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Exam in FFR 105 (Stochastic optimization algorithms), 2016-10-26, 14.00-18.00, M.

The examiner will visit the exam rooms twice, around 15.00 and around 17.00.
It will be possible to review your results (for the exam and the home problems) any day after Nov. 16.

In the exam, it is allowed to use a calculator, as long as it cannot store any text. Furthermore, mathematical tables (such as Beta, Standard Math etc.) are allowed, provided that no notes have been added. However, it is *not* allowed to use the course book, or any lecture notes from the course, during the exam.

Note! In problems involving computation, show *clearly* how you arrived at your answer, i.e. include intermediate steps etc. Only giving the answer will result in zero points on the problem in question.

There are four problems in the exam, and the maximum number of points is 25.

1. (a) The problem of *overfitting* often appears in optimization problems involving real data sets (which are almost always of limited size). The problem can, to some extent, be avoided using *holdout validation*. Introduce and describe this method in detail. (2p)

   (b) Many stochastic optimization algorithms, for example genetic algorithms and ant colony optimization, are based on biological phenomena, meaning that an understanding of such phenomena is important for understading (and developing further) the algorithms.

      i. In genetic algorithms, the concept of *genes* is central. In the biological counterpart, genes serve the purpose of providing the necessary information for generating proteins, using a two-step process. Name and *describe* the two steps. (2p)

      ii. Ant colony optimization relies on an indirect form of communication, similar to the one used by real ants. Name and *describe* this form of communication. (1p)

   (c) Write down the standard particle swarm optimization (PSO) algorithm and describe all steps in detail, with the relevant equations. Include clear definitions and descriptions of all variables and parameters. In particular, describe how the tradeoff between exploration and exploitation (of the results already found) is handled in PSOs. (4p)

2. (a) Newton-Raphson's method is an iterative method for finding local optima of a twice differentiable function. Use this method to find the minimum of the function $f(x) = 8x - \ln x$, starting from $x \equiv x_0 = 0.075$. First, write down (for this particular function) the expression for x_{j+1} as a function of x_j. Next, make a table with two columns: (1) the index j of the iterate, and (2) the corresponding value x_j. Iterate until the difference between two consecutive iterates (i.e. $|x_{j+1} - x_j|$) drops below 10^{-5}, and enter all the iterates in your table. Next, prove that the point found is really a minimum of $f(x)$. (3p)

   (b) The Lagrange multiplier method is applicable to optimization problems involving equality constraints. Consider the curve implicitly determined by the equation $x_1^2 + x_1 x_2 = 1$. Using (Note!) the Lagrange multiplier method, find the points (there may be more than one) in $\mathbf{R}^2$ on this curve that are closest to the origin of the coordinate system. Specify the *exact* location of these points (rather than an approximation in the form of a decimal number). (4p)

3. Linear genetic programming (LGP) is particularly useful in situations where the size of the evolving system is difficult to determine in advance. Consider a very simple, two-dimensional, grid-based computer game, in which a game character (shown as a filled disc in the left panel of Figure 3 (next page)) can move between grid cells. The character has a specified forward direction of motion (indicated by an arrow in the figure), and there are four possible operators, namely O_1: *Move forward* (in the direction of the arrow), O_2: *Move backward* (in the opposite direction), O_3: *Turn left 90 degrees* (while staying in the same grid cell), thus changing the forward direction, and O_4: *Turn right 90 degrees* (i.e. the opposite of O_3). The character moves according to instructions consisting of two elements each, the operator and an operand determining how many times the operator is applied before moving to the next instruction. Thus, for example, if O_1 is applied twice, the character moves two steps forward. If instead O_3 is applied twice, the character makes a 180 degree right turn in its grid cell. The sequence of instructions carried out by the character is encoded in an LGP chromosome.

