ncm_nag

August 8, 2016

1 Nearest Correlation Matrix with NAG

Import required modules and set print options

```
In [1]: import numpy as np
        import nag4py.g02 as nag_g02
        import nag4py.util as nag_util
        import matplotlib.pyplot as plt
        "Plot inline"
        %matplotlib inline
        "Set the print precision."
        np.set_printoptions(precision=4)
```

1.1 Start with an incomplete matrix P

```
In [2]: "Define a 2-d array and us np.nan to set the NaNs."
        P = np.array([[59.875, 42.734, 47.938, 60.359, 54.016, 69.625, 61.500, 62.125],
                      [53.188, 49.000, 39.500, np.nan, 34.750, np.nan, 83.000, 44.500],
                      [55.750, 50.000, 38.938, np.nan, 30.188, np.nan, 70.875, 29.938],
                      [65.500, 51.063, 45.563, 69.313, 48.250, 62.375, 85.250, np.nan],
                      [69.938, 47.000, 52.313, 71.016, np.nan, 59.359, 61.188, 48.219],
                      [61.500, 44.188, 53.438, 57.000, 35.313, 55.813, 51.500, 62.188],
                      [59.230, 48.210, 62.190, 61.390, 54.310, 70.170, 61.750, 91.080],
                      [61.230, 48.700, 60.300, 68.580, 61.250, 70.340, np.nan, np.nan],
                      [52.900, 52.690, 54.230, np.nan, 68.170, 70.600, 57.870, 88.640],
                      [57.370, 59.040, 59.870, 62.090, 61.620, 66.470, 65.370, 85.840]])
```

```
In [3]: def cov_bar(P):
            """Returns an approximate sample covarience matrix"""
            "P.shape returns a tuple (m, n) that we unpack to m and n."
            m, n = P.shape
            "Initialise an nxn zero matrix."
            S = np.zeros((n, n))
            "i = 0, ..., 7."
            for i in range(0, n):
                "Take the ith column."
                xi = P[:, i]
                "j = 0, ..., i"
                for j in range(0, i+1):
                    "Take the jth column, where j <= i."
                    xj = P[:, j]
                    """masked_array masks elements marked as True; this is the opposite behaviour of
        the MATLAB script. Therefore, we need ~(~np.isnan(xi) & ~np.isnan(xj)), which I
```

```
        have simplified below and will label notp."""
                    "Set mask such that all nans are True."
                    notp = np.isnan(xi) | np.isnan(xj)
                    "Apply the mask to xi"
                    xim = np.ma.masked_array(xi, mask=notp)
                    "Apply the mask to xj"
                    xjm = np.ma.masked_array(xj, mask=notp)
                    S[i, j] = np.ma.dot(xim - np.mean(xim), xjm - np.mean(xjm))
                    """As we used notp as our mask, we must take the sum over ~notp to give the
        same result as the MATLAB script when normalising."""
                    S[i, j] = 1.0 / (sum(~notp) - 1) * S[i, j]
                    S[j, i] = S[i, j]
            return S
```

```
In [4]: def cor_bar(P):
            """Returns an approximate sample correlation matrix"""
            S = cov_bar(P)
            D = np.diag(1.0 / np.sqrt(np.diag(S)))
            "This is will only work in Python3"
            return D @ S @ D
```

1.2 Calculate the correlation matrix of P.

```
In [5]: G = cor_bar(P)
        print(G)
```

```
[[ 1.     -0.325   0.1881  0.576   0.0064 -0.6111 -0.0724 -0.1589]
 [-0.325   1.      0.2048  0.2436  0.4058  0.273   0.2869  0.4241]
 [ 0.1881  0.2048  1.     -0.1325  0.7658  0.2765 -0.6172  0.9006]
 [ 0.576   0.2436 -0.1325  1.      0.3041  0.0126  0.6452 -0.321 ]
 [ 0.0064  0.4058  0.7658  0.3041  1.      0.6652 -0.3293  0.9939]
 [-0.6111  0.273   0.2765  0.0126  0.6652  1.      0.0492  0.5964]
 [-0.0724  0.2869 -0.6172  0.6452 -0.3293  0.0492  1.     -0.3983]
 [-0.1589  0.4241  0.9006 -0.321   0.9939  0.5964 -0.3983  1.    ]]
```

