BEHAVIOR OF DIFFERENT NUMERICAL SCHEMES FOR POPULATION GENETIC DRIFT PROBLEMS

MINXIN CHEN∗, CHUN LIU†, SHIXIN XU‡, XINGYE YUE§, AND RAN ZHANG ¶

Abstract. In this paper, we focus on numerical methods for the genetic drift problems, which is governed by a degenerated convection-dominated parabolic equation. Due to the degeneration and convection, Dirac singularities will always be developed at boundary points as time evolves. In order to find a complete solution which should keep the conservation of total probability and expectation, three different schemes based on finite volume methods are used to solve the equation numerically: one is a upwind scheme, the other two are different central schemes. We observed that all the methods are stable and can keep the total probability, but have totally different long-time behaviors concerning with the conservation of expectation. We prove that any extra infinitesimal diffusion leads to a same artificial steady state. So upwind scheme does not work due to its intrinsic numerical viscosity. We find one of the central schemes introduces a numerical viscosity term too, which is beyond the common understanding in the convection-diffusion community. Careful analysis is presented to prove that the other central scheme does work. Our study shows that the numerical methods should be carefully chosen and any method with intrinsic numerical viscosity must be avoided.

Key words. Genetic drift equation, finite volume method, upwind scheme, degenerate parabolic equation

AMS subject classifications. 35K65 65M06 92D10

1. Introduction. The number of a particular gene (allele) of one locus in the population varies randomly from generation to generation. This process is a kind of stochastic process and named as genetic drift, which was first introduced by one of the founders in the field of population genetics, S. Wright [16]. Genetic drift plays an important role in mutation, selection and molecular evolution [1, 10]. Mathematical descriptions of genetic drift are typically built upon the Wright-Fisher model [4, 17] or its diffusion limit [5, 6, 8]. The Wright-Fisher model describes the dynamics of a gene with two alleles, A or B in a population of fixed size, N. The model is formulated as a discrete-time Markov chain. If $X_k$ denotes the number of A in $k_{th}$ generation, then $N - X_k$ is the number of B and the transition probabilities are the following binomial distribution:

$$P(X_{n+1} = j|X_n = i) = C_{N}^{j} \left( \frac{i}{N} \right)^{j} \left( 1 - \frac{i}{N} \right)^{N-j}.$$ (1.1)

The first and second conditional moments of the Wright-Fisher process satisfy [2]

$$E[X_{k+1}|X_k] = X_k,$$ (1.2)

$$Var[X_{k+1}|X_k] = X_k \left( 1 - \frac{X_k}{N} \right).$$ (1.3)
The first condition expresses the neutrality. A basic phenomenon of neutral Wright-Fisher model without mutation is that, either all copies of allele A are lost from the population or all the individuals carry allele A. This is the phenomenon of fixation. And the allele will fix with probability equal to its initial frequency. For a fixed population size, Wright-Fisher model works well, but if the size of the population changes over time, the diffusion approximation come to its own right. In [4] and [17], the diffusion approximation is first introduced to model the genetic drift, Moran [5] and Kimura [6] substantially extended and developed this approach. If we describe the process by $x(t)$, the fraction of type A genes at time $t$, and $f(x,t)$ denotes the probability density of $x$ at time $t$, Kimura [6, 9, 18] showed that $f(x,t)$ obeys the following diffusion equation,

$$ \frac{\partial f(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0, $$

where the quantity $j(x,t)$ is the current that characterizes the flow of probability density, with the form as

$$ j(x,t) = R(x)f(x,t) - \frac{1}{4N} \frac{\partial}{\partial x}(x(1-x)f(x,t)), $$

$R(x)$ represents the deterministic part of gene frequency dynamics and is typically taken as a polynomial in $x$ whose coefficients depend on mutation rates, migration rates and selection coefficients. At the first step, we will consider the simplest case, where the only evolutionary force acting on a randomly mating diploid population is diffusion, thus $R(x) = 0$. By rescaling of the time, we can get the model introduced by Crow and Kimura [1],

$$ \frac{\partial f(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0, $$

where the quantity $j(x,t)$ is the current that characterizes the flow of probability density, with the form as

$$ j(x,t) = -\frac{\partial}{\partial x}(x(1-x)f(x,t)), $$

and the zero current boundary conditions as ([12])

$$ j(0,t) = 0, \quad j(1,t) = 0. $$

In [14], Tran et al. defined that a distribution $f \in H$ is called as a weak solution of problem (1.4)-(1.6) with a initial state $f(x,0) = f_0(x) \in H$, if

$$ (f_t, \phi) = (f, x(1-x)\frac{\partial^2 \phi}{\partial x^2}), \quad \forall \phi \in C^\infty[0,1], $$

where $H = \{ f : [0,1] \rightarrow [0,\infty] \mid \int_0^1 f g dx < \infty, \forall g \in C^\infty[0,1] \}$ is the set of all general distribution functions on $[0,1]$. They also proved the existence and uniqueness of the weak solution.

In the definition (1.7), if we set $\phi = 1$, we can find that problem (1.4)-(1.6) conserve the total probability, for any time $t > 0$,

$$ \int_0^1 f(x,t) \, dx = \int_0^1 f(x,0) \, dx = 1 $$
Furthermore, if we chose $\phi = x$ in (1.7), then we get the conservation of the mean gene frequency (expectation), i.e.

