SYMBOLIC COMPUTATION TO THE AID OF STATISTICAL MECHANICS

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Abstract. We suggest that symbolic computation is a powerful tool in theoretical physics, that is currently not as widely used as it should be. We illustrate it by a bit of "alternative history", how the celebrated and extremely complicated Onsager solution could (at least in principle, but probably also in pratice) could have been conjectured, using symbolic computation. Hopefully, the same methodology would be helpful to make progress on till open problems, like the 2D Ising model with a magnetic field, and the 3D Ising model.

1. Prologue

Until about thirty years ago, physics consisted of **two** parts: theoretical and experimental. Then a new kid came to the block, *computational physics*, that used a computer to 'pretend' that it is nature, and perform many experiments that would be too expensive, and usually impossible to perform in the real world. Alas, computational physics, with a few pioneering exceptions, used *numerical* computations (mostly simulations). We believe that there is room for yet another 'kid', symbolic computations. Very impressive applications of Symbolic Computation to high energy physics are described, for example, in [1]. Here we hope to illustrate the usefullness of symbolic computation to statistical mechanics, by focusing, as a *case study*, on the celebrated *Ising model* (e.g. [5]).

2. A crash course in statistical mechanics

The general scenario of *statistical mechanics* consists of very many possible *configurations*, each with a certain *energy*. Not all configurations are created equal, and some are much more likely than others, as first realized by the Austrian scientific giant, Ludwig Boltzmann. The probability of a configuration C, whose energy is $E(C)$ is **proportional** to

$$e^{\frac{-E(C)}{kT}} \quad ,$$

where k is **Boltzmann's constant**, and T is the **absolute temperature**.

It follows that the higher the energy, the less likely it is to show up, the decay being *exponential*.

In order to get *macroscopic* (thermodynamic) (average) information, we form the famous **Gibbs Partition function**

$$\mathcal{Z} = \sum_{C \in configurations} e^{\frac{-E(C)}{kT}} \quad ,$$

and the 'average' energy (that physicists call *internal energy*) is obtained by taking the *logarithmic derivative*. Other quantities of interest are obtained by taking higher order derivatives.

(Note that in taking the logarithmic derivative, $\mathcal{Z}$ shows up in the denominator, and this makes sense, in order to normalize the sum of the probabilities to be 1).

Statistical mechanicians are fond of *toy models* that 'simplify' nature, and try to preserve the *qualitative* features of the real world. Unfortunately, even these *toy* models are extremely difficult, and with rare exceptions, intractable (or at least wide open), and people resort to *approximations*, using **numerical** methods, sophisticated brilliant (but non-rigorous) renormalization theory calculations, and most often, *simulations* (aka "Monte Carlo methods").

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In this article we will show how symbolic computation may give a new approach to tackling these difficult models.

3. The grandaddy of all models: The (two dimensional) Ising Model

Fix positive integers m and n, and let $\mathcal{M}(m,n)$ be the set (of cardinality 2^{mn}) of all $m \times n$ matrices whose entries are -1 or 1 (called 'spin down' and 'spin up', respectively).

Let

$$x = e^{\frac{J}{kT}} \quad , \quad y = e^{\frac{H}{kT}}$$

where J is the so-called *coupling constant* (and hence a (physical) **constant**) and H is another input variable (in addition to T) called the (strength of the) *external magnetic* field.

The *energy* associated to a specific matrix $M \in \mathcal{M}(m,n)$ is defined as follows

$$E(M) := -J \left(\sum_{i=1}^{m} \sum_{j=1}^{n} (M_{i,j}M_{i,j+1} + M_{i,j}M_{i,j+1}) \right) - H \left(\sum_{i=1}^{m} \sum_{j=1}^{n} M_{i,j} \right) .$$

Here we use the 'periodic' convention that $M_{m+1,j} = M_{1,j}$ and $M_{i,n+1} = M_{i,1}$.

