Some Notes on Euler's Method

- We all know that

$$\lim_{n \longrightarrow \infty} \left(1 + \frac{1}{n}\right)^n = e$$

- One might ask, however, *What is the* **rate** at which this expression converges?

- That is, for $n < \infty$, what is $e - \left(1 + \frac{1}{n}\right)^n$?

- Equivalently, what is r in the following expression?

$$e - \left(1 + \frac{1}{n}\right)^n \sim Cn^r$$

Notes on Euler's Method, continued

- Consider $\tilde{y}' = \lambda \tilde{y}$ on the interval $t \in [0, 1]$ with IC $\tilde{y}(0) = 1$.

- The exact solution to this problem is $\tilde{y}(t) = e^{\lambda t}$ and, for $\lambda = 1$, we have $\tilde{y}(1) = e$

- Consider Euler forward applied to $y' = \lambda y$ on the interval $t \in [0, 1]$,

- Starting with $y_0 = 1$, we have

$$y_k \;=\; (1 + h\lambda) y_{k-1} \;=\; (1 + h\lambda)^k y_0 \;=\; (1 + h\lambda)^k$$

- Taking $\lambda = 1$ and $h = 1/n$, we have

$$y_n \;=\; \left(1 + \frac{1}{n}\right)^n \;\approx\; e$$

Notes on Euler's Method, continued

- However, we have a more precise estimate than $y_n \approx e$.

- We know that EF is $O(h)$ accurate, so we expect

$$e - \left(1 + \frac{1}{n}\right)^n = e - y_n = Ch + O(h^2)$$

- That is, the convergence rate $O(h) = O(n^{-1})$

- Moreover, from the Taylor series expansion for y, we have

$$y_{k+1} - y_k = hy' + \frac{h^2}{2} f''(\xi), \quad \xi \in [0, 1]$$

so we expect the constant to be bounded by $e/2$,

$$\left| e - \left(1 + \frac{1}{n}\right)^n \right| \leq \frac{e}{2} h$$

- `est_e.m`

- est_e.m

```
e=exp(1);
for k=1:11; n=2^k;
    h = 1/n;
    yn = (1+h)^n;
    en = abs(e-yn);
    model = h*(e/2);
    disp([k h n e en model])
end;
```

Richardson Extrapolation

- Suppose we have a sequence of $y_n = \left(1 + \frac{1}{n}\right)^n$ values for $n = 2, 4, 8, \ldots$

- We can apply one or two rounds of Richardson extrapolation to get better estimates of e

- Let

$$\begin{aligned} z_n &= 2y_{2n} - y_n \sim 2(e - c_1\frac{h}{2} + O(h^2)) - (e - c_1 h + O(h^2)) \\ &\sim e + c_2 h^2 \end{aligned}$$

- Repeating, with $q_n = (4z_{2n} - z_n)/3$, will eliminate the $O(h^2)$ error, etc.

- `est_rich.m`

- Of course, none of these are as rapidly convergent as the Taylor series for e,

$$e = \sum_{k=0}^{\infty} \frac{1}{k!}$$

- est_rich.m

```
e=exp(1);

for k=1:11; n=2^k;
    h = 1/n;
    yn = (1+h)^n;
    en = abs(e-yn);
    model = h*(e/2);
    disp([k h n e en model])
    ynk(k) = yn;
end;

% Richardson

pause; disp('First Round of Richardson')
n=length(ynk); m=n-1; yr=zeros(m,1);
for k=1:m
    yr(k) = 2*ynk(k+1) - ynk(k);
    er(k) = abs(e-yr(k));
    erk   = er(k)
end;


pause; disp('Second Round of Richardson')
n=length(yr); m=n-1; yr2=zeros(m,1);
for k=1:m
    yr2(k) = (4*yr(k+1) - yr(k))/3;
    er2(k) = abs(e-yr2(k));
    erk    = er2(k)
end;
```

Chapter 10: ODEs–Boundary Value Problems

ODEs: Boundary Value Problems

- For solution of IVPs, we had all "boundary conditions" prescribed at the same initial timepoint, t_0

- For *boundary value problems* (BVPs), we prescribe conditions at more than one point

- For a kth-order ODE, we require a total of k conditions

- For ODE-BVPs, conditions are generally specified at endpoints of interval of interest, $[a, b]$, so we have a *two-point boundary value problem* with boundary conditions (BCs) at a and b

- As this is still an *ordinary differential equation*, as opposed to partial differential equation, there is still only one independent variable, which we will typically denote by x, but occasionally by t.

Examples of Two-Point BVPs

- 1D "Poisson" equation:

$$-\tilde{u}'' \;=\; f(x) \text{ on } \Omega = [0, L], \qquad \tilde{u}(0) = \tilde{u}(L) = 0$$

- 1D *advection-diffusion* equation:

$$-\nu\tilde{u}'' + c\,\tilde{u}' \;=\; f(x) \text{ on } \Omega = [0, L], \qquad \tilde{u}(0) = \tilde{u}(L) = 0$$

- Blasius equation - 3rd-order *nonlinear* BVP on $\Omega = [0, \infty]$,

$$\tilde{u}''' + \frac{1}{2}\tilde{u}(x)\tilde{u}''(x) \;=\; 0, \qquad \tilde{u}(0) = \tilde{u}'(0) = 0, \;\; \tilde{u}'(x) \longrightarrow 1 \;\text{ as } x \longrightarrow \infty$$

Boundary Conditions

- Prescribed boundary values at either a or b are termed *Dirichlet boundary conditions*

- If $\tilde{u}(a) = 0$ it is a *homogeneous* Dirichlet condition, otherwise it is an *inhomogeneous* Dirichlet condition

- If we prescribe the slope $\tilde{u}'(a)$ (or $\tilde{u}'(b)$, as in the Blasius example) the boundary condition is a *homogeneous Neumann condition* if $\tilde{u}'(a) = 0$ and an *inhomogeneous* Neumann condition if $\tilde{u}'(a) \neq 0$

- We can also have *mixed* or *Robin* conditions, such as

$$\alpha\tilde{u}'(L) + \beta\tilde{u}(L) = \gamma$$

Robin conditions are well posed under either of the two conditions

$$\begin{cases} \alpha \neq 0 \quad \text{and} \quad \alpha\beta \geq 0, & \text{(general Robin condition)} \\ \text{or} & \\ \alpha = 0, \quad \beta \neq 0, & \text{(Dirichlet at } x = L\text{)} \end{cases}$$

ODEs: Boundary Value Problems in 1D

Consider linear ODE of the form $L\tilde{u} = f(x)$, with $\tilde{u}(x)$ satisfying given BCs.

Here, we consider three basic approaches to find $u \approx \tilde{u}$.

- **Finite difference methods (FDM):**
  - Essentially, approximate differential equation at multiple points, x_i, $i = 1, \ldots, n$.
  - **Note:** *we will use either n or $n+1$ points according to what makes the most sense in the given context.*

- **Collocation methods:**
  - Use an expansion to represent a **numerical solution**,

$$u(x) := \sum_{j=1}^{n} u_j \phi_j(x).$$

  - Solve for **coefficients** u_j such that the ODE is satisfied at a c
    collocation points, x_i, along with the boundary conditions.
  - That is, the **residual**,

$$r(x) := (L\tilde{u} - Lu),$$

    is forced to be zero at $x = x_i$, $i = 1, \ldots, n$.