$$
\int_0^1 xf(x, t) \, dx \equiv \int_0^1 xf(x, 0) \, dx.
$$

McKane and Waxman ([12]) gave a closed form of the singular solution to the above genetic drift problem as

$$(1.10) \quad f(x, t) = \Pi_0(t)\delta(x) + \Pi_1(t)\delta(1 - x) + f_r(x, t),$$

where $\Pi_0(t)$, $\Pi_1(t)$ and $f_r(x, t)$ are smooth functions and $f_r(x, t)$ is in a form of infinite series. (1.10) means the solution has three parts: two singular part $\Pi_0(t)\delta(x)$, $\Pi_1(t)\delta(1 - x)$ and one smooth part $f_r$. Specifically, if we solve this equation (1.4) subject to the condition that all replicate populations initially have the gene frequency of $p$, so $f(x, 0)$ corresponds to an initial distribution where only the single frequency $p$ is present,

$$
(1.11) \quad f(x, 0) = \delta(x - p), \quad 0 < p < 1,
$$

which is a Dirac delta function at $x = p$. In this case, by the conservation of total probability (1.8) and the conservation of expectation (1.9), Mckane and Waxman proved that

$$
(1.12) \quad \lim_{t \to \infty} f(x, t) = (1 - p)\delta(x) + p\delta(1 - x)
$$
in the sense of distribution. This is just the fixation phenomenon corresponding to the Wright-Fisher model. However, it is not easy to compute the infinite series in (1.10), and for more complex situations, e.g. $R(x) \neq 0$, one can hardly derive the closed form solutions as above, thus direct numerical simulation is also necessary for this problem.

The numerical scheme should be design to find a complete solution [18], which should keep the conservations of total probability (1.8) and expectation (1.9). Among various numerical methods, we choose finite volume method (FVM) [3] since it is easy to keep the conservation laws numerically. Actually it is a convection-dominated diffusion equation. This can be seen if we rewrite (1.4) as

$$
(1.13) \quad \frac{\partial f(x, t)}{\partial t} - \frac{\partial}{\partial x} \left( x(1 - x) \frac{\partial f}{\partial x} \right) + \frac{\partial}{\partial x}((2x - 1)f) = 0
$$

with diffusion term $-\frac{\partial}{\partial x} \left( x(1 - x) \frac{\partial f}{\partial x} \right)$ and convection term $\frac{\partial}{\partial x}((2x - 1)f)$. It is clear that (1.13) is convection-dominated near boundaries $x = 0$ and $x = 1$, where convection velocity is up to 1 while diffusion coefficient is down to 0.

**Remark 1.1.** At the boundary points, (1.13) is degenerated to a pure convection problem. Whether or not a boundary condition should be imposed is the key point to obtain a well-posed solution. For problem (1.13), the situation is that we can get a unique regular solution without any boundary condition imposed. But this solution is not a complete one: it does not keep the conservation of probability (1.8). So the no-flux boundary condition (1.6) is imposed and of course we can not expect to obtain a regular solution now. See the discussions on the boundary condition in the appendix of [18].
In general, a upwind FVM (UFVM) scheme is a better choice for the convection-dominated diffusion problem to achieve stability due to its intrinsic numerical viscosity. It does give us a stable numerical solution. But we find that we always get the same long-time behavior no matter what the initial state is. This is obviously wrong for gene drift (See (1.12)) because it can not keep the conservation of the expectation (1.9).

To see what’s wrong here, we appeal to the method of vanishing viscosity, i.e., a small viscosity term is first added, then the limit behavior of the solution is considered when the added viscosity tends to zero. We see that the limitation of the steady state solution is uniquely determined and thus it has nothing to do with the initial conditions. This means that the long time behavior of the original problem will be changed by any added infinitesimal viscosity. That is the reason why the upwind scheme does not work for the genetic drift problem.

When we turn to the central difference FVM, we have two choices: in the first method, the central difference is applied to discrete the fluxes induced by the diffusion \(-\frac{\partial}{\partial x}(x(1-x)\frac{\partial f}{\partial x})\) and convection \(\frac{\partial}{\partial x}((2x-1)f)\) respectively (this is referred to Scheme 2 in next section); in the other scheme, we keep the flux (1.5) as a whole, which is also discretized by the central difference (this is referred to Scheme 3). We find that both Schemes 2 and 3 are stable, which is a surprising since we are solving a convection-dominated problem by central schemes. We also observe that the steady-state of Scheme 2 is the same as UFVM (ref. to Scheme 1 in next section) but it takes a much longer time for Scheme 2 to achieve the steady state than for Scheme 1. Scheme 3 is the simplest one and we find it gives us a complete solution. Dirac singularities develop at both boundary points with proper weights rather than for Schemes 1 and 2, Dirac singularities with same weight always develop at both ends. For an explanation, we give a careful analysis to show that Scheme 3 always converges to the right solution and Scheme 2 is equivalent to Scheme 3 plus a 2nd order \(O(h^2)\) viscosity term though it is a central difference scheme itself. That is the reason why it takes a much longer time for Scheme 2 to achieve the steady state than for Scheme 1, which, as we all have known, is equivalent to Scheme 2 plus a much bigger first order \(O(h)\) viscosity term.

This paper is organized as follows. We present three different finite volume schemes for genetic drift problem in Section 2. Numerical results and analysis for three methods are presented in Section 3. The final section gives some concluding remarks.

2. Numerical Methods. In order to keep the total probability, we start from the finite volume method (FVM) [3]. A uniform grid, with grid spacing \(h = 1/M\) and grid points \(x_k = ih, \ i = 0, \ldots, M\), is used to discretize the space domain \([0, 1]\). Likewise, the time domain is uniformly discretized with step size \(\tau\). Let \(j^n_i\) and \(f^n_i\) be the numerical approximations of \(j(x_i, t_n)\), \(f(x_i, t_n)\), respectively. For inner mesh point \(x_i\) (1 \(\leq i \leq M - 1\), the control volume is

\[
D_i = \{x| x_{i-\frac{1}{2}} \leq x \leq x_{i+\frac{1}{2}}\},
\]

where \(x_{i+\frac{1}{2}} = (i + \frac{1}{2})h\). By FVM, we have

\[
\frac{f^{n+1}_i - f^n_i}{\tau} + \frac{j^{n+1}_{i+\frac{1}{2}} - j^n_{i+\frac{1}{2}}}{h} = 0.
\]

