Contents

Part I
MATH 572

1 Course Notes

1.1 01/01/16

What is an algorithim? - sequence of steps to accomplish a given task. Numerical alogrithim: differntiating, integration, solving differential equations $f = u^{''}$. Finite difference methods (FDM): They are straight foward to impliment, but they suffer from several drawbacks. This course is mainly about FD methods and the analysis.

1.1.1 Floating Point Numbers

There are a finite amount of numbers

$$x = \pm(0.d_1 d_2 ... d_n)\beta^{\pm e}, \tag{1}$$

where $(0.d_1 d_2 ... d_n)$is the manttisum, β is the base, and e is the exponent. $d_1 \neq 0$ by convention. Example of how bits are given in a number are shown in Table 1

Machine	Sign	Exponential sign	Mantisson	Exponent
32-bit	$\pm$	$\pm$	n=23	m=7
64-bit	$\pm$	$\pm$	n=52	m=10

Table 1: Ploating point numbers for different machines

Example: Consider a computer with $\beta = 2$, $n = 4$, and $m = 3$. What is $x_{max} =$?

$$\begin{aligned} x_{max} &= (0.1111) \cdot 2^3 \\ &= [1 \times 2^{-1} + 1 \times 2^{-2} + 1 \times 2^{-3} + 1 \times 2^{-4}] \cdot 2^3 \\ &= 4 + 2 + 1 + \frac{1}{2} = 7.5, \end{aligned} \tag{2}$$

and $x_{min} =$?

$$\begin{aligned} x_{min} &= (0.1000) \cdot 2^{-3} \\ &= 2^{-4} = \frac{1}{32} = 0.0625. \end{aligned} \tag{3}$$

Shaded area is where we can represent numbers, but not all the numbers in the shaded area can be represented. ***Add in figure to show this*** Roundoff Error:

$$|x - \text{fl}(x)|. \tag{4}$$

This is from loss of signifigant digits, and techniques to overcome, etc...

1.1.2 Finite Difference Approximation:

Given $u(x)$, find $u^{'}(x)$

$$u(x) = sin(x) \rightarrow u^{'}(x) = cos(x). \tag{5}$$

What if u is complicated or what if $u(x)$ is not given analytically? ***insert picutres***

$$D_{+}u(x) = \frac{u(x+h) - u(x)}{h} \tag{6}$$

for some small parameter. Similarly we can define

$$D_{-}u(x) = \frac{u(x) - u(x-h)}{h}. \tag{7}$$

Both $D_{+}u$ and $D_{-}u$ are first order accurate approximations to $u^{'}(x)$, that is

$$\lim_{h\to 0} |D_{+}u(x) - u^{'}(x)| = \mathcal{O}(h), \tag{8}$$

if h goes down by $\frac{1}{2}$ then error goes down by $\frac{1}{2}$ as well. Define

$$D_0 u = \frac{D_{+}u + D_{-}u}{2} = \frac{u(x+h) - u(x-h)}{2h}. \tag{9}$$

$$\lim_{h\to 0} |D_0 u(x) - u^{'}(x)| = \mathcal{O}(h^2), \tag{10}$$

where the error reduction in this case is by a factor of h^2.

1.1.3 Truncation Errors:

Take a Taylor series expansion of $u(x+h)$

$$u(x+h) = u(x) + hu^{'}(x) + \frac{h^2}{2!}u^{''}(x) + ... \tag{11}$$

and of $u(x-h)$

$$u(x-h) = u(x) - hu^{'}(x) + \frac{h^2}{2!}u^{''}(x) + ... \tag{12}$$

From Eqn. 11 we get:

$$D_{+}u(x) = \frac{u(x+h) - u(x)}{h} = u^{'}(x) + \frac{h^2}{2!}u^{''}(x) + ... \tag{13}$$

$$u^{'}(x) = D_{+}u(x) - \frac{h^2}{2!}u^{''}(x) + ... \tag{14}$$

$$u^{'}(x) = D_{+}u(x) + \mathcal{O}(h) \tag{15}$$

and from Eqn. 12 we get:

$$D_{-}u(x) = \frac{u(x) - u(x-h)}{h} = u^{'}(x) - \frac{h^2}{2!}u^{''}(x) + ..., \tag{16}$$

therfore

$$u^{'}(x) = D_{-}u(x) + \mathcal{O}(h). \tag{17}$$

Then we have

$$D_0 u(x) = \frac{u(x+h) - u(x-h)}{2h} = u^{'}(x) + 2\cdot\frac{h^3}{3!\cdot 2h}u^{'''}(x) + ... = u^{'}(x) + \frac{h^2}{3!}u^{'''}(x) + ..., \tag{18}$$

therfore we have

$$u^{'}(x) = D_0 u(x) + \mathcal{O}(h^2), \tag{19}$$

which is second order accurate. This is also known as a center difference scheme. Deriving finite difference formulas.

