Experiments on Estimation of the Parameters of Gielis Super-formula by Simulated Annealing Method of Optimization

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Introduction: The Gielis superformula given as

$$r(\theta)=f(\theta).\left[\left|\tfrac{1}{a}\cos(\tfrac{m}{4}\theta)\right|^{n_2}+\left|\tfrac{1}{b}\sin(\tfrac{m}{4}\theta)\right|^{n_3}\right]^{(-n_1^{-1})}=f(\theta).g(\theta)\ ;\ a,\ b,\ m>0 \qquad \dots (1)$$

describes almost any closed curve in terms of the deformed circle (or ellipse), $g(\theta)$, and another function, $f(\theta)$, and their parameters (Gielis, 2003; Gielis and Gerats, 2004). The function $f(\theta)$ may be considered as a modifier of the Gielis function, $g(\theta)$. We find in nature a variety of interesting shapes that may possibly be described by the super-formula.

The Gielis super-formula is not the first attempt to seek for a mathematical pattern in nature. D'Arcy Thompson (1917) demonstrated that mathematical formulas and procedures can describe the forms of many living organisms, plant leaves and flowers. The history of such efforts go as far back in the past as to the 13th Century when Fibonacci observed mathematical regularity in nature (Szpiro, 2006). A number of other scientists also attempted to explain the observed mathematical regularities in the natural objects.

Estimation of Gielis Parameters: For a scientific purpose, Gielis parameters need to be estimated from empirical data. Presently, we are concerned with the possibilities of the same. Let the n true points be $[z_i=(x_i,y_i);\ i=1,2,...,n]$, of which the corresponding observed values are $z'=(x_i',y_i')$, possibly with errors of measurement and displacement of origin by (c_x,c_y), unknown to us. Let $(\tilde{c}_x,\tilde{c}_y)$ be the approximate or assumed values of (c_x,c_y). Let us denote by $\tilde{z}_i=(\tilde{x}_i,\tilde{y}_i)=(x_i'-\tilde{c}_x,y_i'-\tilde{c}_y)$. From these values we obtain $\tilde{r}_i=\sqrt{(\tilde{x}_i^{\,2}+\tilde{y}_i^{\,2})}$. We also obtain $\tilde{\theta}_i=\tan^{-1}(\tilde{y}_i/\tilde{x}_i)$. On the other hand, we obtain $\hat{r}_i=g(\tilde{\theta}_i,\tilde{a},\tilde{b},\tilde{m},\tilde{n}_1,\tilde{n}_2,\tilde{n}_3).f(\tilde{\theta})$, where $g(.)$ is the Gielis super-formula defined in (4) and $f(\theta)$ is variously defined. The wavy bar on the arguments of $g(.)$ and $f(.)$ indicates that all parameters have taken on some assumed values, which may not be the correct values. The deviation of assumed values of parameters from their true values gives rise to $d_i=abs(\tilde{r}_i-\hat{r}_i)$ and consequently $S^2=\sum_{i=1}^{n}d_i^2\ge 0$. Only if the assumed values of parameters are the true values, S^2 can be zero, but smaller it is, closer are the assumed values of the parameters from their true values (assuming empirical uniqueness of the parameters to a given set of data). Thus we have to find the values of Gielis parameters in $g(.)$ and $f(.)$ such that S^2 is minimum.

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Minimization of S^2 poses formidable problems due to two reasons. First, the Gielis parameters are possibly not unique to data. The three parameters, n_1, n_2 and n_3 of the deformed circle, $g(\theta)$, interact with each other even if we assume that the parameters of the modifying function, $f(\theta)$, do not influence them. However, that is not the case. As a matter of fact, all of them interact with each other. In econometric literature, the multi-collinearity problem presents an instance of such interaction among the parameters (resulting into non-zero covariances among them). This fact apart, the parameters span a highly nonlinear surface of S^2, which has innumerably many local minima. The author has observed that a highly adaptive direct search methods such as the Nelder-Mead algorithm and the Box algorithm (Nelder and Mead, 1964; Box, 1965) are often caught into local optima while finding the globally optimal values of the Gielis parameters. Although Box's algorithm strews random numbers over the entire surface of the optimand function that endows it with a great power to escape the local optimum points, it has no good strategy to come out of the trap if it is caught in a local optimum. Multiple starting points occasionally succeed, but often fail to give a desirable result.

As it is well known, most of the nonlinear optimization procedures that were developed in the 1960's or before are extremely prone to be caught in the local optima if the surface to be optimized is substantially irregular, ridged and multi-modal. In the due course, researchers in the field of operations research turned to learning from nature and imitating the process in which natural processes attain a minimum. Understanding the process of adaptation of living beings to their environment for a survival led to development of the 'genetic algorithm' (Holland, 1975) and the optimization method based on adaptation (Goldberg, 1989; Wright, 1991). This method mimics the process of survival of the fittest. On the other side, researchers learned from physics – the process of annealing in metallurgy (Kirkpatrick et al., 1983) and the method of 'simulated annealing' was developed.

