TODO TITLE

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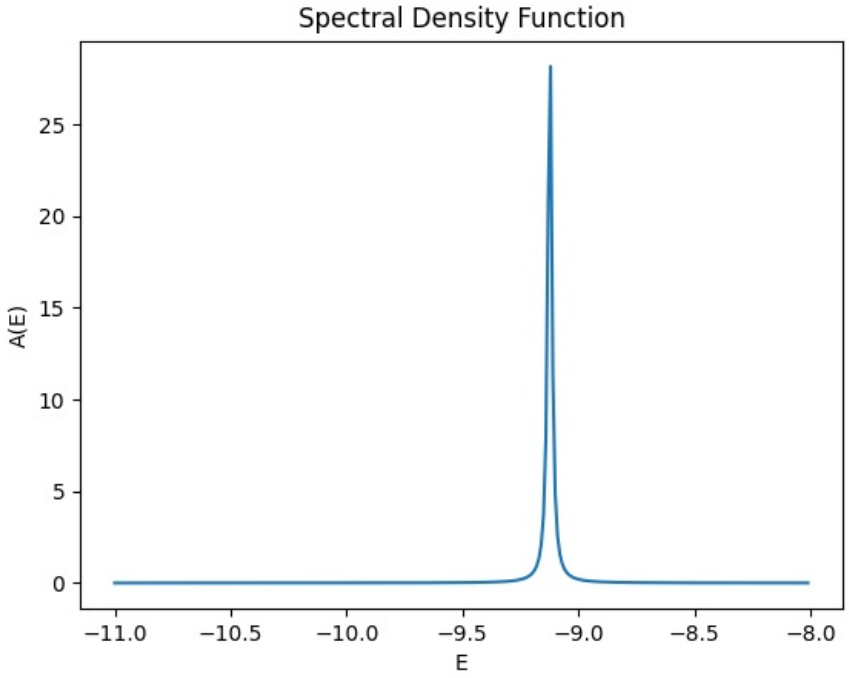
1 Background

In one of my condensed matter physics research projects, I am looking to fit a vector of paramters $\mathbf{v}$ to describe the interactions of a quantum mechanical system (the system is parametrized by $\mathbf{v}$). There is another vector of real numbers $\mathbf{k}$ (the system's momentum) that also parametrizes the system. Now, the system's ground state energy $E_0(\mathbf{v}, \mathbf{k})$ is to be matched with target energies $E_T(\mathbf{k})$. This is done by interpolating for a finite number of $\mathbf{k}$ points (in practice this seems to match $E_T(\mathbf{k})$ for all $\mathbf{k}$ quite well). One way to find an appropriate $\mathbf{v}$ is to use gradient descent on the cost function

$$J(\mathbf{v}) = ||\mathbf{E_0}(\mathbf{v}) - \mathbf{E_T}||_2$$

Here $\mathbf{E_0}$ and $\mathbf{E_T}$ are vectors with entries that are energy values at various $\mathbf{k}$ values. In short, we use a least squares fit. $E_0(\mathbf{v}, \mathbf{k})$ can computed as the energy where the *spectral density function* $A(E)$ spikes. For example, in the following figure, we see that $E \approx -9.1$:



Numerically, we restrict ourselves to an interval I with N evenly spaced grid points to evaluate $A(E)$. We thus have

$$E_0(\mathbf{v}, \mathbf{k}) = \arg\max_{E \in I} A(E, \mathbf{v}, \mathbf{k})$$

There is another parameter η, which controls the spikes width, that is set equal to the grid spacing dE to ensure that the spike will be detected. Locally, this spike is symmetric (a Lorentzian, in fact) in the limit $\eta \to 0^+$. So the error in this method is roughly bounded by $dE/2$. This error propagates to the $J(\mathbf{v})$ function to also produce an error bound of $dE/2$ if we use a dimensionality-agnostic 2-norm (i.e. divide by the square root of the dimension of the energy vectors).

In the following analyses, we consider single-variable functions for simplicity. Let $f(x)$ be such a function that we are interested in and $g(x) = f(x) + \delta(x)$ be a noisy function with $|\delta(x)| \leq \Delta$ for some positive error bound Δ (e.g. $\Delta = dE/2$).

To motivate this project, I seek to answer the question of how Δ should be scaled relative to the other numerical parameters to obtain the best accuracy for the least computation time. I will therefore be determining the asymptotic errors for various numerical methods for a given number of computations.