For the boundary points \(x_0 = 0\) and \(x_M = 1\), the control volumes are

\[
D_0 = \{x| 0 \leq x \leq x_{\frac{1}{2}}\}, \quad \text{and } D_M = \{x| x_{M-\frac{1}{2}} \leq x \leq 1\}.
\]
By the boundary conditions $j(0, t) = j(1, t) = 0$, we have
\begin{equation}
\frac{f_{i+1}^{n+1} - f_i^n}{\tau} + \frac{j_{i+1}^{n+1} - 0}{h/2} = 0 \quad \text{and} \quad \frac{f_M^{n+1} - f_M^n}{\tau} + \frac{0 - j_{M-\frac{1}{2}}^{n+1}}{h/2} = 0.
\end{equation}

To get a fully discrete scheme, we still need to approximate the term $j_{i+\frac{1}{2}}^{n+1}$, for $i = 0, \ldots, M - 1$. It is treated differently by the following three FVM schemes:

- **Scheme 1**: approximate $j(x, t) = -x(1 - x) \frac{\partial f}{\partial x} + (2x - 1)f$ at point $x_{i+\frac{1}{2}}$ by upwind scheme

\begin{equation}
j_{i+\frac{1}{2}}^{n+1} = \begin{cases} 
-x_{i+\frac{1}{2}}(1 - x_{i+\frac{1}{2}}) \frac{f_{i+1}^{n+1} - f_i^{n+1}}{h} + (2x_{i+\frac{1}{2}} - 1)f_{i+1}^{n+1}, & 2x_{i+\frac{1}{2}} - 1 < 0, \\
-x_{i+\frac{1}{2}}(1 - x_{i+\frac{1}{2}}) \frac{f_{i+1}^{n+1} - f_i^{n+1}}{h} + (2x_{i+\frac{1}{2}} - 1)f_i^{n+1}, & 2x_{i+\frac{1}{2}} - 1 > 0.
\end{cases}
\end{equation}

- **Scheme 2**: approximate $j(x, t) = -(x(1 - x) \frac{\partial f}{\partial x} + (2x - 1)f$ at point $x_{i+\frac{1}{2}}$ by central scheme

\begin{equation}
j_{i+\frac{1}{2}}^{n+1} = -x_{i+\frac{1}{2}}(1 - x_{i+\frac{1}{2}}) \frac{f_{i+1}^{n+1} - f_i^{n+1}}{h} + (2x_{i+\frac{1}{2}} - 1)\frac{f_{i+1}^{n+1} + f_i^{n+1}}{2}.
\end{equation}

- **Scheme 3**: approximate $j(x, t) = -\frac{\partial}{\partial x}(x(1 - x)f(x, t))$ at point $x_{i+\frac{1}{2}}$ by central scheme

\begin{equation}
j_{i+\frac{1}{2}}^{n+1} = -x_{i+1}(1 - x_{i+1}) \frac{f_{i+1}^{n+1} - f_i^{n+1}}{h} - x_i(1 - x_i) \frac{f_{i+1}^{n+1} - f_i^{n+1}}{h}.
\end{equation}

Scheme 3 was recently used in [18] for a numerical investigation on the random genetic problems, where some applications can be found on more complicated topics such as time-dependent probability of fixation for a neutral locus or in the presence of selection effect within a population of constant size; probability of fixation in the presence of selection and demographic change. In this paper, we confine ourself to the simplest case to see the behaviors of different schemes.

3. **Numerical Results and Analysis.**

3.1. **Numerical Results.** The numerical results of different schemes for the genetic drift problem (1.4), (1.5), (1.6) and (1.11) are shown in this section. In the numerical simulation, we first approximate the initial state Dirac delta function (1.11) by a normal distribution function:

\begin{equation}
f(x, 0) \sim N(p, \sigma^2)
\end{equation}

with $\sigma << 1$. Later, we will show the dependence on the mean value $p$ of the results. In Figs. 1-6 the numerical probability density at different time with various space grid sizes and initial states, are shown for all three methods. These figures show that, for all schemes, the probability density vanishes in the interval $(0, 1)$ and forms two peaks at the boundary $(x = 0$ and $x = 1)$ as time evolves. But the heights of the peaks at the boundary at the steady state are different. For Scheme 3, the heights of the two peaks at the boundary of steady-state solution are depended on the mean of initial probability density. For Schemes 1 and 2, the heights are equals and has no relations to the expectation of initial condition. This means Schemes 1 and 2 can not keep the conservation of expectation and can not give a complete solution.
Fig. 7 shows that Scheme 3 preserves the expectation while Schemes 1 and 2 do not. This means only Scheme 3 can yield the complete solution. And it can be found that it takes a much longer time for Scheme 2 to achieve the steady state than for Scheme 1.

Table 1 presents the probability density and probability at the boundaries \( f^n_0, f^n_M \) and \( \frac{1}{2}f^n_0, \frac{1}{2}f^n_M \), for Scheme 3 using different space grid sizes \( h = \frac{1}{100}, \frac{1}{1000}, \frac{1}{10000} \) and different initial states \( f(x, 0) \sim N(0.4, 0.01^2) \) and \( N(0.7, 0.01^2) \) at \( t=6, \tau = 0.0001 \). It is shown that the probabilities at the boundary ends of the steady-state solution are independent of the space grid size \( h \). This verifies that the Dirac delta singularities do develop at the boundary points. It is also shown that the probabilities at the boundary points are depended on the expectation of the initial condition, and conservations of probability and expectation are always kept. In Table 2, for fixed grid spacing \( h = 1/1000 \) and two different initial states \( f_0 \sim N(0.4, 0.01^2) \) and \( f_0 \sim N(0.7, 0.01^2) \), the time step \( \tau \) is changed from \( \frac{1}{10} \) to \( \frac{1}{10000} \). The results shows that Scheme 3 can get the same steady state and keep the conservation of total property and expectation for different mesh ratio \( \gamma = \frac{\tau}{h^2} \). This means that the Scheme 3 for the genetic drift problem (1.4), (1.5), (1.6) and (1.11) is stable and independent of the mesh ratio \( \gamma \), i.e. unconditional stable.

