

(\*Die Bestimmung der Konstanten K1,K2 und K3 mittels einer gestörten Datenbasis\*)

(\*die stochiometrische Matrix: \*)

S := {{-2, -2, -1}, {-1, 0, -1}, {0, 1, -1}}

(\*die Funktion  $\rho$ : \*)

$\rho[\{x_, y_, z_}, K_, L_, M_] := S.\{K*x^2*y, L*x^2, M*x*y*z\} + \{x, y, z\}$

$\rho[\{x, y, z\}, K, L, M];$

$\rho\rho[\{x_, y_, z_}, K_, L_, M_] := \rho[\rho[\{x, y, z\}, K, L, M], K, L, M];$

$\rho\rho[\{x_, y_, z_}, K_, L_, M_];$

(\* Der nächste Vektor enthält alle Monome in K\_1,  
K\_2 und K\_3, die in wenigstens einer der drei Zeilen von  
 $\rho\rho$  als Koeffizienten der Polynome in x,y und z auftreten \*)

Konstantenvektor := {1, K1, K1<sup>2</sup>, K1<sup>3</sup>, K1<sup>4</sup>, K2, K1 K2, K1<sup>2</sup> K2, K1<sup>3</sup> K2, K2<sup>2</sup>,  
K1 K2<sup>2</sup>, K1<sup>2</sup> K2<sup>2</sup>, K2<sup>3</sup>, K3, K1 K3, K1<sup>2</sup> K3, K1<sup>3</sup> K3, K2 K3, K1 K2 K3, K1<sup>2</sup> K2 K3, K2<sup>2</sup> K3,  
K1 K2<sup>2</sup> K3, K3<sup>2</sup>, K1 K3<sup>2</sup>, K1<sup>2</sup> K3<sup>2</sup>, K2 K3<sup>2</sup>, K1 K2 K3<sup>2</sup>, K2<sup>2</sup> K3<sup>2</sup>, K3<sup>3</sup>, K1 K3<sup>3</sup>, K2 K3<sup>3</sup>, K3<sup>4</sup>}

(\* Dies sind die Polynome in x,y,z der drei Zeilen von  $\rho\rho$ ,  
vor denen die Konstanten K1, K2 und K3 auftreten: \*)

