NA13 Metoda najmanjih kvadrata

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1 Metoda najmanjih kvadrata

Neka je zadan sustav s više jednadžbi od nepoznanica:

$$Ax = b, \quad m > n.$$

Ako sustav ima rješenje, tada je je $Ax - b = 0$, odnosno $\|Ax - b\| = 0$ za svaku vektorsku normu. Ako sustav nema rješenje, tada je prirodno tražiti rješenje za koje je

$$\|Ax - b\|_{1,2,\infty} \to \min$$

za odabranu vektorsku normu.
Ako je rang $A = n$, tada se *jedinstveno* rješenje x za koje

$$\|Ax - b\|_2 \to \min$$

dobije rješavanjem sustava *normalnih jednadžbi*:

$$A^T Ax = A^T b. \tag{*}$$

Dokaz: Definirajmo

$$Q(x) = \|Ax - b\|_2^2 = (x^T A^T - b^T)(Ax - b) = x^T A^T Ax - 2x^T A^T b + b^T b.$$

Vrijedi

$$\begin{aligned}
Q(x + h) &= (x^T + h^T)A^T A(x + h) - 2(x^T + h^T)A^T b + b^T b \\
&= Q(x) + 2h^T(A^T Ax - A^T b) + h^T A^T Ah \\
&= Q(x) + \|Ah\|_2^2 \\
&\geq Q(x),
\end{aligned}$$

pa se minimum zaista postiže u x.

Rješenje je jedinstveno jer $Q(x) = Q(y)$ povlači $\|Ax\|_2 = 0$ pa je ili $h = 0$ ili rang $A < n$ što je kontradikcija. *QED*

Geometrijsko značenje: Vektori Ax i $Ax - b$ su međusobno okomiti,

$$(Ax)^T \cdot (Ax - b) = x^T(A^T Ax - A^T b) = 0.$$

Dakle, Ax je ortogonalna projekcija vektora b na skup $\{Ay : \ y \text{ proizvoljan}\}$.

Kvaliteta prilagodbe: Rješenje x zove se *kvadratična prilagodba* sustavu $Ax = b$ u smislu najmanjih kvadrata. Kvalitetu prilagodbe mjerimo s

$$q = \sqrt{\frac{Q(x)}{Q(0)}} = \frac{\|Ax - b\|_2}{\|b\|_2}.$$

1.1 Primjer

Riješimo sustav

$$\begin{aligned} x + y &= 0 \\ y + z &= 1 \\ x + z &= 0 \\ -x + y + z &= 1 \\ -x - z &= 0 \end{aligned}$$

u smislu najmanjih kvadrata.

```
In [1]: A=[1//1 1 0;0 1 1;1 0 1;-1 1 1;-1 0 -1]
```

```
Out[1]: 5×3 Array{Rational{Int64},2}:
          1//1  1//1   0//1
          0//1  1//1   1//1
          1//1  0//1   1//1
         -1//1  1//1   1//1
         -1//1  0//1  -1//1
```

```
In [2]: b=collect([0//1,1,0,1,0])
```

```
Out[2]: 5-element Array{Rational{Int64},1}:
         0//1
         1//1
         0//1
         1//1
         0//1
```

```
In [3]: x=(A'*A)\(A'*b)
```

```
Out[3]: 3-element Array{Rational{Int64},1}:
         -10//29
          12//29
          11//29
```

```
In [4]: using LinearAlgebra
        # Kvaliteta prilagodbe
        q=sqrt(norm(A*x-b)/norm(b))
```

```
Out[4]: 0.430923819458906
```

Ako je sustav predefiniran, standardna naredba odmah računa kvadratičnu prilagodbu, pri čemu se koristi QR rastav:

```
In [5]: x1=float(A)\float(b)
```

```
Out[5]: 3-element Array{Float64,1}:
         -0.3448275862068966
          0.4137931034482762
          0.37931034482758635
```

```
In [6]: float(x)
```

```
Out[6]: 3-element Array{Float64,1}:
         -0.3448275862068966
          0.41379310344827586
          0.3793103448275862
```

1.2 Primjer

```
In [7]: import Random
        Random.seed!(123);
        A=rand(20,10)
        b=rand(20);
```

```
In [8]: x=A\b
```

```
Out[8]: 10-element Array{Float64,1}:
          0.09126520276532538
          0.23253293726975455
         -0.23867707369510557
         -0.16294801609881096
          0.08926547724020181
          0.2631846339836788
          0.5435390650803672
         -0.11240823390574475
         -0.045249764335415894
         -0.01306538784642609
```

```
In [9]: q=sqrt(norm(A*x-b)/norm(b))
```

```
Out[9]: 0.680981882736473
```

1.3 Točnost

Osjetljivost problema najmanjih kvadarata dana je sljedećim ocjenama (vidi Matrix Computations, poglavlje 5):

Za matricu A *kondiciju* definiramo na sljedeći način:

$$\kappa_2(A) = \sqrt{\kappa(A^T A)} = \|A\|_2 \|(A^T A)^{-1} A^T\|_2.$$

Neka su x i $\hat x$, kvadratične prilagodbe sustava $Ax = b$ i $(A + \delta A)\hat x = b + \delta b$. *Reziduali* su definirani s

$$\begin{aligned} r &= Ax - b \\ \hat r &= (A + \delta A)\hat x - (b + \delta b). \end{aligned}$$