Example: Given $u(x)$, $u(x-h)$, and $u(x+h)$, let

$$D_2u(x) = au(x) + bu(x-h) + cu(x+h), \tag{20}$$

find a, b, c that gives best possible approximations to $u^{'}(x)$. Subsititute the Taylor series expanision for $u(x-h)$, $u(x-2h)$ about the point x :

$$D_2u(x) = (a+b+c)\,u(x) - (b+2c)\,hu^{'}(x) + \frac{1}{2}\,(b+4c)\,h^2u^{''}(x) - \frac{1}{6}\,(b+8c)\,h^3u^{'''}(x) + ... \tag{21}$$

Then we enforce that

$$\begin{cases} a+b+c & = 0 \\ -\,(b+2c)\,h & = 1 \\ \frac{1}{2}\,(b+4c)\,h^2 & = 0 \end{cases}, \tag{22}$$

then solve for the coefficients to get

$$\begin{cases} a & = \frac{3}{2}h \\ b & = -\frac{2}{h} \\ b & = \frac{1}{2}h \end{cases}. \tag{23}$$

We cannot enforce anything else becauase we only have three unkowns, therefore

$$D_2u(x) = \frac{1}{2h}\left[3u(x) - 4u(x-h) + u(x-2h)\right]. \tag{24}$$

Order of accuracy is ?? Leading order term

$$= -\frac{1}{6}\,(b+8c)\,h^3u^{'''}(x) = -\frac{1}{6}\left(-\frac{2}{h} + 8\cdot\frac{1}{2h}\right)h^3u^{'''}(x) = \frac{1}{3}h^2u^{'''}(x), \tag{25}$$

therefore

$$u^{'}(x) = D_2u(x) + \mathcal{O}(h^2). \tag{26}$$

Function evaluations are always expensive. Use first order method with not the most accurate data set. Need to way both accuracy and stability of algorithim.

1.2 01/12/16

1.2.1 Method of Undetermined coefficients

- Suppose $u(x_1)$, $u(x_2)$, $u(x_3)$ are given
- Find an interpolating polynomial $p(x)$
- Compute $p^{'}(x) \approx u^{'}(x)$

Second order derivative $u^{''}(x)$

$$D^2u = \begin{cases} D_-\left(D_+u(x)\right) \\ D_+\left(D_-u(x)\right) \\ \hat{D}_0\left(\hat{D}_0u(x)\right) \end{cases} \tag{27}$$

is $\mathcal{O}(h^2)$formulas give the same F.D. forumulas, central difference approximation.

$$\begin{aligned}
D_-\left(D_+u(x)\right) &= \frac{D_+u(x)-D_+u(x-h)}{h}\\
&= \frac{1}{h}\left[\frac{u(x+h)-u(x)}{h}-\frac{u(x)-u(x-h)}{h}\right]\\
D^2u(x) &= \frac{1}{h^2}\left[u(x+h)-2u(x)+u(x-h)\right].
\end{aligned} \tag{28}$$

Note that

$$\hat{D}_0u(x)=\frac{u(x+\frac{h}{2})-u(x-\frac{h}{2})}{h}. \tag{29}$$

Using Taylor series we can derive that

$$D^2u(x)=u^{''}(x)+\frac{1}{12}h^2u^{''}(x)+\mathcal{O}(h^4). \tag{30}$$

Similarly we can apply other combinations (D_+D_+, D_-D_-)to get other formulas for second derivatives, But order of accuracy will be different, which can be derived again using Taylor series. Now we find an interpolating polynomial $p(x)$. Compute $p^{''}(x)\approx u^{''}(x)$. Using polynomials is not good if given in uniform points. Finding the polynomial can be done in Newton Form, Larange Form, or any other forms. All will give the same results for a given $\{x_i\}_{i=1}$ (set of data points).

1.2.2 Higher Derivatives

Reduce to lower order derivatives e.g. $u^{'''}(x)\approx D_-\left(D^2u(x)\right)$. Then find a interpolating polynomial $p(x)$, and compute $p^{(k)}(x)\approx u^{(k)}(x)$. The Method of undetermined coefficeints, given u at $\{x_1,x_2,...,x_n\}$ compute $u^{(k)}(x)$. We require that $n>k$, but we asusme that $n>k+1$. Let

$$c_1u(x_1)+c_2u(x_2)+...+c_nu(x_n)=u^{(k)}(x)+\mathcal{O}(h^p), \tag{31}$$

and Taylor series will give

$$u(x_i)=u(x)+(x_i-x)u^{'}(x)+\frac{(x_i-x)^2}{2}u^{''}(x)+...+\frac{1}{k!}(x_i-x)^ku^{(k)}(x)+..., \tag{32}$$

where x_i is very very close to x. Subsitiuting in the above expression and equating all the coefficients, except the one corresponising to $u^{(k)}$, to zero we get:

$$\frac{1}{(i-1)!}\sum_{j=1}^{n}(x_j-x)^n=\begin{cases}1 & \text{,if } i-1=k\\ 0 & \text{,otherwise}\end{cases}. \tag{33}$$

Corresponding to $i=1,...,n$ we get n equations or the unknowns $\{c_1,c_2,...,c_n\}$:

$$\begin{bmatrix} \\ \\ \\ \\ \\ \end{bmatrix}\begin{bmatrix}c_1\\c_2\\ \vdots\\ \vdots\\ c_n\end{bmatrix}=\begin{bmatrix}0\\ \vdots\\ 1\\ \vdots\\ 0\end{bmatrix}, \tag{34}$$

where the empty matrix is a Vandermode matirx, which is ill condition matrix, which is bad for large n, and the 1 value is obtained for position $i=k+1$.

