

List of pdfcomments

GAJ - What does this say about our overall stability? 5

AJR - Have to shift the j by 0, ±1 in these sums and then massive
cancellation to show the operator is self-adjoint. AT least it all cancels
except at the ends: which is why periodic is so nice because the ends
then also cancel. 6

GAJ - Counter example?: 2 intervals ⇒ $[r]_1 = (U_0 + U_2)V_1 - (V_0 + V_2)U_1$. Assume material conservation at boundaries, i.e. $u'=v'=0$.
Then $R = -[r]_1 \neq 0$ 6

GAJ - Try $[u']_0 = 0 \Rightarrow U_{-1} = 2U_0 - U_1$, $[u']_2 = 0 \Rightarrow U_3 = 2U_2 - U_1$.
So $R = -[r]_0 - [r]_1 - [r]_2 = -U_{-1}V_0 + V_{-1}U_0 - U_3V_2 + V_3U_2 = U_1V_0 - V_1U_0 + U_1V_2 - V_1U_2 = -[r]_1$ 6

AJR - Check the following. 6

Notes on the Diffusion Equation

Tuesday 29th October, 2013

1 Introduction

Consider an arbitrary solution $u : \mathbb{X} \times \mathbb{T} \mapsto \mathbb{R}$ to the simple diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}. \quad (1)$$

A computationally feasible approach would be to first establish $|\mathbb{J}|$ discrete grid-points, $\vec{X} = [X_j]_{j \in \mathbb{J}}$, and thence partition the spatial domain \mathbb{X} into contiguous intervals $\mathbb{I}_j := (X_{j-1}, X_j]$. The coarse dynamics at the grid-points are then summarised by $\vec{U} = [U_j]_{j \in \mathbb{J}}$, where $U_j(t) = u(X_j, t)$ for all $t \in \mathbb{T}$, according to some temporal evolution

$$\dot{\vec{U}}(t) = \vec{g}(\vec{U}(t)). \quad (2)$$

Consequently, a link from the coarse dynamics \vec{U} back to the continuum dynamics u might be provided by choosing an appropriate spatial mapping of the form

$$u := u(x, \vec{U}(t)). \quad (3)$$

Under this scheme, the linear diffusion equation (1) becomes

$$\frac{\partial u}{\partial \vec{U}} \cdot \vec{g} = \frac{\partial^2 u}{\partial x^2}. \quad (4)$$

Observe that the evolution of u now has nonlinear interactions with \vec{U} .

2 Centre Manifold Approximation

The original diffusion equation (1) admits physically-realisable eigensolutions of the form

$$u(x, t) = e^{-k^2 t \pm i k x}, \quad (5)$$

with real eigenvalues $\lambda = -k^2 \leq 0$ for eigenmode wavenumbers $\pm k$. As a consequence, the transient solutions corresponding to $\lambda < 0$ decay rapidly to the centre manifold corresponding to $\lambda = 0$.

This centre manifold can be found in practice by iteratively refining approximations to u . In particular, consider a series expansion of the form

$$u \sim \hat{u}_0 + \gamma \hat{u}_1 + \gamma^2 \hat{u}_2 + \cdots, \quad (6)$$

for some parameter $0 \leq \gamma \leq 1$. Without loss of generality, let $\hat{u}_0 = 0$ be the trivial stationary solution to equation (1).

In addition, the constant eigensolution for $\lambda = 0$ implies a slow evolution for the coarse dynamics given by equation (2), which therefore admits a series expansion of the form

$$\dot{\vec{U}} \sim \gamma \vec{g}_1 + \gamma^2 \vec{g}_2 + \cdots. \quad (7)$$

Hence, equation (4) may be decomposed at each order ℓ of the series parameter γ , giving

$$\frac{\partial^2 \hat{u}_1}{\partial x^2} = 0, \quad (8)$$

$$\frac{\partial^2 \hat{u}_\ell}{\partial x^2} = \sum_{m=1}^{\ell-1} \frac{\partial \hat{u}_m}{\partial \vec{U}} \cdot \vec{g}_{\ell-m}, \quad \text{for } \ell = 2, 3, \dots. \quad (9)$$