![Fig. 1](image.png)

**Fig. 1.** Numerical results of Scheme 1 with initial state \( f(x, 0) \sim N(0.4, 0.01^2) \) at different time \( t = 0.01, 0.05, 1, 50 \). The step sizes are \( h = 1/1000 \), \( \tau = 1/1000 \).

### 3.2. Analysis of Results.

#### 3.2.1. Analysis of Schemes 1 and 2.

As shown in Figs. 1-4, in the results of the first two schemes, the values of steady-state solutions at boundaries \( x = 0 \) and \( x = 1 \) are of the same height with different initial states. This is not consistent with the steady state of the singular solutions given in (1.12), and also does not satisfy the conservation of the expectation. Generally, compared to schemes without upwind technique, the upwind scheme is a better choice for the convection-diffusion problem because it is more stable due to its intrinsic numerical viscosity. It is not this case for the problem here. So we first check the effect of the numerical viscosity. To
this purpose, we consider a procedure of viscosity-vanishing. First, an infinitesimal diffusion is added to the corresponding steady-state problem, then the limit behavior of the steady-state solution is investigated. Consider the following problem, for a small $\epsilon > 0$,

$$\begin{align*}
\frac{d^2}{dx^2} \left( (x(1-x) + \epsilon)f_x \right) &= 0, \quad x \in (0, 1), \\
\left. \frac{d}{dx} \left( (x(1-x) + \epsilon)f_x \right) \right|_{x=0,1} &= 0,
\end{align*}$$

(3.2)
Fig. 4. Numerical results of Scheme 2 with initial state $f(x,0) \sim N(0.7, 0.01^2)$ at different time $t = 0.01, 1, 100, 10000$. The step sizes are $h = 1/1000$, $\tau = 1/1000$.

Fig. 5. Numerical results of Scheme 3 with initial state $f(x,0) \sim N(0.4, 0.01^2)$ at different time $t = 0.01, 0.05, 1, 6$. The step sizes are $h = 1/1000$, $\tau = 1/1000$.

with a constraint $\int_0^1 f_\epsilon \, dx = 1$. Integrating the problem (3.2), we get

\begin{equation}
(3.3) \quad f_\epsilon = \frac{a_\epsilon x + b_\epsilon}{x(1 - x) + \epsilon}
\end{equation}
Fig. 6. Numerical results of Scheme 3 with initial state $f(x,0) \sim N(0.7,0.01^2)$ at different time $t = 0.01, 0.05, 1, 6$. The step sizes are $h = 1/1000$, $\tau = 1/1000$.

Fig. 7. Expectation produced by different schemes with initial state $f(x,0) \sim N(0.4,0.01^2)$ under the logarithm time scale.

| space step $h$ | $N(0.4,0.01^2)$ | $N(0.7,0.01^2)$ |
|----------------|------------------|------------------|
| 1/100          | $f_0^n$          | $f_M^n$          |
|                | $f_0^n$          | $f_M^n$          | $\frac{h}{\pi} f_0^n$ | $\frac{h}{\pi} f_M^n$ |
| 1/1000         | 1.199991153e-01  | 7.99991154e-01  | 0.59999558  | 0.39999558  |
| 1/10000        | 1.199991153e-02  | 7.99991154e-02  | 0.59999557  | 0.39999557  |

Table 1
Numerical results of Scheme 3 at the boundaries at steady state ($t = 6$, time step $\tau = 1/10000$) with different initial states and space grid sizes.
where \( a_\epsilon \) and \( b_\epsilon \) are related to \( \epsilon \). From the boundary condition, we get \( a_\epsilon = 0 \). The constraint on the total probability yields that

\[
\frac{b_\epsilon}{c_\epsilon^+} = \frac{c_\epsilon^+}{\ln \frac{c_\epsilon^+ + 1/2}{c_\epsilon^+ - 1/2}}
\]

where \( c_\epsilon^+ = \sqrt{\frac{1}{4} + \epsilon} \). It is easy to verify that when \( \epsilon \to 0 \),

\[
f_\epsilon \to \begin{cases} 0 & x \in (0, 1) \\ \infty & x = 0, 1, \end{cases}
\]

(see Fig. 6 for \( f_\epsilon \)).

It is expected that \( f_\epsilon \) converges to \( \frac{1}{2}\delta(x) + \frac{1}{2}\delta(x - 1) \) in the sense of distribution. Actually we have the following theorem.

**Theorem 3.1.** Take a zero extension of \( f_\epsilon \) and still denote by \( f_\epsilon \),

\[
f_\epsilon = \begin{cases} \frac{b_\epsilon}{x(1-x) + \epsilon} & x \in [0, 1] \\ 0 & \text{otherwise}, \end{cases}
\]

then \( \lim_{\epsilon \to 0} \int_{-\infty}^{+\infty} f_\epsilon \varphi \, dx = \frac{1}{2}\varphi(0) + \frac{1}{2}\varphi(1), \quad \forall \varphi \in C_0^\infty(-\infty, \infty) \).

**Proof.** For any \( \varphi \in C_0^\infty(-\infty, \infty) \), \( \int_{-\infty}^{+\infty} f_\epsilon \varphi \, dx = \int_0^1 f_\epsilon \varphi \, dx \)

First, choosing \( \varphi \in C_0^\infty(-\infty, \frac{1}{2}) \), we have

\[
\lim_{\epsilon \to 0} \int_{-\infty}^{+\infty} f_\epsilon \varphi \, dx = \int_0^1 f_\epsilon \varphi \, dx
\]

where \( \tau = (0.4, 0.01^2) \) and \( h = 1/1000 \).

