Least Squares Fitting of Chacón-Gielis Curves by the Particle Swarm Method of Optimization

SK Mishra
Dept. of Economics
NEHU, Shillong (India)

Introduction: Johan Gielis (2003) showed that his superformula

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

describes almost any closed curve in terms of the deformed circle, $g(\theta)$, and another function, $f(\theta)$, and their parameters. The function $f(\theta)$ may be considered as a modifier of the Gielis function, $g(\theta)$.

Ricardo Chacón (2004) pointed out that Gielis' superformula [$g(\theta)$ in eqn-1 above] is inherently linear. Hence it can generate only idealized (Platonic) rather than real-world forms. However, natural shapes and patterns emerge as a result of nonlinear dynamic processes and should therefore be expressed in terms of related nonlinear functions. In view of this, Gielis' superformula can be reformulated and generalized in which the trigonometric functions in $g(\theta)$ would be replaced by the Jacobian elliptic functions. The use of elliptic parameters on the angle coordinate is the key feature providing diverse variations of a given initial shape. The rate and nature of such variations on an initial theme (pattern) can be controlled by changing the parameters. Thus, one can obtain sequences that mimic transformations of biological shapes, including growth processes.

One of the generalizations of Gielis' superformula, $g(\theta)$, suggested by Chacón is:

$$r(\theta) = f(\theta).\left[\left|\tfrac{1}{a}\cos(\phi(\theta))\right|^{n_2} + \left|\tfrac{1}{b}\sin(\psi(\theta))\right|^{n_3}\right]^{(-n_1^{-1})} = f(\theta).\gamma(\theta) \qquad \ldots (2)$$

where,

$$\phi(\theta) = am\left[\frac{K(\mu)}{2\pi}(m\theta+\varphi);\mu\right] \ \ and \ \ \psi(\theta) = am\left[\frac{K(\mu)}{2\pi}(m\theta+\varphi');\mu\right] \qquad \ldots (3)$$

In the expressions above, $am[u;\mu]$ is the Jacobian elliptic function (JEF) of the parameter μ, $K(\mu)$ is the complete elliptic integral of the first kind, and (φ, φ') are additional parameters (Whittaker and Watson, 1996; Abramowitz and Stegun, 1964). The parameter m signifies rotational symmetry as in the Gielis superformula. The function $\gamma(\theta)$ degenerates into $g(\theta)$ for $\mu = \varphi = \varphi' = 0$ and in this sense the Chacón-Gielis superformula in (2) is a generalization of the Gielis superformula in (1).

Estimation of Chacón-Gielis Parameters: For a scientific purpose, Chacón-Gielis parameters in (2) and (3) above 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 $\tilde{z}_i = (\tilde{x}_i, \tilde{y}_i) = (x_i' - \tilde{c}_x, y_i' - \tilde{c}_y)$. We obtain $\tilde{r}_i = \sqrt{(\tilde{x}_i^2 + \tilde{y}_i^2)}$ from these values. We also obtain $\tilde{\theta}_i = \tan^{-1}(\tilde{y}_i / \tilde{x}_i)$. On the other hand, we obtain $\hat{r}_i = \gamma(\tilde{\theta}_i, \tilde{a}, \tilde{b}, \tilde{m}, \tilde{n}_1, \tilde{n}_2, \tilde{n}_3, \tilde{\mu}, \tilde{\varphi}, \tilde{\varphi}').f(\tilde{\theta})$, where $\gamma(.)$, the generalized form of Gielis' $g(\tilde{\theta})$, is the Chacón-Gielis super-formula defined in (2) and $f(\theta)$ may be defined variously. The wavy bar on the arguments of $\gamma(.)$ and $f(.)$ indicates that all parameters have taken on some arbitrary values, which may not be the correct values. The deviation of arbitrary values of parameters from their true values gives rise to $d_i = abs(\tilde{r}_i - \hat{r}_i)$ and consequently $S^2 = \sum_{i=1}^{n} d_i^2 \geq 0.$ 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 Chacón-Gielis parameters in $\gamma(.)$ and $f(.)$ such that S^2 is minimum.

Minimization of S^2 poses formidable problems due to two reasons. First, the Chacón-Gielis parameters are not unique to data. The parameters of $\gamma(\theta)$, and the modifying function, $f(\theta)$, interact among themselves. Moreover, the parameters span a highly nonlinear surface of S^2, which has innumerably many local minima (Mishra, 2006 (a), (b) & (c)). The minima (local as well as global) are located in the valleys or deep trenches. Therefore, estimation of the parameters in question is elusive to almost all methods of global optimization. Our experience with the Particle Swarm method of global optimization has elsewhere (Mishra, 2006(d)) been quite satisfactory in fitting the Gielis curves. We use this method for fitting the Chacón-Gielis curve here. The Generalized Simulated Annealing method did not work so well in this case too.