1.2.3 Solving Boundary Value Problems (B.V.P.'s)

Starting with

$$u^{''}(x) = f(x);\ u(0) = \alpha :\ u(1) = \beta. \tag{35}$$

We first discreteize the domain,

$$x_j = jh,\ \text{for } j = 0, 1, ..., m+1, \tag{36}$$

then write the difference equations and let

$$u_j = u(x_j) = u(jh), \tag{37}$$

given u_0, u_m, f, compute $\{u_1, u_2, ..., u_m\}$. Since the PDE is valid at all points in the domain, each interior node will give one equation. Then we get m equations and unknowns that can be solved for. Consider x_j, conver the differential equation into a difference equation using F.D. approximation.

$$u^{''} = f\Big|_{x=x_j} \rightarrow \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} = f_j, \tag{38}$$

which is valid for all $j = 1, 2, ..., m$. Consider $j = 1$ the D.E. is

$$f_1 = \frac{u_2 - 2u_1 + u_0}{h^2},\ u_0 = \alpha \tag{39}$$

then we get

$$\frac{u_2 - 2u_2}{h^2} = f_1 - \frac{\alpha}{h^2}, \tag{40}$$

and similarly

$$\frac{-2u_m + u_{m+1}}{h^2} = f_m - \frac{\beta}{h^2}. \tag{41}$$

Convert these D.E.'s into a matrix equation

$$\frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_m \end{bmatrix} = \begin{bmatrix} f_1 - \frac{\alpha}{h^2} \\ f_2 \\ \vdots \\ \vdots \\ f_m - \frac{\beta}{h^2} \end{bmatrix}, \tag{42}$$

which is in the form of $AU = F$, where A is a tridiagonal matrix, and this is formed with Dirichlet Boundary conditions. We need to look at

- local truncation error
- Global truncation error $|u(x) - U(x)|$, where $u(x)$ is the exact solution and $U(x)$ is the computed solution.
- Stability
- Consistancy
- Convergence.

1.3 01/14/16

1.3.1 Continuation from 01/12/16

Neumann's B.C.'s are

$$u''(x) = f(x);\ u'(0) = \alpha;\ u'(1) = \beta. \tag{43}$$

Then discretize the domain

$$0,\ h,\ 2h,\ (m+1)h \tag{44}$$

with the Difference equations: at $x_j = jh$

$$\frac{1}{h^2}\left[U_{j+1} - 2U_j + U_{j-1}\right] = f_j \tag{45}$$

and at $x_0 = 0$

$$u'(0) = \alpha \tag{46}$$

Use a first order Finite Difference approximation on u'

$$\frac{u_1 - u_0}{h} = \alpha \tag{47}$$

or use a second order approximation for u' (or apply polynomial approximation, or method of undertemined coeffecients on u_0, u_1, u_2)

Similarly at x_{m+1}

$$\frac{u_{m+1} - u_m}{h} = \beta \tag{48}$$

or apply the second order approx. The matrix equation is

$$\frac{1}{h^2}\begin{bmatrix} -h & h & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & -2 & 1 & & & & \vdots \\ 0 & 1 & -2 & 1 & & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & 1 & -2 & 1 \\ 0 & \cdots & \cdots & \cdots & 0 & -h & h \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ \vdots \\ \vdots \\ u_m \\ u_{m+1} \end{bmatrix} = \begin{bmatrix} \alpha \\ f_1 \\ \vdots \\ \vdots \\ \vdots \\ f_m \\ \beta \end{bmatrix} \tag{49}$$

$$AU = f. \tag{50}$$

A matrix is not invertable in this form (it had a null space), therfore this is a problem.

1.3.2 Local Truncation Error (L.T.E)

Loosely speaking, error due to truncating Talyor series, $u" = f$, with τ being the notatoin for the L.T.E. In vetor form

$$\tau = A\hat{U} - f \tag{51}$$

at x_j

$$\tau = \frac{1}{h^2}\left[u(x_{j-1}) - 2u(x_j) + u(x_{j+1})\right] - f(x_j) \tag{52}$$

$$\tau = \left[u"(x_j) + \frac{1}{12} h^2 u''''(x_j + \mathcal{O}\left(h^4\right) \right] - f(x_j). \tag{53}$$

By expanding $u(x_{j-1})$ and $u(x_{j+1})$ via Taylor series about x_j therefore

$$\tau_j = \frac{1}{12} h^2 u''''(x_j) + \mathcal{O}(h^4) \implies \tau_j = \mathcal{O}(h^4). \tag{54}$$

1.3.3 Global Error

The global error is defined by

$$E = U - \hat{U}, \tag{55}$$

where E is the global error, U is the numerical approximate solution and $\hat{U}$ is the exact solution

$$\hat{U} = \begin{bmatrix} u(x_1) \\ u(x_2) \\ \vdots \\ u(x_m) \end{bmatrix}. \tag{56}$$

Recall from before that $\tau = A\hat{U} - f$

Question: If we know τ exactly, can we obtain E?

$$AE = AU - A\hat{U}$$

$$AE = f - A\hat{U}$$

$$AE = -\tau, \tag{57}$$

which can be used for multigrid and deferred correction methods. If A is invertible then we can find E. Deferred correction methods estimate τ to find the error, then use the found error to imporve the solution.

$$AE = -\tau$$

can be integrated as

$$u" = f, \tag{58}$$

with $u(0) = \alpha$ and $u(1) = \beta$. Then we have

$$e" = -\tau, \tag{59}$$

such that $e(0) = e(1) = 0$. For this Dirichlet Problem

$$\tau_j = \frac{1}{12} h^2 u''''(x_j) + \mathcal{O}(h^4) \tag{60}$$

$$\implies \tau_j = \frac{1}{12} h^2 f"(x_j) + \mathcal{O}(h^4). \tag{61}$$

Therefore we know approximatley what τ_j is.

