

# Series expansions from the corner transfer matrix renormalization group method

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# What is the CTMRG method?

The corner transfer matrix renormalization group method is an efficient algorithm for calculating thermodynamical quantities in statistical mechanical models.

It can be used to either calculate numerically, or evaluate series expansions of these quantities, the latter purpose of which is the focus of this talk.

To understand the method fully, it is instructive to look at its history and predecessors.

# CTM equations and method

The origin of the corner transfer matrix came from Baxter (1978) and Baxter and Enting (1979).

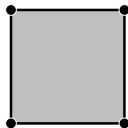
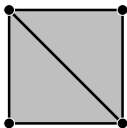
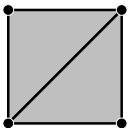
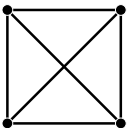
In these papers, which spawned a small series of other papers, they devised the CTM equations, which form the basis of all corner transfer matrix-related methods.

We will first examine these equations in detail.

## Interaction round a face

Firstly, we note that the CTM equations apply for a large class of statistical mechanical models which can be expressed in terms of *interaction round a face* (or IRF).

This means that the Boltzmann weight of a configuration can be expressed as the product (over all cells) of weights of a single cell.



## Interaction round a face (examples)

A classic example is the (2-d square lattice, spin- $\frac{1}{2}$ ) Ising model.

$$\begin{aligned} Z &= \sum_{\sigma} \exp \left( \beta J \sum_{\langle ij \rangle} \sigma_i \sigma_j + \beta H \sum_i \sigma_i \right) \\ &= \sum_{\sigma} \prod_{\langle ij, k, l \rangle} \omega \begin{pmatrix} \sigma_i & \sigma_j \\ \sigma_k & \sigma_l \end{pmatrix} \end{aligned}$$

where

$$\begin{aligned} \omega \begin{pmatrix} \sigma_i & \sigma_j \\ \sigma_k & \sigma_l \end{pmatrix} &= \exp \left( \frac{\beta J}{2} (\sigma_i \sigma_j + \sigma_j \sigma_l + \sigma_k \sigma_l + \sigma_i \sigma_k) \right. \\ &\quad \left. + \frac{\beta H}{4} (\sigma_i + \sigma_j + \sigma_k + \sigma_l) \right). \end{aligned}$$

## Interaction round a face (examples)

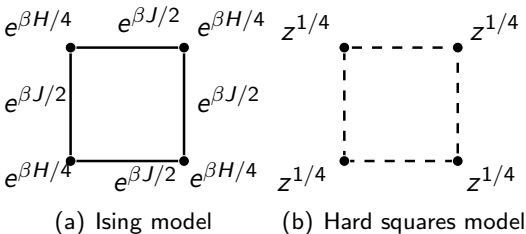
The test case that we used was the simpler hard squares model. We let the spin values be 0 and 1 and prohibit two neighbouring '1' spins. We use  $z$  as the fugacity of a '1' spin.

$$\begin{aligned}
 Z &= \sum_{\sigma} \begin{cases} 0 & \text{if } \sigma_i \sigma_j = 1 \text{ for some } \langle i, j \rangle \\ z^{\sum_i \sigma_i} & \text{otherwise} \end{cases} \\
 &= \sum_{\sigma} \prod_{\langle i, j, k, l \rangle} \omega \begin{pmatrix} \sigma_i & \sigma_j \\ \sigma_k & \sigma_l \end{pmatrix}
 \end{aligned}$$

where

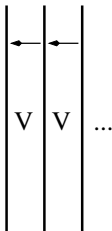
$$\omega \begin{pmatrix} \sigma_i & \sigma_j \\ \sigma_k & \sigma_l \end{pmatrix} = \begin{cases} 0 & \text{if } \sigma_i \sigma_j, \sigma_j \sigma_l, \sigma_k \sigma_l \text{ or } \sigma_i \sigma_k = 1 \\ z^{(\sigma_i + \sigma_j + \sigma_k + \sigma_l)/4} & \text{otherwise.} \end{cases}$$

# Interaction round a face (examples)



# Transfer matrices and the partition function

Consider a traditional (column) transfer matrix,  $V$ .



The elements of this matrix are the weight of a column of the lattice.



# Transfer matrices and the partition function

We can build the partition function of the entire lattice this way:

$$Z_{m \times n} = \text{Tr } V^n \approx \Lambda^n$$

where  $\Lambda$  is the maximum eigenvalue of  $V$ .