- **Weighted residual technique (WRT):**
  - Approximate the solution by an expansion,

$$u(x) \;:=\; \sum_{j=1}^{n} u_j \phi_j(x),$$

    and solve for coefficients u_j such that the ODE is satisfied in some weighted sense.
  - That is, rather than enforcing $r(x) = 0$ at isolated points, we require $r(x)$ to be orthogonal to a set of weight functions, $\psi_i(x)$:

$$\int_a^b \psi_i(x)\, r(x)\, dx \;=\; \int_a^b \psi_i(x)\, \left(L(u) - L(\tilde{u})\right)\, dx \;=\; 0, \quad \text{or}$$

$$\int_a^b \psi_i(x)\, L(u)\, dx \;=\; \int_a^b \psi_i(x)\, L(\tilde{u})\, dx \;=\; \int_a^b \psi_i(x)\, f(x)\, dx$$

    for $i = 1, 2, \ldots$
  - Note that if $\psi_i(x) = \delta(x - x_i)$ (Dirac delta function), we recover collocation.
  - Most often, the *test-space* and *trial space* are the same: $\psi_i := \phi_i$. (Galerkin case.)
  - Finite element, spectral, spectral element methods are examples of WRTs.

  - WRTs have many advantages over collocation in terms of flexibility of basis functions, application of boundary conditions, etc., and are generally preferred over collocation.

- **Weighted residual technique (WRT):**
  - Approximate the solution by an expansion,

$$u(x) \;:=\; \sum_{j=1}^{n} u_j \phi_j(x),$$

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$$\int_a^b \psi_i(x)\, r(x)\, dx \;=\; \int_a^b \psi_i(x)\, \left(L(u) - L(\tilde{u})\right)\, dx \;=\; 0, \quad \text{or}$$

$$\int_a^b \psi_i(x)\, L(u)\, dx \;=\; \int_a^b \psi_i(x)\, L(\tilde{u})\, dx \;=\; \int_a^b \psi_i(x)\, f(x)\, dx$$

    for $i = 1, 2, \ldots$
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  - Most often, the *test-space* and *trial space* are the same: $\psi_i := \phi_i$. (Galerkin case.)
  - Finite element, spectral, spectral element methods are examples of WRTs.

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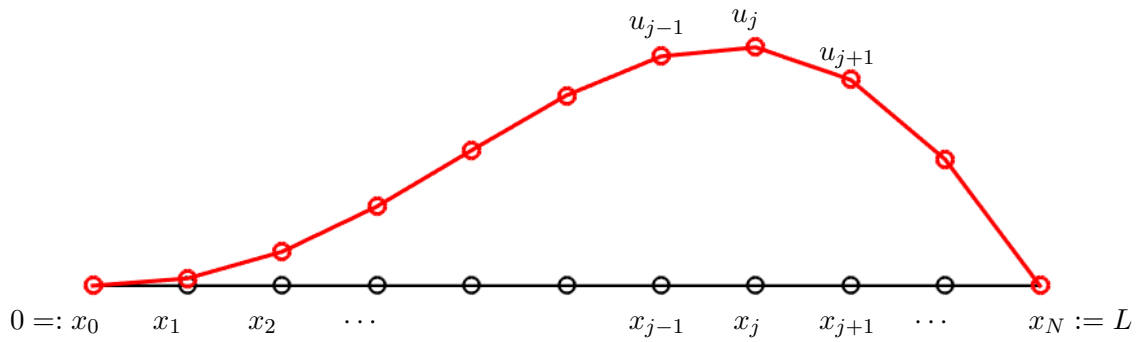
Finite Difference Method (FDM)

- *Finite difference methods* replace derivatives of continuous functions by finite difference approximations to derivatives on *discrete* grids



- For example, to solve two-point BVP

$$\tilde{u}''(x) = f(t, \tilde{u}, \tilde{u}'), \quad a < x < b$$

with BC

$$\tilde{u}(a) = \alpha \quad \tilde{u}(b) = \beta,$$

introduce mesh points $x_j = a + ih$, $i = 0, 1, \ldots, n+1$, where the uniform grid spacing is $h = \Delta x = (b-a)/(n+1)$

- Let $u_j \approx \tilde{u}(x_j)$ on interior points.

- Boundary values $u_0 = \tilde{u}(a)$ and $u_{n+1} = \tilde{u}(b)$ are already known, so we have n unknowns, u_j, $j = 1, \ldots, n$

Finite Difference Method, continued

- Replace derivatives by finite difference approximations on grid

- For example, centered differences on a uniform grid yields

$$\tilde{u}'(x_j) = \frac{\tilde{u}_{j+1} - \tilde{u}_{j-1}}{2h} + O(h^2) \approx \frac{u_{j+1} - u_{j-1}}{2h}$$
$$\tilde{u}''(x_j) = \frac{\tilde{u}_{j+1} - 2\tilde{u}_j + \tilde{u}_{j-1}}{h^2} + O(h^2) \approx \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2}$$

- Leads to system of equations to be solved for unknowns, u_i, $i = 1, \ldots, n$,

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = f\left(x_i, u_i, \frac{u_{j+1} - u_{j-1}}{2h}\right)$$

- System may be linear or nonlinear, depending on f

- If *linear*, this tridiagonal system can be solved in $\approx 8n$ operations

- Note: we typically work with $-\tilde{u}'' = f$, which leads to an SPD system matrix if f does not depend on $\tilde{u}$

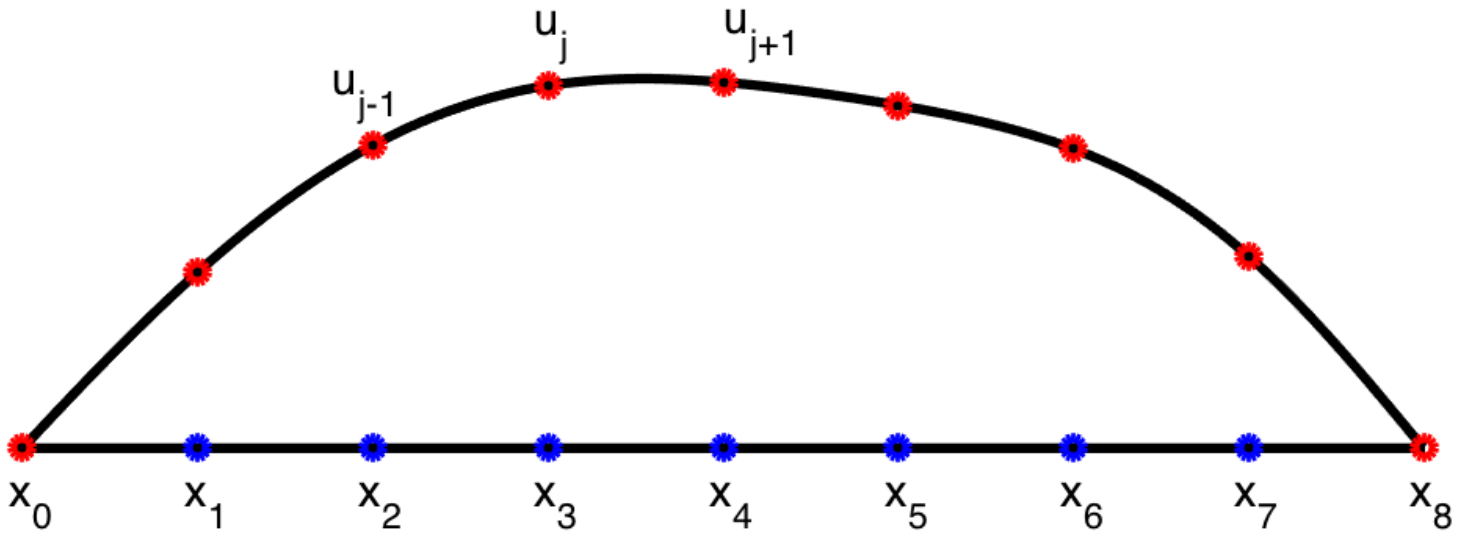
Example: Convection-Diffusion Equation

$$-\nu \frac{d^2u}{dx^2} + c\frac{du}{dx} = f, \quad u(0) = u(1) = 0,$$

Apply finite difference: $L\mathbf{u} = A\mathbf{u} + C\mathbf{u} = \mathbf{f}$

$$A = \frac{\nu}{\Delta x^2}\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix} \qquad C = \frac{c}{2\Delta x}\begin{bmatrix} 0 & 1 & & & \\ -1 & 0 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & -1 & 0 \end{bmatrix}$$

- A is symmetric positive definite.
- C is skew-symmetric.
- $L = A + C$ is neither SPD nor skew-symmetric.



