In [1]:
```
%matplotlib notebook
from matplotlib.pylab import *

from numpy import *
```

Homework #8

This homework will cover issues related to numerical errors that arise when solving $A\mathbf{x} = \mathbf{b}$. In particular, you will look at how the error, residual and condition number are related.

For this homework, you will use standard solvers available in NumPy/SciPy for solving linear systems. The codes below essentially show you how to do this.

Problem #1

Let A be a square, nonsingular matrix, and let $||A||$ be an induced matrix norm on a vector p-norm. Show that

$$\frac{||\mathbf{x}||}{||A\mathbf{x}||} \leq ||A^{-1}|| \tag{1}$$

Solution

Since $||A||$ is an induced matrix norm on a vector p-norm, then the inequality below holds;

$$||A\mathbf{x}|| \leq ||A||\,||\mathbf{x}|| \tag{2}$$
$$\Rightarrow \frac{||A\mathbf{x}||}{||\mathbf{x}||} \leq ||A|| \tag{3}$$

Taking the inverse of the above equation, we get;

$$\frac{||\mathbf{x}||}{||A\mathbf{x}||} \leq ||A||^{-1} \tag{4}$$

But for a square, nonsingular matrix A, $||A||^{-1} = ||A^{-1}||$

$$\therefore \frac{||\mathbf{x}||}{||A\mathbf{x}||} \leq ||A^{-1}|| \tag{5}$$

Problem #2

Show that for square, non-singular matrices

$$\kappa(A) = \|A\|\|A^{-1}\| \geq 1 \tag{6}$$

Hint: Let $\mathbf{b} = A\mathbf{x}$ for some $\mathbf{x}$. Then show that $\|A\mathbf{x}\| \leq \kappa(A)\|\mathbf{b}\|$.

Solution (Try using the hint)

Since A is a square, nonsingular matrix and $\|A\|$ is an induced matrix norm on a vector p-norm, then the inequality below holds;

$$\begin{aligned} \|A^{-1}A\| &\leq \|A^{-1}\|\|A\| && (7)\\ &\leq \|A\|\|A^{-1}\| && (8)\\ \Rightarrow \kappa(A) = \|A\|\|A^{-1}\| &\geq \|A^{-1}A\| && (9) \end{aligned}$$

But $\|\|A^{-1}A\| = \|I\| = 1$

$$\begin{aligned} \Rightarrow \kappa(A) = \|A\|\|A^{-1}\| &\geq \|I\| && (10)\\ \therefore \kappa(A) = \|A\|\|A^{-1}\| &\geq 1 && (11) \end{aligned}$$

Problem #3

When solving a linear system $A\mathbf{x} = \mathbf{b}$, the error in the numerical solution (arising from round-off error or catastrophic cancellation) and the residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$ are related through the condition number $\kappa(A)$ of A.

The goal of this problem is to investigate how the error in solving a linear system, the residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$ and the condition number $\kappa(A)$ of A are related.

Error and residual

Let $\overline{\mathbf{x}}$ be the exact solution to the $A\mathbf{x} = \mathbf{b}$ problem in exact arithmetic, and let $\mathbf{x}$ be a numerical solution computed using some numerical algorithm (e.g. QR or Gaussian Elimination).

We can then define the *error* and *residual* in solving the system $A\mathbf{x} = \mathbf{b}$ as

- The error is defined as $\mathbf{e} = \overline{\mathbf{x}} - \mathbf{x}$.
- The residual is defined as $\mathbf{r} = \mathbf{b} - A\mathbf{x}$.

We can relate the error to the residual as follows

$$A\mathbf{e} = A\left(\bar{\mathbf{x}} - \mathbf{x}\right) = A\bar{\mathbf{x}} - A\mathbf{x} = \mathbf{b} - A\mathbf{x} = \mathbf{r} \tag{12}$$

so that $A\mathbf{e} = \mathbf{r}$ is a new problem we can solve (in theory) for the error $\mathbf{e}$. We will use this equation to relate $\mathbf{e}$, $\mathbf{r}$ and the condition number $\kappa(A)$ of A.

NOTE: In this problem, we use N to define the size of square matrix A, instead of using m.

