Computer Simulation II- PYU44C01 Linear algebra assignment 1

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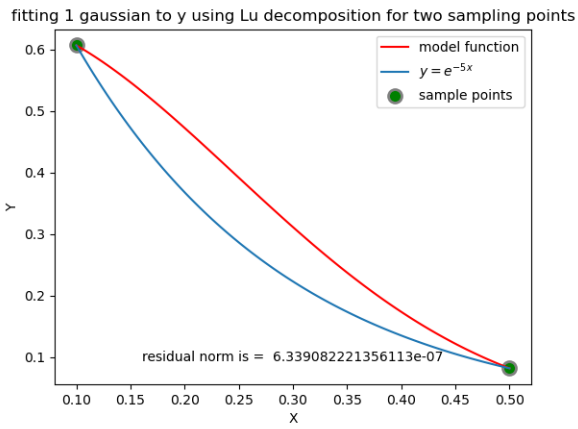
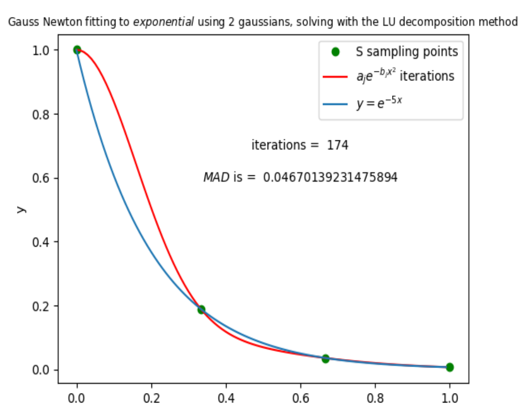
0.1 Initial fitting to two points(near exact fitting of sample points as required) but a large difference in functions

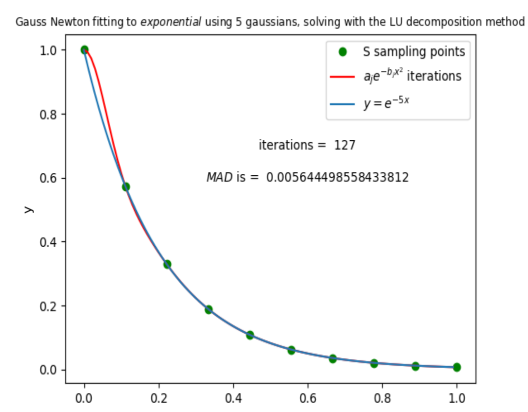


0.2 Generalising to an NxN matrix and taking samples for N = 2, 5 and 6 as examples with one QR graph as comparison(12x12)(3 more next page)

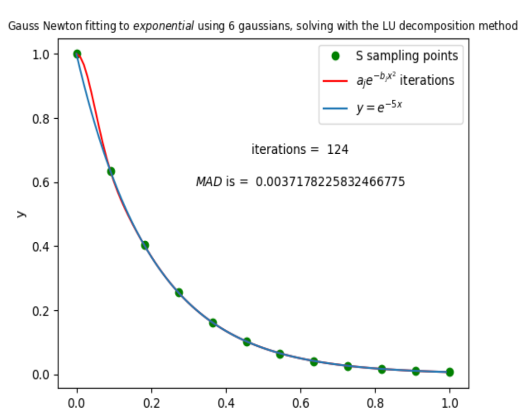
0.3



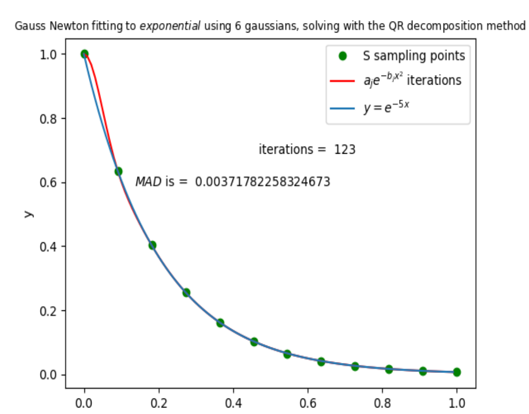
(a) 2 Gaussians fitted to $y = e^{-5x}$ using LU method