**Table 2.** Numerical results of Scheme 3 at the boundaries at steady state \( (t = 6) \) with same space grid sizes \( h = 1/1000 \).

| \( \tau \) | \( f_0^n \) | \( f_M^n \) | \( \frac{\tau}{2} f_0^n \) | \( \frac{\tau}{2} f_M^n \) |
|---|---|---|---|---|
| 1/10 | 1.19997448e3 | 1.39997767e3 | 0.29999884 | 0.69999884 |
| 1/100 | 5.99991298e2 | 1.39999130e3 | 0.29999565 | 0.69999565 |
| 1/1000 | 5.99992177e2 | 1.39999218e3 | 0.29999608 | 0.69999608 |
| 1/10000 | 5.99992260e2 | 1.39999226e3 | 0.29999613 | 0.69999613 |
Now we need to prove that \( \lim_{\epsilon \to 0} \int_0^1 f_\epsilon (\varphi(x) - \varphi(0)) \, dx = 0 \). Denoting by \( c_\epsilon^- = \sqrt{\frac{1}{2} - \epsilon} \) and \( D(x) = x(1-x) \), we have

\[
\int_0^1 f_\epsilon (\varphi(x) - \varphi(0)) \, dx = \int_0^{c_\epsilon^-} f_\epsilon (\varphi(x) - \varphi(0)) \, dx \\
+ \int_{c_\epsilon^-}^1 f_\epsilon (\varphi(x) - \varphi(0)) \, dx \\
\triangleq I_1 + I_2,
\]

where

\[
|I_1| = \left| b_\epsilon \int_0^{c_\epsilon^-} \frac{1}{D(x) + \epsilon} (\varphi(x) - \varphi(0)) \, dx \right| \\
\leq b_\epsilon M_1 \int_0^{c_\epsilon^-} \frac{x}{D(x) + \epsilon} \, dx \quad (M_1 = \max_{x \in [0, \frac{1}{2}]} |\varphi'(x)|) \\
\leq b_\epsilon M_1 c_\epsilon^- \frac{c_\epsilon^-}{c_\epsilon^- (1 - c_\epsilon^-) + \epsilon} \to 0, \quad \text{as } \epsilon \to 0
\]

and

\[
|I_2| = \left| b_\epsilon \int_{c_\epsilon^-}^1 \frac{1}{D(x) + \epsilon} (\varphi(x) - \varphi(0)) \, dx \right| \\
\leq M_2 b_\epsilon \int_{c_\epsilon^-}^1 \frac{1}{D(x) + \epsilon} \, dx \quad (M_2 = \max_{x \in [0, \frac{1}{2}]} |\varphi(x) - \varphi(0)|) \\
= b_\epsilon M_2 \frac{1}{2c_\epsilon} \ln \frac{c_\epsilon^+ - c_\epsilon^- + \frac{1}{2}}{c_\epsilon^+ + c_\epsilon^- - \frac{1}{2}} \to 0, \quad \text{as } \epsilon \to 0.
\]

Thus

\[
(3.4) \quad \lim_{\epsilon \to 0} < f_\epsilon, \varphi > = \frac{1}{2} \varphi(0).
\]
Similarly, choosing \( \varphi \in C_0^\infty(\frac{1}{2}, \infty) \), we get

\[
(3.5) \lim_{\epsilon \to 0} < f_\epsilon, \varphi > = \frac{1}{2} \varphi(1).
\]

Combining together, it can be proved that \( \lim_{\epsilon \to 0} < f_\epsilon, \varphi > = \frac{1}{2} \varphi(0) + \frac{1}{2} \varphi(1) \), for \( \forall \varphi(x) \in C_0^\infty(-\infty, \infty) \). The proof is completed. ■

We see that the long time behavior of the original problem will be changed by any extra infinitesimal viscosity since the steady-state solution always is \( \delta(x)/2 + \delta(1-x)/2 \), no matter what the initial state is. It means that the conservation of expectation must be destroyed by any extra viscosity. This is consistent with the results showed in Figs. 1 and 2 for Scheme 1, since we know that the upwind scheme always introduces a first order viscosity into a central difference scheme.

However, numerical results in Figs. 3 and 4 show that the central difference scheme (Scheme 2) is stable for this convection-dominated problem and the values of steady-state solutions at boundaries \( x = 0 \) and \( x = 1 \) are of the same height with different initial states, which also destroy the conservation of the expectation. Turning to Figs 5 and 6, for the other central scheme (Scheme 3), we have stable and correct long time behavior. In the next subsection, we will prove the stability and long-time convergence for Scheme 3. Taking the difference between these schemes, we will get the answer for these different observations.

**Theorem 3.2.** Scheme 2: (2.1), (2.2) and (2.4) can be rewritten in the following form as

\[
(3.6) \quad \frac{f^n_i - f^{n-1}_i}{\tau} - \frac{D_{i+1}f^n_{i+1} - 2D_if^n_i + D_{i-1}f^n_{i-1}}{h^2} + \Lambda = 0
\]

and Scheme 1: (2.1), (2.2) and (2.3) can be rewritten in the following form as

\[
(3.7) \quad \frac{f^n_i - f^{n-1}_i}{\tau} - \frac{D_{i+1}f^n_{i+1} - 2D_if^n_i + D_{i-1}f^n_{i-1}}{h^2} + \Lambda + \tilde{\Lambda} = 0,
\]

with

\[
\Lambda = -\frac{h^2 f^n_{i+1} - 2f^n_i + f^n_{i-1}}{4}, \quad \tilde{\Lambda} = -\frac{h}{2} \left( |b_{i+\frac{1}{2}}| f^n_{i+1} - (|b_{i+\frac{1}{2}}| + |b_{i-\frac{1}{2}}|) f^n_{i} + |b_{i-\frac{1}{2}}| f^n_{i-1} \right),
\]

where \( D(x) = x(1-x) \) and \( b(x) = D_x = 1 - 2x. \)

Theorem 3.2 tells us that Scheme 2 is just Scheme 3 plus a second order (of \( O(h^2) \)) viscosity term and for Scheme 1, another first order viscosity term is introduced in. That is the reason why Scheme 2 is also stable and it takes a much longer time for Scheme 2 than for Scheme 1 to achieve the same wrong steady state.