In the infinite (thermodynamic) limit, this gives the partition function per site:

$$\kappa = \lim_{m \rightarrow \infty} \Lambda^{\frac{1}{m}}.$$

# Calculating the partition function

To find the maximum eigenvalue of  $V$ , we use the Courant-Fischer theorem:

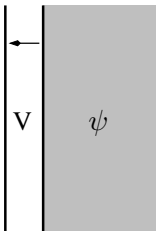
$$\Lambda = \max_{\psi} \frac{\psi^T V \psi}{\psi^T \psi},$$

where  $\psi$  is a vector with the same dimension as  $V$ .

We also know that the maximising  $\psi$  is the corresponding eigenvector of  $V$ .

# Calculating the partition function

The optimal  $\psi$  can be interpreted as the partition function of half a plane, given the spins on the border:



# A variational approximation

In the infinite limit,  $\psi$  is also infinite-dimensional, so maximising over all  $\psi$  is quite hard!

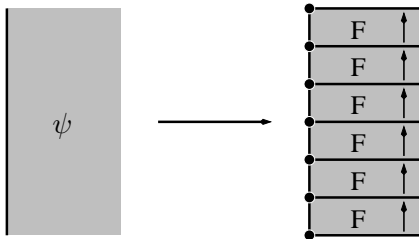
We instead choose to maximise over a subset of all possible  $\psi$ , which have a certain form:

$$\psi(\sigma_1, \sigma_2, \dots, \sigma_m) = \text{Tr } F(\sigma_1, \sigma_2)F(\sigma_2, \sigma_3) \dots F(\sigma_m, \sigma_1),$$

where  $F(a, b)$  is a square matrix of arbitrary dimension.

# Calculating the partition function

$F$  has a graphical interpretation as a 'half-row' transfer matrix.



# Calculating the partition function

Maximising over this subset gives us an approximation for  $\Lambda$ , and therefore  $\kappa$ .

The larger the  $F$ s are, the better the approximation.

It can be shown that in the infinite-dimensional limit (of  $F$ ), the approximation is exact.

# The CTM equations

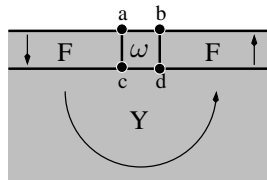
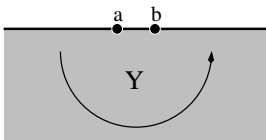
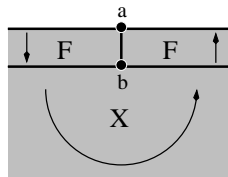
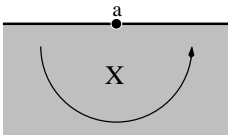
It is now possible to write  $\psi^T \psi$  and  $\psi^T V \psi$  as  $m$ th powers of the largest eigenvalues of 'full-row' transfer matrices consisting of two  $F$ s, or two  $F$ s and a  $\omega$ .

The eigenvalue equations, re-cast in terms of  $F$ , are

$$\sum_b F(a, b) X(b) F(b, a) = \xi X(a)$$
$$\sum_{c, d} \omega \begin{pmatrix} a & b \\ c & d \end{pmatrix} F(a, c) Y(c, d) F(d, b) = \eta Y(a, b).$$

# Interpreting the CTM equations

Both these equations have the graphical interpretation of adding a row to the 'half-plane' transfer matrices  $X$  and  $Y$ .





# Calculating the partition function

We now calculate  $\kappa$  by

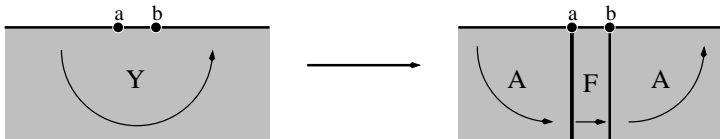
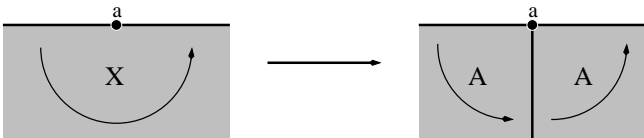
$$\kappa = \lim_{m \rightarrow \infty} \left( \frac{\psi^T V \psi}{\psi^T \psi} \right)^{\frac{1}{m}} = \frac{\eta}{\xi}.$$

It can be shown that this expression is maximised with respect to  $F$  if we also satisfy the equations

$$\begin{aligned} X(a) &= A^2(a) \\ Y(a, b) &= A(a)F(a, b)A(b), \end{aligned}$$

# The CTM equations

These equations can be pictured as breaking down  $X$  and  $Y$  into 'corner' transfer matrices.



