L_Bijman_S_Gijsbers_HW3

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1 Homework set 3

Please **submit this Jupyter notebook through Canvas** no later than **Mon Nov. 20, 9:00**. **Submit the notebook file with your answers (as .ipynb file) and a pdf printout. The pdf version can be used by the teachers to provide feedback. A pdf version can be made using the save and export option in the Jupyter Lab file menu.**

Homework is in **groups of two**, and you are expected to hand in original work. Work that is copied from another group will not be accepted.

2 Exercise 0

Write down the names + student ID of the people in your group.

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Run the following cell to import NumPy and Pyplot.

[ ]:
```
import numpy as np
import matplotlib.pyplot as plt
import scipy
import math
```

3 Exercise 1

In this exercise you will study the accuracy of several methods for computing the QR decomposition. You are asked to implement these methods yourself. (However, when testing your implementation you may compare with an external implementation.)

3.1 (a)

Implement the classical and modified Gram-Schmidt procedures for computing the QR decomposition.

Include a short documentation using triple quotes: describe at least the input and the output, and whether the code modifies the input matrix.

[ ]:
```python
def classical_gram_schmidt(A):
    '''
    Input: matrix A (mxn) as numpy array
    Output: matrices Q (mxn), R(nxn), derived by Gram-Schmidt procedures for QR␣
 ↪decomposition:
    Q orthogonal matrix and R upper triangular.
    Input matrix A is not modified in the process (as is seen in the output).
    '''
    n_rows,n_columns = A.shape
    Q = np.zeros((n_rows,n_columns))
    R = np.zeros((n_columns,n_columns))

    for k in range(n_columns):
        Q[:,k] = A[:,k]
        # loop over previous columns
        for j in range(0,k):
            # create new column k in Q orthogonal to A[:,k]
            r_jk = np.dot(A[:,k],Q[:,j])
            Q[:,k] -= r_jk*Q[:,j]
            R[j,k] = r_jk

        # check for if columns are linearly dependent
        if np.linalg.norm(Q[:,k]) == 0:
            # note: this check only checks if ||Q[:,k]|| is exactly equal to␣
 ↪zero, does not work for floats very close to zero
            # a solution would be to set abs(||Q[:,k]||)< c, but it is hard to␣
 ↪determine c in such a way that it works
            raise ValueError('Rkk = 0')
        else:
            Q[:,k] = list(Q[:,k]/np.linalg.norm(Q[:,k]))
            R[k,k] = np.dot(A[:,k],Q[:,k])

    return Q, R, A

def modified_gram_schmidt(A):
    '''
    Input: matrix A (mxn) as numpy array
    Output: matrices Q (mxn), R(nxn), derived by QR decomposition with modified␣
 ↪Gramm-Schmidt:
    Q orthogonal matrix and R upper triangular
    Input matrix A is modified in the process (as is seen in the output).
    '''
    Q = A.astype(float)
    A = A.astype(float)
    _,n = A.shape
    R = np.zeros((n,n))
```

```python
    for k in range(n):
        rkk = np.linalg.norm(A[:,k], ord=2)
        R[k,k] = rkk
        # check for linear dependence
        if rkk == 0: # see comment in classical Gram-Schmidt
            raise ValueError('Rkk = 0')
        Q[:,k] = A[:,k]/rkk

        # loop over following columns
        for j in range(k+1,n):
            rkj = np.inner(Q[:,k], A[:,j])
            R[k,j] = rkj
            A[:,j] -= rkj*Q[:,k]
    return Q, R, A

A = np.array([[1,1,0,1],[1,0,1,0],[0,1,1,1]]).T
Qc, Rc, Ac = classical_gram_schmidt(A)
Qm, Rm, Am = modified_gram_schmidt(A)

print(f'Input A: \n {A}')
print('Classical:')
print(f'Q: \n{Qc}')
print(f'R: \n {Rc}')
print(f'A: \n {Ac}')
print('---------------------------------------------')

print('Modified: ')
print(f'Q: \n {Qm}')
print(f'R: \n {Rm}')
print(f'A: \n {Am}')
```

```
Input A:
 [[1 1 0]
 [1 0 1]
 [0 1 1]
 [1 0 1]]
Classical:
Q:
[[ 0.57735027  0.51639778 -0.63245553]
 [ 0.57735027 -0.25819889  0.31622777]
 [ 0.          0.77459667  0.63245553]
 [ 0.57735027 -0.25819889  0.31622777]]
R:
 [[1.73205081 0.57735027 1.15470054]
 [0.         1.29099445 0.25819889]
 [0.         0.         1.26491106]]
A:
```

