Mean field variational framework for integer optimization

Arturo Berrones, Jonás Velasco, and Juan Banda,

Abstract—A principled method to obtain approximate solutions of general constrained integer optimization problems is introduced. The approach is based on the calculation of a mean field probability distribution for the decision variables which is consistent with the objective function and the constraints. The original discrete task is in this way transformed into a continuous variational problem. In the context of particular problem classes at small and medium sizes, the mean field results are comparable to those of standard specialized methods, while at large sized instances is capable to find feasible solutions in computation times for which standard approaches can’t find any valuable result. The mean field variational framework remains valid for widely dimensional nonlinear combinatorial optimization tasks.

Index Terms—variational mean field, combinatorial optimization, heuristics, statistical mechanics.

I. INTRODUCTION

Besides of its practical importance and of the progress made in the solution of integer linear programs in the last decades [11], integer optimization is still a very challenging subject. Practical methods for nonlinear problems are rare and mostly limited to small to medium sized problems [2], [1], [3], even in special cases such as convex integer programming [3], [4], [5]. Heuristic approaches consequently play a major role in the field, either hybridized with deterministic algorithms [6], [7], or like stochastic approximate solution strategies on their own right [8], [9], [10], [11], [12], [13], [14], [15], [16].

An essential ingredient in any heuristic is a rule by which candidate solutions are generated. In this contribution we introduce a very general framework to construct probabilistic solution generators that are consistent with the underlying integer optimization task.

II. MEAN FIELD FRAMEWORK

The method is principled and firmly based on the fundamental rules of probability. More precisely, any possible solution for an integer optimization problem can be viewed like a random string drawn from some probability distribution. It is desirable that such a distribution generates deviates that are typically in the feasibility region and close to the optima. To proceed, consider the following class of optimization problems,

\[
\min f(\overline{x}) \quad \text{s.t.} \quad g_k(\overline{x}) \leq 0, \quad h_i(\overline{x}) = 0,
\]

where \( \overline{x} \) is a vector of binary decision variables, \( g_k(k=1,...,K) \) are inequality constraint functions and \( h_i(i=1,...,L) \) are equality constraints. The optimization task (1) can in principle be represented by a potential function \( V(\overline{x}) \) which includes the objective and the constraints. A probability distribution can be associated to such a potential by the transformation \([10],[17]\).

\[
P(\overline{x}) = \frac{1}{Z} \exp \left( -\frac{V}{kT} \right),
\]

where \( Z \) is a normalization factor (or partition function) and \( kT \) is a constant. The Eq. (2) gives the maximum entropy distribution which is consistent with the condition \( \langle V \rangle_P = \int V P d\overline{x} \) [18]. However, \( P \) is in general intractable. Moreover, in our setup is not even known, because the explicit definition of \( V \) would require the knowledge of suitable “barrier” terms that exactly represent the constraints. Is therefore proposed the following mean field probabilistic model for the decision variables,

\[
Q(\overline{x}) = \prod_{i=1}^{N} p(x_i),
\]

Mean field techniques, which have first emerged in statistical mechanics [19], have been already successfully applied to discover fundamental features of combinatorial problems and valuable solution strategies, although focused on particular combinatorial problem classes [20]. Our purpose in this contribution is to develop a practical mean field framework to find good candidate solutions to linear and nonlinear integer problems in the constrained situation (1). The most general form for the independent marginals is,

\[
p(x_i) = 1 + (2m_i - 1)x_i - m_i.
\]

The \( m \)'s are continuous mean field parameters, \( m \in [0,1] \). These parameters can be selected by the minimization of the Kullback-Leibler divergence between distributions \( Q \) and \( P \) [21],

\[
D_{KL}(Q||P) = \langle \ln Q \rangle - \langle \ln P \rangle,
\]

where the brackets represent averages with respect to the tractable distribution \( Q \). Introducing the entropy \( S_Q = -kT \langle \ln Q \rangle \), is obtained the variational problem \( \min F_Q \), where

\[
F_Q = \frac{1}{kT} \left[ \langle V \rangle - S_Q \right]
\]

is the variational “free energy” of the distribution \( Q \) [21]. Without loss of generality, the constant \( kT \) can be set \( kT = 1 \). In first instance we consider the class of combinatorial optimization problems in which all the involved functions

