Numerical Analysis (CS 450)

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Part 1: Use Arnoldi to solve linear systems → GMRES

(a) In the variant of the Arnoldi process shown in Algorithm 4.9 in the text, let Q_k be the matrix consisting of the first k columns of Q, and let H_k be the top-left $(k+1) \times k$ submatrix of H. Show that after q_{k+1} is added to Q in the algorithm, at iteration k, the identity $Q_{k+1}^T A Q_k = H_k$ holds. Does the 'reverse' identity $A = Q_{k+1} H_k Q_k^T$ hold as well?

Proof. From the line $h_{jk} = q_j^T u_k = q_j^T A q_k$ for $j = 1, 2, ..., k$. If $j = k+1$, then the algorithm says that

$$q_{k+1} = \frac{1}{h_{k+1,k}} \left(A q_k - \sum_{j=1}^{k} h_{jk} q_j \right).$$

Since q_i are all unit vectors, then

$$h_{k+1,k} = q_{k+1}^T \left(A q_k - \sum_{j=1}^{k} h_{jk} q_j \right) = q_{k+1}^T A q_k - \sum_{j=1}^{k} h_{jk} q_{k+1}^T q_j.$$

But since q_i are orthnormal, the terms in the sum vanish and this reduces to $h_{k+1,k} = q_{k+1}^T A q_k$. If $i > j+1$, then $h_{ij} = 0$ and $q_i^T A q_j = 0$ because $A q_j \in \text{span}\{q_0, ..., q_{j+1}\}$ and $q_i^T q_\ell = 0$ for all $\ell \leq j+1$. We conclude that $h_{ij} = q_i^T A q_j$ for all $j \leq k, i \leq k+1$. Thus, $H_k = Q_{k+1}^T A Q_k$.

The reverse identity does not hold generically since the rank of $Q_{k+1} H_k Q_k^T$ is at most $\text{rank}(Q_k) \leq k$ and the rank of A could be larger. □

(b) If $x_k \in K_k = \text{span}\{b, ..., A^{k-1} b\}$ is the vector that minimizes the residual $r_k = A x_k - b$ in the 2-norm and $x_k = Q_k y_k$, show that $\|r_k\|_2 = \|H_k y_k - \|b\|_2 e_1\|_2$.

Proof. First, by part (a), $H_k y_k = Q_{k+1}^T A Q_k y_k = Q_{k+1}^T A x_k$. In addition, $Q_{k+1}^T b = \|b\|_2 e_1$ since the columns of Q_k are orthogonal to b except for the first one which is b normalized. Thus,

$$\|H_k y_k - \|b\|_2 e_1\|_2 = \|Q_{k+1}^T A x_k - Q_{k+1}^T b\|_2 = \|Q_{k+1}^T (A x_k - b)\|_2 = \|A x_k - b\|_2 = \|r_k\|_2$$

since $Q_{k+1} Q_{k+1}^T = I$. □

(c) Describe a procedure to find x_k, using a linear least-squares problem with H_k as a building block.

Solution. Since x_k minimizes $\|r_k\|_2$, then if we can find y_k which minimizes $\|H_k y_k - \|b\|_2 e_1\|_2 = \|r_k\|_2$, x_k can be obtained by just multiplying Q_k to y_k. So, we solve the linear least squares problem $H_k y_k \approx \|b\|_2 e_1$ for y_k and let $x_k = Q_k y_k$. □