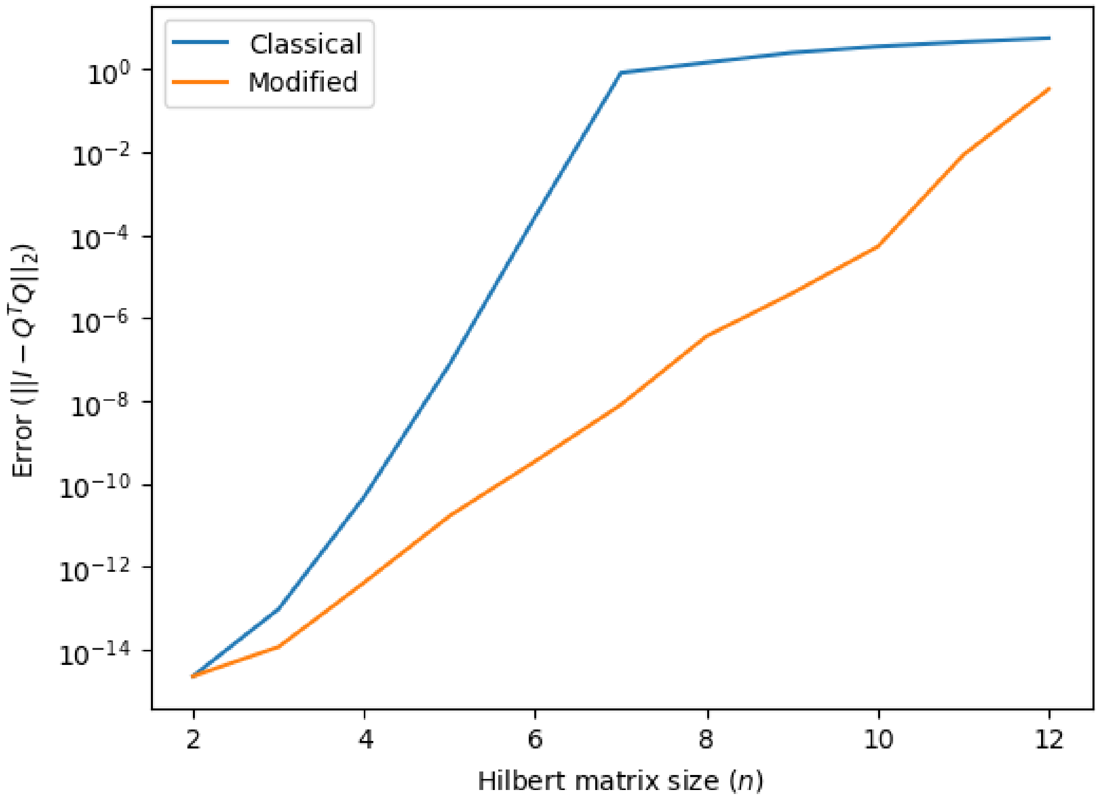
```
 [[1 1 0]
 [1 0 1]
 [0 1 1]
 [1 0 1]]
--------------------------------------------
Modified:
Q:
 [[ 0.57735027  0.51639778 -0.63245553]
 [ 0.57735027 -0.25819889  0.31622777]
 [ 0.          0.77459667  0.63245553]
 [ 0.57735027 -0.25819889  0.31622777]]
R:
 [[1.73205081 0.57735027 1.15470054]
 [0.         1.29099445 0.25819889]
 [0.         0.         1.26491106]]
A:
 [[ 1.          0.66666667 -0.8       ]
 [ 1.         -0.33333333  0.4       ]
 [ 0.          1.          0.8       ]
 [ 1.         -0.33333333  0.4       ]]
```

3.2 (b) (a+b 3.5 pts)

Let H be a Hilbert matrix of size n (see Computer Problem 2.6). Study the quality of the QR decompositions obtained using the two methods of part (a), specifically the loss of orthogonality. In order to do so, plot the quantity $\|I - Q^T Q\|$ as a function of n on a log scale. Vary n from 2 to 12.

