Numerical solutions of a one-dimensional sub-diffusive Gierer-Meinhardt model with controlled precision

Nehemie Nguimbous [1] Juan Pablo Ortiz Gil[2] Yana Nec [1]

[1]Thompson Rivers University [2]Universidad de Antioquia

Subdiffusive Gierer-Meinhardt Model

This study focuses on sub-diffusion with Gierer-Meinhardt reaction kinetics. The Gierer-Meinhardt model is a mathematical model that describes the formation of spatial patterns in biological systems. The sub-diffusive Gierer-Meinhardt model is given by

$$\partial_t^\gamma a = \epsilon^{2\gamma} a_{xx} - a + \frac{a^p}{h^q}, \qquad \tau \partial_t^\gamma h = D h_{xx} - h + \epsilon^{-\gamma}\frac{a^m}{h^s}, \quad -1 < x < 1, \quad t > 0, \tag{1}$$

$$a_x(\pm 1, t) = h_x(\pm 1, t) = 0, \quad a(x,0) = a_0(x), \quad h(x,0) = h_0(x), \tag{2}$$

where $a(x,t)$ and $h(x,t)$ are, respectively, the concentrations of the activator and inhibitor at position x and time t. Here, $\epsilon^{2\gamma}$ and D denote the constant diffusivities, τ is the reaction time constant, γ a real number such that $0 \le \gamma \le 1$ and the exponents (p, q, m, s) satisfy

$$p > 1,\ q > 0,\ m > 0,\ s \ge 0,\ \tfrac{p-1}{q} < \tfrac{m}{s+1}.$$

Solving the System: Matched Asymptotic Expansion

In order to fully capture the behavior of the activator and inhibitor, we scaled both the time and position variables, respectively from

$$t \ \text{ to } \ \sigma = \epsilon^{\gamma+1} t, \text{ and } x \ \text{ to } \ y_i = \frac{x - x_i(\sigma)}{\epsilon^\gamma},$$

where the x_is represent the positions where the activator and the inhibitor significantly interact. Matched asymptotic expansion involves the following steps:

- Approximate the concentrations a and h with power series:

$$A(y_i,\sigma) = a(x_i + \epsilon^\gamma y_i, \epsilon^{-\alpha}\sigma) = A_i^{(0)}(y_i,\sigma) + \epsilon^\gamma A_i^{(1)}(y_i,\sigma) + \epsilon^{2\gamma} A_i^{(2)}(y_i,\sigma) + \cdots \tag{3a}$$

$$H(y_i,\sigma) = h(x_i + \epsilon^\gamma y_i, \epsilon^{-\alpha}\sigma) = H_i^{(0)}(y_i,\sigma) + \epsilon^\gamma H_i^{(1)}(y_i,\sigma) + \epsilon^{2\gamma} H_i^{(2)}(y_i,\sigma) + \cdots \tag{3b}$$

- Substitute these approximations into the original system and truncate the resulting equations at a specific order (second order in our case):

$$\epsilon^{\alpha\gamma}\partial_\sigma^\gamma\left(A_i^{(0)} + \epsilon^\gamma A_i^{(1)}\right) \sim \partial_{y_i}^2\left(A_i^{(0)} + \epsilon^\gamma A_i^{(1)}\right) - \left(A_i^{(0)} + \epsilon^\gamma A_i^{(1)}\right) + \frac{A_i^{(0)p}}{H_i^{(0)q}} - q\epsilon^\gamma \frac{A_i^{(0)p}}{\left(H_i^{(0)q}\right)^2} H_i^{(1)} + p\epsilon^\gamma \frac{A_i^{(1)}}{H_i^{(0)q}}. \tag{4a}$$

$$\tau\epsilon^{\alpha\gamma}\partial_\sigma^\gamma\left(H_i^{(0)} + \epsilon^\gamma H_i^{(1)}\right) \sim \epsilon^{-2\gamma} D \partial_{y_i}^2\left(H_i^{(0)} + \epsilon^\gamma H_i^{(1)}\right)\left(H_i^{(0)} + \epsilon^\gamma H_i^{(1)}\right) + \epsilon^{-\gamma}\frac{A_i^{(0)m}}{H_i^{(0)s}}\left\{1 + \epsilon^\gamma\left(m\frac{A_i^{(1)}}{A_i^{(0)}} - s\frac{H_i^{(1)}}{H_i^{(0)s}}\right)\right\}. \tag{4b}$$

- Collect terms of the same order: the first and second order terms are collected separately to form the first and second order problems.