Monomvektor =

{ {x, -4 x<sup>2</sup> y, 2 x<sup>4</sup> y + 8 x<sup>3</sup> y<sup>2</sup>, -8 x<sup>5</sup> y<sup>2</sup> - 8 x<sup>4</sup> y<sup>3</sup>, 8 x<sup>6</sup> y<sup>3</sup>, -4 x<sup>2</sup>, 16 x<sup>3</sup> y, -8 x<sup>5</sup> y - 24 x<sup>4</sup> y<sup>2</sup>, 16 x<sup>6</sup> y<sup>2</sup>,  
8 x<sup>3</sup>, -24 x<sup>4</sup> y, 8 x<sup>6</sup> y, -8 x<sup>4</sup>, -2 x y z, 3 x<sup>3</sup> y z + 6 x<sup>2</sup> y<sup>2</sup> z, -14 x<sup>4</sup> y<sup>2</sup> z - 8 x<sup>3</sup> y<sup>3</sup> z, 16 x<sup>5</sup> y<sup>3</sup> z,  
-x<sup>3</sup> y + 6 x<sup>2</sup> y z, x<sup>5</sup> y + 2 x<sup>4</sup> y<sup>2</sup> - 10 x<sup>4</sup> y z - 16 x<sup>3</sup> y<sup>2</sup> z, -2 x<sup>6</sup> y<sup>2</sup> + 24 x<sup>5</sup> y<sup>2</sup> z, 2 x<sup>4</sup> y - 8 x<sup>3</sup> y z,  
-2 x<sup>6</sup> y + 8 x<sup>5</sup> y z, x<sup>2</sup> y<sup>2</sup> z + x<sup>2</sup> y z<sup>2</sup> + x y<sup>2</sup> z<sup>2</sup>, -x<sup>4</sup> y<sup>2</sup> z - 2 x<sup>3</sup> y<sup>3</sup> z - 7 x<sup>3</sup> y<sup>2</sup> z<sup>2</sup> - 2 x<sup>2</sup> y<sup>3</sup> z<sup>2</sup>,  
2 x<sup>5</sup> y<sup>3</sup> z + 10 x<sup>4</sup> y<sup>3</sup> z<sup>2</sup>, x<sup>4</sup> y z - x<sup>3</sup> y<sup>2</sup> z - 2 x<sup>3</sup> y z<sup>2</sup> - 2 x<sup>2</sup> y<sup>2</sup> z<sup>2</sup>, -x<sup>5</sup> y<sup>2</sup> z + 8 x<sup>4</sup> y<sup>2</sup> z<sup>2</sup>,  
-2 x<sup>5</sup> y z, -x<sup>3</sup> y<sup>2</sup> z<sup>2</sup> - x<sup>2</sup> y<sup>3</sup> z<sup>2</sup> - x<sup>2</sup> y<sup>2</sup> z<sup>3</sup>, 3 x<sup>4</sup> y<sup>3</sup> z<sup>2</sup> + 2 x<sup>3</sup> y<sup>3</sup> z<sup>3</sup>, x<sup>4</sup> y<sup>2</sup> z<sup>2</sup>, x<sup>3</sup> y<sup>3</sup> z<sup>3</sup> },  
{y, -2 x<sup>2</sup> y, x<sup>4</sup> y + 4 x<sup>3</sup> y<sup>2</sup>, -4 x<sup>5</sup> y<sup>2</sup> - 4 x<sup>4</sup> y<sup>3</sup>, 4 x<sup>6</sup> y<sup>3</sup>, 0, 4 x<sup>3</sup> y, -4 x<sup>5</sup> y - 8 x<sup>4</sup> y<sup>2</sup>,  
8 x<sup>6</sup> y<sup>2</sup>, 0, -4 x<sup>4</sup> y, 4 x<sup>6</sup> y, 0, -2 x y z, 2 x<sup>3</sup> y z + 4 x<sup>2</sup> y<sup>2</sup> z, -8 x<sup>4</sup> y<sup>2</sup> z - 4 x<sup>3</sup> y<sup>3</sup> z,  
8 x<sup>5</sup> y<sup>3</sup> z, -x<sup>3</sup> y + 2 x<sup>2</sup> y z, x<sup>5</sup> y + 2 x<sup>4</sup> y<sup>2</sup> - 6 x<sup>4</sup> y z - 4 x<sup>3</sup> y<sup>2</sup> z, -2 x<sup>6</sup> y<sup>2</sup> + 12 x<sup>5</sup> y<sup>2</sup> z, 2 x<sup>4</sup> y,  
-2 x<sup>6</sup> y + 4 x<sup>5</sup> y z, x<sup>2</sup> y<sup>2</sup> z + x<sup>2</sup> y z<sup>2</sup> + x y<sup>2</sup> z<sup>2</sup>, -x<sup>4</sup> y<sup>2</sup> z - 2 x<sup>3</sup> y<sup>3</sup> z - 5 x<sup>3</sup> y<sup>2</sup> z<sup>2</sup> - x<sup>2</sup> y<sup>3</sup> z<sup>2</sup>,  
2 x<sup>5</sup> y<sup>3</sup> z + 5 x<sup>4</sup> y<sup>3</sup> z<sup>2</sup>, x<sup>4</sup> y z - x<sup>3</sup> y<sup>2</sup> z - 2 x<sup>3</sup> y z<sup>2</sup>, -x<sup>5</sup> y<sup>2</sup> z + 4 x<sup>4</sup> y<sup>2</sup> z<sup>2</sup>, -2 x<sup>5</sup> y z,  
-x<sup>3</sup> y<sup>2</sup> z<sup>2</sup> - x<sup>2</sup> y<sup>3</sup> z<sup>2</sup> - x<sup>2</sup> y<sup>2</sup> z<sup>3</sup>, 3 x<sup>4</sup> y<sup>3</sup> z<sup>2</sup> + x<sup>3</sup> y<sup>3</sup> z<sup>3</sup>, x<sup>4</sup> y<sup>2</sup> z<sup>2</sup>, x<sup>3</sup> y<sup>3</sup> z<sup>3</sup> },  
{z, 0, 0, 0, 0, 2 x<sup>2</sup>, -4 x<sup>3</sup> y, 4 x<sup>4</sup> y<sup>2</sup>, 0, -4 x<sup>3</sup>, 8 x<sup>4</sup> y, 0, 4 x<sup>4</sup>, -2 x y z,  
x<sup>3</sup> y z + 2 x<sup>2</sup> y<sup>2</sup> z, -2 x<sup>4</sup> y<sup>2</sup> z, 0, -x<sup>3</sup> y, x<sup>5</sup> y + 2 x<sup>4</sup> y<sup>2</sup> - 2 x<sup>4</sup> y z + 4 x<sup>3</sup> y<sup>2</sup> z,  
-2 x<sup>6</sup> y<sup>2</sup>, 2 x<sup>4</sup> y + 4 x<sup>3</sup> y z, -2 x<sup>6</sup> y, x<sup>2</sup> y<sup>2</sup> z + x<sup>2</sup> y z<sup>2</sup> + x y<sup>2</sup> z<sup>2</sup>,  
-x<sup>4</sup> y<sup>2</sup> z - 2 x<sup>3</sup> y<sup>3</sup> z - 3 x<sup>3</sup> y<sup>2</sup> z<sup>2</sup>, 2 x<sup>5</sup> y<sup>3</sup> z, x<sup>4</sup> y z - x<sup>3</sup> y<sup>2</sup> z - 2 x<sup>3</sup> y z<sup>2</sup> + x<sup>2</sup> y<sup>2</sup> z<sup>2</sup>,  
-x<sup>5</sup> y<sup>2</sup> z, -2 x<sup>5</sup> y z, -x<sup>3</sup> y<sup>2</sup> z<sup>2</sup> - x<sup>2</sup> y<sup>3</sup> z<sup>2</sup> - x<sup>2</sup> y<sup>2</sup> z<sup>3</sup>, 3 x<sup>4</sup> y<sup>3</sup> z<sup>2</sup>, x<sup>4</sup> y<sup>2</sup> z<sup>2</sup>, x<sup>3</sup> y<sup>3</sup> z<sup>3</sup> } };

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(* Wir erzeugen uns nun ein paar Daten in dreier-Tupeln;
   der Einfachheit halber durchrastern wir den
   Würfel in 0.1 er Schritten *)

Eingabedaten =
  Flatten[Table[{x, y, z}, {x, 0, 1.8, 0.1}, {y, 0, 1.8, 0.1}, {z, 0, 1.8, 0.1}], 2];

(* Die Anzahl der 3-Tupel: *)

Length[Eingabedaten]

6859

(* In den folgenden paar Zeilen werden diejenigen Eingabedaten entfernt,
   auf denen die Funktion  $\rho$  negative Werte annimmt *)

Xi0 = Table[ $\rho$ [Part[Eingabedaten, n], 2, 4, 3], {n, 1, Length[Eingabedaten], 1}];

Hilf0 = x * Xi0;

Hilf2 = b * Eingabedaten;

Hilf0 + Hilf2;

Hilf3 = Cases[Hilf0 + Hilf2,
  {x * (g_ /; g > 0) + b * h_, x * (k_ /; k > 0) + b * l_, x * (j_ /; j > 0) + b * m_}];

(* Leider haben nun die Ausgabedaten verschiedene Größenordnungen,
   so dass der LEAST-SQUARE
   ALGORITHMUS, den wir später anwenden wollen,
   nicht richtig arbeiten kann. Wir sortieren also
   noch die Werte raus, deren Größenordnung nicht zwischen  $10^2$  und  $10^3$  liegt *)

Hilf4 = Cases[Hilf3,
  {x * (g_ /; g > 100) + b * h_, x * (k_ /; k > 100) + b * l_, x * (j_ /; j > 100) + b * m_}];

Length[Hilf4]

1743

Hilf5 = Cases[Hilf4,
  {x * (g_ /; g < 1000) + b * h_, x * (k_ /; k < 1000) + b * l_, x * (j_ /; j < 1000) + b * m_}];

