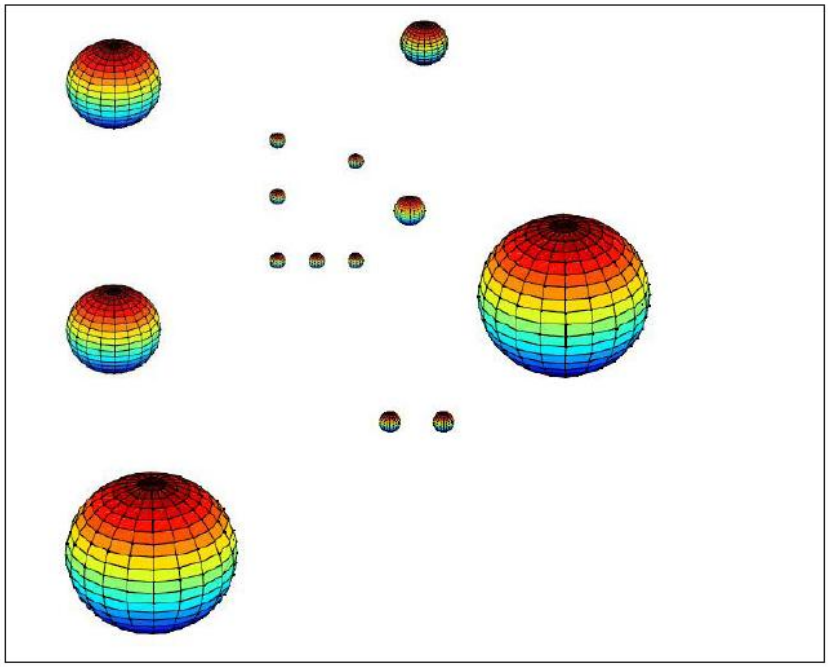


$$f_{12} = f_{21} = G * \frac{m_1 * m_2}{x_1 - x_2^{\ 2}}$$

(b) Spherical Nsol = 2



(c) Spherical Nsol = 3



Nsol >3

Fig 1: Gravitational pull and force amongst multiple bodies/agents/solutions (Nsol)

Translation of forces in nature (Grav) into mathematical methods

Gravitational algorithm : Rashedi et al. [1, 2] introduced gravitational algorithm into the bandwagon of nature inspired software implementable optimization/search tools. It is a swarm type heuristic stochastic approach like ant colony optimization (ACO), particle swarm optimization (PSO), simulated annealing algorithm (SAA) etc.

Artificial agents with Gravitational pull

Mass of agent: The masses of agents in fact represent quality or fitness function (Chart 2). A heavy mass, here, the agent with higher performance index, has a greater (large) effective attraction or pull radius resulting in a faster convergence. Hence, other agents with lesser performance move towards the heavier one and form a neighborhood. In other words, as agents tend to move toward the best agent, the inertia mass is against the motion and so makes its movement slow. The agents with heavy inertia mass move slower and hence search the space more locally. But, slower motion of agents in the search space results in a more precise search. Thus, it can be considered as an adaptive learning or information sharing/transfer. The gravitational and the inertia masses are assumed to be same, in spite of the fact that they are of different magnitude in certain applications.

Chart 2: Data structure of Grav.alg

(a) Variables and free parameters of Grav.alg:

Vector

$mass:\ m_1 \quad m_2 \quad m_i \quad m_{nsol}\ ^T$

Matrix

$$position: \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,d} \\ x_{2,1} & x_{2,2} & x_{2,d} \\ x_{i,1} & x_{i,2} & x_{i,d} \\ x_{nsol,1} & x_{nsol,2} & x_{nsol,d} \end{bmatrix} = \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \boldsymbol{x}_i \\ \boldsymbol{x}_{nsol} \end{bmatrix}$$

Nsol : Number of solutions

x_{id} : Coordinates of i^{th} position in d^{th} dimension

$\boldsymbol{x}_i$: $\begin{bmatrix} x_{i,1} & x_{i,2} & x_{i,d} \end{bmatrix}$ i^{th} position vector in d dimensions