- Let's look at a simple example in more detail.

$$-\nu \frac{d^2\tilde{u}}{dx^2} \;=\; f(x), \;\; \tilde{u}(0) \;=\; \tilde{u}(1) \;=\; 0,$$

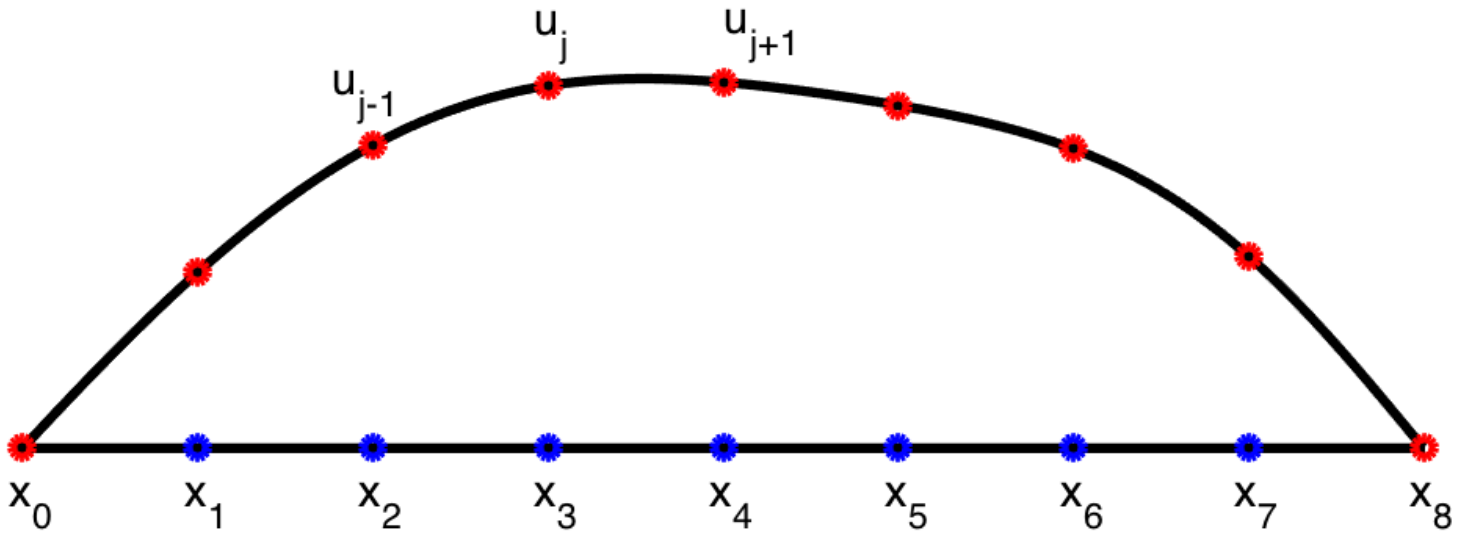
  where $\tilde{u}(x)$ is analytical solution.

- For points with uniform spacing $h := 1/(n+1)$, define:

$$x_j = j \cdot h, \quad j = 0 \ldots, n+1, \text{ as the grid points,}$$

$$f_j = f(x_j) \quad \text{as the } \textit{data} \text{ (the rhs), and}$$

$$u_j \approx \tilde{u}(x_j) \quad \text{as the unknowns.}$$



- The system of equations for $i = 1, \ldots, n$ is

$$\frac{\nu}{\Delta x^2} \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_n \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ \vdots \\ f_n \end{pmatrix}.$$

- Note that, for $i = 1, \ldots, n$, the i**th equation** is

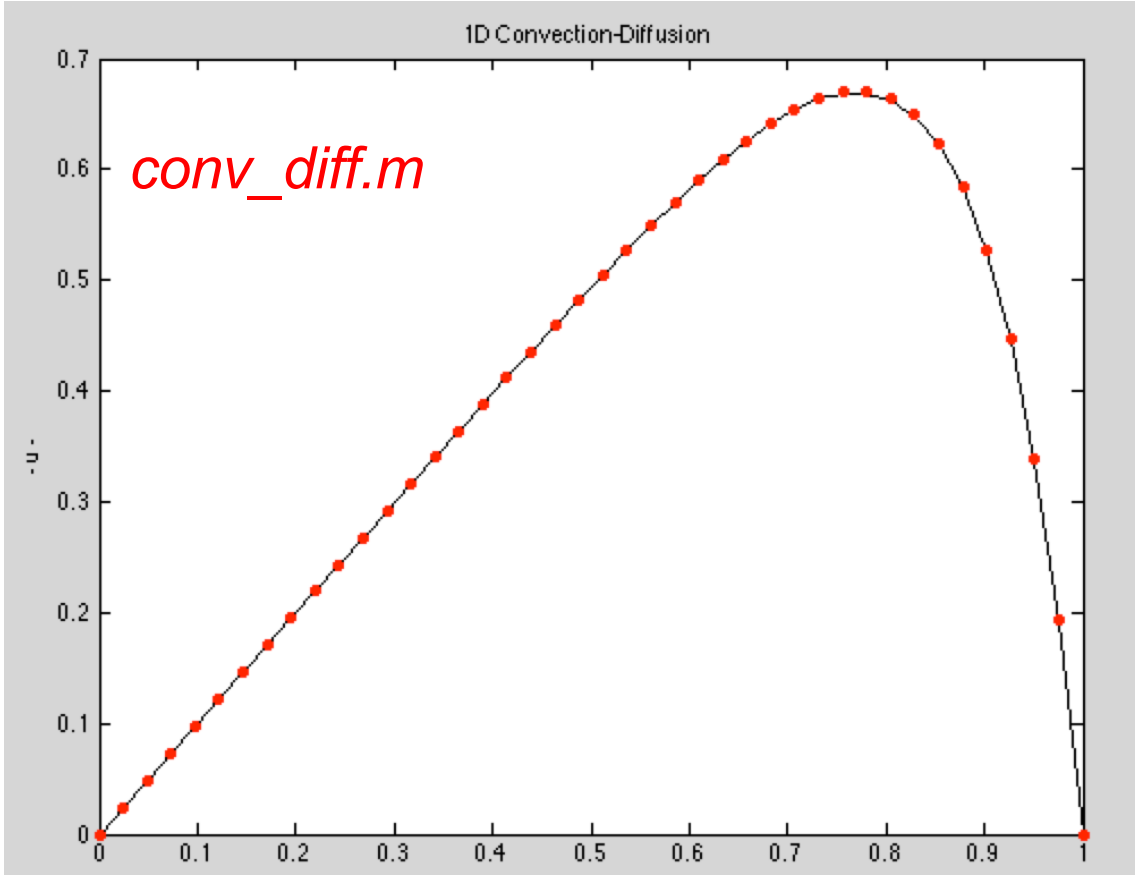
$$-\frac{\nu}{\Delta x^2} [u_{i-1} - 2u_i + u_{i+1}] = f_i,$$

which holds even at $i = 1$ and n since $u_0 = 0$ and $u_{n+1} = 0$.

