Solution of the Neutral Kimura equation with two integral constraints

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Abstract

The Kimura equation is a degenerated partial differential equation of drift-diffusion type used in population genetics. Its solution is required to satisfy not only the equation but a series of conservation laws formulated as integral constraints. In this work, we consider a population of two types evolving without mutation or selection, the so-called neutral evolution. We obtain explicit solutions in terms of Gegenbauer polynomials. To satisfy the integral constraints it is necessary to prove new relations satisfied by the Gegenbauer polynomials. The long-term in time asymptotics is also studied.

Keywords: Neutral Kimura equation; degenerated diffusion; integral constraints; fixation probability; Gegenbauer polynomials.

MSC: 92Dxx; 60J60; 33C47.

1 Introduction

The Kimura equation is a partial differential equation of drift-diffusion type introduced in [1] in the framework of population genetics. The solution of the Kimura Equations, \( p(x, t) \), represents the probability density of finding that, at time \( t > 0 \), a fraction \( x \in [0, 1] \) of individuals carries a given allele, in a population in which two alleles are present. The solution of the neutral case (i.e., when the two alleles do not present any reproductive difference) is known to be written in terms of Gegenbauer polynomials, cf. [2, 3, 4, 5, 6, 7].

In [7] and [8] the Kimura equation was formally derived as the large population, small time-step limit, limit of the Moran and the Wright-Fisher processes, two well-known finite population Markov processes used in population genetics. See [9] and references therein for the definition of these two processes.

In the preceding paragraph, by the author and collaborator, generalized the original Kimura equation to allow arbitrary interaction among individuals in the population; see (7) below. However, to obtain the correct solution, two additional conservation laws had to be introduced into the model.

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The finite population Markov processes referred above are associated with a number of conservation laws to be satisfied by their solutions. Most notably, the solution of the Markov process should satisfy the conservation of probability, but, in fact, the number of conservation laws is equal to the number of different alleles modeled by the associated Markov process. In the present paper, we will consider only the case of two alleles (and therefore, the state of the population will be identified by a single variable, \( x \in [0, 1] \), that indicates the presence of the focal allele). The
correct solution of the continuous models, in the sense of being a continuous approximation of
the discrete process, is a measure that not only satisfy the Kimura equation (7) but also the two
conservation laws given by Eqs. (9).

The present work aims to explicitly present the solution of the neutral Kimura equation that
satisfies the associated conservation laws. The main difference between this and previous works
on the same subject is that the conservation laws are taken into consideration. The construction
of the correct solution will require proof of what is, to the best of our knowledge, a new formula
involving integrals of Gegenbauer polynomials. See Eqs. (3)–(6).

1.1 Outline

In Section 2 we review some well-known results for the Gegenbauer polynomials and some results
from the author and collaborators on the Kimura equation. This section will also fix the notation,
as even in the case of Gegenbauer polynomials the notation seems to not be used in consistently.

We state the new formulas for \( \int_{-1}^{1} C_{2n}^{\alpha}(x)dx \) and \( \int_{-1}^{1} xC_{n}^{\alpha}(x)dx \), but the proofs are deferred to the
Appendix A.

In Section 3, we obtain the explicit solution of the Kimura equation that satisfies both conser-
vation laws and derive asymptotic expressions for \( t \to \infty \).

2 Preliminaries

2.1 Gegenbauer polynomials

Gegenbauer polynomials \( C_n^{\alpha} : [-1, 1] \to \mathbb{R}, \Re \alpha > -\frac{1}{2}, \) \( n \in \mathbb{N} \), are solutions of the Gegenbauer
differential equation

\[
(1 - x^2)y'' - (2\alpha + 1)x y' + n(n + 2\alpha)y = 0 .
\]

See [11]. The set \( \{C_n^{\alpha}\}_{n \in \mathbb{N}} \) is orthogonal, with appropriate weight:

\[
\int_{-1}^{1} C_{\alpha}^{\alpha}C_{\alpha}^{\alpha}(1 - x^2)^{\alpha - \frac{1}{2}}dx = \delta_{nm} \frac{\pi^{1 - 2\alpha} \Gamma(n + 2\alpha)}{n!(n + \alpha)\Gamma(\alpha)^2} .
\]

where \( \delta_{nm} \) is the Kronecker delta. The generating function is given by

\[
\frac{1}{(1 - 2xt + t^2)^{\alpha}} = \sum_{n=0}^{\infty} C_{\alpha}^{\alpha}(x)t^n .
\]

