

*Keywords:* Diffusion equation, regular bounded domain

## 1 Motivation

## 2 Solution on $\Omega \subset \mathbb{R}$

In this Section we will demonstrate the method outlined in Section 1 where the solution is defined on a bounded interval on  $\mathbb{R}$ . In this case, we have the true solution to the diffusion equation. We will compare the asymptotic expansion to the true solution.

The PDE we will solve is the following BC/IC problem

$$\frac{\partial}{\partial t} q(x, t) = \frac{1}{2} \sigma^2 \frac{\partial^2}{\partial x^2} q(x, t), \quad (1)$$

$$q(x, 0) = \delta_{x_0}(x), \quad (2)$$

$$q(a, t) = q(b, t) = 0. \quad (\text{i.e. } \Omega = [a, b]) \quad (3)$$

Without loss of generality we will assume

$$a = 0,$$

$$b = 1.$$

Problem (1) - (3) can be solved in a variety of ways. We will use the method of images, which repeatedly reflects the fundamental solution

$$q_{\text{fundamental}}(x, t) = \frac{1}{\sqrt{2\pi\sigma^2 t}} \exp \left\{ -\frac{1}{2\sigma^2 t} (x - x_0)^2 \right\}$$

about the boundary points  $a$  and  $b$ . The steps for the full solutions are as follows:

Step 1: Select a kernel  $f(x|t)$  for the basis expansion,

Step 2: Perform Gram-Schmidt orthogonalization on the polynomials basis,

Step 3: Compute the weight for each basis element,

Step 4: Profit.

### 2.1 A suitable kernel for the basis elements

As noted in the motivating Section 1, the kernel we will use must be in  $C^\infty(a, b)$ , and it must obey the boundary conditions. Moreover, the basis kernel must be chosen such that

- i) derivatives  $f'(x)$  can be computed easily,
- ii) integrals  $\int_{\Omega} x^m f(x|t)^2 dx$  can be computed easily

Consideration i) suggests that  $f(x|t)$  should be of polynomial form. Consideration ii) suggests that  $f(x|t)$  should be a known pdf over  $[a, b]$ , taking on zero at  $a$  and  $b$ . Given these requirements, the Beta distribution comes to mind:

$$f(x|t, \alpha, \beta) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1},$$

where  $B(\alpha, \beta)$  is the beta function. Our choice for  $\alpha$  and  $\beta$  is not very restricted. However, we will outline a few heuristics by which we can choose these parameters. Note that there may exist an optimal choice for  $(\alpha, \beta)$  in terms of the accuracy of the asymptotic expansion with respect to the true solution  $q(x, t)$ . However, we will not prove anything in this vein here.

**First**, as long as

$$\alpha, \beta > 1, \quad (4)$$

the mode for the distribution is guaranteed to exist, so that the boundary conditions are met.

Aside from  $\alpha > 1$  and  $\beta > 1$ , we can pick any  $(\alpha, \beta)$  pair for our kernel. However, given that  $f(x|t)$  can be thought of as implicitly dependent upon  $t$ , and that the variance of the fundamental solution is  $\sigma^2 t$ , a first, reasonable guess for  $(\alpha, \beta)$  can be given by the solution to the equation:

$$\text{Var}[X] := \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)} = \sigma^2 t, \quad (5)$$

$$p(X \in dx) = f(x|t, \alpha, \beta).$$

By the same logic, noting the mean for the fundamental solution, we can require

$$\mathbb{E}[X] := \frac{\alpha}{\alpha+\beta} = x_0, \quad (6)$$

$$p(X \in dx) = f(x|t, \alpha, \beta).$$

Finally, we may require that  $\alpha, \beta \in \mathbb{Z}$ , since this will guarantee that

$$\frac{\partial^k}{\partial x^k} f(x|t, \alpha, \beta) = 0$$

for large enough  $k$ . [georgid: This may not prove important, but I will keep it here anyway]

Thus, to set  $\alpha$  and  $\beta$ , we simultaneously solve (5) and (6), then round  $\alpha$  and  $\beta$  to the closest integer greater than or equal to 2. Since  $\alpha$  and  $\beta$  are dependent upon  $t$ , we will keep  $t$  in our notation for  $f$ , albeit implicitly. In other words, once we choose  $\alpha$  and  $\beta$ , we will not be able to take derivatives of  $f$  with respect to  $t$ . We will denote the kernel as  $f(x|\alpha, \beta; t)$ .

