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Sobolev Gradient Approach for Huxley and Fisher Models for Gene Propagation

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ABSTRACT

The application of Sobolev gradient methods for finding critical points of the Huxley and Fisher models is demonstrated. A comparison is given between the Euclidean, weighted and unweighted Sobolev gradients. Results are given for the one dimensional Huxley and Fisher models.

Keywords: Sobolev Gradient; Huxley and Fisher Models; Descent Methods

1. Introduction

The numerical solution of nonlinear problems is a topic of basic importance in numerical mathematics, as stated in [1]. It has been a subject of extensive investigation in the past decades, thus having vast literature [2-5]. The most widespread way of finding numerical solutions is first discretizing the given problem, then solving the arising system of algebraic equations by a solver which is generally some iterative method. For nonlinear problems most often Newton's method is used. However, when the work of compiling the Jacobians exceeds the advantage of quadratic convergence, one may prefer gradient type iterations including steepest descent or conjugate gradients. An important example in this respect is the Sobolev gradient technique, which is relying on descent methods. The Sobolev gradient technique presents a general efficient preconditioning approach where the preconditioners are derived from the representation of the Sobolev inner product.

Sobolev gradients have been used for ODE problems [6,7] in a finite-difference setting, PDEs in finite-difference [7,8] and finite-element settings [9], minimizing energy functionals associated with Ginzburg-Landau models in finite-difference [10] and finite-element [11,12] settings and related time evolutions [13], the electrostatic potential equation [1], nonlinear elliptic problems [14], semilinear elliptic systems [15], simulation of Bose-Einstein condensates [16], inverse problems in elasticity [17] and groundwater modelling [18].

A detailed analysis regarding the construction and the application of Sobolev gradients can be found in [6]. For a quick overview of Sobolev gradients, applications and some open problems in the subject we refer to [19].

Sobolev gradients are also useful for preconditioning for linear and nonlinear problems. Sobolev preconditioning [20] has been tested on some first order and second order linear and nonlinear problems and it is found comparable in terms of efficiency and stability with other methods such as Newton's method and Jacobi method. For differential equations with nonuniform behavior on long intervals, "Sobolev gradients have proved to be effective if we divide the interval of interest into pieces and take a recursive approach (cf. [21])". Sobolev gradients have interesting applications in the field of geometric modelling [22]. It has been proved therein that the Sobolev gradient is a very useful tool for minimizing functionals that pertain to the length of curves, curvatures, surface area etc. Recently, the paper [23] has shown the possible applications of Sobolev gradient technique for systems of Differential Algebraic Equations.

The idea of a weighted Sobolev gradient has been introduced by W. T. Mahavier in [7]. The weighted Sobolev gradient has successfully exhibited its effectiveness in dealing with linear and nonlinear singular differential equations with regular and some typically irregular singularities. Weighted gradients have also been used for DAEs and it turns out that weighted Sobolev gradients outperform unweighted Sobolev gradients in many situations.

In the field of gene technolog, Modelling of gene frequencies is of the prospective area of research. Its applications can be seen in livestocks and agricultural crops. By the modification of their genes, they can be made more resistive to infection and to produce more yield. To derive historical patterns of migration, archaeologists are expecting that study of the entire human genetic material, will facilitate to map geographical distribution of signature genes. By using gene technology, many bacteria have been developed to prescribed antibiotics. From medical point of view, it is important to study the genetic background of diseases, with implications in diagnosis, treatment and drug development. In order to make use of genetic population data, we need to understand the dynamics of gene patterns through the population.

2. Fisher and Huxley Models

In the 1930s, number of authors proposed reaction-diffusion equations to model changing gene frequencies in a population. One of the earliest and best known such equations was that of Fisher. In his paper in 1937 [24], he proposed a reaction-diffusion equation with quadratic source term that models the spread of a recessive advantageous gene through a population *i.e.*;

$$p_t = \kappa p_{xx} + mp(1-p) \tag{1}$$

where p is the frequency of the new mutant gene, κ is the coefficient of diffusion, and m is the intensity of selection in favor of the mutant gene. The equation predicts a wave front of increasing allele frequency, propagating through a population. The quadratic logistic term of Fisher's equation is more appropriate for asexual species.