[ ]:
```python
error_class, error_mod = [], []

n_list = range(2,13)
for n in n_list:
    # create Hilbert matrix
    H = scipy.linalg.hilbert(n)

    Q_class = classical_gram_schmidt(H)[0]
    error_class.append(np.linalg.norm(np.identity(n) - np.matmul(Q_class.
 ↪T,Q_class)))

    Q_mod = modified_gram_schmidt(H)[0]
    error_mod.append(np.linalg.norm(np.identity(n) - np.matmul(Q_mod.T,Q_mod)))

plt.plot(n_list,error_class, label = 'Classical')
plt.plot(n_list,error_mod, label = 'Modified')
plt.yscale('log')
plt.xlabel('Hilbert matrix size ($n$)')
plt.ylabel('Error ($||I - Q^TQ||_2$)')
plt.legend()
```

```
plt.show()
```

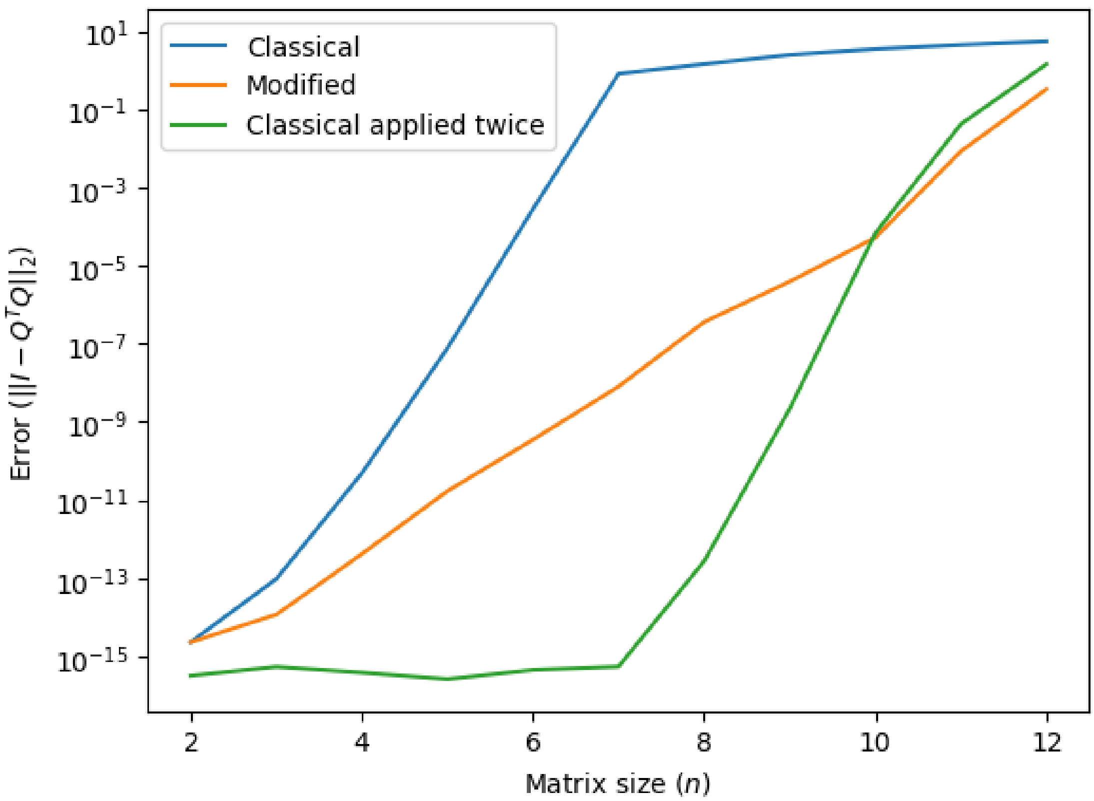


3.3 (c) (1.5 pts)

Try applying the classical procedure twice. Plot again the loss of orthogonality when computing the QR decomposition of the Hilbert matrix of size n as in (b).

