2 Pieces of Mathematics

1 Dissipation, Dispersion and Discrete Models

For linear PDEs (1 dimension here), one can look for exponential solutions $e^{\lambda t+ik}$. Notice of course if λ is has positive real part, the equation is unstable and possibly ill-posed. For standard examples of linear equations

Equation	Phase relation
$\partial_t u+\partial_x u=0$	$\lambda=-ik$
$\partial_t u={\partial_x}^2 u$	$\lambda=-k^2$
$\partial_t u=\partial_x^3 u$	$\lambda=-ik^3$

Now consider a standard argument for passing from a discrete collection of blocks joined by springs to the continuum. Imagine a typical formulation

$$\partial_t^2 y \;=\; \partial_x[T(\partial_x y)] \tag{1}$$

The usual expansion would read

$$\partial_t^2 u_j \;=\; \frac{T(u_{j+1})-2T(u_j)+T(u_{j-1})}{h^2} \tag{2}$$

where $u_j=(y_j-y_{j-1})/h$, y_j is the displacement of the j^{th} particle, and h is the equilibrium interparticle distance. Expanding the RHS,

$$\partial_t^2 u_j \;=\; \partial_x^2 T(u_j) \;+\; \frac{h^2}{12}\partial_x^4 T(u_j) \;+\; O(h^4) \tag{3}$$

Usually one simply passes to the limit $h\to 0$ and thats it. However if T is nonlinear - in particular, non-harmonic - the higher order term provides useful information about the continuum behavior. Set $u_j=u$ and assume T is linear. Then one has

$$\lambda^2 \;=\; -\,k^2 \;+\; \frac{h^2}{12}k^4 \tag{4}$$

and the dispersion term leads to ill-posedness. (Note: Considering wave propagation in one direction only lead to the KdV equation.)
[From Rosenau, *Phys Rev D* **36** (1987)] A way around the short wave blow-up is to reconsider (3) and recall the Chapman-Enskog expansion we saw earlier

$$\partial_t^2 u \;=\; \mathcal{L}\partial_x^2[T(u)] \tag{5}$$

where $\mathcal{L}=1+\frac{h^2}{12}\partial_x^2+O(h^4)$. This operator can be inverted, and we write

$$\mathcal{L}^{-1} \;=\; 1-\frac{h^2}{12}\partial_x^2+O(h^4)$$

Apply to (5) yields

$$\partial_t^2 u \;=\; \partial_x^2 T(u) \;+\; \frac{h^2}{12}\partial_x^2\partial_t^2 T(u) \tag{6}$$

Now the linearized dispersion relation is $\lambda^2 = -k^2 - \frac{h^2}{12}k^2\lambda^2$ or

$$\lambda^2 \;=\; \frac{-k^2}{1+\frac{h^2}{12}k^2} \tag{7}$$

Now the high frequency modes asymptote to an imaginary constant, while low frequency waves behave much as they had earlier, with eigenvalue $\lambda \approx \pm ik$.

It is worth returning to a linearized version of the discrete equation (2) again, and look at the action of the discrete shift operator $\sigma u_j = u_{j+1}$ so $\sigma u_j = \sigma e^{\lambda t + ik(j+1)h} = e^{ikh}u_j$. In the equation we have

$$\lambda^2 \;=\; \frac{1}{h^2}(e^{ikh} - 2 + e^{-ikh}) \;=\; -\frac{2}{h^2}\sin^2(kh) \tag{8}$$

The usual Taylor expansion of the sin gives the ill-posed result of (4). An expansion by rational functions leads to (7).

2 Variation of Parameters

[Estep and Neckels, *J. Comp. Phys* **213** (2006)] The second issue we tackle is to investigate the variation of a parameter on the output of a system of equations. We illustrate with a finite dimensional example first, then examine an ODE example. The methodology carries over to PDEs directly.

2.1 A Nonlinear System

So imagine we want to solve

$$f(\mathbf{x},\lambda) \;=\; b \tag{9}$$

where $x \in \Re^N$ and where $\lambda \in \Re^d$ is a parameter. We asume f is as smooth as we need it to be. If we think of f as the action of an experiment, we often are not able to monitor all of f on output, but only a functional of it - perhaps an average, or only one component of the solution. By the Riesz representation theorem, there is a vector $\psi \in \Re^N$ such that $< \mathbf{x}, \psi >$ yields the functional of interest. For example, $\psi = \frac{1}{N}(1, 1, \ldots, 1)^T$ is the average.

