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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

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

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 eigensolutions of the form

$$u(x, t) = e^{\lambda t + i k x}, \quad (5)$$

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

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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

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

Similarly, the smoothness condition (13) implies that

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

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

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

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 $c = \cos \kappa \leq 1$ 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 $\kappa = n\pi$, $n = 0, 1, 2, \dots$. 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

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

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

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

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

$$\langle u'', v \rangle = \langle u, v'' \rangle + R, \quad (22)$$

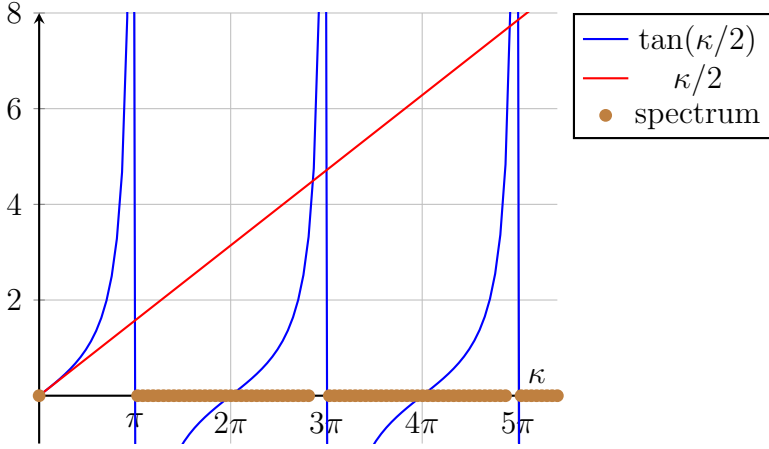


Figure 1: The equilibrium spectrum determined by the forbidding condition (20).

with residual

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

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

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

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:

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

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

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

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

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

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 convenience. 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

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

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

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

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

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

Spatial integration then gives

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

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

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

$$\hat{u}_\ell|_{X_j} = 0 \quad \text{for } \ell = 1, 2, \dots \quad (33)$$

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

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

However, the smoothness condition (13) gives

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

and hence

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

This solution can also be obtained 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).

Consequently, as a first approximation, the coarse dynamics evolve according to

$$\dot{\vec{U}} = \frac{\gamma}{H^2} S \delta^2 \vec{U} + \mathcal{O}(\gamma^2), \quad (37)$$

from equations (2) and (7), where, for convenience, we let $S = (1 + \frac{1}{6} \delta^2)^{-1}$. Now, recall from Section 2 that the eigensolution $u = e^{\lambda t + i k x}$ to the diffusion equation (1) has the exact spectrum $\lambda = -k^2$. It can further be shown that this eigensolution satisfies the relation $\delta^2 u = -2(1 - \cos kH)u$. Hence, the spectrum of the first-order approximation with $\gamma = 1$ is given by

$$\lambda = -\frac{6(1 - \cos kH)}{H^2(2 + \cos kH)} \sim -k^2 - \frac{1}{12} H^2 k^4 + \mathcal{O}(H^4 k^6), \quad (38)$$

which reveals an error of size $\mathcal{O}(H^2 k^4)$ in comparison to the exact spectrum. The behaviour of this approximate spectrum is shown in Figure 2.

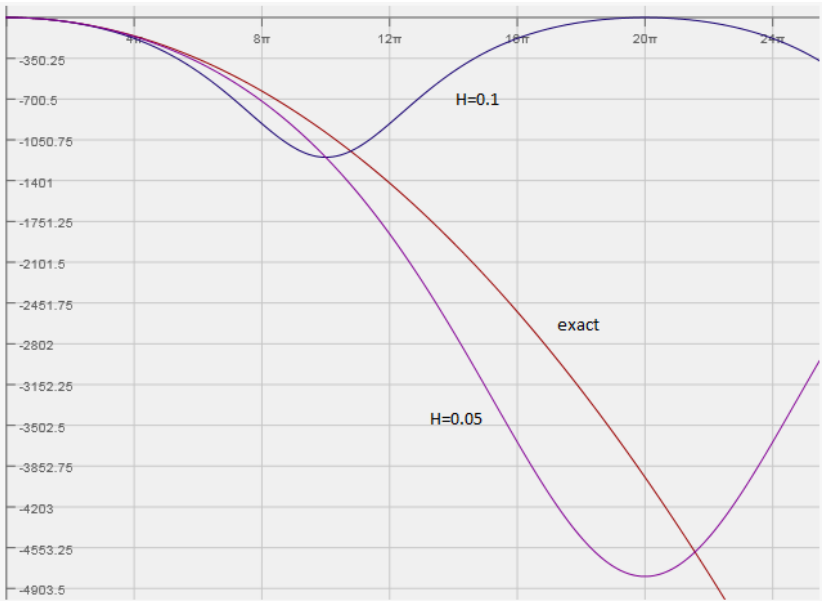


Figure 2: The exact spectrum (λ versus k) of the linear diffusion equation, compared to a first-order approximation with $H = 0.1$ and $H = 0.05$, respectively, for $\gamma = 1$.