conv_diff.m

Example: Convection-Diffusion Equation

```
format compact

a = 1; b=-2; c=1;
e = ones(n,1);
A = spdiags([a*e b*e c*e],-1:1, n,n);

a =-1; b=0; c=1;
e = ones(n,1);
C = spdiags([a*e b*e c*e],-1:1, n,n);

h = 1./(n+1);

nu = .1; c=0.001;
nu = .01; c=1;
nu = .001; c=1;

A = -(nu/(h*h))*A;
C = (c/(2*h))*C;

L = A+C;

f = ones(n,1);

u = L\f;

x = (1:n)*h; x=x';
x=[ 0; x ; 1];
u=[ 0; u ; 0];

ue = (x - (exp(c*x/nu)-1)/(exp(c/nu)-1) )/c;
ue = (x - ( exp(c*(x-1)/nu)-exp(-c/nu) )/(1-exp(-c/nu)) )/c;

plot(x,ue,'k-',x,u,'r.-')
title('1D Convection-Diffusion')
xlabel(' - x - ')
ylabel(' - u - ')

norm(ue-u)/norm(ue)
```



Note: It is critical that A & C be defined as ***sparse matrices.***
Otherwise, the cost will be $O(n^3)$ instead of $O(n)$!

Comments About Computing Error Norms

- We test the convergence of FD by computing $e_j := \tilde{u}(x_j) - u_j$, where $\tilde{u}$ solves a known problem.
- Be careful with the l_2 vector norm*!*
- Even though $\max |e_i| \longrightarrow 0$ with $n \longrightarrow \infty$, we can still have $||\mathbf{e}||$ grow with n. Why?
- When solving differential equations, it is better to use norms that approximate their continuous counterparts.

$$||e||_2 \;=\; \left[\int_\Omega e^2\,dx\right]^{\frac{1}{2}} \;\approx\; \underbrace{\left[\frac{1}{n}\sum_{i=1}^{n}|e_i|^2\right]^{\frac{1}{2}}}_{n \text{ scales out}}$$

- The issue can also be resolved by measuring *relative error:*

$$error \;:=\; \frac{||\mathbf{e}||}{||\mathbf{u}||}$$

  for some appropriate vector norm.
- Still, it's best to use a norm that doesn't scale with n.

Convection-Diffusion Equation

- Consider 1D convection-diffusion with $c = 1$ and $f = 1$:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} + f$$

$$u(0) = 0, \quad u(1) = 0.$$

- Assume steady-state conditions $u_t = 0$

$$-\nu u_{xx} + c\, u_x = 1, \quad u(0) = u(1) = 0.$$

- If $\nu = 0$, we have:

$$c\, u_x = 1, \quad u(0) = u(1) = 0 \text{ ???}$$

  Too many boundary conditions!

Convection-Diffusion Equation

- The issue is that $\nu \longrightarrow 0$ is a *singular perturbation.*
- This is true whenever the *highest-order derivative* is multiplied by a small constant.
- As the constant goes to zero, the number of boundary conditions changes.
- Here,
  - We go from one boundary condition when $\nu = 0$,
  - to two boundary conditions when $\nu > 0$ (even for $\nu \ll 1$).
- An example that is *not* a singular perturbation is

  $$-u_{xx} + \epsilon\, u_x = 1, \quad u(0) = u(1) = 0, \quad \epsilon \longrightarrow 0.$$

  This is called a *regular perturbation.*

Regular / Singular Perturbations You're Familiar With

- Consider solutions to the quadratic equation: $ax^2 + bx + c = 0.$

Example 1: $x^2 + \epsilon x = 1:$ Two roots as $\epsilon \longrightarrow 0.$ *Regular perturbation.*

Example 2: $\epsilon x^2 + x = 1:$ *Equation changes to first order when ε=0.*

$$
\begin{aligned}
x &= -\frac{1}{2\epsilon} \pm \frac{1}{2\epsilon}\sqrt{1+4\epsilon} \\
x_1 &= \frac{1}{2\epsilon}\left(\sqrt{1+4\epsilon} - 1\right) \\
&= \frac{1}{2\epsilon}\left(1 + 2\epsilon - 1 + O(\epsilon^2)\right) \\
&= 1 + O(\epsilon).
\end{aligned}
$$

$$
x_2 = -\frac{1}{2\epsilon}\left(2 + O(\epsilon)\right) \longrightarrow -\infty. \quad \textit{Singular perturbation.}
$$

Convection-Diffusion Equation

- Exact solution for our 1D model problem:

$$u = \frac{x}{c} - \frac{L}{c}\left[\frac{e^{cx/\nu} - 1}{e^{cL/\nu} - 1}\right]$$

$$= \frac{1}{c}\left[x - \frac{e^{c(x-L)/\nu} - e^{-cL/\nu}}{1 - e^{-cL/\nu}}\right].$$

- In the convection-dominated limit ($cL \gg \nu$), one of these is computable in IEEE floating point, one is not.

- Which is which?

Nonlinear Example: The Bratu Equation

- Consider 1D diffusion with nonlinear right-hand side:

$$-\frac{d^2u}{dx^2} \;=\; q(x,u) \;=\; \sigma\, e^u, \;\; u(0) = u(1) = 0.$$

- Discretizing with finite differences (say),

$$A\mathbf{u} = \sigma\, e^{\mathbf{u}}.$$

- Nonlinear system:

$$\mathbf{f}(\mathbf{u}) \;=\; 0, \quad \mathbf{f}(\mathbf{u}) \;=\; A\mathbf{u} - \sigma\, e^{\mathbf{u}}.$$

- Newton's method:

$$\begin{aligned} \mathbf{u}^{k+1} &= \mathbf{u}^k + \mathbf{s}^k \\ \mathbf{s}^k &= -\left[J^k\right]^{-1} \mathbf{f}(\mathbf{u}^k). \end{aligned}$$

$$\left(J^k\right)_{ij} := \frac{\partial f_i^k}{\partial u_j^k}.$$

- ith equation:

$$f_i^k = \sum_{j=1}^{n} A_{ij}\, u_j^k - \sigma e^{u_i^k} \quad \longrightarrow \quad (J_k)_{ij} = \frac{\partial f_i}{\partial u_j} = A_{ij} - \sigma \delta_{ij} e^{u_i}.$$

- If $b = -1$ and $a_j = 2 - h^2\sigma e^{u_j}$, then

$$J = \frac{1}{h^2}\begin{pmatrix} a_1 & b & & & \\ b & a_2 & b & & \\ & b & \ddots & \ddots & \\ & & \ddots & \ddots & b \\ & & & b & a_n \end{pmatrix},$$