2 Derivatives

2.1 First Derivative: Central Difference

Suppose we want to compute the derivative of $f(x)$ but only have access to evaluating the noisy function $g(x)$. A central difference yields:

$$f'(a) \approx \frac{g(a+k) - g(a-k)}{2k}$$

The error in this method is

$$\begin{aligned} f'(a) - \frac{g(a+k) - g(a-k)}{2k} &= f'(a) - \frac{f(a+k) - f(a-k)}{2k} - \frac{\delta(a+k) - \delta(a-k)}{2k} \\ &= -\frac{1}{12} f'''(\xi) k^2 + \frac{1}{12} f'''(\zeta) k^2 - \frac{\delta(a+k) - \delta(a-k)}{2k} \end{aligned}$$

for some $\xi \in (a, a+k)$ and $\zeta \in (a-k, a)$. A bound for this error $E(k, \Delta)$ is then

$$E(k, \Delta) = \frac{1}{6} K_3 k^2 + \frac{\Delta}{k}$$

where K_3 is a bound on the absolute value of the third derivative of $f(x)$. Note that Taylor analysis is not applied to $\delta(x)$ because it is not continuous–$\delta(x)$ is discretized, for example, in the spectral density function case.

Now, the computation time $C(k, \Delta)$ is independent of k because only a single finite difference is computed. $C(k, \Delta)$ is inversely proportional to Δ in the spectral density function scenario,

however, because the number of $A(E)$ evaluations for a given interval size $|I|$ is approximately $|I|/dE$:

$$\boxed{C(k,\Delta) \sim \Delta^{-1}}$$

The optimal k that produces a minimal error bound given a fixed $C(k,\Delta)$ and therefore fixed Δ is given by

$$\frac{dE}{dk} = \frac{\partial E}{\partial k} = \frac{1}{3}K_3 k - \frac{\Delta}{k^2} = 0$$

This is indeed a minimum by the second derivative test:

$$\frac{d^2E}{dk^2} = \frac{\partial^2 E}{\partial k^2} = \frac{1}{3}K_3 + \frac{2\Delta}{k^3} > 0$$

So the optimal k-Δ relationship is

$$\boxed{\Delta = \frac{1}{3}K_3 k^3}$$

The cubic relationship makes sense because the $\frac{1}{6}K_3k^2$ and $\frac{\Delta}{k}$ terms in $E(k,\Delta)$ should scale the same–if they did not, the term that vanishes the slowest would become a bottleneck and could be made smaller for faster error convergence. The error bound is then

$$\boxed{E(k,\Delta) = \frac{1}{2}K_3k^2 = \frac{3^{2/3}}{2}K_3^{2/3}\Delta^{2/3}}$$

The error bound therefore scales with the comptuation time as:

$$\boxed{E \sim C^{-2/3}}$$

2.2 Second Derivative

We now consider the task of estimating $f''(a)$:

$$f''(a) \approx \frac{g(a+k) - 2g(a) + g(a-k)}{k^2}$$

The error in this method is

$$\begin{aligned} f''(a) - \frac{g(a+k) - 2g(a) + g(a-k)}{k^2} &= f''(a) - \frac{f(a+k) - 2f(a) + f(a-k)}{k^2} \\ &\quad - \frac{\delta(a+k) - 2\delta(a) + \delta(a-k)}{k^2} \\ &= -\frac{1}{24}f''''(\xi)k^2 + \frac{1}{24}f''''(\zeta)k^2 - \frac{\delta(a+k) - 2\delta(a) + \delta(a-k)}{k^2} \end{aligned}$$

for some $\xi \in (a, a+k)$ and $\zeta \in (a-k, a)$. A bound for this error $E(k,\Delta)$ is then

$$E(k,\Delta) = \frac{1}{12}K_4k^2 + \frac{4\Delta}{k^2}$$

where K_4 is a bound on the absolute value of the fourth derivative of $f(x)$. Again, the computation time is scaled as such:

$$\boxed{C(k, \Delta) \sim \Delta^{-1}}$$

The optimal k-Δ relationship is given by:

$$\frac{dE}{dk} = \frac{\partial E}{\partial k} = \frac{1}{6} K_4 k - \frac{8\Delta}{k^3} = 0$$