7 Second-order Approximation

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

$$\begin{aligned} \hat{u}_2'' &= \frac{\partial \hat{u}_0}{\partial \vec{U}} \cdot \vec{g}_2 + \frac{\partial \hat{u}_1}{\partial \vec{U}} \cdot \vec{g}_1 \\ &= \sum_{j \in \mathbb{J}} \chi_j \{ \xi_j + (1 - \xi_j) \sigma^{-1} \} g_{2,j} \\ &\quad + \frac{1}{6} \sum_{j \in \mathbb{J}} \chi_j \xi_j (1 - \xi_j) \{ (\xi_j - 2) \sigma^{-1} - (\xi_j + 1) \} S \delta^2 g_{1,j}, \end{aligned} \quad (39)$$

using equations (10), (32), and (36). Next, observe from equations (29), (13) and (33) that

$$\langle \hat{u}_\ell'', \hat{v}_0^{[j]} \rangle = 0 \quad \text{for } \ell = 2, 3, \dots \quad (40)$$

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

$$\langle \hat{u}_2'', \hat{v}_0^{[j]} \rangle = H S^{-1} g_{2,j} - \frac{H}{6} \left(\frac{7}{60} \delta^2 + \frac{1}{2} \right) S \delta^2 g_{1,j}, \quad (41)$$

from equations (28) and (39). Hence, as a second approximation, the coarse dynamics evolve according to

$$\dot{\vec{U}} = \frac{\gamma}{H^2} S \delta^2 \vec{U} + \frac{\gamma^2}{60 H^2} (7 - 2S) S^2 \delta^4 \vec{U} + \mathcal{O}(\gamma^3), \quad (42)$$

using the fact that $S \delta^2 = 6(1 - S)$. Thus, following Section 6, the approximate spectrum for $\gamma = 1$ is now

$$\lambda = -\frac{1}{5H^2} \frac{96 + 27c - 72c^2 - 51c^3}{8 + 12c + 6c^2 + c^3} \sim -k^2 - \frac{1}{180} H^4 k^6 + \mathcal{O}(H^6 k^8), \quad (43)$$

where, as previously in Section 4, $c := \cos kH$. Observe that the $O(H^2 k^4)$ error term from the first-order approximation (38) has now been completely eliminated by the second-order correction, in favour of an $O(H^4 k^6)$ error.

The behaviour of this corrected, approximate spectrum is shown in Figure 3. Observe that the approximation becomes untenable from the first turning point, at which $k \approx \frac{\pi}{H}$.

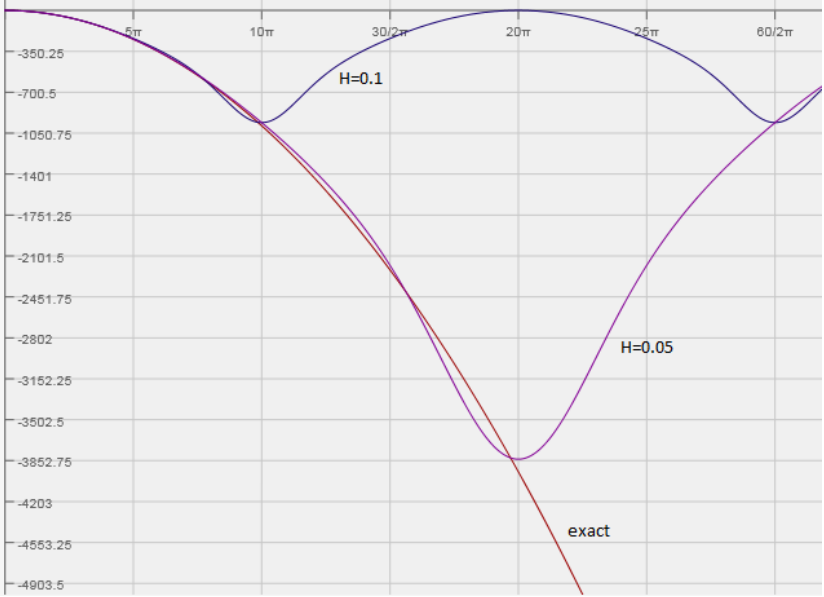


Figure 3: The exact spectrum (λ versus k) of the linear diffusion equation, compared to a second-order approximation with $H = 0.1$ and $H = 0.05$, respectively, for $\gamma = 1$.