**Proof of Theorem 3.2.** \( \Lambda \) is the difference between Schemes 2 and 3. We have
after direct computation that

\[
\Lambda = \frac{1}{h^2} \left( (D_{i+1} - D_i) f^n_{i+1} + (D_i - D_{i-1}) f^n_i + (D_{i-1} - D_{i-2}) f^n_{i-1} \right)
\]

\[
- \frac{2h}{b_i+\frac{1}{2}} f^n_{i+1} + (b_{i+\frac{1}{2}} - b_{i-\frac{1}{2}}) f^n_i - b_{i-\frac{1}{2}} f^n_{i-1}
\]

\[
= \frac{1}{h^2} \left( (D_{i+1} - D_i) f^n_{i+1} + (D_i - D_{i-1}) f^n_i + (D_{i-1} - D_{i-2}) f^n_{i-1} \right)
\]

\[
+ \frac{1}{h^2} \left( (D_{i+\frac{1}{2}} + D_i - \frac{1}{2} D_i - (b_{i+\frac{1}{2}} - b_{i-\frac{1}{2}})) f^n_i \right)
\]

\[
= \frac{1}{h^2} \left( \frac{h^2}{8} D_{xx} f^n_{i+1} + \frac{h^2}{8} D_{xx} f^n_i - \frac{h^2}{4} D_{xx} f^n_{i-1} \right)
\]

(3.8) = \frac{-h^2 f^n_{i+1} - 2 f^n_i + f^n_{i-1}}{h^2},

where we have used the facts that \( D_{xx} = -2 \) and \( \frac{\partial f^n_i}{\partial x} D = 0, \ n > 2. \)

Note that \( \tilde{\Lambda} \) is the difference between Schemes 1 and 2, which, as we have known, is a first order viscosity term introduced by a upwind scheme ([11]). For completeness, we derive it again. There are only 3 situations to check.

**Case 1:** \( 0 \leq b_i - \frac{1}{2} < b_i + \frac{1}{2}. \)

\[
\tilde{\Lambda} = \frac{b_i+\frac{1}{2} f^n_{i+1} + (b_{i+\frac{1}{2}} - b_{i-\frac{1}{2}}) f^n_i - b_{i-\frac{1}{2}} f^n_{i-1}}{2h} - \frac{b_{i+\frac{1}{2}} f^n_{i+1} - b_{i-\frac{1}{2}} f^n_{i}}{h}
\]

\[
= \frac{-b_{i+\frac{1}{2}} f^n_{i+1} + (b_{i+\frac{1}{2}} - b_{i-\frac{1}{2}}) f^n_i - b_{i-\frac{1}{2}} f^n_{i-1}}{2h}
\]

(3.9) = \frac{-h^2 f^n_{i+1} - 2 f^n_i + f^n_{i-1}}{h^2}.

**Case 2:** \( b_i - \frac{1}{2} < b_i + \frac{1}{2} \leq 0. \)

(3.10) \(
\tilde{\Lambda} = \frac{-h^2 f^n_{i+1} - 2 f^n_i + f^n_{i-1}}{h^2}.
\)

**Case 3:** \( b_i - \frac{1}{2} \leq 0 \leq b_i + \frac{1}{2}. \)

(3.11) \(
\tilde{\Lambda} = \frac{-h^2 f^n_{i+1} - 2 f^n_i + f^n_{i-1}}{h^2}.
\)

Combining all together, we get

\[
\tilde{\Lambda} = \frac{-h^2 |b_{i+\frac{1}{2}}| f^n_{i+1} - (|b_{i+\frac{1}{2}}| + |b_{i-\frac{1}{2}}|) f^n_i + |b_{i-\frac{1}{2}}| f^n_{i-1}}{h^2}.
\]

The proof is completed. ■

**3.2.2. Analysis of Scheme 3.** In this section, we will prove the stability and long-time convergence for Scheme 3. (2.1), (2.2) and (2.5) can be split into three independent parts. For inner points, \( i = 1, \ldots, M - 1, \)

\[
\frac{f^{n+1}_i - f^n_i}{\tau} - \frac{1}{h^2} \left( D_{i+1} f^{n+1}_{i+1} - 2 D_i f^{n+1}_i + D_{i-1} f^{n+1}_{i-1} \right) = 0,
\]

(3.12)
with $D_i = x_i(1 - x_i)$. For the boundary points, it yields,

\begin{align}
&f_0^{n+1} = f_0^n + 2D_1 \gamma f_1^{n+1}, \\
&f_M^{n+1} = f_M^n + 2D_{M-1} \gamma f_{M-1}^{n+1},
\end{align}

with the mesh ratio $\gamma = \frac{\tau h}{2}$.

Due to $D_0 = D_M = 0$, the unknowns at inner points $f_1^{n+1}, \cdots, f_{M-1}^{n+1}$ form a closed linear system which can be solved first. Then the boundary points $f_0^{n+1}, f_M^{n+1}$ can be updated by the inner points $f_1^{n+1}, f_{M-1}^{n+1}$ respectively.