1.3.4 Deferred Correction Method:

1. Solve $AU = f \to \mathcal{O}(h^2)$ scheme
2. Solve $AE = \frac{1}{12}h^2 f"$
3. Set $U \to U + E$

with $\to A$ on the $\mathcal{O}(h^2)$ scheme. The price paid is solving $AE = (\,)$, can we avoid this? For this example, yes! Add 1) and 2) to get:

$$A(U+E) = f + \frac{1}{12}h^2 f", \tag{62}$$

but in general this can not be avoided.

1.3.5 Stablilty:

$$A^h E^h = -\tau^h \tag{63}$$

and we want $E^h \to 0$ as $h \to 0$.

Definition: we say that our F.D. method is stable if $(A^h)^{-1}$ exists for all h sufficiantly small ($h < h_0$) and if there exists a constant c such that

$$||(A^h)^{-1}|| \leq c \ \ \forall\, h < h_0 \tag{64}$$

which is defined for by any norm type.

1.3.6 Consistancy:

Conistancy is for error truncation. Our F.D. method is consistnet with the differential equation and boundary conditions if $||\tau^h|| \to 0$ as $h \to 0$. Typically

$$||\tau^h|| \sim \mathcal{O}(h^p) \tag{65}$$

where p is the power. As long as truncation error is something like this then consitancy of our method is met.

1.3.7 Convergence:

Convergnce is important in regards to global error. Our F.D. method is convergent if $||E^h|| \to 0$ as $h \to 0$. The Fundamental theorem of Finite Difference Method is

$$\text{Consitancy} + \text{Stability} = \text{Convergence}. \tag{66}$$

If we have stability and consitany, then our method will have convergence. Proof:

$$A^h E^h = -\tau^h \tag{67}$$

$$E^h = -(A^h)^{-1}\tau^h, \tag{68}$$

since $(A^h)^{-1}$exists

$$||E^h|| = ||(A^h)^{-1}\tau^h|| \tag{69}$$

$$||E^h|| \leq ||(A^h)^{-1}|| \cdot ||\tau^h|| \tag{70}$$

and from the stability condition in Eqn. 64 we get

$$||E^h|| \leq c \cdot ||\tau^h|| \tag{71}$$

therefore

$$||E^h|| \to 0 \text{ as } h \to 0 \tag{72}$$

because $||\tau^h|| \to 0$ as $h \to 0$ due to the consitancy condition. More importantly,

$$\mathcal{O}(h^p) \text{ L.T.E. } + \text{Stability} \implies \mathcal{O}(h^p) \text{ for global error.}$$

1.4 01/19/16

1.4.1 Continuatoin from 01/14/2016

$$\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 2 \end{bmatrix} \text{ is a symmetric and negative definite matrix.}$$

1.4.2 More General P.D.E.'s

Starting with

$$f(x) = (k(x)u'(x))'; \; u(0) = \alpha; \; u(1) = \beta \tag{73}$$

Fromt this we get that

$$f = ku'' + k'u' \tag{74}$$

which is similar to our previous strategy and at x_i

$$u''(x_i) = \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} \tag{75}$$

$$u'(x_i) = \frac{u_{i+1} - u_{i-1}}{2h} \tag{76}$$

At whih $x_1$we get the following difference equation, and we imply k is a given quantity, therefore

$$f_i = k_i \left(\frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} \right) + k_i^{'} \left(\frac{u_{i+1} + u_{i-1}}{2h} \right), \tag{77}$$

where $k_i = k(x_i)$, and $f_i = f(x_i)$. From this we can set up the matrix equation, $AU = F$, where

$$A = \frac{1}{h^2} \begin{bmatrix} -2k_1 & k_1 + h\frac{k_1^{'}}{2} & & & \\ k_2 - h\frac{k_2^{'}}{2} & -2k_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & -2k_n \end{bmatrix}, \tag{78}$$

which is not a symmetric matrix. If we consider halfway points inbetween $i-1, i,$ and $i+1$we can have the following

$$f=(ku^{'})^{'}, \tag{79}$$

where

$$k_{i+1/2}u^{'}(x_{i+1/2})=k_{i+1/2}\left(\frac{u_{i+1}-u_{1}}{h}\right), \tag{80}$$

and

$$k_{i-1/2}u^{'}(x_{i-1/2})=k_{i-1/2}\left(\frac{u_{i}-u_{i-1}}{h}\right). \tag{81}$$

Now we can apply the difference scheme at $x_i$to get

$$f(x_i)=\frac{k_{i+1/2}u^{'}(x_{+1/2})-k_{i-1/2}u^{'}(x_{i-1/2})}{h}, \tag{82}$$

then we can get

$$f_i=\frac{1}{h^2}\left[k_{i+1/2}\left(u_{i+1}-u_i\right)-k_{i-1/2}\left(u_i-u_{i+1}\right)\right], \tag{83}$$

$$f_i=\frac{1}{h^2}\left[k_{i+1/2}u_{i+1}-\left(k_{i+1/2}+k_{i-1/2}\right)u_i+k_{i-1/2}u_{i-1}\right]. \tag{84}$$

This then gives us the following A matrix

$$A=\frac{1}{h^2}\begin{bmatrix} -\left(k_{1+1/2}+k_{1-1/2}\right) & k_{1+1/2} & & & \\ k_{2-1/2} & -\left(k_{2+1/2}+k_{2-1/2}\right) & k_{2+1/2} & & \\ & k_{3-1/2} & \ddots & \ddots & \\ & & \ddots & \ddots & k_{n-1+1/2} \\ & & & k_{n-1/2} & -\left[k_{n+1/2}+k_{n-1/2}\right] \end{bmatrix}, \tag{85}$$

which is a symmetric and negative definite matrix, all eigen values are negative.

