## Optimization Theory Applied Mathematics

Laboratory assignments

NLP1. An environmental scientist wants to find out whether the temperatures or their amplitudes in his country have an increasing trend. In order to do that he tries to fit the curve (showing theoretical dependence of average monthly temperature T on time in months t)

$$T(t) = (\alpha(t - t_0) + \beta) \sin\left(\frac{2\pi(t - t_0)}{12}\right) + \gamma t + \delta$$

(with  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\delta$  and  $t_0$  being the parameters of the curve) to the average monthly temperatures given in the table below:

$\operatorname{month}$	jan	feb	$\operatorname{mar}$	apr	may	jun	jul	aug	$\operatorname{sep}$	$\operatorname{oct}$	nov	$\operatorname{dec}$
2013	1.0	1.3	3.5	7.8	12.5	15.1	17.9	15.7	12.9	9.1	4.5	2.1
2014	1.3	0.7	3.2	6.7	12.7	14.9	15.9	16.3	14.5	9.0	4.1	1.2
2015	0.1	1.2	3.8	5.3	11.5	14.5	16.1	17.8	15.1	8.0	3.2	1.9
2016	0.9	1.6	5.1	7.9	10.2	14.2	16.3	19.8	12.5	9.3	6.0	3.2
2017	1.9	2.3	4.5	8.4	12.0	15.9	17.8	18.9	13.0	8.7	6.3	3.0
2018	2.1	0.2	3.9	7.3	11.6	15.7	18.5	19.9	12.7	8.1	4.2	2.8
2019	1.9	0.9	4.5	8.9	13.8	16.8	17.9	18.1	15.6	7.4	6.9	2.3
2020	1.5	1.5	5.4	9.1	15.1	15.3	18.8	20.0	14.1	8.5	5.3	1.7
2021	2.4	1.7	5.0	6.1	13.7	17.2	20.1	18.7	14.8	7.9	7.7	3.5
2022	1.4	2.6	5.9	8.4	12.9	18.3	19.7	20.5	15.7	9.6	3.7	2.6

Write a procedure allowing you to find the parameters of the function T minimizing the sum of the squares of the deviations between the real and the predicted (given by T) values of the temperatures. Your program is supposed to compute them using Newton's method with Armijo rule used for the stepsize selection.

NLP2. A chain of stores wants to build a distribution center to provide its retail outlets with articles to sell. The data available are the locations of the retail outlets  $(x_i, y_i)$ ,  $i = 1, \ldots, 8$  and the amounts of articles sold at each outlet  $w_i$ ,  $i = 1, \ldots, 8$  as well as the locations of production centers  $(x_i^P, y_i^P)$  and amounts produced in each of them,  $w_i^P$ , i = 1, 2. Find the location for the distribution center  $(x_0, y_0)$ , which minimizes the approximate transportation expenses of the chain, that is, it minimizes the weighted sum of Euclidean distances from the center to the outlets (with  $w_i$  serving as weights) and Euclidean distances from the center to the production centers (with  $w_i^P$  serving as weights). Do it using Newton's method with stepsize chosen using Armijo rule. The data for the problem is given in the tables below.

Outlet number	$x_i$	$y_i$	$w_i$		
1	-9	55	3000		
2	37	40	3100		
3	14	10	1500		
4	87	35	4500		
5	52	-12	5000		
6	-10	-34	1500		
7	25	-11	2200		
8	45	-20	3200		
			Į.		
Prod. center number $ x_i^P y_i^P  = w_i^P$					

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	1	00
$2 \qquad  -8  20  1400$	2	00

Repeat your computations for other values of  $w_1^P$  and  $w_2^P$  summing up to 24000. Find those that minimize the transportation costs of the company using golden-section search.

NLP3. An investor tries to figure out which of the two industries to invest in. He knows that the number of employees available in the local market is very small, so he wants to choose the industry with higher capital output elasticity/labor output elasticity ratio. He thus needs to estimate the elasticities for the three industries from

the available data. It is known that the following Cobb-Douglas formula should approximately hold for each of the industries:

$$y = \alpha c^{\beta_1} l^{\beta_2},$$

where l is the labor input (the total number of person-hours worked in a year), c is the capital input (the real value of all machinery, equipment, and buildings), y is the total production (these values are known for many firms in each industry), while  $\alpha$  (productivity factor),  $\beta_1$  (capital output elasticity) and  $\beta_2$  (labor output elasticity) are unknown.

Estimate  $\alpha$ ,  $\beta_1$  and  $\beta_2$  for each industry from the following experimental data by minimizing the sum of the squares of the deviations between the experimental and predicted values of y: Tobacco industry:

y	c	l
75	7.0	10.5
36.8	8.3	6.2
142.5	2.5	18.0
171	15.0	13.5
131	21.5	9.2
1.7	4.8	0.5
y	c	l
224	9.0	14.0
75	4.0	4.0
516.5	23.0	13.5
135	16.5	3.5
80	2.5	8.5
164	5.0	10.0
57.5	7.0	3.0
431	22.5	11.0
280	12.5	9.7
375	9.4	17.9

Food and beverage industry:

Do it using Newton's method with Armijo rule used for the stepsize selection. Choose which industry should be invested in.

