Scientific Computation HW2

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September 2022

Exercise 2.1 *(inverse matrix and Green's functions)*

(a) Write out the 5×5 matrix A from (2.43) for the boundary value problem $u''(x) = f(x)$ with $u(0) = u(1) = 0$ for $h = 0.25$.

Using the form of the matrix in (2.43) for $h = 0.25$, we get

$$A = \frac{1}{0.25^2}\begin{bmatrix} 0.25^2 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0.25^2 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 16 & -32 & 16 & 0 & 0 \\ 0 & 16 & -32 & 16 & 0 \\ 0 & 0 & 16 & -32 & 16 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

(b) Write out the 5×5 inverse matrix A^{-1} explicitly for this problem.

Solving for the inverse of A, we find

$$A^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 3/4 & -3/64 & -1/32 & -1/64 & 1/4 \\ 1/2 & -1/32 & -1/16 & -1/32 & 1/2 \\ 1/4 & -1/64 & -1/32 & -3/64 & 3/4 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

(c) If $f(x) = x$, determine the discrete approximation to the solution of the boundary value problem on this grid and sketch this solution and the five Green's functions whose sum gives this solution.

We will approximate x on the interval $[0, 1]$ by the following sum of Dirac Delta functions: $x \approx 0\delta(x) + \frac{1}{4}\delta(x - 1/4) + \frac{1}{2}\delta(x - 1/2) + \frac{3}{4}\delta(x - 3/4) + \delta(x - 1)$. That is, we are approximating x on $[0, 1]$ with a mesh grid of mesh width $1/4$. Using this approximation, our differential equation turns into

$$U''(x) = \frac{1}{4}\delta(x - 1/4) + \frac{1}{2}\delta(x - 1/2) + \frac{3}{4}\delta(x - 3/4) + \delta(x - 1)$$

Where $U(x)$ denotes the approximate solution and $u(x)$ denotes the exact solution.

And we know that for any linear operator $\mathcal{L}$, $\mathcal{L}(G(x,\bar{x})) = \delta(x-\bar{x})$ and by the superposition principle, we have

$$\mathcal{L}(G(x,\bar{x}_1) + G(x,\bar{x}_2) + \cdots + G(x,\bar{x}_n)) = h\delta(x-\bar{x}_1) + h\delta(x-\bar{x}_2) + \cdots + h\delta(x-\bar{x}_n)$$

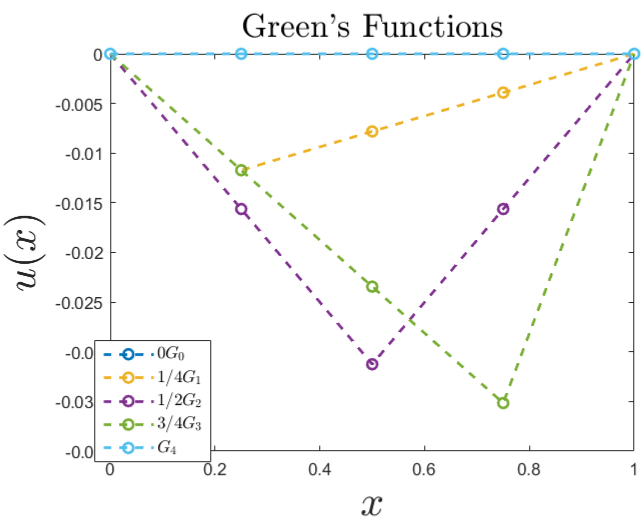
So we expect that our solution to our discretized differential equation will be of the form

$$U(x) = h\frac{1}{4}G(x,1/4) + h\frac{1}{2}G(x,1/2) + h\frac{3}{4}G(x,3/4) + hG(x,1)$$

