Testing QR algorithm

Test problem

A test program qr_test.c was programmed for testing the accuracy of the QR and Householder algorithms. Similar or same test problems were used as was with NNLS algorithm (see modelling report TPCMOD0020). There a least squares problem $\min\|Ep - f\|$ was introduced, where values for the elements of f were calculated from some polynomial. Now values of $p_1 \ldots p_n$ are estimated with QR algorithm instead of NNLS. Results are compared to the results given by NNLS algorithm.

Test results

Problems of the first four tables are the same as presented in report TPCMOD0020. Both NNLS and QR algorithm give the right results in these cases. Now more problems were created to check how the QR algorithm performs when some of the parameters are to be negative. In table 5 we see an example of this kind of problem. Algorithm NNLS was also tested for this problem, but it was obvious to give wrong result because it doesn't accept negative values for model parameters. Algorithm QR gave right negative values.

Table 1. 2-parameter estimation.
```
qr_test 0.1  (c) 2003 by Turku PET Centre
Matrix A:
1 1
2 4
3 9
4 16
Vector b:
0.6 2.2 4.8 8.4
Result vector:0.1 0.5

nnls_test 0.1  (c) 2003 by Turku PET Centre
Matrix E:
1 1
2 4
3 9
4 16
Vector f:
0.6 2.2 4.8 8.4
Result vector:0.1 0.5
```

Table 2. 3-parameter estimation.

```
qr_test 0.1  (c) 2003 by Turku PET Centre
Matrix A:
1 1 1
2 4 8
3 9 27
4 16 64
Vector b:
0.73 3.24 8.31 16.72
Result vector:0.1 0.5 0.13

nnls_test 0.1  (c) 2003 by Turku PET Centre
Matrix E:
1 1 1
2 4 8
3 9 27
4 16 64
Vector f:
0.73 3.24 8.31 16.72
Result vector:0.1 0.5 0.13
```

Table 3. 4-parameter estimation, where the fourth parameter is zero.

```
qr_test 0.1  (c) 2003 by Turku PET Centre
Matrix A:
1 1 1 1
2 4 8 16
3 9 27 81
4 16 64 256
Vector b:
0.73 3.24 8.31 16.72
Result vector:0.1 0.5 0.13 1.75196e-16

nnls_test 0.1  (c) 2003 by Turku PET Centre
Matrix E:
1 1 1 1
2 4 8 16
3 9 27 81
4 16 64 256
Vector f:
0.73 3.24 8.31 16.72
Result vector:0.1 0.5 0.13 0
```

Table 4. 3-parameter estimation, where the second parameter is zero.

```
qr_test 0.1  (c) 2003 by Turku PET Centre
Matrix A:
1 1 1
2 4 8
3 9 27
4 16 64
Vector b:
0.23 1.24 3.81 8.72
Result vector:0.1 -4.31099e-16 0.13


nnls_test 0.1  (c) 2003 by Turku PET Centre
Matrix E:
1 1 1
2 4 8
3 9 27
4 16 64
Vector f:
0.23 1.24 3.81 8.72
Result vector:0.1 7.26423e-16 0.13
```

Table 5. 2-parameter estimation for negative parameter value.
```
qr_test 0.1  (c) 2003 by Turku PET Centre
Matrix A:
1 1
2 4
3 9
4 16
Vector b:
1 6 15 28
Result vector:-1 2


nnls_test 0.2  (c) 2003 by Turku PET Centre
Matrix A:
1 1
2 4
3 9
4 16
Vector b:
1 6 15 28
Result vector:0 1.71751
```