We will prove at Appendix A that for \( \alpha \neq 1 \),

\[
\int_{-1}^{1} C_{2n+1}^{\alpha}(x)dx = 0 ,
\]

\[
\int_{-1}^{1} xC_{2n}^{\alpha}(x)dx = \frac{1}{\alpha - 1} \left(\frac{2\alpha + 2n - 2}{2n + 1}\right)
\]

and

\[
\int_{-1}^{1} xC_{2n}^{\alpha}(x)dx = 0 ,
\]

\[
\int_{-1}^{1} xC_{2n+1}^{\alpha}(x)dx = \frac{2(\alpha + n)}{(\alpha - 1)(2n + 3)} \left(\frac{2\alpha + 2n - 2}{2n + 1}\right) .
\]

\footnote{For example, in [10] and in the references cited in the introduction, the \( \alpha \)-Gegenbauer polynomials are called \( T_{\alpha}^{n} \). On the other hand, in [11] they are referred as \( C_{\alpha}^{n} \), with \( T_{\alpha}^{n} = C_{\alpha}^{n + \frac{1}{2}} \). In this work, we use the \( C_{\alpha}^{n} \) notation, which is also used in large reference websites, such as Wikipedia and Wolfram MathWorld.}
The singularity $\alpha = 1$ at the right hand side of Eqs. (3)–(6) are removable and the equations can easily be extended to that case.

To the best of our knowledge, Eqs. (3)–(6) are new. For $\alpha < \frac{3}{2}$, the right hand side of Eqs. (3)–(6) are identically zero.

2.2 The Kimura equation

The Kimura equation is a degenerated partial differential equation of drift-diffusion type (Fokker-Planck), introduced as a model for the evolution of allele frequencies in a given population:

$$\partial_t p = \kappa \partial_x^2 (x(1-x)p) - \partial_x (x(1-x)\psi(x)p) .$$

(7)

In the above equation, $p$ is the probability density that a given allele is present in a fraction $x \in [0, 1]$ of individuals in a population, at time $t$, and $\psi : [0, 1] \to \mathbb{R}$ is the fitness difference between the focal type and the alternative type, as a function of the presence of the focal type.

Eq. (7) has a classical solution $r \in C^\infty(0,1, \mathbb{R})$, discussed in [12]; see also [13, 14]. When $\psi = 0$, we call Equation (7) as the neutral Kimura equations.

However, the classical solution decay in the limit $t \to \infty$, and therefore cannot be the correct solution from the modeling point of view. Namely, it cannot be a continuous approximation of a given stochastic model, when the number of interacting individuals in a population is very large. In [13], solutions of measure type were considered, including Dirac deltas supported on the boundaries of the domain, $x = 0$ and $x = 1$. More precisely,

$$p(x,t) = a(t)\delta_0(x) + r(x,t) + b(t)\delta_1(x) ,$$

(8)

where $a, b : \mathbb{R}_+ \to \mathbb{R}$ are such that two conservation laws derived directly from the discrete process are satisfied: $\partial_t \int_0^1 p(x,t)dx = \partial_t \int_0^1 \varphi(x)p(x,t)dx = 0$, where $\varphi$ is the solution of $\varphi'' + \psi \varphi' = 0$, $\varphi(0) = 0, \varphi(1) = 1$. See [8] for further discussions. In the neutral case $\psi = 0$, and therefore, the two conservation laws are

$$\partial_t \int_0^1 p(x,t)dx = \partial_t \int_0^1 xp(x,t)dx = 0 ,$$

(9)