## 2.2 Gram-Schmidt orthogonalization on the polynomials basis

The family of (polynomial) functions  $\{x^m f(x|\alpha, \beta; t)\}_{m=0}^\infty$  spans the space of  $L^2([a, b])$  functions. We generate the basis elements  $\{u_m(x|\alpha, \beta; t)\}_{m=0}^\infty$  by setting

$$v_0(x|\alpha, \beta; t) = f(x|\alpha, \beta; t),$$

$$u_0(x|\alpha, \beta; t) = \frac{f(x|\alpha, \beta; t)}{\|f(x|\alpha, \beta; t)\|}, \quad (7)$$

$$\|f(x|\alpha, \beta; t)\| \equiv \left( \int_{\Omega} f(x|\alpha, \beta; t)^2 dx \right)^{1/2}. \quad (8)$$

The integral in (8) is easy to compute because of the form we have chosen for the kernel  $f$ :

$$\begin{aligned} \int_{\Omega} f(x|\alpha, \beta; t)^2 dx &= \int_{\Omega} \left( \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1} \right)^2 dx, \\ &= \int_{\Omega} \frac{1}{B(\alpha, \beta)^2} x^{(2\alpha-1)-1} (1-x)^{(2\beta-1)-1} dx, \\ &= \frac{B(2\alpha-1, 2\beta-1)}{B(\alpha, \beta)^2}, \\ \left( \int_{\Omega} f(x|\alpha, \beta; t)^2 dx \right)^{1/2} &= \sqrt{\frac{B(2\alpha-1, 2\beta-1)}{B(\alpha, \beta)^2}}. \end{aligned}$$

Next, for  $u_1(x|\alpha, \beta; t)$ ,

$$v_1(x|\alpha, \beta; t) = x f(x|\alpha, \beta; t) - \langle x f(x|\alpha, \beta; t) | u_0(x|\alpha, \beta; t) \rangle u_0(x|\alpha, \beta; t) \quad (9)$$

$$= \left( x - \frac{\langle x f(x|\alpha, \beta; t) | u_0(x|\alpha, \beta; t) \rangle}{\|f(x|\alpha, \beta; t)\|} \right) f(x|\alpha, \beta; t) \quad (10)$$

$$\langle x f(x|\alpha, \beta; t) | u_0(x|\alpha, \beta; t) \rangle = \int_{\Omega} \frac{x f(x|\alpha, \beta; t)^2}{\|f(x|\alpha, \beta; t)\|} = \frac{1}{\|f(x|\alpha, \beta; t)\|} \int_{\Omega} \frac{1}{B(\alpha, \beta)^2} x^{2\alpha-1} (1-x)^{(2\beta-1)-1} dx \quad (11)$$

$$u_1(x|\alpha, \beta; t) = \frac{v_1(x|\alpha, \beta; t)}{\|v_1(x|\alpha, \beta; t)\|} \quad (12)$$

$$\|v_1(x|\alpha, \beta; t)\| = \int_{\Omega} \left( x - \frac{\langle x f(x|\alpha, \beta; t) | u_0(x|\alpha, \beta; t) \rangle}{\|f(x|\alpha, \beta; t)\|} \right)^2 f(x|\alpha, \beta; t)^2 dx \quad (13)$$

$$u_1(x|\alpha, \beta; t) = \frac{v_1(x|\alpha, \beta; t)}{\|v_1(x|\alpha, \beta; t)\|} = p_1(x) f(x|\alpha, \beta; t), \quad (14)$$

where  $p_1(x)$  is a first-order polynomial. In general,

$$v_m(x|\alpha, \beta; t) = x^m f(x|\alpha, \beta; t) - \sum_{m'=0}^{m-1} \langle x^m f(x|\alpha, \beta; t) | u_{m'}(x|\alpha, \beta; t) \rangle u_{m'}(x|\alpha, \beta; t)$$

$$u_m(x|\alpha, \beta; t) = \frac{v_m(x|\alpha, \beta; t)}{\|v_m(x|\alpha, \beta; t)\|} \equiv p_m(x|\alpha, \beta; t) f(x|\alpha, \beta; t)$$