(d) See `my_gmres_d` in `gmres.py` for my code. Here is my function:

```
def my_gmres_d(A_func, b, tol=1e-10):
    """Solve Ax = b to an absolute residual norm of at most tol.

    Returns a tuple (x, num_iterations).

    Solution to Part 2(d) of the project assignment.
    """
    if la.norm(b) < tol:
        return 0 * b, 0
    if la.norm(A_func(b)) == 0:
        print "Warning: Krylov subspaces are trivial."
        return 0 * b, 0

    n = len(b)
    H = np.empty((1, 0))
    Q = np.empty((n, 1))
    Q[:, 0] = b / la.norm(b)
    x = b * np.dot(b, A_func(b)) / np.dot(A_func(b), A_func(b))
    y = np.empty((2, 1))
    vec = np.array([la.norm(b)])

    for k in xrange(n):
        print "performing iteration %d of GMRES..." % (k+1)
        H = np.column_stack((H, np.zeros(k + 1)))
        H = np.row_stack((H, np.zeros(k + 1)))
        u = A_func(Q[:, k])
        for j in xrange(k + 1):
            H[j, k] = np.dot(Q[:, j], u)
            u = u - H[j, k] * Q[:, j]
        H[k + 1, k] = la.norm(u)
        if H[k + 1, k] == 0:
            break
        Q = np.column_stack((Q, u / H[k + 1, k]))

        vec = np.append(vec, 0)
        y = la.lstsq(H, vec)[0]
        x = np.dot(Q[:, :-1], y)
        res = la.norm(b - A_func(x)) / la.norm(b)
        if res < tol:
            break

    if la.norm(b - A_func(x)) / la.norm(b) >= tol:
        print "Warning: tolerance was not met."
    return x, k + 1
```

Here's my output:

```
----------------------------------------
part(d)
----------------------------------------
converged after 13 iterations
residual: 6.63889e-11
error: 8.8999e-10
```

(e) See `my_gmres_e` in `gmres.py` for my code. Here is my function:

```
def my_gmres_e(A_func, b, tol=1e-10):
    """Solve Ax = b to an absolute residual norm of at most tol.

    Returns a tuple (x, num_iterations).

    Solution to Part 2(e) of the project assignment.
    """
    if la.norm(b) < tol:
        print "Solution is trivial."
        return 0 * b, 0
    if la.norm(A_func(b)) == 0:
        print "Warning: Krylov subspaces are trivial."
        return 0 * b, 0

    n = len(b)
    H = np.empty((1, 0))
    Q = np.empty((n, 1))
    Q[:, 0] = b / la.norm(b)
    x = b * np.dot(b, A_func(b)) / np.dot(A_func(b), A_func(b))
    givens = []
    y = np.empty((2, 1))
    R = np.empty((1, 0))
    vec = np.array([la.norm(b)])

    for k in xrange(n):
        print "performing iteration %d of GMRES..." % (k+1)
        H = np.column_stack((H, np.zeros(k + 1)))
        H = np.row_stack((H, np.zeros(k + 1)))
        u = A_func(Q[:, k])
        for j in xrange(k + 1):
            H[j, k] = np.dot(Q[:, j], u)
            u = u - H[j, k] * Q[:, j]
        H[k + 1, k] = la.norm(u)
        if H[k + 1, k] == 0:
            break
        Q = np.column_stack((Q, u / H[k + 1, k]))

        vec = np.append(vec, 0)
        R = np.row_stack((R, np.zeros(k)))
        R = np.column_stack((R, H[:, -1]))
        # Apply previous Givens rotations to new column of H
        for i in xrange(k):
            R[i:i + 2, -1] = np.dot(givens[i], R[i:i + 2, -1])
        [c, s] = R[-2:, -1] / la.norm(R[-2:, -1])
        givens.append(np.array([[c, s], [-s, c]]))
        R[-2:, -1] = np.dot(givens[k], R[-2:, -1])
        vec[-2:] = np.dot(givens[k], vec[-2:])
        y = sla.solve_triangular(R[:-1, :], vec[:-1])
        res = abs(vec[-1]) / la.norm(b)
        if res < tol:
            x = np.dot(Q[:, :-1], y)
            break

    if la.norm(b - A_func(x)) / la.norm(b) >= tol:
        print "Warning: tolerance was not met."
    return x, k + 1
```

Here is my output:

```
----------------------------------------
part(e)
----------------------------------------
converged after 13 iterations
residual: 1.65026e-11
error: 3.71017e-10
```

Part 2: Derive an integral equation for a second-order boundary value problem

(a) For any φ, show that if

$$u(x) = \tau(x)u_a + (1-\tau(x))u_b + \frac{1}{L}\left((b-x)\int_a^x \varphi(z)(a-z)\,dz + (a-x)\int_x^b \varphi(z)(b-z)\,dz\right),$$

$u(a) = u_a$ and $u(b) = u_b$, where $\tau(x) = 1-(x-a)/L$, $L = b-a$.