   (a) Consider now the situation in the figure in which the character starts at the cell $(x, y) = (4, 3)$, and where the chromosome takes the form $c_1 = 11311241223211$. Decode the chromosome, write down a the movement steps in a list, and plot the entire trajectory of the character. (3p)

   (b) At the end of a generation, chromosome c_1 is crossed with a chromosome $c_2 = 22113121$, using two-point crossover such that the first crossover point (in both chromosomes) occurs after the first *instruction* and the second crossover point (in both chromosomes) occurs just before the last instruction. After crossover, two new chromosomes are formed. Find and plot the entire trajectory for the shorter of the two new chromosomes (again starting from $(x, y) = (4, 3)$). (2p)

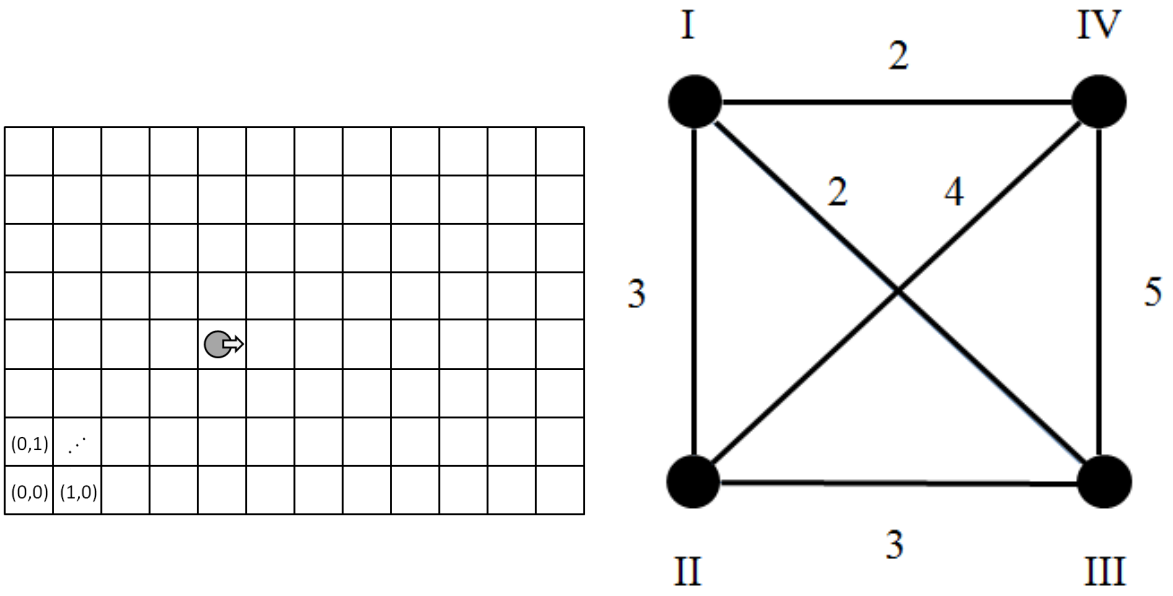

Figure 1: Left panel: The grid for Problem 3. In the situation shown here, the character is located at $(4, 3)$*, and the direction of movement is to the right. Right panel: The graph for Problem 4.*

4. Ant colony optimization can, for example, be used in routing problems. Consider the problem illustrated in the right panel of Fig. 3. The figure shows a number of locations that are to be visited by a delivery truck. The aim is to find the best path, using the Ant system (AS) algorithm. Here, the visibility η_{ij} of the nodes depend not only on the distance between the nodes, but also on the level of traffic along the various parts of the road, and similar factors. The numbers associated with each edge in the figure determine the visibility η_{ij} in a given situation (such that, moreover, $\eta_{ji} = \eta_{ij}$).

   (a) Assuming that the pheromone levels (on all edges) are equal to 1, compute the probability of selecting the path I $\rightarrow$ II $\rightarrow$ III $\rightarrow$ IV (with a return to location I implied in the final step), given that the artificial ant generates the path using AS, using the parameters $\alpha = \beta = 1$. Let $p(e_{ij}|S)$ denote the probability of taking a step from node j to node i, given a path fragment S. Show clearly how you arrive at the probabilities for each step of the computation. (2p)

   (b) Determine the pheromone levels on all edges after *one* ant has traversed the path described above, assuming that the value of the objective function (to be maximized) is equal to 0.5 for this path, and that the pheromone evaporation rate is also equal to 0.5. Show clearly how you arrive at your answer. (2p)

Stochastic optimization methods (FFR 105), 2016
Solutions to the exam (2016-10-26)

1. (a) In holdout validation one divides the data set into three subsets: A training set, a validation set, and a test set. The training set is used for giving feedback to the algorithm during training. At the same time, the performance over the validation set is also measured (but not provided to the training algorithm). Training continues until there is a significant drop in the validation performance. At that point, the training is stopped, and the system with the best *validation* performance is selected. Next, the performance over the previously unused test set is measured, and can be taken as the true performance of the system. A typical percentage division between training, validation, and test is 60-20-20.