In finding the basis, we will have to perform two main types calculations:

- 1) polynomial multiplication:  $p_m(x|\alpha, \beta; t) p_n(x|\alpha, \beta; t)$
- 2) integration of the form:  $\int_{\Omega} x^m f(x|\alpha, \beta; t)^2 dx$

In  $\mathbb{R}$ , the package `mpoly` will be used to handle 1). Calculation 2) can be performed relatively easily due to the form of  $f(x|\alpha, \beta; t)$ , as show in (15).

$$\int_{\Omega} x^m f(x|\alpha, \beta; t)^2 dx = \int_{\Omega} x^m \frac{1}{B(\alpha, \beta)^2} x^{2\alpha-2} (1-x)^{2\beta-2} dx = \frac{1}{B(\alpha, \beta)^2} \int_{\Omega} x^{2\alpha+m-2} (1-x)^{2\beta-2} dx = \frac{B(2\alpha+m-1, 2\beta-1)}{B(\alpha, \beta)^2} \quad (15)$$

### 2.3 Computing the Weights of the Basis Elements

Given the set of orthonormal functions  $\{u_m(x|\alpha, \beta; t)\}_{m=0}^{\infty}$  spanning  $L^2([a, b])$ , and assuming that  $q(x, t) \in L^2([a, b])$ , we can write down

$$q(x, t) = \sum_{m=0}^{\infty} c_m u_m(x|\alpha, \beta; t), \quad (16)$$

$$\text{with } c_m = \int_{\Omega} q(x, t) u_m(x|\alpha, \beta; t) dx. \quad (17)$$

Since each  $u_m$  is the product of two polynomials,  $u_m(x|\alpha, \beta; t) \in C^{\infty}([a, b])$  and is square-integrable. Therefore, we can write

$$\int_{\Omega} \frac{\partial^k \delta_{x_0}(x)}{\partial x^2} u_m(x|\alpha, \beta; t) dx = (-1)^k \int_{\Omega} \delta_{x_0}(x) \frac{\partial^k u_m(x|\alpha, \beta; t)}{\partial x^k} dx = (-1)^k \left. \frac{\partial^k u_m(x|\alpha, \beta; t)}{\partial x^k} \right|_{x=x_0} \quad (18)$$

Equipped with (18) and that  $q(x, 0) = \delta_{x_0}(x)$ , we can compute the integrals in (17) by using the Taylor expansion of  $q(x, t)$  about  $t = 0$ :

$$\begin{aligned} c_m(t; \alpha, \beta, x_0) &= \int_{\Omega} q(x, t) u_m(x|\alpha, \beta; t) dx = \int_{\Omega} \left[ \underbrace{q(x, 0)}_{\delta_{x_0}(x)} + \sum_{k=1}^{\infty} \frac{t^k}{k!} \left. \frac{\partial^k q(x, t)}{\partial t^k} \right|_{t=0} \right] u_m(x|\alpha, \beta; t) dx \\ &= \int_{\Omega} \delta_{x_0}(x) u_m(x|\alpha, \beta; t) dx + \sum_{k=1}^{\infty} \frac{t^k}{k!} \int_{\Omega} \left. \frac{\partial^k q(x, t)}{\partial t^k} \right|_{t=0} u_m(x|\alpha, \beta; t) dx \\ &= \int_{\Omega} \delta_{x_0}(x) u_m(x|\alpha, \beta; t) dx + \sum_{k=1}^{\infty} \frac{t^k}{k!} \int_{\Omega} \left( \frac{1}{2} \sigma^2 \right)^k \frac{\partial^{2k} \delta_{x_0}(x)}{\partial x^{2k}} u_m(x|\alpha, \beta; t) dx \\ &= u_m(x_0|\alpha, \beta; t) + \sum_{k=1}^{\infty} \frac{t^k}{k!} (-1)^{2k} \left( \frac{1}{2} \sigma^2 \right)^k \int_{\Omega} \delta_{x_0}(x) \frac{\partial^{2k} u_m(x|\alpha, \beta; t)}{\partial x^{2k}} dx \\ &= u_m(x_0|\alpha, \beta; t) + \sum_{k=1}^{\infty} \frac{t^k}{k!} (-1)^{2k} \left( \frac{1}{2} \sigma^2 \right)^k \frac{\partial^{2k} u_m(x_0|\alpha, \beta; t)}{\partial x^{2k}} \\ &= u_m(x_0|\alpha, \beta; t) + \sum_{k=1}^{\infty} \frac{t^k}{k!} \left( \frac{1}{2} \sigma^2 \right)^k \frac{\partial^{2k} u_m(x_0|\alpha, \beta; t)}{\partial x^{2k}}. \end{aligned}$$

