Abstract

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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 solutio.

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

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

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

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

Without loss of generality we will assume

$$a = 0, \qquad b = 1.$$

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

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

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 α and β is not very restricted. However, we will outline a few heuristics by which we can choose these parameters. Note that there may exist and optimal choise for (α,β) 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

$$\alpha, \beta > 1, \tag{4}$$

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 (α,β) 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 (α,β) can be given by the solution to the equation:

$$\begin{aligned} \mathrm{Var}\,[X] &:= \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)} = \sigma^2 t, \\ p(X \in dx) &= f(x|t,\alpha,\beta). \end{aligned} \tag{5}$$

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

$$\begin{aligned} \mathrm{E}\,[X] &:= \frac{\alpha}{\alpha+\beta} = x_0, \\ p(X \in dx) &= f(x|t,\alpha,\beta). \end{aligned} \tag{6}$$

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 α and β, we simultaneously solve (5) and (6), then round α and β to the closest integer greater than or equal to 2. Since α and β are dependent upon t, we will keep t in our notation for f, albeit implicitly. In other words, once we choose α and β, 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

$$\begin{aligned} v_0(x|\alpha,\beta;t) &= f(x|\alpha,\beta;t), \\ u_0(x|\alpha,\beta;t) &= \frac{f(x|\alpha,\beta;t)}{\|f(x|\alpha,\beta;t\|}, \end{aligned} \tag{7}$$

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

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 $u_1(x;\alpha,\beta;t)$,

$$v_1(x|\alpha,\beta;t) = xf(x|\alpha,\beta;t) - \langle xf(x|\alpha,\beta;t)|u_0(x|\alpha,\beta;t)\rangle\, u_0(x|\alpha,\beta;t) \tag{9}$$

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

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

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

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

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

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 calcluations:

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 `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).

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

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

$$q(x,t) = \sum_{m=0}^{\infty} c_m u_m(x|\alpha,\beta;t), \tag{16}$$
$$\text{with } c_m = \int_\Omega q(x,t) u_m(x|\alpha,\beta;t) dx. \tag{17}$$

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

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

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

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

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 choise the bump function

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

In thise 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

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

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

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

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

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 $\phi(x) \in C_0^\infty(\Omega)$,

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

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,

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

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),

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

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

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

Defining

$$\xi(t) = (\xi_1(t), \ldots, \xi_K(t))^T, \qquad \psi(x) = (\psi_1(x), \ldots, \psi_K(x))^T,$$

condition (22) sets up the system of equations

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

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

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

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.

References

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