(* Das ist nun die neue Anzahl von Tripeln: *)

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Length[Hilf5]

343

{ \* Wir erhalten also als neue Eingabedaten : \* }

EingabeNeu = Hilf5 /. {b -> 1, x -> 0};

(\* Auf diesen Werten nimmt  $\rho\rho$  die folgenden positiven Werte an: \*)

AusgabeNeu = Hilf5 /. {b -> 0, x -> 1}

{{112.462, 209.997, 178.454}, {108.398, 212.644, 184.608},  
{155.672, 252.572, 207.246}, {105.086, 204.357, 161.394},  
{123.418, 226.708, 179.025}, {169.097, 263.327, 196.994}, {135.161, 243.784, 193.956},  
{187.671, 285.876, 215.038}, {246.578, 332.283, 237.998}, {139.154, 254.666, 205.615},  
{197.934, 301.872, 229.67}, {264.302, 354.227, 256.028}, {338.647, 411.98, 284.804},  
{134.647, 258.734, 213.595}, {198.856, 310.492, 240.368}, {271.904, 368.278, 269.897},  
{354.267, 432.402, 302.328}, {446.423, 503.177, 337.806}, {121.334, 255.691, 217.667},  
{189.863, 311.246, 246.796}, {268.517, 373.736, 279.153}, {357.876, 443.544, 314.918},  
{458.519, 521.048, 354.273}, {571.024, 606.63, 397.399}, {170.868, 303.993, 248.814},  
{253.781, 370.264, 283.542}, {348.813, 444.851, 322.199}, {456.657, 528.212, 365.009},  
{578.011, 620.807, 412.195}, {713.569, 723.096, 463.98}, {132.118, 248.281, 179.43},  
{179.056, 283.814, 193.766}, {118.474, 247.625, 188.422}, {170.795, 287.711, 205.391},  
{228.979, 331.633, 223.856}, {293.28, 379.553, 243.885}, {139.486, 273.584, 208.046},  
{201.657, 321.154, 228.777}, {271.186, 373.582, 251.492}, {348.412, 431.085, 276.288},  
{433.676, 493.882, 303.262}, {150.616, 291.969, 224.167}, {222.144, 346.721, 248.557},  
{302.666, 407.453, 275.474}, {392.624, 474.451, 305.049}, {492.457, 548., 337.415},  
{602.605, 628.388, 372.704}, {150.331, 301.62, 236.14}, {230.28, 362.94, 263.92},  
{320.979, 431.447, 294.814}, {422.986, 507.506, 328.998}, {536.859, 591.483, 366.645},  
{663.155, 683.744, 407.928}, {802.432, 784.655, 453.021}, {137.763, 301.857, 243.578},  
{224.766, 368.824, 274.313}, {324.359, 444.248, 308.786}, {437.238, 528.586, 347.22},  
{564.099, 622.298, 389.837}, {705.636, 725.843, 436.86}, {862.545, 839.681, 488.513},  
{112.766, 292.509, 246.366}, {205.042, 363.914, 279.471}, {311.798, 445.079, 316.954},  
{433.888, 536.573, 359.095}, {572.166, 638.962, 406.176}, {727.486, 752.814, 458.477},  
{900.701, 878.696, 516.278}, {171.328, 348.301, 279.423}, {283.096, 433.739, 319.19},  
{412.275, 530.94, 364.324}, {559.901, 640.596, 415.174}, {727.007, 763.398, 472.085},  
{914.63, 900.038, 535.405}, {124.628, 322.638, 274.496}, {238.883, 410.613, 315.685},  
{372.609, 511.778, 362.941}, {527.046, 626.963, 416.689}, {703.432, 757., 477.35},  
{903.008, 902.72, 545.349}, {136.321, 276.685, 182.165}, {186.366, 312.248, 192.961},  
{150.677, 300.329, 203.873}, {211.335, 343.824, 218.34}, {277.855, 391.034, 234.09},  
{350.455, 442.097, 251.18}, {135.7, 302.326, 216.719}, {204.643, 352.262, 234.282},  
{281.06, 406.997, 253.618}, {365.259, 466.729, 274.812}, {457.551, 531.657, 297.953},  
{558.244, 601.979, 323.128}, {164.94, 336.313, 239.866}, {247.858, 396.339, 261.83},  
{340.329, 462.559, 286.201}, {442.774, 535.246, 313.105}, {555.616, 614.674, 342.668},  
{679.275, 701.117, 375.015}, {814.174, 794.848, 410.273}, {180.155, 360.085, 258.966},  
{276.447, 429.826, 285.179}, {384.595, 507.308, 314.514}, {505.156, 592.899, 347.143},  
{638.687, 686.964, 383.241}, {785.748, 789.868, 422.981}, {946.895, 901.978, 466.538},  
{179.007, 371.985, 273.239}, {287.408, 450.602, 303.314}, {410.154, 538.639, 337.289},  
{547.966, 636.574, 375.395}, {701.564, 744.881, 417.866}, {871.669, 864.038, 464.933},