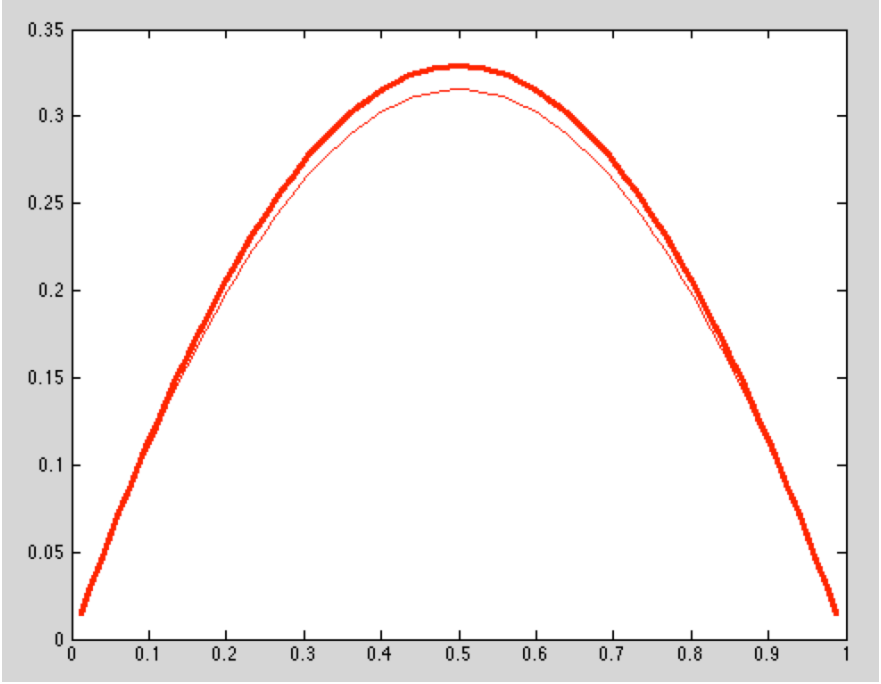
- At *each iteration*, modify the tridiagonal matrix A such that

$$J_k = A + \sigma e^{u_i^k}\delta_{ij},$$

and solve this tridiagonal system in $\approx 8n$ operations.

bratu1a.m

```
format compact; format longe;  close all

n=80; sigma = 2;

h=1./(n+1); b = ones(n,1); x=1:n; x=h*x'; h2i = 1./(h*h);
hold off; plot(x,0*x,'k-'); hold on

a=-2*b;
A = h2i*spdiags([b a b],-1:1, n,n);

c=-2*b + sigma*h*h*exp(x); J = h2i*spdiags([b c b],-1:1, n,n);


u=b*0;

for iter=1:31;

    f=A*u + sigma*exp(u);
    c=-2*b + sigma*h*h*exp(u);
    J = h2i*spdiags([b c b],-1:1, n,n);

    [L,U]=lu(J);

    s = -U\ (L\f);

    u = u+s;

    plot(x,u,'r-'); hold on

    ns = norm(s); nf = norm(f); [ns nf]

end;

plot(x,u,'r-'); hold on
```



Extension of Finite Difference to Variable Coefficients

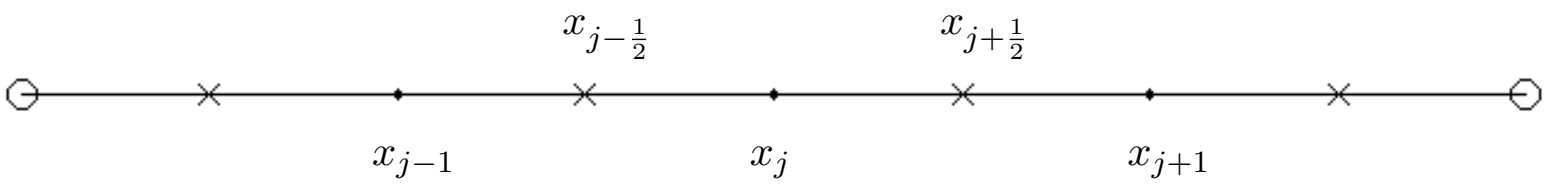


Figure 1: Grid spacing for variable coefficient diffusion operator.

Consider the one-dimesional model problem,

$$-\frac{d}{dx}\,a(x)\frac{du}{dx} \;=\; f(x), \qquad u(0) \;=\; u(1) \;=\; 0. \tag{5}$$

Let

$$u_i \;:=\; u(x_i), \qquad a_{i+\frac{1}{2}} \;:=\; a(x_{i+\frac{1}{2}}), \qquad w_i \;\approx\; \frac{d}{dx}\,a(x)\frac{du}{dx}\bigg|_{x_i}, \tag{6}$$

with $x_i := i\,h$, $i = 0, \ldots, n+1$ and $x_{i+\frac{1}{2}} := (i+\frac{1}{2})\,h$, $i = 0, \ldots, n$, and $h := 1/(n+1)$. Then

$$w_i \;=\; \frac{d}{dx}\,a(x)\frac{du}{dx}\bigg|_{x_i} \;\approx\; \frac{1}{h}\left[\left(a\frac{du}{dx}\right)\bigg|_{x_{i+\frac{1}{2}}} - \left(a\frac{du}{dx}\right)\bigg|_{x_{i-\frac{1}{2}}}\right] \tag{7}$$

$$\approx \frac{1}{h}\left[a_{i+\frac{1}{2}}\left(\frac{u_{i+1}-u_i}{h}\right) - a_{i-\frac{1}{2}}\left(\frac{u_i-u_{i-1}}{h}\right)\right]. \tag{8}$$

Extension of Finite Difference to Variable Coefficients

Assuming $u = 0$ at the domain endpoints, then the finite difference appoximation to $u'_{i+\frac{1}{2}}$, $i = 0, \ldots, n$ can be evaluated as the matrix-vector product, $\underline{v} = D\underline{u}$, where D is the $(n+1) \times n$ finite difference matrix illustrated below.

$$\underline{v} = \begin{pmatrix} v_{\frac{1}{2}} \\ v_{\frac{3}{2}} \\ \vdots \\ v_{n+\frac{1}{2}} \end{pmatrix} = \frac{1}{h} \begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & -1 & \ddots & \\ & & \ddots & 1 \\ & & & -1 \end{bmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} = D\underline{u}. \tag{9}$$

Note that $\frac{1}{h}(u_{i+1} - u_i)$ is generally regarded as a first-order accurate approximation to $\frac{du}{dx}$, it is in fact second-order accurate at the midpoint $x_{i+\frac{1}{2}}$.

Given $v_{i+\frac{1}{2}}$, it remains to evaluate the outer finite difference in (7), which maps data from the $(n+1)$ half-points to the n integer points. Let

$$q_{i+\frac{1}{2}} := a_{i+\frac{1}{2}} v_{i+\frac{1}{2}}. \tag{10}$$

Then

$$\underline{w} = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = \frac{1}{h} \begin{bmatrix} -1 & 1 & & \\ & -1 & 1 & \\ & & \ddots & \ddots \\ & & & -1 \quad 1 \end{bmatrix} \begin{pmatrix} q_{\frac{1}{2}} \\ q_{\frac{3}{2}} \\ \vdots \\ q_{n+\frac{1}{2}} \end{pmatrix} = -D^T \underline{q}. \tag{11}$$