[ ]:
```
error_class_twice = []
n_list = range(2,13)
for n in n_list:
    H = scipy.linalg.hilbert(n)
    # apply the classical procedure twice
    Q_class_1 = classical_gram_schmidt(H)[0]
    Q_class = classical_gram_schmidt(Q_class_1)[0]
    error_class_twice.append(np.linalg.norm(np.identity(n) - np.matmul(Q_class.
  ↪T,Q_class)))

plt.plot(n_list,error_class, label = 'Classical')
plt.plot(n_list,error_mod, label = 'Modified')
plt.plot(n_list,error_class_twice, label = 'Classical applied twice')
plt.yscale('log')
```

```
plt.xlabel('Matrix size ($n$)')
plt.ylabel('Error ($||I - Q^TQ||_2$)')
plt.legend()
plt.show()
```



3.4 (d) (2 pts)

Implement the Householder method for computing the QR decomposition. Remember to include a short documentation.

[ ]:
```
def householder_QR(A):
    """
    Input: matrix A (mxn) as numpy array
    Output: matrices Q (mxn), R(mxn), derived by QR decomposition with the␣
 ↪Householder method:
    Q orthogonal matrix and R upper triangular with rows of zeros below the␣
 ↪upper square
    Input matrix A is modified in the process to become R (as is seen in the␣
 ↪output).
    """
    A = A.astype(float)
```

```python
    n_rows,n_columns = A.shape
    Q = np.eye(n_rows)
    R = np.zeros((n_rows,n_columns))

    for k in range(n_columns):
        alpha_k = -np.sign(A[k,k]) * np.linalg.norm(A[k:n_rows,k])

        ek = np.zeros(n_rows)
        ek[k] = alpha_k

        ak = A[:,k].copy()
        ak[:k] = 0
        vk = ak - ek

        beta_k = np.inner(vk,vk)
        if beta_k != 0:
            for j in range(k,n_columns):
                gamma_j = np.inner(vk,A[:,j])
                A[:,j] -= (2*gamma_j/beta_k)*vk
            for j in range(0,n_columns):
                gamma_j = np.inner(vk,Q[:,j])
                Q[:,j] -= (2*gamma_j/beta_k)*vk

    R[:(n_rows - n_columns)] = A[:(n_rows - n_columns)]
    return Q,R,A

A = np.array([[1,0,0],[0,1,0],[0,0,1],[-1,1,0],[-1,0,1],[0,-1,1]])
print(f"input A:\n {A}")
Q, R, A = householder_QR(A)
print(f"Q:\n {Q}")
print(f"R:\n {R}")
print(f"output A:\n {A}")
```

```
input A:
 [[ 1  0  0]
 [ 0  1  0]
 [ 0  0  1]
 [-1  1  0]
 [-1  0  1]
 [ 0 -1  1]]
Q:
 [[-0.57735027  0.          0.          0.          0.          0.        ]
 [-0.20412415 -0.61237244  0.          0.          0.          0.        ]
 [-0.35355339 -0.35355339 -0.70710678  0.          0.          0.        ]
 [ 0.51133922 -0.48783152 -0.0235077   1.          0.          0.        ]
 [ 0.48783152  0.0235077  -0.51133922  0.          1.          0.        ]
 [-0.0235077   0.51133922 -0.48783152  0.          0.          1.        ]]
```

