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Notes on the Diffusion Equation

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1 Introduction

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

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}\,. \tag{1}$$

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

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

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

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

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

$$\frac{\partial u}{\partial \vec{U}} \cdot \vec{g} = \frac{\partial^2 u}{\partial x^2}\,. \tag{4}$$

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

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

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

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

for some parameter $0 \leq \gamma \leq 1$. Now, 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

$$\dot{\vec{U}} \sim \gamma \vec{g}_1 + \gamma^2 \vec{g}_2 + \cdots\,. \tag{7}$$

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

$$\frac{\partial^2 \hat{u}_0}{\partial x^2} = 0\,, \tag{8}$$

$$\frac{\partial^2 \hat{u}_\ell}{\partial x^2} = \sum_{m=0}^{\ell-1} \frac{\partial \hat{u}_m}{\partial \vec{U}} \cdot \vec{g}_{\ell-m}\,, \qquad \text{for } \ell = 1, 2, \ldots\,. \tag{9}$$

3 Leading Approximation

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

$$\hat{u}_0 = \sum_{j \in \mathbb{J}} \chi_j (\xi_j U_j + (1 - \xi_j) U_{j-1})\,, \tag{10}$$

where $\chi_j(x)$ is an indicator that takes on the value 1 (or 0) inside (or outside) of the jth interval, and $\xi_j(x) = \frac{x - X_{j-1}}{X_j - X_{j-1}}$ is a linear, spatial 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 jth interval, namely:

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

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

$$[\hat{u}_1']_j = \frac{1}{H}(U_{j+1} + U_{j-1} - 2U_j) \;=\; \frac{1}{H}\,\delta^2 \hat{u}_0\big|_{X_j}\,, \tag{12}$$

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 internal boundary condition, namely

$$[u']_j = \frac{1-\gamma}{H}\,\delta^2 u\big|_{X_j}\,. \tag{13}$$

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

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

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

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

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

Similarly, the smoothness condition (13) implies that

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

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

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

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

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

with roots given by

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

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 $kH = n\pi$, $n = 0, 1, 2, \ldots$. 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. More precisely, these unstable regions occur when

$$\frac{kH}{2} < (1-\gamma)\tan\frac{kH}{2}\,, \qquad kH \neq n\pi\,. \tag{20}$$

Thus, for $\gamma = 0$ there is an initial forbidden gap $k \in (0, \frac{\pi}{H})$ adjacent to the centre manifold wavenumber $k = 0$.

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

$$\langle \mathcal{L}u, v\rangle = \langle u, \mathcal{L}v\rangle + R\,, \tag{21}$$

with the residual

$$R \;=\; \sum_{j\in\mathbb{J}} \left[u'v - v'u\right]_{X_{j-1}}^{X_j}\,. \tag{22}$$

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

$$R = r_{\bar{J}} - r_{\underline{J}} - \sum_{j=\underline{J}+1}^{\bar{J}-1} [r]_j \,, \tag{23}$$

for $\underline{J} = \inf \mathbb{J}$ and $\bar{J} = \sup \mathbb{J}$, if there are at least two intervals. Assuming that v also obeys conditions (11) and (13), the j-th residual jump becomes

$$\begin{aligned} [r]_j &= [u']_j V_j - [v']_j U_j \\ &= \frac{1-\gamma}{H} \left[(U_{j+1} + U_{j-1}) V_j - (V_{j+1} + V_{j-1}) U_j \right] . \end{aligned} \tag{24}$$

Observe that terms from adjacent interval boundaries will cancel, leaving

$$\begin{aligned} R &= u'_{\bar{J}} V_{\bar{J}} - v'_{\bar{J}} U_{\bar{J}} - u'_{\underline{J}} V_{\underline{J}} + v'_{\underline{J}} U_{\underline{J}} \\ &\quad - \frac{1-\gamma}{H} \left[U_{\underline{J}} V_{\underline{J}+1} - V_{\underline{J}} U_{\underline{J}+1} + U_{\bar{J}} V_{\bar{J}-1} - V_{\bar{J}} U_{\bar{J}-1} \right] . \end{aligned} \tag{25}$$

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 First-order Approximation

Substituting the leading approximation (10) into the nonlinear diffusion equation (9) for $\ell = 1$ results in the first-order equation

$$\hat{u}_1'' = \sum_{j \in \mathbb{J}} \chi_j (\xi_j g_{1,j} + (1 - \xi_j) g_{1,j-1}) \,. \tag{26}$$

Spatial integration then gives

$$\hat{u}_1' = \frac{H}{2} \sum_{j \in \mathbb{J}} \chi_j (\xi_j^2 g_{1,j} - (1 - \xi_j)^2 g_{1,j-1} + c_{1,j}) \,, \tag{27}$$

$$\hat{u}_1 = \frac{H^2}{6} \sum_{j \in \mathbb{J}} \chi_j (\xi_j^3 g_{1,j} + (1 - \xi_j)^3 g_{1,j-1} + 3\xi_j c_{1,j} + d_{1,j}) \,. \tag{28}$$

Recall from the chosen spatial discretisation that $u|_{X_j} = U_j$ at each grid-point. Observe this is already satified by $\hat{u}_0$ from equation (10), implying from expansion (6) that

$$\hat{u}_\ell\big|_{X_j} = 0 \qquad \text{for } \ell = 1, 2, \ldots . \tag{29}$$

Thus $[\hat{u}_\ell]_j = 0$ at each X_j, satisfying the continuity condition (11). Now, evaluating equation (28) at $\xi_j = 0$ gives $d_{1,j} = -g_{1,j-1}$, and at $\xi_j = 1$ gives $3c_{1,j} = -(g_{1,j} - g_{1,j-1})$. Thus, from equation (27), observe that

$$[\hat{u}_1']_j = -H(1 + \frac{1}{6}\delta^2)g_{1,j}\,, \tag{30}$$

However, the smoothness condition (13) gives

$$[\hat{u}_1']_j = \frac{1}{H}\,\delta^2\hat{u}_1\big|_{X_j} - \frac{1}{H}\,\delta^2\hat{u}_0\big|_{X_j}\,, \tag{31}$$

where, from equation (28),

$$\delta^2\hat{u}_1\big|_{X_j} = , \tag{32}$$

and hence

$$(1 + \frac{1}{6}\delta^2)g_{1,j} = \frac{1}{H^2}\delta^2 U_j\,. \tag{33}$$