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Dual mean field search for large scale linear and quadratic knapsack problems

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HIGHLIGHTS

- Principled heuristic capable to deal with large scale binary optimization problems.
- Running times that are orders of magnitude shorter than state of the art algorithms.
- Search in a dual space which takes into account the effect of the constraints.

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ABSTRACT

An implementation of mean field annealing to deal with large scale linear and non linear binary optimization problems is given. Mean field annealing is based on the analogy between combinatorial optimization and interacting physical systems at thermal equilibrium. Specifically, a mean field approximation of the Boltzmann distribution given by a Lagrangian that encompass the objective function and the constraints is calculated. The original discrete task is in this way transformed into a continuous variational problem. In our version of mean field annealing, no temperature parameter is used, but a good starting point in the dual space is given by a "thermodynamic limit" argument. The method is tested in linear and quadratic knapsack problems with sizes that are considerably larger than those used in previous studies of mean field annealing. Dual mean field annealing is capable to find high quality solutions in running times that are orders of magnitude shorter than state of the art algorithms. Moreover, as may be expected for a mean field theory, the solutions tend to be more accurate as the number of variables grow.

1. Introduction

Discrete optimization is applicable in numerous fields of science and engineering, including biological networks, planning, scheduling and automation, just to indicate a few [1–4]. It represents one of the major challenges for algorithmics,

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deeply related to constraint satisfaction problems in artificial intelligence [5–7]. Besides of its practical importance and of the progress made in the solution of integer linear programs in the last decades, integer optimization is still a very difficult subject [8]. Practical methods for nonlinear problems are rare and mostly limited to small to medium sized problems [9, 8,10], even in special cases such as convex integer programming [10–12]. Heuristic approaches consequently play a major role in the field, either hybridized with deterministic algorithms [13,14], or like stochastic solution strategies on their own right [15–23].

An essential ingredient in any heuristic is a rule by which candidate solutions are generated. In this contribution we introduce a version of mean field annealing to construct probabilistic solution generators that are consistent with the underlying integer optimization task under the basis of the mean field approximation of an associated Boltzmann distribution. The method is given for the class of binary integer programs, which implies that the ideas are general enough to be extended to any combinatorial optimization model in a bounded domain.

2. Mean field framework

Mean field annealing is a deterministic procedure that approximates a stochastic simulated annealing search [24–26]. Simulated annealing emulates the probability distribution,

$$P(\vec{x}) \propto \exp\left(-V/T\right), \tag{1}$$

where T (temperature) is a noise parameter which is diminished from a starting high value following a careful annealing schedule and generating a number of configurations for each temperature [17]. In mean field annealing, the sampling stage is replaced by a step in which a set of coupled mean field equations must be solved at each T, which reduces much of the computational burden of simulated annealing [24–26]. In this contribution we propose a variation of the original mean field annealing method which do not involves an annealing stage but a random search around a good starting point in a dual space. This further reduces the computational burden, allowing the exploration of large instance sizes. Our method is principled and firmly based on the fundamental rules of probability. More precisely, any possible solution for a binary 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,

$$\begin{aligned} &\min f(\vec{x}) \quad \text{s.t.} \\ &g_k(\vec{x}) \leq 0, \qquad h_l(\vec{x}) = 0, \end{aligned} \tag{2}$$

where $\vec{x}$ is a vector of binary decision variables, $g_{k(k=1,\ldots,K)}$ are inequality constraint functions and $h_{l(l=1,\ldots,L)}$ are equality constraints. The optimization task (2) can in principle be represented by a potential function $V(\vec{x})$ which includes the objective and the constraints. A probability distribution can be associated to such a potential by the transformation [17, 27],

$$P(\vec{x}) = \frac{1}{Z}\exp\left(-V\right), \tag{3}$$

where Z is a normalization factor (or partition function). The Eq. (3) gives the maximum entropy distribution which is consistent with the condition $\langle V\rangle_P = \int VPd\vec{x}$ [28]. 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,

$$Q(\vec{x}) = \prod_{i=1}^{N} p(x_i). \tag{4}$$

Mean field techniques, together with other methods which have first emerged in statistical mechanics [29], have been already successfully applied to discover fundamental features of combinatorial problems and valuable solution strategies, although focused on particular combinatorial problem classes [30,31]. Our purpose in this contribution is to develop a practical mean field framework to find good candidate solutions to linear and nonlinear binary problems in the constrained situation (2). The most general form for the independent marginals is,

$$p(x_i) = 1 + (2m_i - 1)x_i - m_i. \tag{5}$$

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 [32],

$$D_{KL}(Q \parallel P) = \langle \ln Q\rangle - \langle \ln P\rangle, \tag{6}$$

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

$$F_Q = \left[\langle V\rangle - S_Q\right] \tag{7}$$