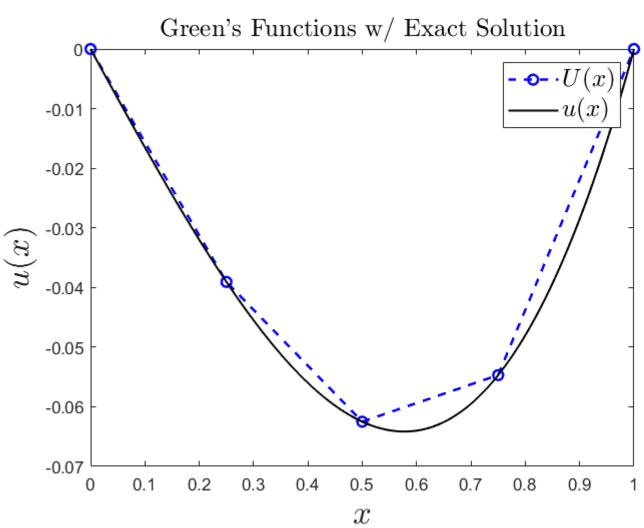
where

$$G(x,\bar{x}) = \begin{cases} x(\bar{x}-1) & 0 \le x \le \bar{x} \\ \bar{x}(x-1) & \bar{x} \le x \le 1 \end{cases}$$

The following figure shows the scaled Green's functions as they appear in the above equation:



And their sum $U(x)$ plotted against the exact solution $u(x) = \frac{1}{6}x^3 - \frac{1}{6}x$:



Exercise 2.2 *(Green's function with Neumann boundary conditions)*

(a) Determine the Green's functions for the two-point boundary value problem $u''(x) = f(x)$ on $0 < x < 1$ with a Neumann boundary condition at $x = 0$ and a Dirichlet condition at $x = 1$, i.e, find the function $G(x, \bar{x})$ solving

$$u''(x) = \delta(x - \bar{x}), \quad u'(0) = 0, \quad u(1) = 0$$

and the functions $G_0(x)$ solving

$$u''(x) = 0, \quad u'(0) = 1, \quad u(1) = 0$$

and $G_1(x)$ solving

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

We wish to find Green's function that satisfies $G''(x, \bar{x}) = \delta(x-\bar{x})$ with boundary conditions $G'(0, \bar{x}) = 0$, $G(1, \bar{x}) = 0$. Integrating the above differential equation, we get

$$G'(x, \bar{x}) = \begin{cases} c_1, & 0 \le x \le \bar{x} \\ c_2 + 1, & \bar{x} \le x \le 1 \end{cases}$$

Evaluating the above expression at $x = 0$, we find $c_1 = 0$ from the given boundary conditions. Now, integrating again, we get the following:

$$G(x, \bar{x}) = \begin{cases} c_3 & 0 \le x \le \bar{x} \\ (c_2 + 1)x + c_4 & \bar{x} \le x \le 1 \end{cases}$$

Evaluating the above expression at $x = 1$, we get $c_2 + 1 + c_4 = 0$ from the given boundary condition. Solving for c_4, we get $c_4 = -(c_2 + 1)$. Substituting this back in, we find

$$G(x, \bar{x}) = \begin{cases} c_3 & 0 \le x \le \bar{x} \\ (c_2 + 1)(x - 1) & \bar{x} \le x \le 1 \end{cases}$$

Additionally, we require that $G'(x, \bar{x})$ must have a jump of 1 at $\bar{x}$. That is,

$$c_2 + 1 - 0 = 1$$

so $c_2 = 0$. Finally, we require $\lim_{x\to\bar{x}^-} G(x, \bar{x}) = \lim_{x\to\bar{x}^+} G(x, \bar{x})$. Doing this, we find

$$c_3 = \bar{x} - 1$$

Putting it all together, we have

$$G(x, \bar{x}) = \begin{cases} \bar{x} - 1 & 0 \le x \le \bar{x} \\ x - 1 & \bar{x} \le x \le 1 \end{cases}$$

Now must find the solutions G_0 and G_1. From the differential equation, it is easy to see that

$$G_0(x) = c_1 x + c_2$$

and from our boundary conditions, we have

$$G_0(x) = x - 1$$

similarly for $G_1(x)$:

$$G_1(x) = 1$$

(b) Using this as guidance, find the general formulas for the elements of the inverse of the matrix in equation (2.54). Write out the 5×5 matrices A and A^{-1} for the case $h = 0.25$.

