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The Fourier Transform of the First Derivative of the Generalized Logistic Growth Curve

Genelleştirilmiş Lojistik Büyüme Eğrisinin Birinci Türevinin Fourier Dönüşümü

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Abstract

The “generalized logistic growth curve” or the “5-point sigmoid” is a typical example for sigmoidal curves without symmetry and it is commonly used for non-linear regression. The “critical point” of a sigmoidal curve is defined as the limit, if it exists, of the points where its derivatives reach their absolute extreme values. The existence and the location of the critical point of a sigmoidal curve is expressed in terms of its Fourier transform. In this work, we obtain the Fourier transform of the first derivative of the generalized logistic growth curve in terms of Gamma functions and we discuss special cases.

Keywords: Logistic growth, Fourier transform, Sigmoidal curve

Öz

Genelleştirilmiş lojistik büyüme eğrisi simetrisi olmayan sigmoid eğrileri için tipik bir örnektir ve genellikle lineer olmayan regresyon için kullanılır. Bir sigmoid eğrisinin “kritik noktası” kısaca, türevlerinin mutlak ekstremum noktalarının (eğer varsa) limiti olarak tanımlanır. Bir sigmoid eğrisinin kritik noktasının varlığı ve konumu Fourier dönüşümü ile ifade edilebilir. Bu çalışmada, genelleştirilmiş lojistik büyüme eğrisinin birinci türevinin Gama fonksiyonları cinsinden Fourier dönüşümü elde edilmiş ve bazı özel durumlar tartışılmıştır.

Anahtar Kelimeler: Lojistik büyüme, Fourier dönüşümü, Sigmoid eğrisi

I. INTRODUCTION

Sigmoidal curves are monotone increasing functions y(t) with horizontal asymptotes as $t \to \pm\infty$, providing mathematical models for transitions between two stable states. In previous work, in a study of (irreversible) chemical gelation phenomena, the transition from liquid state to gel state was described in terms of the “Susceptible-Infected-Removed” (SIR) epidemic model [3]. Later on, in a numerical study for the search for the exact instant of gelation [4], we observed that the points where the higher derivatives of the sigmoidal curve that represents the phase transition reach their extreme values, tend to accumulate at a certain point [5]. This limit point, if it exists, was defined as the “critical point” of the sigmoidal curve. A similar behaviour was observed for the formation of (reversible) physical gels, which was shown to obey a modified form of the “Susceptible-Infected-Susceptible” (SIS) model whose solutions are generalized logistic growth curves [7]. In [6] we expressed sufficient conditions for the existence of a critical point of a sigmoidal curve in terms of the Fourier transform of the first derivative. For the sigmoidal curves that arise as solutions of the SIR model, we could only give numerical evidence for the existence of the critical point. But for the solutions of the SIS model expressed in terms of generalized logistic growth functions, we could express the location of the critical point in terms of the parameters of the generalized logistic growth curve [7] where we used without proof the expression of the Fourier transform of its first derivative.

The standard logistic growth curve is a typical example for a sigmoidal curve with an even first derivative and well known Fourier transform properties. The generalized logistic family provides good examples for sigmoidal curves with no symmetry but the explicit expression of their Fourier transform is not available in the literature. The purpose of this note is to give a detailed derivation of the Fourier transform of the first derivative of the generalized logistic family. The integrals involved

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in the computation of this Fourier transform can be evaluated by certain computer algebra softwares, but we believe that an explicit derivation should be found in the mathematical literature.

The standard logistic growth curve is a sigmoidal curve which is the solution of the differential equation $y'=1-y^2$, $y(0)=0$. This equation can be solved as

$$y(t) = \tanh(t) \tag{1}$$

and its first derivative $y'(t)=sech^2(t)$ is the well known 1-soliton solution of the Korteweg-deVries (KdV) equation. The generalized logistic growth curve with horizontal asymptotes at -1 and 1 is a sigmoidal curve given by

$$y(t) = -1 + \frac{2}{[1+ke^{-\beta t}]^{\frac{1}{\nu}}} \tag{2}$$

where $k > 0$, $\beta > 0$ and $\nu > 0$. The sigmoidal curve (2) reduces to (1) for $\nu = 1$, $k = 1$, $\beta = 2$.