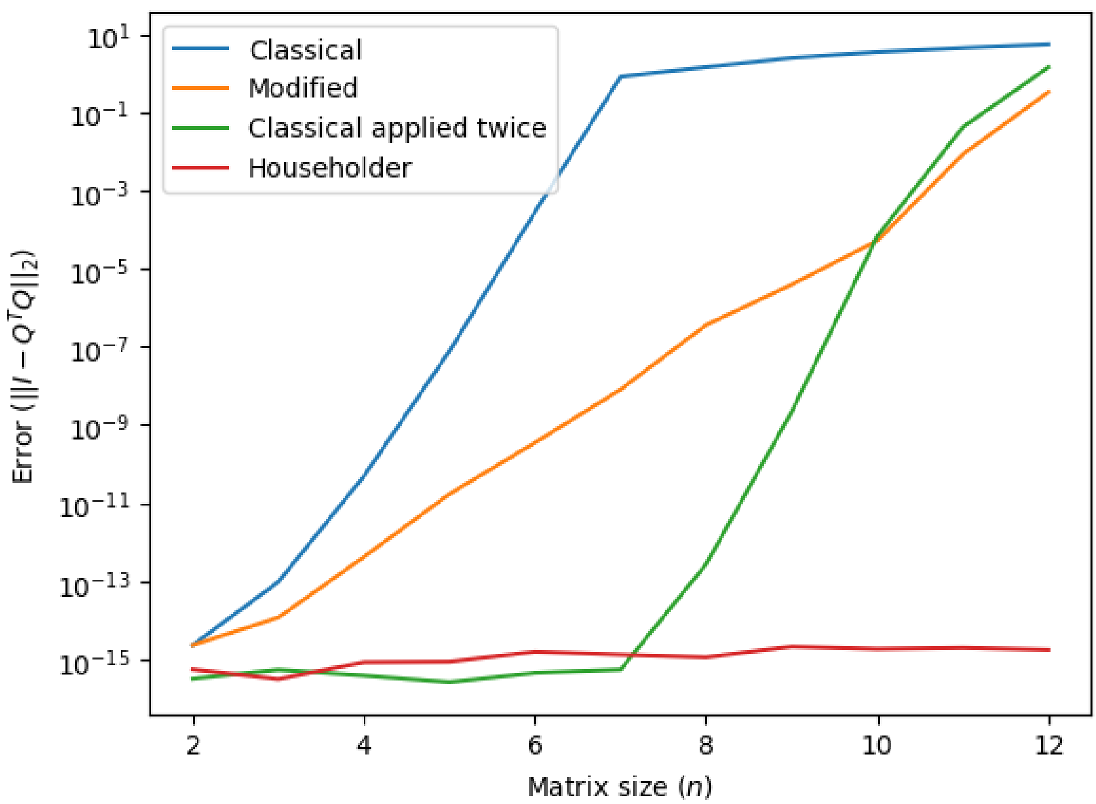
```
R:
 [[-1.73205081  0.57735027  0.57735027]
 [ 0.         -1.63299316  0.81649658]
 [ 0.          0.         -1.41421356]
 [ 0.          0.          0.        ]
 [ 0.          0.          0.        ]
 [ 0.          0.          0.        ]]
output A:
 [[-1.73205081e+00  5.77350269e-01  5.77350269e-01]
 [ 0.00000000e+00 -1.63299316e+00  8.16496581e-01]
 [ 0.00000000e+00  0.00000000e+00 -1.41421356e+00]
 [ 0.00000000e+00  0.00000000e+00  6.93889390e-18]
 [ 0.00000000e+00  0.00000000e+00  1.11022302e-16]
 [ 0.00000000e+00  0.00000000e+00  1.11022302e-16]]
```

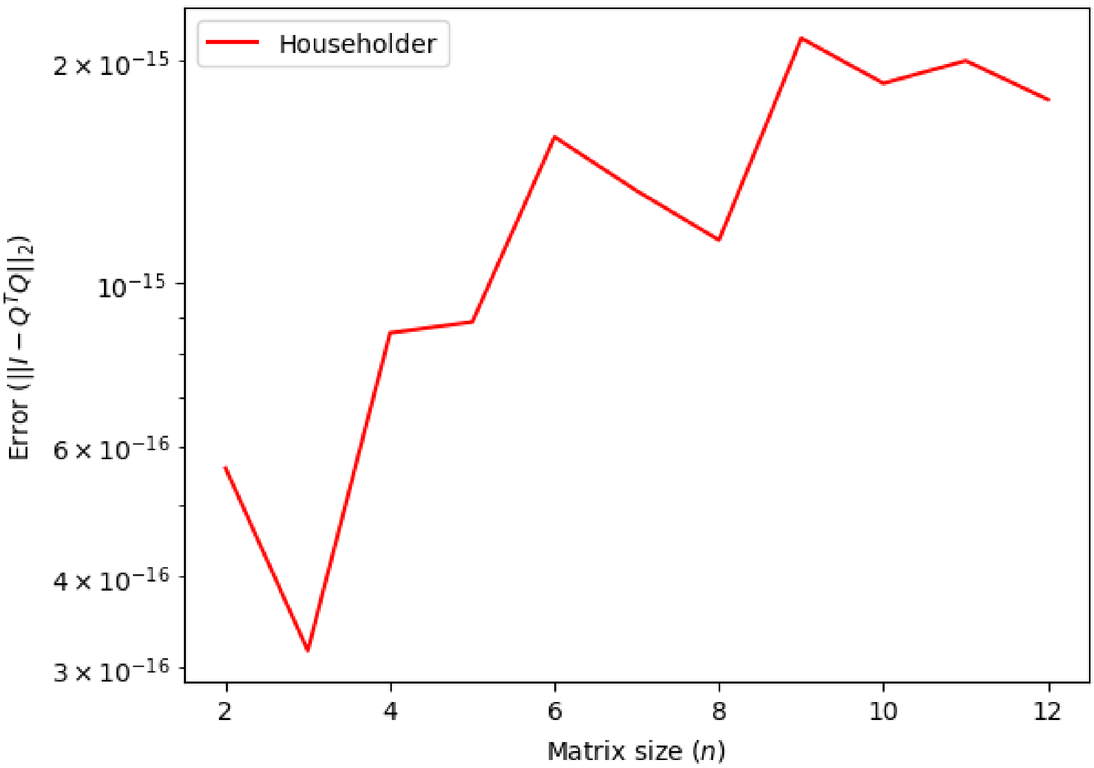
3.5 (e) (2 pts)

