laughlin_justin_mae290a_hw2-1

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0.1.1 MAE 290A: Homework 2 (10/19/17)

0.1.2 Problem 1

In [1]:
```
# Import necessary packages & configure settings
import numpy as np
from scipy.sparse.linalg import gmres
from scipy import linalg
import matplotlib.pyplot as plt
import timeit
import time

%matplotlib inline
fs_med = 14 # medium font size for plots
```

Consider the linear system of equations $Ax = b$, where $A_{i,j} = |i-j|^{-1}$ if $i \neq j$ and $A_{ii} = 10$, and $b_i = i$ for $i = 1...100$.

In [2]:
```
# Construct A using nested for loops
N = 100
A = np.ndarray([N,N], dtype=np.double)
for i in np.arange(N):
    for j in np.arange(N):
        if i == j:
            A[i,j] = 10
        else:
            A[i,j] = (np.abs((i+1)-(j+1)))**(-1)
# Construct b
b = np.arange(1,N+1)
```

In [3]:
```
print('Condition number of (A^T A): %e' % np.linalg.cond(np.dot(A.T,A)))
```

```
Condition number of (A^T A): 4.619571e+00
```

According to https://en.wikipedia.org/wiki/Condition_number a general rule of thumb is that the condition number $\rho(A) = 10^k$ means you may lose up to k digits of accuracy. For residual minimization methods we are effectively solving the equation

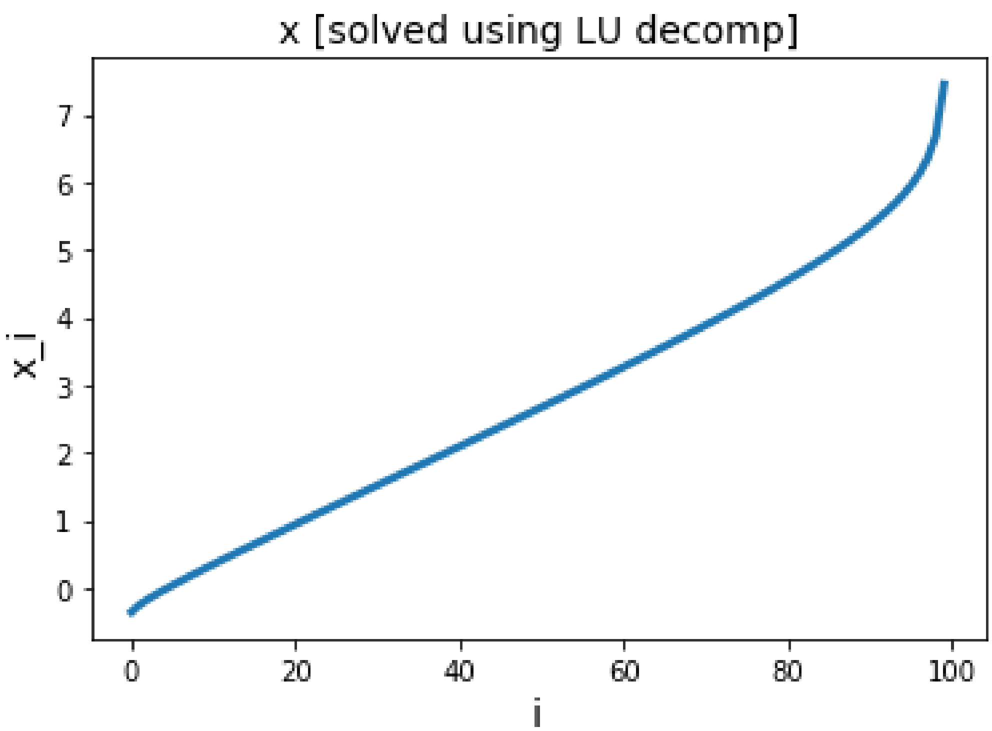
$$A^T \cdot A \cdot x = A^T \cdot b$$

Which means our condition number is $\rho(A^T \cdot A) \sim \rho(A)^2$. Our condition number is ~ 1, which means $k \approx 0$ so our matrix is not ill-conditioned. We can safely invert using residual minimization methods without preconditioning.