First Order Problem

For $\alpha = \gamma + 1$, and upon collecting terms of first order in equations (4a) and (4b), we respectively obtain:

$$\partial_{y_i}^2 A_i^{(0)}(y_i) - A_i^{(0)} + \frac{A_i^{(0)p}}{H_i^{(0)q}} = 0, \qquad \partial_{y_i}^2 H_i^{(0)} = 0, \qquad -\infty < y_i < \infty. \tag{5}$$

Upon solving this system, one obtains

$$H_i^{(0)}(y_i) = \bar{H}_i(\sigma) = g(\sigma), \qquad A_i^{(0)}(\sigma) = \bar{H}_i^{\mathrm{B}}(\sigma) u(y_i), \tag{6}$$

with g being a function of the variable σ, $\mathrm{B} = \dfrac{q}{p-1}$ and

$$u(y) = \left(\frac{p+1}{2}\operatorname{sech}^2\frac{(p-1)y}{2}\right)^{\frac{1}{p-1}}.$$

Second Order Problem

Once collecting terms of second order in equations (4a) and (4b) respectively, and upon post-processing these equations, we obtain the following differential-algebraic system:

$$-\left|\frac{dx_i}{d\sigma}\right|^\gamma \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) = \frac{q b_m}{(p+1)\bar{H}_i}\left(\sum_{\substack{j=1\\ j\neq i}}^{n} \bar{H}_i^{\mathrm{B}\,m-s} G_x(x; x_j) + \bar{H}^{\mathrm{B}\,m-s}\langle G_x\rangle_i\right) f(p;\gamma), \tag{7a}$$

$$\bar{H}_i(\sigma) = h^{(0)}(x,t) = b_m \sum_{i=1}^{n} \bar{H}_i^{\mathrm{B}\,m-s} G(x; x_i), \qquad b_m = \int_{-\infty}^{\infty} u^m dy, \tag{7b}$$

$$f(p;\gamma) = \left(\int_{-\infty}^{\infty} u^{p+1} dy\right) \Big/ \left(\int_{-\infty}^{\infty} \frac{du}{dy}\mathcal{D}_y^\gamma u dy\right). \tag{7c}$$

Here, G is the solution of

$$DG_{xx} - G = -\delta(x - x_i), \quad -1 < x < 1, \quad G_x(\pm 1; x_i) = 0,$$

with D being a constant and

$$\langle G_x\rangle_i = \frac{1}{2}\Big(G_x^-(x_i^-; x_i) + G_x^+(x_i^+; x_i)\Big), \tag{8a}$$

$$\mathcal{D}_y^\gamma u(y) = \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right)\frac{1}{\Gamma(-\gamma)}\int_0^\infty \left\{u(y) - u\left(y + \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right)\xi_1\right)\right\}\left(\frac{1}{\xi_1}\right)^{\gamma+1} d\xi_1, \tag{8b}$$

Solutions

Upon solving the first equation of (7b) at $x = x_i$, and for $i = 1$ (first spike), we have

$$\bar{H}_1 = \left(b_m G(x_1; x_1)\right)^{\frac{-1}{\mathrm{B}\,m-1-s}}.$$

Substituting this result into the second equation in (6) and computing both $A_1^{(0)}$ and $H_1^{(0)} = \bar{H}_1$ lead to the following solutions:

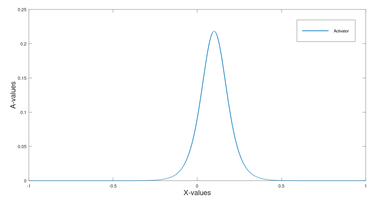

Figure 1. Activator concentration for $p = 2$.

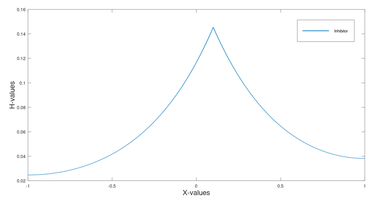

Figure 2. Inhibitor concentration for $p = 2$.