Proof. Simply compute.

$$u(a) = \tau(a)u_a + (1-\tau(a))u_b + \frac{1}{L}\left((b-a)\int_a^a \varphi(z)(a-z)\,dz + (a-a)\int_a^b \varphi(z)(b-z)\,dz\right)$$

$$= 1\cdot u_a + 0\cdot u_b + \frac{1}{L}\left(L\cdot 0 + 0\cdot\int_a^b \varphi(z)(b-z)\,dz\right) = u_a.$$

Similarly,

$$u(b) = \tau(b)u_a + (1-\tau(b))u_b + \frac{1}{L}\left((b-b)\int_a^b \varphi(z)(a-z)\,dz + (a-b)\int_b^b \varphi(z)(b-z)\,dz\right)$$

$$= 0\cdot u_a + 1\cdot u_b + \frac{1}{L}\left(0\cdot\int_a^b \varphi(z)(a-z)\,dz - L\cdot 0\right) = u_b.$$

□

(b) Show that

$$u'(x) = \frac{1}{L}\left(u_b - u_a - \int_a^x \varphi(z)(a-z)\,dz - \int_x^b \varphi(z)(b-z)\,dz\right).$$

Proof. Using the fact that $\tau'(x) = -\frac{1}{L}$ and the fundamental theorem of calculus combined with the chain rule, we obtain

$$u'(x) = -\frac{u_a}{L} + \frac{u_b}{L}$$
$$+\frac{1}{L}\left((-1)\int_a^x \varphi(z)(a-z)\,dz + (b-x)\varphi(x)(a-x) + (-1)\int_x^b \varphi(z)(b-z)\,dz - (a-x)\varphi(x)(b-x)\right)$$
$$= \frac{1}{L}\left(u_b - u_a - \int_a^x \varphi(z)(a-z)\,dz - \int_x^b \varphi(z)(b-z)\,dz\right).$$

□

(c) Show that $u''(x) = \varphi(x)$.

Proof. Using the previous result, we again apply the fundamental theorem of calculus and obtain

$$u''(x) = \frac{1}{L}\left(-\varphi(x)(a-x) + \varphi(x)(b-x)\right) = \frac{\varphi(x)(b-a)}{L} = \varphi(x).$$

□

(d) Show that if u satisfies $u'' + pu' + qu = r$, then φ satisfies the integral equation

$$\varphi(x) + \int_a^b K(x,z)\varphi(z)\,dz = R(x)$$

with the so-called 'kernel'

$$K(x,z) = \begin{cases} \frac{p(x)+(x-b)q(x)}{L}(z-a) & : z \le x \\ \frac{p(x)+(x-a)q(x)}{L}(z-b) & : z > x \end{cases}$$

and the right-hand side

$$R(x) = -\left(q(x)[\tau(x)u_a + (1-\tau(x))u_b] + \frac{p(x)}{L}(u_b - u_a) - r(x)\right).$$

Proof. Plugging u'', u', and u into the differential equation, we obtain

$$u''(x) + p(x)u'(x) + q(x)u(x) = \varphi(x) + \frac{p(x)}{L}\left(u_b - u_a - \int_a^x \varphi(z)(a-z)\,dz - \int_x^b \varphi(z)(b-z)\,dz\right)$$

$$+q(x)\tau(x)u_a + q(x)(1-\tau(x))u_b + \frac{q(x)}{L}\left((b-x)\int_a^x \varphi(z)(a-z)\,dz + (a-x)\int_x^b \varphi(z)(b-z)\,dz\right)$$

