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Weak approximations of Wright–Fisher equation

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Abstract. We construct weak approximations of the Wright-Fisher model and illustrate their accuracy by simulation examples.

 ${\bf Keywords:} \ {\rm Wright-Fisher \ model; \ simulation; \ weak \ approximation}$

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Introduction

We consider Wright-Fisher process defined by the stochastic differential equation

$$dX_t^x = \left(a - bX_t^x\right)dt + \sigma\sqrt{X_t^x\left(1 - X_t^x\right)}dB_t, \quad X_0^x = x,$$
(1)

where B is a standard Brownian motion, $0 \leq a \leq b, \sigma > 0$, and $x \in [0, 1]$.

The Wright–Fisher model (Fisher 1930; Wright 1931) takes the values in the interval [0, 1] and explicitly accounts for the effects of various evolutionary forces – random genetic drift, mutation, selection – on allele frequencies over time. This model can also accommodate the effect of demographic forces such as variation in population size through time and/or migration connecting populations [5].

In this note, we present a simple first-order weak approximation of the solution of Eq. (1) by discrete random variables that take two values at each approximation step. Recall the definition of such an approximation. By a discretization scheme with time step h > 0 we mean any time-homogeneous Markov chain $\hat{X}^h = \{\hat{X}^h_{kh}, k = 0, 1, ...\}$. We say that a family of discretization schemes \hat{X}^h , h > 0, is a first-order weak approximation of the solution X^x of (1) in the interval [0, T] if

$$\left|\mathbb{E}f\left(\widehat{X}_{T}^{h}\right) - \mathbb{E}f\left(X_{T}^{x}\right)\right| \leqslant Ch, \quad h = \frac{T}{N} \leqslant h_{0}, \tag{2}$$

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for a "sufficiently wide" class of functions $f : [0,1] \to \mathbb{R}$ and some constants C and $h_0 > 0$ (depending on the function f), where $N \in \mathbb{N}$. Note that because of the Markovity, the one-step approximation \widehat{X}_h^h completely defines (in distribution) a weak approximation \widehat{X}_{kh}^h , $k = 0, 1, \ldots$ Thus, with some ambiguity, we also call it an approximation and denote it by \widehat{X}_h^x , with x indicating its starting point.

In our context, we introduce the following "sufficiently wide" function class of infinitely differentiable functions with "not too fast" growing derivatives:

$$C^{\infty}_{*}[0,1] := \bigg\{ f \in C^{\infty}[0,1] : \limsup_{k \to \infty} \frac{1}{k!} \sup_{x \in [0,1]} \big| f^{(k)}(x) \big| < \infty \bigg\}.$$

We easily see that all functions from this class can be expanded by the Taylor series in the interval [0, 1] around arbitrary $x_0 \in [0, 1]$ (which, in fact, converges on the whole real line \mathbb{R}) and contain, for example, all polynomials and exponential functions.

Approximation

Let us first construct an approximation for the "stochastic" part of Wright–Fisher equation, that is, the solution S_t^x of Eq. (1) with a = b = 0. Similarly to [4] (see also [3]), we look for an approximation \hat{S}_h^x as a two-valued discrete random variable taking values $x_{1,2} \in [0, 1]$ with probabilities $p_{1,2}$ such that

$$\mathbb{E}\left(\hat{S}_{h}^{x}-x\right)=0, \quad x\in[0,1],\tag{3}$$

$$\mathbb{E}(\hat{S}_{h}^{x}-x)^{2} = \sigma^{2}x(1-x)h + O(h^{2}), \quad x \in [0,1],$$
(4)

$$\left|\mathbb{E}(\hat{S}_{h}^{x}-x)^{3}\right| = O(h^{2}), \quad x \in [0,1],$$
(5)

$$\mathbb{E}[(\hat{S}_{h}^{x} - x)^{4}] = O(h^{2}), \quad x \in [0, 1].$$
(6)

By solving the equation system (3)–(4) with respect to x_1, x_2, p_1, p_2 , we get the solution

$$x_1 = x + (1-x)\sigma^2 h - \sqrt{\left(x + (1-x)\sigma^2 h\right)(1-x)\sigma^2 h}, \quad x \in [0,1],$$
(7)

$$x_2 = x + (1-x)\sigma^2 h + \sqrt{\left(x + (1-x)\sigma^2 h\right)(1-x)\sigma^2 h}, \quad x \in [0,1]$$
(8)

with $p_{1,2} = \frac{x}{2x_{1,2}}$. It also satisfies conditions (5)–(6). However, for the values of x near 1, the values of x_2 a slightly greater than 1, which is unacceptable. We overcome this problem by using the symmetry of the solution of the stochastic part with respect to the point $\frac{1}{2}$; to be precise, $S_t^x \stackrel{d}{=} 1 - S_t^{1-x}$. Therefore, in the interval [0, 1/2], we can use the values $x_{1,2}$ defined by (7)–(8), whereas in the interval (1/2, 1], we use the values corresponding to the process $1 - \hat{S}_t^{1-x}$, that is,