Note that

$$\begin{aligned}
u_m^{(k)}(x|\alpha, \beta; t) &= \sum_{j=0}^k \binom{k}{j} p_m^{(j)}(x|\alpha, \beta; t) f^{(k-j)}(x|\alpha, \beta; t) \\
f'(x|\alpha, \beta; t) &= \frac{1}{B(\alpha, \beta)} \left[ (\alpha-1)x^{\alpha-2}(1-x)^{\beta-1} + (\beta-1)x^{\alpha-1}(1-x)^{\beta-2} \right] \\
&= \frac{1}{B(\alpha, \beta)} [(\alpha-1)B(\alpha-1, \beta)f(x|\alpha-1, \beta; t) + (\beta-1)B(\alpha, \beta-1)f(x|\alpha, \beta-1; t)]
\end{aligned}$$

The  $k^{th}$  order derivative of the polynomial  $p_m(x|\alpha, \beta; t)$  can be computed on the fly with `mpoly`. The recursive definition of

### 3 Another Kernel Choice

Another suitable kernel choose the bump function

$$f(x) = \begin{cases} \exp\left\{-\frac{1}{1-x^2}\right\}, & \text{if } |x| < 1 \\ 0, & \text{otherwise} \end{cases} \quad (19)$$

In this case,  $f \in C^\infty(-1, 1)$ . As outlined perviously, we need to compute

$$f^{(k)}(x), \int_{-1}^1 x^m f(x)^2 dx$$

For the first calculation, note that

$$f'(x) = f(x)(1-x^2)^{-2}(-2x) \equiv f(x)P_{1,0}(x)^{-1}P_{1,1}(x)$$

Assuming that

$$f^{(k)}(x) = f(x)P_{k,0}(x)^{-1}P_{k,1}(x),$$

we have that

$$\begin{aligned}
f^{(k+1)}(x) &= f'(x)P_{k,0}(x)^{-1}P_{k,1}(x) \\
&\quad + f(x) \left[ -P_{k,0}(x)^{-2}P'_{k,0}(x)P_{k,1}(x) + P_{k,0}(x)^{-1}P'_{k,1}(x) \right] \\
&= (f(x)P_{1,0}(x)^{-1}P_{1,1}(x))P_{k,0}(x)^{-1}P_{k,1}(x) \\
&\quad + f(x)P_{k,0}(x)^{-2} \left[ -P'_{k,0}(x)P_{k,1}(x) + P_{k,0}(x)P'_{k,1}(x) \right] \\
&= f(x) (P_{k,0}(x)P_{1,0}(x))^{-1}P_{1,1}(x)P_{k,1}(x) \\
&\quad + f(x)P_{k,0}(x)^{-2} \left[ -P'_{k,0}(x)P_{k,1}(x) + P_{k,0}(x)P'_{k,1}(x) \right]
\end{aligned}$$

$$f^{(k+1)}(x) = f(x) \left[ P_{k,0}(x)P_{1,0}(x)P_{k,0}(x)^2 \right]^{-1} \left( P_{1,1}(x)P_{k,1}(x)P_{k,0}(x)^2 + P_{k,0}(x)P_{1,0}(x) \left[ -P'_{k,0}(x)P_{k,1}(x) + P_{k,0}(x)P'_{k,1}(x) \right] \right)$$

$$\boxed{P_{k+1,0} = P_{k,0}(x)P_{1,0}(x)P_{k,0}(x)^2}$$

$$\boxed{P_{k+1,1} = P_{1,1}(x)P_{k,1}(x)P_{k,0}(x)^2 + P_{k,0}(x)P_{1,0}(x) \left[ -P'_{k,0}(x)P_{k,1}(x) + P_{k,0}(x)P'_{k,1}(x) \right]}$$