1.2.1 Some of the eigenvalues are negative and therefore the matrix is not semi-positive definite.

```
In [6]: print("The sorted eigenvalues of G {}".format(np.sort(np.linalg.eig(G)[0])))
```

```
The sorted eigenvalues of G [-0.2498 -0.016   0.0895  0.2192  0.7072  1.7534  1.9611  3.5355]
```

1.3 Use g02aa to calculate the nearest correlation matrix in the Frobenius norm

```
In [7]: order = nag_util.Nag_RowMajor
        Gflat = G.flatten()
        n = G.shape[0]
        pdg = n
        errtol = 0.0
        maxits = 0
        maxit = 0
        Xflat = np.empty_like(Gflat)
        pdx = n
        itr = np.array([0])
        feval = np.array([0])
```

```
        nrmgrd = np.array([0.0])
        fail = nag_util.noisy_fail()
        nag_g02.g02aac(order, Gflat, pdg, n, errtol, maxits,
                       maxit, Xflat, pdx, itr, feval, nrmgrd, fail)
```

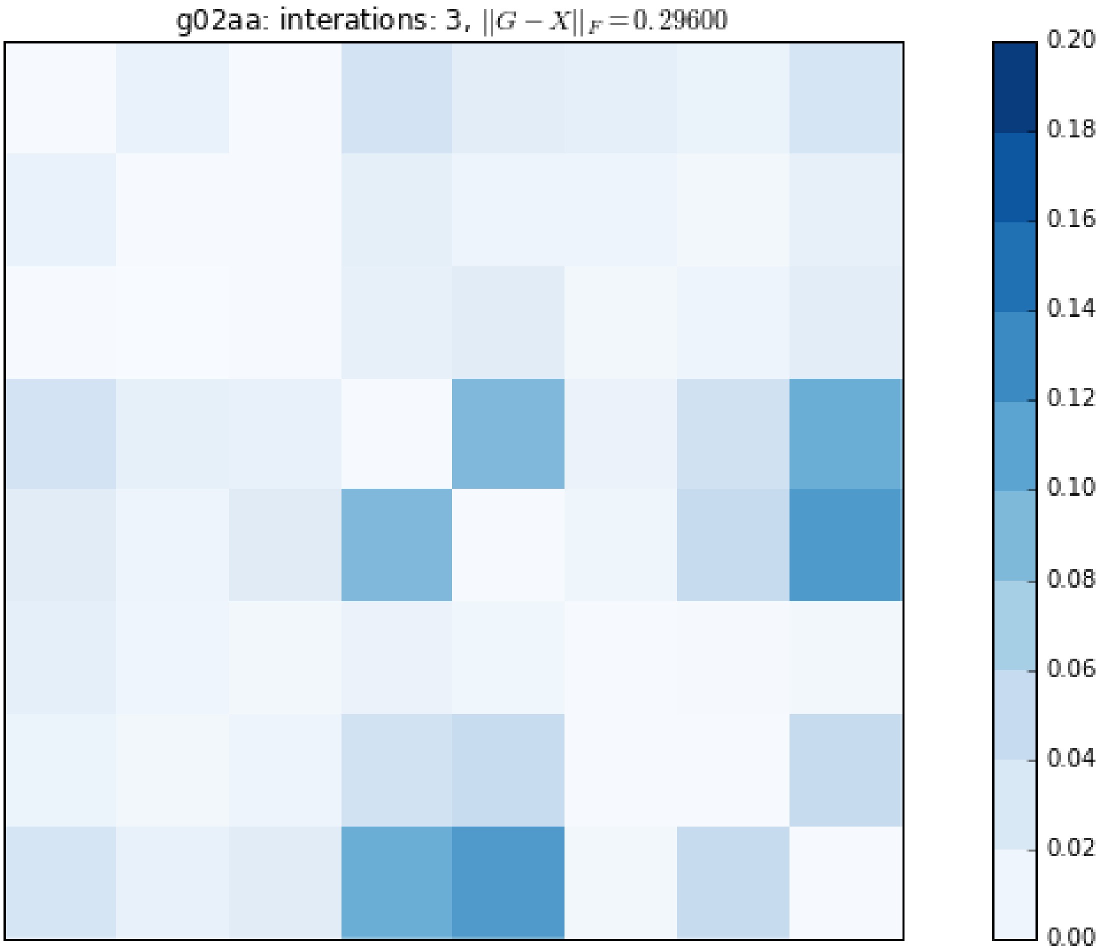
```
In [8]: "Unflatten X to have the same shape as G for comparison."
        X = np.reshape(Xflat, G.shape)
        print(X)
```

```
[[ 1.     -0.3112  0.1889  0.5396  0.0268 -0.5925 -0.0621 -0.1921]
 [-0.3112  1.      0.205   0.2265  0.4148  0.2822  0.2915  0.4088]
 [ 0.1889  0.205   1.     -0.1468  0.788   0.2727 -0.6085  0.8802]
 [ 0.5396  0.2265 -0.1468  1.      0.2137  0.0015  0.6069 -0.2208]