Extension of Finite Difference to Variable Coefficients

Finally, note that if A is an $(n+1) \times (n+1)$ diagonal matrix with entries $(a_{\frac{1}{2}}, a_{\frac{3}{2}}, \ldots a_{n+\frac{1}{2}})$, then (10) can be expressed as $\underline{q} = A\underline{v}$, and the finite-difference approximation (7) can be compactly expressed in matrix form as

$$\underline{w} = -D^T A D \underline{u} \tag{12}$$

Assuming $a_{i+\frac{1}{2}} > 0$, it is easy to show that the matrix

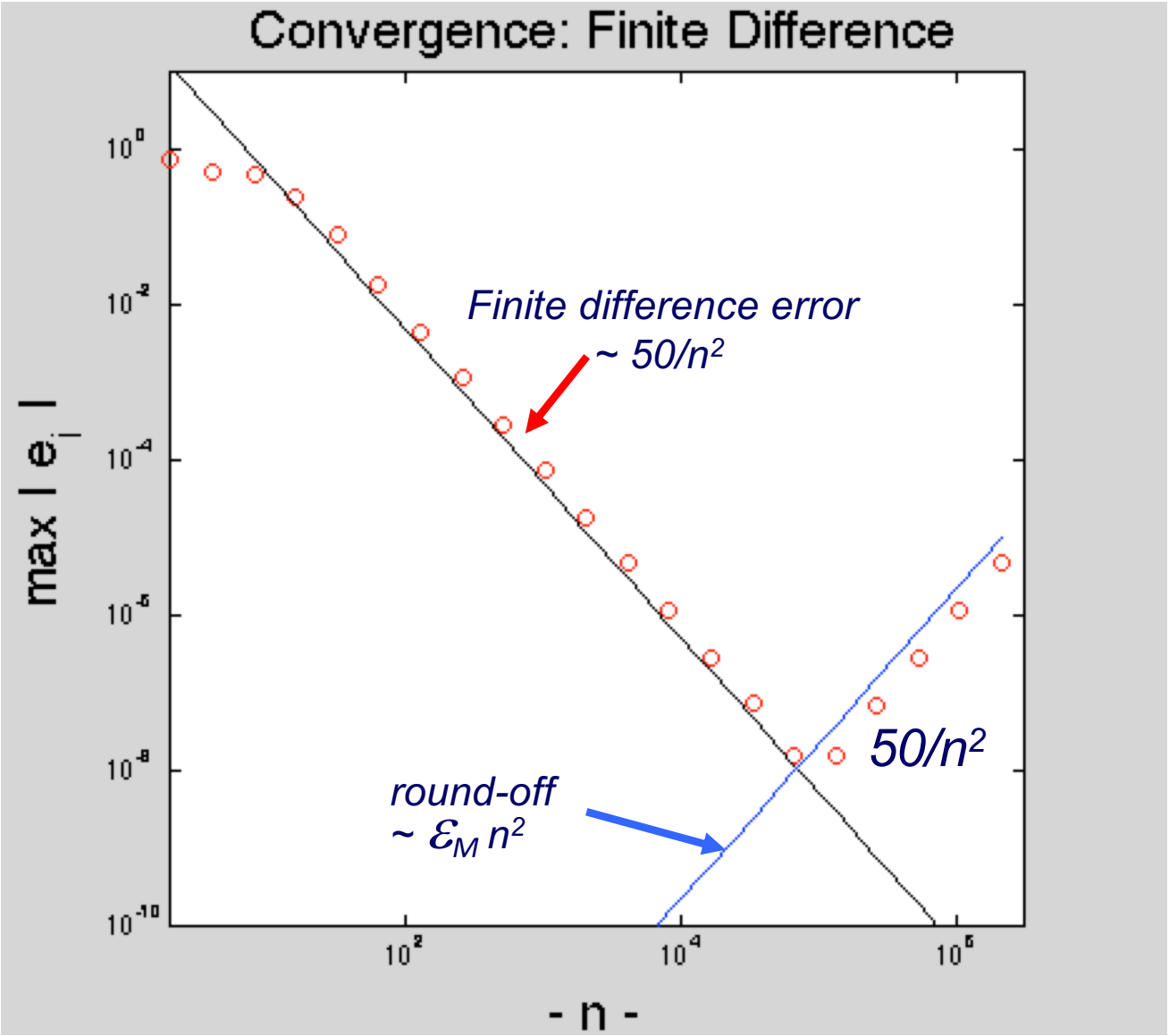
$$L \quad := \quad D^T A D \tag{13}$$

is symmetric positive definite, which is a requirement if the system is to be solved with conjugate gradient iteration or Cholesky factorization. Fortunately, this property carries over into the multidimensional case, which we consider in the next section. We further remark that L is a map from data $(u_1 \ldots u_j \ldots u_n)$ to $(w_1 \ldots w_j \ldots w_n)$. That is, once defined, it does not generate data at the half gridpoint locations. This is a particularly attractive feature in multiple space dimensions where having multiple grids leads to an explosion of notational difficulties.

Convergence Behavior: Finite Difference

- In differential equations, we are interested in the rate of convergence – i.e., the rate at which the error goes to zero vs. n, the number of unknowns in the system.
- For finite difference methods and methods using Lagrangian interpolants, n is the number of gridpoints (but, depends on the type of boundary conditions…..)
- The next figure shows the error vs. n for a 2^{nd}-order (i.e., $O(h^2)$) finite difference solution of the steady-state convection-diffusion equation in 1D.
- For $n > \sim \varepsilon_M^{-1/3}$, the error goes up, due to round-off associated with the approximation to the 2^{nd}-order derivative.
- As we've seen in past homework assignments, the minimum error is around $\varepsilon_M^{-1/2}$

Finite Difference Convergence Rate



Properties of Finite Difference Methods

- Pros
  - Easy to formulate (for simple problems)
  - Easy to analyze "
  - Easy to code "
  - Closed-form expressions for eigenvalues/eigenvectors for uniform grid with constant coefficients.

- Cons –
  - Geometric complexity for 2D/3D is not as readily handled as FEM.
  - Difficult to extend to high-order (because of boundary conditions).
  - Do not always (e.g., because of BCs) get a symmetric matrix for

$$\frac{d^2u}{dx^2} \qquad \text{or} \qquad \frac{d}{dx}\nu(x)\frac{du}{dx}$$

Eigenvalues, Continuous and Discrete

- One of the great features of finite difference methods is that one can readily compute the eigenvalues of the discrete operators and thus understand their spectrum and convergence rates.
- The latter is important for understanding accuracy.
- The former is important for understanding stability of time-stepping schemes in the case of PDEs, which we'll see in the next chapter.
- The reason it is easy to find the eigenvalues for finite difference methods is that, for the constant coefficient case, they often share the same eigenfunctions as their continuous counterparts.

Eigenvalue Example:

- Consider the analytical (i.e., continuous) eigenvalue problem

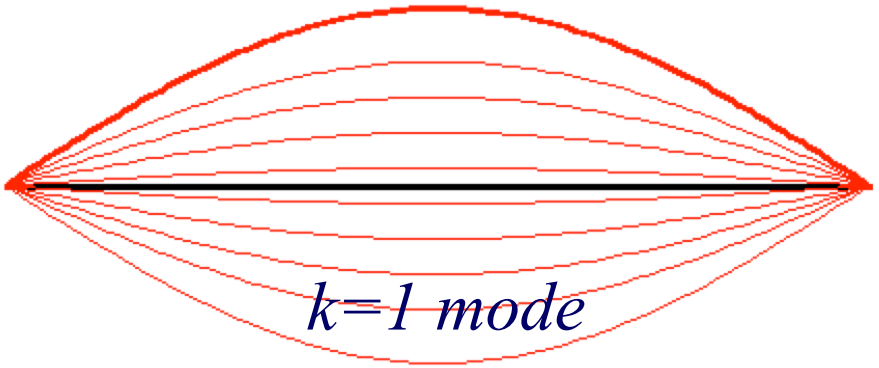
$$-\frac{d^2\tilde{u}}{dx^2} = \tilde{\lambda}\,\tilde{u}, \qquad \tilde{u}(0) = \tilde{u}(1) = 0.$$