(b) 5 Gaussians fitted to $y = e^{-5x}$ using LU method



(c) 6 Gaussians fitted to $y = e^{-5x}$ using LU method

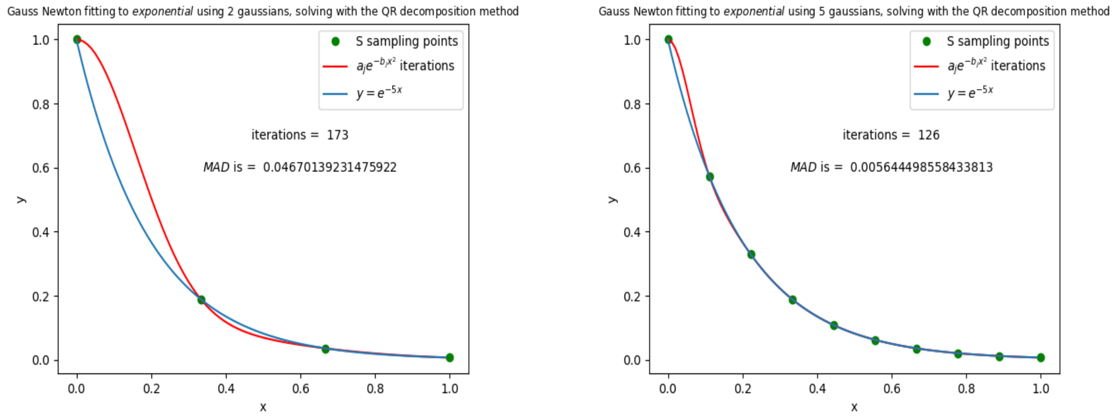


(d) 6 Gaussians fitted to $y = e^{-5x}$ using QR method

Figure 1: Relevant fitting data for 3 LU graphs and a 4th QR method graph for comparison

0.4 Generalising to an NxN matrix and taking samples for N = 2, 5 for the QR method

0.5



(a) 2 Gaussians fitted to $y = e^{-5x}$ using QR method

(b) 5 Gaussians fitted to $y = e^{-5x}$ using QR method

Figure 2: Relevant fitting data for QR N=2,5

0.6 QR decomposition

In the case of LU decomposition we are solving for x in the form Ax = B where A is the jacobian and B is - residual at any given set of parameters. In the method of QR decomposition we tweak this by first setting A = QR where Q is an orthogonal matrix and R is a square upper triangular matrix. This allows us to obtain

$$Q^T Q = QQ^T = I, Q^T = Q^{-1}$$

i.e we can avoid finding the inverse of matrices directly which is bad practice for linear algebra in general

$$Rx = Q^T b$$

So for this problem in particular how we implement it is:
1. compute QR = A
2. compute d where d is taken to be $Q^T b$
3. using back substitution, the equation Rx = d is then solved
4. repeat until parameters are at a desirable tolerance level and good agreement with fit is reached

0.7 QR decomposition vs LU decomposition

LU decomposition works for m x m matrices as we have here but does not function for rectangular m x n matrices which QR decomposition is particularly suited for. There is no major difference between the fittings returned by LU and QR methods since we are working on square matrices both towards an optimal function. However it was noted that while allowing the simulation to run indefinitely, the smallest values of residual for LU and QR respectively were 10^{-18} and 10^{-17} which would seem to be the machine precision difference in them.

0.8 Final error results - satisfactory?

As the number of sampling points and parameters for gaussians increases, it is clear that so too does the accuracy of the fit. We can see there is still room for improvement in the fit as the model and exact functions are not perfectly matched for the 12x12 matrix as shown by the mean absolute difference values. This could be solved by expanding the matrix and employing hessian terms(similar to jacobian matrix but for 2nd derivatives as opposed to first).