Fisher's assumptions for a sexually reproducing species lead to a Huxley reaction-diffusion equation, with cubic logistic source term for the gene frequency of a mutant advantageous recessive gene. Huxley's equation is given by

$$p_t = \kappa p_{xx} + \alpha p^2(1-p). \tag{2}$$

3. Review of Sobolev Gradient Methods

In this section we discuss the Sobolev gradient and steepest descent. A detailed analysis regarding the construction of Sobolev gradients can be seen in [6].

Let us consider n is a positive integer and G is a real valued C^1 function on R^n. We can define its gradient ∇G as

$$\lim_{t\to 0}\frac{1}{t}\big(G(x+th)-G(x)\big) = G'(x)h = \langle h, \nabla G(x)\rangle_{R^n},\ x,h\in R^n. \tag{3}$$

For G as above, but with $\langle .,.\rangle_S$ an inner product on R^n different from the standard inner product $\langle .,.\rangle_{R^n}$, there is a function $\nabla_S G : R^n \to R^n$ so that

$$G'(x)h = \langle h, \nabla_S G(x)\rangle_S\ x,h\in R^n. \tag{4}$$

The linear functional $G'(x)$ can be represented using any inner product on R^n. Let us call $\nabla_S G$ is the gradient of G with respect to the inner product $\langle .,.\rangle_S$ and it can be seen that $\nabla_S G$ has the same properties as ∇G.

By applying a linear transformation, we have

$$A : R^n \to R^n,$$

we can relate these two inner products

$$\langle x, y\rangle_S = \langle x, Ay\rangle_{R^n}$$

for $x, y \in R^n$, and by a reflection

$$(\nabla_S G)(x) = A^{-1}\nabla G(x),\ x\in R^n. \tag{5}$$

For each $x\in R^n$ an inner product is assciated

$$\langle .,.\rangle_x$$

on R^n. Thus for $x \in R^n$, define $\nabla_x G : R^n \to R^n$ such that

$$G'(x)h = \langle h, \nabla_x G(x)\rangle_x\ x,h\in R^n. \tag{6}$$

When gradient is defined in a finite or infinite dimensional Sobolev space we call it Sobolev gradient. Steepest descent can be classified into two categories: the one is discrete and other continuous steepest descent. Let G be a real-valued C^1 function, defined on a Hilbert space H and $\nabla_S G$ be its gradient with respect to the inner product $\langle .,.\rangle_S$ defined on H. Discrete steepest descent method is a process of constructing a sequence $\{x_i\}$ so that x_0 is given and

$$x_i = x_{i-1} - \delta_i(\nabla G)(x_{i-1}),\ i = 1,2,\cdots. \tag{7}$$

where for each i, δ_i is chosen so that

$$G\big(x_{i-1} - \delta_i(\nabla G)(x_{i-1})\big) \tag{8}$$

is minimal in some appropriate sense. In continuous steepest descent we construct a function $z:[0,\infty)\to H$ so that

$$\frac{\mathrm{d}z}{\mathrm{d}t} = -\nabla G(z(t)),\ z(0) = z_{\text{initial}}. \tag{9}$$

Under suitable conditions on G, $z(t)\to z_\infty$ where $G(z_\infty)$ is the minimum value of G.

Continuous steepest descent is interpreted as a limiting case of discrete steepest descent. So (7) can be considered as a numerical method for approximating solutions to (9). Continuous steepest descent gives a theoretical starting point for proving convergence of discrete steepest descent. Using (7) one seeks $u=\lim_{i\to\infty} x_i$, so that

$$G=0 \text{ or } (\nabla_S G)(u)=0 \tag{10}$$

and using (9) one seeks $u=\lim_{t\to\infty} z_t$ so that (10) holds. Two groups of problems can be cast in terms of determining the functional G. The first group deals with those problems where G serves as an energy functional. For cases of the use of G as an energy functional see [6,10,12,13].

