Vertical Derivative Math for iWave

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1 What is a Square Root?

For a number x, the square root is designated $\sqrt{x}$. Its meaning comes from its definition, which is

$$(\sqrt{x})^2 = x \tag{1}$$

This is the fundamental definition, and it can be used for defining the square root of objects other than numbers.

2 Square Root of a Matrix

Consider a square $N \times N$ matrix M which is have eigenvalues and eigenvectors. Denote the eigenvalues by $m_\alpha, \alpha = 1, \ldots N$, and the orthonormal eigenvectors $\hat{e}_\alpha$. The eigenvectors satisfy

$$\hat{e}^*_\alpha \cdot \hat{e}_\beta = \delta_{\alpha\beta} \tag{2}$$

We can expand the matrix as

$$M = \sum_{\alpha=1}^{N} m_\alpha \ \hat{e}_\alpha \otimes \hat{e}^*_\alpha \tag{3}$$

and we can directly verify that

$$M \cdot \hat{e}_\alpha = m_\alpha \ \hat{e}_\alpha \tag{4}$$

Using the definition for the square root $(\sqrt{M})^2 = M$, we can directly verify that

$$\sqrt{M} = \sum_{\alpha=1}^{N} \sqrt{m_\alpha} \ \hat{e}_\alpha \otimes \hat{e}^*_\alpha \tag{5}$$

and in particular that

$$\sqrt{M} \ \cdot \hat{e}_\alpha = \sqrt{m_\alpha} \ \hat{e}_\alpha \tag{6}$$

How do we use the square root of a matrix on a vector in N space. Since all such vectors can be expanded in terms of the orthonormal eigenbasis, we can write an arbitrary vector $\vec{v}$ as

$$\vec{v} = \sum_{\alpha=1}^{N} v_\alpha \; \hat{e}_\alpha \tag{7}$$

the application of the square root matrix is

$$\sqrt{M} \cdot \vec{v} = \sum_{\alpha=1}^{N} \sqrt{m_\alpha} \; v_\alpha \; \hat{e}_\alpha \tag{8}$$

As a side note, if you know the eigenvalues of a matrix, then a good way of computing the exponential of that matrix is

$$e^M = \sum_{\alpha=1}^{N} e^{m_\alpha} \; \hat{e}_\alpha \otimes \hat{e}_\alpha^* \tag{9}$$

3 Eigenbasis for derivative operators - One dimensional case

When we go to looking at derivatives as operators, the eigenvalue/eigenvector approach carries over, but the eigenvalues are continuous instead of discrete, so there is some additional mathematical machinery to put in place. We begin with one dimensional problems for this.

Consider functions $f(x)$ of a single variable x. The deriviative d/dx is an operator on those functions. You can directly verify that d/dx has eigenvectors

$$\hat{e}_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} \tag{10}$$

and the eigenvalues are ik, for k real-valued. The eigenvectors are orthonormal in the continuous sense, i.e.

$$\int_{-\infty}^{\infty} dx \; \hat{e}_k^*(x) \; \hat{e}_q(x) \;\; = \;\; \delta(k-q) \tag{11}$$

So now lets look at the operator $-d^2/dx^2$. Since

$$-\frac{d^2}{dx^2} \; \hat{e}_k(x) = k^2 \; \hat{e}_k(x) \tag{12}$$

we can see that $\hat{e}_k(x)$ is an eigenvector and k^2 is the corresponding eigenvalue for $-d^2/dx^2$. Following the process used for matrices, the square root acts like

$$\sqrt{-\frac{d^2}{dx^2}} \; \hat{e}_k(x) \;\; = \;\; |k| \; \hat{e}_k(x) \tag{13}$$

Since any function $f(x)$ has a Fourier representation

$$f(x) = \int_{-\infty}^{\infty} dk\ \hat{e}_k(x)\ \tilde{f}(k) \tag{14}$$

the square root operator looks like this:

$$\sqrt{-\frac{d^2}{dx^2}}\ f(x) = \int_{-\infty}^{\infty} dk\ \hat{e}_k(x)\ \tilde{f}(k)\ |k| \tag{15}$$

4 Two Dimensions

The two dimensional case is a straightforward extension of the 1D case. Now positions are $\vec{x} = (x, z)$ and the eigenvalue label is $\vec{k} = (k_x, k_z)$. The eigenvectors are

$$\hat{e}_{\vec{k}}(\vec{x}) \ = \ \frac{1}{2\pi} e^{i\vec{k}\cdot\vec{x}} \tag{16}$$

and are properly normalized:

$$\int d^2x\ \hat{e}^*_{\vec{k}}(\vec{x})\ \hat{e}_{\vec{q}}(\vec{x}) \ = \ \delta(\vec{k} - \vec{q}) \tag{17}$$

Following the same procedure as above, we can verify directly that

$$\sqrt{-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right)}\ \hat{e}_{\vec{k}}(\vec{x}) = |\vec{k}|\ \hat{e}_{\vec{k}}(\vec{x}) \tag{18}$$