Now let us solve the system using LU decomposition (which is not a residual minimization method!) and plot the solution. This will serve as somewhat of a baseline for the methods we use later.

In [4]:
```
# Forward substitution
# Solves Ly=f when L is lower diagonal
def fsub(L,f):
    # Initialize
    N = len(f)
    y = np.ndarray((N,), dtype=np.double)
    y[0] = f[0]/L[0,0]

    # Forward sub
    for j in np.arange(1,N):
        y[j] = (f[j] - np.dot(L[j,0:j],y[0:j]))/L[j,j]

    return y

# Backward substitution
# Solves Ux=y when U is upper diagonal
def bsub(U,y):
        # Initialize
    N = len(y)
    x = np.ndarray((N,), dtype=np.double)
    x[-1] = y[-1]/U[N-1,N-1]

    # Backward sub
    for j in np.arange(N-2,-1,-1):
        x[j] = (y[j] - np.dot(U[j,(j+1):],x[(j+1):]))/U[j,j]

    return x

# Solve Ax=f using LU decomposition
def LUsolve(A,f):
    # Perform LU decomposition. In scipy's implementation A = PLU
    P, L, U = linalg.lu(A)
    F = np.dot(P.T,f)
    y = fsub(L,F)
    x = bsub(U,y)

    return x
```

```
In [5]: xlu = LUsolve(A,b)
        plt.plot(np.arange(N),xlu,linewidth=3)
        plt.xlabel('i',fontsize=fs_med)
        plt.ylabel('x_i',fontsize=fs_med)
        plt.title('x [solved using LU decomp]',fontsize=fs_med)

Out[5]: <matplotlib.text.Text at 0x11b709e80>
```



0.1.3 Solve Ax=b using conjugate gradient method

Now, let us verify that we can solve this system using a conjugate gradient method.

There is a special case we can use when A is a symmetric positive-definite matrix. We know that A is symmetric because of its definition. We also suspect that A is positive-definite because it is diagonally dominant. Showing that A is positive-definite is equivalent to showing that all eigenvalues are positive; however solving for eigenvalues is typically a $\mathcal{O}(N^3)$ operation... Let's use the Gershgorin Circle Theorem (https://en.m.wikipedia.org/wiki/Gershgorin_circle_theorem) to show that all eigenvalues are positive (cheaply!) so that we may use the special case routine.

According to the Gershgorin Circle Theorem if A is a complex $n \times n$ matrix, for $i \in 1, ..., n$, $R_i = \sum_{j,j\neq i}^{N} = |a_{ij}|$ is the sum of absolute values of the non-diagonal entries in the ith row. Let $D(a_{ii}, R_i)$ be the closed disk centered at a_{ii} with radius R_i; every eigenvalue of A lies within at least one of the discs $D(a_{ii}, R_i)$.

Thus, if we can show that the sum of values along each row (excluding the entry on the diagonal) is less than the diagonal value, all eigenvalues must be positive!

```
In [6]: pd_bool = True # positive-definite boolean
        # loop over rows, check if R>D
        for i in np.arange(N):
            R = A[i,np.arange(len(A))!=i].sum()
            D = A[i,i]
            if R>D:
                print('A is NOT positive-definite...sad days :(')
                pd_bool = False
        # if for all rows D>R, A is positive-definite
        if pd_bool == True:
            print('A is positive-definite! Nice!')
```