3 Solution of the Kimura equation

Consider a smooth initial condition $p^I$ such that $\text{supp} \ p^I \subset (0,1)$. The Gegenbauer polynomials $C_\alpha^n(2x-1)$ are solution of $x(1-x)f'' + (\alpha + \frac{1}{2}) (1-2x)f' + n(n+2\alpha)f = 0$. It is clear that

$$r(x,t) = \sum_{n=0}^\infty d_n e^{-(n+1)(n+2)t} C_{3/2}^n(2x-1)$$

is a classical solution of the neutral Kimura equation, for any choice of the coefficients $d_n$, $n \in \mathbb{N}$. Let $p$ be given by (5), such that conservation laws (9) are satisfied. Therefore:

$$a(t) + b(t) + \int_0^1 r(x,t)dx = \int_0^1 p^I(x)dx = 1 ,$$

and

$$b(t) + \int_0^1 xr(x,t)dx = \int_0^1 xp^I(x)dx .$$

We note that for $\alpha = \frac{3}{2}$

$$\int_0^1 C_{3/2}^n(2x-1)dx = \begin{cases} 1, & n \in 2\mathbb{N} , \\ 0, & n \in 2\mathbb{N} + 1 , \end{cases}$$

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and \( \int_0^1 x C_n^{3/2}(2x - 1)dx = \frac{1}{2} \) for all \( n \in \mathbb{N} \).

The initial condition is given by \( p^1(x) = \sum_{n=0}^{\infty} d_n C_n^{3/2}(2x-1) \). From the orthogonality property of the Gegenbauer polynomials, we find the coefficients \( (d_n)_{n \in \mathbb{N}} \)

\[
d_n = \frac{4(2n + 3)}{(n+1)(n+2)} \int_0^1 C_n^{3/2}(2x-1)p^1(x)(1-x)dx .
\]

On the other hand,

\[
1 = \int_0^1 p^1(x)dx = \sum_{n=0}^{\infty} d_{2n} ,
\]

and

\[
\int_0^1 xp^1(x)dx = \frac{1}{2} \sum_{n=0}^{\infty} d_{n+1}.
\]

Finally, the time-dependent fixation probability is given by

\[
b(t) = \int xp^1(x)dx - \int_0^t xr(x,t)dx = \frac{1}{2} \sum_{n=0}^{\infty} d_{n+1} \left( 1 - e^{-(n+1)(\alpha+2)t} \right),
\]

and time-dependent extinction probability is given by

\[
a(t) = 1 - \int_0^1 r(x,t)dx - b(t) = \sum_{n \in 2\mathbb{N}} d_n - \sum_{n \in 2\mathbb{N}} d_ne^{-(n+1)(\alpha+2)t} - \frac{1}{2} \sum_{n=0}^{\infty} d_n \left( 1 - e^{-(n+1)(\alpha+2)t} \right)
\]

\[
= \frac{1}{2} \sum_{n=0}^{\infty} (-1)^n d_n \left( 1 - e^{-(n+1)(\alpha+2)t} \right).
\]

When \( t \to \infty \),

\[
b(t) \approx \int_0^1 xp^1(x)dx - 3 \left[ \int_0^1 p^1(x)(1-x)dx \right] e^{-2t} ,
\]

where it was used that \( C_0^0(x) = 1 \). If we assume (in the sense of distributions) that \( p^1 = \delta_{x_0} \), i.e., an initial condition of Dirac-delta type, we conclude that \( b(t) \approx x_0 - 3x_0(1-x_0)e^{-2t} \), when \( t \to \infty \).

## A Properties of Gegenbauer polynomials

Let us define

\[
f(\alpha, t) = \int_{-1}^{1} \frac{dx}{(1-2xt+t^2)^{\alpha}}, \quad \alpha \neq 1.
\]

The value of \( f \) will be determined using Feynmann’s trick for integral calculation\(^2\). Differentiating with respect to \( \alpha \), and, after one integration by parts, one finds:

\[
\partial_\alpha f(\alpha, t) = - \int_{-1}^{1} \frac{\log(1-2xt+t^2)}{(1-2xt+t^2)^\alpha} dx
\]

\[
= - \left[ \frac{\log(1-2x+t^2)}{(\alpha-1)2t(1-2xt+t^2)^{\alpha-1}} \right]_{x=-1}^{x=1} - \frac{1}{\alpha-1} \int_{-1}^{1} \frac{dx}{(1-2xt+t^2)^\alpha}.
\]