Particle Swarm Method of Global Optimization: A swarm of birds or insects or a school of fish searches for food, protection, etc. in a very typical manner. If one of the members of the swarm sees a desirable path to go, the rest of the swarm will follow up quickly. Every member of the swarm searches for the best in its locality - learns from its own experience. Additionally, each member learns from the others, typically from the best performer among them. Even human beings show a tendency to learn from their own experience, their immediate neighbours and the ideal performers.

The Particle Swarm method of optimization mimics the said behaviour (see Wikipedia : http://en.**wikipedia**.org/wiki/Particle_**swarm**_optimization). Every individual of the swarm is considered as a particle in a multidimensional space that has a position and a velocity. These particles fly through hyperspace and remember the best position that they have seen. Members of a swarm communicate good positions to each other and adjust their own position and velocity based on these good positions. There are two main ways this communication is done: (i) "swarm best" that is known to all (ii) "local bests" are known in neighborhoods of particles. Updating the position and velocity is done at each iteration as follows:

- $x \leftarrow x + v$
- $v \leftarrow wv + c_1 r_1(\hat{x} - x) + c_2 r_2(\hat{x}_g - x)$
  - w is the inertial constant. Good values are usually slightly less than 1.
  - c_1 and c_2 are constants that say how much the particle is directed towards good positions. Good values are usually right around 1.
  - r_1 and r_2 are random values in the range [0,1].
  - $\hat{x}$ is the best the particle has seen.
  - $\hat{x}_g$ is the global best seen by the swarm. This can be replaced by $\hat{x}_l$, the local best, if neighborhoods are being used.

The Particle Swarm method (Eberhart and Kennedy, 1995) has many variants; (Parsopoulos and Vrahatis, 2002). Among them, the Repulsive Particle Swarm (RPS) method of optimization (see Wikipedia, http://en.wikipedia.org/wiki/RPSO) is particularly effective in finding out the global optimum in very complex search spaces (although it may be slower on certain types of optimization problems). Other variants use a dynamic scheme (Liang and Suganthan, 2005; Huang et al., 2006).

In RPS the future velocity, v_{next} of a particle at position $\mathbf{x}$ with a recent velocity $\mathbf{v}$ is calculated by

$$\mathbf{v}_{\text{next}} = \omega \mathbf{v} + a\ \chi_1\ (-\mathbf{x} + \hat{\mathbf{x}}) + b\ \chi_2\ \omega(-\mathbf{x} + \hat{\mathbf{y}}) + c\ \chi_3\ \omega\ \mathbf{z}$$

where,

- χ_1, χ_3, χ_3 : random numbers $\in (0,1)$
- ω : inertia weight $\in (0.01, 0.7)$
- $\hat{\mathbf{x}}$: best position of a particle
- $\hat{\mathbf{y}}$: best position of a randomly chosen other particle from within the swarm
- $\mathbf{z}$: a random velocity vector
- a,b,c : constants

The future x that is, x_{next} is defined as $x_{next} = x + v_{next}$. Occasionally, when the process is caught in a local optimum, some perturbation of v may be needed.

The Simulation Experiments: We have experimented with four different models. All these models are instances of $\gamma(.)$ modified by different modifier functions, $f(.)$. Two typical instances of $\gamma(.)$ have been chosen. The parameters of $\gamma(.)$ are given in table A.1. Three typical modifier functions are chosen, as given below. The chosen values of n_4 and n_5 are also given in table-A.1.

Model-1 modifier : $f_1(\theta) = r = [n_4(3\cos(t) - \cos(3t))^2 + n_5(3\sin(t) - \sin(3t))^2]^{0.5}$
Model-2 modifier: $f_2(\theta) = r = n_4 + n_5 \cos(t)$; Model-3 modifier: $f_2(\theta) = r = n_4 + n_5 \cos(t)$
Model-4 modifier: $f_3(\theta) = r = n_4 - n_5 \cos(t) + abs(\cos(t))^3$
In all 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 $\gamma(.)$ and $f(.)$. The Repulsive Particle Swarm method of optimization (RPS) has been applied to estimate the parameters. The jointly estimated parameters of $\gamma(.)$ and $f(.)$ are presented in table-A.1. Their graphs are presented in Fig.A.1. The red points are those generated by the true parameters, the blue ones are generated by using the RPS-estimated parameters. For each model, the RPS-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 and Observations: Our experience of fitting the Chacón-Gielis curves to simulated data has been less satisfactory than fitting the simple Gielis curves by the Particle swarm method (see Mishra, 2006(d)). The reasons may lie in the severity of non-linearity introduced by elliptic functions into the original Gielis curves.