{160.173, 371.066, 282.271}, {278.758, 457.266, 315.589}, {414.321, 554.663, 353.632},  
{567.773, 663.864, 396.701}, {740.027, 785.475, 445.099}, {931.994, 920.103, 499.127},  
{123.43, 357.154, 286.048}, {249.643, 449.208, 321.773}, {395.556, 554.296, 363.071},  
{562.302, 673.176, 410.328}, {751.017, 806.609, 463.926}, {962.833, 955.352, 524.25},  
{200.395, 426.645, 322.059}, {353.55, 537.315, 365.582}, {530.542, 663.805, 416.004},  
{732.761, 807.05, 473.807}, {961.596, 967.984, 539.47}, {132.545, 390.627, 317.067},  
{289.261, 504.377, 361.592}, {472.805, 635.964, 413.942}, {684.859, 786.523, 474.708},  
{927.105, 957.19, 544.478}, {204.899, 457.011, 351.973}, {390.738, 590.797, 404.829},  
{608.317, 745.734, 467.1}, {859.649, 923.182, 539.501}, {152.953, 331.715, 199.157},  
{214.177, 372.578, 207.82}, {280.273, 416.397, 217.295}, {118.761, 326.045, 216.988},  
{189.489, 374.089, 228.685}, {266.814, 426.22, 241.664}, {350.968, 482.584, 255.986},  
{442.181, 543.327, 271.712}, {540.685, 608.596, 288.903}, {103.364, 332., 234.176},  
{185.682, 388.423, 249.066}, {276.681, 450.303, 265.814}, {376.7, 517.858, 284.52},  
{486.079, 591.306, 305.279}, {605.155, 670.866, 328.19}, {734.27, 756.756, 353.35},  
{873.762, 849.194, 380.857}, {138.413, 372.366, 259.085}, {238.937, 441.298, 278.478},  
{350.813, 517.446, 300.489}, {474.52, 601.12, 325.26}, {610.533, 692.631, 352.938},  
{759.33, 792.29, 383.667}, {921.388, 900.408, 417.594}, {155.012, 399.978, 279.972},  
{273.084, 480.992, 303.658}, {405.507, 571.198, 330.823}, {552.927, 671.024, 361.671},  
{715.994, 780.897, 396.409}, {895.353, 901.242, 435.243}, {149.883, 412.653, 296.013},  
{283.906, 504.676, 323.466}, {435.557, 608.059, 355.345}, {605.691, 723.368, 391.931},  
{795.16, 851.171, 433.505}, {121.197, 409.206, 306.881}, {268.636, 510.534, 337.268},  
{437.2, 625.531, 373.09}, {627.989, 754.934, 414.719}, {842.105, 899.478, 462.525},  
{226.116, 497.854, 344.99}, {408.302, 622.245, 383.665}, {616.646, 763.642, 429.293},  
{852.537, 922.981, 482.353}, {156.889, 467.096, 347.133}, {348.488, 598.041, 387.283},  
{570.282, 748.656, 435.544}, {823.997, 920.109, 492.522}, {259.195, 553.999, 384.77},  
{489.411, 710.439, 434.012}, {755.977, 890.64, 493.246}, {143.654, 492.419, 377.537},  
{376.455, 650.755, 425.878}, {649.981, 835.724, 485.429}, {235.697, 572.627, 412.921},  
{509.508, 757.872, 470.635}, {831.295, 974.57, 541.783}, {114.616, 359.169, 205.353},  
{182.271, 401.458, 209.371}, {254.81, 446.616, 214.033}, {332.365, 494.724, 219.369},  
{181.998, 424.948, 240.686}, {271.895, 481.937, 249.143}, {369.04, 543.307, 258.828},  
{473.653, 609.196, 269.798}, {585.954, 679.744, 282.111}, {706.161, 755.088, 295.824},  
{199.037, 457.716, 268.514}, {309.197, 528.208, 281.024}, {429.363, 604.859, 295.474},  
{559.875, 687.888, 311.958}, {701.073, 777.512, 330.576}, {853.294, 873.95, 351.425},  
{157.6, 451.995, 286.645}, {283.581, 533.139, 302.047}, {422.612, 622.41, 320.182},  
{575.188, 720.132, 341.201}, {741.806, 826.629, 365.256}, {922.962, 942.225, 392.498},  
{193.011, 495.378, 311.964}, {344.289, 592.958, 331.937}, {512.493, 701.179, 355.683},  
{698.316, 820.499, 383.426}, {902.455, 951.379, 415.389}, {199.187, 519.768, 332.685},  
{374.251, 632.74, 356.647}, {570.558, 759.157, 385.551}, {789.048, 899.647, 419.71},  
{172.509, 522.967, 348.349}, {368.5, 649.386, 375.297}, {590.422, 792.295, 408.454},  
{839.514, 952.525, 448.243}, {111.552, 504.271, 359.217}, {324.288, 641.314, 387.75},  
{567.923, 798.065, 423.815}, {844.052, 975.601, 467.969}, {241.264, 608.566, 394.652},  
{501.348, 775.608, 431.874}, {799.48, 967.036, 478.678}, {121.553, 552.849, 397.431},  
{391.561, 725.807, 433.709}, {705.276, 926.801, 481.039}, {242.033, 651.293, 431.213},  
{563.658, 856.713, 476.608}, {379.562, 760.402, 467.783}, {160.519, 643.211, 457.716},  
{535.043, 880.699, 507.284}, {139.08, 433.492, 205.664}, {215.841, 477.805, 203.86},  
{297.18, 524.704, 202.468}, {103.707, 443.918, 246.595}, {199.993, 500.988, 247.772},  
{303.302, 562.174, 249.901}, {413.82, 627.594, 253.028}, {531.734, 697.364, 257.201},  
{657.23, 771.601, 262.466}, {790.495, 850.422, 268.87}, {151.368, 500.332, 279.456},  
{275.269, 574.74, 284.303}, {409.428, 655.309, 290.86}, {554.156, 742.237, 299.214},  
{709.761, 835.722, 309.453}, {876.553, 935.964, 321.665}, {126.106, 511.556, 305.628},