Now we solve these problems by using various descent techniques.

3.1. Using Second Order Operators

Consider Fisher's equation

$$p_t=\kappa p_{xx}+mp(1-p) \tag{11}$$

in the space domain Ω which is the interval [0,2]. We use Neumann boundary conditions, *i.e.* $p_x=0$.

Now a suitable finite difference discretization will be done. We work with a finite-dimensional vector $p\in R^M$ on the interval. We will denote by L_2 the vector space R^M equipped with the usual inner product $\langle p,q\rangle=\sum_i p(i)q(i)$. The operators $D_0,D_1,D_2:R^M\to R^{M-2}$ are defined by

$$D_0(p)(i)=p(i+1) \tag{12}$$

$$D_1(p)(i)=\frac{p(i+2)-p(i)}{2\delta_x} \tag{13}$$

$$D_2(p)(i)=\frac{\left(p(i+2)-2p(i+1)+p(i)\right)}{\delta_x^2} \tag{14}$$

for $i=1,2,\cdots,M-2$ and where $\delta_x=\dfrac{2}{M-1}$ is the spacing between the nodes. D_0 just picks up the points in the grid which are not on the endpoints. D_1 and D_2 are standard central difference formulas for estimating the first and second derivatives. The choice of difference formula is not central to the theoretical development in this paper, other choices would also work. The numerical version of the problem of evolving from one time t to a time $t+\delta_t$ is to solve

$$\frac{p-f}{\delta_t}=\kappa p_{xx}+mp(1-p) \tag{15}$$

where f in the equation is p at the previous time and p is the p desired at the next time level. In terms of operators problem can be written as

$$D_0\left((1-m\delta_t)p+m\delta_t p^2-f\right)-\kappa\delta_t D_2(p)=0. \tag{16}$$

The time-step δ_t must be prescribed small enough ti have $1-m\delta_t$. We can put the solution of this problem in other terms of minimizing a functional via steepest descent. Define $L\in R^{M-2}$ by

$$L(p)=D_0\left((1-m\delta_t)p+m\delta_t p^2-f\right)-\kappa\delta_t D_2(p) \tag{17}$$

which is zero when the we have the desired p. The functional

$$F(p)=\frac{\langle L(p),L(p)\rangle}{2} \tag{18}$$

has a minimum of zero when $L(p)$ is zero so we will look for the minimum of this functional. This functional is a convex functional that guarantees global minima in Ω, a solution to problem (11). The aim is to find the gradient of a convex functional $F(p)$ associated with the problem and use this gradient in steepest descent minimization process to finding the zero of the functional, that is the minimum of $F(u)$ and the solution of the original problem.

3.2. Gradients and Minimization

The gradient $\nabla F(p)\in R^M$ of a functional $F(p)$ in L_2 is found by solving

$$F(p+h)=F(p)+\langle\nabla F(p),h\rangle+O(h^2) \tag{19}$$

for test function h. The gradient points in the direction of greatest increase of the functional. The direction of greatest decrease of the functional is $-\nabla F(p)$. This is the basis of steepest descent algorithms. One can reduce $F(p)$ by replacing an initial p with $p-\lambda\nabla F(p)$ where the step size λ is a positive number. This can be done repeatedly until either $F(p)$ or $\nabla F(p)$ is less than some specified tolerance. We desire a finite-dimensional analogue to the original problem in which $u_x=0$ on the endpoints of the interval. So, we use a projection $\pi:R^M\to R^M$ which projects vectors in R^M onto the subspace in which the gradient vanishes at the boundary. Rather than using $\nabla F(p)$, we will use $\pi\nabla F(p)$. The steepest descent algorithm in this new space now looks like

1) Calculate $\nabla F(p)$;

2) Update p by $p\to p-\lambda\pi\nabla F(p)$ where λ is some fixed positive number;

3) Repeat.