A. Berrones, J. Velasco and J. Banda are with Universidad Autónoma de Nuevo León, Facultad de Ingeniería Mecánica y Eléctrica Postgrado en Ingeniería de Sistemas, AP 126, Cd. Universitaria, San Nicolás de los Garza, NL 66450, México e-mail: arturo@yalma.fime.uanl.mx.

\[\text{arXiv:1305.1593v1 [math.OC] 5 May 2013}\]
(objective and constraints) are polynomial, e.g. \( f(\vec{x}) = a_0 + \sum_i b_i x_i + \sum_i \sum_j c_{ij} x_i x_j + \sum_i \sum_j r_i x_i x_j + \ldots \).

In such case \( f(\vec{x}) = f(\langle \vec{x} \rangle), (g(\vec{x})) = g(\langle \vec{x} \rangle) \) and \( h(\vec{x}) = h(\langle \vec{x} \rangle) \). Therefore, the continuous relaxation of the problem \((\text{I})\) is equivalent to its average under the mean field distribution,

\[
\min f(\langle \vec{m} \rangle \, s.t. \quad g_k(\vec{m}) \leq 0, \quad h_l(\vec{m}) = 0.
\]

An expression for \( \langle V \rangle \) can be constructed in terms of the Lagrangian,

\[
\langle V \rangle = \mathcal{L} = f(\langle \vec{m} \rangle) + \sum_i \lambda_i h_i(\langle \vec{m} \rangle) + \sum_k \mu_k g_k(\langle \vec{m} \rangle),
\]

where the constants \( \lambda_i \) and \( \mu_k \geq 0 \) are the Karush-Kuhn-Tucker (KKT) multipliers \([22]\). The entropy of \( Q \), on the other hand, is given by,

\[
S_Q = -\sum_i [(1 - m_i) \ln(1 - m_i) + m_i \ln m_i],
\]

so the variational problem for the \( m_i \)’s is written like,

\[
\min F_Q(\langle \vec{m} \rangle) = \min \{ f(\langle \vec{m} \rangle) + \sum_i \lambda_i h_i(\langle \vec{m} \rangle) + \sum_k \mu_k g_k(\langle \vec{m} \rangle) \}
\]

\[
+ \sum_i [(1 - m_i) \ln(1 - m_i) + m_i \ln m_i].
\]

Equations \((3), (4)\) and \((10)\) give a general probabilistic model for combinatorial optimization problems with binary decision variables. Any continuous and differentiable nonlinearities in the objective or the constraints can be expanded in a Taylor series under the condition \( m_i < 1 \, \forall \, i \). Due to independence under the mean field, \( \langle V \rangle \) is therefore given by Eq. \((8)\) for any problem \((\text{I})\), provided that the stated conditions are met. Stationarity applied to \( F_Q \) with respect to the mean field parameters reduce the variational problem to a set of self-consistency equations for \( \vec{m} \),

\[
m_i = \frac{1}{1 + \exp[\alpha \mathcal{L}_{\vec{m}, \mu}(\vec{m})]},
\]

The generation of valid solutions of \((\text{I})\) from the mean field model can then be tackled by the following numerical scheme,

1. Give initial values for the KKT multipliers.
2. Solve Eq. \((11)\).
3. Evaluate the objective and constraints, either rounding the mean field (MF) solution or drawing a point from the resulting MF distribution. Update the KKT multipliers and repeat from stage 2 until suitable stopping criteria are met.