 [ 0.0268  0.4148  0.788   0.2137  1.      0.658  -0.2812  0.8762]
 [-0.5925  0.2822  0.2727  0.0015  0.658   1.      0.0479  0.5932]
 [-0.0621  0.2915 -0.6085  0.6069 -0.2812  0.0479  1.     -0.447 ]
 [-0.1921  0.4088  0.8802 -0.2208  0.8762  0.5932 -0.447   1.    ]]
```

```
In [9]: print("The sorted eigenvalues of X [{0}]".format(''.join(
                      ['{:.4f} '.format(x) for x in np.sort(np.linalg.eig(X)[0])])))
```

```
The sorted eigenvalues of X [-0.0000 -0.0000 0.0380 0.1731 0.6894 1.7117 1.9217 3.4661 ]
```

```
In [10]: fig1, ax1 = plt.subplots(figsize=(14, 7))
         cax1 = ax1.imshow(abs(X-G), interpolation='none', cmap=plt.cm.Blues, vmin=0, vmax=0.2)
         cbar = fig1.colorbar(cax1, ticks = np.linspace(0.0, 0.2, 11, endpoint=True),
                              boundaries=np.linspace(0.0, 0.2, 11, endpoint=True))
         cbar.set_clim([0, 0.2])
         ax1.tick_params(axis='both', which='both',
                         bottom='off', top='off', left='off', right='off',
                         labelbottom='off', labelleft='off')
         ax1.set_title(r'g02aa: interations: {0}, $||G-X||_F = {1:.5f}$'.format(itr[0],
                                                                               np.linalg.norm(X-G)))
         plt.show()
```