### 4 Mesh-Free Finite Element Method

Here we take a similar approach, where we seek the *weak solution* of the PDE (1) - (3). A weak solution is any function  $q_{weak}(x, t)$  where, for any  $\phi(x) \in C_0^\infty(\Omega)$ ,

$$\int_{\Omega} \partial_t q_{weak}(x, t) \phi(x) dx - \frac{1}{2} \sigma^2 \int_{\Omega} \partial_x^2 q_{weak}(x, t) \phi(x) dx = 0. \quad (20)$$

We can relax the definition of a weak solution in the following way. Consider a countable family of functions, or elements,  $\{\psi_k(x)\}_{k=1}^{\infty}$  dense in the space of all  $L_2(\Omega)$  functions. It can be shown that a function is a weak solution to the problem if (20) holds for each  $\psi_k(x)$ . In other words,

$$\int_{\Omega} \partial_t q_{weak}(x, t) \psi_k(x) dx - \frac{1}{2} \sigma^2 \int_{\Omega} \partial_x^2 q_{weak}(x, t) \psi_k(x) dx = 0. \quad (21)$$

It should be noted that each element  $\psi_k(x)$  need not be  $C_0^{\infty}(\Omega)$ . In fact, under the Ritz method,  $\psi_k(x) \in C_0^1(\Omega)$  in the weak sense. As long as the basis elements are dense in  $L_2$  and they satisfy the boundary conditions, we can solve the problem in the weak formulation. This can be proved using Friedrichs' mollification (See exercise 2.12 in Zeidler [1998]). Furthermore, we can show that the weak solution converges to the classical solution. In application, we restrict ourselves to a subset of  $\{\psi_k(x)\}_{k=1}^{\infty}$ :

$$\{\psi_k(x)\}_{k=1}^K,$$

applying (21) only to elements  $\psi_1(x)$  through  $\psi_K(x)$ . For the purposes of this section, we will work with a finite family of basis elements which are orthonormal (this can be achieved by following the Gram-Schmidt procedure outlined above). Further, we impose the form for the approximate solution  $q_K(x, t)$ :

$$q_K(x, t) = \sum_{k=1}^K \xi_k(t) \psi_k(x).$$

Plugging into (21),

$$\begin{aligned} \int_{\Omega} \sum_{k=1}^K (\partial_t \xi_k(t)) \psi_k(x) \psi_l(x) dx - \frac{1}{2} \sigma^2 \int_{\Omega} \sum_{k=1}^K \xi_k(t) (\partial_x^2 \psi_k(x)) \psi_l(x) dx &= 0, \\ \sum_{k=1}^K (\partial_t \xi_k(t)) \int_{\Omega} \psi_k(x) \psi_l(x) dx - \frac{1}{2} \sigma^2 \sum_{k=1}^K \xi_k(t) \int_{\Omega} (\partial_x^2 \psi_k(x)) \psi_l(x) dx &= 0. \end{aligned}$$

Using the boundary conditions and integration by parts,

$$\int_{\Omega} (\partial_x^2 \psi_k(x)) \psi_l(x) dx = - \int_{\Omega} \partial_x \psi_k(x) \partial_x \psi_l(x) dx.$$

Using the orthonormality of  $\psi_k(x)$ ,

$$\int_{\Omega} \psi_k(x) \psi_l(x) dx = \delta(k-l).$$

The solution condition then becomes

$$\sum_{k=1}^K (\partial_t \xi_k(t)) \delta(k-l) + \frac{1}{2} \sigma^2 \sum_{k=1}^K \xi_k(t) \int_{\Omega} \partial_x \psi_k(x) \partial_x \psi_l(x) dx = 0. \quad (22)$$

Defining

$$\xi(t) = (\xi_1(t), \dots, \xi_K(t))^T, \quad \Psi(x) = (\psi_1(x), \dots, \psi_K(x))^T,$$

condition (22) sets up the system of equations

$$\partial_t \xi(t) = -\frac{1}{2} \sigma^2 A \xi(t), \quad [A]_{ij} = \int_{\Omega} \partial_x \psi_i(x) \partial_x \psi_j(x) dx. \quad (23)$$