$$= \varphi(x) + \int_a^x \frac{p(x)+(x-b)q(x)}{L}(z-a)\varphi(x)\,dz + \int_x^b \frac{p(x)+(x-a)q(x)}{L}(z-b)\varphi(x)\,dz$$

$$+\left(q(x)[\tau(x)u_a + (1-\tau(x))u_b] + \frac{p(x)}{L}(u_b - u_a)\right)$$

$$= \varphi(x) + \int_a^b K(x,z)\varphi(z)\,dz + \left(q(x)[\tau(x)u_a + (1-\tau(x))u_b] + \frac{p(x)}{L}(u_b - u_a)\right) = r(x).$$

Thus, moving the third summand to the right hand side, we obtain

$$\varphi(x) + \int_a^b K(x,z)\varphi(z)\,dz = R(x).$$

□

Part 3: Build a BVP solver

(a) See `apply_kernel` in `bvp.py`. Here is my code:

```
def apply_kernel(a, b, mesh, kernel, density):
    def trapz(f, mesh):
        return np.dot((f[1:] + f[:-1]) / 2, mesh[1:] - mesh[:-1])

    temp = np.zeros(len(mesh))
    for i in xrange(len(mesh)):
        left = trapz(kernel(mesh[i], mesh[:i + 1], -1) * density[:i + 1], mesh[:i + 1])
        right = trapz(kernel(mesh[i], mesh[i:], +1) * density[i:], mesh[i:])
        temp[i] = left + right
    return temp
```

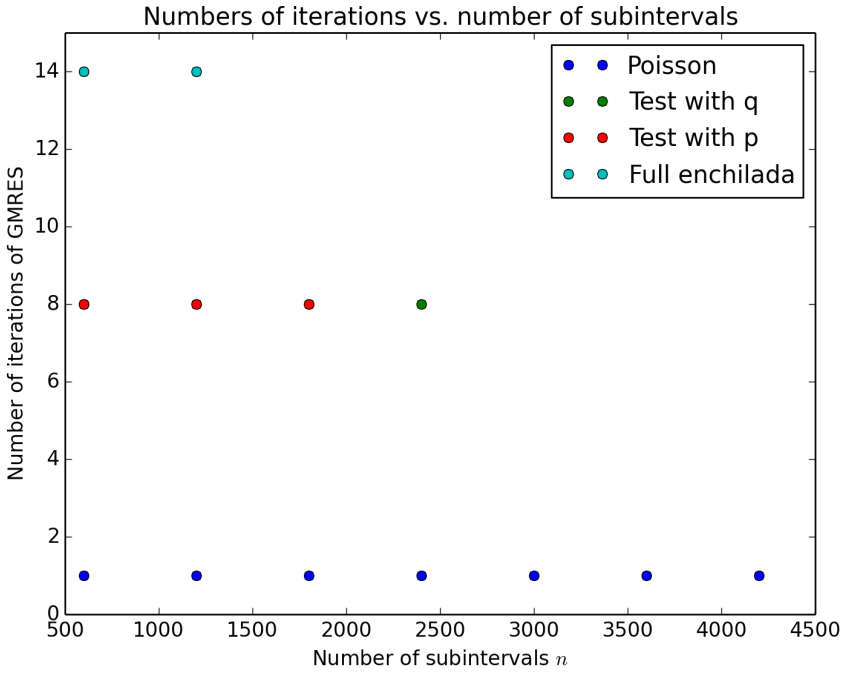
(b) See `solve_bvp` in `bvp.py`. Here is my code:

```
def solve_bvp(mesh, p, q, r, ua, ub):
    x = mesh
    a, b = mesh[0], mesh[-1]
    L = b - a

    def tau(x):
        return 1 - (x - a) / L

    def R(x):
        return -(q(x) * (tau(x) * ua + (1 - tau(x)) * ub) + p(x) * (ub - ua) / L - r(x))

    def K(x, z, sign):
        temp = np.empty(len(z))
        if sign == -1:
            temp[z <= x] = (p(x) + (x - b) * q(x)) * (z[z <= x] - a) / L
            temp[z > x] = (p(x) + (x - a) * q(x)) * (z[z > x] - b) / L
        if sign == +1:
            temp[z < x] = (p(x) + (x - b) * q(x)) * (z[z < x] - a) / L
            temp[z >= x] = (p(x) + (x - a) * q(x)) * (z[z >= x] - b) / L
        return temp

    def K2(x, z, sign):
        temp = np.empty(len(z))
        if sign == -1:
            temp[z <= x] = (x - b) * (z[z <= x] - a) / L
            temp[z > x] = (x - a) * (z[z > x] - b) / L
        if sign == +1:
            temp[z < x] = (x - b) * (z[z < x] - a) / L
            temp[z >= x] = (x - a) * (z[z >= x] - b) / L
        return temp

    def A_func(phi):
        return phi + apply_kernel(a, b, mesh, K, phi)

    phi, its = my_gmres_e(A_func, R(x))
    print "Solution found. For n = %d, GMRES took %g iteration(s)." % (len(x), its)
    print
    u = tau(x) * ua + (1 - tau(x)) * ub + apply_kernel(a, b, mesh, K2, phi)
    return u
```

