

Determining the Critical Point of a Sigmoidal Curve via its Fourier Transform

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Abstract. A sigmoidal curve $y(t)$ is a monotone increasing curve such that all derivatives vanish at infinity. Let t_n be the point where the n th derivative of $y(t)$ reaches its global extremum. In the previous work on sol-gel transition modelled by the Susceptible-Infected-Recovered (SIR) system, we observed that the sequence $\{t_n\}$ seemed to converge to a point that agrees qualitatively with the location of the gel point [2]. In the present work we outline a proof that for sigmoidal curves satisfying fairly general assumptions on their Fourier transform, the sequence $\{t_n\}$ is convergent and we call it “the critical point of the sigmoidal curve”. In the context of phase transitions, the limit point is interpreted as a junction point of two different regimes where all derivatives undergo their highest rate of change.

1. Introduction

Let $y(t)$ be a monotone increasing function with horizontal asymptotes y_1 and y_2 as $t \rightarrow \pm\infty$ and with $\lim_{t \rightarrow \pm\infty} y^{(n)}(t) = 0$ for all $n \geq 1$, i.e, a sigmoidal curve. Let t_n be the point where the n th derivative of $y(t)$ reaches its global extremum. If the sequence $\{t_n\}$ converges, its limit is called the “critical point” of the sigmoidal curve $y(t)$.

The present work is motivated by an observation on the behaviour of the derivatives of sigmoidal curves representing gelation phenomena, modelled by the Susceptible-Infected-Removed (SIR) system of differential equations [2]. We have seen that the points t_n where higher order derivatives reach their absolute extreme values seemed to accumulate at a point in between the zeros of the second and first derivatives. The location of this accumulation point agreed qualitatively with the so-called “gel point”. Later on, we computed higher order derivatives for a number of different sigmoidal functions and we observed the same type of accumulation behaviour interpreted as the existence of a critical point in the sense defined above. For odd sigmoidal curves, we observed that the critical point was always located at $t = 0$, i.e, at the zero of the first derivative, as expected, but we were unable to prove this even for the simplest functions. After trying numerous techniques we could explain the existence of the critical point in terms of the Fourier transform of the first derivative of the sigmoidal curve. In this paper, we outline the steps leading to the proof of the existence of the critical point. Complete proofs that are quite technical and lengthy will be presented elsewhere.



2. Preliminaries

We briefly outline basic properties of Fourier transform. For simplicity assume that $f(t)$ is in L^1 . Then its Fourier transform $\mathcal{F}(f) = F$ and the inverse transform $\mathcal{F}^{-1}(F) = f$ are defined by

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

respectively. The effect of differentiation in the time domain is multiplication by $i\omega$ in the frequency domain, i.e., $\mathcal{F}(f^{(n)}(t)) = (i\omega)^n F(\omega)$. Multiplication and convolution in the time and frequency domains are related by $\mathcal{F}(f(t)g(t)) = \frac{1}{\sqrt{2\pi}} F(\omega)G(\omega)$. The “modulation” of low frequency signal in the time domain is the multiplication of this signal by a sinusoidal function of fixed (usually high) angular frequency ω_0 . In the frequency domain, the Fourier transform of the low frequency function is convolved with the Fourier transform of the sinusoid. The Fourier transform of a pure sinusoid is represented by Dirac δ functions occurring at $\pm\omega_0$ and convolution carries the spectrum of the low frequency signal to the frequencies $\pm\omega_0$. It follows that multiplication in the time domain by a complex exponential results in a shift in the frequency domain. Similarly, multiplication by a linear phase factor in the frequency domain leads to a shift in the time domain, as given below:

$$\mathcal{F}(f(t)e^{i\omega_0 t}) = F(\omega - \omega_0), \quad \mathcal{F}^{-1}(e^{-i\alpha\omega} F(\omega)) = f(t - \alpha).$$

(See [3, 4] for more details.)