$\boldsymbol{x}_{nsol}$: Coordinates of $nsol^{th}$ position (row) vector

superscript ^{T}: Transpose of vector/matrix/tensor

(b) Intermediate variables

MT =	[m1, m2, m3]
MMT =	[m1^2, m1*m2, m1*m3] [m1*m2, m2^2, m2*m3] [m1*m3, m2*m3, m3^2]

$$Dist = \begin{bmatrix} dist_{1,1} & dist_{1,2} & dist_{1,nsol} \\ dist_{2,1} & dist_{2,2} & dist_{2,nsol} \\ dist_{i,1} & dist_{i,2} & dist_{i,nsol} \\ dist_{nsol,1} & dist_{nsol,2} & dist_{nsol,nsol} \end{bmatrix}$$

MMT./dist^2 =

$$\begin{bmatrix} m1*m1/dist_{1,1}^2 & m1*m2/dist_{1,2}^2 & m1*m3/dist_{1,3}^2 \\ m2*m1/dist_{2,1}^2 & m2*m2/dist_{2,2}^2 & m2*m3/dist_{2,3}^2 \\ m3*m1/dist_{3,1}^2 & m3*m2/dist_{3,2}^2 & m3*m3/dist_{3,3}^2 \end{bmatrix}$$

MMT./dist^{power} =

$$\begin{bmatrix} \frac{m1*m1}{dist_{1,1}^p} & \frac{m1*m2}{dist_{2,1}^p} & \frac{m1*m3}{dist_{3,1}^p} \\ \frac{m2*m1}{dist_{2,1}^p} & \frac{m2*m2}{dist_{2,2}^p} & \frac{m2*m3}{dist_{2,3}^p} \\ \frac{m\,\mathrm{nsol}*m1}{dist_{\mathrm{nsol},1}^p} & \frac{m\,\mathrm{nsol}*m2}{dist_{\mathrm{nsol},2}^p} & \frac{m\,\mathrm{nsol}*m\,\mathrm{nsol}}{dist_{\mathrm{nsol},\mathrm{nsol}}^p} \end{bmatrix}$$

- Diagonal elements are attraction of ith mass by itself
- Symmetric $(a_{ij} = a_{ji})$

Distance between pair of agents: Each agent experiences the feel of all others. It sees the neighboring ones of same mass with more force than those at a longer distance. Thus, it sees the space around it like electrons in quantum chemistry. Although, Euclidian distance is employed generally, Hamming distance is made use in binary gravitational method.

Force between pair of agents: Gravitational force contains information of masses of two agents and Euclidean distance between them. If power = 1, force vector is directly proportional to the product of qualities of the two solutions and thus, independent of their inter distance [3]. The force between a pair of agents (i,j) is rendered stochastic by multiplying it with a random number. The position and velocity of each agent in the iteration (it) (Eqn. 1) are also random variables.

Eqn 1: Refinement of velocity and position of approximate solution tensor

	Eqn. Number		Eqn. Number
$G(it) = G_0 * \left(1 - \frac{it}{Tot\_it}\right)$	1	$worst(it) = \max \; fitrand(it)$	6
$mnorm_j \; it = \frac{m_j \; it}{\sum_{k=1}^{nsol} m_k \; it}$	2	$\mathrm{m}(it) = \left(\frac{fitrand(it) - worst(it)}{best(it) - worst(it)}\right)$	7
$fit_{ij} \; it = \frac{mnorm_i * mnorm_j}{x_i - x_j \; ^{power-1}}$	3	$acc_i \; it = \frac{fitrand_i \; it}{nmorm_i \; it}$	8
$fitrand \; it = \sum_{j=1} rand_j \; it * fit_j \; it$	4	$vel_i \; it+1 = urand_i * vel_i \; it + dist_i(it)$	9
$best(it) = \min \; fitrand(it)$	5	$x_i \; it+1 = x_i \; it+1 + vel_i \; it+1$	10

G0 : Constant; [set to 100]

Power : 2

Tot_it : Total number of iterations (i.e. total age of system)

Gravitational constant: Gravitational constant adjusts the accuracy of the search, so it decreases with time similar to the temperature in a simulated annealing algorithm. In binary.grav. alg, the gravitational constant is assumed to be a linear decreasing function (Eqn. 1)

Artificial Grav mimicking algorithm : The gravitational coefficient and number of effective agents (or approximate solutions) are two key parameters influencing the convergence of GravAlg. Gravitational Search in floating point space module finds place in continuous Single (S) or multiple (M) object (function) optimization (OO) [SOO, MOO], no matter with or without constraints. Binary gravitational search is in arsenal of the feature selection tools.