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{273.542, 600.702, 313.085}, {434.952, 698.368, 323.144}, {610.814, 804.864, 335.951},
{801.605, 920.5, 351.65}, {186.709, 573.93, 333.049}, {368.345, 684.143, 344.669},
{568.685, 805.892, 360.074}, {788.424, 939.636, 379.488}, {210.432, 613.648, 357.104},
{425.226, 744.124, 372.282}, {664.104, 889.576, 392.608}, {191.019, 627.076, 377.222},
{436.092, 775.797, 394.804}, {711.202, 943.3, 419.041}, {125.134, 612.543, 393.762},
{395.76, 776.28, 412.06}, {702.847, 962.895, 438.617}, {302.269, 744.858, 424.898},
{635.158, 946.392, 451.636}, {157.05, 683.077, 435.206}, {507.751, 894.161, 459.497},
{323.844, 808.965, 464.697}, {514.224, 948.857, 496.688}, {233.16, 807.519, 497.148},
{394.664, 930.056, 525.134}, {129.185, 490.155, 183.57}, {128.016, 533.997, 245.374},
{235.574, 593.09, 238.641}, {349.561, 655.819, 232.535}, {470.116, 722.271, 227.087},
{597.38, 792.531, 222.329}, {731.492, 866.685, 218.294}, {148.288, 582.388, 287.431},
{288.143, 660.877, 283.169}, {437.95, 745.184, 280.279}, {597.964, 835.472, 278.831},
{768.439, 931.903, 278.893}, {182.395, 635.451, 320.64}, {358.746, 735.548, 318.837},
{549.484, 844.233, 319.397}, {755.032, 961.781, 322.446}, {111.709, 627.368, 350.251},
{317.946, 744.786, 349.026}, {543.625, 873.955, 351.304}, {159.479, 685.643, 374.906},
{409.512, 828.415, 375.899}, {685.37, 986.957, 381.903}, {153.414, 712.928, 398.032},
{444.787, 879.202, 399.957}, {415.116, 892.469, 421.055}, {316., 866.312, 440.336},
{147.41, 801.783, 460.283}, {365.194, 955.286, 478.884}, {267.367, 962.995, 515.823},
{123.867, 611.34, 220.686}, {234.406, 667.01, 204.473}, {350.129, 725.465, 188.48},
{471.121, 786.756, 172.725}, {183.884, 693.878, 277.683}, {337.06, 773.993, 262.848},
{499.145, 859.153, 248.934}, {670.326, 949.474, 235.988}, {165.662, 728.286, 324.454},
{360.691, 831.99, 309.957}, {569.359, 943.641, 297.338}, {165.162, 768.105, 359.021},
{406.608, 897.539, 344.308}, {298.476, 877.729, 379.676}, {366.117, 951.183, 401.329},
{354.732, 981.42, 423.986}, {256.131, 964.826, 449.229}, {195.385, 795.592, 241.358},
{350.997, 870.726, 214.861}, {513.681, 949.685, 188.747}, {215.744, 865.678, 305.267},
{426.426, 970.601, 277.305}, {127.948, 872.988, 361.639}, {170.762, 986.009, 416.008},
{158.945, 866.939, 159.74}, {301.525, 928.824, 122.044}, {252.753, 999.329, 255.358}
```

(\* Die Anzahl der Daten \*)

```
Length[EingabeNeu]
```

```
343
```

```
matA1 =
```

```
Flatten[Table[Monomvektor /. {x -> EingabeNeu[[1]][[1]], y -> EingabeNeu[[1]][[2]],
z -> EingabeNeu[[1]][[3]]}, {1, 1, Length[EingabeNeu], 1}, 1];
```

```
system1 = Transpose[matA1].matA1;
```

```
AusNeu = Flatten[AusgabeNeu];
```

```
absolute1 = Transpose[matA1].AusNeu;
```

```
ErgebnGest = LinearSolve[system1, absolute1]
```

```
{1., 2., 4., 8., 16., 4., 8., 16., 32., 16., 32., 64., 64., 3., 6., 12., 24.,
12., 24., 48., 48., 96., 9., 18., 36., 36., 72., 144., 27., 54., 108., 81.}
```

(\* Dies ist der Vektor der gesuchten Konstanten,  
in der Form des obigen "Konstantenvektors", im  
ungestörten Fall. Wie man leicht ablesen kann,  
erhalten wir also wieder K1=2, K2=4 und K3=3 zurück. \*)

```
{1., 2., 4., 8., 16., 4., 8., 16., 32., 16., 32., 64., 64., 3., 6., 12., 24.,  
12., 24., 48., 48., 96., 9., 18., 36., 36., 72., 144., 27., 54., 108., 81.}
```

(\* Wir stören nun die Daten ein wenig und versuchen dann erneut den Vektor  
der Konstanten, insbesondere also auch K1, K2 und K3 zu bestimmen.

Die Störung ist so gewählt,

dass der relative Fehler jedes einzelnen Wertes 0.1 Prozent ist. Es werden sowohl  
Ausgabe- als auch Eingabedaten gestört \*)

AusNeu;

```
AusDatengest = AusNeu + AusNeu * Table[0.001 * Random[], {Length[AusNeu]}]
```