(c) See `bvp.py` for my code. Here is the output upon running `test_bvp.py`.

```
h=0.0301003 err=0.270672
h=0.003001 err=0.00268591
test_poisson: EOC: 2.00074

h=0.0301003 err=0.426333
h=0.003001 err=0.00386274
test_with_p: EOC: 2.04019

h=0.0301003 err=2.07232
h=0.003001 err=0.0187981
test_with_q: EOC: 2.03968

h=0.0301003 err=0.332962
h=0.003001 err=0.00303815
test_full_enchilada: EOC: 2.03713
```

(d) See `test_bvp.py` for my code. I observe that the number of iterations it takes for GMRES to solve does not depend on the number of subintervals for each test. The test with q only shows up for one size n because it takes 8 iterations for both the test with p and the test with q. Here is my plot:



Part 4: A toolkit for composite high-order discretization

(a) See `__init__` in `legendre_discr.py`. Here is my code:

```
def __init__(self, intervals, order):
    self.intervals = intervals
    self.nintervals = len(intervals) - 1
    self.npoints = order + 1
    self.mid_pts = (self.intervals[1:] + self.intervals[:-1]) / 2
    self.scales = (self.intervals[1:] - self.intervals[:-1]) / 2
    self.sample_nodes = sp.legendre(self.npoints).weights[:, 0].real
    self.sample_weights = sp.legendre(self.npoints).weights[:, 1].real
    # taking real part because sometimes sp.legendre is returning
    # complex numbers with zero imaginary part and displaying a warning

    nodes = (self.mid_pts + np.outer(self.sample_nodes, self.scales)).T
    self.nodes = np.reshape(nodes, -1)
    weights = np.outer(self.scales, self.sample_weights)
    self.weights = np.reshape(weights, -1)

    monos = np.array([self.sample_nodes ** k for k in range(self.npoints)])
    integrals = np.array([(self.sample_nodes ** (k + 1) - (-1) ** (k + 1)) / (k + 1)
                          for k in range(self.npoints)])
    self.spec_int_mat = la.solve(monos, integrals)
```

(b) See `integral` in `legendre_discr.py`. Here is my code:

```
def integral(self, f):
    return np.dot(f, self.weights)
```

(c) See `left_indefinite_integral` and `right_indefinite_integral` in `legendre_discr.py`. Here is my code:

```
def left_indefinite_integral(self, f):
    d = self.npoints
    n = self.nintervals
    f = f.reshape((n, d))
    weights = self.weights.reshape((n, d))
    integrals = np.cumsum(np.einsum('ij,ij->i', f, weights))
    integrals = np.roll(integrals, 1)
    integrals[0] = 0
    indef = np.dot((f.T * self.scales).T, self.spec_int_mat)
    indef = (integrals + indef.T).T
    indef = np.reshape(indef, -1)
    return indef

def right_indefinite_integral(self, f):
    return self.integral(f) - self.left_indefinite_integral(f)
```

