**Abstract**

*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 solutio.

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

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

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

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

**Without loss of generality we will assume**

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

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 $\alpha$ 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 and optimal choise 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

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

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 $(\alpha, \beta)$ 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:

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

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

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

$$\mathrm{E}[X] := \frac{\alpha}{\alpha+\beta} = x_0, \tag{6}$$

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

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

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

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

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

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

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

$$= \int_\Omega \frac{1}{B(\alpha, \beta)^2} x^{(2\alpha-1)-1}(1-x)^{(2\beta-1)-1} dx,$$

$$= \frac{B(2\alpha-1, 2\beta-1)}{B(\alpha, \beta)^2},$$

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

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

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

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

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

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

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

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

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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).

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

$$(15)$$

## 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 $t=0$:

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

$$= \int_\Omega \delta_{x_0}(x) u_m(x|\alpha,\beta;t) dx + \sum_{k=1}^\infty \frac{t^k}{k!} \int_\Omega \left. \frac{\partial^k q(x,t)}{\partial t^k} \right|_{t=0} u_m(x|\alpha,\beta;t) dx$$

$$= \int_\Omega \delta_{x_0}(x) u_m(x|\alpha,\beta;t) dx + \sum_{k=1}^\infty \frac{t^k}{k!} \int_\Omega \left( \frac{1}{2}\sigma^2 \right)^k \frac{\partial^{2k} \delta_{x_0}(x)}{\partial x^{2k}} u_m(x|\alpha,\beta;t) dx$$

$$= u_m(x_0|\alpha,\beta;t) + \sum_{k=1}^\infty \frac{t^k}{k!} (-1)^{2k} \left( \frac{1}{2}\sigma^2 \right)^k \int_\Omega \delta_{x_0}(x) \frac{\partial^{2k} u_m(x|\alpha,\beta;t)}{\partial x^{2k}} dx$$

$$= u_m(x_0|\alpha,\beta;t) + \sum_{k=1}^\infty \frac{t^k}{k!} (-1)^{2k} \left( \frac{1}{2}\sigma^2 \right)^k \frac{\partial^{2k} u_m(x_0|\alpha,\beta;t)}{\partial x^{2k}}$$

$$= u_m(x_0|\alpha,\beta;t) + \sum_{k=1}^\infty \frac{t^k}{k!} \left( \frac{1}{2}\sigma^2 \right)^k \frac{\partial^{2k} u_m(x_0|\alpha,\beta;t)}{\partial x^{2k}}.$$

Note that

$$u_m^{(k)}(x|\alpha,\beta;t) = \sum_{j=0}^{k} \binom{k}{j} p_m^{(j)}(x|\alpha,\beta;t) f^{(k-j)}(x|\alpha,\beta;t)$$

$$f'(x|\alpha,\beta;t) = \frac{1}{B(\alpha,\beta)} \left[ (\alpha-1)x^{\alpha-2}(1-x)^{\beta-1} + (\beta-1)x^{\alpha-1}(1-x)^{\beta-2} \right]$$

$$= \frac{1}{B(\alpha,\beta)} \left[ (\alpha-1)B(\alpha-1,\beta)f(x|\alpha-1,\beta;t) + (\beta-1)B(\alpha,\beta-1)f(x|\alpha,\beta-1;t) \right]$$

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

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

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

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

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

## 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 $\{\psi_k(x)\}_{k=1}^\infty$ dense in $C_0^\infty(\Omega)$ under the $L_2$ norm. 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,

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

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.

In application, we restrict ourselves to a subset of $\{\psi_k(x)\}_{k=1}^\infty$:

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