NLP4. Michaelis-Menten enzyme kinetics is described by the following equation:

$$v = \frac{V_{\max}S}{K_M + S}$$

where S is the concentration of substrate, v is the initial velocity of reaction,  $V_{\text{max}}$  is the saturation velocity and  $K_M$  is Michaelis-Menten constant. Write a procedure to determine  $V_{\text{max}}$  and  $K_M$  from a vector of measurements of v as function of S which will minimize the least-square error

$$Err = \sum_{i=1}^{N} \left( v_i - \frac{V_{\max}S_i}{K_M + S_i} \right)^2$$

using steepest descent method with Armijo rule used for stepsize selection. Apply it to determine the values of  $V_{\text{max}}$  and  $K_M$  for the data of Wong [W75]:

Compare it to the results obtained in [JK05] (available online), where the problem was reduced to a onedimensional one.

[W75] J.T.-F. Wong, Kinetics of Enzyme Mechanisms, Academic Press, New York (1975)

[JK05] Ž. Jeričević and Ž. Kušter, Non-linear optimization of parameters in Michaelis-Menten kinetics. Croatica Chemica Acta 78(4) 519–523 (2005)

NLP5. The cost of refined oil when shipped via the Malacca Straits to Japan in dollars per kiloliter was given in [U68] as the linear sum of the crude oil cost, the insurance, customs, freight cost for the oil, loading and

unloading cost, sea berth cost, submarine pipe cost, storage cost, tank area cost, refining cost, and freight cost of products as

$$c = c_c + c_i + c_x + \frac{2.09 \times 10^4 t^{-0.3017} + 5.042 \times 10^3 q^{-0.1899} + 0.1049 q^{0.671}}{360} + \frac{1.064 \times 10^6 a t^{0.4925} + 4.242 \times 10^4 a t^{0.7952} + 1.813i p (nt + 1.2q)^{0.861} + 4.25 \times 10^3 a (nt + 1.2q)}{52.47q (360)}$$

where a is annual fixed charges percentage,  $c_c$  is crude oil price (in k/kl),  $c_i$  – insurance cost (in k/kl),  $c_x$  – customs cost (in k/kl), i – interest rate, n – number of ports, p – land price (in  $k/m^2$ ), q – refinery capacity (in bbl/day) and t – tanker size (in kl). Write a procedure to compute the minimum cost of oil and the optimum tanker size t and refinery size q by Newton's method using Armijo rule to choose the stepsize. Apply it to the following data:

$$\begin{array}{c|ccccccccccccc} a & c_c & c_i & c_x & i & n & p \\ \hline 0.20 & 12.5 & 0.5 & 0.9 & 0.1 & 2 & 7000 \end{array}$$

[U68] T. Uchiyama, Best Size for Refinery and Tankers. Hydrocarbon Process. 47(12) 85–88 (1968)

## In the following 5 problems one may consult the textbook:

[AnLu07] A. Antoniou, W.-S. Lu, Practical Optimization, Springer Science+Business Media, LLC, 2007. It is available online.

NLP6. Write procedures allowing to find an unconstrained minimum of any given function using two methods:

- (a) Newton's method with search method based on quadratic interpolation used to find the stepsize;
- (b) Fletcher-Reeves conjugate gradient method with search method based on quadratic interpolation used to determine the stepsize.

Apply the two methods (with different starting points) to the Rosenbrock function

$$f(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

and to some nonquadratic convex function of a large number of variables. Compare their speed of convergence in terms of time and in terms of the number of iterations taken to obtain a good approximation.

- NLP7. Write procedures allowing to find an unconstrained minimum of any given function using two methods:
  - (a) Newton's method with search method based on quadratic interpolation used to find the stepsize;
  - (b) Partan method with search method based on quadratic interpolation used to determine the stepsize.

Apply the two methods (with different starting points) to the Rosenbrock function (see problem NLP6.) and to some nonquadratic convex function of a large number of variables. Compare their speed of convergence in terms of time and in terms of the number of iterations taken to obtain a good approximation.

## NLP8. Write procedures allowing to find an unconstrained minimum of any given function using two methods:

- (a) Newton's method with search method based on quadratic interpolation used to find the stepsize;
- (b) Powell method with search method based on quadratic interpolation used to determine the stepsize.

Apply the two methods (with different starting points) to the Rosenbrock function (see problem NLP6.) and to some nonquadratic convex function of a large number of variables. Compare their speed of convergence in terms of time and in terms of the number of iterations taken to obtain a good approximation.

NLP9. Write procedures allowing to find an unconstrained minimum of any given function using two methods:

- (a) Newton's method with search method based on quadratic interpolation used to find the stepsize;
- (b) Davidon-Fletcher-Powell method with search method based on quadratic interpolation used to determine the stepsize.

Apply the two methods (with different starting points) to the Rosenbrock function (see problem NLP6.) and to some nonquadratic convex function of a large number of variables. Compare their speed of convergence in terms of time and in terms of the number of iterations taken to obtain a good approximation.

- NLP10. Write procedures allowing to find an unconstrained minimum of any given function using two methods:
  - (a) Newton's method with search method based on quadratic interpolation used to find the stepsize;
  - (b) Broyden-Fletcher-Goldfarb-Shanno method with search method based on quadratic interpolation used to determine the stepsize.

Apply the two methods (with different starting points) to the Rosenbrock function (see problem NLP6.) and to some nonquadratic convex function of a large number of variables. Compare their speed of convergence in terms of time and in terms of the number of iterations taken to obtain a good approximation.