III. RESULTS

The probabilistic setup \((3), (4), (10)\) and \((11)\) is now tested on specific examples. We first consider here the classical Knapsack Problem (KP),

\[
\min -\vec{q} \cdot \vec{x} \quad s.t. \quad \vec{w} \cdot \vec{x} - d \leq 0,
\]

where \( d \) is the capacity of the knapsack, \( \vec{q} \) are the gains and \( \vec{w} \) the weights of a collection of \( i = 1, \ldots, N \) objects. The set of self-consistency equations for the mean field parameters is in this case independent, with solution,

\[
m_i = \frac{1}{1 + \exp(-q_i + \mu w_i)},
\]

where \( \mu \) is the KKT multiplier associated to the single constraint. When this constraint is inactive, \( \mu = 0 \) and \( m_i \in [\frac{1}{2}, 1] \). In the case in which the constraint is active, \( \mu \geq 0 \). The substitution of Eq. \((13)\) into the complementary slackness condition \( \vec{w} \cdot \vec{m} - d = 0 \) gives,

\[
\sum_{i=1}^{N} (w_i - d) \exp(q_i - \mu w_i)
\]

\[
+ \sum_{i=1}^{N} (w_i + w_{i+1} - d) \exp [(q_i + q_{i+1} - \mu (w_i + w_{i+1})]
\]

\[
+ \sum_{i=1}^{N} (w_i + w_{i+1} + w_{i+2} - d) \exp [(q_i + q_{i+1} + q_{i+2} - \mu (w_i + w_{i+1} + w_{i+2})]
\]

\[
+ \ldots + \left( \sum_{i=1}^{N} w_i \right) - d \exp (\sum_{i=1}^{N} q_i - \mu N w_i) = d,
\]

where \( q_{i+j} = w_{i+j} = 0 \) if \( (i+j) > N \). The overlines represent averages over the distributions from which the instance parameters (weights and gains) are drawn. The index \( \tau = 1, \ldots, N \) counts the terms in the left side of Eq. \((14)\). The finite sums over the instance parameters that appear in the expression are rewritten in terms of the estimators,

\[
\frac{1}{\tau} \sum_{i=1}^{\tau} w_{i+\tau} = \bar{w} + \epsilon_{\tau},
\]

\[
\frac{1}{\tau} \sum_{i=1}^{\tau} q_{i+\tau} = \bar{q} + \epsilon'_{\tau},
\]

where the \( \epsilon \)’s are estimation errors, which in general go to zero as \( \tau \rightarrow \infty \). For the problem to be feasible, \( \bar{w} < d \) if \( N \gg 1 \). This imply that for large \( N \), the terms of the left side of Eq. \((14)\) with small \( \tau \) are typically negative, and should be cancelled out. Therefore,

\[
\alpha (N \bar{w} - d) \exp [N(\bar{q} - \mu \bar{w})] \approx d, \quad \alpha \geq 1,
\]

from which it follows that,

\[
\mu \approx \frac{\bar{q}}{\bar{w}} - \frac{1}{\alpha N} \ln \left( \frac{d}{N \bar{w} - d} \right).
\]

In the limit \( N \rightarrow \infty, \mu = \frac{\bar{q}}{\bar{w}} \). This result gives an important insight: for active constraints, the multipliers are such that the distribution \((4)\) actually represents the “competition” between the objective and the constraints. Good starting points of the search scheme for the multipliers can be obtained on this basis. For KP, we have implemented the following procedure,

1. The multiplier is initially set like \( \mu = \frac{\bar{q}}{\bar{w}} \).
2. Evaluate Eq. \((13)\)
3) Update $\mu$ by the minimization of $(\tilde{w} \cdot \tilde{m} - d)^2$. Evaluate $\tilde{w} \cdot \tilde{m} - d = \epsilon$. Given a predefined tolerance $tol$, if $|\epsilon| > tol$, then go to step 2 using a new initial value for the multiplier drawn at random from a neighborhood around $\tilde{m}$. Else, end.

At each iteration the resulting mean field parameters are rounded, the feasibility is checked and the objective is evaluated, keeping track of the best feasible solution. The random initial values for the multiplier are taken from an interval of 10% around the $\mu$ value associated to the current best rounded solution at each iteration. Some numerical results and comparisons are presented in Table 1. In the reported experiments, $tol = 0.0001$. A maximum of 1000 iterations is allowed. The scheme is terminated if $|\epsilon| \leq tol$ or the total number of permitted iterations is completed. The best found rounded feasible solution and its objective value is reported.