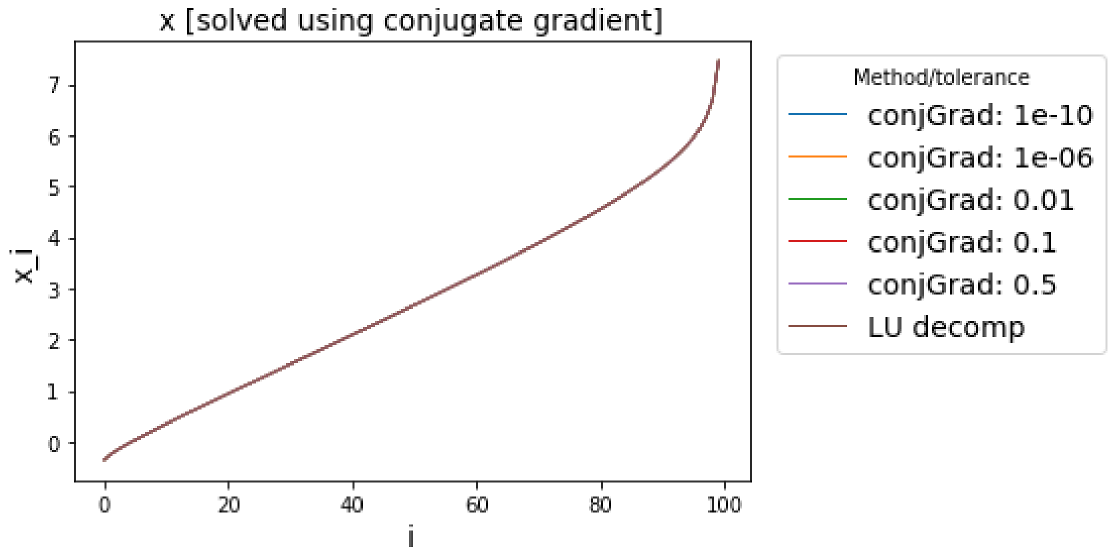
```
A is positive-definite! Nice!
```

Now let's code the conjugate gradient method:

```
In [7]: # Conjugate gradient method to solve Ax=b
        # x0: initial guess
        # tol: tolerance
        def conjGrad(A,b,x0,tol):
            rvec = [] # list of residues
            tvec = [] # time per iteration
            x = x0 # initial guess
            r = b-np.dot(A,x0) # initial residue
            p = r # initial search direction
            rnorm = np.linalg.norm(r)

            # main loop
            while rnorm >= tol:
                rvec.append(rnorm)
                alpha = np.dot(r,r)/(np.dot(np.dot(p,A),p))
                x = x + alpha*p
                rnew = r - alpha*np.dot(A,p)
                beta = np.dot(rnew,rnew)/np.dot(r,r)
                p = rnew + beta*p
                r = rnew

                # check tolerance
                rnorm = np.linalg.norm(r)
                # check time
                tvec.append(time.time())
            rvec.append(rnorm)
            tvec.append(time.time())
            # convert to arrays
            tvec = np.asarray(tvec) - tvec[0]
            rvec = np.asarray(rvec)
            return x, rvec, tvec
```

Plot x when solved using conjugate gradient and compare between different tolerances used. Compare with solution from LU decomposition as a baseline.

```
In [8]: tolvec = np.array(([1e-10, 1e-06, 1e-02, 1e-01, 5e-01]))
        for tol in tolvec:
            x,rvec,tvec = conjGrad(A,b,np.ones((N,)),tol)
            plt.plot(np.arange(N),x,linewidth=1,label='conjGrad: ' + str(tol))
        plt.xlabel('i',fontsize=fs_med)
        plt.ylabel('x_i',fontsize=fs_med)
        plt.title('x [solved using conjugate gradient]',fontsize=fs_med)
        plt.plot(np.arange(N),xlu,linewidth=1, label='LU decomp')
        plt.legend(bbox_to_anchor=(1.02, 1), loc=2, fontsize=fs_med, title='Method/tolerance')

Out[8]: <matplotlib.legend.Legend at 0x11b7ba668>
```