1.4.3 More General Boundary Value Problems

Similarly F.D.M. can be applied to more general boundray value problems (B.V.P.'s), such as:

$$f(x)=a(x)u^{"}(x)+b(x)u^{'}(x)+c(x)u(x). \tag{86}$$

Higher order method

$$f=u^{"};\ u(0)=\alpha:\ u(1)=\beta. \tag{87}$$

Simply apply as higher order approximation to all the derivatives inovolved. Here,$u^{"}(x)$ is a 4^{th}order approximation

$$\frac{1}{12h^2}\left[-u_{1-2}+16u_{i-1}-30u_i+16u_{i+1}-u_{i+2}\right] \tag{88}$$

1.4.4 Extrapolation Method:

We have two grids, one course grid and one fine grid, where $u_j$are points on the course grid and $v_j$are points on the fine grid. Starting from $f = u"$; $u(0) = \alpha$; $u(1) = \beta$, we know that $u_j$solved via central difference shcemes satisfies the estimate:

$$\text{for } j = 1, 2, ..., m \tag{89}$$

$$u_j - u(jh) = c_2h^2 + c_4h^4 + c_6h^6 + ... = \text{Error Equation}, \tag{90}$$

and

$$v_{2j} - u(jh) = c_2\left(\frac{h}{2}\right)^2 + c_4\left(\frac{h}{2}\right)^4 + c_6\left(\frac{h}{2}\right)^6 + ..., \tag{91}$$

which the error is reduced be a factor of $\frac{1}{4}$ for the fine gird. Multiply Eqn. 91 by 4 and we get

$$4v_{2j} - 4u(jh) = c_2h^2 + 4c_4\left(\frac{h}{2}\right)^4 + 4c_6\left(\frac{h}{2}\right)^6 + ... \tag{92}$$

Now subtract Eqn. 92 from Eqn. 90 and we get

$$u_j - 4v_{2j} + 3u(jh) = c_4\left(1 - \frac{1}{4}\right)h^4 + \mathcal{O}(h^6), \tag{93}$$

then divide by -3

$$\frac{4v_{2j} - u_j}{3} - u(jh) = -\frac{1}{3}c_4\frac{3}{4}h^4 + \mathcal{O}(h^6), \tag{94}$$

where $\bar{u}_j = \frac{4v_{2j}-u_j}{3}$,therefore $\bar{u}_j$is a $\mathcal{O}(h^4)$ accurate solution, so for the Extrapolation algorithim

- solve for u_j on the course grid using central difference scheme
- sovle for $v_j$on the fine grid using central difference scheme
- set $\bar{u}_j = \frac{4v_{2j}-u_j}{3}$

We can also use nonuniform course and fine grids. What happens if all the date points are used for each difference equation? Use the spectral method. Higher the order, steeper the slope.

$$f(x) = \sum_{j=0}^{n} c_j x^i \tag{95}$$

is an unstable approximatoin. In general, approximately data given on a regular grid with monic polynomial represented leads to inaccurate approximations $\rightarrow$Rungle phenomenon??

1.5 01/26/15

1.5.1 Continuation

Starting from u_{xx} in which is $\triangle u$ in 1D

$$-\triangle u = f(x), \tag{96}$$

and u and f are periodic on $[0,1]$. This means $u(0)=u(1)$ and $f(0)=f(1)$. The FD

$$f_i = -\left(\frac{u_{i-1}-2u_i+u_{i+1}}{h^2}\right), \tag{97}$$

and the unknowns are $\{u_0, u_1, ..., u_m\}$. Since $u_{m+1}=u_m$ due to the periodic nature, we have at $i=0$ *** insert picute***

$$f_0 = -\left(\frac{u_m-2u_0+u_1}{h^2}\right), \tag{98}$$

and this i s $\mathcal{O}(h^2)$ algorithm.

1.5.2 Spectral Method

Assume $u(x)$ and $f(x)$ are smooth and periodic on $[0,2\pi]$, so we get $\{..., e^{-2ix}, e^{-ix}, 1, e^{ix}, e^{2ix}, ...\}$, which is a basis for all smooth, periodic functions on $[0,2\pi]$,then

$$u(x) = \sum_{n=-\infty}^{\infty} \hat{u_n} e^{-nx}, \tag{99}$$

which is the Fourier series representaion of a function, and $\hat{u_n}$is the n^{th}Fourier coefficeint of $u(x)$. This can be approximated by

$$u(x) \approx \sum_{n=-N}^{N} u_n \hat{e^{-inx}}, \tag{100}$$

which is the truncated Fourier series expansion. The accuracy of this approximation is super-algebraic as long as u is smooth and periodic. **This is better than any polynomial order** How to compute $\hat{u}$?