$$\hat{x}_{1,2} = \hat{x}_{1,2}(x,h) := 1 - x_{1,2}(1-x,h) = x - x\sigma^2 h \pm \sqrt{(1-x+x\sigma^2 h)x\sigma^2 h}$$
(9)

with probabilities $\hat{p}_{1,2} = \frac{1-x}{2x_{1,2}(1-x,h)}$. Thus we obtain a correct (i.e., with values in [0, 1]) approximation \hat{S}_h^x taking the values

$$\tilde{x}_{1,2} := \begin{cases} x_{1,2}(x,h) \text{ with probabilities } p_{1,2} = \frac{x}{2x_{1,2}(x,h)}, & x \in [0,1/2], \\ 1 - x_{1,2}(1-x,h) \text{ with probabilities } p_{1,2} = \frac{1-x}{2x_{1,2}(1-x,h)}, & x \in (1/2,1]. \end{cases}$$

Now for the initial equation (1), we obtain an approximation \widehat{X}_h^x by a simple "splitstep" procedure (again, see, e.g., [4] or [3]):

$$\widehat{X}_{h}^{x} := \widehat{S}_{h}^{x} e^{-bh} + \frac{a}{b} \left(1 - e^{-bh} \right).$$
(10)

Now we can state the following:

Theorem 1. Let \hat{X}_t^x be the discretization scheme defined by one-step approximation (10). Then \hat{X}_t^x is a first-order weak approximation of equation (1) for functions $f \in C_*^{\infty}[0, 1].$

Backward Kolmogorov equation

The constructed approximation is in fact a so-called *potential* first-order weak approximation of Eq. (1) (for a definition, see, e.g., Alfonsi [1], Section 2.3.1). The proof that, indeed, it is a first-order weak approximation, is based on the following:

Theorem 2. Let $f \in C^{\infty}_{*}[0,1]$. The $u(t,x) := \mathbb{E}f(X^{x}_{t})$ is a C^{∞} function on $[0,1] \times \mathbb{R}$ that solves the backward Kolmogorov equation

$$\partial_t u(t,x) = Au(t,x), \quad x \in [0,1], \ t \ge 0.$$

In particular,

$$\forall T > 0, \ \forall l, m \in \mathbb{N}, \ \exists C_{l,m} : \left| \partial_l \partial_m u(t, x) \right| \leq C_{l,m}, \ t \in [0, T], \ x \in [0, 1].$$

Such theorem is stated for $f \in C^{\infty}[0, 1]$ in [1, Thm. 6.1.12], based on the results of [2]. Our class of functions f is slightly narrower, but our proof of the theorem is significantly simpler and is based on the estimates of the moments of X_t^x , which show that they grow slower than factorials. The recurrent relations of the moments $\mathbb{E}[(X_t^x)^k]$ show that they are infinitely differentiable with respect to t and x, which allows us to infinitely differentiate the series

$$u(t,x) = \mathbb{E}f(X_t^x) = \sum_{k=0}^{\infty} c_k \mathbb{E}[(X_t^x)^k]$$

termwise with respect to t and x, where $f(x) = \sum_{k=0}^{\infty} c_k x^k$ is the Taylor expansion of f.

Simulation examples

We illustrate our approximation for $f(x) = x^4$ and $f(x) = \exp\{-x\}$. Since we do not explicitly know the moments $\mathbb{E} \exp\{-X_t^x\}$, we use the approximate equality $\exp\{-x\} \approx 1 - x + \frac{x^2}{2} - \frac{x^3}{6} + \frac{x^4}{24}$. In Figs. 1 and 2, we compare the moments $\mathbb{E}f(\widehat{X}_t^x)$ and $\mathbb{E}f(X_t^x)$ as functions of t (left plots, h = 0.001) and as functions of discretization step h (right plots, t = 1). As expected, the approximations agree with exact values pretty well.



Fig. 1. Comparison of $\mathbb{E}f(\widehat{X}_t^x)$ and $\mathbb{E}f(X_t^x)$ as functions of t and h for $f(x) = x^4$: x = 0.815, $\sigma^2 = 0.5$, a = 4, b = 5, the number of iterations N = 500.000.



Fig. 2. Comparison of $\mathbb{E}f(\hat{X}_t^x)$ and $\mathbb{E}f(X_t^x)$ as functions of t and h for $f(x) = \exp\{-x\}$: x = 0.36, $\sigma^2 = 0.6$, a = 3, b = 4, N = 100.000.

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REZIUMĖ

Wright–Fisher lygties silpnosios aproksimacijos

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Sukonstruota silpnoji pirmos eilės aproksimacija stochastinei Wright–Fisher lygčiai. Pavyzdžiais iliustruojamas jos tikslumas.

Raktiniai žodžiai: Wright-Fisher modelis; modeliavimas; silpnoji aproksimacija