Exploration versus exploitation: During the initial phase of iteration process (Chart 3), comparatively larger numbers of widely spread approximate solutions are considered to perform exploration extensively to avoid trapping in local minima. As the refinement proceeds towards true solution, exploration must fade away with simultaneous onset of fade in of exploitation process. Now, k-best solutions attract each other forming a nearest neighbor shell driving towards global optimum at least as nearer as possible to the true one. The advantages and limitations of GravAlg are cited in Chart 4.

Chart 3(a): Gravitational search algorithm

Initiation
Search space identification
Randomized initialization (generation) of binary agents

Do until convergence
- Fitness evaluation of agents
- Updating G(t), best(t), worst(t) and Mi(t) for i=1, 2,…, N
- total force in different directions
- Refining acceleration and velocity, position

EndDo

Chart 3(b): KB of binary.Grav.alg

$v_{max} = 6.0$

If $ABS\ v\ i,d,it\ > v_{max}$

Then $vid\ i,d,it\ = v_{max}$

$\text{probfn}(v(i,d,it)) = |\tanh\ d(v,i,it)\ |$

If $Rand\ < probfn\ v(i,d,it+1)$

Then $x(i,d,it+1) = \text{compliment}\ x\ i,d,it$

Else $xid(it+1) = xid\ it$

Chart 4: Advantages and limitations of Grav.alg.

\+ GSA is memory-less
\+ easy implementation
\+ fast convergence
\+ low computational cost

– Convergence speed slows down in final search phase
– Easy to fall into local optimum solution
▶ Remedy: Immunity-based Gravitational Search

APPLICATIONS

GravAlg is used in the optimization of connection strengths (W) matrix of Fuzzy-ARTMAP-neural network (NN) [4,5] training of feed forward- (FF-) NNs and parameter identification of a chaotic system [6]. It is successfully applied to optical character recognition (OCR), decision function estimation without requirement to prior knowledge in supervised clustering [7], face classification of instances in multi-class data sets and rule discovery in classification. Electric power systems are another area of multi-object optimization (MOO) in dynamic economic dispatch of power system operation and solving MO-optimal reactive power dispatch task. The bi-objective task is minimization of transmission loss while maximizing the quality of voltage [8]. The tri-objective issue is simultaneous minimization of active power loss, improvement of voltage profile and enhancement of voltage stability [9]. The other fields of potential use are in communication and managing the demand supply chain [10].

Chemical tasks: Grav. Algoritm is used to minimize the emission due to oxides of nitrogen (NO_x), considering both thermal and wind generators [11]. Quantitative Structure X (X: activity/property/ response/sequence/toxicity/ Biodegradability) relationships ([Q] SXR) formerly popular as QSAR spread their wings beyond the prediction of mechanism of toxicity, mode of action of compounds and onset of diseases like diabetes in health care. SXR are credible tools providing complementary, supplementary and otherwise-not-obtainable information to experimental scientists involved in drug discovery, pharmaceutical chemistry, toxicology and synthetic preparation of any type of materials with conventional and nano-chemistry/technology. The databases contain more than 10^6 small organic molecules and of course the theoretically possible number is up to 10^{100}. The investigations over years used from 20 to more than 30,000 compounds in the research study.