In this particular case,

$$\pi\nabla F(p)=\pi\left[\left(1-m\delta_t+2m\delta_t p^2\right)D_0^t L(p)-\kappa\delta_t D_2^t L(p)\right] \tag{20}$$

gives the desired gradient for steepest descent in L_2. The operators $D_0^t,D_2^t:R^{M-2}\to R^M$ are the adjoints of D_0 and D_2 respectively. The Sobolev gradient approach to the problem of minimizing functionals is to do the minimization in Sobolev spaces which correspond to the problem. In this paper only discrete Sobolev spaces are used. We define two such spaces in which the minimization can be compared to minimization in L_2. We are prompted to consider the space H_2^2 which is R^M with the inner product

$$(p,q)_s = \langle D_0(p), D_0(q)\rangle + \langle D_1(p), D_1(q)\rangle + \langle D_2(p), D_2(q)\rangle \tag{21}$$

because $L(p)$ and $F(p)$ have D_{11} in them. We also follow the technique of Mahavier for solving differential equations for this we define a new inner product $\hat{H}_2^2$ as R^M equipped with the inner product

$$(p,q)_w = (1-m\delta_t)^2 \langle D_0(p), D_0(q)\rangle + \langle D_1(p), D_1(q)\rangle + (\kappa\delta_t)^2 \langle D_2(p), D_2(q)\rangle \tag{22}$$

because this takes into account the coefficients of D_1 and D_0 in $L(p)$ and $F(p)$. The desired Sobolev gradients $\pi\nabla_s F(p)$, $\pi\nabla_w F(p)$ in H_2^2 and $\hat{H}_2^2$ are found by solving

$$\pi\left(D_0^t D_0 + D_1^t D_1 + D_2^t D_2\right)\pi\nabla_s F(p) = \pi\nabla F(p) \tag{23}$$

$$\pi\left((1-m\delta_t)^2 D_0^t D_0 + D_1^t D_1 + (\delta_t)^2 D_2^t D_2\right)\pi\nabla_w F(p) = \pi\nabla F(p) \tag{24}$$

respectively. Here D_1^t is the adjoint of D_1. Following the same line we construct the gradients for Huxley's model.

Numerical experiments for the solution of Fisher and Huxley's equations were conducted as follows. A system of M nodes was set up with $p(0,x) = 0.2\exp(-4x^2)$ *i.e.* the initial conditions. The internodal spacing was δ_x. The value of κ was set to 1 for all the experiments. We chose $m = \frac{16\alpha}{27}$ with $\alpha = 1$ so that both source functions has the same maximum value. The function p was then evolved. The updated value of p for a given time step was considered to be correct when the infinity norm of $\pi L(p)$ was less than 10^{-7}. We set $\delta_t = 0.4$ for the time increment. For the gradients in H_2^2 and $\hat{H}_2^2$ we used the same step size regardless of the nodal spacing. The total number of minimization steps for fifteen time steps, the largest value of λ that can be used and CPU time were recorded in **Tables 1** and **2**.

From the tables we see that the results in H_2^2 are far better than L_2, in fact there is no L_2 convergence for $M \geq 101$. The best results are in the weighted Sobolev space $\hat{H}_2^2$. When we perform minimization in $\hat{H}_2^2$ the convergence is three times faster for solving Huxley's model than from that H_2^2.

3.3. Using the Associated Functional

Here we suggest another approach, in order to avoid second order operators. Once again consider the problem

$$p_t = \kappa p_{xx} + mp(1-p) \tag{25}$$

with Neumann boundary conditions. We think of the M nodes as dividing up [0,2] into $M-1$ subintervals. The

Table 1. Numerical results of steepest descent in L_2, H_2^2, $\hat{H}_2^2$ using $\delta_t = 0.4$ over 15 time steps using second order operators for Fisher's model.