This is indeed a minimum by the second derivative test:

$$\frac{d^2E}{dk^2} = \frac{\partial^2 E}{\partial k^2} = \frac{1}{6} K_4 + \frac{24\Delta}{k^4} > 0$$

The ideal k-Δ relationship is thus

$$\boxed{\Delta = \frac{1}{48} K_4 k^4}$$

Similar to the central difference case, the $\frac{1}{12} K_4 k^2$ and $\frac{4\Delta}{k^2}$ terms scale the same under this relationship. The error bound is then

$$\boxed{E(k, \Delta) = \frac{1}{6} K_4 k^2 = \frac{2}{\sqrt{3}} K_4^{1/2} \Delta^{1/2}}$$

The error bound therefore scales with the comptuation time as:

$$\boxed{E \sim C^{-1/2}}$$

3 Finit Difference Methods

3.1 1-Periodic $-u'' + u = f$

Consider the following 1-periodic ODE:

$$-u''(x) + u(x) = f(x)$$

We may solve this problem using finite differences by discretizing the interval $[0, 1)$ into N uniformly-spaced grid points, with $k = 1/N$ being the grid spacing. Now let $\mathbf{u}$ be $u(x)$ evaluated at these points and $\mathbf{U}$ be our numerical estimation of $\mathbf{u}$. Then

$$A\mathbf{U} = \mathbf{G} = \mathbf{F} + \delta$$
$$A\mathbf{u} = \mathbf{F} - \tau$$

Here $A = -D_2 + I$ (and A is nonsingular), $\mathbf{F}$ is $f(x)$ evaluated at the grid points, $\mathbf{G}$ is our noisy evaluation of $\mathbf{F}$ with error δ, where $||\delta||_2 \leq \Delta$, and τ is the truncation error in the (non-noisy) finite difference approximation. This numerical recipe takes the following steps to complete:

1. $\mathbf{G}$ needs to be constructed. There are $N = k^{-1}$ entries, each of which require $O(\Delta^{-1})$ computations. This step has a runtime of $O(k^{-1}\Delta^{-1})$.

2. A needs to be constructed. Since A is sparse, this step takes $O(N) = O(k^{-1})$ computations.
3. The system $A\mathbf{U} = \mathbf{G}$ needs to be solved. Since A is sparse, this step also has a runtime of $O(k^{-1})$.

The bottleneck occurs in the first step, giving a total runtime of

$$\boxed{C \sim k^{-1}\Delta^{-1}}$$

Meanwhile, the error $\mathbf{E} = \mathbf{u} - \mathbf{U}$ is given by

$$\begin{aligned} A\mathbf{E} &= A\mathbf{u} - A\mathbf{U} = -\tau - \delta \\ \mathbf{E} &= -A^{-1}\tau - A^{-1}\delta \end{aligned}$$

We know that $\left|\left|A^{-1}\right|\right|_2 = 1$ from von Neumann analysis. The truncation error $\tau = \mathbf{F} - A\mathbf{u}$ is bounded by the non-noisy finite difference error bound:

$$||\tau||_2 \leq \frac{1}{12}K_4 k^2$$

This bounds the error as:

$$||\mathbf{E}||_2 \leq ||\tau||_2 + ||\delta||_2 = \frac{1}{12}K_4 k^2 + \Delta$$

For a fixed $C(k, \Delta) = k^{-1}\Delta^{-1}$, we can treat Δ as a function of k: $\Delta = C^{-1}k^{-1}$. Then optimizing the error bound gets us:

$$\begin{aligned} E(k, \Delta) &= \frac{1}{12}K_4 k^2 + \Delta \\ \frac{dE}{dk} &= \frac{\partial E}{\partial k} + \frac{\partial E}{\partial \Delta}\frac{d\Delta}{dk} = \frac{1}{6}K_4 k - C^{-1}k^{-2} = \frac{1}{6}K_4 k - k^{-1}\Delta = 0 \end{aligned}$$

$$\boxed{\Delta = \frac{1}{6}K_4 k^2}$$

Again, both error terms scale the same in this relationship. Finally, we verify that this is indeed a minimum:

$$\begin{aligned} \frac{d^2E}{dk^2} &= \frac{\partial^2 E}{\partial k^2} + \frac{\partial^2 E}{\partial \Delta^2}\left(\frac{d\Delta}{dk}\right)^2 + \frac{\partial^2 E}{\partial \Delta \partial k}\frac{d\Delta}{dk} + \frac{\partial E}{\partial \Delta}\frac{d^2\Delta}{dk^2} \\ &= \frac{\partial^2 E}{\partial k^2} + \frac{\partial E}{\partial \Delta}\frac{d^2\Delta}{dk^2} = \frac{1}{6}K_4 + 2C^{-1}k^{-2} > 0 \end{aligned}$$