Problem 3(a)

Use the equation $A\mathbf{e} = \mathbf{r}$ to show that

$$\frac{||\mathbf{e}||}{||\mathbf{x}||} \leq \kappa(A)\frac{||\mathbf{r}||}{||\mathbf{b}||} \tag{13}$$

where $\kappa(A) = ||A||||A^{-1}||$. Assume that the matrix norm $||A||$ is induced from a vector p-norm.

This inequality provides a crucial connection between the error in solving linear systems and the conditioning of the system. Many numerical methods aim to make the *residual* $\mathbf{r}$ as small as possible, but this inequality above demonstrates that a small residual can only reliably lead to a small error if the condition number of the linear system is small.

Solution

Suppose A is a square non singular, then $\mathbf{e} = A^{-1}\mathbf{r}$ and this implies that $||e|| = ||A^{-1}\mathbf{r}||$.

Using consistency of the induced norm, the inequality below holds;

$$\begin{align} ||A^{-1}r|| \leq ||A^{-1}||||r|| \tag{14} \\ \tag{15} \\ \Rightarrow ||e|| \leq ||A^{-1}||||r|| \qquad (1) \tag{16} \end{align}$$

Similary, for the linear system $\mathbf{b} = A\mathbf{x}$ we have that;

$$\begin{align} ||b|| \leq ||A||||\mathbf{x}|| \tag{17} \\ \tag{18} \\ \Rightarrow \frac{1}{||\mathbf{x}||} \leq ||A||\frac{1}{||\mathbf{b}||} \qquad (2) \tag{19} \end{align}$$

Combining equations (1) and (2), we get;

$$\begin{align} \frac{||e||}{||\mathbf{x}||} \leq ||A||||A^{-1}||\frac{||r||}{||\mathbf{b}||} \tag{20} \\ \tag{21} \\ \therefore \frac{||\mathbf{e}||}{||\mathbf{x}||} \leq \kappa(A)\frac{||\mathbf{r}||}{||\mathbf{b}||} \tag{22} \end{align}$$

Problem 3(b)

A matrix that arises often in numerical methods is the matrix

$$A = \begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix} \tag{23}$$

This is a banded matrix with three diagonal "bands". Entries in the lower and upper bands are all 1s, and the main diagonal is all -2s. This is an example of a *tridiagonal* matrix.

We will use this matrix to investigate the relationship between error and condition number you established in **3(a)**.

Tasks

1. Use Numpy to compute the condition number $\kappa(A)$ for the matrix A above for a range of N values. Store these values in vectors `Nv_data` and `kv_data`. *(This step is already done for you in code below)*

2. Use the data you computed above and stored in `Nv_data` and `kv_data` to estimate parameters p and C for the model

$$\kappa(A) \approx CN^p. \tag{24}$$

   Use a QR decomposition to solve the resulting least squares system. **Note:** Do not use any other fitting routines available in NumPy or SciPy. You may, however, use the NumPy `qr` routine, rather than your own routine.

   Hint: Take the log of both sides of the model equation and use QR to solve a linear least squares problem for $\log(C)$ and p.

1. Plot the condition number data computed using Numpy, along with your model equation based on parameters C and p you found above. Plot your model equation over the range $N = N_0 2^p$, $N_0 = 8$ and $p = 0, 1, 2, \ldots 14$. **Hint:** Use a loglog plot.

2. In a legend, show the model parameter p that relates $\kappa(A)$ to N.

Question

How does the condition number for this matrix increase with N? Give an example of a matrix whose condition number does not increase with N.

In [2]:
```python
def set_xticks(P):
```

```
    p0 = np.log2(P[0])
    p1 = np.log2(P[-1])
    pv = list(range(int(p0),int(p1)+1))
    Pstr = ([r"$2^{%d}$" % p for p in pv])
    xlim([2**(p0-1), 2**(p1+1)])
    xticks(P,Pstr)
```

Construct data needed to estimate model parameters

In [3]:

```
N0_data = 8      # Size of smallest matrix A
m_data = 5       # Number of observations to construct
kv_data = zeros(m_data)
Nv_data = zeros(m_data)
print("{:>8s} {:>12s}".format("N","k(A)"))
print("{:s}".format('-'*21))
for p in range(m_data):
    N = N0_data*2**p
    Nv_data[p] = N

    # Construct A by add diagonal matrices
    #A  = eye(N)
    A = diag(ones(N-1),k=-1) + diag(-2*ones(N)) + diag(ones(N-1),k=1)

    kv_data[p] = linalg.cond(A)
    print("{:8d} {:12.2f}".format(N,kv_data[p]))
```

```
       N         k(A)
---------------------
       8        32.16
      16       116.46
      32       440.69
      64      1711.66
     128      6743.68
```