The instances were created with the Pisinger generator \[23\], under the conditions of strong linear correlations between $q_i$ and $w_i$, being $w_i$ randomly distributed in the interval $[1, 1000]$. It has been argued that for these type of instances the integer solution is usually far from the continuous relaxation solution \[23\]. The exact solutions have been found using the branch and bound algorithm provided by Cplex \[2\], which is a widely accepted state of the art standard for linear and quadratic integer problems. A general purpose Genetic Algorithm (GA) is also tested on the instances. The Cplex version is Ibm Ilog Cplex 12.4. For the GA the R package Genalg \[24\], version 0.1.1 was used, with all the defaults except a rule which stops GA evolution if there is no change in best objective value after 500 generations or a time limit of 5000 seconds of CPU time is exceeded. The experiments were run on an Intel I7-3820 processor with 4 cores, 3.60 GHz and 32 GB RAM. For each problem dimension, 10 instances are drawn from the Pisinger generator, running each instance 10 times from different initial conditions. Averages and standard deviations of the objective values and computation times for the MF and GA algorithms are reported. For the considered instances, Cplex found the exact solutions in CPU times < 1 second. Although GA and MF are comparable at small problem sizes, for large problems the mean field heuristic finds higher quality solutions at a computation time that is orders of magnitude below of GA. The effectiveness of the formulation in nonlinear cases has been tested on the Quadratic Knapsack Problem (QKP), which is stated as follows \[24\],

$$\min \quad -x^T Q x \quad s.t. \quad \tilde{w} \cdot \tilde{x} - d \leq 0,$$

where $Q$ is a symmetric matrix with coefficients $q_{i,j} \geq 0 \quad \forall \quad i, j$. QKP has a graph-theoretic interpretation in terms of the Clique problem \[24\]. Moreover, QKP is in general NP-hard in the strong sense, meaning that admits no polynomial-time approximation scheme unless $P = NP$ \[24\]. The mean field Lagrangian reads,

$$L = -\tilde{m}^T Q \tilde{m} + \mu(\tilde{w} \cdot \tilde{m} - d),$$

from which

$$\partial_i L_\mu = -2q_i m_i - \sum_{j \neq i} q_{i,j} m_j + \mu w_i. \tag{20}$$

The initial value of the multiplier is taken like,

$$\mu = \frac{1}{Nw} \left[2 \sum_i q_{i,i} + \sum_{i,j} q_{i,j} \right]. \tag{21}$$

Due to nonlinearity, the algebraic system \[11\] is now coupled. At fixed $\mu$, it can be efficiently solved by iterating the equations \[11\]. Besides this, the numerical procedure is almost the same followed for the KP example. More precisely, the step 2 of the procedure now involves the iteration of the mean field equations \[11\] from a starting random initial $\tilde{m}$. In our experiments, we have used only one iterating step. Results in instances of 200 variables taken from the benchmark provided by Billionet and Soutif \[25\] are reported in Table 2. Even in these relatively small instances Cplex is unable to find optimality certificates in short times. Therefore we now include the branch and bound method in the comparison, focusing on solution quality and computation times. The equipment is the same as that used for the KP experiments. A maximum CPU time of 100 seconds is allowed for the mean field and the branch and bound algorithms, while for the GA is imposed a limit of 5000 seconds. The averages and standard deviations of the ratio between the best value found with respect the known optimum is reported. Each instance has been run 10 times, while the benchmark includes 10 examples of each of the quadratic coefficients matrix densities of 25%, 50% and 100%. Therefore the statistics is computed from a total of 300 runs per method. Both the branch and bound and the mean field methods have an average solution quality above 99% with respect to the known exact optimum, while the GA shows considerable inferior performance. Larger instances are studied using the QKP generator provided by Pisinger \[3\]. Comparisons are in this case only between the mean field and branch and bound by computing the ratio between the best solutions found by MF and Cplex. A total of 10 instances is generated for each problem size, with matrix density of 100%. Each instance was run 10 times from different initial conditions, giving a total statistics of 100 runs for each problem size per method. For problem sizes of 1000 the performance between both methods appear to be similar, however at size 2000 Cplex is unable to find integer solutions in some cases. These are discarded until the 10 examples are completed. For sizes of 5000 and above, the branch and bound is unable to find any integer solution in the 100 seconds computation time limit. In fact, by further tests it have turned out that Cplex is unable to give integer solutions for these cases even after several days of CPU time in our equipment. We have tested the mean field up to instances of size 20000, always giving integer feasible solutions, although with an increasing variance of the best objectives values. Figure 1 shows that the variance is however reduced and the overall solution quality incremented when larger computation times are allowed, which indicates that