The Fourier transform of a function f, $F(\omega)$, is defined as

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t)\, e^{-i\omega t}\, dt$$

for all $\omega \in \mathbb{R}$ provided that the integral exists in the sense of Cauchy principal value [9]. If f is in L^1, then its Fourier transform exists. Since the sigmoidal functions (in particular the standard and generalized logistic growths) are finite as $t \to \infty$, their first derivatives are in L^1 and thus their Fourier transform exists.

The Fourier transform of the first derivative of the standard logistic growth solution

$f(t)=y'(t)=\text{sech}^2(t)$
is obtained easily by using the integral formula

$$\int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\cosh^2(t)} dt = \frac{\pi\omega}{\sinh\left(\frac{\pi\omega}{2}\right)}$$

as

$$F(\omega) = \sqrt{\frac{2}{\pi}} \frac{(\pi\omega/2)}{\sinh(\pi\omega/2)}. \tag{3}$$

The first derivative of the generalized logistic growth is a localized pulse but it is not symmetrical and the computation of its Fourier transform is more complicated. In Section II, we obtain this Fourier transform explicitly in terms of Gamma functions (see Equation (7)), pointing out certain interesting relations among these and the hypergeometric functions.

We recall that the hypergeometric function $_2F_1$ is defined by the Gauss series as

$$_2F_1(a,b;c;z) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{z^n}{n!}$$

on the disk $|z| < 1$ (and by analytic continuation elsewhere) where $a,b,c \in \mathbb{C}$, $c \notin \mathbb{Z}^- \cup \{0\}$ and the symbol $(x)_n$ (also known as Pochhammer symbol) is defined by $(x)_0=1$ and $(x)_n=x(x+1)\dots(x+n-1)$
for $1 \le n \in \mathbb{N}$ (see [10] and [2] for more details).

2. THE FOURIER TRANSFORM OF THE FIRST DERIVATIVE OF THE SIGMOIDAL CURVE

The first derivative of the sigmoidal curve (2) is

$$y'(t) = f(t) = \frac{2k\beta}{\nu}\left[1+ke^{-\beta t}\right]^{-\frac{1}{\nu}-1} e^{-\beta t}.$$

Its Fourier transform is defined by the integral

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \frac{2k\beta}{\nu} \int_{-\infty}^{\infty} e^{-i\omega t} e^{-\beta t} \left[1+ke^{-\beta t}\right]^{-\frac{1}{\nu}-1} dt. \tag{4}$$

The definite integral

$$I(\omega) := \int_{-\infty}^{\infty} e^{-i\omega t} e^{-\beta t} \left[1+ke^{-\beta t}\right]^{-\frac{1}{\nu}-1} dt$$

can be expressed as

$$I(\omega) = \frac{1}{\beta} \int_0^{\infty} u^{\frac{i\omega}{\beta}} \left[1+ku\right]^{-\frac{1}{\nu}-1} du$$

by setting $u = e^{-\beta t}$. $I(\omega)$ can be evaluated in terms of the hypergeometric functions using the integral equality

$$\int_0^{\infty} x^{\lambda-1} (1+x)^{\eta} (1+\alpha x)^{\mu}\, dx =$$

$$B(\lambda, -\eta-\mu-\lambda) \times {}_2F_1(-\mu, \lambda; -\mu-\eta; 1-\alpha) \tag{5}$$

which holds for $|arg(\alpha)| < \pi$, $-\text{Re}(\mu+\eta) > \text{Re}(\lambda) > 0$ (see [8, p.317]).

