

Testing NNLS algorithm

Test problem

A test program test_nnls.c was programmed for testing the accuracy of the NNLS algorithm. We introduced a problem $\min \|Ep - f\|$, where the values in f are calculated from some polynomial. For example the values of polynomial $y(x) = p_1x + p_2x^2$ are calculated at points $x=1,2,3,4$ with fixed p_1 and p_2 . Then the columns of E hold the values of polynomial $y(x)=x$ and polynomial $y(x) = x^2$ at points $x=1,2,3,4$. The values of p_1 and p_2 are then estimated with NNLS.

Test results

Tables 1-4 show output of the test program in four different occasions. In the first problem (Table 1.) values of vector f were calculated from polynomial $y(x)=0.1x+0.5x^2$ and the columns of matrix E hold the values of $y(x)=x$ and $y(x) = x^2$ at points $x=1,2,3,4$. Last row of Table 1. shows that values of parameters p_1 and p_2 were estimated correctly.

In the second problem (Table 2) a third column was added to matrix E . It contained values of polynomial $y(x) = x^3$. Values of vector f were now calculated from polynomial $y(x) = 0.1x + 0.5x^2 + 0.13x^3$. The estimates were correct also in this case.

Table 1. 2-parameter estimation.

```
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.

```
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
```

Of course NNLS should work also when some of the parameter values are to be zero. This was verified by adding one parameter to problem of Table 2, thus adding matrix E one column containing the values of polynomial $y(x) = x^4$, but keeping the vector f unaltered. The results are shown in Table 3.

The fourth problem (Table 4.) is a three-parameter estimation, where matrix E is the same as in problem 2 but values of vector f are calculated from polynomial $y(x) = 0.1x + 0.13x^3$. Now the zero result was found with the accuracy of 16 decimals.

The differences between zero results in tables 3 and 4 are due to basic functioning of the algorithm. It processes parameters in two sets P and Z , which were described together with the flow chart (Figure 1). In problem 3, algorithm has interpreted parameter p_4 to be in the set Z but in problem 4 it doesn't put parameter p_2 in set Z although we do interpret it as zero.

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

```
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.

```
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
```