It follows that the *weight* of a matrix is

$$weight(M) := exp(-\frac{E(M)}{kT}) = x^{\sum_{i=1}^{m} \sum_{j=1}^{n} (M_{i,j}M_{i,j+1} + M_{i,j}M_{i,j+1})} \cdot y^{\sum_{i=1}^{m} \sum_{j=1}^{n} M_{i,j}} \quad .$$

Our first (modest!) goal is just to compute, for as large m and n that our computers and human ingenuity would allow, the (Gibbs) *Partition function* (i.e. *weight enumerator* of the set $\mathcal{M}(m,n)$).

$$\mathcal{Z}_{m,n}(x,y) := \sum_{M \in \mathcal{M}(m,n)} weight(M) \quad ,$$

a certain *Laurent polynomial* in the variables x (of degree $2mn$ and low-degree $\geq -2mn$) and y (of degree mn and low-degree $-mn$).

Later on we would be especially interested in the 'square case' ($m = n$), and the semi-infinite strip case ($n = \infty$).

4. Transfer matrices

A *direct* [4] way to compute $\mathcal{Z}_{m,n}(x,y)$ is to simply construct the set $\mathcal{M}(m,n)$ consisting of all 2^{mn} whose entries are drawn from the set $\{-1,1\}$ matrices, compute the weight for each and every one of them, and add them all up. But there is a much more efficient way [5, 6], called the *transfer-matrix method*.

Let's associate for each integer i between 0 and $2^m - 1$ the m-dimensional $\{-1,1\}$ column vector $v(i) := (2b_0 - 1, \ldots, 2b_{m-1} - 1)$, where $i = \sum_{j=0}^{m-1} b_j 2^j$ is the binary representation of i.

Define the $2^m \times 2^m$ transfer matrix

$$\mathbf{T}(m) := (T_{ij})_{0 \leq i,j \leq 2^m - 1} \quad ,$$

where the typical entry T_{ij} is as follows.

$$T_{ij} := x^{\sum_{l=1}^{m} v(i)_l v(j)_l + \sum_{l=1}^{m-1} v(j)_l v(j)_{l+1} + v(j)_m v(j)_1} \cdot y^{\sum_{l=1}^{m} v(j)_l} \quad .$$

Using the transfer matrix, the desired polynomial $\mathcal{Z}_{m,n}(x,y)$ can be expressed very succinctly as

$$\mathcal{Z}_{m,n}(x,y) = \mathrm{Tr}\left[\, \mathbf{T}(m)^n \,\right] \quad .$$

It is well-known (and easy to see!) that *exponentiation* of a matrix is really fast (poly-log time, using $A^{2k} = (A^k)^2$, $A^{2k+1} = A^{2k}A$ rather than $A^k = A^{k-1}A$), but for a *numeric* matrix. Here we have a *symbolic* matrix, and a naive approach, (once m gets larger) would be unfeasible. But with the method of *homomorphic images*, we can go pretty far.

5. The Functions that physicists care about

For the finite (torodial) $m \times n$ lattice, one is interested in the *Free energy*, $\mathcal{F}$

$$\mathcal{F} = -kT \log \mathcal{Z} \quad ,$$

Internal Energy, U

$$U = kT^2 \frac{\partial}{\partial T} \log \mathcal{Z} \quad ,$$

and *Specific heat*

$$C = \frac{\partial U}{\partial T} \quad .$$

Physicists are also very interested in the *Magnetization*, M

$$M = -\frac{\partial \mathcal{F}}{\partial H} \quad ,$$

and the *Isothermal susceptibilty*

$$\chi_T = \frac{\partial M}{\partial H} \quad .$$

At the "end of the day", people take the limit as **both** m and n go to infinity, but one can already get a rough idea on what is going on for small values of m and n, as we hope to show soon.

6. The Data for $\mathcal{Z}_{m,n}(x,y)$

For $\mathcal{Z}_{n,n}(x,y)$ for $1 \leq n \leq 9$ see:

`http://www.math.rutgers.edu/~zeilberg/tokhniot/ising/Polys`

Very impressively, Per Hakan Lundow[3], has already computed these for $n \leq 16$

For $\mathcal{Z}_{m,n}(x,y)$ for $1 \leq m \leq 5 \quad , \quad 1 \leq n \leq 11$ see:

`http://www.math.rutgers.edu/~zeilberg/tokhniot/ising/Polys1`

7. The Semi-Infinite case

Physicists are not really interested in the polynomials $\mathcal{Z}_{m,n}(x,y)$ for their own sake but in the logarithm

$$\log \mathcal{Z}_{m,n} \quad .$$

But, physicists (and chemists) that believe in the (fictional!) infinity, are *really* interested in the *free energy* $\mathcal{F}(x,y)$

$$\mathcal{F} := -kT \lim_{m \to \infty} \lim_{n \to \infty} (mn)^{-1} \log \mathcal{Z}_{m,n}(x,y) \quad .$$

For the case $y = 1$ (zero magnetic field), this is known *explicitly*, thanks to the **mathematical** *tour de force* (using very abstract representation theory!) of 1968 **Chemistry** Nobelist, **physicist** Lars Onsager. For general y this is a wide-open, possibly impossible, problem. So all we can hope for, so far, is getting 'close to infinity'.

But, following Onsager, we can try and do the semi-inifite case, and get *explicit* expressions for

$$A_m(x,y) := \frac{1}{m} \lim_{n \to \infty} n^{-1} \log \mathcal{Z}_{m,n}(x,y) \quad .$$

It is well known [5] (and easy to see) that $A_m(x,y)$ is the largest root of the *characteristic equation* of the transfer matrix $\mathbf{T}(m)$

$$\det(\mathbf{T}(m) - \lambda I) = 0 \quad .$$

Hence, it is a solution of an *algebaric* equation (by an appropriate change of independent and dependent variables, it could be viewed as *formal power series*). It also follows that the *logarithm* (and of course, its derivatives with respect to both variables) are *holonomic* formal power series (or functions) in both variables.

8. How Onsager's solution could have been conjectured via the C-finite ansatz

Onsager's solution was an amazing *tour de force* using human ingenuity and lots of ad hoc tricks to find an 'explicit' expression for the largest eigenvalue of the transfer matrix for the $k \times infinity$ case for *any* (symbolic) k. It turned out this (at most) algebraic function of degree 2^k can be expressed as some explicit product of k algebraic functions of degree 2. Using the methods in our previous paper [2], this fact could be deduced automatically, and we believe that with a little more effort, the actual Onsager factorization would be automatically derivable for $k \leq 9$, from which it would be immediate to **conjecture** the Onsager factoriziation for *symbolic* (i.e. general k). Of course, this would not be a rigorous proof, in the mathematical sense, but definitely good enough for physicists.

9. How Onsager's solution would be conjectured via the Holonomic ansatz

The exact value of the largest eigenvalue $\lambda_1^{(m)}$ of the $2^m \times 2^m$ transition matrix, is only a stepping stone for the free energy, the limit of $\log \lambda_1^{(m)}/m$ as m goes to infinity, viewed as a function of the continuous parameter x (right now are only considering the zero magnetic field case, i.e. $y = 1$). It follows from general theory, that for each m $\log \lambda_1^{(m)}$ is *holonomic* (aka D-finite) in the variable x, i.e. satisfies a linear differential equation with *polynomial* coefficients.

Alas, as m gets larger and larger, these differential equations get more and more complicated, (to see them for $2 \leq m \leq 6$) go to the webpage of this article.

Suprisingly the case of interest $m = \infty$ satisfies a reasonale differential equation.

As is standard in the theory (see [5], Ch. 6), it is convenient to perform the change of variable

$$v = \frac{x - x^{-1}}{x + x^{-1}} \quad .$$

In terms of this the free energy satisfies the linear differential equation

$$(-13\,v^6 + 70\,v^5 - 251\,v^4 + 16\,v^3 + 69\,v^2 + 2\,v - 5)\frac{d}{dv}f(v) - v(v-1)(55\,v^5 - 309\,v^4 + 328\,v^3 + 220\,v^2 - 87\,v + 1)\frac{d^2}{dv^2}f(v) - v^2(33\,v^4 - 172\,v^3 - 10\,v^2 + 116\,v - 15)(v-1)^2\frac{d^3}{dv^3}f(v) -4\,v^3v + 1)(v^2 - 6\,v + 1)(v-1)^3\frac{d^4}{dv^4}f(v) = 0 \quad .$$

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