Numerical Analysis (CS 450)

Homework Set 3, Bill Karr

Problem 1: QR iteration with Shifts (11 points)

See `cs450hw3p1.py` for my code. My results were:

```
Matrix =
[[ 2  3  2]
 [10  3  4]
 [ 3  6  1]]
Computed eigenvalues:  [ 11.  -3.  -2.]
Actual eigenvalues:  [ 11.  -2.  -3.]
Matrix =
[[6 2 1]
 [2 3 1]
 [1 1 1]]
Computed eigenvalues:  [ 7.28799214  2.13307448  0.57893339]
Actual eigenvalues:  [ 7.28799214  2.13307448  0.57893339]
```

Problem 2: Lanczos Iteration and Convergence of Ritz Values (31 points)

(a) Prove that, in the case of A symmetric and real-valued, Arnoldi iteration reduces to Lanczos iteration.

Proof. We know that both iterations output matrices H and Q, given A, where H is in upper Hessenberg form, Q is an orthogonal matrix, and $H = Q^T AQ$.

However, notice that $H^T = (Q^T AQ)^T = Q^T A^T (Q^T)^T = Q^T AQ = H$. Thus, H is symmetric.

In addition, since H is upper Hessenberg and symmetric, the entries above the first super-diagonal are zeros since the entries below the first sub-diagonal are zeros.

Finally, since the entries above the first super-diagonal are zero, then the j loop in Arnoldi iteration, as show in Algorithm 4.9 in the book, is trivial except when $j = k - 1$ and $j = k$ since $h_{jk} = 0$ whenever $|j - k| > 1$. Hence, only two iterations are needed in the j loop.

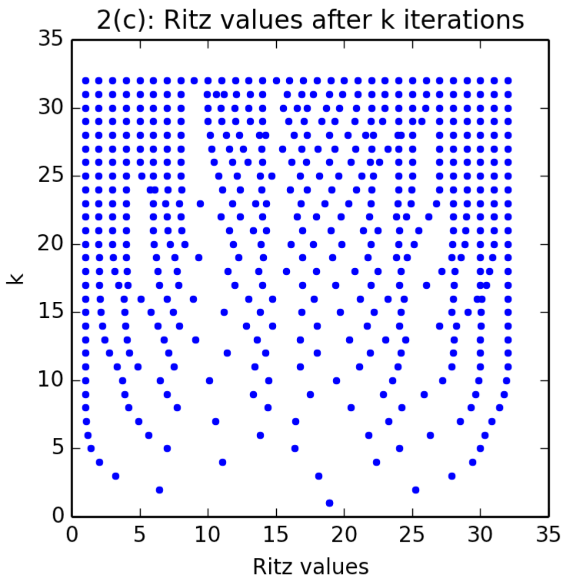
This is exactly what the Lanczos algorithm produces, so Arnoldi reduces to Lanczos when A is symmetric. □

(b) See `cs450hw3p2.py` for my code. My results were:

```
size(A) = 25 by 25
|QQ.T - I| = 7.21487455622e-07
|Q.T*A*Q - H|/|A| = 3.02974383378e-07
```

It's worth noting that these errors are not very small even though A is only a 25 by 25 matrix, demonstrating the numerical instability of Lanczos iteration.

(c) See `cs450hw3p2.py` for my code. See the figure below for the plots of the Ritz values.



Problem 3: Reduction to Hessenberg form (25 points)

(a) Let $A \in \mathbb{R}^{n\times n}$ be a matrix. Also, let H be a Householder reflector designed to annihilate rows $3, ..., n$ of the first column of A.

Show that the matrix $B = HAH^T$ has the form

$$B = \begin{pmatrix} * & * & \cdots & * \\ * & * & \cdots & * \\ 0 & * & \cdots & * \\ \vdots & \vdots & \ddots & \vdots \\ 0 & * & \cdots & * \end{pmatrix} \tag{1}$$

i.e. it has zeros below the second diagonal of the first column. You may assume that HA has the non-zero pattern in (1).

Proof. The vector v used to compute the Householder transformation is of the form

$$v = \begin{pmatrix} 0 \\ 0 \\ * \\ \vdots \\ * \end{pmatrix}.$$

Thus, $H = I - 2\frac{vv^T}{v^Tv}$ is of the form

$$H = \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & 0 \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & * & \cdots & * \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & * & \cdots & * \end{pmatrix}$$

Furthermore, since $H^T = H$ and HA is of the form in (1), we use matrix multiplication and find that HAH^T is of the form

$$HAH^T = (HA)H = \begin{pmatrix} * & * & * & \cdots & * \\ * & * & * & \cdots & * \\ 0 & * & * & \cdots & * \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & * & * & \cdots & * \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & * & \cdots & * \end{pmatrix} = \begin{pmatrix} * & * & * & \cdots & * \\ * & * & * & \cdots & * \\ 0 & * & * & \cdots & * \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & * & * & \cdots & * \end{pmatrix}$$

This completes the proof. □

(b) See `cs450hw3p3.py` for my code.