$$\hat{u}_n =< u, e^{inx} >= \int_0^{2\pi} u(x)e^{-inx}dx, \tag{101}$$

and from this we can compute this in a summation form of

$$= \sum_{k=1}^{N} u_k e^{-ink2\pi/2N} \cdot \frac{2\pi}{2N}, \tag{102}$$

therefore

$$\hat{u}_n = \frac{\pi}{N} \sum_{k=1}^{2N} u_k e^{-\pi ink/N}, \tag{103}$$

for $u=-N,-N+1,...,N-1$ and $u_k :$ for $k=1,2,...,2N$ and $\hat{u}_n : n=-N,...N-1$.This is$\mathcal{O}(N^2)$ opperations, which is neccesary to compute \ensuremath$\hat{u}_n$ to and $\mathcal{O}(N^2)$ to evaluate $u(x)$ at a single point. This reduces to $\mathcal{O}(Nlog(N))$ when using FFT for the $\hat{u}_n$ calculations and $\mathcal{O}(N\log(N)$ using IFFT for computing a point at $u(x)$, where IFFT is Inverse ...???... Tranfer. How to solve the PDE

$$-u_{xx} = f(x). \tag{104}$$

Now subsitute the Fourier representation of u into this equation

$$
\begin{aligned}
-\left(\sum_{n=-N}^{N-1} \hat{u}_n e^{inx}\right)_{xx} &= f(x) \\
-\sum_{n=-N}^{N-1} \left(\hat{u}_n e^{-inx}\right)_{xx} &= f(x) \\
-\sum_{n=-N}^{N-1} \hat{u}_n \left(e^{inx}\right)_{xx} &= f(x) \\
\sum_{n=-N}^{N-1} \hat{u}_n \cdot n^2 e^{inx} &= f(x), \qquad (105)
\end{aligned}
$$

now taking the inner product of both sides with e^{-imx} we get

$$\sum_{n=-N}^{N-1} n^2 \hat{u}_n < e^{inx}, e^{-imx} >=< f(x), e^{-imx} >, \qquad (106)$$

where

$$< e^{inx}, e^{-inx} >= \begin{cases} 1 & , \text{ if } n = m \\ 0 & , \text{ otherwise} \end{cases}, \qquad (107)$$

therefore

$$n^2 \hat{u}_n =< f, e^{-inx} >= \hat{f}_n, \qquad (108)$$

where $\hat{f}_n$ is the Fourier transform of f. From this we have

$$\hat{u}_n = \frac{1}{n^2} \hat{f}_n, \;\; n \neq 0. \qquad (109)$$

The order of opperations for this spectral method is

$$\boxed{f_k} \xrightarrow[\mathcal{O}(N\log(N))]{\text{FFT}} \boxed{\hat{f}_n} \xrightarrow[1/n^2]{\text{multiply by}} \boxed{\hat{u}_n} \xrightarrow[\mathcal{O}(N\log(N))]{\text{IFFT}} \boxed{u_k}$$

Note: you can set $\hat{u}_0$to some arbitrary constant, (say $= 0$).

- Computational complexity $= \mathcal{O}(N\log(N))$
- Order of accuracy is <u>spectral</u>

Using all the data points you may get spectral.

1.5.3 Non-periodic Functions

Startign from

$$-u_{xx} = f(x); \;\; u(0) = \alpha, \;\; u(1) = \beta, \tag{110}$$

Let

$$u(x) = \sum_{k=0}^{N} c_k \phi_k(x), \tag{111}$$

where $\{\phi(x)\}_0^{N-1}$ are the basis functions that span all smooth functions defined on $[0, 1]$.

e.g.: $\{\phi_k(x)\} = \{T_k(x)\}$, where T_k are chebyshev polynomials.

Where should $u(x)$ be specified? At the roots of the chebyshev polynomial of highest degree. ***insert figure*** Discretizes uniformly. At endpoints, densely spaced and at midpoints sparsely spaced. $x_i's$ are roots of the highest degree chebyshev polynomial.

$$u(x) = \sum_{k=0}^{N-1} c_k T_k(x), \tag{112}$$

and then substitute in the PDE

$$\sum_{k=0}^{N-1} c_k \left(T_k(x)\right)_{xx} = f_{xx}, \tag{113}$$

where the pseudo-spectral method(collocation) or galerkin method can be used to solve this. By taking the inner product with respect to T_k's we get a set of equations to solve for c_k's. In the Fourier: Both of these are the same(collocation and galerkin).

- If you can always go with galerkin.
- In the end both will give spectral method.

Get notes that were missed and insert figs***

1.6 01/28/16

1.6.1 Boundary Layers

Consider:

$$\epsilon u^{''} - u^{'} = f; \;\; u(0) = \alpha, \;\; u(1) = \beta, \tag{114}$$

which is the steady state advection-diffusion equation. $u^{'}$ is the advection term, and $u^{''}$ is the diffusion term. If we only have

$$-u^{'} = f; \;\; u(0) = \alpha, \;\; u(1) = \beta, \tag{115}$$

this equation is over specified. This same issue happens for Eqn. 114, when $\epsilon \to 0$.

i) Singularly perturbed Equatoin

$$\epsilon u^{''} - u^{'} = f; \; u(0) = \alpha, \;\; u(1) = \beta, \tag{116}$$

and ϵ is small. ϵ multiplies the term with the highest order derivative. The soltion u in this case will have boundary-layers. *If we have

$$u^{''} - \epsilon u^{'} = f, \tag{117}$$

then the problem doesn't have issues as $\epsilon \to 0$. Other examples:

- Navier-Stokes (high Re)
- Reaction-Diffusion (reaction dominates region)

ii) Regularly - Perturbed Equations

$$u^{''} - au^{'} = f; \;\; u(0) = \alpha, \;\; u(1) = \beta, \tag{118}$$

where a̲ is a small parameter. As $a \to 0$ our solution equation is diffusion dominated. Interior Layers

$$\epsilon u^{''} - u(u^{'} - 1) = 0; \;\; u(0) = \alpha, \;\; u(1) = \beta, \tag{119}$$

with $0 < \epsilon < 1$. Let $\epsilon = 0 \implies u(u' - 1) = 0$ which gives us

$$u(x) = \begin{cases} x + \alpha & \text{if left B.C. is enforced} \\ x + \beta - 1 & \text{if right B.C. is enforced} \end{cases}. \tag{120}$$

insert figure Perturbation theory will tell us exactly where the switch happens and the width of the layers. What happens if we apply FDM with a regular grid? ***insert figures***

L.T.E (local truncation error)

$$\tau \propto h^2 u^{'''}(x) + \mathcal{O}(h^3), \tag{121}$$

Near the boundary layer, $u^{'''}(x)$ is very large therefore we expect τ to be large. What we need is an estimate on the global error E.

$$AE = -\tau \implies E = -A^{-1}\tau, \tag{122}$$

where A is a dense matrix. The matrix system $-A^{-1}\tau = E$:

$$\begin{bmatrix} \# & \cdots & \cdots & \cdots & \# \\ \vdots & & & & \vdots \\ \vdots & & \text{dense} & & \vdots \\ \vdots & & & & \vdots \\ \# & \cdots & \cdots & \cdots & \# \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ \text{non-} \\ \text{zeros} \end{bmatrix} = \begin{bmatrix} \# \\ \# \\ \# \\ \# \\ \# \end{bmatrix}, \tag{123}$$

From this we get a value of error in every row of the E (global error) matrix. Even though L.T.E. error is small in some regions, because A matrix is dense, so multipling $A^{-1}$by some L.T.E. error, will give global error everywhere.

We could make a non-uniform grid, where it is more course in smooth areas, and a fine grid in the boundary layer. ***Insert figure***

$X(z)$ is a smooth function that maps a regular grid in z to a non-uniform gird in x. This tells us to set up a gird like this for FDM on the x axis. *** insert fig***

$$u^{''}(x_i) \backsimeq c_1 u(x_{i-1}) + c_2 u(x_i) + c_3 u(x_{i+1}), \tag{124}$$

where the grid is not unifrom.

$$c_1 u(x_{i-1}) + c_2 u(x_i) + c_3 u(x_{i+1}) - u^{''}(x_i) = \frac{1}{3}(h_2 - h_1) u^{'''}(x_i) + () u^{''''}(x_i) + ..., \tag{125}$$

where

$$\begin{aligned} h_2 - h_1 &= (x_{i+1} - x_i) - (x_i - x_{i-1}) \\ &= X(z_{i+1}) - 2X(z_i) + X(z_{i-1}) \\ &= \mathcal{O}(h^2) X^{''}(z_i), \end{aligned} \tag{126}$$

therefore we get

$$c_1 u(x_{i-1}) + c_2 u(x_i) + c_3 u(x_{i+1}) - u^{''}(x_i) = \mathcal{O}\left(h^2\right)[\quad] + ... \tag{127}$$

From previous class ***inserft fig***

- Break domain into non-uniform intervals
- use a fixed-degree ,say p, polynomial to representent functions in each interval
- Pseudo-spectral method.

Adaptive Mesh Refinement (AMR): Even before solving the PDE, can we predict where the solution is changing rapidly?

1.6.2 Continuation Method

Starting from the following equation:

$$\epsilon u^{''} - u^{'} = f; \;\; u(0) = \alpha, \;\; u(1) = \beta, \tag{128}$$

and we start with a large ϵ **insert fig*** Therefore the final solution is okay on a regular gird. Then we make the grid slightly smaller *** insert fg*** We need to refine a portion of the gird. ****Insert fig*** as ϵ goes down we get a more curvy plot.

From pseudo spectral method last class

$$u(x) = \sum_{j=0}^{\phi} c_j \phi_j(x) = c_0 + c_1 x + c_2 x^2, \tag{129}$$

which is a second degree monomial, and we combine this with spectral coefficients. This doesn't combine with FDM.

1.7 02/02/16

1.7.1 B.V.P.'s

Consider Elliptic Equations:

2D

$$(k u_x)_x + (k u_y)_y = f, \tag{130}$$

whichis the steady heat/diffusion equation. If k is constant we get

$$u_{xx} + u_{yy} = f; \;\; \text{assume } k = 1, \tag{131}$$

and this is the Poisson Equation.

$$u_{xx} + u_{yy} = 0, \tag{132}$$

which is the Laplace Equation, or another notation is

$$\Delta u = 0, \tag{133}$$

where $\triangle$ is the Laplacian opprerator

$$\Delta = \nabla \cdot (\nabla u), \tag{134}$$

where $\nabla \cdot (\;)$ is the divergence and $(\nabla u)$is the gradient.

$$\nabla \vec{u} = \begin{bmatrix} u_x \\ u_y \end{bmatrix}, \;\; \nabla \cdot \vec{u} = u_{1x} + u_{2y}. \tag{135}$$

In complex analysis:

$$f(z) = u(z) + iv(z) = u(x,y) + iv(x,y), \tag{136}$$

from which we get the Cauchy-Riemman Equations:

$$\begin{cases} u_x & = v_y \\ u_y & = v_x \end{cases} \rightarrow \begin{cases} u_{xx} + u_{yy} & = 0 \\ v_{xx} + u_{yy} & = 0 \end{cases}, \tag{137}$$

If this is true, then we say that $f(z)$ is analytic u, v are harmonic functions.