Great! It seems like the conjugate gradient method for all tolerances chosen provides a solution that is indistinguishable from LU decomposition when graphed. Let's now compare the computational time between tolerances for the conjugate gradient method and LU decomposition:

```
In [9]: # This wrapper allows functions such as LUsolve() to be timed by timeit.timeit() so we c
        def wrapper(func, *args, **kwargs):
            def wrapped():
                return func(*args, **kwargs)
            return wrapped

In [10]: nrun = 2000 # number of times to run inversion algorithms for benchmarking
         print("Time to solve using LUsolve() %d times:\t\t\t %.4f" % (nrun, timeit.timeit(wrapp
         for tol in tolvec:
             t = timeit.timeit(wrapper(conjGrad,A,b,np.ones((N,)),tol), number = nrun)
             print("Time to solve using conjGrad() %d times (tol=%.10f):\t %.4f" % (nrun,tol,t),
```

```
Time to solve using LUsolve() 2000 times:                                1.7953 s
Time to solve using conjGrad() 2000 times (tol=0.0000000001):           1.3556 s
Time to solve using conjGrad() 2000 times (tol=0.0000010000):           0.6709 s
Time to solve using conjGrad() 2000 times (tol=0.0100000000):           0.4245 s
Time to solve using conjGrad() 2000 times (tol=0.1000000000):           0.5061 s
Time to solve using conjGrad() 2000 times (tol=0.5000000000):           0.3907 s
```

As expected, in all cases conjGrad() solves the system faster than LUsolve()! For symmetric positive-definite matrices the conjugate gradient method is the fastest iterative solver.

0.1.4 Solve Ax=b using GMRES

GMRES stands for Generalized Minimal RESidual. Let us define our function to minimize as the squared L_2 norm of the residual (other norms could be used as well):

$$f(x) = \frac{1}{2}||r||^2 = \frac{1}{2}||Ax - b||^2$$

The $\frac{1}{2}$ term in front is simply to make the final expression for $f'(x)$ cleaner as we will see. We can expand $f(x)$ out by noting that the squared L_2 norm of a vector is simply the dot product of the vector by itself.

$$f(x) = \frac{1}{2}(Ax - b)^T (Ax - b) = \frac{1}{2}\left[x^T A^T Ax - x^T A^T b - b^T Ax + b^T b\right]$$

Now we will use two matrix calculus identities to find the gradient of $f(x)$:

$$\frac{\partial x^T Ax}{\partial x} = (A + A^T)x, \quad \frac{a^T x}{\partial x} = \frac{\partial x^T a}{\partial x} = a$$

Take the derivative of $f(x)$ w.r.t. x:

$$f'(x) = \frac{1}{2}\left[(A^T A + A^T A)x - A^T b - A^T b\right] = A^T Ax - A^T b$$

Setting the gradient to 0 gives us an equation to solve for:

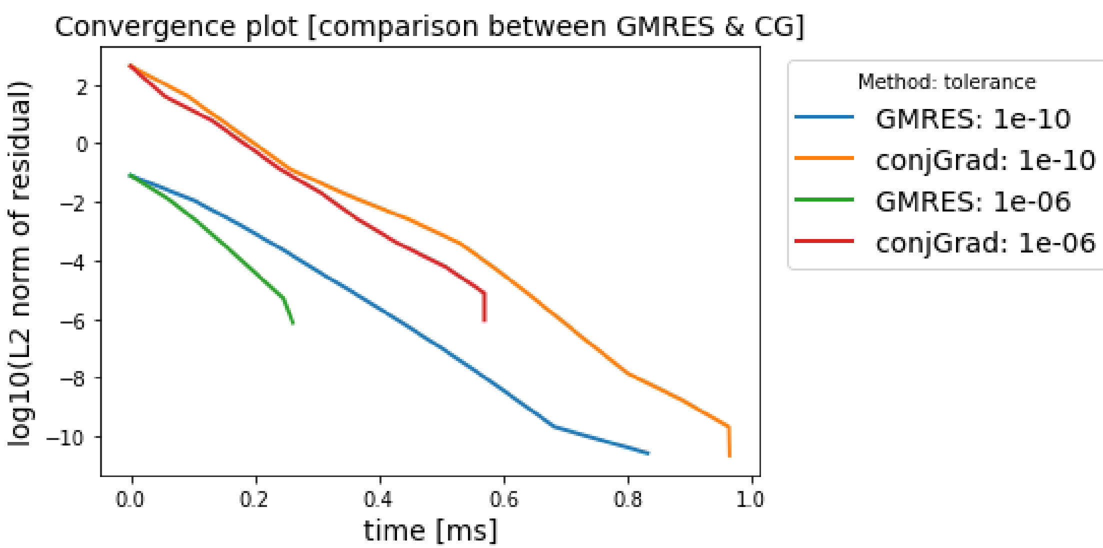
$$f'(x) = 0 \rightarrow A^T Ax = A^T b$$