Putting $x = u$, $\lambda = 1 + \frac{i\omega}{\beta}$, $\alpha = k$, $\mu = -\frac{1}{\nu} - 1$ and $\eta = 0$ in (5) we obtain

$$I(\omega) = \frac{1}{\beta} B\left(1+\frac{i\omega}{\beta}, \frac{1}{\nu} - \frac{i\omega}{\beta}\right) \times {}_2F_1\left(\frac{1}{\nu}+1, 1+\frac{i\omega}{\beta}; \frac{1}{\nu}+1; 1-k\right),$$

where B is the well-known Beta function. It is known that

$$B(x,y) = \frac{\Gamma(x)\,\Gamma(y)}{\Gamma(x+y)}$$

provided $\text{Re}(x)>0$ and $\text{Re}(y)>0$, and

$$ {}_2F_1\left(\frac{1}{\nu}+1, 1+\frac{i\omega}{\beta}; \frac{1}{\nu}+1; 1-k\right) = k^{-1-\frac{iw}{\beta}} $$

since

$$ {}_2F_1(b,a;b;z) = {}_2F_1(a,b;b;z) = (1-z)^{-b} $$

(see [1, p.556]).

Thus we have

$$ I(\omega) = \frac{1}{\beta} \frac{\Gamma\left(1+\frac{iw}{\beta}\right)\Gamma\left(\frac{1}{\nu}-\frac{iw}{\beta}\right)}{\Gamma\left(1+\frac{1}{\nu}\right)} k^{-1-\frac{iw}{\beta}}. \qquad (6) $$

Substituting (6) in (4) we get

$$ \begin{aligned} F(\omega) &= \frac{1}{\sqrt{2\pi}} \frac{2k\beta}{\nu} I(\omega) \\ &= \sqrt{\frac{2}{\pi}} \frac{k^{-\frac{iw}{\beta}}}{\nu} \frac{\Gamma\left(1+\frac{iw}{\beta}\right)\Gamma\left(\frac{1}{\nu}-\frac{iw}{\beta}\right)}{\Gamma\left(1+\frac{1}{\nu}\right)} \end{aligned} $$

and using the equality

$$ \Gamma\left(1+\frac{1}{\nu}\right) = \frac{1}{\nu}\Gamma\left(\frac{1}{\nu}\right) $$

we can express the Fourier transform of the first derivative of the generalized logistic curve as

$$ F(\omega) = \sqrt{\frac{2}{\pi}} k^{-\frac{i\omega}{\beta}} \frac{\Gamma\left(1+\frac{i\omega}{\beta}\right)\Gamma\left(\frac{1}{\nu}-\frac{iw}{\beta}\right)}{\Gamma\left(\frac{1}{\nu}\right)}. \qquad (7) $$

3. SPECIAL CASES

We rewrite the Fourier transform pair for the first derivative as, displaying the dependence on the parameters k and ν as

$$ f(t,k,\nu) = \frac{2k\beta}{\nu}\left[1+ke^{-\beta t}\right]^{-\frac{1}{\nu}-1} e^{-\beta t}, $$

$$ F(\omega,k,\nu) = \sqrt{\frac{2}{\pi}} \frac{1}{\Gamma\left(\frac{1}{\nu}\right)} e^{-i\left(\frac{\ln k}{\beta}\right)\omega} \Gamma\left(1+\frac{i\omega}{\beta}\right)\Gamma\left(\frac{1}{\nu}-\frac{iw}{\beta}\right). \qquad (8) $$

Substituting $\nu=1$, $k=1$, $\beta=2$ in (7) and using the property

$$ \Gamma(x)\,\Gamma(1-x) = \frac{\pi}{\sin(\pi x)} $$

together with $\sin(ix)=i\sinh(x)$, we get the Fourier transform of the standard logistic growth function as given in (3).

Differentiating $f(t,k,\nu)$ with respect to t and setting it equal to zero we obtain the location of the maximum of $f(t,k,\nu)$, that we denote by $tm(k,\nu)$ as

$$ t_m(k,\nu) = \frac{\ln(k/\nu)}{\beta}. $$

We recall that a shift of the origin in the time domain by an amount α corresponds to the multiplication of the Fourier transform by a factor $e^{-i\alpha\omega}$, i.e, if $F(\omega)$ is the Fourier transform of $f(t)$, then $e^{-i\alpha\omega}F(\omega)$ is the Fourier transform of $f(t-\alpha)$. Thus the parameter k has the effect of shifting the origin of the time axis. For $k=1$, and $\nu=1$, the peak of the first derivative of the standard logistic growth is located at $t=0$. For $k=1$, and $\nu>1$, the peak shifts left while for $\nu<1$ it shifts right.