The Simulated Annealing Method of Optimization: The simulated annealing method mimics the annealing process in metallurgy. In an annealing process a metal in the molten state (at a very high temperature) is slowly cooled so that the system at any time is approximately in thermodynamic equilibrium. As cooling proceeds, the system becomes more ordered – the liquid freezes or the metal re-crystallizes – attaining the ground state at T=0. This process is simulated through the Monte Carlo experiment (Metropolis et al. 1953). If the initial temperature of the melt is too low or cooling is done unduly fast the metal may become 'quenched' due to being trapped in a local minimum energy state (meta-stable state) forming defects or freezing out.

The simulated annealing method of optimization makes very few assumptions regarding the function to be optimized, and therefore, it is quite robust with respect to irregular surfaces. In this method, the mathematical system describing the problem mimics the thermodynamic system. The current solution to the problem mimics the current state of the thermodynamic system, the objective function mimics the energy equation for the thermodynamic system, and the global minimum mimics the ground state (Kirkpatrick et al., 1983; Cerny, 1985). However, nothing in the numerical optimization problem directly mimics the temperature, T, in the thermodynamic system underlying the metallurgical process of annealing. Therefore, a complex abstraction mimics it. An arbitrary choice of initial value of a variable called 'temperature', how many iterations are performed at each 'temperature', the step length at which the decision variables are adjusted, and the rate of fall of 'temperature' at each step as 'cooling' proceeds, together make an 'annealing schedule'. This schedule mimics the cooling process. At a high 'temperature' the step lengths at which the decision variables are adjusted are larger than those at a lower 'temperature'. Whether the system is trapped into local minima (quenching takes place) or it attains the global minimum (faultless crystallization) is dependent on the said annealing schedule. A wrong choice of the initial 'temperature', or the rate of fall in the 'temperature' leads to quenching or entrapment of the solution in the local minima. The method does not provide any clear guideline as to the choice of the 'annealing schedule' and often requires judgment or trial and error. If the schedule is properly chosen, the process attains the global minimum. It is said that using this method is an art and requires a lot of experience and judgment.

The Simulation Experiments: We have experimented with twelve different models. All these models are instances of a deformed circle, $g(.)$, modified by different modifier functions, $f(.)$. Three typical instances of $g(.)$ have been chosen. Their graphs are presented in Figures (M-01, M-02 and M-03). The parameters of $g(.)$ are given in table A.1. Four typical modifier functions are chosen. Their graphs are presented in M-10, M-20, M-30 and M-40 and their functional forms are given below. The chosen values of n_4 and n_5 are also given in table-A.1.

Model 10: $f_{10}(\theta) = r = [n_4(3\cos(t) - \cos(3t))^2 + n_5(3\sin(t) - \sin(3t))^2]^{0.5}$: (Nephroid) … (2)

Model 20: $f_{20}(\theta) = \mathrm{r} = \mathrm{n}_4 + \mathrm{n}_5 \cos(\mathrm{t})$: (Limaçon) … (3)

Model 30: $f_{30}(\theta) = \mathrm{r} = \mathrm{n}_4 - \mathrm{n}_5 \cos(\mathrm{t}) + \mathrm{abs}(\cos(\mathrm{t}))^3$ …(4)

Model 40: $f_{40}(\theta) = \mathrm{r} = \mathrm{n}_4 \exp(\mathrm{n}_5\, \mathrm{abs}(\sin(\mathrm{t})))$ … (5)

In all the four modifier functions, n_4 and n_5 are parameters and $0 \le t \le 2\pi$.

In case of each model, hundred uniformly distributed random points have been generated with the parameters specified in the relevant $g(.)$ and $f(.)$. The simulated annealing method of optimization has been repetitively applied to estimate the parameters with different values of initial temperature, T. This method requires the bounds (the lower and the upper limits; LL and UL) on the parameters to be specified. For all the 12 models we have used the identical set of bounds, specified in table-A.1. The jointly estimated parameters of $g(.)$ and $f(.)$ are presented in table-A.1. Their graphs are presented in Fig. $M_{ij} (i = 1, 2, ..., 4;\ j = 1, 2, 3)$. The red points are those generated by the true parameters while the blue ones are generated by using the estimated parameters. For each model, the estimated (blue) points are superimposed on the generated (red) points to facilitate a visual assessment of the quality of fit, which is quantitatively represented by the value of S^2.