3. The existence and non-existence of the critical point

We will use the generalized logistic growth family of curves and its limiting function the Gompertz curve to illustrate the existence and the nonexistence of the critical point and its location. The generalized logistic growth curve with horizontal asymptotes at -1 and 1 is given by

$$y(t) = -1 + 2 \left[1 + ke^{-\beta t} \right]^{-1/\nu},$$

where $k > 0$, $\beta > 0$ and $\nu > 0$. The parameter k can be adjusted by a time shift, β corresponds to a scaling of time and ν is the key parameter that determines the shape of the growth. For $\nu = 1$, $k = 1$ and $\beta = 2$ we obtain the standard logistic growth $y(t) = \tanh(t)$. The Gompertz curve obtained as the limit of the generalized logistic family for $k = 1/n$, $\nu = 1/n$, as $n \rightarrow \infty$ is the function

$$y(t) = -1 + 2e^{-e^{-\beta t}}.$$

We present the behavior of the derivatives of these functions in Figure 1. The critical point of the standard logistic curve is located at $t = 0$; the choice $k = 1$ ensures that the critical point of the generalized logistic curve is also located at the same point. The Gompertz curve has no critical point, because the points t_n move to negative infinity.

One ingredient for the existence of a critical point is the fact that higher derivatives of the sigmoidal function behave as localized humps modulated by sinusoids of increasingly high frequencies and these wave packets accumulate near a certain point, as shown below in Figure 2 (see [1] for the Fourier transform of the first derivative of the generalized logistic curve).

The wave packet behavior in the time domain corresponds to the band-pass property of its Fourier transform. That is, if higher derivatives resemble more and more closely sinusoids of increasing frequencies, their Fourier transforms become more and more localized humps located at higher and higher frequencies. The wave packet behavior is not sufficient to ensure the existence of the critical point, as in the case of the Gompertz functions these wave packets move to negative infinity. These wave packets should be agglomerate as the order of differentiation

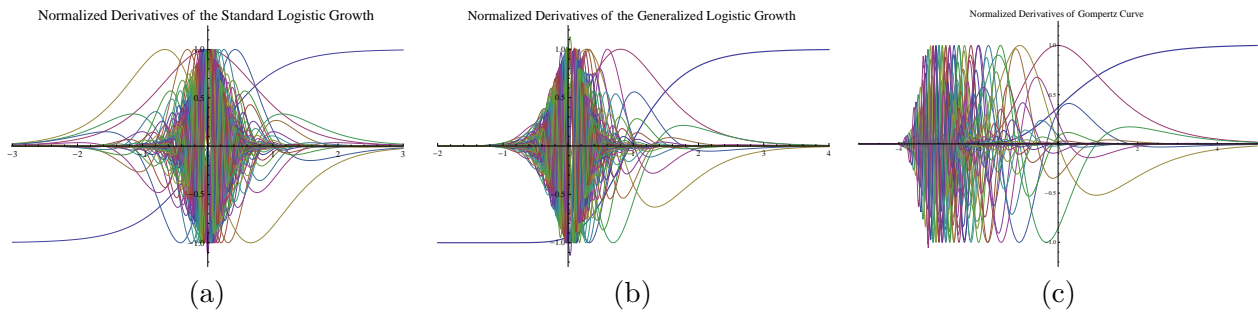


Figure 1. (a) Normalized derivatives of the standard logistic growth; (b) Normalized derivatives of the generalized logistic growth ($\beta = 1, k = 1, \nu = 1/5$) up to order 30. The behavior of the generalized logistic is more or less the same except that the zeros of even derivatives are not fixed. (c) The Gompertz function is the limit of the generalized logistic family, the critical point move to negative infinity.