What if you could solve (9) easily for some value μ of the parameter, but wanted to know the solution (or an estimate of it) for nearby values. Let $\mathbf{y}$ be the solution of $f(\mathbf{y}, \mu) \;=\; b$. Let $A = D_x f(\mathbf{y}, \mu)$. Then there is a Green's function ϕ such that

$$A^T\phi \;=\; \psi$$

so

$$< \mathbf{x}, \psi > \;=\; < \mathbf{x}, A^T\phi > \;=\; < A\mathbf{x}, \phi > \tag{10}$$

Now compute a Taylor expansion around $(\mathbf{y}, \mu)$

$$f(\mathbf{x}, \lambda) = f(\mathbf{y}, \mu) + D_x f(\mathbf{y}, \mu)(x - y) + D_\lambda f(\mathbf{y}, \mu)(\lambda - \mu) + R \tag{11}$$

where R is the remainder. Now the f's both equal b, so

$$< A\mathbf{x}, \phi > = < A\mathbf{y}, \phi > - < D_\lambda f(\mathbf{y}, \mu)(\lambda - \mu), \phi > - < R, \phi > \tag{12}$$

Drop the remainder, we find

$$< \mathbf{x}, \psi > \approx < \mathbf{y}, \psi > - < D_\lambda f(\mathbf{y}, \mu)(\lambda - \mu), \phi > \tag{13}$$

2.2 Example 1

Consider the system

$$\begin{aligned} \lambda_1 x_1^2 + x_2^2 &= 1 \\ x_1 - \lambda_2 x_2 &= 1 \end{aligned} \tag{14}$$

For simplicity, choose $\psi = (1, 0)^T$ so $< \mathbf{x}, \psi >= x_1$, and lets look near $\mu_1 = \mu_2 = 1$ and the solution $y_1 = 1$, $y_2 = 0$.

$$D_x = \begin{pmatrix} 2\lambda_1 x_1 & 2x_2 \\ 1 & \lambda_2 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 1 & 1 \end{pmatrix} \tag{15}$$

$$D_\lambda = \begin{pmatrix} x_1^2 & 0 \\ 0 & -x_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{16}$$

Putting it all together then,

$$< \mathbf{x}, \psi >= x_1 \approx < (1, 0), \psi > - < \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda_1 - 1 \\ \lambda_2 - 1 \end{pmatrix}, \phi > \tag{17}$$

2.3 Example 2

Here is a scalar ODE

$$\begin{aligned} \dot{x}(t, \lambda) &= f(x(t, \lambda), \lambda_1) \quad 0 \le t \le T \\ x(0) &= \lambda_0 \end{aligned} \tag{18}$$

where for simplicity take $x \in \Re^1$, and λ_1, λ_0 both 1-dimensional also. Here I am thinking of $\lambda = \lambda(\omega)$ as a random variable with some distribution. A solution $x(t, \lambda(\omega))$ is a stochastic process. We need to make enough assumptions on x so the solution exists for the time of interest.

Functionals: $\psi(s) = \delta(s - t)$ gives the solution at time t; $\psi(s) = 1/T$ is the average of the solution over $[0, T]$.

So the quantity of interest

$$q(\lambda(\omega)) = \int_0^T < x(s,\lambda(\omega)), \psi(s) > ds$$

We are really trying to get an idea of the distribution of the solution as λ varies.

The Green's function solves the adjoint problem

$$\begin{aligned} -\dot{\phi}(t) - A^T(t)\phi(t) &= \psi(t) \quad T \geq t \geq 0 \\ \phi(T) &= 0 \end{aligned} \tag{19}$$

and of course $A(t) = D_x f(y(t), \mu_1)$ where y is the solution of the deterministic problem with reference values (μ_0, μ_1).

One can show

$$q(\lambda) = \int_0^T < x, \psi > ds \approx \int_0^T < y, \psi > ds + < \lambda_0 - \mu_0, \phi(0) > + \int_0^T < D_{\lambda_1} f(y, \mu_1)(\lambda_1 - \mu_1), \phi(s) > ds$$

So if our problem is

$$\begin{aligned} \dot{x}(t,\lambda) &= \lambda x(t,\lambda) \quad 0 \leq t \leq T \\ x(0) &= x_0 \end{aligned} \tag{20}$$

with λ random, and $\psi(s) = \delta(s-t)$, then

$$q(\lambda) = x(t,\lambda) \approx y(t,\mu) + (\lambda - \mu) \int_0^t e^{\mu(t-s)} y(s,\mu)\, ds$$

The approximation is

$$y(t,\lambda) = a(t) + \lambda b(t)$$

with

$$a(t) = x_0(1-\mu t)e^{\mu t} \qquad b(t) = x_0 t e^{\mu t}$$

What happens if λ is normally distributed about 0? What is it is the initial data that varies, at a fixed value of λ_1?