λ			iterations			CPUs			M
L_2	H_2^2	$\hat{H}_2^2$	L_2	H_2^2	$\hat{H}_2^2$	L_2	H_2^2	$\hat{H}_2^2$	-
1.5×10^{-7}	1.2	0.7	>164 100	487	238	>6 403.4	1.140	0.562	51
-	1.2	0.7	-	431	193	-	5.827	2.734	101
-	1.2	0.7	-	398	186	-	36.525	17.622	201
-	1.2	0.7	-	369	172	-	246.32	123.32	401

Table 2. Numerical results of steepest descent in L_2, H_2^2, $\hat{H}_2^2$ using $\delta_t = 0.4$ over 15 time steps using second order operators for Huxley's model.

λ			iterations			CPUs			M
L_2	H_2^2	$\hat{H}_2^2$	L_2	H_2^2	$\hat{H}_2^2$	L_2	H_2^2	$\hat{H}_2^2$	-
1.2×10^{-5}	1.6	1.2	>2164 100	337	87	>4 003.4	0.828	0.234	51
-	1.6	1.2	-	273	88	-	4.093	1.281	101
-	1.6	1.2	-	257	81	-	27.011	8.311	201
-	1.6	1.2	-	249	81	-	186.14	59.46	401

operators $D_0 : R^M \to R^{M-1}$ estimates p on the interval by

$$D_0(p)(i) = \frac{1}{2}\big(p(i) + p(i+1)\big) \tag{26}$$

for $i = 1, 2, \cdots, M-1$. $D_1 : R^M \to R^{M-1}$ estimates the first derivative on the intervals by

$$D_1(p)(i) = \frac{1}{\delta_x}\big(p(i+1) - p(i)\big) \tag{27}$$

for $i = 1, 2, \cdots, M-1$ and where δ_x is the internodal spacing. The associated functional for a finite dimensional version of the problem with discrete time steps is given by

$$G(p) = \left\langle D_0\left(p^2/2 - fp\right), 1\right\rangle + m\delta_t\left\langle D_0\left(p^3/3 - p^2/2\right), 1\right\rangle + \delta_t\frac{\kappa}{2}\left\langle D_1(p), D_1(p)\right\rangle \tag{28}$$

and we wish to minimize the functional $G(p)$ until $\pi\nabla G(p)$ is smaller than some set tolerance. $G(p)$ has a minimum when the gradient

$$\pi\nabla G(p) = \pi D_0^t D_0\left(p - f + m\delta_t p^2 - m\delta_t p\right) - \kappa\delta_t D_1^t D_1(p) \tag{29}$$

is equal to zero, and this might be considered the condition for finding p at the next time step. Here $D_0^t, D_1^t : R^{M-1} \to R^M$ are the adjoins of D_0, D_1 respectively. We want to minimize this functional in L_2, and also in some new inner product spaces H_1^2, $\dot{H}_1^2$, defined via

$$\langle p, q\rangle_s = \langle D_0 p, D_0 q\rangle + \langle D_1 p, D_1 q\rangle. \tag{30}$$

$$\langle p, q\rangle_w = (1 - m\delta_t)\langle D_0 p, D_0 q\rangle + \kappa\delta_t\langle D_1 p, D_1 q\rangle. \tag{31}$$

Once again numerical experiments are conducted by using the same parameters as defined earlier. for solution of Fisher and Huxley models were conducted as follows. The updated value of p for a given time step was considered to be correct when the infinity norm of $\pi\nabla G(p)$ was less than 10^{-7}. We set $\delta_t = 0.4$ for the time increment. For the gradients in H_1^2 and $\dot{H}_1^2$ we used the same step-size regardless of the nodal spacing. The total number of minimization steps for fifteen time steps, the largest value of λ that can be used and CPU time were recorded in **Tables 3** and **4**.