From (2.54) for $h = 0.25$, we find

$$A = \begin{bmatrix} -4 & 4 & & & \\ 16 & -32 & 16 & & \\ & 16 & -32 & 16 & \\ & & 16 & -32 & 16 \\ & & & 0 & 1 \end{bmatrix}$$

We may easily compute A^{-1} in MATLAB, but we may also compute A^{-1} by using what we found for $G(x, \bar{x})$. To do so, notice from (2.54) that

$$\begin{bmatrix} U_0 \\ U_1 \\ U_2 \\ U_3 \\ U_4 \end{bmatrix} = A^{-1} \begin{bmatrix} \sigma \\ f(x_1) \\ f(x_2) \\ f(x_3) \\ \beta \end{bmatrix}$$

Additionally, if we approximate our differential equation with Dirac Delta functions, we may say

$$U''(x) = h(f(x_1)\delta(x - x_1) + f(x_2)\delta(x - x_2) + f(x_3)\delta(x - x_3) + f(x_4)\delta(x - x_4))$$

I exclude the point x_0 since the value of $U'(x_0)$ is prescribed, not $U(x_0)$. Then we find the general solution to be given by

$$U(x) = h(f(x_1)G(x, x_1) + f(x_2)G(x, x_2) + f(x_3)G(x, x_3) + f(x_4)G(x, x_4)) + \sigma G_0(x) + \beta G_1(x)$$

Now, let's evaluate $U(x)$ at each x_j and $U'(x)$ at x_0:

$$U'(x_0) = \sigma$$

$$\begin{aligned} U(x_1) &= h(f(x_1)G(x_1, x_1) + f(x_2)G(x_1, x_2) + f(x_3)G(x_1, x_3) + f(x_4)G(x_1, x_4)) + \sigma(x_1 - 1) + \beta \\ &= -\frac{3}{16}f(x_1) - \frac{1}{2}f(x_2) - \frac{1}{8}f(x_3) - \frac{1}{16}f(x_4) - \sigma + \beta \end{aligned}$$

$$\begin{aligned} U(x_2) &= h(f(x_1)G(x_2, x_1) + f(x_2)G(x_2, x_2) + f(x_3)G(x_2, x_3) + f(x_4)G(x_2, x_4)) + \sigma(x_2 - 1) + \beta \\ &= -\frac{3}{16}f(x_1) - \frac{1}{8}f(x_2) - \frac{1}{16}f(x_3) - \frac{3}{4}\sigma + \beta \end{aligned}$$

$$\begin{aligned} U(x_3) &= h(f(x_1)G(x_3, x_1) + f(x_2)G(x_3, x_2) + f(x_3)G(x_3, x_3) + f(x_4)G(x_3, x_4)) + \sigma(x_3 - 1) + \beta \\ &= -\frac{1}{8}f(x_1) - \frac{1}{8}f(x_2) - \frac{1}{16}f(x_3) - \frac{1}{2}\sigma + \beta \end{aligned}$$

$$\begin{aligned} U(x_4) &= h(f(x_1)G(x_4, x_1) + f(x_2)G(x_4, x_2) + f(x_3)G(x_4, x_3) + f(x_4)G(x_4, x_4)) + \sigma(x_4 - 1) + \beta \\ &= \beta \end{aligned}$$

Knowing that this linear system must be equal to $A^{-1}\mathbf{f}$, we find the following expression for A^{-1}:

$$A^{-1} = \begin{bmatrix} -1 & -3/16 & -1/8 & -1/16 & 1 \\ -3/4 & -3/16 & -1/8 & -1/16 & 1 \\ -1/2 & -1/8 & -1/8 & -1/16 & 1 \\ -1/4 & -1/16 & -1/16 & -1/16 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Exercise 2.3 *(solvability condition for Neumann problem)*

Determine the null space of the matrix A^T, where A is given in equation (2.58), and verify that the condition (2.62) must hold for the linear system to have solutions.