   (b) i. The two steps are called transcription and translation. In transcription, the information in a gene (in the form of a sequence of bases, from the alphabet A, C, G, and T) is read by RNA polymerase, resulting in an mRNA molecule, containing the same information (albeit coded slightly differently) as the gene. In translation, the mRNA molecule is used as a template when forming a chain of amino acids (i.e. a protein). Each codon, i.e. a sequence of three bases in the mRNA molecule, e.g. CAA, encode a particular amino acid. Some codons encode the start and stop command. Once the stop command has been reached the amino acid chain is complete.

   ii. The form of communication is referred to as stigmergy. This is a process of indirect communication by means of local modification of the environment, in which an ant deposits a volatile hydrocarbon (a pheromone) that other ants can perceive. Ants tend to move in the direction of highest pheromone scent. Note that the pheromones will evaporate after a while, unless the path is replenished by additional ants.

   (c) Description of PSO, see the course book, pp. 121-123. The tradeoff between exploration and exploitation is handled by the inertia weight (w). If w takes a value above 1, exploration is favoured since, in that case, the particle's acceleration is dominated by a component its current direction of motion. If instead $w < 1$, exploitation is favoured. Typically w is initialized around 1.4, and is then allowed to drop by a constant factor (0.99, say) in each iteration, until it reaches around 0.3-0.4, after which point w is kept constant.

2. (a) Iterates are formed as

$$x_{j+1} = x_j - \frac{f'(x)}{f"(x)}. \tag{1}$$

In this case,

$$f'(x) = 8 - \frac{1}{x}, \tag{2}$$

and

$$f"(x) = \frac{1}{x^2}. \tag{3}$$

Thus,

$$x_{j+1} = x_j - \frac{8 - \frac{1}{x}}{\frac{1}{x^2}} = 2x_j - 8x_j^2. \tag{4}$$

Starting from $x_0 = 0.075$, the following table is obtained

j	x_j
0	0.07500000
1	0.10500000
2	0.12180000
3	0.12491808
4	0.12499994
5	0.12499999

In the last step, the difference between the two successive iterates is less than 10^{-7}. From the value obtained, it easy to guess that the true minimum x^* is at $0.125 = 1/8$. One can easily check that indeed $f'(1/8) = 0$. Moreover, since $f"(1/8) = 64 > 0$, the optimum is a minimum.

(b) Rather than minimizing the distance, one can (equivalently) minimize the distance squared. Thus, function to minimize will be

$$f(x_1, x_2) = x_1^2 + x_2^2, \tag{5}$$

with the constraint

$$h(x_1, x_2) = x_1^2 + x_1 x_2 - 1 = 0. \tag{6}$$

Thus L takes the form

$$L(x_1, x_2, \lambda) = x_1^2 + x_2^2 + \lambda(x_1^2 + x_1 x_2 - 1), \tag{7}$$

so that

$$\begin{aligned}\frac{\partial L}{\partial x_1} &= 2x_1 + \lambda(2x_1 + x_2) = 0,\\ \frac{\partial L}{\partial x_2} &= 2x_2 + \lambda x_1 = 0\\ \frac{\partial L}{\partial \lambda} &= = x_1^2 + x_1 x_2 - 1 = 0.\end{aligned} \tag{8}$$

From the first two equations, one finds $2x_1 = -\lambda(2x_1 + x_2)$ and $2x_2 = -\lambda x_1$, so that

$$x_1(4 + 4\lambda - \lambda^2) = 0. \tag{9}$$

The solution $x_1 = 0$ does not satisfy the constraint. Thus, instead, one must have $4 + 4\lambda - \lambda^2 = 0$, so that

$$\lambda_{1,2} = 2 \pm 2\sqrt{2} \tag{10}$$

Considering first $\lambda_1 = 2 + 2\sqrt{2}$, using $2x_2 = -\lambda x_1$, one can then write (using the constraint)

$$x_1^2 - \frac{\lambda_1}{2} x_1^2 = 1, \tag{11}$$

so that

$$x_1^2 = \frac{2}{2 - \lambda_1} \rightarrow x_1 = \pm \frac{1}{\sqrt[4]{2}} \approx \pm 0.8498964153. \tag{12}$$

and

$$x_2 = \ldots = \pm \frac{-1 + \sqrt{2}}{\sqrt[4]{2}} = \pm 0.3483106995. \tag{13}$$

If one instead tries with λ_2, one obtains imaginary values, so those solutions can be excluded. Thus, there are two possible solutions, namely

$$(x_1^\star, x_2^\star) = \pm(\frac{1}{\sqrt[4]{2}}, \frac{-1 + \sqrt{2}}{\sqrt[4]{2}}). \tag{14}$$

Both points are equidistant from the origin.