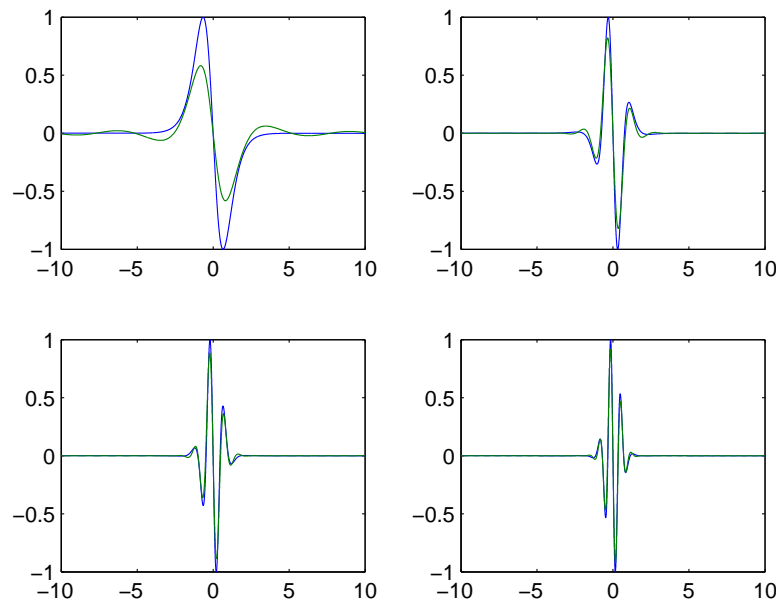


Figure 2. Comparison of the derivatives $f^{(n)}(t)$ of the standard logistic function with sinusoids of frequency ω_n .

increases. The property that ensures this is the “asymptotically constant phase” condition, given in Proposition 1 below.

The main result is the proposition below, whose proof will be published elsewhere. We claim that if $f(t)$ satisfies asymptotically constant phase and band-pass hypotheses, to be specified below, then the critical point is located at $t = 0$. Note that the asymptotically constant phase condition is trivially satisfied when $f(t)$ is even.

Proposition 1 *Let $f(t)$ be the first derivative of a sigmoidal curve $y(t)$ and $f^{(n)}(t)$ be its n th derivative. If*

the Fourier transform of $f(t)$ has the form $F(\omega) = |F(\omega)|e^{-i\alpha\omega}e^{i\psi(\omega)}$ where α is a constant

and $\psi(\omega)$ has horizontal asymptotes,

ii for $\omega > 0$, $\omega^n |F(\omega)|$ has a single maximum at ω_n and ω_n 's are unbounded,

iii the spectrum is localized in the sense that there are constants ω_a and ω_b (depending on n), such that

$$\lim_{n \rightarrow \infty} \int_{|\omega| < \omega_a} \omega^n |F(\omega)| d\omega = \lim_{n \rightarrow \infty} \int_{|\omega| > \omega_b} \omega^n |F(\omega)| d\omega = 0,$$

then the sigmoidal curve $y(t)$ has a critical point located at $t = \alpha$.

The first condition is the key “asymptotically constant phase” assumption. If $F(\omega)$ is as in (i), then an appropriate shift in time eliminates this phase factor and the phase of $F(\omega)$ becomes asymptotically constant. The requirement of the existence of a single maximum in (ii) is technical; what we need is ensure that, as n goes to infinity, the the Fourier spectrum of the n th derivatives be shifted to the region where the phase is nearly constant. Finally (iii) is again a technical assumption to ensure that the spectrum of the n th derivative is localized. The proof consists of expressing $|f^n(t)|$ using the Fourier inversion formula and proving that for large n , it is less than $|f^n(0)|$. Intermediate steps include the determination of the location of the spectrum of the n th derivative, from the equality $\omega/n = F(\omega)/F'(\omega)$. The behavior of the solutions is shown in Figure 3, for the standard logistic growth.

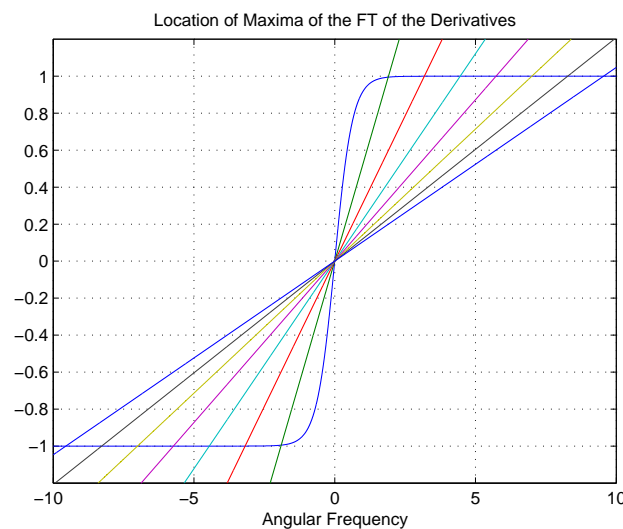


Figure 3. Graphical solution of the equation $\omega/n = F(\omega)/F'(\omega)$ for the standard logistic growth.

Finally we note that the asymptotically constant phase assumption leads to an intrinsic definition of even and odd components of a function $f(t)$, by choosing the origin of the time axis in such a way that the Fourier transform has asymptotically constant phase.

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