In [4]:

```
# Estimate parameters p and C using linear least squares.  Use data in Nv_data,
b = array( [log(kv_data)]).T
G = hstack((ones((len(Nv_data),1)),array([log(Nv_data)]).T))
q, r = linalg.qr(G)
x = dot(linalg.inv(r), dot(q.T, b))
P= x[1]
C = exp(x[0])
print("C = ", C)
print("p = ", P)
#Define a function you can use to approximate the condition number of A for larg
def condition_number(m,N0,C,P):
    Nv = zeros(m)
    kv = zeros(m)
    for p in range(m):
        Nv[p] = N0_data*2**p
        kv[p] = C*(Nv[p])**P
    return kv
kv = condition_number(14,8,C,P)
```

```
C =  [0.56343708]
p =  [1.9301416]
```

In [8]:

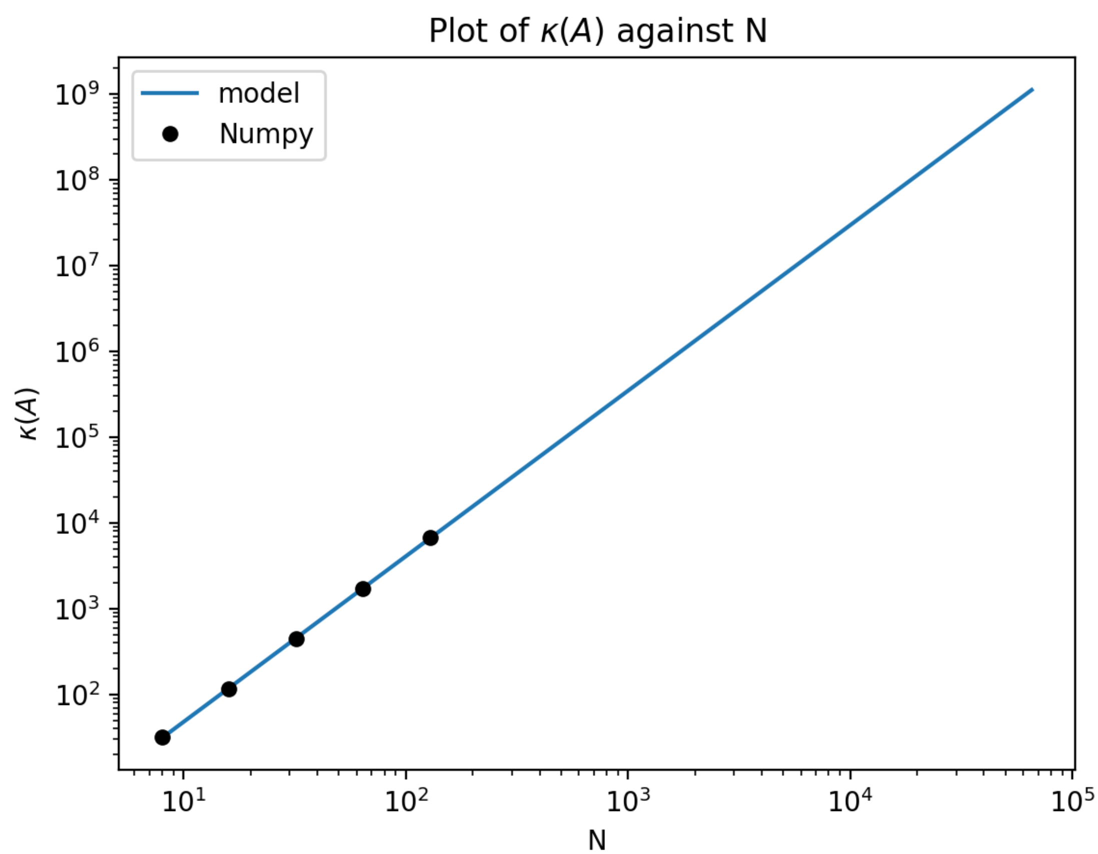
```
figure(1)
```

```
clf()


N0 = 8
Nv = N0*2**arange(14)
plot(Nv,kv)
plot(Nv_data,kv_data,'k.',markersize=10,label='Computed data')
title('Plot of $\kappa(A)$ against N')
xlabel('N')
ylabel('$\kappa(A)$')
legend(['model','Numpy'])
gca().set_xscale('log')
gca().set_yscale('log')

set_xticks(2**arange(14)) # Fix tick marks so they look like 2^p.

show()
```



Soltion

The condition number for matrix A increases with increase in N.