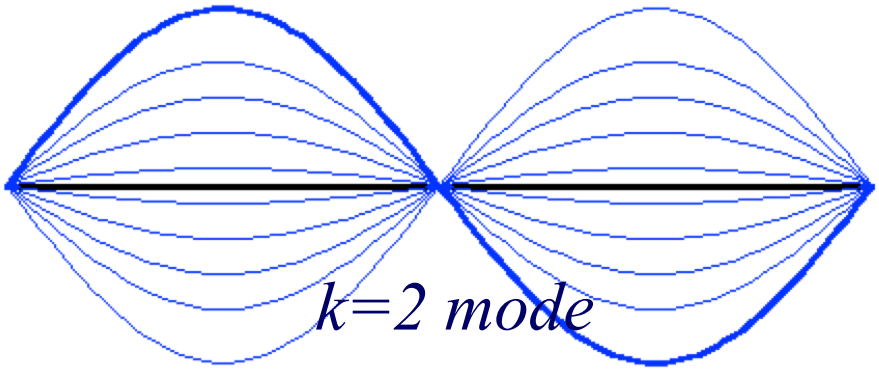
- The eigenfunctions/eigenvalues for the continuous problem are

$$\tilde{u} = \sin(k\pi x):$$

$$-\tilde{u}'' = k^2\pi^2 \sin(k\pi x) = k^2\pi^2\,\tilde{u} = \tilde{\lambda}_k\,\tilde{u}$$

$$\tilde{\lambda}_k = k^2\pi^2$$





The modes are like the vibrations of a guitar string.
Higher wavenumbers, k, correspond to higher frequency.
Here, the k=2 mode would be a harmonic – one octave higher.

Finite Difference Eigenvectors/values:

- Consider $\mathbf{s} = [\sin(k\pi x_j)]^T$:

$$
\begin{aligned}
A\mathbf{s}|_j &= \frac{-1}{\Delta x^2}\left[\sin k\pi x_{j+1} - 2\sin k\pi x_j + \sin k\pi x_{j-1}\right] \\
&= \frac{-1}{\Delta x^2}\left[\sin(k\pi x_j + \Delta x) - 2\sin(k\pi x_j) + \sin(k\pi x_j - \Delta x)\right]
\end{aligned}
$$

- Use the identity:

$$
\sin(a+b) = \sin a\,\cos b + \cos a\,\sin b
$$

$$
\begin{aligned}
\sin(k\pi x_{j+1}) &= \sin k\pi x_j\,\cos k\pi\Delta x + \cos k\pi x_j\,\sin k\pi\Delta x \\
\sin(k\pi x_{j-1}) &= \sin k\pi x_j\,\cos k\pi\Delta x - \cos k\pi x_j\,\sin k\pi\Delta x \\
\text{SUM} &= 2\,\sin k\pi x_j\,\cos k\pi\Delta x
\end{aligned}
$$

- $$
A\mathbf{s}|_j = \frac{-1}{\Delta x^2}\left[s_{j+1} - 2s_j + s_{j-1}\right] = -\frac{1}{\Delta x^2}\left[2\cos k\pi\Delta x - 2\right]\sin k\pi x_j
$$

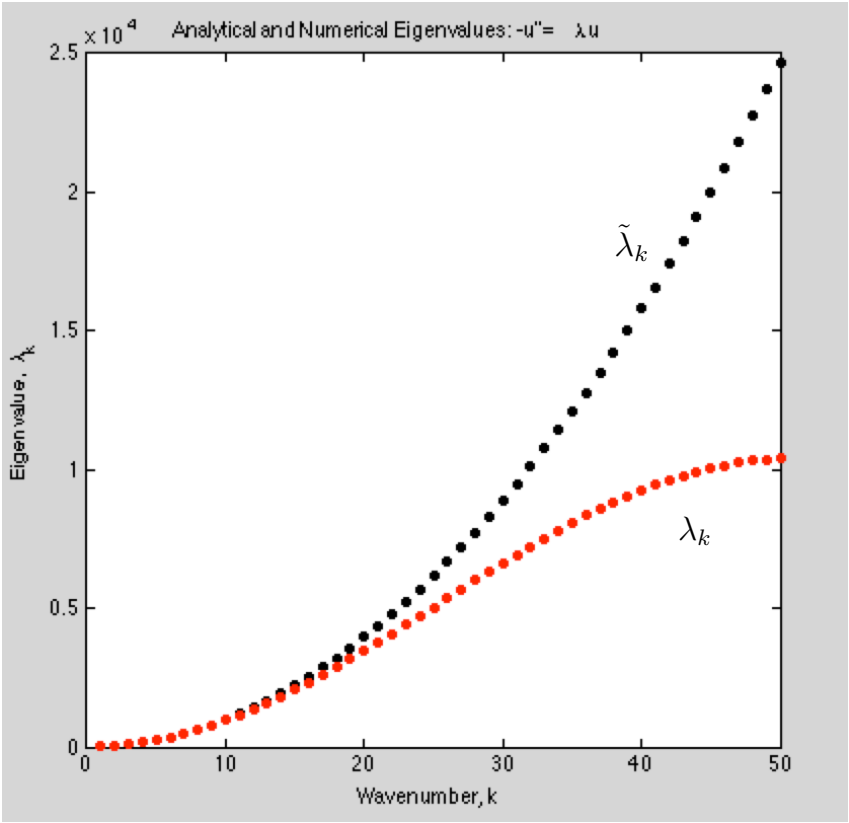
$$
= \lambda_k \mathbf{s}|_j
$$

$$
\boxed{\lambda_k = \frac{2}{\Delta x^2}\left[1 - \cos k\pi\Delta x\right].}
$$

Eigenvalue Properties for $-u'' = \lambda u$, $u(0) = u(1) = 0$:

- $\max \lambda_k \sim Cn^2$ $\qquad\qquad \dfrac{\tilde{\lambda}_n}{\lambda_n} \sim \dfrac{\pi^2}{4}$
- For $k\Delta x \ll 1$, (with $\theta := k\Delta x$):