1.4 Use g02ab to calculate the nearest correlation matrix with row and column weighting

1.4.1 Define the weights as follows

```
In [11]: W = np.array([10, 10, 10, 1, 1, 1, 1, 1], dtype = np.float64)
```

```
In [12]: order = nag_util.Nag_RowMajor
         Gflat = G.flatten()
         n = G.shape[0]
         opt = nag_util.Nag_Both
         alpha = 0.001
         pdg = n
         errtol = 0.0
         maxits = 0
         maxit = 0
         Xflat = np.empty_like(Gflat)
         pdx = n
         itr = np.array([0])
         feval = np.array([0])
```

```
        nrmgrd = np.array([0.0])
        fail = nag_util.noisy_fail()
        nag_g02.g02abc(order, Gflat, pdg, n, opt, alpha, W, errtol, maxits,
                       maxit, Xflat, pdx, itr, feval, nrmgrd, fail)
```

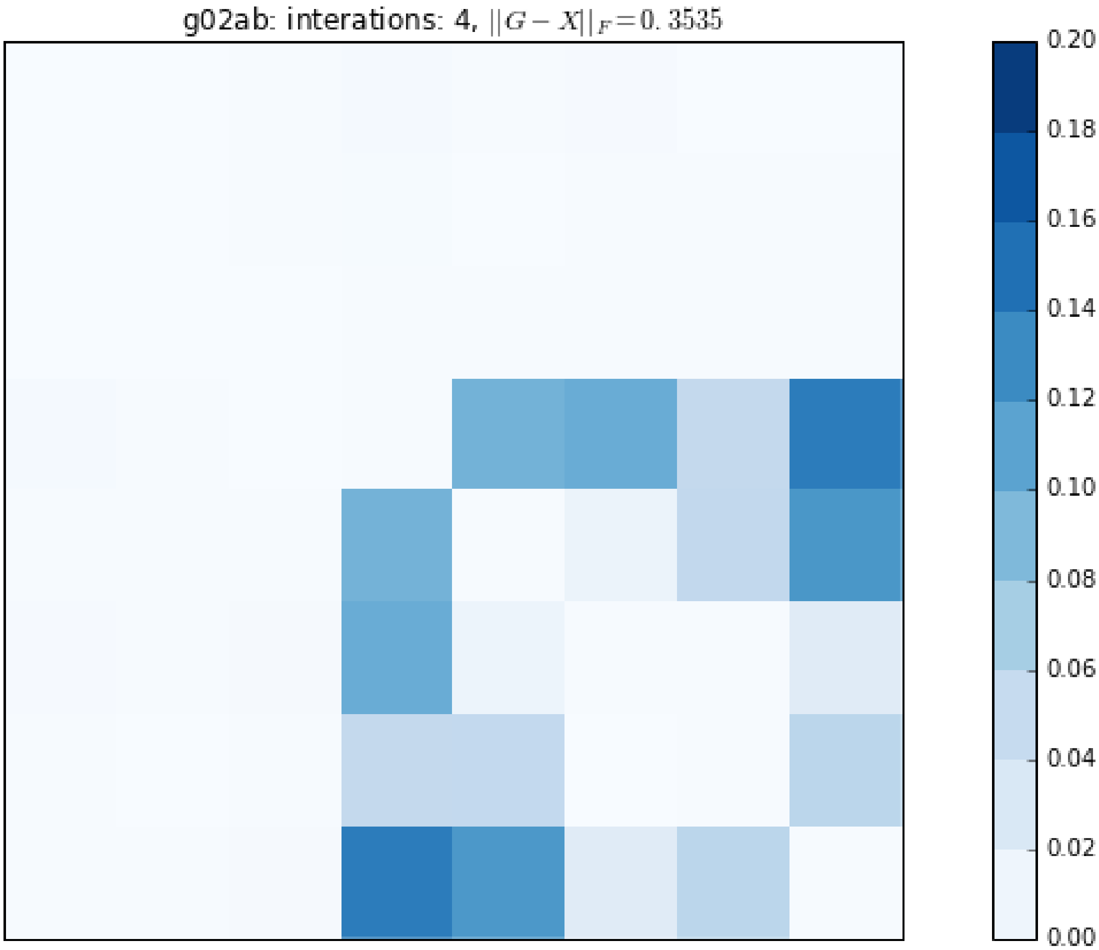
```
In [13]: X = np.reshape(Xflat, G.shape)
         print(X)
```

```
[[ 1.     -0.3247  0.1879  0.5733  0.0067 -0.609  -0.0721 -0.1596]
 [-0.3247  1.      0.2046  0.2423  0.4056  0.2735  0.2867  0.4232]
 [ 0.1879  0.2046  1.     -0.1321  0.7654  0.2756 -0.6164  0.8995]
 [ 0.5733  0.2423 -0.1321  1.      0.2083 -0.0889  0.5948 -0.1804]
 [ 0.0067  0.4056  0.7654  0.2083  1.      0.655  -0.2777  0.8748]
 [-0.609   0.2735  0.2756 -0.0889  0.655   1.      0.049   0.574 ]
 [-0.0721  0.2867 -0.6164  0.5948 -0.2777  0.049   1.     -0.4545]
 [-0.1596  0.4232  0.8995 -0.1804  0.8748  0.574  -0.4545  1.    ]]
```

```
In [14]: print("The sorted eigenvalues of X [{0}]".format(''.join(
                     ['{:.4f} '.format(x) for x in np.sort(np.linalg.eig(X)[0])])))
```

```
The sorted eigenvalues of X [0.0020 0.0020 0.0315 0.1655 0.6767 1.7708 1.8901 3.4614 ]
```

```
In [15]: fig1, ax1 = plt.subplots(figsize=(14, 7))
         cax1 = ax1.imshow(abs(X-G), interpolation='none', cmap=plt.cm.Blues, vmin=0, vmax=0.2)
         cbar = fig1.colorbar(cax1, ticks = np.linspace(0.0, 0.2, 11, endpoint=True),
                              boundaries=np.linspace(0.0, 0.2, 11, endpoint=True))
         cbar.set_clim([0, 0.2])
         ax1.tick_params(axis='both', which='both',
                         bottom='off', top='off', left='off', right='off',
                         labelbottom='off', labelleft='off')
         ax1.set_title(r'g02ab: interations: {0}, $||G-X||_F = {1:.4f}$'.format(itr[0],
                                                                               np.linalg.norm(X-G)))
         plt.show()
```