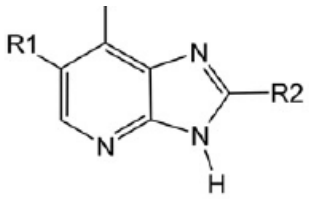
Dataset.SXR: DRAGON outputs a (65x1497) matrix of 65 rows representing compounds under study [12] and 1497 columns corresponding to molecular descriptors (Table 2). In yesteryears, the experimental approach for the three dimensional (3D-) structure of a chemical molecule/compound was from measurements on a single crystal with X-ray instrument. The structural data was represented as the set of coordinates in XYZ space. NMR and neutron diffraction techniques opened new vistas in crystal structure studies of even macromolecules. Under the task of geometric optimization, computational quantum chemistry (CQC) packages like G03 (or G09), GAMESS etc. compute (without any experiment/instrument) a set of (floating point real) numerical values of bond lengths (BL), bond angles (BA) and dihedral angles (DA) pooled into what is called a Z-matrix. Now, Z-matrix and XYZ coordinates are inter-convertible through mathematical transformation.PM3, a semi empirical molecular orbital (SEMO) quantum chemistry (QC) procedure is used to calculate stationary geometry of the molecules using Gaussian 03 software. This tradeoff between more accurate ab intio (DFT and HF) and SEMO probes is a good enough compromise for a follow up calculation of molecular descriptors with available commercial packages viz. CODESSA, DRAGON etc.

Feature (dimension/explanatory variable/multi-response) reduction : A high pair-wise correlation ($r \geq 0.9$) between two columns indicates that one of them is sufficient from mathematical statistics stand point as otherwise the design matrix becomes singular or ill conditioned. The problem can be alleviated iff (i.e. if and only if) one of the variables is eliminated, because both were not truly needed in the sense that pruned one does not offer any more additional information for a model. The preliminary pruning with heuristics (Table 2) leaves 329 descriptors for further analysis. The popular statistical methods (forward selection and backward elimination), soft mathematical approaches (principle component analysis, partial least squares), nature inspired mathematical tools (genetic algorithm) are in vogue in selection of prospective variables without losing gross information content. This task is known as feature selection. Here, GravAlg, a nature mimicking strategy, selects seven descriptors through its binary search in the (molecular descriptors') feature space. The descriptors in the optimum model are number of acceptor

atoms for H-bonds (N, O, F), number of CH3X groups, Moran autocorrelation (lag 4 and lag 6 weighted by atomic masses), H autocorrelation of lag 7/weighted by atomic polarizabilities, 3D-MoRSE—signal 25/unweighted and 1st component accessibility directional WHIM index/weighted by atomic electrotopological states.

The data driven hybrid modeling approach **([Grav_binary]** + **[Baysian_Regul + NN])** resulted (Table 3) in higher explainability (reflected in R^2) and lower value of a function of residual (RMSE) [12] between experimentally measured and model calculated pIC_{50} (i.e. –log(Inhibition concentration for 50% effect)).
Chemical industry: The constituents of synthesis gas (or Syngas) -- a fuel -- are hydrogen, carbon monoxide and a little of carbon dioxide. Ganesan et.al [13] reported the use of gravitational algorithm along with particle swarm optimization (PSO) and normal boundary intersection in MOO of combined carbon dioxide reforming and partial oxidation of methane.

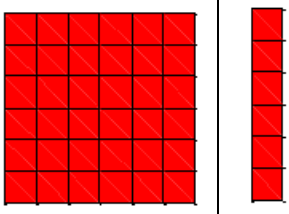
Table 2: Modeling of SXR



Imidazo[4,5-b]pyridine skelton

R1	R2	pIC_{50}	
		Expt	GrAlg
CN	4-Dimethylamino-phenyl	7.301	7.194
Br	Ph	7.092	7.112
Cl	Pyrazol-1-ylmethyl	8.000	8.059

(a) Data structure



X y

(b) Functional model (No apriori knowledge)

$$\text{Re}\,sponse = fn\left(\begin{array}{c} \\ Features \\ \\ Ncompunds \end{array}\right)^{Ndescriptors}$$

X : Features; matrix size : Ncompounds x Ndescriptors
y : Response vector size : Ncompounds x 1

(c) Pruning of descriptor set by linear correlation

If desj ≈ 0.0 or constant
Then Eliminate desj from the set

If r(desj, desk) >= 0.9
Then Eliminate desj or desk from the set
+ Number of influencing variables in model decreases
– Descriptor eliminated may be physically significant
– Descriptor retained may not have physical significance