We note that the finer the spacing the less CPU time the Sobolev gradient technique uses in comparison to the usual steepest descent method. The step size for minimization in L_2 has to decrease as the spacing is refined. From the tables one can see that the results in H_1^2 are far better than L_2 and results in the space $\dot{H}_1^2$ are the best.

3.4. Using First Order Operators

Once again consider the problem

$$p_t = \kappa p_{xx} + mp(1-p).$$

Table 3. Numerical results of steepest descent in L_2, H_1^2, $\dot{H}_1^2$ using $\delta_t = 0.4$ over 15 time steps using the associated functional for the Fisher's model.

λ			iterations			CPUs			M
L_2	H_1^2	$\dot{H}_1^2$	L_2	H_1^2	$\dot{H}_1^2$	L_2	H_1^2	$\dot{H}_1^2$	-
2.0×10^{-3}	1.2	0.9	88 135	144	99	0.750	0.078	0.047	51
5.0×10^{-4}	1.2	0.9	349 444	141	97	4.718	0.2343	0.156	101
1.2×10^{-4}	1.2	0.9	1449 408	143	97	36.197	0.8904	0.547	201
3.0×10^{-5}	1.2	0.9	5784 213	142	96	260.55	3.328	2.046	401

Table 4. Numerical results of steepest descent in L_2, H_1^2, $\dot{H}_1^2$ using $\delta_t = 0.4$ over 15 time steps using the associated functional for the Huxley's model.

λ			iterations			CPUs			M
L_2	H_1^2	$\dot{H}_1^2$	L_2	H_1^2	$\dot{H}_1^2$	L_2	H_1^2	$\dot{H}_1^2$	-
2.0×10^{-3}	1.2	1.0	54 621	113	63	0.4686	0.0624	0.0312	51
5.0×10^{-4}	1.2	1.0	215 093	113	62	2.9213	0.203	0.1249	101
1.2×10^{-4}	1.2	1.0	892 470	113	61	22.51	0.7498	0.4218	201
3.0×10^{-5}	1.2	1.0	3570 492	113	61	163.55	2.796	1.5622	401

Let us write this as a system of two equations

$$p_t = mp - mp^2 + \kappa q_x \quad (32)$$

$$q - p_x = 0. \quad (33)$$

A finite-dimensional version which is first order in time is to solve

$$D_0\left(\left(1-m\delta_t\right)p + m\delta_t p^2 - f\right) - \kappa\delta_t D_1\left(q\right) = 0 \quad (34)$$

$$D_1\left(p\right) - D_0\left(q\right) = 0. \quad (35)$$

We define functions

$$S = D_0\left(\left(1-\delta_t\right)p + \delta_t p^2 - f\right) - \kappa\delta_t D_1\left(q\right) \quad (36)$$

$$T = D_1\left(p\right) - D_0\left(q\right). \quad (37)$$

The functional for the problem is

$$F\left(p,q\right) = \frac{1}{2}\langle S,S\rangle + \frac{1}{2}\langle T,T\rangle. \quad (38)$$

The problem is considered to be solved when $F\left(p,q\right)$ has been minimized, that is, when $S = T = 0$ or infinity norms of S and T are less than some desired tolerance. The L_2 gradients are

$$\nabla F_p\left(p,q\right) = \pi\left[\left(\left(1-m\delta_t\right) + 2m\delta_t p\right)D_0^t\left(S\right) + D_1^t\left(T\right)\right] \quad (39)$$

$$\nabla F_q\left(p,q\right) = -\kappa\delta_t D_1^t\left(S\right) - D_0^t\left(T\right). \quad (40)$$

The Sobolev gradients in H_1^2 are found by solving

$$\pi\left(D_0^t D_0 + D_1^t D_1\right)\nabla_s F_p\left(p,q\right) = \pi\nabla F_p\left(p,q\right) \quad (41)$$

$$\left(D_0^t D_0 + D_1^t D_1\right)\nabla_s F_q\left(p,q\right) = \nabla F_q\left(p,q\right). \quad (42)$$