1.5 Use g02aj to calculate the nearest correlation matrix with element-wise weighting

In [16]:
```
H = np.ones([n, n])
H[0:3, 0:3] = 100
```

In [17]:
```
Gflat = G.flatten()
n = G.shape[0]
alpha = 0.001
Hflat = H.flatten()
pdg = n
pdh = n
errtol = 0.0
maxits = 0
maxit = 500
Xflat = np.empty_like(Gflat)
pdx = n
itr = np.array([0])
norm = np.array([0.0])
fail = nag_util.noisy_fail()
```

```
         nag_g02.g02ajc(Gflat, pdg, n, alpha, Hflat, pdh, errtol,
                        maxit, Xflat, pdx, itr, norm, fail)
```

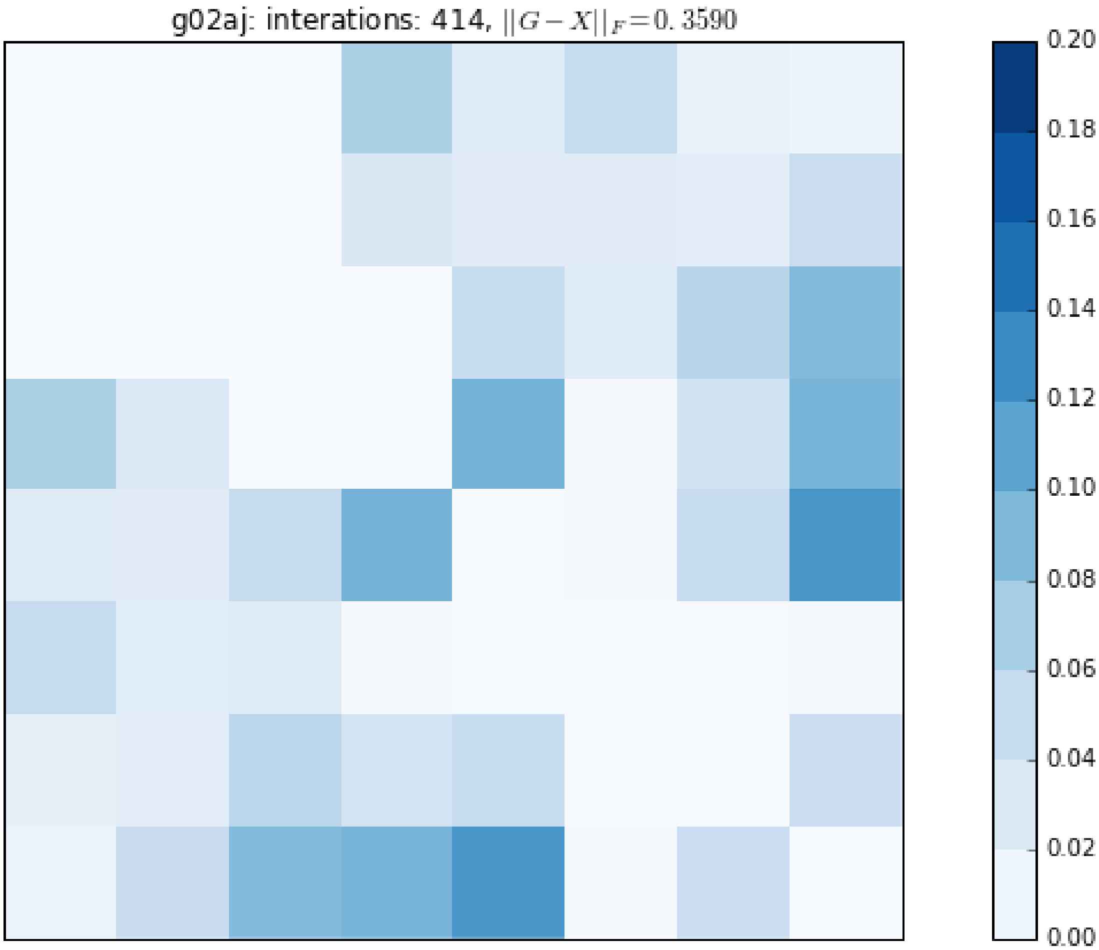
In [18]:
```
X = np.reshape(Xflat, G.shape)
print(X)
```

```
[[ 1.     -0.3247  0.188   0.5091  0.0306 -0.5611 -0.0569 -0.1701]
 [-0.3247  1.      0.2047  0.2146  0.3837  0.2504  0.2676  0.3781]
 [ 0.188   0.2047  1.     -0.1331  0.7175  0.2534 -0.5607  0.812 ]
 [ 0.5091  0.2146 -0.1331  1.      0.2081  0.0145  0.6079 -0.2272]
 [ 0.0306  0.3837  0.7175  0.2081  1.      0.6622 -0.282   0.8732]
 [-0.5611  0.2504  0.2534  0.0145  0.6622  1.      0.0482  0.5982]
 [-0.0569  0.2676 -0.5607  0.6079 -0.282   0.0482  1.     -0.4438]
 [-0.1701  0.3781  0.812  -0.2272  0.8732  0.5982 -0.4438  1.    ]]
```