If $\nu=\frac{1}{n}$, where n is a positive integer greater than 1, we use the property

$$ \Gamma(1+x) = x\,\Gamma(x) $$

to express $F\left(\omega,1,\frac{1}{n}\right)$ in terms of $F(\omega,1,1)$ as

$$ F(\omega,1,1/n) = \frac{1}{\Gamma(n)}\left(1-\frac{i\omega}{\beta}\right)\left(2-\frac{i\omega}{\beta}\right)\cdots\left(n-1-\frac{i\omega}{\beta}\right) F(\omega,1,1). $$

This expression is a polynomial multiple of the standard logistic growth. Since the Fourier transform of the nth derivative of $f(t)$ is $(i\omega)^n F(\omega)$, it follows that $f(t,1,1/n)$ is a polynomial in the derivatives of $f(t)$.

For arbitrary values of ν, the (complex) Gamma function with complex arguments can be computed numerically. In our case, as we are interested in the Fourier transform $F(\omega)$ for fixed values of the parameters, we need to obtain the graphs of the real and imaginary parts of $F(\omega,1,\nu)$ on vertical lines in the complex plane. It is known that the Gamma functions falls of faster than any polynomial in the imaginary direction, it follows that the Fourier transform of all higher derivatives are rapidly decreasing functions. For the cases $\nu=\frac{1}{n}$ and $\nu=n$, we present the plot of the first derivatives of the generalized logistic growth in Figure 1 and the plot of the magnitudes of the Fourier transform of the first derivatives in Figure 2 for the values of n=1,4,8,12 (with $k=1$, $\beta=2$). By continuity of the Gamma function with respect to real part of its argument, the parametric plot of the complex Fourier transform for $n<\frac{1}{\nu}<n+1$ fill the region between the curves corresponding to the integer values of $\frac{1}{\nu}$, as shown in Figure 3.

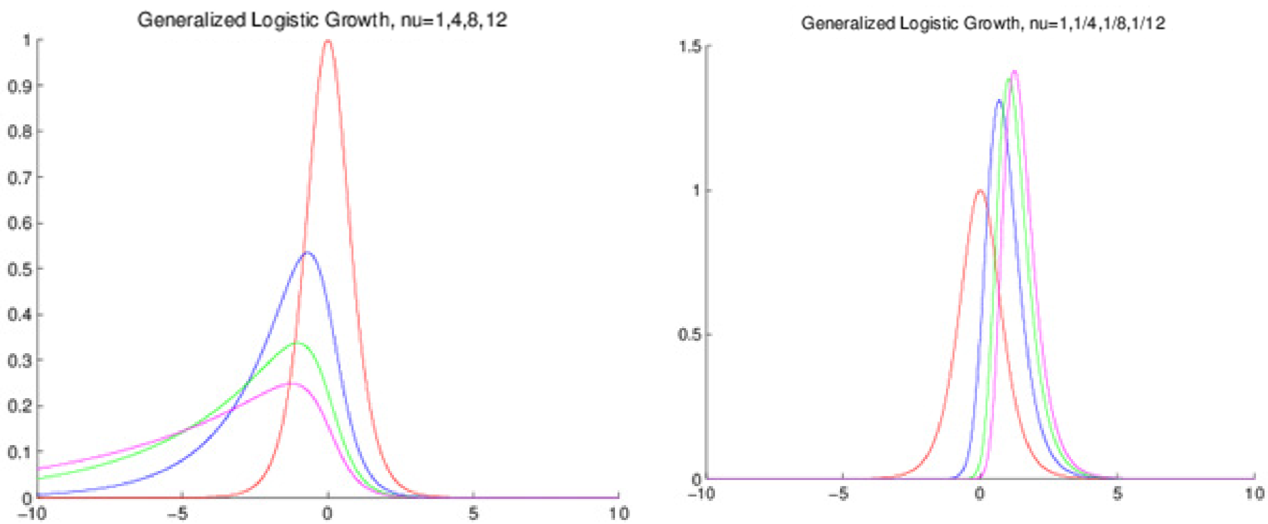

Figure 1: Time domain plots of the first derivative of the generalized logistic growth: a) for $\frac{1}{\nu} = 1, \frac{1}{4}, \frac{1}{8}, \frac{1}{12}$ (left), b) for $\frac{1}{\nu} = 1, 4, 8, 12$ (right)

