Assignment 7.

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Due Friday, Feb. 16.

1. The conjugate gradient method for solving a symmetric positive definite linear system $Ax = b$ can be written as below:

> Given x_0, compute $r_0 = b - Ax_0$, and set $p_0 = r_0$.
> For $k = 1, 2, \ldots,$
> Compute Ap_{k-1}.
> Set $x_k = x_{k-1} + a_{k-1}p_{k-1}$, where $a_{k-1} = \frac{\langle r_{k-1}, r_{k-1}\rangle}{\langle p_{k-1}, Ap_{k-1}\rangle}$.
> Compute $r_k = r_{k-1} - a_{k-1}Ap_{k-1}$.
> Set $p_k = r_k + b_{k-1}p_{k-1}$, where $b_{k-1} = \frac{\langle r_k, r_k\rangle}{\langle r_{k-1}, r_{k-1}\rangle}$.
> Endfor

   (a) Show that the residual vectors $r_0, \ldots, r_k$ are orthogonal to each other ($\langle r_i, r_j\rangle = 0$ if $i \neq j$) and that the direction vectors $p_0, \ldots, p_k$ are A-orthogonal ($\langle p_i, Ap_j\rangle = 0$ if $i \neq j$). [Hint: First show that $\langle r_1, r_0\rangle = \langle p_1, Ap_0\rangle = 0$ and then use induction on k.]

   Solution:

$$\langle r_1, r_0\rangle = \langle r_0 - a_0 Ap_0, r_0\rangle = \langle r_0, r_0\rangle - \frac{\langle r_0, r_0\rangle}{\langle p_0, Ap_0\rangle}\langle Ap_0, r_0\rangle$$

$$r_0 = p_0$$

$$\langle r_1, r_0\rangle = \langle r_0, r_0\rangle - \langle r_0, r_0\rangle = 0$$

$$\langle p_1, Ap_0\rangle = \langle r_1 + b_0 p_0, Ap_0\rangle = \langle r_1, Ap_0\rangle + \langle b_0 p_0, Ap_0\rangle$$

$$= \langle r_1, Ap_0\rangle + \frac{1}{a_0}\langle r_1, r_1\rangle$$

$$= \langle r_1, Ap_0\rangle + \frac{1}{a_0}\langle r_1, r_0 - a_0 Ap_0\rangle$$

$$= \langle r_1, Ap_0\rangle + \frac{1}{a_0}\langle r_1, r_0\rangle - \langle r_1, Ap_0\rangle$$

$$= 0$$

Assume for j from 1 to k,

$$\langle r_j, r_{k+1}\rangle = 0, \langle p_j, Ap_{k+1}\rangle = 0$$

$$\langle r_{k+2}, r_{k+1}\rangle = \langle r_{k+1} - a_{k+1}Ap_{k+1}, r_{k+1}\rangle = \langle r_{k+1}, r_{k+1}\rangle - \frac{\langle r_{k+1}, r_{k+1}\rangle}{\langle p_{k+1}, Ap_{k+1}\rangle}\langle Ap_{k+1}, r_{k+1}\rangle$$

$$\begin{aligned}\langle r_{k+2}, r_{k+1}\rangle &= \langle r_{k+1}, r_{k+1}\rangle - \frac{\langle r_{k+1}, r_{k+1}\rangle}{\langle p_{k+1}, Ap_{k+1}\rangle}\langle Ap_{k+1}, p_{k+1}\rangle + \frac{\langle r_{k+1}, r_{k+1}\rangle}{\langle p_{k+1}, Ap_{k+1}\rangle}\langle Ap_{k+1}, b_k p_k\rangle \\ &= \langle r_{k+1}, r_{k+1}\rangle - \langle r_{k+1}, r_{k+1}\rangle + a_{k+1}b_k\langle Ap_{k+1}, p_k\rangle \\ &= 0\end{aligned}$$

For j from 1 to k,

$$\begin{aligned}\langle r_{k+2}, r_j\rangle &= \langle r_{k+1}, r_j\rangle - a_{k+1}\langle Ap_{k+1}, p_j\rangle + a_{k+1}b_k\langle Ap_{k+1}, b_k p_{j-1}\rangle \\ &= 0 + 0 + 0 = 0\end{aligned}$$

$$\begin{aligned}\langle p_{k+2}, Ap_{k+1}\rangle &= \langle r_{k+2}, Ap_{k+1}\rangle + b_{k+1}\langle p_{k+1}, Ap_{k+1}\rangle \\ &= \langle r_{k+2}, Ap_{k+1}\rangle + \frac{1}{a_{k+1}}\langle r_{k+2}, r_{k+2}\rangle \\ &= \frac{1}{a_{k+1}}\langle r_{k+2}, r_{k+1} - r_{k+2}\rangle + \frac{1}{a_{k+1}}\langle r_{k+2}, r_{k+2}\rangle \\ &= \frac{1}{a_{k+1}}\langle r_{k+2}, r_{k+1}\rangle - \frac{1}{a_{k+1}}\langle r_{k+2}, r_{k+2}\rangle + \frac{1}{a_{k+1}}\langle r_{k+2}, r_{k+2}\rangle \\ &= 0\end{aligned}$$