The error bound is now

$$\boxed{E(k, \Delta) = \frac{1}{4}K_4 k^2 = \frac{3}{2}\Delta}$$

The runtime under this k-Δ relationship scales as $C \sim k^{-3} \sim \Delta^{-3/2}$. The error therefore scales with runtime as

$$\boxed{E \sim C^{-2/3}}$$

4 Time Stepping

4.1 Forward Euler

4.1.1 Error Analysis

Consider the initial value problem:

$$u'(t) = f(u,t), \quad u(0) = u_0, \quad t \in [0, \infty)$$

We can approximate $u(t)$ numerically up to a cutoff time T using Euler's method. This is done by estimating $u(t)$ at evenly-spaced time intervals of k. Let U_n denote the estimate of $u(nk)$. Then $U^0 = u_0$ and

$$U_{n+1} = U_n + kg(U_n, nk)$$

where $g(u,t) = f(u,t) + \delta(u,t)$ and $|\delta| \leq \Delta$. We find the local error by assuming $U_n = u(nk)$:

$$\begin{aligned} u((n+1)k) - U_{n+1} &= u((n+1)k) - u(nk) - ku'(nk) - k\delta(u(nk), nk) \\ &= -\frac{k^2}{2} f''(\xi) - k\delta(u(nk), nk) \end{aligned}$$

We can then bound the local error by:

$$|u((n+1)k) - U_{n+1}| \leq L(k, \Delta) = \frac{1}{2} K_2 k^2 + k\Delta$$

where K_2 is a bound on $|u''(t)|$. As a rough estimate, the global error scales as $k^{-1}L(k,\Delta)$. We shall therefore minimize the following global error estimate for a fixed number of computations:

$$E(k, \Delta) = \frac{1}{2} K_2 k + \Delta$$

Regarding the computational complexity of this method, there are T/k time steps, and each time step requires $O(\Delta^{-1})$ evaluations of $g(u,t)$. The computation time thus scales as

$$\boxed{C \sim k^{-1}\Delta^{-1}}$$

Next we optimize

$$\begin{aligned} E &= \frac{1}{2} K_2 k + C^{-1} k^{-1} \\ \frac{dE}{dk} &= \frac{1}{2} K_2 - C^{-1} k^{-2} = \frac{1}{2} K_2 - k^{-1}\Delta = 0 \end{aligned}$$

We thus obtain the relationship

$$\boxed{\Delta = \frac{1}{2} K_2 k}$$

We also verify the second derivative test:

$$\frac{d^2 E}{dk^2} = 2C^{-1}k^{-3} > 0$$

The global error thus scales as:

$$\boxed{E \sim K_2 k \sim \Delta}$$

In terms of time complexity, we have $C \sim k^{-2} \sim \Delta^{-2}$. That means

$$\boxed{E \sim C^{-1/2}}$$

4.1.2 Stability

To investigate the stability of Forward Euler for a noisy function, we consider the test problem

$$u' = \lambda u \ \therefore \ u(t) = e^{\lambda t}$$

Then

$$U_{n+1} = U_n + k f(U_n, nk) + k\delta(U_n, nk) = \left(1 + k\lambda + \frac{k\delta}{U_n}\right) U_n$$

We attain stability when

$$\left|1 + k\lambda + \frac{k\delta}{U_n}\right| \leq 1$$

By the triangle inequality, this condition is satisfied when

$$\boxed{|1 + k\lambda| + \frac{k\Delta}{|U_n|} \leq 1}$$

In the case of minimal error, we have $\Delta = \frac{1}{2} K_2 k$, so the stability condition becomes

$$|1 + k\lambda| + \frac{K_2 k^2}{2\,|U_n|} \leq 1$$

As k vanishes (for a fixed T and therefore maximal $|U_n|$), the $\frac{K_2 k^2}{2|U_n|}$ term becomes negligible compared to the $k\lambda$ term. So the region of stability in the $z = k\lambda$ plane remains roughly the same in the limit of small k.