(c) See `cs450hw3p3.py` for my code. My results were

```
|Q.T*U*Q - A|/|A| = 6.53919429383e-16
```

(d) See `cs450hw3p3.py` for my code. My results were

```
|Q.T*U*Q - A|/|A| = 8.03225086772e-16
|QQ.T - I| = 1.5667118603e-15 <-- when this is small, Q is orthogonal
|U.T - U|/|U| = 7.97339107923e-17 <-- when this is small, U is symmetric
```

Thus, U is upper Hessenberg, but it is also symmetric and therefore also in "lower Hessenberg" form. It's a tridiagonal symmetric matrix.

Problem 4: Newton's method in 1D (18 points)

(a) Newton's method for solve a scalar nonlinear equation $f(x) = 0$ requires computation of the derivative of f at each iteration. Suppose that we instead replace the true derivative with a constant value d, that is, we use the iteration scheme:

$$x_{k+1} = x_k - f(x_k)/d.$$

(i) Under what conditions on the value of d will this scheme be locally convergent.

Solution. By Taylor's theorem, we can approximate f near the root x^* so that for small ε, we have

$$f(x^* + \varepsilon) = f'(x^*)\varepsilon + O(\varepsilon^2).$$

Thus,

$$x_{k+1} - x^* = x_k - x^* - \frac{f'(x^*)(x_k - x^*) + O((x_k - x^*)^2)}{d}$$

$$\Rightarrow e_{k+1} = e_k \left(1 - \frac{f'(x^*)}{d}\right) + O(e_k^2) \Rightarrow \left|\frac{e_{k+1}}{e_k}\right| = \left|1 - \frac{f'(x^*)}{d} + O(e_k)\right|$$

In order to converge locally we must have, $\left|1 - \frac{f'(x^*)}{d}\right| < 1$ so $0 < \frac{f'(x^*)}{d} < 2$ or equvalently $\frac{d}{f'(x^*)} > \frac{1}{2}$. Thus, d must have the same sign as the derivative at the root $f'(x^*)$ and it cannot be too small relative to the derivative. □

(ii) What will be the convergence rate in general?

Solution. By the above, we have

$$\frac{|e_{k+1}|}{|e_k|} \approx \left|1 - \frac{f'(x^*)}{d}\right| + O(|e_k|),$$

so in general, this method should have a linear convergence rate. □

(iii) Is there any value of d that would still yield quadratic convergence?

Solution. Notice that if the linear convergence rate $\left|1 - \frac{f'(x^*)}{d}\right|$ is zero, then we actually have quadratic convergence. This happens exactly when $d = f'(x^*) \neq 0$. So, we d is the derivative of f at the root and the root is order 1, then this method yields quadratic convergence, locally. □

(b) See `cs450hw3p4.py` for my code. My code prints out a list of r values, one computed at each iteration. The last few r values printed should show the true r value. I used the following formula for r at each iteration:

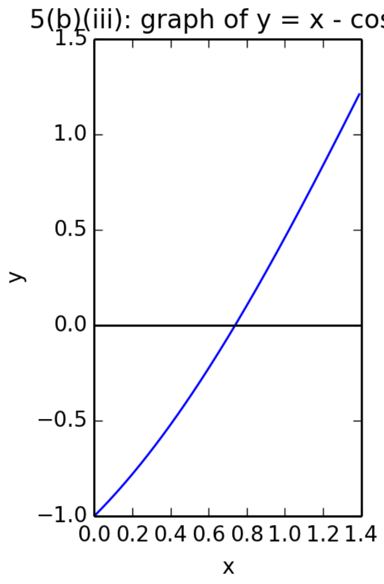
$$r = \frac{\log(e_{k+1}/e_k)}{\log(e_k/e_{k-1})}$$

where $e_k = |x_k - x^*|$.

(i) For $f(x) = x^2 - 1$, the observed convergence rate is quadratic, i.e. $r = 2$. The reason is because the root it's converging to is $x^* = 1$ which has multiplicity 1. Thus, Newton's method has quadratic convergence.

(ii) For $f(x) = (x-1)^4$, the observed convergence rate is linear, i.e. $r = 1$. This is because it is converging to $x* = 1$ which has multiplicity 4 which is larger than 1. Thus, Newton's method has linear convergence in this case.