3 First-order Approximation

Now, the leading equation (8) admits any spatially piecewise linear function as a solution. Hence, in keeping with the discretisation imposed by the coarse dynamics, consider the linear approximation

$$\hat{u}_1 = \sum_{j \in \mathbb{J}} \chi_j (\xi_j U_j + (1 - \xi_j) U_{j-1}), \quad (10)$$

where $\chi_j(x)$ is an indicator that takes on the value 1 (or 0) inside (or outside) of the j th interval, and $\xi_j(x) = (x - X_{j-1})(X_j - X_{j-1})$ is a spatial, linear interpolator. This particular approximation is chosen to be continuous across the boundaries of each interval. In general, it suffices to impose a continuity condition at the right-hand end of each arbitrary j th interval, namely:

$$[u]_j := \lim_{\epsilon \rightarrow 0^+} u(X_j + \epsilon, t) - u(X_j - \epsilon, t) = 0. \quad (11)$$

Unfortunately, this linear approximation is not smooth at the interval boundaries. For convenience, consider regular grid spacings of size $X_j - X_{j-1} = H$. Then, denoting $\partial u / \partial x$ as u' , observe that

$$[\hat{u}'_1]_j = \frac{1}{H}(U_{j+1} + U_{j-1} - 2U_j) = \frac{1}{H} \delta^2 \hat{u}_1|_{X_j}, \quad (12)$$

for the centred difference $\delta u(x, t) := u(x + \frac{H}{2}, t) - u(x - \frac{H}{2}, t)$. However, this non-smoothness may be corrected at higher order by imposing a further segment boundary condition, namely

$$[u']_j = \frac{1 - \gamma}{H} \delta^2 u|_{X_j}. \quad (13)$$

Consequently, smooth approximations are found in the limit as $\gamma \rightarrow 1$.

4 Linear Eigenmode Analysis

Consider a single eigenmode of the form (5) for some fixed wavenumber $k > 0$. Thus, allowing for the partitioning of \mathbb{X} , let

$$u \sim \sum_{j \in \mathbb{J}} \chi_j a_j e^{ikH\xi_j} + \text{c.c.}, \quad (14)$$

for arbitrary, time-varying, complex coefficients $a_j = A_j + iB_j$. We now seek the ‘spatial’ evolution from interval to interval for the given wavenumber. The continuity condition (11) implies that

$$a_{j+1} - a_j e^{ikH\xi_j} + \text{c.c.} = 0. \quad (15)$$

Similarly, the smoothness condition (13) implies that

$$ika_{j+1} - ika_j e^{ikH} + \text{c.c.} = \frac{1 - \gamma}{H} (a_{j+1} e^{ikH} + a_j - 2a_j e^{ikH}) + \text{c.c.}, \quad (16)$$

where continuity has also been invoked at the left-hand of the j th interval. In coefficient form, the update from the j th to $(j + 1)$ th segment is


$$\begin{bmatrix} 1 & 0 \\ fc & 1 - fs \end{bmatrix} \begin{bmatrix} A_{j+1} \\ B_{j+1} \end{bmatrix} = \begin{bmatrix} c & -s \\ s + f(2c - 1) & c - 2fs \end{bmatrix} \begin{bmatrix} A_j \\ B_j \end{bmatrix}, \quad (17)$$

where $c + is := e^{ikH}$ and $f := \frac{1-\gamma}{kH}$. Now, letting $a_{j+1} = \mu a_j$, the characteristic equation for the growth factor μ is

$$(1 - fs) \left[\mu^2 - 2 \frac{c - fs}{1 - fs} \mu + 1 \right] = 0, \quad (18)$$

with roots given by

$$\mu = \beta \pm \sqrt{\beta^2 - 1} \quad \text{for } \beta = \frac{c - fs}{1 - fs}. \quad (19)$$

Observe that $\beta \leq 1$ since $c = \cos kH \leq 1$ and $1 - fs = 1 - (1 - \gamma) \frac{\sin kH}{kH} \geq 0$. Thus, for $|\beta| < 1$, the factors are complex with magnitude $|\mu| = 1$, indicating marginally stable evolution of a_j . This includes the limiting case of $\gamma = 1$ ($f = 0$), for which $\mu = c \pm is = e^{\pm ikH}$. Likewise, $\mu = \pm 1$ for $\beta = \pm 1$, corresponding to $kH = n\pi$, $n = 0, 1, 2, \dots$. Finally, for small regions near each $kH = (2n + 1)\pi$, it is found that $\beta < -1$, resulting in two real factors, $\mu < -1$ and $-1 < \mu < 0$, indicating unstable (saddle) evolution. 