For j from 1 to k,

$$\begin{aligned}\langle p_{k+2}, Ap_j\rangle &= \langle r_{k+2}, Ap_j\rangle + b_{k+1}\langle p_{k+1}, Ap_j\rangle \\ &= \langle r_{k+2}, Ap_j\rangle + 0 \\ &= \frac{1}{a_j}\langle r_{k+2}, r_j - r_{j+1}\rangle \\ &= \frac{1}{a_{k+1}}\langle r_{k+2}, r_j\rangle - \frac{1}{a_j}\langle r_{k+2}, r_{j+1}\rangle \\ &= 0 + 0 = 0\end{aligned}$$

Since the induction step works, it is thus proved that all k+1 residual vectors are orthogonal.

(b) If A is the $N \times N$ matrix of the 5-point operator for Poisson's equation on a square, count the number of operations (additions, subtractions, multiplications, and divisions) performed in each iteration. (Show how you arrive at your result.)

Solution:

Multiplying one row of A with a vector is 5 multiplications and 4 additions. Thus, Ap takes 9 N operations. Similarly, an inner product takes $2N - 1 \approx 2N$ operations. Vector additions and scalar vector multiplication take N operations. a_{k-1} takes 4N but b_{k-1} takes 2N because one inner product has been done before.

$9N$	Compute Ap_{k-1}.
$6N = N + N + 4N$	Set $x_k = x_{k-1} + a_{k-1}p_{k-1}$, where $a_{k-1} = \frac{\langle r_{k-1}, r_{k-1}\rangle}{\langle p_{k-1}, Ap_{k-1}\rangle}$.
$2N$	Compute $r_k = r_{k-1} - a_{k-1}Ap_{k-1}$.
$4N = N + N + 2N$	Set $p_k = r_k + b_{k-1}p_{k-1}$, where $b_{k-1} = \frac{\langle r_k, r_k\rangle}{\langle r_{k-1}, r_{k-1}\rangle}$.

Thus, CG has a total of 21 N operations.

(c) Compare your operation count in (b) to that of a Gauss-Seidel iteration applied to the same N by N 5-point matrix A. Also compare to the operation count for a multigrid V-cycle, using one Gauss-Seidel iteration on each visit to each grid level. (Again, show how you derive your operation counts.)

Solution:

Gauss Seidel iteration:

$$u^{k+1} = M^{-1}Nu_k + M^{-1}f$$

M is lower triangular with diagonal terms. To find its inverse, we have to solve these equations, which I do with back substitution.

$$\begin{bmatrix} a & 0 & 0 & 0 \\ b & c & 0 & 0 \\ d & e & f & 0 \\ g & h & i & j \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix}$$

The first line would take 1 operation(division). The second line would take 3(2 divisions and 1 subtraction). The third line would be 5 operations. The fourth 7. The Nth would take 2N-1. So, totally, it would take N^2 operations (the sum of the first N odd numbers).

However if you have the lower triangular part of the Poisson matrix, the number of operations would in each line would 1,3,5,5,5,5,.... Thus, total number of operations needed would be 5N.

N has two elements on each row. So, Nu_k would be 3N operations. (2 multiplications and 1 addition on every line)

Thus, total number of operations needed for Gauss-Seidel would be 13 N ($M^{-1}Nu_k = 5N + 3N = 8N$ and $M^{-1}F = 5N$).

V-cycle:

- Going Down:
  Gauss Seidel :

$$13N + 13\frac{N}{4} + 13\frac{N}{16} + \ldots \approx 13\frac{4}{3}N = 17.33N$$

  Projection : Projection involves one multiplication in each row. So, N operations

$$N + \frac{N}{4} + \frac{N}{16} + \ldots \approx \frac{4}{3}N$$

- Bottom Level :
  Operations : c (Constant)
- Going Up: Gauss Seidel :

$$13N + 13\frac{N}{4} + 13\frac{N}{16} + \ldots \approx 13\frac{4}{3}N = 17.33N$$

  Interpolation : Projection involves two multiplications in each row. So, N operations

$$2N + \frac{2N}{4} + \frac{2N}{16} + \ldots \approx \frac{8}{3}N$$

- Final Step

$$x_k = x_{k-1} + e$$

  N operations.