Neka je

$$\epsilon = \max \left\{ \frac{\|\delta A\|_2}{\|A\|_2}, \frac{\|\delta b\|_2}{\|b\|_2} \right\}$$

i neka je

$$q = \frac{\|r\|_2}{\|b\|_2} \equiv \sin\theta < 1.$$

Vrijedi:

$$\begin{aligned} \frac{\|\hat x - x\|_2}{\|x\|_2} &\leq \epsilon \left[\frac{2\,\kappa_2(A)}{\cos\theta} + \tan\theta\, \kappa_2^2(A) \right] + O(\epsilon^2), \\ \frac{\|\hat r - r\|_2}{\|b\|_2} &\leq \epsilon\,[1 + 2\,\kappa_2(A)](m - n) + O(\epsilon^2). \end{aligned}$$

Vidimo da je rezidual manje osjetljiv od samog mjesta na kojem se postiže.

```
In [10]: cond(A)
```

```
Out[10]: 17.55193806289537
```

```
In [11]: δA=1e-4*(rand(20,10).-0.5)
```

```
Out[11]: 20×10 Array{Float64,2}:
           3.70804e-5  -1.46483e-5   3.78108e-5  …  -3.40051e-6   2.97237e-7
          -2.92476e-5  -3.01169e-5  -7.11582e-7     -3.10979e-5  -7.3709e-6
          -3.62478e-5  -4.62203e-5  -2.18e-5         3.34273e-5   1.22474e-5
          -1.4055e-5   -2.2101e-5    2.47534e-5     -3.17975e-5  -2.09256e-5
           9.99739e-6  -3.74349e-5   4.32239e-5     -2.72284e-5  -4.57705e-5
          -1.5921e-5   -4.15485e-5   4.53109e-6  …  -1.20715e-5   1.95729e-5
           1.56878e-5  -3.85177e-6   2.79167e-6     -3.39768e-5  -4.07255e-6
          -2.53126e-5   2.53036e-5  -8.00883e-6     -5.53739e-6  -1.31477e-5
           2.30285e-5   2.34625e-5  -1.08889e-5      3.90731e-6  -2.69901e-5
           2.9528e-5   -1.62549e-6   4.34735e-5     -4.67067e-5   3.4356e-5
           4.91776e-6  -1.25858e-5   2.52665e-5  …   1.57212e-5  -3.02322e-5
          -6.00838e-6  -1.4645e-5   -3.7536e-5       1.70556e-5   3.07931e-5
          -3.54482e-5  -4.57917e-5   4.34059e-5     -2.36215e-5  -7.05426e-6
           1.69838e-6  -3.42984e-5   4.95414e-5     -1.88728e-5  -3.29889e-5
           4.96909e-5   4.42417e-5  -1.32862e-6     -3.70811e-5   2.87517e-5
           3.80923e-5   3.61648e-5   6.22363e-6  …  -3.25223e-5   1.18442e-5
          -4.28172e-5   1.33864e-5   3.72266e-5      2.20163e-5   3.23573e-5
          -4.69022e-6   1.68004e-5   3.71808e-5     -4.6524e-6    5.6063e-6
          -2.18221e-5  -8.96464e-6  -2.35e-5         8.03785e-6   1.71421e-5
          -4.7337e-5    3.4914e-5    3.55016e-5      4.07858e-5   4.00353e-5
```

```
In [12]: x1=(A+δA)\b
```

```
Out[12]: 10-element Array{Float64,1}:
           0.09124152035466916
           0.23255326896117634
          -0.23868978883842978
          -0.16295402718226268
           0.08928215497482153
           0.2631596591254608
           0.543496075864643
          -0.11242053952020302
          -0.04521690131702883
          -0.012995050999963656
```

```
In [13]: r=A*x-b
         r1=(A+δA)*x-b
```

```
Out[13]: 20-element Array{Float64,1}:
           0.2803107040893482
          -0.0017144735606671735
           0.03004676820080543
           0.1517928600635049
           0.1353865009669705
          -0.17325632694031823
           0.23916745374473725
```

```
 0.40511466709329863
-0.06326100077670932
-0.03770546855670237
-0.3342609373365829
-0.05250034421081984
 0.1680616083026139
-0.024255067059543278
-0.207203911044531
-0.21422109905026337
-0.09908169394354915
 0.10596216301245184
-0.27006014566494485
-0.457322890886751
```

```
In [14]: norm(x1-x)/norm(x), norm(r1-r)/norm(b)
```

```
Out[14]: (0.00013760412992742412, 4.6690121366230774e-5)
```

Napomena: Ako je rang $A = n$, matrica $A^T A$ je simetrična i pozitivno definitna pa se sustav (*) može riješiti metodom Choleskog.

Za izračunato rješenje $\hat{x}$ vrijedi

$$(A^T A + E)\hat{x} = A^T b,$$

gdje je

$$\|A\|_2 \approx \varepsilon \|A^T A\|_2,$$

pa za relativnu pogrešku vrijedi ocjena

$$\frac{\|\hat{x} - x\|_2}{\|x\|_2} \approx \varepsilon \kappa_2(A^T A) = \varepsilon \kappa_2^2(A).$$

Dakle, relativna pogreška rješenja dobivenog pomoću metode normalnih jednadžbi ovisi o *kvadratu kondicije* pa je bolje koristiti QR rastav.