5 Linear Dual Space

The linear diffusion equation (1) is seperable into the temporal operator $\partial/\partial t$ and the spatial operator $\mathcal{L} = \partial^2/\partial x^2$. Assuming a spatially square-integrable field over \mathbb{X} , the inner product can be shown to obey

$$\langle \mathcal{L}u, v \rangle = \langle u, \mathcal{L}v \rangle + R, \quad (20)$$

with the residual

$$R = \sum_{j \in \mathbb{J}} [u'v - v'u]_{X_{j-1}}^{X_j}. \quad (21)$$

Now, letting $r = u'v - v'u$, the residual becomes

$$R = r_{\text{right}} - r_{\text{left}} - \sum_{j=\text{left}+1}^{\text{right}-1} [r]_j, \quad (22)$$

if there are at least two intervals. Assuming that v also obeys conditions (11) and (13), the j -th residual jump becomes

$$\begin{aligned} [r]_j &= [u']_j V_j - [v']_j U_j \\ &= \frac{1-\gamma}{H} [(U_{j+1} + U_{j-1})V_j - (V_{j+1} + V_{j-1})U_j] . \end{aligned} \quad (23)$$

Observe that terms from adjacent interval boundaries will cancel, leaving

$$\begin{aligned} R &= u'_{\text{right}} V_{\text{right}} - v'_{\text{right}} U_{\text{right}} - u'_{\text{left}} V_{\text{left}} + v'_{\text{left}} U_{\text{left}} \\ &\quad - \frac{1-\gamma}{H} [U_{\text{left}} V_{\text{left}+1} - V_{\text{left}} U_{\text{left}+1} + U_{\text{right}} V_{\text{right}-1} - V_{\text{right}} U_{\text{right}-1}] \end{aligned} \quad (24)$$



where there are three main boundary conditions on a finite domain:

periodic easy;

Dirichlet setting $u = 0$ on the bdry, that is, $U_{\text{bdry}} = 0$, means we get cancellation in R if correspondingly $v = V = 0$ on the bdry;

Neumann requiring $u' = 0$ on the bdry is more complicated, but it appears that setting on the bdry $u' = \frac{1-\gamma}{H}(U_{\text{next}} - U_{\text{bdry}})$, means we get cancellation in R if correspondingly for v on the bdry interval..

6 Second-order Approximation

Substituting the first-order approximation (10) into the nonlinear diffusion equation (9) for $\ell = 2$ gives

$$\hat{u}_2'' = \sum_{j \in \mathbb{J}} \chi_j (\xi_j g_{1,j} + (1 - \xi_j) g_{1,j-1}) . \quad (25)$$

Spatial integration then gives

$$\hat{u}_2' = \frac{H}{2} \sum_{j \in \mathbb{J}} \chi_j (\xi_j^2 g_{1,j} - (1 - \xi_j)^2 g_{1,j-1} + c_j) , \quad (26)$$

$$\hat{u}_2 = \frac{H^2}{6} \sum_{j \in \mathbb{J}} \chi_j (\xi_j^3 g_{1,j} + (1 - \xi_j)^3 g_{1,j-1} + 3c_j \xi_j + d_j) . \quad (27)$$

Note that the two constants of integration form piecewise linear terms that properly belong with the first-order approximation, and hence may be neglected. Consequently, the jump across adjacent intervals gives

$$[\hat{u}_2]_j = 0 , \quad [\hat{u}_2']_j = -H g_{1,j} , \quad (28)$$

such that \hat{u}_2 satisfies the continuity condition (11). The smoothness condition (13) then implies that

$$[\hat{u}'_2]_j = \frac{1}{H} \delta^2 \hat{u}_2|_{X_j} - \frac{1}{H} \delta^2 \hat{u}_1|_{X_j} = \frac{H}{6} \delta^2 g_{1,j} - \frac{1}{H} \delta^2 U_j, \quad (29)$$

and hence

$$(1 + \frac{1}{6} \delta^2) g_{1,j} = \frac{1}{H^2} \delta^2 U_j. \quad (30)$$