```
{112.54, 210.099, 178.484, 108.407, 212.792, 184.76, 155.71, 252.68, 207.374, 105.094,  
204.551, 161.436, 123.52, 226.884, 179.028, 169.209, 263.563, 196.996, 135.165,  
244.023, 194.102, 187.82, 286.148, 215.061, 246.593, 332.386, 238.183, 139.156,  
254.76, 205.715, 198.04, 302.049, 229.843, 264.41, 354.433, 256.112, 338.961, 412.239,  
284.965, 134.737, 258.742, 213.727, 198.962, 310.704, 240.435, 272.128, 368.492,  
270.053, 354.344, 432.625, 302.571, 446.674, 503.605, 337.815, 121.367, 255.94,  
217.688, 189.981, 311.46, 246.956, 268.563, 374.107, 279.187, 358.227, 443.606,  
315.036, 458.79, 521.203, 354.577, 571.338, 606.636, 397.685, 170.977, 304.004,  
248.866, 253.821, 370.557, 283.544, 349.139, 444.933, 322.422, 456.834, 528.342,  
365.206, 578.312, 621.051, 412.246, 713.966, 723.371, 463.989, 132.188, 248.345,  
179.523, 179.139, 283.962, 193.871, 118.579, 247.732, 188.481, 170.86, 287.737,  
205.478, 229.066, 331.698, 223.945, 293.292, 379.603, 244.046, 139.608, 273.761,  
208.048, 201.677, 321.315, 228.922, 271.316, 373.896, 251.739, 348.469, 431.499,  
276.372, 433.719, 494.243, 303.458, 150.756, 291.971, 224.235, 222.203, 346.973,  
248.708, 302.746, 407.508, 275.493, 392.91, 474.743, 305.088, 492.934, 548.125,  
337.748, 602.994, 628.467, 372.797, 150.455, 301.827, 236.334, 230.314, 362.974,  
263.93, 321.268, 431.507, 295.047, 423.311, 507.592, 329.173, 537.141, 591.857,  
366.681, 663.688, 684.367, 408.135, 802.539, 785.107, 453.44, 137.882, 301.859,  
243.658, 224.789, 368.89, 274.364, 324.418, 444.251, 308.83, 437.364, 528.608,  
347.296, 564.308, 622.37, 390.036, 706.124, 726.379, 436.867, 863.154, 840.337,  
488.626, 112.866, 292.547, 246.578, 205.118, 364.233, 279.695, 312.034, 445.164,  
317.173, 434.157, 536.974, 359.114, 572.397, 639.331, 406.391, 727.981, 753.03,  
458.508, 901.455, 879.524, 516.419, 171.39, 348.321, 279.622, 283.206, 433.839,  
319.253, 412.417, 531.212, 364.481, 560.149, 640.693, 415.514, 727.596, 763.929,  
472.131, 915.01, 900.245, 535.494, 124.68, 322.679, 274.54, 238.962, 410.808,  
315.955, 372.908, 511.917, 363.219, 527.293, 627.321, 416.72, 703.729, 757.724,  
477.418, 903.579, 902.964, 545.424, 136.367, 276.944, 182.196, 186.5, 312.28,  
193.109, 150.791, 300.507, 204.064, 211.429, 343.92, 218.501, 277.893, 391.1,  
234.211, 350.549, 442.347, 251.203, 135.713, 302.42, 216.811, 204.738, 352.551,  
234.323, 281.086, 407.211, 253.783, 365.424, 467.19, 275.02, 457.961, 532.114,  
297.968, 558.418, 602.351, 323.168, 165.091, 336.361, 239.891, 248.07, 396.477,  
261.843, 340.332, 462.811, 286.465, 443.035, 535.347, 313.221, 556.078, 614.713,
```

342.852, 679.9, 701.708, 375.131, 814.696, 794.895, 410.599, 180.334, 360.094,  
259.209, 276.691, 430.192, 285.442, 384.626, 507.58, 314.765, 505.616, 593.216,  
347.355, 638.823, 687.46, 383.303, 786.359, 789.987, 423.059, 947.126, 902.82,  
466.93, 179.104, 372.053, 273.277, 287.651, 450.835, 303.389, 410.26, 539.175,  
337.49, 548.058, 637.035, 375.468, 702.046, 745.352, 417.913, 872.524, 864.872,  
465.15, 160.227, 371.375, 282.491, 278.821, 457.449, 315.902, 414.42, 554.686,  
353.724, 567.855, 664.341, 397.016, 740.029, 785.591, 445.153, 932.578, 920.36,  
499.603, 123.483, 357.509, 286.096, 249.886, 449.419, 321.942, 395.884, 554.374,  
363.322, 562.472, 673.466, 410.39, 751.355, 806.819, 464.004, 962.84, 956.05,  
524.495, 200.428, 427.011, 322.255, 353.847, 537.792, 365.912, 530.635, 664.366,  
416.305, 733.444, 807.618, 473.958, 962.453, 968.75, 539.479, 132.547, 390.808,  
317.27, 289.424, 504.758, 361.698, 473.104, 636.494, 414.062, 684.945, 787.132,  
474.814, 927.52, 957.418, 544.952, 204.91, 457.286, 352.155, 391.104, 591.002,  
404.944, 608.697, 745.843, 467.254, 859.879, 923.334, 539.774, 153.07, 331.885,  
199.331, 214.364, 372.926, 207.867, 280.483, 416.439, 217.449, 118.853, 326.211,  
217.037, 189.613, 374.154, 228.912, 266.892, 426.353, 241.879, 351.097, 482.654,  
256.237, 442.456, 543.438, 271.885, 540.802, 608.662, 288.999, 103.443, 332.095,  
234.384, 185.791, 388.681, 249.209, 276.711, 450.337, 265.93, 377.046, 518.342,  
284.543, 486.148, 591.664, 305.293, 605.588, 671.536, 328.395, 734.581, 757.142,  
353.478, 874.118, 849.46, 380.925, 138.496, 372.411, 259.196, 239.078, 441.711,  
278.63, 350.926, 517.713, 300.639, 474.818, 601.352, 325.401, 610.751, 692.645,  
353.058, 759.876, 792.573, 383.82, 922.234, 900.595, 418.01, 155.166, 400.22,  
279.981, 273.193, 481.409, 303.712, 405.684, 571.463, 330.93, 553.4, 671.642, 362.02,  
716.492, 781.263, 396.603, 895.898, 901.85, 435.298, 149.999, 412.756, 296.095,  
283.965, 504.961, 323.548, 435.682, 608.427, 355.535, 606.209, 723.67, 392.099,  
795.237, 851.503, 433.546, 121.267, 409.277, 307.012, 268.743, 510.587, 337.5,  