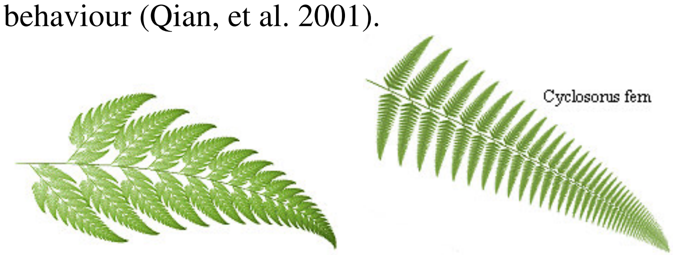
So far as the closeness of estimated parameters to the true parameters (used to generate the data) is concerned, our observation on the lack of empirical uniqueness of these parameters to data is corroborated once again. A lack of empirical uniqueness, or otherwise, of estimated parameters, $\hat{\alpha}$, of any function, say, $\wp(x \mid \alpha) = \wp(x_1, x_2, ..., x_p \mid \alpha_1, \alpha_2, ..., \alpha_p)$ by minimization of any specified norm, say, $\hat{\sigma} = \|\wp(x \mid \alpha) - \hat{\wp}(\hat{x} \mid \hat{\alpha})\|$ depends on the surface of $\hat{\sigma}$. The true surface of σ spanned by the true parameters, α, itself may have multiple global optima, in which case, a lack of uniqueness is inherent. An extravagant use of parameters in specification of the optimand function often may lead to this problem. But an inherent lack of uniqueness is not ubiquitous. The true surface may have unique σ. However, this true value may not be achievable on account of several reasons. Numerical approximation in the process of search is one of the reasons. Secondly, no global optimization method can ensure its immunity to entrapment by local optima, especially in the vicinity of the true global optimum. Such local optima may attribute non-uniqueness to estimated parameters. These local optima themselves may be a creation of numerical approximation in computing. In general, global optimization of complicated functions is an extremely difficult exercise and no method developed so far can ensure that it will unfailingly obtain the global optimum on an arbitrarily defined surface.

The ultimate utility of estimated parameters, nevertheless, lies in interpretability that suggests the process by which a particular shape might have been generated in nature. Fitness of a curve to data is only an index that guides us to this objective. But if fitness is not uniquely related to parameters through data, we cannot proceed to explanation of the process of generation of the concerned data in any reliable manner. Unfortunately, this lack of uniqueness has been observed in estimating the Gielis parameters and we obtain the same thing in estimating the parameters of Chacón-Gielis curves as well. Thus, interpretability or indication to sequences that mimic transformations of biological shapes, including growth processes, continues to elude our efforts.

It is well-known that the Jacobian elliptic functions may profitably be replaced by *Weierstrass's elliptic functions*. The latter are simpler and elegant for developing a general theory of non-linear processes. However, irrespective of the fact whether elliptic functions (Jacobian or Weierstrass's) or trigonometric functions are used to parametrize the real shapes in nature, a scientic explanation of the process of their genearation would remain elusive due to lack of uniqueness of parameters to data. In this sense, Gielis' or Chacón-Gielis superformula will continue to be interesting only for graphics.

Finally, a pertinent question arises. Is nature basically as complicated or complex as postulated by Gielis or Chacon-Gielis superformulas? Or, nature is intrinsically simple and the observed complexities are only apparent! This question was addressed in the late 1940's by John von Neumann in his theory of automata. This question was also addressed by S. Ulam in his theory of cellular automata. Since then, researches on identification of very simple rules underneath the apparent complexities observed in nature have progressed substantially.

Along with this, the mathematics of fractals (that had a beginning in the 19th Century) and the theory of Chaos developed (Peitgen, et al. 1992). In the recent past, the traditional theory of automata was supplemented with self-improving functions. This led to the development of Learning Cellular Automata as an emergent system having some collective behaviour (Qian, et al. 2001).



http://www.home.aone.net.au/~byzantium/ferns/fractal.html

Barnsley's fern (1993) is an instance of generating a pattern, with simple fractal procedure, closely resembling natural fern. That gives us a hope that other patterns (a cyclosorus fern leaf, for example) also may be generated similarly.