The condition number of an identity matrix does not increase with N.

Problem 3(c)

In this problem, we will compute the numerical error that arises from solving a linear system using the matrix A above. To compute these errors, we solve

$$A\mathbf{x} = \mathbf{b} \tag{25}$$

where the vector $\mathbf{b} = A\overline{\mathbf{x}}$ and $\overline{\mathbf{x}}$ is a vector of random values in $[0, 1]$. We will try to see how well a standard solver (e.g. Gaussian elimination) recovers the value $\overline{\mathbf{x}}$.

Tasks

1. Given a vector $\overline{\mathbf{x}}$ of random values, compute $\mathbf{b} = A\overline{\mathbf{x}}$
2. Solve the linear system $A\mathbf{x} = \mathbf{b}$ over a range of N values $N_0 2^p$, $p = 0, 1, \ldots m$. Setting $m = 14$ is a good value to choose. This corresponds to $N = 16384$.
3. For each N, compute the norm of the error $\mathbf{e} = \overline{\mathbf{x}} - \mathbf{x}$.
4. For each N, compute the norm of the residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$.
5. For each N, compute $\kappa(A)\|\mathbf{r}\|$. **Note:** Use your model approximation to compute $\kappa(A)$. Do not try to compute the condition number from A directly. This will take forever for larger values of N!

Question

How does this plot you created relate to the inequality you showed in **3(a)**?

In [10]:

```
import scipy
from scipy.sparse import spdiags
from scipy.sparse.linalg import spsolve


m = 14   # Number of matrices to consider
Nv = N0*2**arange(m)

# Create vector of approximate condition number values
kv = condition_number(14,8,C,P)

# Store error, residual and k(A)*residual
ev = zeros(m)
rv = zeros(m)
krv = zeros(m)
print("{:>8s} {:>12s} {:>12s} {:>12s}".format("N","e(N)","r(N)","k(A)*r(N)"))
print("{:s}".format('-'*47))
for p in range(m):
    N = Nv[p]

    # Construct sparse matrix A
    z = ones(N)
    data = vstack((z, -2*z, z))
    diags = array([-1,0,1])
    A_sparse = spdiags(data,diags,N,N).tocsr()

    # Vector of random values
```

```
    xbar = random.rand(N,1)
    #right hand side matrix b using xbar
    b = A_sparse @xbar

    #Solve linear system using sparse solver
    x = spsolve(A_sparse,b)
    x = reshape(x,(N,1))    # the sparse result needs to be reshaped.

    # norm of the error
    e = xbar - x
    ev[p] = norm(e)
    #Compute norm of the residual
    r = b- (A_sparse@x)
    rv[p] = norm(r)

    #Compute kappa(A)*(norm of the residual)
    krv[p] = kv[p]*rv[p]
    print("{:8d} {:12.2e} {:12.2e} {:12.2e}".format(N,ev[p],rv[p],krv[p]))
```