(d) Upon running `test_legendre_discr.py`, here is the output.

```
 ---------------------------------
 ORDER 2
---------------------------------
 h=0.1 err=0.118027
 h=0.0333333 err=0.00168249
 <lambda>: EOC: 3.8691

 h=0.1 err=0.141862
 h=0.0333333 err=0.0016825
 <lambda>: EOC: 4.03652

---------------------------------
 ORDER 3
---------------------------------
 h=0.1 err=0.0455367
 h=0.0333333 err=0.000125478
 <lambda>: EOC: 5.36508

 h=0.1 err=0.0456416
 h=0.0333333 err=0.000125478
 <lambda>: EOC: 5.36718

---------------------------------
 ORDER 5
---------------------------------
 h=0.1 err=0.00221849
 h=0.0333333 err=5.46588e-07
 <lambda>: EOC: 7.56285

 h=0.1 err=0.00221849
 h=0.0333333 err=5.46588e-07
 <lambda>: EOC: 7.56285

---------------------------------
 ORDER 7
---------------------------------
 h=0.1 err=6.48553e-05
 h=0.0333333 err=1.47309e-09
 <lambda>: EOC: 9.73278

 h=0.1 err=6.48553e-05
 h=0.0333333 err=1.47309e-09
 <lambda>: EOC: 9.73278
```

Part 5: Build a fast and accurate BVP solver

(a) See `fast_bvp.py`. The code for my `apply_kernel` function is:

```
def apply_kernel(discr, fl, gl, fr, gr, density):
    """
    :arg discr: an instance of
        :class:`legendre_discr.CompositeLegendreDiscretization`
    :arg fl,gl,fr,gr: functions of a single argument
    """
    x = discr.nodes
    Gl = discr.left_indefinite_integral(gl(x) * density)
    Gr = discr.right_indefinite_integral(gr(x) * density)
    result = fl(x) * Gl + fr(x) * Gr
    return result
```

(b) See `fast_bvp.py`. The code for my `solve_bvp` function is:

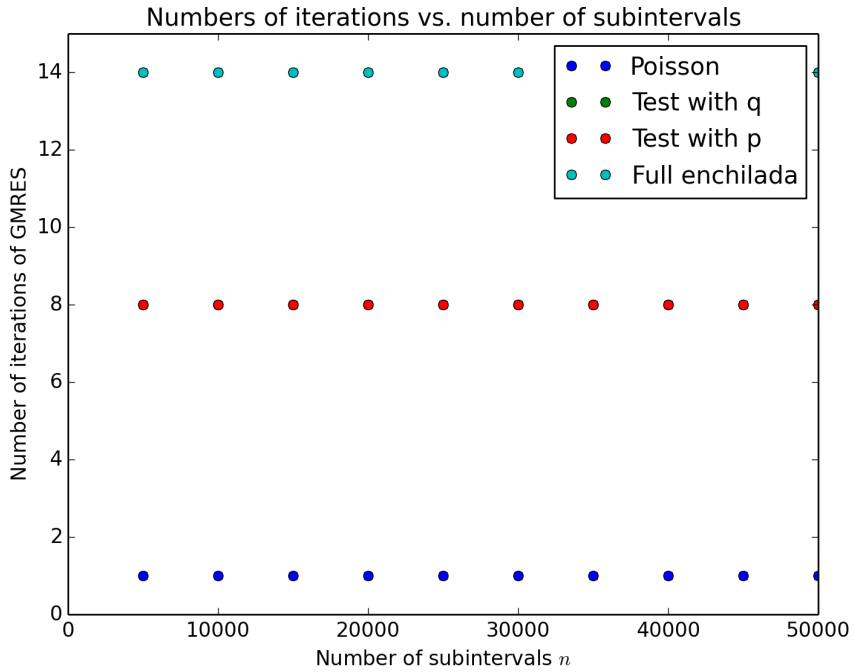
```
def solve_bvp(discr, p, q, r, ua, ub):
    """
    :arg discr: an instance of
        :class:`legendre_discr.CompositeLegendreDiscretization`
    """
    a, b = discr.intervals[0], discr.intervals[-1]
    L = b - a

    def tau(x):
        return 1 - (x - a) / L

    def R(x):
        return -(q(x) * (tau(x) * ua + (1 - tau(x)) * ub) + p(x) * (ub - ua) / L - r(x))

    def fl(x):
        return (p(x) + (x - b) * q(x)) / L

    def fr(x):
        return (p(x) + (x - a) * q(x)) / L

    def gl(x):
        return x - a

    def gr(x):
        return x - b

    def fl2(x):
        return (x - b) / L

    def fr2(x):
        return (x - a) / L

    def A_func(phi):
        return phi + apply_kernel(discr, fl, gl, fr, gr, phi)

    x = discr.nodes
    phi, its = my_gmres_e(A_func, R(x))
    u = tau(x) * ua + (1 - tau(x)) * ub + apply_kernel(discr, fl2, gl, fr2, gr, phi)

    return u
```