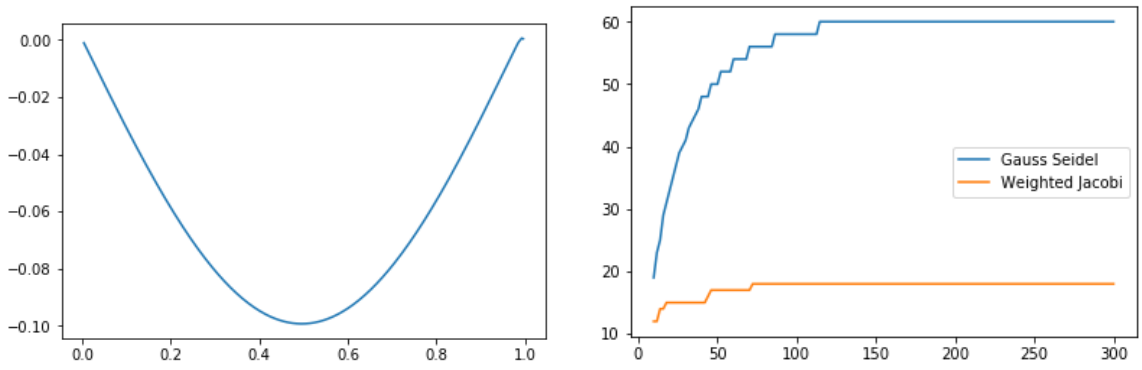
Total number of operations for a V-cycle = 38.66 N +c .

2. Implement a 2-grid method for solving the 1D model problem with homogeneous Dirichlet boundary conditions:

$$u_{xx} = f(x), \quad u(0) = u(1) = 0.$$

Use linear interpolation to go from the coarse grid with spacing $2h$ to the fine grid with spacing h. Take the projection matrix I_h^{2h}, going from the fine grid to the coarse grid, to be 0.5 times the transpose of the interpolation matrix: $I_h^{2h} = \frac{1}{2}(I_{2h}^h)^T$. Use a multigrid V-cycle with 1 smoothing step on each visit to each grid level. Try weighted Jacobi and Gauss-Seidel as the smoothing step. Try several different values of the mesh spacing h and show that you achieve convergence to a fixed tolerance in a number of cycles that is independent of the mesh size.

Solution:



(a) Solution (b) Iterations needed

Figure 1: $u_{xx} = \sin(\pi x)$

The number of cycles needed becomes independent of mesh size

```
import numpy as np
import scipy
import matplotlib.pyplot as plt

def pmatrix(n):
    #n internal points to n/2
    L = np.zeros((int(n/2),n))
    for i in range(int(n/2)):
        p = int(2*(i+1)-1)
        L[i,p]=1
    return L
def imatrix(n):
    #n/2 to n internal points
    L = np.zeros((n,int(n/2)))
    L[0,0] = 0.5
    for i in range(1,int(n/2)):
        a = 2*i-1
        b = i-1
        L[a,b]=1
        L[a+1,b]=0.5
        L[a+1,b+1]=0.5
    L[-1,-1]=1
    return L
n = 10

def jacobi_step(u,A,f):
    p = np.diag(A)
    M  = np.diag(p)
    invM = np.diag(1/p)
    N = M - A
    G = np.dot(invM,N)
```

```
    c = np.dot(invM,f)
    return np.dot(G,u)+c

def GS_step(u,A,f):
    M  = np.tril(A)
    #invM = np.diag(1/p)
    N = M - A
    G = scipy.linalg.solve(M,N)
    c = scipy.linalg.solve(M,f)
    return np.dot(G,u)+c

def weighted_step(u,A,f,w=2/3):
    u_n = jacobi_step(u,A,f)
    return (1-w)*u+w*u_n
def tridiag(a, b, c, k1=-1, k2=0, k3=1):
    return np.diag(a, k1) + np.diag(b, k2) + np.diag(c, k3)
def multigrid(f,x_0,smoother):
    n = len(f)
    h = 1/(n+1)
    A = makeA(n)
    A_c = makeA(int(n/2))
    pmat = pmatrix(n)
    imat = imatrix(n)
    x = x_0
    for i in range(100):
        #print(len(x))
        x = smoother(x,A,f)
        r = f - np.dot(A,x)
        r_c = np.dot(pmat,r)
        e_c = np.linalg.solve(A_c,r_c)
        e = np.dot(imat,e_c)
        x = x+e
        if np.linalg.norm(e, np.inf) < 0.001:
            #print(i)
            return x,i
    return x
n=70
x_0 = 2*np.ones(n)
x1 = np.linspace(0,1,n+2)

f = np.sin(np.pi*x1[1:-1])

def makeA(N):
    a = np.ones(N)
    b = np.ones(N-1)
    A = ((N+1)**2)*tridiag(b,-2*a,b)
    return A
```

```
g = []
for n in range(10,300,2):
        x_0 = 2*np.ones(n)
        x1 = np.linspace(0,1,n+2)
        f = np.sin(np.pi*x1[1:-1])
        g+= [multigrid(f,x_0,GS_step)[1]]

s = []
for n in range(10,300,2):
        x_0 = 2*np.ones(n)
        x1 = np.linspace(0,1,n+2)
        f = np.sin(np.pi*x1[1:-1])
        s+= [multigrid(f,x_0,weighted_step)[1]]


x = np.linspace(10,300,145)
plt.plot(x,g,label = 'Gauss Seidel')
plt.plot(x,s,label = 'Weighted Jacobi')
plt.legend()
```