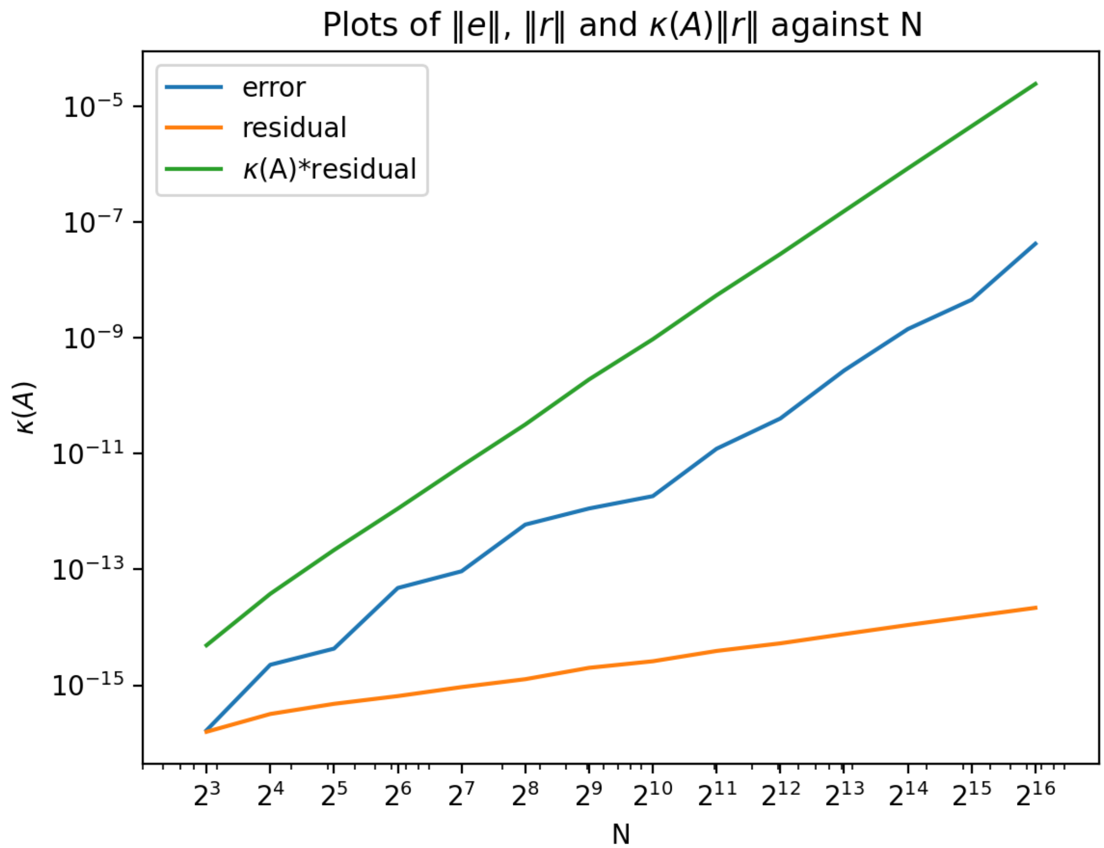
```
       N         e(N)         r(N)     k(A)*r(N)
------------------------------------------------
       8     1.67e-16     1.57e-16     4.90e-15
      16     2.26e-15     3.19e-16     3.79e-14
      32     4.29e-15     4.78e-16     2.16e-13
      64     4.78e-14     6.50e-16     1.12e-12
     128     9.29e-14     9.29e-16     6.11e-12
     256     5.95e-13     1.27e-15     3.19e-11
     512     1.13e-12     2.00e-15     1.91e-10
    1024     1.84e-12     2.59e-15     9.45e-10
    2048     1.21e-11     3.91e-15     5.42e-09
    4096     4.04e-11     5.29e-15     2.80e-08
    8192     2.72e-10     7.64e-15     1.54e-07
   16384     1.42e-09     1.10e-14     8.42e-07
   32768     4.54e-09     1.54e-14     4.52e-06
   65536     4.21e-08     2.17e-14     2.42e-05
```

In [11]:

```
figure(2)
clf()
e1=array([ev]).T
r1=array([rv]).T
krv1=array([krv]).T
N = array([Nv]).T

#Plot error, residual and k(A)*residual
plot(N,e1)
plot(N,r1)
plot(N,krv1)
# TODO : add title, legend and x and y axis labels.
title('Plots of $\Vert e \Vert$, $\Vert r\Vert$ and $\kappa(A)\Vert r \Vert$ aga
xlabel('N')
ylabel('$\kappa(A)$')
legend(['error','residual','$\kappa$(A)*residual'])
gca().set_xscale('log')
gca().set_yscale('log')
set_xticks(Nv)

show()
```



Question

- How does your plot in **3(c)** relate to the inequality you showed in **3(a)**?

  ### Solution.

  The plots for the error is below that of κ(A)*residual and this clearly shows that $\|e\| < \kappa(A)\|r\|$ which relates to 3(a).

- If we solve $A\mathbf{u} = A\overline{\mathbf{u}}$ numerically, do we automatically get $\mathbf{u} = \overline{\mathbf{u}}$? Why or why not?

  ### Solution. No we don't automatically get $\mathbf{u} = \overline{\mathbf{u}}$ because of rounding errors during the computations.

```
In [ ]:
```