In the following, we prove FVM keeps discrete total probability and Scheme 3 also preserves the expectation. The discrete total probability and expectation at step $n$ are defined as follows.

\begin{align}
P_n &= \frac{h}{2} f_0^n + \frac{h}{2} f_M^n + \sum_{i=1}^{M-1} f_i^n h, \\
E_n &= \frac{h}{2} x_0 f_0^n + \frac{h}{2} x_M f_M^n + \sum_{i=1}^{M-1} x_i f_i^n h,
\end{align}

**Lemma 3.3.** For the genetic drift problem (1.4), (1.5), (1.6) and (1.11), the finite volume method (2.1), (2.2) keep the discrete total probability, $P_{n+1} = P_n$. Furthermore, the central finite volume method (2.5) yields a complete solution, which preserves the discrete expectation, $E_{n+1} = E_n$.

**Proof.** By the definition of $P_n$, it yields,

\begin{align}
P_{n+1} - P_n &= \frac{h}{2} (f_0^{n+1} - f_0^n) + \frac{h}{2} (f_M^{n+1} - f_M^n) + \sum_{i=1}^{M-1} (f_i^{n+1} - f_i^n) h.
\end{align}

Using (2.1) and (2.2), we have

\begin{align}
P_{n+1} - P_n &= -\tau \sum_{i=1}^{M-1} (j_i^{n+1} - j_i^n) - \tau j_0^{n+1} + \tau j_M^{n+1} = 0.
\end{align}

On the other hand,

\begin{align}
E_{n+1} - E_n &= \frac{h}{2} x_0 (f_0^{n+1} - f_0^n) + \frac{h}{2} x_M (f_M^{n+1} - f_M^n) + \sum_{i=1}^{M-1} x_i (f_i^{n+1} - f_i^n) h.
\end{align}

Using (2.1) and (2.2), we have

\begin{align}
E_{n+1} - E_n &= -\tau \sum_{i=1}^{M-1} x_i (j_i^{n+1} - j_i^n) + \tau x_M j_M^{n+1} \\
&= h \tau \sum_{i=1}^{M-1} j_i^{n+1}.
\end{align}

Combining with (2.5), we get

\begin{align}
\sum_{i=1}^{M-1} j_i^{n+1} = 0.
\end{align}
Thus, for Scheme 3, \( E_{n+1} = E_n \). The proof is completed. ■

**Lemma 3.4.** Let \( f^n_i \) be the solution of Scheme 3: (2.1), (2.2) and (2.5). Then,

\[
\sum_{i=1}^{M-1} x_i f^{n+1}_i h \leq \sum_{i=1}^{M-1} f^{n+1}_i h \leq \frac{e^{-\tau^{n+1}}}{4h(1-h)} \sum_{i=1}^{M-1} f^0_i h, \quad t_{n+1} = (n+1)\tau.
\]

**Proof.** Since \( D_i = x_i(1-x_i) > 0 \) for \( i = 1, \ldots, M-1 \), by setting \( v^n_i = D_if^n_i \), Scheme 3 for inner points (3.12) can be rewritten as

\[
\frac{1}{D_i} \frac{v^{n+1}_i - v^n_i}{\tau} - \frac{v^{n+1}_{i+1} - 2v^{n+1}_i + v^{n+1}_i}{h^2} = 0.
\]

It is obviously that the discrete maximum principle is valid. So we have

\[
v^n_i \geq 0, \quad f^n_i \geq 0, \quad i = 1, \ldots, M-1, \quad n > 1,
\]

since the initial value is nonnegative.

Multiplying by \( v^{n+1}_i h \) on both sides of (3.22), summing from \( i = 1 \) to \( M-1 \), using Hölder inequality and \( D(x) \leq \frac{1}{4} \), it yields that

\[
2\|v^{n+1}\|^2_h \leq \sum_{i=1}^{M-1} \left( \frac{v^{n+1}_{i+1} - 2v^n_i + v^{n+1}_i}{h^2} \right) v^{n+1}_i h \leq 2\|v^n\|^2_h,
\]

where \( \|v^n\|^2_h = \left( \sum_{i=1}^{M-1} |v^n_i|^2h \right)^{1/2} \) is the discrete \( L^2 \) norm of \( v^n \).

Denote by \( \Delta_h w_i = \frac{w_{i-1} - 2w_i + w_{i+1}}{h^2} \) the discrete Laplacian. We know that the minimum eigenvalue of the problem

\[-\Delta_h w_i = \lambda w_i, \quad i = 1, \ldots, M-1, \quad w_0 = w_M = 0,
\]

is \( \lambda_0 = \frac{\pi^2}{h^2} \sin^2\left( \frac{\pi}{2M} \right) \). Then from (3.24),

\[
2\|v^{n+1}\|^2_h + \lambda_0\|v^n\|^2_h \leq 2\|v^n\|^2_h.
\]

So we get the estimate

\[
\|v^{n+1}\|^2_h \leq \left( \frac{1}{1 + \frac{2\lambda_0}{\tau}} \right) \|v^n\|^2_h \leq e^{-\tau^{n+1}/2}\|v^0\|^2_h, \quad t_{n+1} = (n+1)\tau.
\]

By Hölder inequality, above formula means,

\[
\sum_{i=1}^{M-1} v^{n+1}_i h \leq \left( \sum_{i=1}^{M-1} |v^{n+1}_i|^2 h \right)^{1/2} = \|v^{n+1}\|_h \leq e^{-\tau^{n+1}/2}\|v^0\|_h.
\]

For fixed grid spacing \( h, \ h(1-h) \leq D_i \leq \frac{1}{4}, \ i = 1, \ldots, M-1 \). Thanks to \( v^{n+1}_i = D_if^{n+1}_i \), \( f^{n+1}_i \) can be estimated as follows:

\[
\sum_{i=1}^{M-1} f^{n+1}_i h \leq \frac{e^{-\tau^{n+1}}}{4h(1-h)} \sum_{i=1}^{M-1} f^0_i h.
\]
At the same time, since $x \in (0, 1)$, by (3.28), we can directly obtain,

$$
(3.29) \quad \sum_{i=1}^{M-1} x_i f_i^{n+1} h \leq \sum_{i=1}^{M-1} f_i^{n+1} h \leq \frac{e^{-x^2(n+1)}}{4h(1-h)} \sum_{i=1}^{M-1} f_i^0 h.
$$