\[http://www.diku.dk/~pisinger/generator.c\]
\[http://www-01.ibm.com/software/commerce/optimization/cplex-optimizer/index.html\]
\[http://cran.r-project.org/web/packages/genalg/\]
\[http://www.diku.dk/~pisinger/testqkp.c\]
the mean field procedure scales robustly for large problem dimensions.

IV. CONCLUSION

Under mild assumptions on the statistical properties of the linear KP, an explicit mean field solution has been found in the infinite size limit, expressed by the equations (13) and (17). In the experiments presented in Table 1, the ratio between the initial value of \( \mu \) given by \( \mu = \frac{q}{2} \) and the final value obtained after the iterations of the numerical scheme has been found to be \( 1 \pm 0.003 \). This kind of “thermodynamic limit” might exist in other linear constrained problems as well. The nonlinear constrained case studied here also points out in a similar direction. In all the considered problems, the heuristically proposed initial multiplier always give an integer valid solution, despite that it is hard to achieve by a branch and bound search from random initial conditions.

The mean field framework presented in this contribution appears to be highly competitive with respect to standard approaches. For the test problems considered, there exist other more specialized deterministic and stochastic methods besides the GA and branch and bound used here for comparisons. However, the available literature on these other algorithms is mainly focused on small to medium problem sizes [13], [14], [15], [16]. We have used therefore two popular stochastic and deterministic methods as a way to assess the scalability of our framework with respect to what is often done in practice. Moreover, our interest is the development of a general paradigm. The implementation for almost arbitrary nonlinear problem structures should follow essentially the same steps used here for the QKP example. Clearly, the application of our framework to different integer optimization problem classes is one of the research lines opened by the present work. Other is the design of novel heuristics based on the mean field or its hybridization with existing algorithms. Also could be valuable to explore corrections to the mean field equations, by the use of cavity, replica or related approaches [19], [21].

ACKNOWLEDGMENT

This work was partially supported by the National Council of Science and Technology of Mexico under grant CONACYT CB-167651 and by the Autonomous University of Nuevo Leon support to research program under grant UANL-PAICYT IT795-11.