Notice that we now have a $A^T A$ term, which squares the significance of the condition number for A. This is why we checked at the beginning of this problem that $\rho(A)$ was sufficiently small to apply residual minimization techniques.

```
In [11]: # hack solution to obtaining residual; bad to use a global definition.
         def giveres(r):
             global gmres_rvec
             if not ('gmres_rvec' in vars() or 'gmres_rvec' in globals()):
                 gmres_rvec = []
                 print('gmres_rvec initialized')
             gmres_rvec.append(r)
             t_gmres.append(time.time())
             #print('gmres(): residual = %e' % r)
```

Plot residual norm vs time (scaled using $\log_{10}$ due to the drastic difference in residual norms). Compare between GMRES and conjugate gradient for tolerances $1e{-10}$ and $1e{-6}$:

```
In [12]: def convergencePlot(axesLabels):
             global gmres_rvec
             global t_gmres
             for tol in [1e-10, 1e-6]:
                 gmres_rvec = []
                 t_gmres = []
                 x = gmres(A,b,tol=tol,callback=giveres)
                 t_gmres = np.asarray(t_gmres) - t_gmres[0]
                 plt.plot(t_gmres * 1e+3, np.log10(np.asarray(gmres_rvec)),linewidth=2,label='GM
                 xcg,rvec,tvec = conjGrad(A,b,np.ones((N,)),tol)
                 plt.plot(tvec * 1e+3, np.log10(rvec), linewidth=2, label='conjGrad: ' + str(tol
             if axesLabels == True:
                 plt.xlabel('time [ms]',fontsize=fs_med)
                 plt.ylabel('log10(L2 norm of residual)',fontsize=fs_med)
                 plt.title('Convergence plot [comparison between GMRES & CG]',fontsize=fs_med)
                 plt.legend(bbox_to_anchor=(1.02, 1), loc=2, fontsize=fs_med, title='Method: tol

         convergencePlot(True)
```



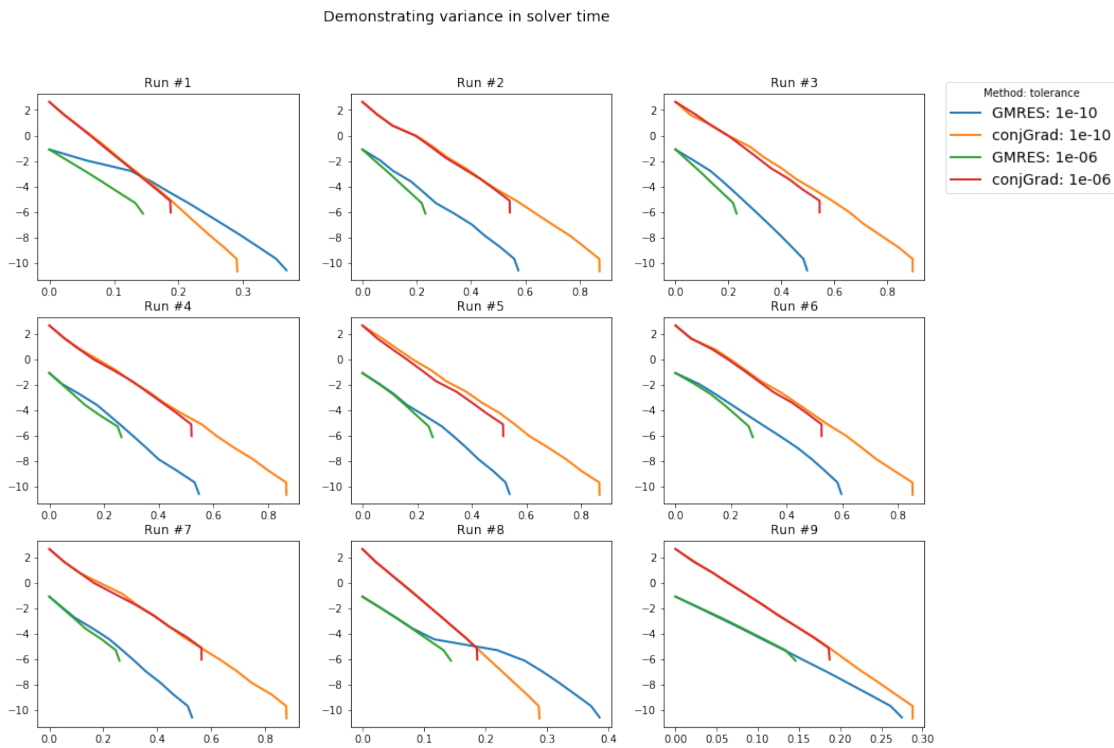
As expected, a lower tolerance corresponds to a quicker convergence. In general, conjugate gradient and GMRES seem to perform similarly in terms of speed (there is a large variance in runtimes, which I will demonstrate below by re-creating the same plot many times...)

