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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 eigensolutions of the form

$$u(x,t) = e^{\lambda t \pm \sqrt{\lambda} x}, \tag{5}$$

which are physically realisable for real eigenvalues $\lambda = -k^2 \leq 0$ for corresponding 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

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

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

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

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

with indicator $\chi_j(x) = 1$ (or 0) for $x \in \mathbb{I}_j$ (or $x \notin \mathbb{I}_j$), and interpolator $\xi_j(x) = \frac{x - X_{j-1}}{X_j - X_{j-1}}$. This particular approximation is chosen to be continuous across the boundaries of each interval $\mathbb{I}_j$. In general, it suffices to impose a continuity condition at the right-hand end of each $\mathbb{I}_j$, 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

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

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, non-dimensionalised wavenumber $\kappa = kH > 0$. Thus, allowing for the partitioning of $\mathbb{X}$, let

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

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

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

Similarly, the smoothness condition (13) implies that

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

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 $c+is := e^{i\kappa}$ and $f := \frac{1-\gamma}{\kappa}$. 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 $c = \cos\kappa \leq 1$ and $1 - fs = 1 - (1-\gamma)\frac{\sin\kappa}{\kappa} \geq 0$. 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 $\mu = c \pm is = e^{\pm i\kappa}$. Likewise, $\mu = \pm 1$ for $\beta = \pm 1$, corresponding to $\kappa = n\pi$, $n = 0, 1, 2, \ldots$. Finally, for small regions near each $\kappa = (2n+1)\pi$, 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

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

Thus, at equilibrium ($\gamma = 0$) there is an initial forbidden gap $\kappa \in (0, \pi)$ adjacent to the centre manifold wavenumber $\kappa = 0$ (see Figure 1), indicating that transient solutions decay to the centre manifold at a rate of at least $\lambda = -\frac{\kappa^2}{H^2} = -\frac{\pi^2}{H^2}$. It is this gap that provides robustness to nonlinear perturbations of the system about the equilibrium.

5 Linear Dual Space

Suppose the domain $\mathbb{X}$has been discretised to have outer boundaries $X_{\underline{J}}$ and $X_{\bar{J}}$ for indices $\underline{J} = \inf\mathbb{J}$ and $\bar{J} = \sup\mathbb{J}$. Assume for convenience that $|\mathbb{J}| > 2$. Then an appropriate inner product for spatially square-integrable fields u and v is given by

$$\langle u, v\rangle = \int_{X_{\underline{J}}}^{X_{\bar{J}}} uv\; dx = \sum_{j=\underline{J}+1}^{\bar{J}} \int_{\mathbb{I}_j} uv\; dx\,. \tag{21}$$

It can then be shown, for twice-differentiable fields, that

$$\langle u'', v\rangle = \langle u, v''\rangle + R\,, \tag{22}$$

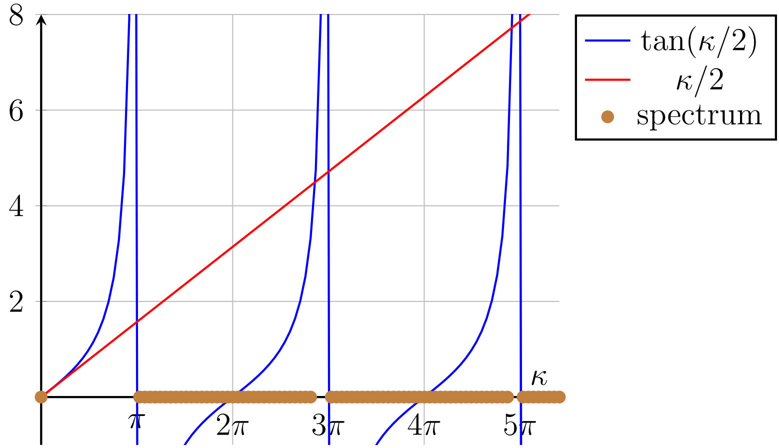

Figure 1: The equilibrium spectrum determined by the forbidding condition (20).

with residual

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

for $r = u'v - v'u$. Now, assuming that both u and v obey conditions (11) and (13), the residual jump at X_j 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 intervals $\mathbb{I}_{j-1}$ and $\mathbb{I}_{j+1}$ will cancel terms from $\mathbb{I}_j$, leaving only contributions from the outermost boundary intervals $\mathbb{I}_{\underline{J}+1}$ and $\mathbb{I}_{\bar{J}}$; consequently:

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

On a finite domain, there are three main outer boundary conditions that lead to a zero residual:

periodic Having period $\bar{J} - \underline{J}$ corresponds to $U_{\bar{J}} = U_{\underline{J}}$. Furthermore, by joining the domain cylindrically at $X_{\underline{J}}$ and $X_{\bar{J}}$, it can be shown that

$$u'_{\underline{J}} - u'_{\bar{J}} = [u']_{\bar{J}} = \frac{1-\gamma}{H} (U_{\underline{J}+1} + U_{\bar{J}-1} - 2U_{\bar{J}}) \,, \tag{26}$$

using condition (13). Hence, $R = 0$ if correspondingly v is periodic with period $\bar{J} - \underline{J}$.

Dirichlet Setting $u = 0$ at the boundaries corresponds to $U_{\underline{J}} = U_{\bar{J}} = 0$, giving $R = 0$ if correspondingly $v = 0$ on the boundaries.