4.2 Improved Euler

4.2.1 Error Analysis

The Improved Euler uses the following recursion:

$$U_{n+1} = U_n + \frac{k}{2}\left(g(U_n, nk) + g(U_n + kg(U_n, nk), (n+1)k)\right)$$

Again, the computational complexity scales as

$$\boxed{C \sim k^{-1}\Delta^{-1}}$$

although with thrice as many evaluations of $g(u,t)$ at each time step as the Forward Euler method. Elsewhere, the local error is

$$\begin{aligned}
u((n+1)k) - U_{n+1} &= u((n+1)k) - u(nk) \\
&\quad - \frac{k}{2}\left(f(u(nk),nk) + f(u(nk)+kg(u(nk),nk),(n+1)k)\right) \\
&\quad - \frac{k}{2}\left(\delta(u(nk),nk) + \delta(u(nk)+kg(u(nk),nk),(n+1)k)\right) \\
&= u((n+1)k) - u(nk) \\
&\quad - \frac{k}{2}\left(f(u(nk),nk) + f(u(nk)+kf(u(nk),nk),(n+1)k)\right) \\
&\quad - \frac{k}{2}\left(\delta(u(nk),nk)\left(1+kf_u+O(k^2)\right) + \delta(u(nk)+kg(u(nk),nk),(n+1)k)\right) \\
&= u((n+1)k) - u(nk) \\
&\quad - \frac{k}{2}\left(2f + k(f_u f + f_t) + \frac{k^2}{2}(f_{uu}f^2 + f_{tt} + 2f_{ut}f) + O(k^3)\right) \\
&\quad - \frac{k}{2}\left(\delta(u(nk),nk)\left(1+kf_u+O(k^2)\right) + \delta(u(nk)+kg(u(nk),nk),(n+1)k)\right) \\
&= \frac{1}{6}\ddot{f}k^3 - \frac{1}{4}(f_{uu}f^2 + f_{tt} + 2f_{ut}f)k^3 \\
&\quad - \frac{k}{2}\left(\delta(u(nk),nk)\left(1+kf_u+O(k^2)\right) + \delta(u(nk)+kg(u(nk),nk),(n+1)k)\right)
\end{aligned}$$

Now let B be an upper bound on the second derivatives of f as such:

$$\left|\frac{1}{6}\ddot{f} - \frac{1}{4}(f_{uu}f^2 + f_{tt} + 2f_{ut}f)\right| \leq B$$

Then the local error is bounded by

$$|u((n+1)k) - U_{n+1}| \leq Bk^3 + k\Delta$$

Factoring out k^{-1} gives us an estimate for global error:

$$E(k,\Delta) = Bk^2 + \Delta$$

Differentiating,

$$\begin{aligned}
E &= Bk^2 + C^{-1}k^{-1} \\
\frac{dE}{dk} &= 2Bk - C^{-1}k^{-2} = 0 \\
\frac{d^2E}{dk^2} &= 2B + 2C^{-1}k^{-3} > 0
\end{aligned}$$

The first derivative test yields

$$\boxed{\Delta \sim k^2}$$

This gives an error that scales as

$$\boxed{E \sim k^2 \sim \Delta \sim C^{-2/3}}$$

4.2.2 Stability

Again considering the test problem $u' = \lambda u$, we have

$$\begin{aligned} U_* &= U_n + kg(U_n, nk) = \left(1 + k\lambda + \frac{k\delta(U_n, nk)}{U_n}\right) U_n \\ U_{n+1} &= U_n + \frac{k}{2}\left(g(U_n, nk) + g(U_*, (n+1)k)\right) \\ &= U_n + \frac{k\lambda}{2}\left(2 + k\lambda + \frac{k\delta(U_n, nk)}{U_n}\right) U_n + \frac{k}{2}\left(\delta(U_n, nk) + \delta(U_*, (n+1)k)\right) \end{aligned}$$

So the method is stable when

$$\boxed{\left|1 + k\lambda + \frac{k^2\lambda^2}{2}\right| + \frac{k\Delta}{2\left|U_n\right|}\left(1 + \left|1 + k\lambda\right|\right) \leq 1}$$

If we scale $\Delta \sim k^2$, we again see that this approaches the non-noisy stability condition $\left|1 + k\lambda + \frac{k^2\lambda^2}{2}\right| \leq 1$ when we neglect terms of order k^3 or higher.