So for any function $\phi(\vec{x})$ that has a Fourier representation $\tilde{\phi}(\vec{k})$,

$$\sqrt{-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right)}\ \phi(\vec{x}) = \int d^2k\ \hat{e}_{\vec{k}}(\vec{x})\ \tilde{\phi}(\vec{k})\ |\vec{k}| \tag{19}$$

5 Conversion to Convolution

Through a series of manipulations of the identities associated with the eigenvectors, we can convert equation 19 to an equation for a convolution. First, we insert an integral over the Dirac function:

$$\begin{aligned} \sqrt{-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right)}\ \phi(\vec{x}) \ &= \ \int d^2k\ \hat{e}_{\vec{k}}(\vec{x})\ |\vec{k}|\ \int d^2q\ \tilde{\phi}(\vec{q})\ \delta(\vec{k} - \vec{q}) \qquad (20) \\ &= \ \int d^2k\ \hat{e}_{\vec{k}}(\vec{x})\ |\vec{k}|\ \int d^2q\ \tilde{\phi}(\vec{q})\ \int d^2y\ \hat{e}^*_{\vec{k}}(\vec{y})\ \hat{e}_{\vec{q}}(\vec{y}) \end{aligned}$$

Since we assume that all of the integral converge and are well behaved, we can move the order of integration around and rewrite this as

$$\int d^2y\ \int d^2k\ \hat{e}_{\vec{k}}(\vec{x})\ |\vec{k}|\ \hat{e}^*_{\vec{k}}(\vec{y})\ \int d^2q\ \tilde{\phi}(\vec{q})\ \hat{e}_{\vec{q}}(\vec{y}) \tag{21}$$

The integral over $\vec{q}$ we can recognize is just $\phi(\vec{x})$. If we define

$$G(\vec{x}-\vec{y}) \;\equiv\; \int d^2k\; \hat{e}_{\vec{k}}(\vec{x})\; |\vec{k}|\; \hat{e}^*_{\vec{k}}(\vec{y}) \tag{22}$$

then everything assembles to

$$\sqrt{-\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}\right)}\;\phi(\vec{x}) \;=\; \int d^2y\; G(\vec{x}-\vec{y})\;\phi(\vec{y}) \tag{23}$$

which is a convolution of ϕ by the convolution kernel G.

6 Grid Discretization

The next step is to convert equation 23 to living on a 2D rectangular grid. So we assume that we want to evaluate things on a grid consisting of vertices at points $\vec{x}_{ij}$. The function $\phi(\vec{x})$ exists only at the grid points, and we label it $\phi_{ij} \equiv \phi(\vec{x}_{ij})$. Then we rewrite the continuous convolution in 23 as

$$\left\{\sqrt{-\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}\right)}\;\phi(\vec{x})\right\}_{ij} = \sum_{IJ} G(\vec{x}_{ij}-\vec{x}_{IJ})\;\phi_{IJ} \tag{24}$$

There is actually a normalization issue here, because I haven't put in anything for the integration measure d^2y. Instead, I am going to lump all of the normalization problems into the free parameters in the problem, like the gravity coefficient and the time step, and instead normalize by G(0). So I am going to replace this with

$$\left\{\sqrt{-\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}\right)}\;\phi(\vec{x})\right\}_{ij} \;\to\; \frac{\sum_{IJ}\; G(\vec{x}_{ij}-\vec{x}_{IJ})\;\phi_{IJ}}{G(0)} \tag{25}$$

And so the weights in iWave are

$$w_{ijIJ} = \frac{G(\vec{x}_{ij}-\vec{x}_{IJ})}{G(0)} \tag{26}$$

The next order of business is to note that the definition of G in equation 22 is divergent. But since we are only simulating on a grid, we don't need spatial frequencies higher than the grid resolution. A simple way to handle this is to insert a "soft-cutoff" in the form of an gaussian term, and redefine G to be

$$G(\vec{x}-\vec{y}) \;\equiv\; \int d^2k\; \hat{e}_{\vec{k}}(\vec{x})\; |\vec{k}|\; e^{-|\vec{k}|^2\sigma^2}\; \hat{e}^*_{\vec{k}}(\vec{y}) \tag{27}$$

The parameter σ acts as a controllable cutoff. In practice, a value of $\sigma = 1$ works well, but others can too.

We can make further reductions of the the expression for G by using polar coordinates and evaluating the integral over the polar angle exactly. With the switch to polar coordinates, G looks like

$$
\begin{aligned}
G(\vec{x}) &= \int_0^\infty dk\ k^2 e^{-k^2\sigma^2} \int_0^{2\pi} d\theta\ e^{ik|\vec{x}|\cos\theta} &\quad (28)\\
&= \int_0^\infty dk\ k^2 e^{-k^2\sigma^2} J_0(k|\vec{x}|) &\quad (29)
\end{aligned}
$$