We want to minimize this functional in L_2, H_1^2 and also in the new inner product spaces $\tilde{H}_1^2$ and $\breve{H}_1^2$. To define these new inner products we follow the technique of Mahavier [7] for singular differential equations and use weighted Sobolev spaces $\tilde{H}_1^2$ and $\breve{H}_1^2$ such that

$$\langle p,q\rangle_{\tilde{S}} = \left\langle\left(1-\delta_t\right)D_0\left(p\right),\left(1-\delta_t\right)D_0\left(q\right)\right\rangle + \left\langle D_1\left(p\right),D_1\left(q\right)\right\rangle \quad (43)$$

$$\langle p,q\rangle_{\breve{S}} = \left\langle D_0\left(p\right),D_0\left(q\right)\right\rangle + \left\langle \kappa\delta_t D_1\left(p\right),\kappa\delta_t D_1\left(q\right)\right\rangle \quad (44)$$

and new gradients $\nabla_{w1}F\left(p,q\right),\nabla_{w2}F\left(p,q\right)$ are found by solving

$$\pi\left(\left(1-m\delta_t\right)^2 D_0^t D_0 + D_1^t D_1\right)\pi\nabla_{w1}F_p\left(p,q\right) = \pi\nabla F_p\left(p,q\right) \quad (45)$$

$$\left(D_0^t D_0 + \left(\kappa\delta_t\right)^2 D_1^t D_1\right)\nabla_{w2}F_q\left(p,q\right) = \nabla F_q\left(p,q\right). \quad (46)$$

Numerical experiments are conducted by using the same parameters as defined in Section 2.2. The updated value of p for a given time step was considered to be correct when the infinity norms of both s and T were less than 10^{-7}. We set $\delta_t = 0.4$ for the time increment. The total number of minimization steps for fifteen time steps, the largest value of λ that can be used and CPU time were recorded in **Tables 5** and **6**.

Table 5. Numerical results of steepest descent in L_2, H_1^2 and $\tilde{H}_1^2$, $\breve{H}_1^2$ using $\delta_t = 0.4$ over 15 time steps using first order operators for the Fisher's model.

λ			iterations			CPUs			M
L_2	H_1^2	$\tilde{H}_1^2$, $\breve{H}_1^2$	L_2	H_1^2	$\tilde{H}_1^2$, $\breve{H}_1^2$	L_2	H_1^2	$\tilde{H}_1^2$, $\breve{H}_1^2$	-
8.0×10^{-4}	0.9	0.7	2745 683	30 494	16 221	47.34	3.359	2.7	51
2.0×10^{-4}	0.9	0.7	20436 186	95 571	43 389	578.48	17.33	11.16	101
5.0×10^{-5}	0.9	0.7	-	212 550	47 415	-	92.172	49.48	201
1.2×10^{-5}	0.9	0.7	-	59 348	39 556	-	507.45	258.75	401

Table 6. Numerical results of steepest descent in L_2, H_1^2 and $\tilde{H}_1^2$, $\breve{H}_1^2$ using $\delta_t = 0.4$ over 15 time steps using first order operators for the Huxley's model.

λ			iterations			CPUs			M
L_2	H_1^2	$\tilde{H}_1^2$, $\breve{H}_1^2$	L_2	H_1^2	$\tilde{H}_1^2$, $\breve{H}_1^2$	L_2	H_1^2	$\tilde{H}_1^2$, $\breve{H}_1^2$	-
8.0×10^{-4}	0.9	0.5	2500 498	36 675	20 125	46.83	3.125	2.25	51
2.0×10^{-4}	0.9	0.5	17169 941	72 158	47 371	525.14	12.03	8.61	101
5.0×10^{-5}	0.9	0.5	-	115 047	80 785	-	55.83	36.45	201
1.2×10^{-5}	0.9	0.5	-	42 214	1 21 167	-	351.94	169.25	401

We note that the finer the spacing the less CPU time the Sobolev gradient technique uses in comparison to the usual steepest descent. For the Fisher and Huxley model the same step size λ can be used for all spacings δ when minimizing in the appropriate Sobolev space. The step-size for minimization in L_2 has to decrease as the spacing is refined.