\(^2\)It is not easy to find classical references to Feynmann’s trick. Two online references that discuss this technique in detail are [http://fy.chalmers.se/~tfkhj/FeynmanIntegration.pdf](http://fy.chalmers.se/~tfkhj/FeynmanIntegration.pdf) (Anonymous) and [https://courses.grainger.illinois.edu/PHYS487/sp2021/homework/Hwk04Assistance-Feynman%27sTrick.pdf](https://courses.grainger.illinois.edu/PHYS487/sp2021/homework/Hwk04Assistance-Feynman%27sTrick.pdf), by Saavanth Velury. (Both consulted on June 21, 2022.)
Therefore, \( f \) satisfies

\[
\partial_\alpha f + \frac{1}{\alpha - 1} f = - \frac{1}{(\alpha - 1)t} \left[ \frac{\log(1-t)}{(1-t)^{2\alpha-2}} - \frac{\log(1+t)}{(1+t)^{2\alpha-2}} \right],
\]

with initial condition \( f(0,t) = 2 \) for all values of \( t \).

The solution of the differential equation is given by

\[
f(\alpha,t) = \frac{1}{\alpha - 1} \left[ C(t) - \frac{1}{2t} \left( \frac{1}{(1+t)^{2\alpha-2}} - \frac{1}{(1-t)^{2\alpha-2}} \right) \right],
\]

for a certain \( \alpha \)-independent function \( C \). Using the boundary conditions, we conclude that

\[
f(\alpha,t) = -\frac{1}{(\alpha - 1)2t} \left[ \frac{1}{(1+t)^{2\alpha-2}} - \frac{1}{(1-t)^{2\alpha-2}} \right].
\]

From the Taylor expansion

\[
\frac{1}{(1+t)^\beta} = \sum_{n=0}^{\infty} (-1)^n \binom{\beta + n - 1}{n} t^n,
\]

we conclude that

\[
f(\alpha,t) = \frac{1}{\alpha - 1} \sum_{n=0}^{\infty} \binom{2\alpha + 2n - 2}{2n + 1} t^{2n}.
\]

and this proves equations (3) and (4). In particular, if \( \alpha < \frac{3}{2} \), \( \alpha \neq 1 \) (including the case of Legendre’s polynomials, \( \alpha = \frac{1}{2} \)), then \( \int_1^1 C_n^\alpha(x) = 0 \) for all \( n \in \mathbb{N} \).

Differentiating \( f(\alpha,t) \) with respect to \( t \):

\[
\partial_t f(\alpha,t) = 2\alpha \int_{-1}^{1} \frac{(x-t) \, dx}{(1-2xt + t^2)^{\alpha+1}} = 2\alpha \int_{-1}^{1} \frac{x \, dx}{(1-2xt + t^2)^{\alpha+1}} - 2\alpha tf(\alpha+1,t),
\]

we conclude that

\[
\int_{-1}^{1} \frac{x \, dx}{(1-2xt + t^2)^\alpha} = \frac{1}{2(\alpha - 1)} \partial_\alpha f(\alpha - 1,t) + tf(\alpha,t)
\]

\[
= \frac{1}{2(\alpha - 1)(\alpha - 2)} \sum_{n=0}^{\infty} 2n \left( \frac{2\alpha + 2n - 4}{2n + 1} \right) t^{2n-1} + \frac{1}{\alpha - 1} \sum_{n=0}^{\infty} \left( \frac{2\alpha + 2n - 2}{2n + 1} \right) t^{2n+1}
\]

\[
= \frac{1}{\alpha - 1} \left[ \sum_{n=0}^{\infty} \frac{n+1}{\alpha - 2} \left( \frac{2\alpha + 2n - 2}{2n + 3} \right) t^{2n+1} + \left( \frac{2\alpha + 2n - 2}{2n + 1} \right) t^{2n+1} \right]
\]

\[
= \frac{1}{\alpha - 1} \sum_{n=0}^{\infty} \frac{2(\alpha+n)}{2n + 3} \left( \frac{2\alpha + 2n - 2}{2n + 1} \right) t^{2n+1}.
\]

This proves equations (5) and (6). All expressions for \( f \) can be analytically extended to the case \( \alpha = 1 \).

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