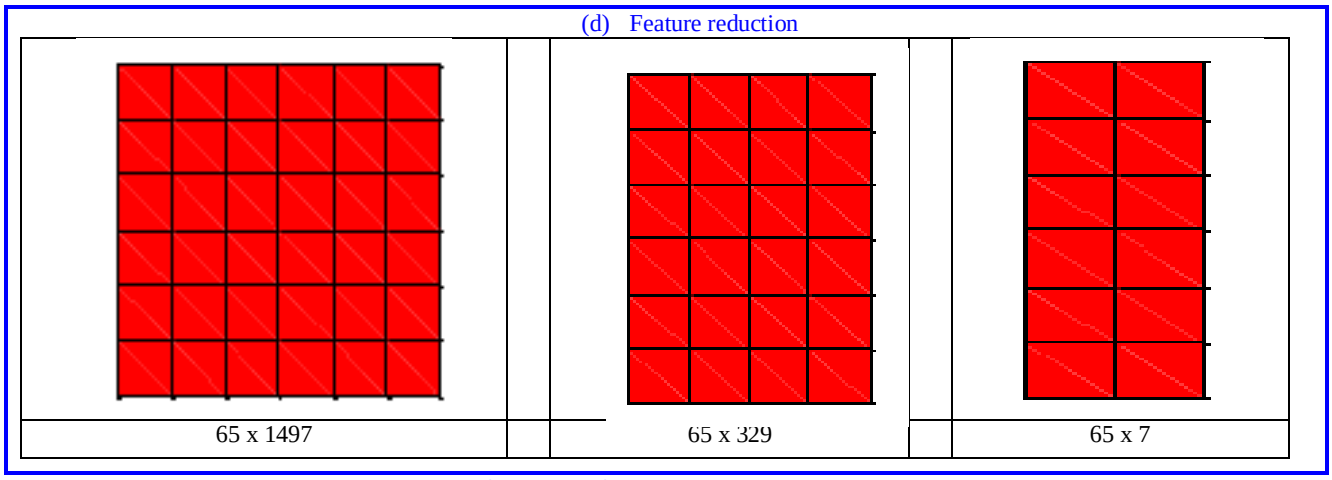


Table 3: Relative performance of Grav_alg with NN and hard modeling MLR

Hybrid		Training		External validation	
Alg-1	Alg-2	R^2	RMSE	R^2	RMSE
Stepwise-MLR		0.942	0.272	0.738	0.716
MLR	Baysian_Regul_NN	0.958	0.231	0.882	0.429
Grav_binary_alg	Baysian_Regul_NN	**0.990**	**0.131**	**0.982**	**0.214**

The three objectives are methane conversion, carbon monoxide selectivity and optimum hydrogen to carbon monoxide ratio.

Mathematical functions

A large number of standard test (SO, MO) functions have been proposed in literature to assess the efficacy of a proposed algorithm and also to compare its results with an arsenal of earlier reported methods. The functions of more than two variables are either fix or variable dimension. They may be unimodal or multimodal with several local minima.

Function.binary: In binary search space, functions have only two values (zero or 1) unlike continuous functions with any floating point value. Fig. 2a shows profiles for a grid of multi-integer (0 to 6) range on x and y axis.

Function.uniModal: Fig. 2b is a popular unimodal single object quadratic function in two (variable) dimensions.

Function.multiModal: Three dimensional surfaces (Fig.2c, 2d) exhibit multiple modes for a polynomial and trigonometric functions.

Gravitational algorithm successfully found optima of these and other test functions endorsing the applicability of the approach.

Similarity of GravAlg with other nature mimicking swarm approaches: The agents representing approximate solutions move in search space and finally reach the true/nearly true solution. The strategies are different and thus CPU times are also obviously not same. Chart 5 compares the philosophy of GravAlg with PSO. The results are compared with particle swarm optimization (PSO), evolutionary programming (EP), genetic algorithm (GA) and hybrid tabu search with simulated annealing algorithm (SAA).

Recent advances

Fuzzy system is designed for intelligently updating the effective parameters of GSA. GSA is employed to construct a novel decision function estimation algorithm from feature space [14].