REFERENCES

[1] R. Hemmecke, M. Köppe, J. Lee, R. Weismantel, “Nonlinear integer programming”. In 50 Years of Integer Programming 1958-2008. The Early Years and State-of-the-Art Surveys, eds Jinger M, Liebling T, Naddef D, Nemhauser G, Pulleyblank W, Reinhart G, Rinaldi G, Wolsey L. A Springer, Heidelberg, 2009.
[2] C. DAmбросio, A. Lodi, "Mixed integer nonlinear programming tools: a practical overview". Journal of Operations Research 9:329-349, 2011.
[3] C. Buchheim, A. Caprara, A. Lodi, “An effective branch-and-bound algorithm for convex quadratic integer programming”. Math. Program., Ser. A 135:369-395, 2012.
[4] P. Bonami, M. Kilinc, J. Linderoth, “Algorithms and Software for Convex Mixed Integer Nonlinear Programs”. In Mixed Integer Nonlinear Programming, The IMA Volumes in Mathematics and its Applications 154:1-39, Eds: J. Lee, S. Leyffer, Springer, 2012.
[5] A. Sipahioglu, T. Sarac, “The Performance of the Modified Subgradient Algorithm on Solving the 0-1 Quadratic Knapsack Problem”. Informatica, 20(2):293-304, 2009.
[6] P. Belotti, C. Kirches, S. Leyffer, J. Linderoth, J. Luedtke, A. Mahajan, “Mixed-integer nonlinear optimization”. Acta Numerica 22:1131, 2012.
[7] A. Lodi, “The Heuristic (Dark) Side of MIP Solvers”. In Hybrid Metaheuristics. Studies in Computational Intelligence 434:273-284. Ed. E. Talbi, Springer, 2013.
[8] A. Hartmann, M. Weigt. Phase transitions in combinatorial optimization problems. Wiley, 2005.
[9] A. Colorni, M. Dorigo, F. Maffioli, V. Maniezzo, G. Righini, M. Trubian, “Heuristics from nature for hard combinatorial optimization problems”. International Transactions in Operational Research 3(1):1-21, 1996.
[10] S. Kirkpatrick, C. D. Gelatt Jr., M. P. Vecchi, Optimization by Simulated Annealing. Science 220:671-680, 1983.
[11] D. Goldberg. Genetic Algorithms in Search, Optimization and Machine Learning. Addison-Wesley, 1989.
[12] A. E. Eiben, J. E. Smith. Introduction to Evolutionary Computing. Springer, 2003.
[13] Y. Lin, “A hybrid method of evolutionary algorithms for mixed-integer nonlinear optimization problems”. In Proceedings of the 1999 Congress on Evolutionary Computation 3:2166, 1999.
[14] Z. Yang, G. Wang, F. Chu, “An effective GRASP and tabu search for the 0-1 quadratic knapsack problem”. Computers & Operations Research 40:11761185, 2013.
[15] X. Xie, J. Liu, “A mini-swarm for the quadratic knapsack problem”. In Proceedings of the 2007 IEEE Swarm Intelligence Symposium (SIS 2007), 2007.
[16] A. Narayan, C. Patvardhan, “A novel quantum evolutionary algorithm for quadratic knapsack problem”. In Proceedings of the 2009 IEEE International Conference on Systems, Man, and Cybernetics, 2009.
[17] N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, E. Teller, “Equation of state calculations by fast computing machines”. Journal of Chemical Physics 21:1087-1092, 1953.
[18] E. T. Jaynes, “Information Theory and Statistical Mechanics”. Physical Review 106:620-630, 1957.
[19] G. Parisi. Statistical Field Theory. Addison-Wesley, 1988.
[20] O. C. Martin, R. Monasson, R. Zecchina, “Statistical mechanics methods and phase transitions in optimization problems”. Theoretical Computer Science 265(1-2):3-67, 2001.
[21] Eds: M. Opper, D. Saad. Advanced Mean Field Methods: Theory and Practice. MIT Press, 2001.
[22] E. K. P. Chong, S. H. Zak. An Introduction to Optimization, fourth edition. Wiley, 2013.
[23] D. Pisinger, “Where are the hard knapsack problems?” Computers and Operations Research 32(9):2271-2284, 2005.
[24] D. Pisinger, “The quadratic knapsack problem-a survey”. Discrete Applied Mathematics 155:623-648, 2007.
[25] A. Billionnet, E. Soutif. “Using a Mixed Integer Programming Tool for Solving the 0-1 Quadratic Knapsack Problem”. INFORMS Journal on Computing 16(2):188-197, 2004.
TABLE I

CLASSICAL KNAPSACK PROBLEM. STATISTICS OF THE RATIO OF THE BEST VALUES OBTAINED BY GA AND MF WITH RESPECT TO THE KNOWN OPTIMUM (FOUND BY THE BRANCH AND BOUND ALGORITHM IMPLEMENTED IN CPLEX) AND OF THE CPU TIMES PER RUN (IN SECONDS) IS COMPUTED FROM 10 INSTANCES FOR EACH PROBLEM SIZE, RUNNING EACH INSTANCE 10 TIMES FROM RANDOM AND INDEPENDENT INITIAL CONDITIONS FOR BOTH METHODS. ON THESE AND THE FOLLOWING REPORTED EXPERIMENTS, ALL THE RUNS WERE PERFORMED ON THE SAME EQUIPMENT UNDER THE SAME CONTROLLED CONDITIONS.