From the table one can see that the results in H_1^2 are far better than L_2 and results in the space $\tilde{H}_1^2$, $\breve{H}_1^2$ are the best.

4. Summary and Conclusions

In this paper, we have presented minimization schemes for the Huxley and Fisher's models based on the Sobolev gradient technique [6]. The Sobolev gradient technique is computationally more efficient than the usual steepest descent method as the spacing of the numerical grid is made finer. Choosing an optimal inner product can improve the performance with respect to which the Sobolev gradient works better. it is still an open question what the absolutely optimal inner product is, and it is possible that different inner products might not make large differences in computational performance in all cases. One advantage of steepest descent is that it converges even for a poor initial guess. The Sobolev gradient methods presented here converge even for rough initial guess or jumps in the initial guess.

In **Figures 1** and **2**, we display the numerical solution of two models with the same localized Gaussian clump of the mutant alleles, contained within the region $0 \le x \le 2$ by zero flux boundary conditions *i.e.*; $p_x = 0$. We choose $m = \frac{16\alpha}{27}$ with $\alpha = 1$ and diffusion coefficient $\kappa = 0.005$ so that the differences in the source term can be highlighted in comparison to the diffusion effects. For both models the mutant gene frequency can be seen to increase at the origin and then spread throughout the range. As expected mutant take over is greatly retarded in the Huxley model compared to the Fisher model. So, for asexually reproducing population, a cubic source term is more appropriate than a quadratic source term and for sexually reproducing population, Fisher's equation is more appropriate.

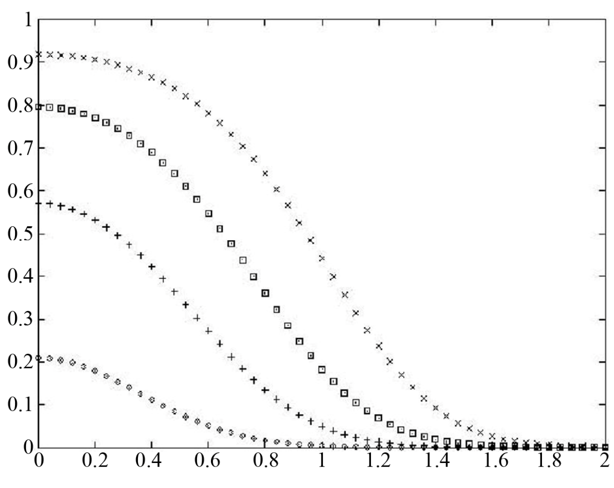

Figure 1. Graph of solution of Fisher's equation for *t* = 0.1, 3, 5, 7.

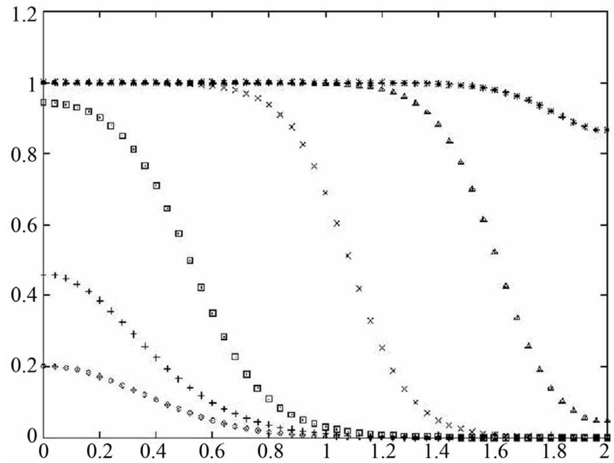

Figure 2. Graph of solution of Huxley's equation for *t* = 0.1, 5, 10, 20, 30, 37.

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