The matrix  $A$  is symmetric, so that an eigendecomposition for it exists. Moreover, the solution to the system of ODEs in (23) is given by

$$\xi(t) = e^{-\frac{1}{2} \sigma^2 A t} \xi(0), \quad \xi_k(0) = \int_{\Omega} \psi_k(x) \delta(x - x_0) dx = \psi_k(x_0), \quad q_K(x, t) = \Psi(x)^T \xi(t) = \Psi(x)^T \left( e^{-\frac{1}{2} \sigma^2 A t} \right) \xi(0). \quad (24)$$

The definition for  $\xi(0)$  can be derived from the orthonormality of  $\{\psi_k(x)\}_{k=1}^K$ . Obviously, sparsity in  $\{\psi_k(x)\}_{k=1}^K$  makes calculating the solution easy.

## 4.1 Basis Element Choice

It is known that the family of Gaussian pdfs is dense in  $L_2(\mathbb{R})$  (See exercise 3.6 in Zeidler [1998]). This motivates the choice for the family of basis elements that we will use for this problem:

$$\{(x-a)(b-x)\phi(x|\mu_k, \sigma_k^2)\}_{k=1}^K, \quad \phi(x|\mu_k, \sigma_k^2) = \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left\{-\frac{1}{2\sigma_k^2}(x-\mu_k)^2\right\}. \quad (25)$$

Multiplying the Gaussian densities  $\phi$  by  $(x-a)(b-x)$  ensures that each basis element obeys the boundary conditions. We have to prove the the above family of basis elements is dense in  $L_2(\Omega)$ .

The choice of  $(\mu_k, \sigma_k^2)$  is up to us. However, for a fixed  $K$ , we can choose a (locally) optimum sequences of  $(\mu_k, \sigma_k^2)_{k=1}^K$  in the following way. Given  $(\mu_k, \sigma_k^2)_{k=1}^K$ , we can first follow Gram-Schmidt to make the basis elements orthonormal, then use the solution in (24) to compute the weak solution  $q_K(x, t)$  for each  $x \in \Omega$ . Then we can compute

$$\left\| \partial_t q_K(x, t) - \frac{1}{2} \sigma^2 \partial_x^2 q_K(x, t) \right\|_{2, \Omega}. \quad (26)$$

This norm will tell us approximately how closely the weak solution  $q_K(x, t)$  solves the original problem in the classical sense. We can then use R's `optim` to search over the space  $(\mu_k, \sigma_k^2)_{k=1}^K$  for the best sequence by minimizing (26), given some starting point. In this case, the starting point for  $\mu_k$  are evenly spaced points on the domain  $[a, b]$ , including the boundaries. The starting point for the basis variances are all  $\sigma_k^2 = 0.05$ . We can see in Figure (1) that already for  $K = 6$  the approximate solution reaches a qualitatively reasonable accuracy, and certainly good enough for effective maximum likelihood estimation.

## 4.2 Path-Integral Formulation and Differentiation With Respect to Boundaries

The Taylor expansion of the semigroup operator in (24) can be used to obtain the path-integral form for this problem:

$$\begin{aligned} \xi(t + \Delta t) &= e^{-\frac{1}{2} \sigma^2 A \Delta t} \xi(t) \approx \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \xi(t), \\ \Rightarrow q(x, t + \Delta t) &\approx \psi^T(x) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \xi(t), \end{aligned} \quad (27)$$

for a small enough  $\Delta t$ . We will lend (27) a *probabilistic* interpretation. First, if we recall that the elements in  $\psi(x)$  are orthonormal, we will notice that the matrix

$$\int_{\Omega} \psi(x) \psi^T(x) dx = I.$$

Therefore, we can re-write (27) as

$$\begin{aligned} q(x, t + \Delta t) &\approx \psi^T(x) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \xi(t), \\ &= \psi^T(x) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) e^{-\frac{1}{2} \sigma^2 A t} \xi(0), \\ &= \int_{\Omega} \psi^T(x) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \psi(y) \psi^T(y) e^{-\frac{1}{2} \sigma^2 A t} \xi(0) dy, \end{aligned}$$