437.557, 625.984, 373.455, 628.565, 755.36, 414.904, 842.752, 899.796, 462.669,  
226.153, 497.935, 345.273, 408.488, 622.707, 383.946, 617.092, 763.691, 429.571,  
852.673, 923.487, 482.662, 156.928, 467.12, 347.432, 348.775, 598.354, 387.313,  
570.821, 748.85, 435.577, 824.25, 920.654, 492.989, 259.432, 554.079, 385.067,  
489.652, 710.561, 434.191, 756.013, 891.02, 493.504, 143.691, 492.665, 377.834,  
376.558, 650.885, 426.149, 650.608, 836.352, 485.489, 235.86, 573.031, 413.2,  
509.924, 757.949, 470.992, 831.928, 975.225, 541.962, 114.647, 359.381, 205.407,  
182.322, 401.795, 209.385, 254.812, 446.966, 214.044, 332.629, 495.125, 219.4,  
182.014, 424.966, 240.852, 272.018, 482.121, 249.234, 369.36, 543.498, 258.989,  
473.94, 609.316, 269.804, 586.162, 679.754, 282.375, 706.684, 755.477, 296.105,  
199.221, 458.154, 268.638, 309.244, 528.269, 281.253, 429.523, 604.927, 295.601,  
560.077, 688.57, 312.191, 701.466, 777.518, 330.698, 853.414, 874.269, 351.772,  
157.602, 452.052, 286.768, 283.651, 533.404, 302.101, 422.824, 622.59, 320.193,  
575.201, 720.41, 341.364, 742.295, 827.382, 365.605, 923.071, 942.855, 392.563,  
193.087, 495.432, 312.058, 344.298, 592.976, 331.978, 512.641, 701.809, 355.897,  
698.928, 821.149, 383.703, 902.543, 951.937, 415.704, 199.327, 520.137, 332.722,  
374.288, 633.238, 356.916, 571.124, 759.484, 385.791, 789.332, 900.441, 419.765,  
172.612, 523.139, 348.614, 368.81, 649.84, 375.57, 590.944, 792.333, 408.853,  
840.043, 952.809, 448.373, 111.583, 504.734, 359.285, 324.35, 641.63, 387.813,  
568.034, 798.672, 424.184, 844.731, 975.906, 468.264, 241.33, 608.855, 394.87,  
501.744, 776.052, 432.197, 800.015, 967.753, 478.963, 121.567, 553.055, 397.611,  
391.685, 725.952, 433.788, 705.461, 927.565, 481.056, 242.272, 651.62, 431.624,  
563.789, 857.291, 477.024, 379.821, 760.977, 467.84, 160.532, 643.281, 457.72,  
535.286, 880.999, 507.544, 139.204, 433.527, 205.847, 215.883, 478.137, 204.043,

297.366, 524.9, 202.601, 103.801, 443.974, 246.699, 200.079, 501.105, 247.835,  
 303.526, 562.551, 249.929, 413.891, 627.989, 253.195, 532.085, 697.944, 257.231,  
 657.735, 772.048, 262.713, 791.222, 850.485, 269.053, 151.416, 500.605, 279.572,  
 275.482, 574.85, 284.338, 409.833, 655.661, 291.132, 554.37, 742.474, 299.341,  
 710.304, 836.355, 309.657, 877.224, 936.837, 321.871, 126.219, 511.651, 305.931,  
 273.739, 601.194, 313.243, 435.245, 698.492, 323.274, 611.261, 805.253, 335.968,  
 801.935, 920.678, 351.842, 186.834, 573.982, 333.305, 368.633, 684.764, 344.818,  
 568.686, 806.575, 360.17, 788.849, 940.402, 379.814, 210.546, 614.09, 357.215,  
 425.304, 744.396, 372.401, 664.489, 890.2, 392.731, 191.193, 627.318, 377.28,  
 436.374, 776.431, 395.048, 711.468, 943.998, 419.203, 125.211, 612.865, 393.949,  
 396.096, 776.902, 412.335, 703.501, 963.018, 438.832, 302.415, 745.279, 425.241,  
 635.737, 947.132, 451.749, 157.192, 683.436, 435.479, 508.058, 894.234, 459.914,  
 323.926, 809.665, 465.02, 514.373, 949.548, 496.882, 233.358, 807.914, 497.179,  
 394.846, 930.726, 525.658, 129.26, 490.594, 183.738, 128.027, 534.422, 245.532,  
 235.577, 593.424, 238.681, 349.575, 656.431, 232.688, 470.546, 722.398, 227.141,  
 597.6, 792.678, 222.504, 731.777, 867.446, 218.321, 148.336, 582.778, 287.684,  
 288.301, 661.16, 283.384, 438.297, 745.743, 280.5, 598.408, 835.662, 278.993,  
 769.012, 932.658, 279.051, 182.516, 635.813, 320.823, 358.818, 735.902, 319.087,  
 549.584, 844.507, 319.511, 755.379, 962.273, 322.589, 111.799, 627.388, 350.515,  
 318.154, 744.832, 349.111, 543.632, 874.328, 351.472, 159.559, 685.782, 375.227,  
 409.844, 829.185, 376.136, 685.819, 987.282, 381.959, 153.483, 713.164, 398.419,  
 445.091, 880.026, 400.312, 415.183, 893.053, 421.132, 316.074, 866.397, 440.516,  
 147.436, 802.429, 460.568, 365.526, 956.212, 479.338, 267.583, 963.937, 515.998,  
 123.903, 611.633, 220.87, 234.615, 667.653, 204.577, 350.181, 726.156, 188.495,  
 471.286, 787.145, 172.858, 184.04, 694.051, 277.707, 337.261, 774.021, 263.013,  
 499.233, 859.691, 248.956, 670.876, 949.662, 236.056, 165.793, 728.534, 324.572,  
 360.834, 832.68, 310.215, 569.482, 944.061, 297.561, 165.242, 768.659, 359.264,  
 406.977, 897.749, 344.527, 298.5, 878.494, 379.906, 366.286, 951.614, 401.644,  
 355.01, 981.677, 424.056, 256.385, 965.254, 449.632, 195.535, 795.723, 241.506,  
 351.236, 871.008, 214.95, 513.746, 950.596, 188.869, 215.853, 866.451, 305.366,  
 426.668, 971.215, 277.385, 128.058, 873.088, 361.946, 170.848, 986.603, 416.403,  
 159.081, 866.989, 159.852, 301.58, 929.467, 122.098, 252.759, 1000.19, 255.43}

(\* Im nächsten Schritt kann man ebenfalls die Eingabedaten stören  
 (indem man die "0.0000" ändert), was aber in unserem Fall nicht getan wurde\*)