Yatapanage's (2003) work is another interesting attempt in simulating nature by simple rules. The quest for simplicity undeneath the apparent complexity in nature has been so encouraging that Wolfram (2002) looks at nature and science from an entirely new angle. In view of all these facts, it would possibly be more rewarding to explain natural shapes in terms of simple rules than complicated nonlinear equations.

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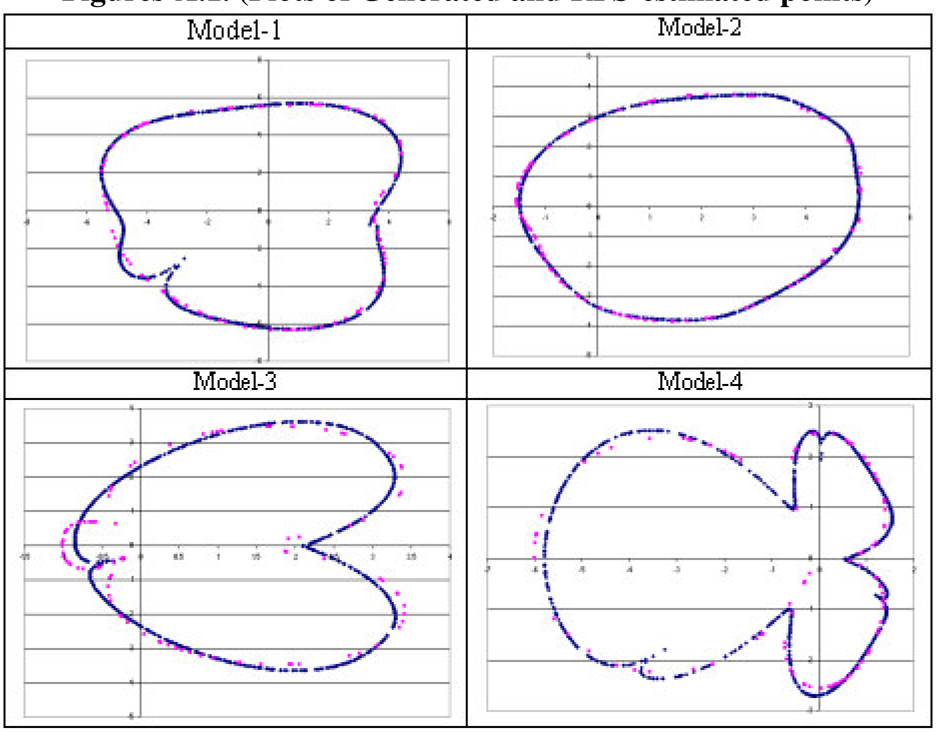
Appendix

Table-A.1. True and Estimated Chacón-Gielis Parameters (Modified Curves)

Parameters	Model-1		Model-2		Model-3		Model-4	
	True	Estimated	True	Estimated	True	Estimated	True	Estimated
c_x	0.0000	-1.4847	0.0000	2.6874	0.0000	0.6768	0.0000	-0.0212
c_y	0.0000	-0.7819	0.0000	0.1766	0.0000	0.0011	0.0000	-0.0109
a	1.0000	-0.0885	1.0000	3.6048	1.0000	0.8992	1.0000	-0.4045
b	1.0000	1.1816	1.0000	1.0225	1.0000	0.0078	1.0000	-1.2066
$\mathbf{n_1}$	0.6000	3.7602	0.6000	3.7730	8.0000	1.5566	8.0000	0.9241
$\mathbf{n_2}$	2.0000	-0.7625	2.0000	0.0085	4.0000	2.6696	4.0000	0.8672
$\mathbf{n_3}$	3.0000	4.0648	3.0000	7.0168	-4.0000	0.4337	-4.0000	-0.0492
m	3.0000	2.1139	3.0000	3.8572	6.0000	2.7388	6.0000	5.9588
$\mathbf{n_4}$	3.0000	2.7802	3.0000	3.8158	3.0000	1.3808	3.0000	2.9282
$\mathbf{n_5}$	2.0000	1.6498	2.0000	-1.0791	2.0000	0.6222	2.0000	1.9049
μ	0.5000	-0.9817	0.5000	0.9993	0.0000	0.4421	0.2000	1.0000
φ	0.3142	-2.3663	0.3142	4.0068	0.0000	4.0216	0.0314	0.2830
φ'	0.6283	-0.3029	0.6283	8.3493	0.0000	2.8652	0.1571	3.4126
S^2	0.0000	1.5028	0.0000	0.2697	0.0000	3.5440	0.0000	2.8337

Figures-A.1. (Plots of Generated and RPS-estimated points)



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Author's Contact: mishrasknehu@hotmail.com Ph: 913642550102 (R), 913642723175 (O)