Chart 5: Comparison of GravAlg with PSO

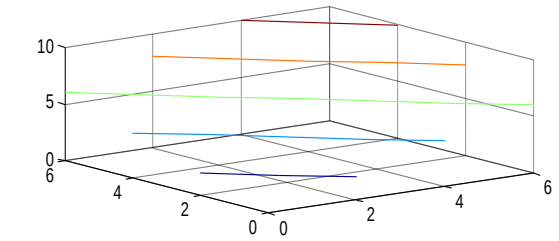
	Grav.alg	PSO
Direction of agent	The agent direction is calculated based on the overall force obtained by all other agents	Direction of an agent is calculated using only two best positions, pbesti and gbest.
Updating/ refining	The force is proportional to the fitness value and so the agents see the search space around themselves in the influence of force.	Updating is performed without considering the quality of the solutions, and the fitness values are not important in the updating procedure
Velocity	Memory-less and only the current position of the agents plays a role in the updating procedure	A kind of memory for updating the velocity (due to pbesti and gbest).
Distance between agents	Force is reversely proportional to the distance between solutions.	Updating is performed without considering the distance between solutions
Inspiration	Physical phenomena	Simulates the social behavior of birds

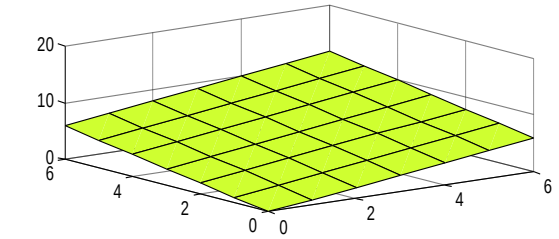
Hybrid systems

The binary hybrid systems of GravAlg are proposed using another nature mimicking strategy viz. artificial (honey) bee colony (ABC) [15], Chaos [6,16,17], elitism and CoEvolutionary process [18], convolutional neural networks (CNNs) [19], Fuzzy logic [14,20-22], immune system and self-adaptive mutation technique [23]. The results are noteworthy even when combined with k-means [24], member-satellite algorithm [25], opposition-based learning for population initialization for generation jumping [26], orthogonal array [27], sequential quadratic programming [28] and quantum technique [29-31].

Future scope

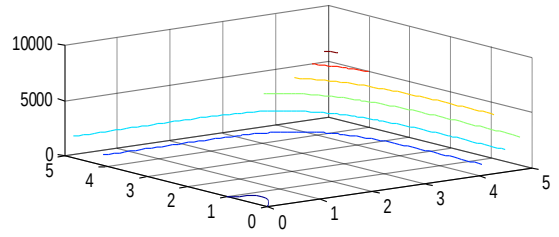
Many other nature inspired —genetic/ immune/evolutionary/firefly/ honeybee mating/ bat/ mosquito/ breeding — algorithms have already been in the forefront of solving chemical engineering /technical/commerce tasks with promising results. Thus, GravAlg also deserves feasibility study and comparison in varied disciplines with standard test data bases. The rigorous mathematical proof of convergence and stability of algorithm is the follow up phase for its unequivocal acceptance. The prospective application of the GravAlg alone and in hybrid form in computation of equilibrium constants, rate n and in chromatography is under way.