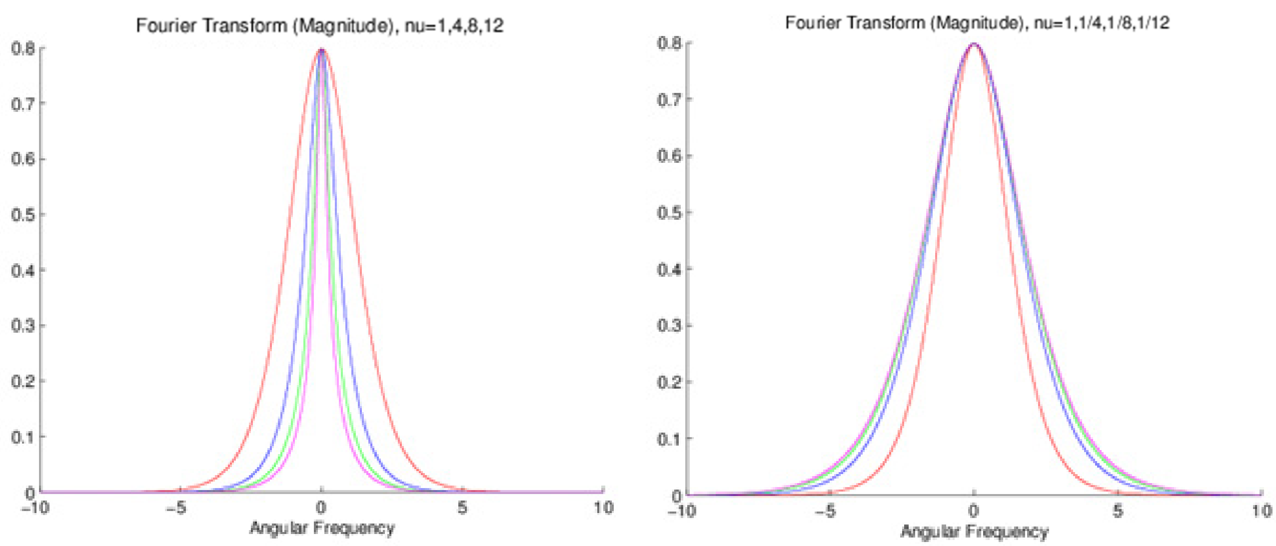

Figure 2: The magnitude of the Fourier transform:a) for $\frac{1}{\nu} = 1, \frac{1}{4}, \frac{1}{8}, \frac{1}{12}$ (left), b) for $\frac{1}{\nu} = 1, 4, 8, 12$ (right)

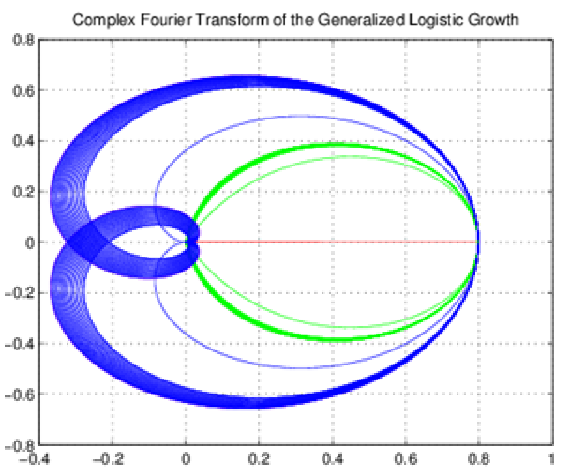

Figure 3: Parametric plot of the complex Fourier transform of the first derivative of the generalized logistic growth (from inside to out) for ν=1, ν=4, ν from 8 to 12, $\nu = \frac{1}{4}$ and ν from $\frac{1}{8}$ to $\frac{1}{12}$ respectively

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