The first and second parts in the integral are the probabilities

$$\begin{aligned} P(X_{t+\Delta t} = x, a < X_t < b, \forall t \in [t, t + \Delta t] | X_t = y) &\approx \psi^T(x) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \psi(y) \\ P(X_t = y, a < X_t < b, \forall t \in [0, t] | X_0 = x_0) &= \psi^T(y) e^{-\frac{1}{2} \sigma^2 A t} \xi(0) \\ \Rightarrow \int_{\Omega} P(X_{t+\Delta t} = x, a < X_t < b, \forall t \in [t, t + \Delta t] | X_t = y) P(X_t = y, a < X_t < b, \forall t \in [0, t] | X_0 = x_0) dy \\ &\approx \int_{\Omega} \psi^T(x) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \psi(y) \psi^T(y) e^{-\frac{1}{2} \sigma^2 A t} \xi(0) dy \end{aligned}$$

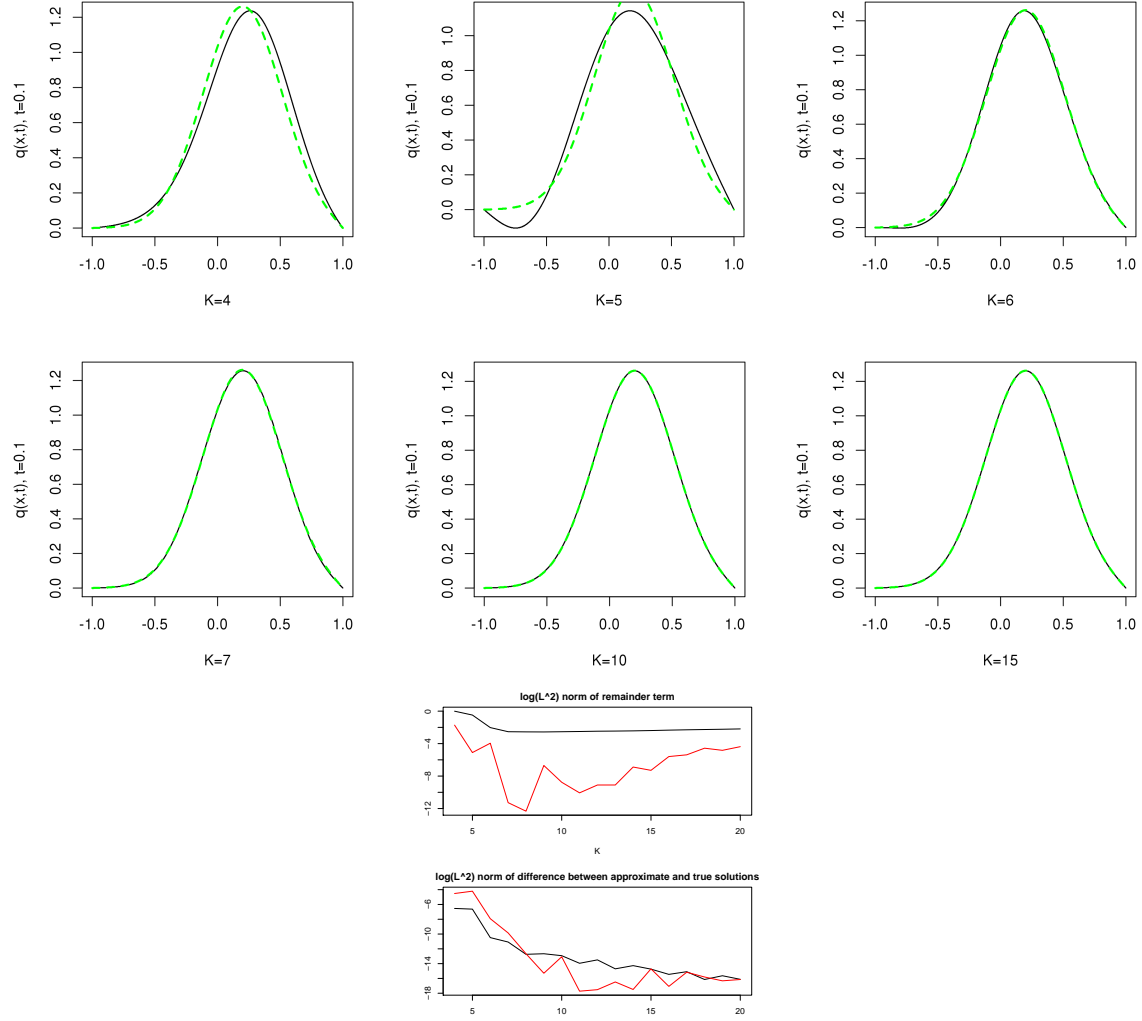


Figure 1: Approximate solution (solid black) and true solution (dashed green) for different number  $K$  of optimally chosen basis elements  $\{(a-x)(b-x)\phi(x|\mu_k, \sigma_k^2)\}_{k=1}^K$ .

In general, again for small enough  $\Delta t$ ,

$$P(X_t = x, a < X_t < b, \forall t \in [0, t] | X_0 = x_0) \approx q_K(x, t) \approx \int_{\Omega} \cdots \int_{\Omega} \left[ \psi^T(x) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \psi(x_n) \right] \left[ \psi^T(x_{n-1}) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \psi(x_{n-2}) \right] \cdots \left[ \psi^T(x_1) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \psi(x_0) \right] dx_n \cdots dx_1 \quad (28)$$

Equation (28) is the **path integral formulation** for the solution to the initial-BV problem. We can reduce (28) to

$$q_K(x, t) \approx \psi^T(x) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right)^{t/\Delta t} \psi(x_0).$$

Before we take derivatives with respect to the boundaries, first note

$$P(X_t = x, a < X_t < b, \forall t \in [0, t] | X_0 = x_0) = P(X_t = x, \max_{t' \in [0, t]} \{X_{t'}\} < b, \min_{t' \in [0, t]} \{X_{t'}\} > a | X_0 = x_0) = q(x, t).$$

Hence,

$$P \left( X_t = x, \max_{t' \in [0, t]} \{X_{t'}\} = b, \min_{t' \in [0, t]} \{X_{t'}\} = a | X_0 = x_0 \right) = -\frac{\partial^2}{\partial a \partial b} q(x, t). \quad (29)$$

