An example of a link between artificial intelligence and statistical physics: exact computation of the partition function of a graphical model on a series-parallel graph

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Context. Computing efficiently the partition function Z of a model of interacting particles like the Ising model has been a challenge for many decades in statistical physics and still is an open problem. It is required for instance to derive an exact dependence of the partition function on an intensive parameter, like temperature. Such a computation is feasible analytically for a very limited number of models only (Baxter, 1982). The problem of computing the partition function is equivalent to that of computing the normalizing constant of an undirected graphical model. Most underlying graphs in statistical physics are regular, like invariant by translation (2D or 3D mesh), or Cayley trees (Eggarter, 1974). In other domains of applications of graphical models, the graph can be a random graph or a scale-free network (like in epidemic or social network), or a graph representing interactions between molecules or atoms in computational protein design. For all these graphs (except Cayley trees) in general exact computation of Z (analytically or even numerically) is out of reach.

The objective of this work is to extend the transfer matrix method from statistical physics (Baxter, 1982) which enables exact computation of Z on a line, to a more complex family of graphs, the family of series-parallel graphs (Duffin, 1965).

The transfer matrix method. Let us consider a graphical model whose attached graph is a line, with homogeneous potential functions. The state of a vertex can be in any discrete space, and the potentials are pairwise, as a function of the two endpoints of an edge. Such a pairwise potential can be represented as a matrix, called a transfer matrix. Then, on a line of length n, the partition function is exactly the sum of the elements of the nth power of the transfer matrix (the global transfer matrix). As the Ising model of statistical mechanics can be interpreted as a graphical model with two states (+1,-1) and a 2×2 transfer matrix, it can be solved this way.

Application to series-parallel graphs. A series parallel graph is defined recursively. It is a graph with two end points, a source and a tip. Two series parallel graph can be combined to build a new one, either in series by merging the tip of one with the source of the other, or in parallel by merging tips and merging sources. A graph with two vertices and one edge in-between is the simpler series-parallel graph.

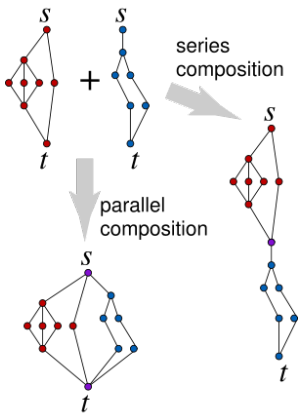

Figure : Constructive definition of a series-parallel graph (from Wikipedia)

We show that for these particular graphs, the transfer-matrix method can be extended and provides an analytical algebraic approach for an exact computation of the partition function. More concretely, we attach to a series-parallel graph a global potential matrix with rows being the states of the tip and columns being the state of the source, such that the sum of its terms is the partition function. We derive a general recursive procedure for computing algebraically the global transfer matrix of a series-parallel graph knowing the matrices attached to the graphs it has been built with. The result is a combination of matrix products, and component wise matrix products. If the potential matrix depends on a parameter as in Ising model, this leads to the analytical dependence of the global transfer matrix on the parameter. It is known that the decomposition tree of a series-parallel graph can be constructed in linear time in the size of the network (Borie et al., 1991). Furthermore, matrix product can be performed in $O(m^3)$ elementary operations (scalar addition/multiplication), if m is the number of states of one node, while component-wise multiplication and matrix sum of elements can be performed in $O(m^2)$. This can be implemented by first computing its decomposition tree and then applying the elementary vertex deletion/edge merging operations specified by this decomposition tree. Therefore, if G is the series-parallel graph of a stochastic graphical model, the associated partition function Z can be computed in $O(|G|\times m^3)$ time in the worst case assuming scalar addition/multiplication have constant time complexity. This upper bound can be significantly reduced in some particular cases. In all cases, Z can be computed in time linear with respect to the size of the graph and polynomial time in m.

Perspectives. This result should be related to results from Artificial Intelligence and Computer Science: in this field it is well known that for a broader family of graphs, namely graphs of bounded treewidth (Bodlaender, 1994), an exact computation of the partition function is possible in polynomial time using variable elimination and dynamical programming (Dechter, 1999). The direct application of this computation method for a graphical model on a tree (BP algorithm) has also been applied in a loopy version in order to obtain an approximation of Z for a general graph, leading to loopy Belief Propagation Algorithms (LBP). A perspective of our work is then to develop a similar loopy version of the transfer matrix method. The motivation of developing such a method is that while BP is exact on trees (treewidth 1), transfer-matrix approaches are exact for Series-parallel graphs, which are of treewidth 2 and include trees. Thus, it is likely that a loopy transfer-matrix approach may improve LBP for some graph structures.

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