We wish to find the null space (kernel) for

$$A^T = \begin{bmatrix} -h & 1 & & & & & \\ h & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & 1 & -2 & 1 & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & 1 & -2 & h \\ & & & & & 1 & -h \end{bmatrix}$$

Essentially, we are looking for all vectors $\mathbf{v}$ such that $A^T\mathbf{v} = \mathbf{0}$. Well, solving row-by-row, we find the following equations:

$$\begin{aligned} hv_1 &= v_2 \\ v_2 &= v_3 \\ v_3 &= v_4 \\ &\vdots \\ v_{n-2} &= v_{n-1} \\ v_{n-1} &= hv_n \end{aligned}$$

That is, for $\mathbf{v} \in \ker(A^T)$,

$$\mathbf{v} = t \begin{bmatrix} 1 \\ h \\ \vdots \\ h \\ 1 \end{bmatrix}$$

where $t \in \mathbb{R}$. Explicitly, we can write the kernel of A^T as

$$\ker(A^T) = \left\{ t \begin{bmatrix} 1 \\ h \\ \vdots \\ h \\ 1 \end{bmatrix} \;\middle|\; t \in \mathbb{R} \right\}$$

Now, recall the Fredholm Alternative Theorem. In order for the system $A\mathbf{x} = \mathbf{b}$ to have a solution, it must be true that $\mathbf{b} \in \ker(A^T)^\perp$. That is, $\mathbf{b}$ must be orthogonal to the null space of A^T. For our problem,

$$\mathbf{b} = \begin{bmatrix} \sigma_0 + \frac{h}{2}f(x_0) \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_m) \\ -\sigma_1 + \frac{h}{2}f(x_{m+1}) \end{bmatrix}$$

Since $\mathbf{b}$ and any vector in $\ker(A^T)$ must be orthogonal, it follows that

$$\mathbf{b} \cdot \mathbf{k} = 0$$

where $\mathbf{k} \in \ker(A^T)$. Well, notice that the dot product with any $\mathbf{k}$ will give us the following equation:

$$\sigma_0 + \frac{h}{2}f(x_0) + hf(x_1) + hf(x_2) + \cdots + hf(x_m) - \sigma_1 + \frac{h}{2}f(x_{m+1}) = 0$$

Moving σ_0 and σ_1 to the right hand side and writing the middle sum in summation notation, we get

$$\frac{h}{2}f(x_0) + h\sum_{i=1}^{m} f(x_i) + \frac{h}{2}f(x_{m+1}) = \sigma_1 - \sigma_0$$

which matches equation (2.62) exactly.

Exercise 2.4 *(boundary conditions in* `bvp` *codes)*

(a) Modify the m-file `bvp2.m` so that it implements a Dirichlet boundary condition at $x = a$ and a Neumann condition at $x = b$ and test the modified program.

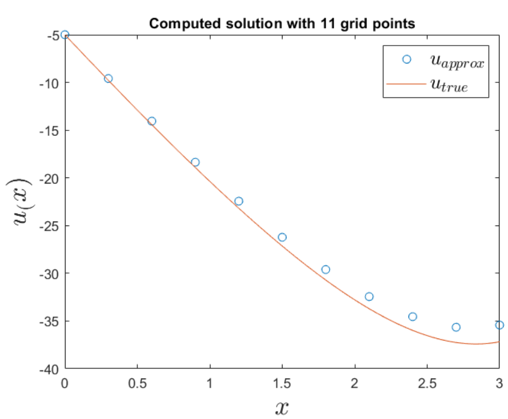
By swapping the first and last rows of the finite difference matrix A, we get the effect of implementing a Neumann condition at $x = b$ and a Dirichlet condition at $x = a$ (see attached codes). For this problem, I kept the same differential equation $u''(x) = e^x$ and kept the same boundary conditions (that is, same values at the boundaries, but the type of boundary condition has changed, obviously). So our new boundary value problem is