Neumann Requiring $u' = 0$ on the boundaries (for $\gamma = 1$) corresponds to

$$u'_{\underline{J}} = \frac{1-\gamma}{H}(U_{\underline{J}+1} - U_{\underline{J}})\,, \qquad u'_{\bar{J}} = \frac{1-\gamma}{H}(U_{\bar{J}} - U_{\bar{J}-1})\,, \tag{27}$$

giving $R = 0$ if correspondingly $v' = 0$ on the boundaries.

Under any of the above three conditions, observe that $\langle \mathcal{L}u, v\rangle = \langle u, \mathcal{L}v\rangle$ for $\mathcal{L} = \partial^2/\partial x^2$, and hence $\mathcal{L}$ is self-adjoint. Furthermore, we are free to choose any dual v, e.g. to satisfy $\mathcal{L}v = 0$ for conenience. In particular, we may specifically target the j-th interval for u, for each $j \in \mathbb{J}$, with $v = \hat{v}_0^{[j]}$, where

$$\hat{v}_0^{[j]} = \chi_j \xi_j + \chi_{j+1}(1 - \xi_{j+1})\,, \tag{28}$$

which satisfies conditions (11) and (13) for $\gamma = 0$. It can then be shown in general that

$$\langle u'', \hat{v}_0^{[j]}\rangle = -[u']_j + \frac{1}{H}\,\delta^2 u\big|_{X_j}\,, \tag{29}$$

for any continuous, twice-differentiable u.

6 First-order Approximation

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

$$\hat{u}''_1 = \sum_{j\in\mathbb{J}} \chi_j(\xi_j g_{1,j} + (1-\xi_j) g_{1,j-1})\,. \tag{30}$$

Spatial integration then gives

$$\hat{u}'_1 = \frac{H}{2}\sum_{j\in\mathbb{J}} \chi_j(\xi_j^2 g_{1,j} - (1-\xi_j)^2 g_{1,j-1} + c_{1,j})\,, \tag{31}$$

$$\hat{u}_1 = \frac{H^2}{6}\sum_{j\in\mathbb{J}} \chi_j(\xi_j^3 g_{1,j} + (1-\xi_j)^3 g_{1,j-1} + 3\xi_j c_{1,j} + d_{1,j})\,. \tag{32}$$

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

$$\hat{u}_\ell|_{X_j} = 0 \qquad \text{for } \ell = 1, 2, \dots . \tag{33}$$

Thus $[\hat{u}_\ell]_j = 0$, satisfying the continuity condition (11), and $\delta^2\hat{u}_\ell|_{X_j} = 0$. Now, evaluating equation (32) 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 (31), observe that

$$[\hat{u}_1']_j = -H\left(1 + \frac{1}{6}\delta^2\right) g_{1,j} \,. \tag{34}$$

However, the smoothness condition (13) gives

$$[\hat{u}_1']_j = \frac{1}{H}\,\delta^2\hat{u}_1\big|_{X_j} - \frac{1}{H}\,\delta^2\hat{u}_0\big|_{X_j} = -\frac{1}{H}\delta^2 U_j \,, \tag{35}$$

and hence

$$\left(1 + \frac{1}{6}\delta^2\right) g_{1,j} = \frac{1}{H^2}\delta^2 U_j \,. \tag{36}$$

This solution can also be otained more directly via the dual space by computing $\langle \hat{u}_1'', \hat{v}_0^{[j]}\rangle$ from equations (28) and (30), and using results (29) and (35).

7 Second-order Approximation

For convenience, consider the shift operator $\sigma u(x,t) := u(x+H,t)$, which commutes with $\delta := \sigma^{\frac{1}{2}} - \sigma^{-\frac{1}{2}}$. Then, from equation (9) for $\ell = 2$, we obtain

$$\begin{aligned}
\hat{u}_2'' &= \frac{\partial \hat{u}_0}{\partial \vec{U}} \cdot \vec{g}_2 + \frac{\partial \hat{u}_1}{\partial \vec{U}} \cdot \vec{g}_1 \\
&= \sum_{j\in\mathbb{J}} \chi_j \left\{\xi_j + (1-\xi_j)\sigma^{-1}\right\} g_{2,j} \\
&\quad + \frac{1}{6}\sum_{j\in\mathbb{J}} \chi_j \xi_j (1-\xi_j)\left\{(\xi_j - 2)\sigma^{-1} - (\xi_j + 1)\right\} S\delta^2 g_{1,j} \,,
\end{aligned} \tag{37}$$

using equations (10) and (32), and equation (36) with $S = (1 + \delta^2/6)^{-1}$. Next, observe from equations (29), (13) and (33) that

$$\langle \hat{u}_\ell'', \hat{v}_0^{[j]}\rangle = 0 \qquad \text{for } \ell = 2, 3, \dots . \tag{38}$$

Hence, it can be shown by direct integration and simplification that

$$\langle \hat{u}_2'', \hat{v}_0^{[j]} \rangle = S^{-1} g_{2,j} - \frac{H}{6} \left(\frac{7}{60} \delta^2 + \frac{1}{2} \right) S \delta^2 g_{1,j} = 0 \,, \tag{39}$$

from equations (28) and (37).