| N     | [(GA best) / (optimum)] (%) | GA time     | [(MF best) / (optimum)] (%) | MF time   |
|-------|----------------------------|-------------|-----------------------------|-----------|
| 100   | 95.44 ± 0.66               | 21.88 ± 5.37| 92.35 ± 9.68                | 0.11 ± 0.05|
| 1000  | 91.34 ± 3.35               | 224.01 ± 65.24| 94.32 ± 2.23               | 4.192 ± 3.66|
| 10000 | 90.43 ± 3.43               | 1098.71 ± 170.05| 96.51 ± 0.62               | 48.19 ± 27.73|

TABLE II

QUADRATIC KNAPSACK PROBLEM. THE PROBLEM SIZE WITH N = 200 DECISION VARIABLES FROM THE BILLIONET AND SOUTIF BENCHMARK IS CONSIDERED. A TOTAL OF 100 SECONDS OF CPU TIME IS ALLOWED FOR MF AND CPLEX, WHILE A 5000 SECONDS OF CPU TIME LIMIT IS IMPOSED TO THE GA. THE BENCHMARK CONSISTS OF 10 INSTANCES OF EACH OF THE QUADRATIC COEFFICIENTS MATRIX DENSITIES OF 25%, 50% AND 100%. STATISTICS WERE COLLECTED BY PERFORMING 10 INDEPENDENT RUNS PER METHOD ON EACH INSTANCE. THE RATIO OF THE BEST VALUES WITH RESPECT TO THE KNOWN OPTIMA IS THEREFORE REPORTED FROM A TOTAL OF 300 RUNS PER METHOD.

| N     | [(GA best) / (optimum)] (%) | [(MF best) / (optimum)] (%) | [(Cplex best) / (optimum)] (%) |
|-------|----------------------------|----------------------------|--------------------------------|
|       | 87.4 ± 0.3                 | 99.4 ± 0.2                 | 99.9 ± 0.1                     |

TABLE III

QUADRATIC KNAPSACK PROBLEM. LARGE PROBLEM DIMENSIONS ARE CONSIDERED BY DRAWING THEM FROM THE PISINGER GENERATOR. NO EXACT OPTIMA ARE KNOWN IN THESE CASES. THE RATIO BETWEEN THE BEST FOUND VALUES OF MF AND CPLEX ARE REPORTED FROM 10 DIFFERENT INSTANCES RAN 10 TIMES BY BOTH METHODS, IMPOSING A LIMIT OF 100 SECONDS OF CPU TIME. AT SIZE N = 2000, CPLEX IS UNABLE TO FIND INTEGER SOLUTIONS FOR SOME CASES. THESE HAVE BEEN DISCARDED UNTIL 10 INSTANCES SOLVABLE BY CPLEX ARE COMPLETED. AT SIZE N = 5000, CPLEX GAVE NONE INTEGER SOLUTION.

| N     | [(MF best) / (Cplex best)] (%) |
|-------|-------------------------------|
| 500   | 99.5 ± 0.4                    |
| 1000  | 100.6 ± 0.9                   |
| 2000  | 101.2 ± 1.6                   |
| 5000  | ∞                             |
Fig. 1. The scalability of the MF procedure is tested by analyzing the relative standard deviation (the ratio of the standard deviation of the best values with respect to the average of the best values, in percent units) of the MF results at different sizes of the QKP. The solid curve reports the behavior with 100 seconds of CPU time while the dashed curve gives the relative standard deviations with 200 seconds of CPU time. The curves show that integer feasible solutions can be found by MF in modest computation times for problem sizes that are intractable by standard methods. The variability of MF decreases by increasing computation times. The ratio between average best values at 200 and 100 seconds is $1.13^{+0.4}_{-0.1}$. Therefore the figure is indicative of an overall increase in solution quality as a consequence of the CPU time increment.