The proof is completed. ■

**Theorem 3.5.** Scheme 3: (2.1), (2.2) and (2.5) is unconditionally stable and for fixed $h$ and $\tau$ and we have, as $n \to \infty$, that

$$
(3.30) \quad \begin{cases} 
  f_i^n \to 0, & \text{for } i = 1, \cdots, M - 1, \\
  \frac{h}{2} f_0^n + \frac{h}{2} f_M^n \to P_0, \\
  \frac{h}{2} x_M f_M^n \to E_0,
\end{cases}
$$

i.e.,

$$(3.31) \quad \begin{cases} 
  \frac{h}{2} f_0^n \to (P_0 - E_0) \approx 1 - p, \\
  \frac{h}{2} f_M^n \to E_0 \approx p.
\end{cases}$$

**Proof.** The unconditional stability is ensured by the discrete maximum principle. The long-time convergence comes from Lemmas 3.3, 3.4 and nonnegative property of the solution (3.23). The proof is completed. ■

**4. Conclusion and discussion.** We have considered three different numerical schemes for genetic drift diffusion equation. Schemes 1 and 2 discretize the flux in convection and diffusion form using upwind and central difference methods, respectively. Scheme 3 discretizes the flux as a whole using central difference method. Numerical experiments show that all the schemes are stable and the first two schemes give an artificial steady state solution while Scheme 3 presents the correct one. Analysis shows that Scheme 3 preserves both of total probability and expectation, so it yields the complete solution. We prove that any extra infinitesimal diffusion leads to a same steady state. We find that Scheme 2, also a central scheme, introduces a second order numerical viscosity term to Scheme 3, while Scheme 1, as a upwind one, introduces another first order numerical viscosity term to Scheme 2. Therefore, both Schemes 1 and 2 yield the same artificial long time behaviors of the numerical solutions, but it takes different time for them to achieve the steady state since they introduce different scales of viscosity terms. Some interesting observations are that a central scheme could be unconditional stable for a convection-dominated problem and a central scheme could also introduce numerical viscosity, which are beyond the common understanding of the convection-diffusion community. All the complexity comes from the diffusion degeneration and convection dominating. For this kind of problem, the numerical methods must be carefully chosen. Any methods with intrinsic numerical viscosity must be avoided. This means that most of stable methods for convection-diffusion problem don’t work since they achieve the stability by introducing the numerical viscosity ([11]).

If a population or species of organisms typically includes multiple alleles at each locus among various individuals, which is called multiple alleles, the problem will be a high dimension problem ([7, 13, 15]). It is a great challenge to find a complete solution. It is a great challenge to find a complete solution since the singularity will always be developed on the boundary surface rather than only two points for 1-D case. The numerical method for the multiple alleles include the fixation phenomena will be our
future work.

Acknowledgments The authors benefitted a great deal from discussions with David Waxman. This work is supported in part by NSF of China under the grants 11271281, 11301368 and 91230106. Minxin Chen, Chun Liu and Shixin Xu are partially supported by NSF grants DMS-1159937, DMS-1216938, DMS-1412005 and DMS-1109107.

REFERENCES

[1] J. F. Crow, M. Kimura, An Introduction to Population Genetics Theory. Harper & Row, New York, 1970.
[2] R. Der, C. L. Epstein, J. B. Plotkin, Generalized population models and the nature of genetic drift, Theor Popul Biol., 80(2):80-99, 2011.
[3] R. Eymard, T. Gallouët, R. Herbin, The finite volume method, Handbook for Numerical Analysis, Ph. Ciarlet J.L. Lions eds, North Holland, 715-1022, 2000.
[4] R. A. Fisher, On the dominance ratio, Proc. R. Soc. Edinburgh 42, 321-431, 1922.
[5] P. A. P. Moran, Random processes in genetics, Proc. Cambridge Philos. Soc. 54: 60-72, 1958.
[6] M. Kimura, Stochastic processes and distribution of gene frequencies under natural selection, Cold Spring Harbour Symp. Quant. Biol., 20, 33-53, 1955.
[7] M. Kimura, Random genetic drift in multi-allelic locus, Evolution, 9(4):419-435, 1955.
[8] M. Kimura, On the probability of fixation of mutant genes in a population, Genetics, 47(6): 713-719, 1962.
[9] M. Kimura, Diffusion models in population genetics. J. Appl. Probab. 1, 177-232, 1964.
[10] M. Kimura, The neutral theory of molecular evolution: a review of recent evidence, Cambridge University Press, 1983.
[11] R. LeVeque, Finite-Volume Methods for Hyperbolic Problems, Cambridge University Press, 2002.
[12] A.J. McKane, D. Waxman, Singular solution of the diffusion equation of population genetics. J. Theor. Biol. 247, 849-858, 2007.
[13] T. D. Tran, J. Hofrichter, J. Jost, A general solution of the Wright-Fisher model of random genetic drift, arXiv:1207.6623.
[14] T. D. Tran, J. Hofrichter, J. Jost, An introduction to the mathematical structure of the Wright-Fisher model of population genetics, Theory Biosci., 132:73-82, 2013.
[15] D. Waxman, Fixation at a locus with multiple alleles: Structure and solution of the Wright Fisher model, J. Theor. Biol., 257: 245C251, 2009.
[16] S. Wright, The evolution of dominance, The American Naturalist, 63(689), 556-561, 1929.
[17] S. Wright, The differential equation of the distribution of gene frequencies. Proc. Natl Acad. Sci. USA, 31, 382-389, 1945.
[18] L. Zhao, X. Yue, D. Waxman, Complete numerical solution of the diffusion equation of random genetic drift, Genetics, 194(4), 973-985, 2013.