This is what we are after. To compute the derivative, we can do

$$-\frac{\partial^2}{\partial a \partial b} q(x, t) \approx -\frac{\partial^2}{\partial a \partial b} \left( \psi(x)^T \left( e^{-\frac{1}{2} \sigma^2 A t} \right) \psi(0) \right) \approx -\frac{\partial^2}{\partial a \partial b} \left( \psi^T(x) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right)^{t/\Delta t} \psi(x_0) \right). \quad (30)$$

The above derivatives are expensive to compute. Moreover, at a first glance, they have no immediate probabilistic interpretation. However, under the path-integral formulation, they do. From (28)

$$-\frac{\partial^2}{\partial a \partial b} q_K(x, t) = \int_{\Omega} \cdots \int_{\Omega} -\frac{\partial^2}{\partial a \partial b} \left( \left[ \psi^T(x) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \psi(x_n) \right] \cdots \left[ \psi^T(x_1) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \psi(x_0) \right] \right) dx_n \cdots dx_1. \quad (31)$$

Note that I have placed the derivatives on the inside of the integral. This follows from the Dominated Convergence Theorem since the derivatives are bounded over  $\Omega$ . This is not cheaper than the other representations, however, consider one of the elements in the sum of derivatives:

$$-\int_{\Omega} \cdots \int_{\Omega} \frac{\partial}{\partial a} \left[ \psi^T(x) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \psi(x_n) \right] \cdots \frac{\partial}{\partial b} \left[ \psi^T(x_1) \left( I - \frac{1}{2} \sigma^2 A \Delta t \right) \psi(x_0) \right] dx_n \cdots dx_1.$$

The above expression is the probability

$$P(X_t = x, \min \{X_t\} = a, \max \{X_t\} = b, \tau_a \in [t_n, t], \tau_b \in [0, t_1] | X_0 = x_0),$$

where  $\tau_a(\tau_b)$  is the time when  $X_t$  reaches boundary  $a$  ( $b$ ),

## References

E. Zeidler. *Applied Functional Analysis, Applications to Mathematical Physics*. Springer Science & Business Media, 1998.