The Findings: First, the simulated annealing method of optimization performs very well in fitting the Gielis curves to data. It performs better than the genetic algorithm in the majority of cases. The author used the genetic algorithm for estimation of Gielis parameters (Mishra, 2006). Difficulties faced with that method prompted the author to switch over to the simulated annealing method of optimization. In this method also, it is not always easy to escape the trappings of local optima. Fittings in M-41 and M-42 are perhaps caught in the sub-optimal traps as indicated by the relatively large values of S^2.

Secondly, a perusal of the magnitudes of exponential parameters (n_1, n_2, n_3) suggests that very often they deviate significantly from the true parameters but they may have a tendency to keep some proportionate relations among themselves. This tendency indicates the lack of empirical uniqueness of the parameters of the Gielis super-formula (Mishra, 2006). The problems are intensified in hybrid models, where $g(.)$ is modified by $f(.)$. On the basis of fitness (alone) one cannot say whether the one estimate (of parameters) is more reliable than the others. Thus, the exponential parameters intermingle with each other as well as with the parameters of the modifier function.

Some Observations: Looking at the shapes of the hybrid models, it is very difficult to guess the specification of $f(.)$ that modifies the deformed ellipse/circle, $g(.)$. In case of $g(.)$ the specification is fixed, only the parameters vary. However, in case of $f(.)$ nothing can be said a-priori. Since estimation depends on the specification of $f(.)$, in practice it would be very difficult to venture upon the task of estimation of Gielis parameters of arbitrary real life shapes. Furthermore, even one estimates the parameters and finds that the fit is acceptably good, how to be sure of the roles of the parameters of $f(.)$ and $g(.)$! A scientific outlook would expect the parameters to be liable to interpretation. That would possibly be a far cry for the enterprise of estimation of the Gielis parameters. It appears that the work of Gielis is suitable for graphics, but it may not have much significance with respect to the secrets of nature. Szpiro (2006) has rightly observed : D'Arcy tried to explain transformation of shapes in terms of forces that might have acted on the body of an organism. But, beyond some approximate description of a number of organic forms, Gielis offers no explanations of the shapes or the parameters of his super-formula.

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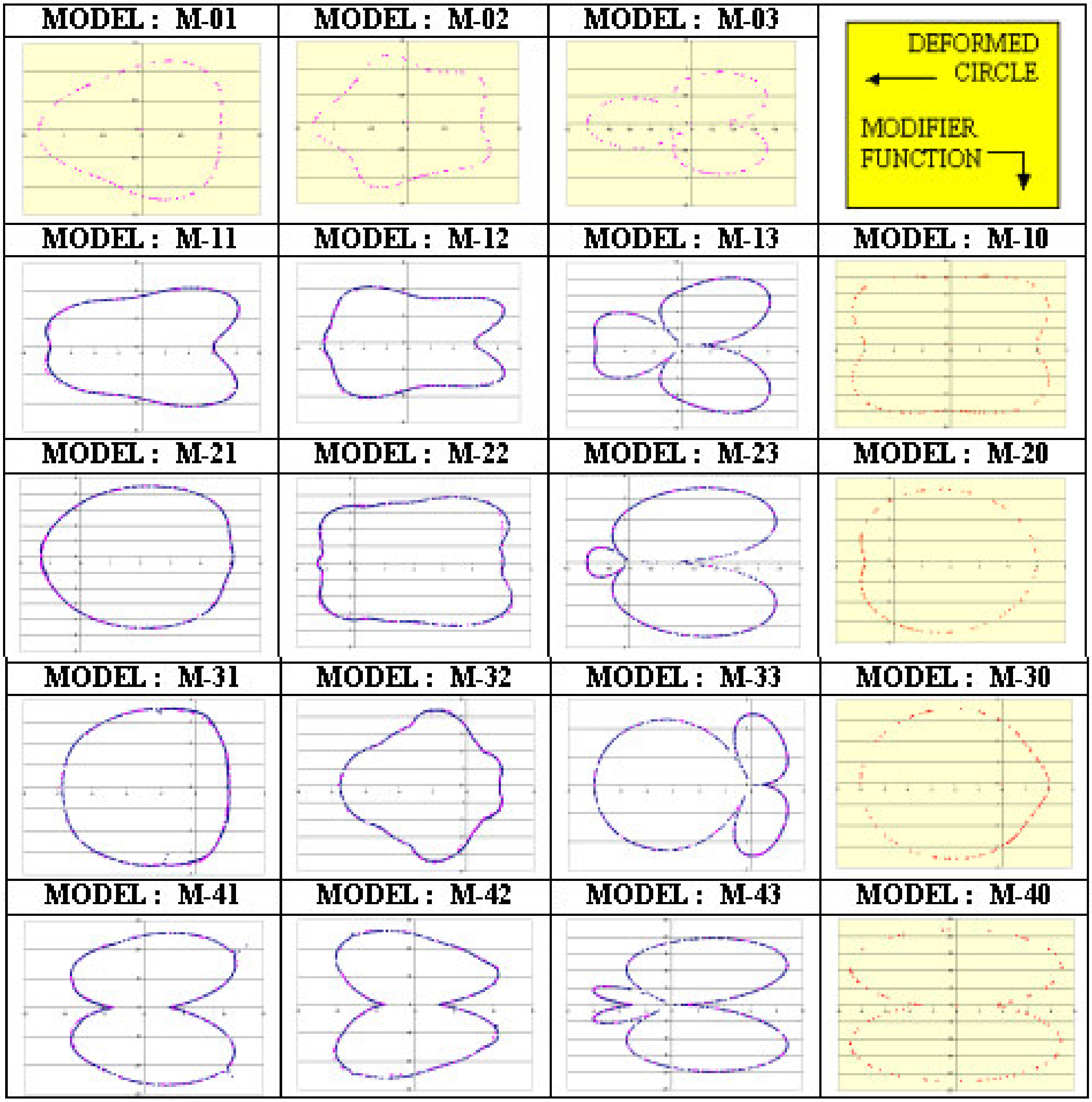
Appendix