1.7.2 F.D.M. for Poisson Equation in 2D

Starting with the following equations, see diagram for more detail **insert fig**

$$\begin{cases} \Delta u = f & \text{in } \Omega \\ u = \xi & \text{on } \Gamma \end{cases}, \tag{138}$$

1) Discretize the Domain: Let

$$h = \frac{1}{m}, \tag{139}$$

insert fig and we get

$$\begin{cases} x_i = ih, & i = 0, 1, ..., m+1 \\ y_i & j = 0, 1, ..., m+1 \end{cases} \tag{140}$$

2)Convert the Difference Equation: We convert the differnce equation to a difference equation at some arbitrary interior point (x_i, y_i)

$$\Delta u \left(x_i, y_j\right) = u_{xx} + u_{yy}\Big|_{(i,j)}, \tag{141}$$

insert fig

$$\begin{aligned} &= \frac{u_{(i-1,j)} - 2u_{ij} + u_{(i+1,j)}}{h^2} + \frac{u_{(i,j-1)} - 2u_{i,j} + u_{(i,j+1)}}{h^2} \\ &= \frac{1}{h^2}\left[u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}\right], \end{aligned} \tag{142}$$

which we call a 5-point stencil. **insert Figure*** Now apply the B.C.'s at the boundary nodes.

3) Form the Matrix Equation: Let's assume row wise ordering. ***insert fig*** We have the matrix sytem of equations $AU = f$

$$\frac{1}{h^2}\begin{bmatrix} T & I & & & \\ I & T & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & I \\ & & & I & T \end{bmatrix}\begin{bmatrix} u^{(1)} \\ u^{(2)} \\ \vdots \\ \vdots \\ u^{(m)} \end{bmatrix} = \begin{bmatrix} \\ f \\ \\ \end{bmatrix}, \tag{143}$$

where

$$\begin{cases} u^{(1)} & = u_1, u_2, ..., u_m \\ u^{(2)} & = u_{m+1}, u_{m+2}, ..., u_{2m} \\ \vdots & \vdots \\ u^{(j)} & = u_{jm+1}, ..., u_{jm} \end{cases}, \tag{144}$$

and $I_{m\times m}$is an identity matrix and

$$T = \begin{bmatrix} -4 & 1 & & & \\ 1 & -4 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -4 \end{bmatrix}. \tag{145}$$

The order of accuracy:

$$\tau_{i,j} = \frac{1}{12}h^2 \left(u_{xxxx} + u_{yyyy}\right)\Big|_{(i,j)} + \mathcal{O}(h^4), \tag{146}$$

where $\tau_{i,j}$ is the L.T.E, therefore we have second order accuracy, with

$$AE = -\tau, \tag{147}$$

therefore

$$\Delta u = \Delta_5^h + \mathcal{O}(h^2), \tag{148}$$

where Δ_5^h is the 5-point discrete Laplacian. We can also have alternating ordering, see figure for scheme **insert fig** and we get the following matrix system of equations

$$\begin{bmatrix} D & H \\ H^T & D \end{bmatrix}\begin{bmatrix} u^{red} \\ u^{black} \end{bmatrix} = \begin{bmatrix} f^{red} \\ f^{black} \end{bmatrix}, \tag{149}$$

where D is a diagonal matrix and

$$D = -\frac{4}{h^2}I, \tag{150}$$

and H is a sparse matrix. We can also have a 9-point stencil **insert fig**

$$\Delta_9^h u = \frac{1}{6h^2}\left[4u_{i+1,j} + 4u_{i-1,j} + 4u_{i,j-1} + 4u_{i,j+1} + ...\right], \tag{151}$$

and

$$\Delta u = \Delta_9^h u + \frac{1}{12} h^2 \left[u_{xxxx} + 2u_{xxyy} + u_{yyyy} \right] + \mathcal{O}(h^2), \tag{152}$$

therefore we have

$$\Delta u = \Delta_9^h u + \mathcal{O}(h^2), \tag{153}$$

and also note that

$$\Delta \left(\Delta u \right) = \Delta^2 u = u_{xxxx} + 2u_{xxyy} + u_{yyyy}, \tag{154}$$

which is the Biharmonic operator.

Case i) Suppose we are showing Laplace Equation

$$\begin{cases} \Delta u = 0, & \text{in } \Omega \\ u = \xi, & \text{in } \Gamma \end{cases} \rightarrow \Delta^2 u = 0, \tag{155}$$

therefore Δ_9^h is fourth order accurate.

Case ii) We have

$$\begin{cases} \Delta u = f, & \text{in } \Omega \\ u = \xi, & \text{on } \Gamma \end{cases} \rightarrow \Delta^2 u = \Delta f, \tag{156}$$

and solve for

$$\Delta_9^h u = f, \tag{157}$$

where

$$\widetilde{f} = f - \frac{1}{12} h^2 \Delta f, \tag{158}$$

which is a fourth order accuate method and Δf is computed with a 5-point or 9-point stencil, but Δu needs to be computed with a 9-point stencil. **insert fig** For cases like these, were the grid has portions that are defined in Γ, we need to modify our method to use the 5-point stencil. We can use methods such as

- Inverse Boundary Method (I.B.M.)
- Inversed Inteface Method (I.I.M)
- Ghost-Fluid-Method (G.F.M)

2 Homework

2.1 Homework #1