3. (a) Consider an iteration of the form

$$x_k = x_{k-1} + M^{-1}(b - Ax_{k-1}),$$

for solving a nonsingular linear system $Ax = b$. Note that the error $e_k := A^{-1}b - x_k$ satisfies

$$e_k = (I - M^{-1}A)e_{k-1} = \ldots = (I - M^{-1}A)^k e_0.$$

Assume that $\|e_0\|_2 = 1$ and that $\|I - M^{-1}A\|_2 = \frac{1}{2}$. Estimate the number of iterations required to reduce the 2-norm of the error below 2^{-20}. Show how you obtain your estimate. Now suppose you know only that the spectral radius $\rho(I - M^{-1}A) = \frac{1}{2}$. Can you give an estimate of the number of iterations required to reduce the 2-norm of the error below 2^{-20}? Explain why or why not.

Solution:

If we know $\|I - M^{-1}A\|_2 = \frac{1}{2}$,

$$||e_k||_2 \leq \|I - M^{-1}A\|_2^k ||e_0||_2 \leq 2^{-k}.$$

To get the error below 2^{-20}, we need 20 iterations.

If $I - M^{-1}A$ is normal, then $\rho(I - M^{-1}A) = \|I - M^{-1}A\|_2$. So, we would only need 20.

If $I - M^{-1}A$ is diagonalizable with condition number κ

$$||e_k||_2 \leq \|I - M^{-1}A\|_2^k ||e_0||_2 \leq \kappa^k$$
$$\kappa^k = 2^{-20}$$

$$k\log(\kappa) = -20\log(2)$$
$$k = \frac{-20\log(2)}{\log(\kappa)}$$

Without the condition number, we cannot determine the bounds.

(b) Consider the GMRES algorithm applied to an n by n matrix A with the sparsity pattern pictured below:

$$\begin{bmatrix} * & * & \cdots & * & * \\ * & * & \cdots & * & 0 \\ 0 & * & \cdots & * & 0 \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & * & 0 \end{bmatrix},$$

where the $*$'s represent nonzero entries. Show that if the initial residual is the nth unit vector $(0, \ldots, 0, 1)^T$, then the algorithm makes no progress until step n. Show that a matrix with this sparsity pattern can have *any* eigenvalues. Conclude that eigenvalue information alone cannot be enough to ensure fast convergence of the GMRES algorithm.

Solution:

$$Ar_0 = \begin{bmatrix} * \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, A^2r_0 = \begin{bmatrix} * \\ * \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

For k = 1: n - 1

$$\langle r_0, A^k r_0 \rangle = 0$$
$$r_k = r_0 - AQy$$

The columns of Q span $[r_0, Ar_0, A^2r_0, \ldots]$.
The columns of AQ span $[Ar_0, A^2r_0, A^3r_0, \ldots]$.

$$r_k = r_0 - \sum_{i=1}^{k} y_i AQ$$
$$r_k = r_0 - \sum_{i=1}^{k} y_i c_i A^i r_0$$

We choose the y that minimizes $||r_k||_2$. For k from 1 to n-1, since r_0 is orthogonal to $A^i r_0$, the y vector is simply zero. Thus, for k from 1 to n-1,

$$r_k = r_0$$

The matrix

$$\begin{bmatrix} a & b & c \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

has the following characteristic polynomial.

$$-a\lambda^2 - b\lambda - c + \lambda^3$$

The matrix

$$\begin{bmatrix} a & b & c & d \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

has the following characteristic polynomial.

$$-a\lambda^3 - b\lambda^2 - c\lambda - d + \lambda^4$$

This patterns extends to bigger and bigger matrices. So, we can assume that it is general. This matrix follows the same sparsity layout as the matrix in the question. Thus, our matrix has the same characteristic polynomial. Since the coefficients of the polynomial can be any number, the eigenvalues can be any number.