Table-A.1. True & Estimated Gielis Parameters (Modified Curves) with Limits on them

	c_x	c_y	a	b	n_1	n_2	n_3	m	n_4	n_5	S^2	
M	0	0	1	1	0.6	2	3	3	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
11	15	15	50	50	80	80	80	10	5	5	UL	
	0.0303	0.0000	0.8178	23.9384	6.1427	3.3738	0.2229	6.0400	3.4583	2.3029	2.0358	E
M	0	0	1	1	2	2	6	5	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
12	15	15	50	50	80	80	80	10	5	5	UL	
	0.0000	0.1021	6.0376	0.8767	-3.8274	-0.0158	2.8309	10.000	2.9837	1.9869	2.5097	E
M	0	0	1	1	8	4	-4	6	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
13	15	15	50	50	80	80	80	10	5	5	UL	
	0.0000	0.0000	0.2717	2.0359	19.7701	9.0342	-9.8961	6.000	4.2797	2.8524	0.0026	E
M	0	0	1	1	0.6	2	3	3	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
21	15	15	50	50	80	80	80	10	5	5	UL	
	0.0428	0.0000	8.5868	0.7304	-8.2281	0.3996	3.5140	6.085	3.3880	2.2219	0.1561	E
M	0	0	1	1	2	2	6	5	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
22	15	15	50	50	80	80	80	10	5	5	UL	
	0.0000	0.0419	6.6620	2.1659	12.8108	3.3245	4.7098	9.940	5.0000	3.3155	0.6219	E
M	0	0	1	1	8	4	-4	6	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
23	15	15	50	50	80	80	80	10	5	5	UL	
	0.0000	0.0000	0.2103	2.0859	30.5799	12.4818	-15.3198	6.000	4.3319	2.8878	0.0010	E
M	0	0	1	1	0.6	2	3	3	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
31	15	15	50	50	80	80	80	10	5	5	UL	
	0.0000	0.0000	0.8375	0.0357	13.1260	5.1005	-0.6757	5.941	3.3011	2.1886	0.4877	E
M	0	0	1	1	2	2	6	5	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
32	15	15	50	50	80	80	80	10	5	5	UL	
	0.0000	0.0000	0.9677	0.4810	-43.4942	-1.8018	12.4391	10.000	3.0442	2.0252	0.5075	E
M	0	0	1	1	8	4	-4	6	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
33	15	15	50	50	80	80	80	10	5	5	UL	
	0.0000	0.0000	0.4977	1.0103	38.5048	16.3313	19.2912	6.000	3.0138	2.0098	0.0015	E
M	0	0	1	1	0.6	2	3	3	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
41	15	15	50	50	80	80	80	10	5	5	UL	
	0.0560	0.0369	47.6023	0.2479	-37.1224	-2.3988	12.7253	6.096	2.4362	1.9796	4.8473	E
M	0	0	1	1	2	2	6	5	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
42	15	15	50	50	80	80	80	10	5	5	UL	
	0.0000	0.1507	39.3609	0.3752	-14.7559	0.5965	5.4151	10.000	2.6299	0.0000	9.1952	E
M	0	0	1	1	8	4	-4	6	3	2	0	T
#	0	0	0	0	-80	-80	-80	1	0	0	LL	
43	15	15	50	50	80	80	80	10	5	5	UL	
	0.0000	0.0004	0.3062	1.8282	33.2615	17.3848	16.6389	6.000	4.0534	1.9993	0.0250	E

M=Model; LL=Lower Limits; UL=Upper Limite; T=True Parameters; E=Estimated Parameters

FIGURES



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