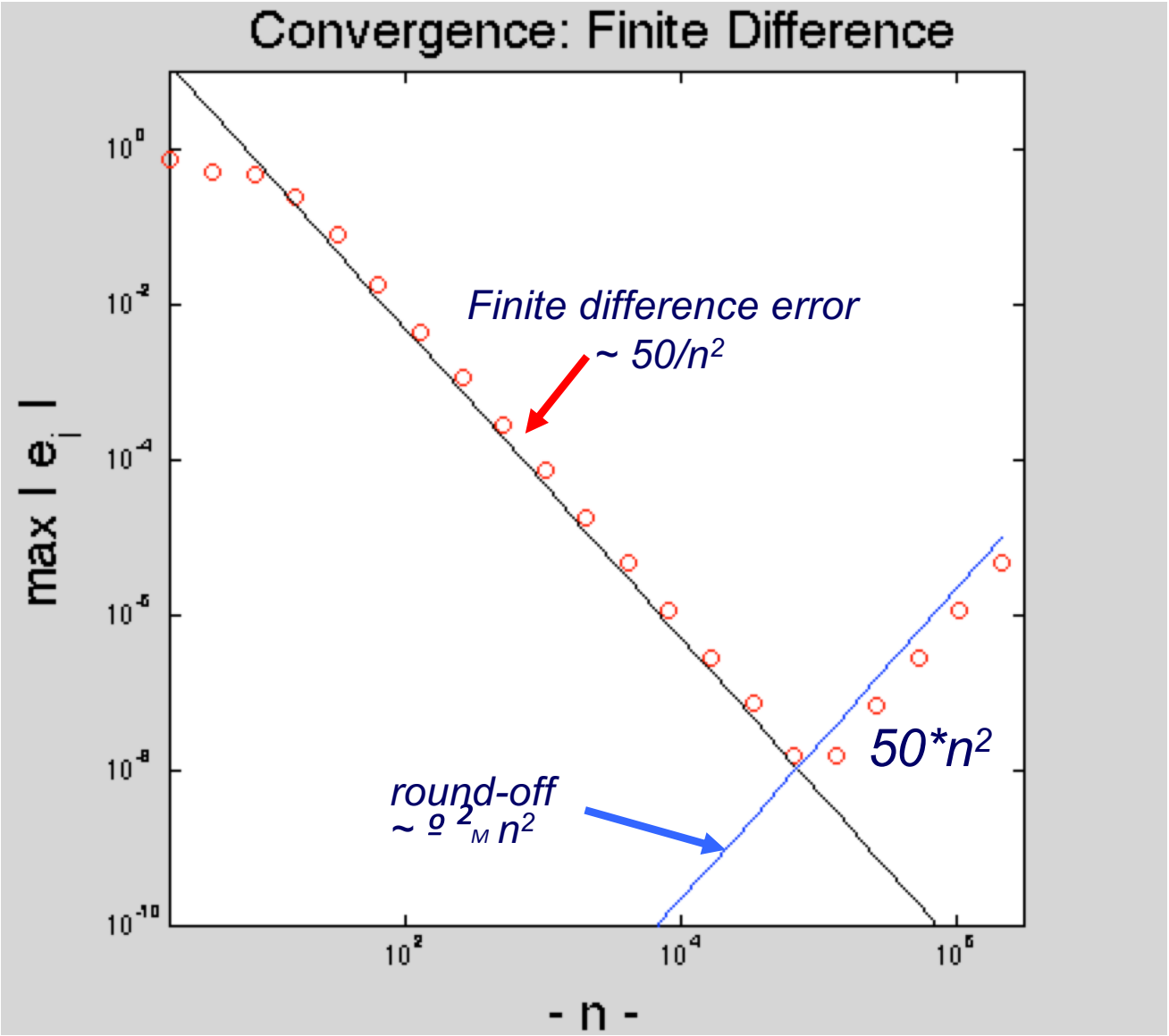
$$\lambda_k \;=\; (k\pi)^2 \left[1 - \frac{(k\pi\Delta x)^2}{12} + \cdots\right]$$



Collocation

- Collocation is essentially the ***method of undetermined coefficients***.
  - Start with
$$u(x) = \sum_{j=0}^{n} \hat{u}_j \phi_j(x)$$
    .
  - Find coefficients $\hat{u}_j$ such that BVP is satisfied at gridpoints x_i.
- Instead of using monomials, $\phi_j = x^j$, could use Lagrange polynomials on Chebyshev or Legendre quadrature points.
- Normally, one would use Gauss-Lobatto-Legendre or Gauss-Lobatto-Chebyshev points, which include ± 1 (i.e., the endpoints of the interval) in the nodal set.
- If the solution is to be zero at those boundaries one would have $u_0 = u_n = 0$.
- In many cases, these methods are exponentially convergent.
- For several reasons conditioning, symmetry, robustness, and ease of boundary condtions, collocation has lost favor to Galerkin methods.

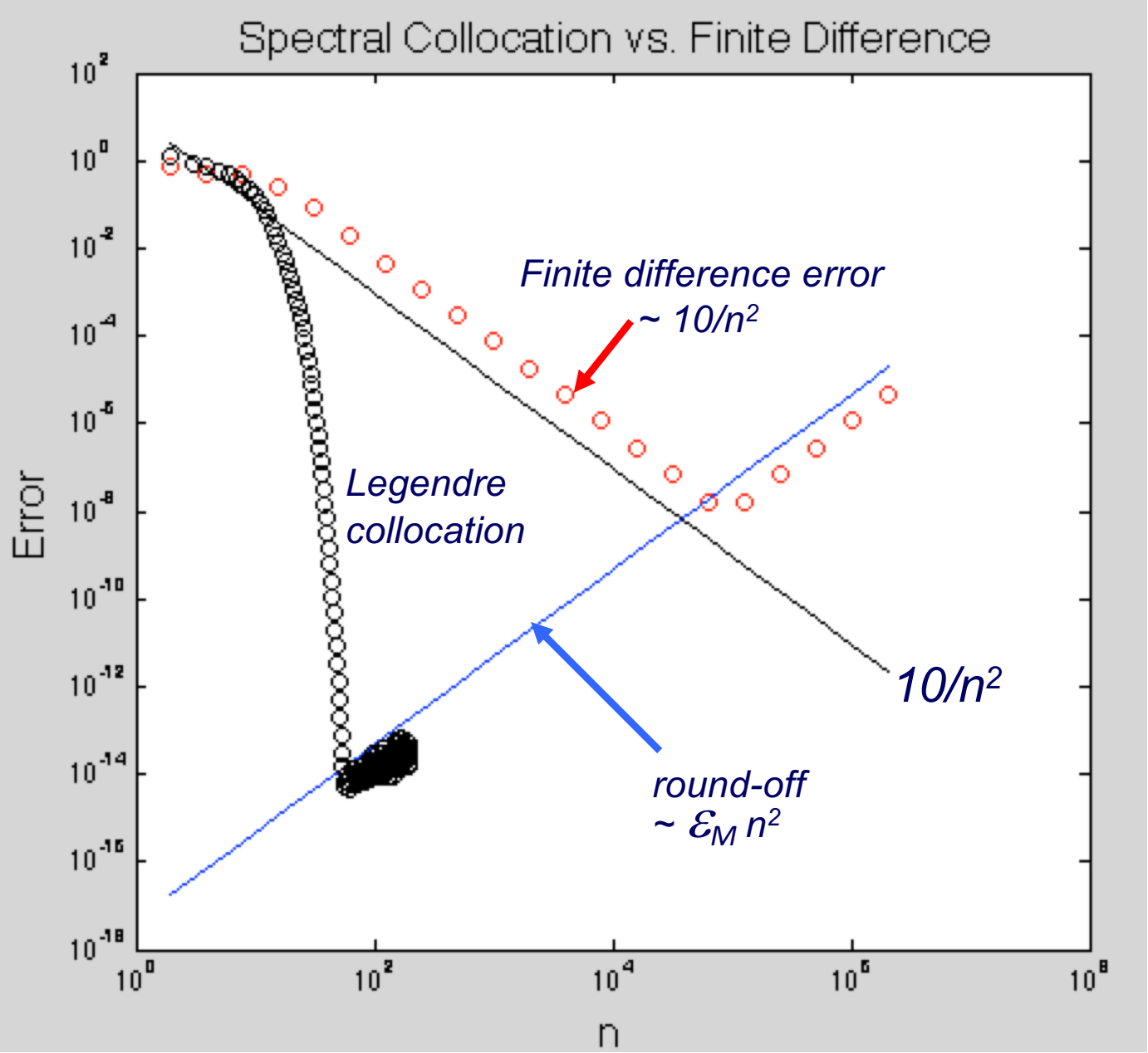
Finite Difference Convergence Rate



Convergence Behavior: High-Order Methods

- The 2^{nd}-order convergence of standard finite difference methods looks reasonable.
- However, higher-order methods are generally much faster in that the same error can be achieved with a lower n, once n is large enough for the asymptotic convergence behavior to apply.
- High-order methods suffer the same round-off issue, with error growing like $\varepsilon_M n^2$.
- However, their truncation error goes to zero more rapidly so that the n where truncation and round-off errors balance is lower and the minimum error is thus much smaller.
- Usually, we are more interested in a small error at small n, rather than realizing the minimum possible error.
- For PDEs on an (n x n x n) grid cost generally scales as n^3, so a small n is a significant win.

Spectral Collocation vs. Finite Difference



Spectral Collocation vs. Finite Difference (semilogy)