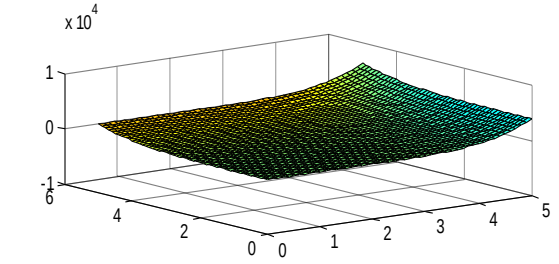




$$\max\_ones = \sum_{i=1}^{2} x_i$$

(a)Function with binary output

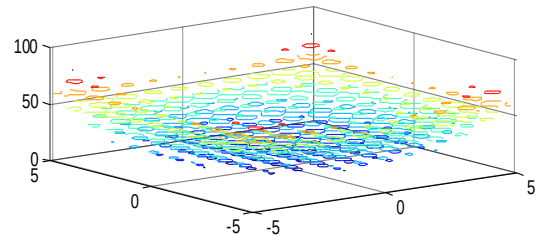




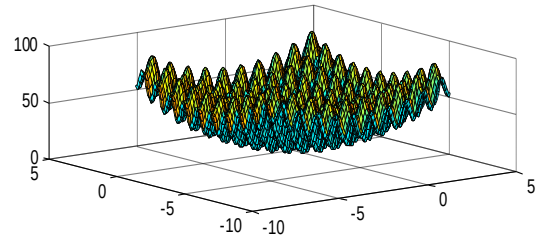
$$f1 = \sum_{i=1}^{2} x_i^2$$

```
range = [-100 100 1]' ;
number = '001';
fn=  'x.^2 + y.^2' ;
[fn001]= fn2object(fn,range,number);
```

(b)Unimodal function of a single variable

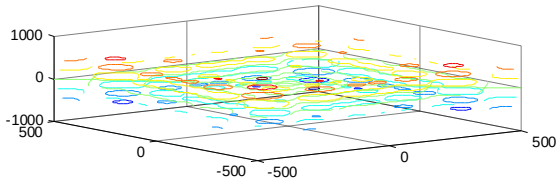


$$f16 = 4*x^2-2.1*x^4+\frac{1}{3}*x^6+x*y-4*y^2+4*y^4$$




```
range = [0 5  .1]' ;
fn = '4*x.^2 -2.1*x.^4
+1./3.*x.^6+x.*y-4.*y.^2+4.*y.^4;';
number = '016';
 [fn016]= fn2object(fn,range,number);
```

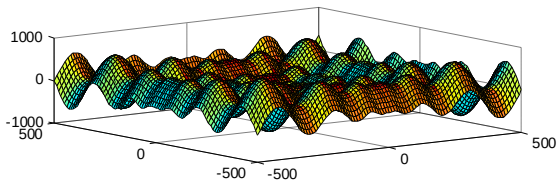
(c)multimodal Function of a single variable



$$f9 = \left[x^2 - 10*cos\ 2\pi x\ +10\right]+ \left[y^2 - 10*cos\ 2\pi y\ +10\right]$$

$$\dim = 2;$$

$$range = [-5.12 : 0.1 : 5.12]^T;$$




```
number = '009';
range = [-5.12 5.12 0.11]'
fn =
[x.^2 -10.*cos(2*pi*x)+10*one]+
[y.^2 -10.*cos(2*pi*y)+10*one];';
[fn009]= fn2object(fn,range,number);
```

(c)Multimodal trigonometric function of a two variables

```
% fn2object.m (R S Rao) Modified 12-4-
13
%
function[fnind]=
fn2object(f,range,number)
fnind = ['fn',num2str(number)];
fnind.number = number;
fnind.fn = f;
```

```
                                        fnind.range = range;
```

```
om_99(MO001);
om_99(MO009);
[MO016]=om_99(MO016);
```

```
function [Fn] = om_99(Fn)
f = Fn.fn;
ll = Fn.rangex(1,1);
ul = Fn.rangex(2,1);
inc = Fn.rangex(3,1);

[x,y,one] = om_xygrid(ll,ul,inc);
om_xyz_surfcont(x,y,f1);
```

```
%
% om_xygrid.m (R S Rao) 30-5-93;
 Modified 12-4-13
%
function [x,y,onex,oney] =
om_xygrid(xinit,xfinal,xinc,
yinit,yfinal,yinc)

if nargin <3
    x1 = [-1:0.5:1]'; x2 = x1;
end
if nargin ==3 | nargin > 3
    x1  = [xinit:xinc:xfinal]'; x2 =
x1;
end

if nargin ==6
   x2  = [yinit:yinc:yfinal]';
end
%
[x,y] = meshgrid(x1,x2);
[rx,cx]=size(x);[ry,cy]=size(y);
onex = ones(rx,cx);oney = ones(ry,cy);
```

```
%
% om_xyz_surfcont.m (R S Rao) 30-5-
93;
%
function   om_xyz_surfcont(x,y,z)
figure, axis square
subplot(2,1,1),contour3(x,y,z)
subplot(2,1,2),surfl(x,y,z)
```

Fig. 2: 2D-contour and 3D-surface plots of unimodal and multimodal functions

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