Conjugate gradient only works on symmetric positive-definite matrices. GMRES is very useful because it is a general method which can be applied to non-symmetric and not positive-definite matrices.

```
In [13]: # Show the variance in runtimes
         fig = plt.figure(figsize=(15, 11))
```

```
for j in np.arange(9):
    plt.subplot(3,3,j+1)
    convergencePlot(False)
    plt.title('Run #'+str(j+1))
plt.legend(bbox_to_anchor=(1.05, 3.5), loc=2, fontsize=fs_med, title='Method: tolerance
plt.suptitle('Demonstrating variance in solver time',fontsize=fs_med)
```

Out[13]: <matplotlib.text.Text at 0x11b9aff98>



In a theoretical computer with no machine error, the conjugate gradient method would converge ($||r|| = 0$) in at most N operations. This means that it is a direct method and

0.1.5 Modifying A (to be non positive-definite)

If the matrix A was modified such that $A_{i,j} = -10 \cdot |ij|^{-1}$ if $i = j$ and $A_{ii} = 10$, instead of choosing the conjugate gradient method I would opt to use GMRES. Under this new condition we cannot guarantee A is positive definite anymore as it is no longer diagonally dominant. The first version of A had N Gershgorin discs centered at $(10, 0)$ and the largest had a radius of:

```
In [14]: R = A[1,np.arange(len(A))!=1].sum()
         print('Largest Gershgorin disc radius: %.3f' % R)
```

```
Largest Gershgorin disc radius: 6.167
```

All discs were in the right hand side of the complex plane, thus proving that all eigenvalues were positive. Under this modification of A the largest disc radius would be 10 times larger; a disc centered at $(10, 0)$ with a radius of 61.67 extends into the left hand plane, meaning negative eigenvalues are a possibility. GMRES provides a general method to solve matrices such as this one.

```
In [15]: A2 = np.ndarray([N,N], dtype=np.double)
         for i in np.arange(N):
             for j in np.arange(N):
                 if i == j:
                     A2[i,j] = 10
                 else:
                     A2[i,j] = -10*(np.abs((i+1)-(j+1)))**(-1)
```

```
In [16]: np.linalg.cond(A2)**2
```

```
Out[16]: 187632.60989463286
```

However, the squared condition number of this modified A is a bit larger now; we may lose a little more than 5 digits of accuracy according to our definition in the beginning ($\rho(A) = 10^k$ means you may lose up to k digits of accuracy). Remember we must check the squared condition number as this is a residual minimization routine.

Since GMRES is fairly fast it would be nice if we could still use it while maintaining our accuracy. To solve this problem I would apply a preconditioner (Jacobi works fairly well, since A is still diagonally dominant) to reduce the condition number as much as possible.