Computing $\mathcal{D}_t^\gamma u$

In order to compute $\dfrac{dx_i}{d\sigma}$ and track the evolution of x_i in (7a), we have to compute $\mathcal{D}_t^\gamma u$. We first start by eliminating the singularity at $\xi_1 = 0$ by regularizing its expression. This leads to

$$\mathcal{D}_t^\gamma u(t) = \frac{t_\infty^{-\gamma}}{\Gamma(1-\gamma)}\Big(u(t) - u(t - t_\infty)\Big) + \frac{t_\infty^{1-\gamma}}{\Gamma(2-\gamma)}u'(t - t_\infty) - \frac{1}{\Gamma(2-\gamma)}\int_t^{t-t_\infty} u''(y)(t-y)^{1-\gamma}\, dy.$$

The first two terms of $\mathcal{D}_t^\gamma u$ are known values, except for the third one, named I, which is the integral of a complex function and is impossible to compute analytically. Moreover, I depends on three parameters: p, γ, and t. The number of subdivisions required to compute I varies with these parameters as well. We aim to predict the number of subdivisions n required to compute I with a precision of 10^{-10}.

Procedure: Finding the Number of Subdivisions Required to Compute I With a Precision of 10^{-10}

1. Establish a correspondence between the number of subdivisions n and the integral I

$$n_{(t,p,\gamma)} \to I_{(t,p,\gamma)}(n).$$

I is computed using the composite Simpson method:

$$\int_a^b f(x)dx \approx \frac{h}{3}\sum_{i=0}^{n/2-1}\Big[f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})\Big], \quad h = \frac{b-a}{n}.$$

2. Our goal being to compute I with a controlled precision, it makes sense to establish a correspondence between the number of subdivisions n and the residual R as well:

$$n_{(t,p,\gamma)} \to R_{(t,p,\gamma)}(n).$$

This calculation is for (t, p, γ) values within the ranges:
$\{0.1, 1, 5\} \times \{1.5, 2, 2.5, \ldots, 4.5\} \times \{0.1, 0.2, 0.3, \ldots, 0.9\}$.

3. However, since the residual function we obtained is not a well-known function, we fit it using a variant of the hyperbolic-arctangent function, denoted $f = c_1 \times \operatorname{atanh}(n) + c_2$, with c_1 and c_2 being parameters used to minimize the distance between the residual and the fitting curve. Consequently,

$$n_{(t,p,\gamma)} \to f_{(t,p,\gamma)}(n) \sim R_{(t,p,\gamma)}.$$

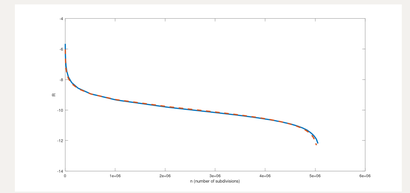

Figure 3. Specific case for $t = 1$, $p = 4$, and $\gamma = 0.8$. The x-axis represents the number of subdivisions and the y-axis the logarithm of the corresponding residuals. The solid curve represents the numerical results while the dashed one represents the fitting curve.

4. To find the number of subdivisions based on a specific residual (the inverse path), we determine the inverse f^{-1} of f such that

$$f_{(t,p,\gamma)}^{-1}(R) \to n_{(t,p,\gamma)},$$

where $n_{(t,p,\gamma)}$ and $R_{(t,p,\gamma)}$ represent the number of subdivisions and the corresponding residual values for specific t, p, and γ values.

Verification of the Accuracy

The table below displays the approximated number of subdivisions obtained using the inverse of the fitting curve for $t = 0.1$ and some discrete values of p and γ.

g/p	1.5	2.0	2.5	3	3.5	4	4.5
0.1	35065	51414	61242	73570	80108	86651	93201
0.3	214565	342453	430919	519457	563799	608143	686814
0.5	1674913	2341552	3365120	3698389	4365537	5033725	5366720
0.7	4662043	28071526	37953058	45866233	54342976	60260601	68207443
0.9	76155108	727802772	1015373018	1025834015	1025841827	1025918580	1025859852

Table 1. Approximated number of subdivisions for $t = 0.1$

As a test for the effectiveness of our method, we computed the absolute value of the difference between $\mathcal{D}_t^\gamma u\Big|_{N=2n}$ and $\mathcal{D}_t^\gamma u\Big|_{N=n}$ for some values of t. This leads to the following table:

t	3.6	3.7	3.8	3.9	4.0
$error$	-1.784137e-010	-1.721758e-010	-1.664409e-010	-1.605218e-010	-1.547047e-010
t	4.1	4.2	4.3	4.4	4.5
$error$	-1.494032e-010	-1.443059e-010	-1.395319e-010	-1.351115e-010	-1.307046e-010

Table 2. Error file for $p = 2$ and $\gamma = 0.7$.

nguimbousn21@mytru.ca