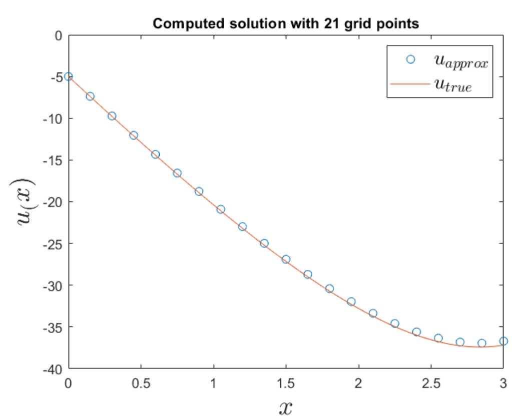
$$u''(x) = e^x, \quad u(0) = -5 \quad u'(3) = 3$$

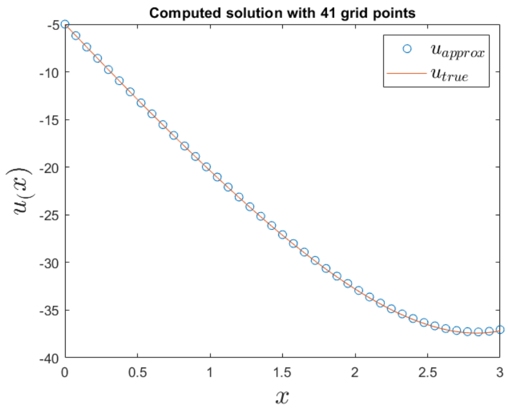
Which has an exact solution of

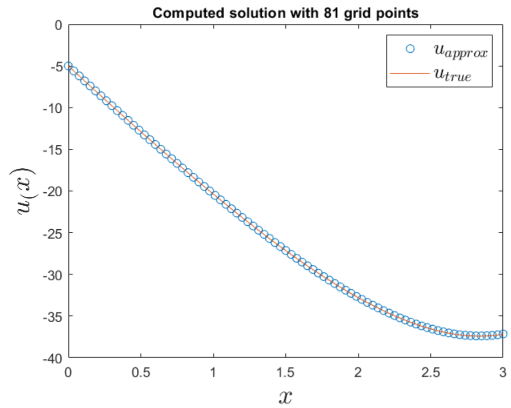
$$u(x) = e^x + (3 - e^3)x - 6$$

Running the code generates the following plots for the approximations of $u(x)$:

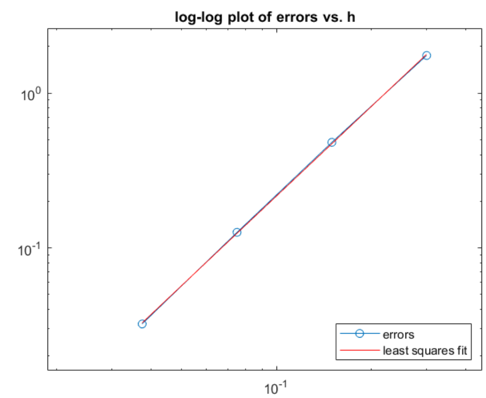








With the following plot and table of the errors:

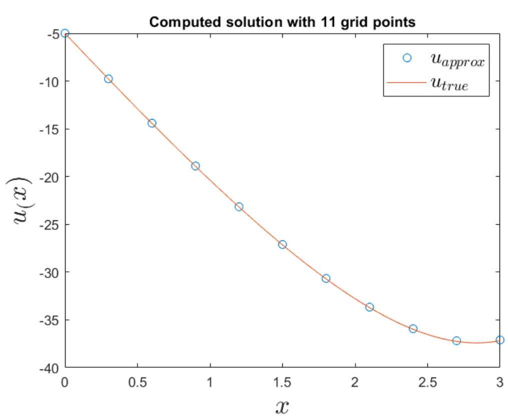


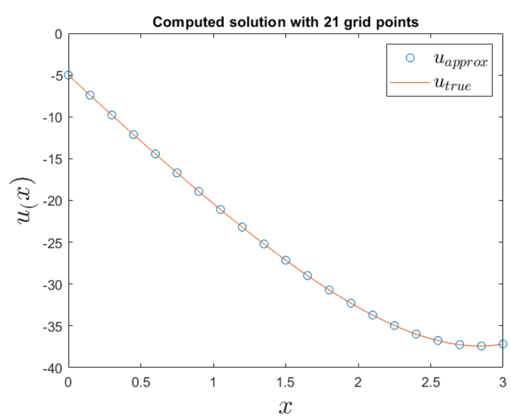

```
   h          error       ratio       observed order
0.30000   1.74886e+00       NaN                  NaN
0.15000   4.80811e-01   3.63732              1.86288
0.07500   1.26086e-01   3.81336              1.93106
0.03750   3.22858e-02   3.90531              1.96544

Least squares fit gives E(h) = 18.0049 * h^1.92092
```

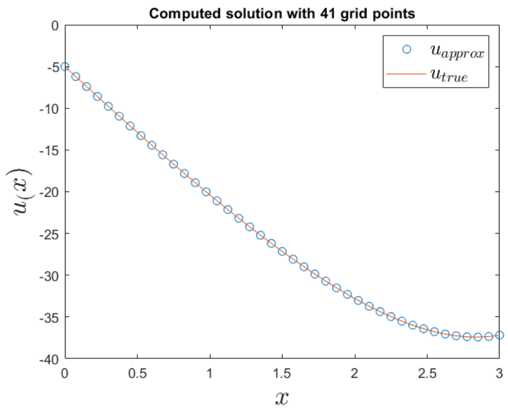
Which shows that the method is approximately $\mathcal{O}(h^2)$ for this problem, as we should expect from a second order method.

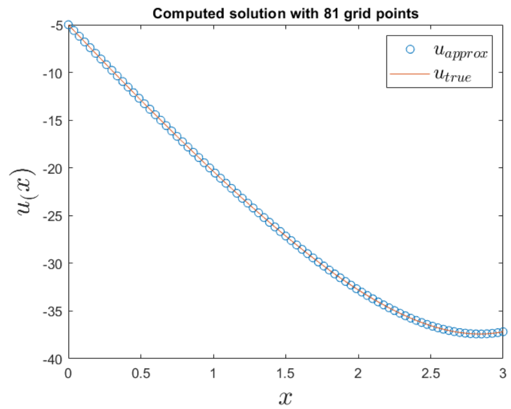
(b) Make the same modification to the m-file `bvp4.m`, which implements a fourth order accurate method. Again test the modified program.

Using the exact same process as in part (a), and utilizing the same boundary value problem, we find the following plots:

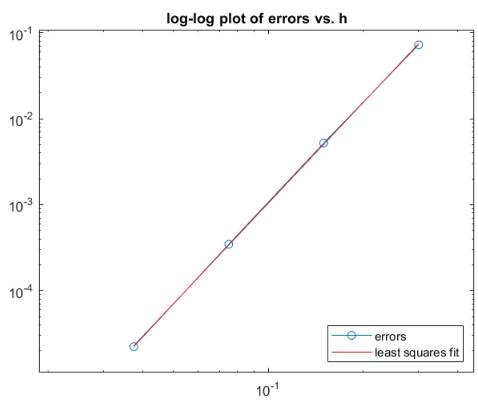








With the following plot and table for the errors:



h	error	ratio	observed order
0.30000	7.22610e-02	NaN	NaN
0.15000	5.21206e-03	13.86421	3.79329
0.07500	3.47061e-04	15.01768	3.90859
0.03750	2.23260e-05	15.54515	3.95839

```
Least squares fit gives E(h) = 8.04934 * h^3.88894
```

We can see that this is roughly of $\mathcal{O}(h^4)$ accuracy, which is also to be expected from a fourth order method.