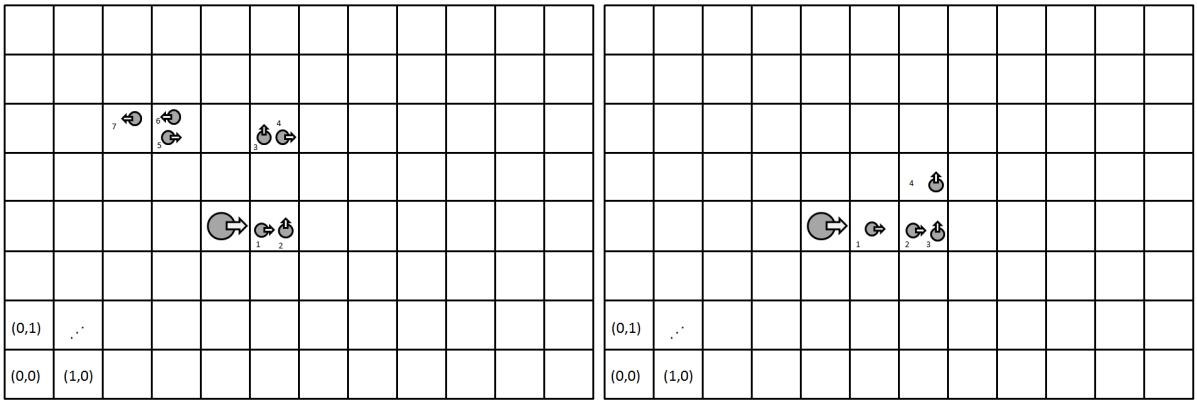

Figure 1: Left panel: The trajectory for Problem 3(a). Right Panel: The trajectory for Problem 3(b).

3. (a) The chromosome $c_1 = 11311241223211$ can be decoded as
   $11 \rightarrow$ Move forward one step
   $31 \rightarrow$ Turn left, 90 degrees
   $12 \rightarrow$ Move forward two steps
   $41 \rightarrow$ Turn right 90 degrees
   $22 \rightarrow$ Move backward, two steps
   $32 \rightarrow$ Turn left $2 \times 90 = 180$ degrees
   $11 \rightarrow$ Move forward one step

   (b) The crossover results in the two chromosomes $c_3 = 11113111$ and $c_4 = 22311241223221$. When decoded, the shorter of the two new chromosomes results in the following sequence of movements:
   $11 \rightarrow$ Move forward one step
   $11 \rightarrow$ Move forward one step
   $31 \rightarrow$ Turn left, 90 degrees
   $11 \rightarrow$ Move forward one step
   The trajectories are shown in Fig. 1.

4. (a) The probabilities are obtained using Eq. (4.3) in the book. Since the pheromone levels are equal on all edges, they will disappear from the equation. The resulting probabilities are thus

$$p(I \rightarrow II) = \frac{3}{3+2+2} = \frac{3}{7}, \tag{15}$$

since the ant can move to any other node (II, III, or IV) from node 1. Continuing, one finds in a similar way

$$p(II \to III) = \frac{3}{4+3} = \frac{3}{7}, \tag{16}$$

$$p(III \to IV) = 1, \tag{17}$$

and

$$p(IV \to I) = 1. \tag{18}$$

Thus, the probability of obtaining the desired path is equal to $9/49 \approx 0.18367$.

(b) The pheromone levels will be

$$\tau_{ij} \leftarrow \tau_{ij}(1-\rho) + f = 1 \times 0.5 + 0.5 = 1, \tag{19}$$

for those (note!) four edges that the ant traversed (listed above). For all other edges (including the reverse edges, e.g. I $\to$ IV etc.), only evaporation will occur, so that $\tau_{ij} \leftarrow 0.5$.