(iii) For $f(x) = x - \cos(x)$, the observed convergence rate is quadratic, i.e. $r = 2$. The reason is because the root it's converging to has multiplicity 1 since $f'(x*) = 1 - \sin(x^*) = 1 \mp \sqrt{1-(x^*)^2} \neq 0$. You can easily see this if you plot the graph of $f(x) = x - \cos(x)$. Thus, Newton's method has quadratic convergence.



Problem 5: Newton's method for a system (15 points)

(a) See `cs450hw3p5.py` for my code.

(b) See `cs450hw3p5.py` for my code.

(c) See `cs450hw3p5.py` for my code.

The relative error is not necessarily small when the relative residual is small. This is because, given a vector in Cartesian coordinates, there are multiple ways to represent the point in spherical coordinates and Newton's method doesn't always converge to the "standard" spherical coordinates; it is only guaranteed to converge to a set of numbers (r, θ, φ) that satisfy $f(r, \theta, \varphi) = 0$ which has infinitely many solutions. For example, if you shift θ by a multiple of 2π or if you shift φ by a multiple of π, you will not change the Cartesian point represented.

Here are my results as printed from my code:

```
Trial 1

Number of iterations of Newton's method: 7
Cartesian vector = [ 0.47298583 -0.68142588  0.2424395 ]

Output using Newton's method = [-0.86419543  1.85515071  2.17755962]
 True spherical coordinates  = [ 0.86419543  2.47917726 -0.96403303]

relative residual = 2.89055198425e-16
relative error = 1.30129251914

Trial 2

Number of iterations of Newton's method: 10
Cartesian vector = [-1.70073563  0.75314283 -1.53472134]

Output using Newton's method = [ -2.41145089   0.88093441 -31.8328049 ]
 True spherical coordinates  = [ 2.41145089  1.25316277  2.72471429]

relative residual = 6.70347104211e-16
relative error = 9.06744023065

Trial 3

Number of iterations of Newton's method: 6
Cartesian vector = [ 0.00512708 -0.12022767 -0.80698188]

Output using Newton's method = [ 0.81590485 -2.99356369  1.61341525]
 True spherical coordinates  = [ 0.81590485  1.71868988 -1.52817741]

relative residual = 4.17291477464e-16
relative error = 2.32083829101

Trial 4

Number of iterations of Newton's method: 9
Cartesian vector = [ 2.87181939 -0.59782292  0.47245699]

Output using Newton's method = [ 2.97118739  1.41110562 -6.48842291]
 True spherical coordinates  = [ 2.97118739  1.77338602 -0.2052376 ]

relative residual = 2.17881143295e-16
relative error = 1.81567932411

Trial 5

Number of iterations of Newton's method: 10
Cartesian vector = [ 1.09595612 -1.2151688   1.34235637]
```

```
Output using Newton's method = [ 2.11652443  0.88378837 -0.83693459]
 True spherical coordinates  = [ 2.11652443  2.18234248 -0.83693459]

relative residual = 1.48365162969e-16
relative error = 0.411819309513

Trial 6

Number of iterations of Newton's method: 6
Cartesian vector = [-0.12214979  1.01251548 -0.91386915]

Output using Newton's method = [ 1.36940315  2.30143914  1.69085604]
 True spherical coordinates  = [ 1.36940315  0.73864059  1.69085604]

relative residual = 1.67137296585e-16
relative error = 0.680130495471

Trial 7

Number of iterations of Newton's method: 6
Cartesian vector = [-1.02953021  1.20979645  0.5018723 ]

Output using Newton's method = [ 1.66595789  1.26479148  2.27586751]
 True spherical coordinates  = [ 1.66595789  0.7580374   2.27586751]

relative residual = 1.88491253438e-16
relative error = 0.173513265511

Trial 8

Number of iterations of Newton's method: 5
Cartesian vector = [ 0.13884618  0.64076111  0.52733267]

Output using Newton's method = [ 0.84138743  0.89343152  1.35740592]
 True spherical coordinates  = [ 0.84138743  0.70509036  1.35740592]

relative residual = 6.26794132391e-13
relative error = 0.107885648614

Trial 9

Number of iterations of Newton's method: 28
Cartesian vector = [-1.15436024 -2.21333348 -1.68175651]

Output using Newton's method = [ -3.00993316  55.57073176 -14.61790418]
 True spherical coordinates  = [ 3.00993316  2.3969691  -2.05153357]

relative residual = 1.13328561435e-15
relative error = 12.6061490462

Trial 10

Number of iterations of Newton's method: 20
```

```
Cartesian vector = [-1.78809425 -2.21853495 -0.64743078]

Output using Newton's method = [ 2.92204466  4.48896712  0.89241981]
 True spherical coordinates  = [ 2.92204466  2.4329418  -2.24917284]

relative residual = 4.5524744551e-14
relative error = 0.849888371936
```