(c) Upon running `test_fast_bvp.py`, my output was:

```
-----------------------------------------------
test_poisson -- order 3
-----------------------------------------------
h=0.02 err=0.00426799
h=0.01 err=0.000129103
get_error: EOC: 5.04697

-----------------------------------------------
test_poisson -- order 5
-----------------------------------------------
h=0.02 err=8.76324e-06
h=0.01 err=6.4139e-08
get_error: EOC: 7.09412

-----------------------------------------------
test_poisson -- order 7
-----------------------------------------------
h=0.02 err=9.53116e-09
h=0.01 err=1.69574e-11
get_error: EOC: 9.13459

-----------------------------------------------
test_with_p -- order 3
-----------------------------------------------
h=0.02 err=1.41895
h=0.01 err=0.0745256
get_error: EOC: 4.25095

-----------------------------------------------
test_with_p -- order 5
-----------------------------------------------
h=0.02 err=0.203782
h=0.01 err=0.00295016
get_error: EOC: 6.11008

-----------------------------------------------
test_with_p -- order 7
-----------------------------------------------
h=0.02 err=0.018239
h=0.01 err=6.41014e-05
get_error: EOC: 8.15245

-----------------------------------------------
test_with_q -- order 3
-----------------------------------------------
h=0.02 err=3.6688
h=0.01 err=0.0760487
get_error: EOC: 5.59224

-----------------------------------------------
test_with_q -- order 5
-----------------------------------------------
```

```
h=0.02 err=0.204061
h=0.01 err=0.00295022
get_error: EOC: 6.11203

---------------------------------------------
test_with_q -- order 7
---------------------------------------------
h=0.02 err=0.0182281
h=0.01 err=6.41023e-05
get_error: EOC: 8.15157

---------------------------------------------
test_full_enchilada -- order 3
---------------------------------------------
h=0.02 err=1.43841
h=0.01 err=0.0744792
get_error: EOC: 4.2715

---------------------------------------------
test_full_enchilada -- order 5
---------------------------------------------
h=0.02 err=0.203789
h=0.01 err=0.00295022
get_error: EOC: 6.11011

---------------------------------------------
test_full_enchilada -- order 7
---------------------------------------------
h=0.02 err=0.0182401
h=0.01 err=6.41023e-05
get_error: EOC: 8.15252
```

(d) Each time GMRES runs, my code outputs the number of iterations. It appears that for a fixed test, the number of iterations it takes to converge does not depend on the matrix size. Here is my plot:



(e) See `timing.py` for my code. Here is a graph of my results for numbers of subintervals $n = 2^9, ..., 2^{20}$. After finding the best fit linear relationship between $\log(t)$ and $\log(n)$ I obtain $t \propto n^{1.04489}$, so the algorithm runs in approximately linear time.