In [19]:
```
print("The sorted eigenvalues of X [{0}]".format(''.join(
                 ['{:.4f} '.format(x) for x in np.sort(np.linalg.eig(X)[0])])))
```

```
The sorted eigenvalues of X [0.0020 0.0129 0.1162 0.2104 0.7367 1.6700 1.8892 3.3627 ]
```

In [20]:
```
fig1, ax1 = plt.subplots(figsize=(14, 7))
cax1 = ax1.imshow(abs(X-G), interpolation='none', cmap=plt.cm.Blues, vmin=0, vmax=0.2)
cbar = fig1.colorbar(cax1, ticks = np.linspace(0.0, 0.2, 11, endpoint=True),
                     boundaries=np.linspace(0.0, 0.2, 11, endpoint=True))
cbar.set_clim([0, 0.2])
ax1.tick_params(axis='both', which='both',
                bottom='off', top='off', left='off', right='off',
                labelbottom='off', labelleft='off')
ax1.set_title(r'g02aj: interations: {0}, $||G-X||_F = {1:.4f}$'.format(itr[0],
                                                                     np.linalg.norm(X-G)))
plt.show()
```



1.6 Use g02an to calculate the nearest correlation matrix with fixed leading block

In [21]:
```
Gflat = G.flatten()
n = G.shape[0]
pdg = n
k = 3
errtol = 0.0
eigtol = 0.0
maxits = 0
maxit = 500
Xflat = np.empty_like(Gflat)
pdx = n
alpha = np.array([0.0])
itr = np.array([0])
eigmin = np.array([0.0])
norm = np.array([0.0])
fail = nag_util.noisy_fail()
nag_g02.g02anc(Gflat, pdg, n, k, errtol, eigtol, Xflat, pdx,
               alpha, itr, eigmin, norm, fail)
```