Perform the analysis of (b) for the Householder method. Discuss the differences between all the methods you have tested so far. Look online and/or in books for information about the accuracy of the different methods and include this in your explanations (with reference).

[ ]:
```
error_class, error_mod, error_house = [], [], []

n_list = range(2,13)
for n in n_list:
    # create Hilbert matrix
    H = scipy.linalg.hilbert(n)

    Q_class = classical_gram_schmidt(H)[0]
    error_class.append(np.linalg.norm(np.identity(n) - np.matmul(Q_class.
 ↪T,Q_class)))

    Q_mod = modified_gram_schmidt(H)[0]
    error_mod.append(np.linalg.norm(np.identity(n) - np.matmul(Q_mod.T,Q_mod)))

    Q_house = householder_QR(H)[0]
    error_house.append(np.linalg.norm(np.identity(n) - np.matmul(Q_house.
 ↪T,Q_house)))

plt.plot(n_list,error_class, label = 'Classical')
plt.plot(n_list,error_mod, label = 'Modified')
plt.plot(n_list,error_class_twice, label = 'Classical applied twice')
plt.plot(n_list,error_house, label = 'Householder')
plt.yscale('log')
plt.xlabel('Matrix size ($n$)')
plt.ylabel('Error ($||I - Q^TQ||_2$)')
plt.legend()
plt.show()
```

```
plt.plot(n_list,error_house, label = 'Householder', color = 'red')
plt.yscale('log')
plt.xlabel('Matrix size ($n$)')
plt.ylabel('Error ($||I - Q^TQ||_2$)')
plt.legend()
plt.show()
```





We observe that the error for both the Gram-Schmidt methods increases as the size of the Hilbert matrix (n) increases. The error for the classical method increases more steeply than the error for the modified version. At $n = 7$, the error of the classical Gram-Schmidt method stabilizes when it is almost equal to 1, and it remains above the error for the modified version for all values of n. When the classical method is applied twice, the error is smaller and mostly stable before $n = 7$, and increases afterwards. The error for the Householder method is small and remains approximately stable.

Heath (2018) states that the orthogonality in the columns of Q is lost due to rounding error [1]. We compute $\mathbf{q}_k = \mathbf{q}_k - r_{jk}\mathbf{q}_j$. Since we do not have $\mathbf{q}_j > 0$ in all cases, there is a risk of cancellation. In the modified version this error is less severe, but loss of orthogonality is still present [1]. This is similar to what we observe. Heath further notes that 'reorthogonalization' can significantly ehhance the orthogonality. We observe this when the classical procedure is applied twice. When $n > 7$, the rounding error starts to impact the orthogonality and the error increases.

For the Householder method, there is less chance of a cancellation error, since we can choose out of subtraction or addition when forming the columns of R. Heath states that the relative error is proportional to $\mathrm{cond(A)} + \|\mathrm{r}\|_2[\mathrm{cond(A)}]^2$. This is the best that can be done, since this is also the sensitivitty for a solution to the least squares problem [1]. Furthermore, the Householder method only breaks down if $\mathrm{cond(A)} \approx 1/\ _{\mathrm{mach}}$ or worse [1].

Reference: [1] Heath, M. T. (2018). Scientific computing: an introductory survey, revised second edition. Society for Industrial and Applied Mathematics.