```
EinDatengest = EingabeNeu +
  EingabeNeu * Table[0.0000 * {Random[], Random[], Random[]}, {Length[EingabeNeu]}];

matA2 = Flatten[
  Table[Monomvektor /. {x -> EinDatengest[[1]][[1]], y -> EinDatengest[[1]][[2]],
    z -> EinDatengest[[1]][[3]]}, {1, 1, Length[EinDatengest], 1}], 1];
system2 = Transpose[matA2].matA2;

absolute2 = Transpose[matA2].AusDatengest;
```

(\* Unser neuer " Konstantenvektor " für den Fall gestörter Daten: \*)

```
Ergebnis = LinearSolve[system2, absolute2]
```

```
{1.00508, 2.64501, 4.36211, 8.11946, 16.1017, 3.44491, 8.01015, 16.0466,  
32.0234, 15.7688, 32.0191, 64.0392, 63.9685, 2.8506, 5.9977, 11.9757,  
23.9777, 11.8814, 23.9794, 48.0646, 48.0946, 96.0212, 9.05876, 18.0526,  
35.9746, 35.9717, 72.0815, 144.128, 27.1185, 54.114, 107.892, 81.1168}
```

```
Length[Ergebnis]
```

```
32
```

```
Length[matA2.Ergebnis]
```

```
1029
```

```
Length[AusDatengest]
```

```
1029
```

```
d = matA2.Ergebnis - AusDatengest;
```

```
Length[d]
```

```
1029
```

```
(* Als nächstes rechnen wir nach,  
dass unser gefundener Vektor " Ergebnis " wirklich  
den Abstand von {(matA2*c) - AusDatengest} für c=  
Ergebnis in der l^2-Norm (d.h. man  
summiert die einzelnen Komponenten im  
Quadrat auf und zieht am Ende die Wurzel) rela-  
tiv klein wird. *)
```

```
Sqrt[Sum[(d[[i]])^2, {i, 1, Length[d]}]]
```

```
4.61182
```

```
(* Zum Vergleich einmal den Abstand für unseren Vektor " ErgebUngest ": *)
```

```
du = matA2.ErgebUngest - AusDatengest;
```

```
Sqrt[Sum[(du[[i]])^2, {i, 1, Length[du]}]]
```

```
9.43397
```

\$Aborted

```
Sum[(Ergebnis[[i]] - ErgebUngest[[i]])^2, {i, 1, Length[Ergebnis]}
```

1.07363

{ \* Wir rechnen nun nach, wie weit die zugehörigen Konstanten K1,  
K2 und K3 voneinander abweichen \* }

```
Datenfehler = (Ergebnis[[2]] - ErgebUngest[[2]])^2 +  
(Ergebnis[[6]] - ErgebUngest[[6]])^2 + (Ergebnis[[14]] - ErgebUngest[[14]])^2
```

0.746477

```
f[K1_, K2_, K3_] = {1, K1, K1^2, K1^3, K1^4, K2, K1 K2, K1^2 K2, K1^3 K2, K2^2, K1 K2^2,  
K1^2 K2^2, K2^3, K3, K1 K3, K1^2 K3, K1^3 K3, K2 K3, K1 K2 K3, K1^2 K2 K3, K2^2 K3,  
K1 K2^2 K3, K3^2, K1 K3^2, K1^2 K3^2, K2 K3^2, K1 K2 K3^2, K2^2 K3^2, K3^3, K1 K3^3, K2 K3^3, K3^4};
```

```
DifferenzListe = f[K1, K2, K3] - Ergebnis
```

```
{-0.0100881, -1.77696 + K1, -3.66035 + K1^2, -7.91953 + K1^3, -15.9433 + K1^4,  
-3.59534 + K2, -8.06771 + K1 K2, -15.9567 + K1^2 K2, -32.0172 + K1^3 K2, -15.6517 + K2^2,  
-32.0464 + K1 K2^2, -64.0037 + K1^2 K2^2, -63.882 + K2^3, -2.95678 + K3, -5.98663 + K1 K3,  
-11.8366 + K1^2 K3, -23.9093 + K1^3 K3, -11.8633 + K2 K3, -24.1273 + K1 K2 K3,  
-48.0621 + K1^2 K2 K3, -47.944 + K2^2 K3, -96.0663 + K1 K2^2 K3, -8.9405 + K3^2,  
-18.1146 + K1 K3^2, -36.0091 + K1^2 K3^2, -35.8989 + K2 K3^2, -72.0884 + K1 K2 K3^2,  
-144.011 + K2^2 K3^2, -26.8444 + K3^3, -54.0805 + K1 K3^3, -107.982 + K2 K3^3, -80.8149 + K3^4}
```

```
Abstand[K1_, K2_, K3_] = Sum[(DifferenzListe[[i]])^2, {i, 1, Length[DifferenzListe]}]
```

$$\begin{aligned}
& 0.00010177 + (-1.77696 + K1)^2 + (-3.66035 + K1^2)^2 + (-7.91953 + K1^3)^2 + (-15.9433 + K1^4)^2 + \\
& (-3.59534 + K2)^2 + (-8.06771 + K1 K2)^2 + (-15.9567 + K1^2 K2)^2 + (-32.0172 + K1^3 K2)^2 + \\
& (-15.6517 + K2^2)^2 + (-32.0464 + K1 K2^2)^2 + (-64.0037 + K1^2 K2^2)^2 + (-63.882 + K2^3)^2 + \\
& (-2.95678 + K3)^2 + (-5.98663 + K1 K3)^2 + (-11.8366 + K1^2 K3)^2 + (-23.9093 + K1^3 K3)^2 + \\
& (-11.8633 + K2 K3)^2 + (-24.1273 + K1 K2 K3)^2 + (-48.0621 + K1^2 K2 K3)^2 + (-47.944 + K2^2 K3)^2 + \\
& (-96.0663 + K1 K2^2 K3)^2 + (-8.9405 + K3^2)^2 + (-18.1146 + K1 K3^2)^2 + (-36.0091 + K1^2 K3^2)^2 + \\
& (-35.8989 + K2 K3^2)^2 + (-72.0884 + K1 K2 K3^2)^2 + (-144.011 + K2^2 K3^2)^2 + \\
& (-26.8444 + K3^3)^2 + (-54.0805 + K1 K3^3)^2 + (-107.982 + K2 K3^3)^2 + (-80.8149 + K3^4)^2
\end{aligned}$$

(\* Als nächstes berechnen wir den Abstand  
- im quadratischen Mittel- des Ergebnis-  
vektors zu dem Graphen von (K1,K2,K3) ->  
Konstantenvektor (siehe oben für die genaue  
Form von dem Konstantenvektor). Dies ist  
der Modellfehler \*)

```
Modellfehler = FindMinimum[Sqrt[Abstand[K1, K2, K3]], {K1, 0}, {K2, 0}, {K3, 0}]
```

```
{0.809235, {K1 -> 2.00057, K2 -> 3.99986, K3 -> 2.99955}}
```

(\* Das ist die Differenz von den ungestörten und um 0,  
1% gestörten Ausgabedaten in der klein 1^2  
Norm\*)

---

```
Sqrt[Sum[(AusNeu[[i]] - AusDatengest[[i]])^2, {i, 1, Length[AusNeu]}]]
```

```
9.43397
```