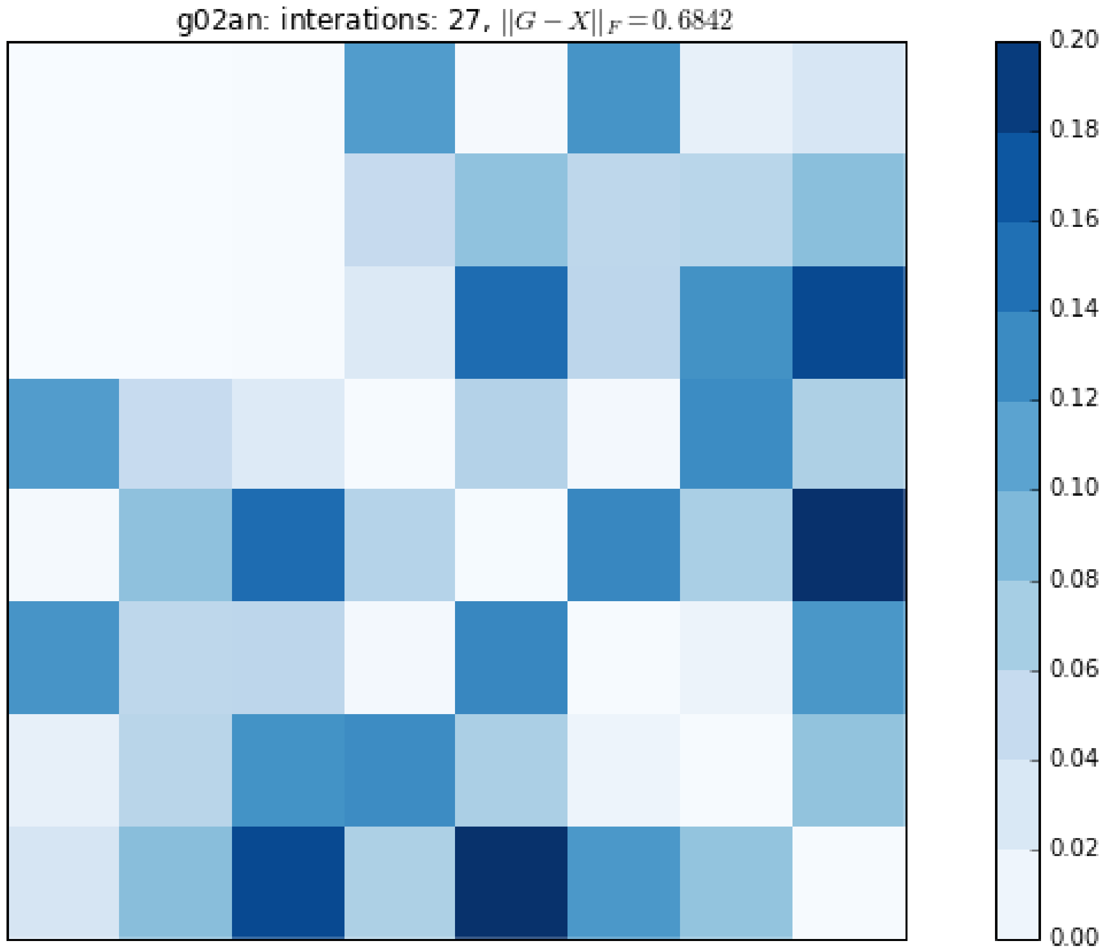
```
In [22]: X = np.reshape(Xflat, G.shape)
         print(X)
```

```
[[ 1.     -0.325   0.1881  0.4606  0.0051 -0.4887 -0.0579 -0.1271]
 [-0.325   1.      0.2048  0.1948  0.3245  0.2183  0.2294  0.3391]
 [ 0.1881  0.2048  1.     -0.106   0.6124  0.2211 -0.4936  0.7202]
 [ 0.4606  0.1948 -0.106   1.      0.2432  0.0101  0.516  -0.2567]
 [ 0.0051  0.3245  0.6124  0.2432  1.      0.532  -0.2634  0.7949]
 [-0.4887  0.2183  0.2211  0.0101  0.532   1.      0.0393  0.4769]
 [-0.0579  0.2294 -0.4936  0.516  -0.2634  0.0393  1.     -0.3185]
 [-0.1271  0.3391  0.7202 -0.2567  0.7949  0.4769 -0.3185  1.    ]]
```

```
In [23]: print("The sorted eigenvalues of X [{0}]".format(''.join(
                     ['{:.4f} '.format(x) for x in np.sort(np.linalg.eig(X)[0])])))
```

```
The sorted eigenvalues of X [0.0000 0.1375 0.2744 0.3804 0.7768 1.6263 1.7689 3.0356 ]
```

```
In [24]: fig1, ax1 = plt.subplots(figsize=(14, 7))
         cax1 = ax1.imshow(abs(X-G), interpolation='none', cmap=plt.cm.Blues, vmin=0, vmax=0.2)
         cbar = fig1.colorbar(cax1, ticks = np.linspace(0.0, 0.2, 11, endpoint=True),
                              boundaries=np.linspace(0.0, 0.2, 11, endpoint=True))
         cbar.set_clim([0, 0.2])
         ax1.tick_params(axis='both', which='both',
                         bottom='off', top='off', left='off', right='off',
                         labelbottom='off', labelleft='off')
         ax1.set_title(r'g02an: interations: {0}, $||G-X||_F = {1:.4f}$'.format(itr[0],
                                                                          np.linalg.norm(X-G)))
         plt.show()
```


g02an: interations: 27, $||G - X||_F = 0.6842$
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00