# The CTM equations

Putting it all together gives us the CTM equations:

$$\sum_b F(a, b)X(b)F(b, a) = \xi X(a)$$
$$\sum_{c,d} \omega \begin{pmatrix} a & b \\ c & d \end{pmatrix} F(a, c)Y(c, d)F(d, b) = \eta Y(a, b)$$
$$X(a) = A^2(a)$$
$$Y(a, b) = A(a)F(a, b)A(b).$$

Solving these equations for infinite-size matrices will solve the model; solving them for finite-size matrices will provide an approximation.

# The CTM method

One of the properties that give corner transfer matrices their power is that even small size matrices tend to give very good approximations.

Moreover, increasing size gives us a non-decreasing number of correct series terms, making the equations an ideal springboard for calculating series expansions.

It is claimed (but as far as we know, not proven) that we need a matrix size of  $O(\alpha^{\sqrt{n}})$  to generate  $n$  terms, making algorithms based on CTM sub-exponential.

# The CTM method

Baxter's original CTM method fixed matrix sizes and iterated through the CTM equations, fixing some matrices and re-calculating others.

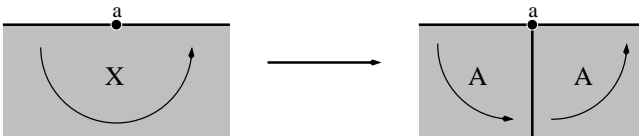
One notable triumph of CTM was Baxter's exact solution of the hard hexagons model, which he derived by finding a pattern in the eigenvalues of the corner transfer matrices.

In practice, however, he transformed the equations using (non-obvious) model-specific transformations, which make it hard to extend or generalise his method. We would like to develop a more general method that does not require these transformations.

# The CTMRG method

Nishino and Okunishi (1996) combined the CTM equations with ideas from the density matrix renormalization group method to form the corner transfer matrix renormalization group method.

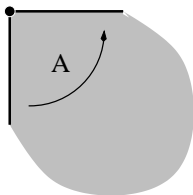
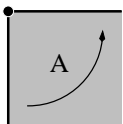
To understand this method, we look closer at the matrices in the CTM equations — in particular,  $A$ .



# The CTMRG method

$A$  is a transfer matrix that carries the weight of a quarter of the plane.

To get exact results, it should be of infinite size; at finite size, the solution to the CTM equations covers as much area as possible, in a sense.



# The CTMRG method

Now we have to figure out how we can calculate such a matrix.

The first step is to recognize that, given  $A$  and  $F$ , we can ‘expand’  $A$  to include one more column and row.

$$A_I(a) = \begin{pmatrix} \sum_b \omega \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} F(0, b) A(b) F(b, 0) & \sum_b \omega \begin{pmatrix} a & 1 \\ 0 & b \end{pmatrix} F(0, b) A(b) F(b, 1) \\ \sum_b \omega \begin{pmatrix} a & 0 \\ 1 & b \end{pmatrix} F(1, b) A(b) F(b, 0) & \sum_b \omega \begin{pmatrix} a & 1 \\ 1 & b \end{pmatrix} F(1, b) A(b) F(b, 1) \end{pmatrix}$$



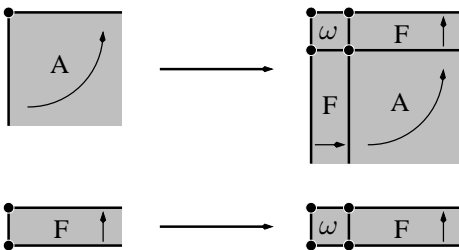
# The CTMRG method

We can also expand  $F$  by a cell.

$$F_I(a, b) = \begin{pmatrix} \omega \begin{pmatrix} b & 0 \\ a & 0 \end{pmatrix} F(0, 0) & \omega \begin{pmatrix} b & 1 \\ a & 0 \end{pmatrix} F(0, 1) \\ \omega \begin{pmatrix} b & 0 \\ a & 1 \end{pmatrix} F(1, 0) & \omega \begin{pmatrix} b & 1 \\ a & 1 \end{pmatrix} F(1, 1) \end{pmatrix}$$

# The CTMRG method

These equations have an obvious graphical interpretation.



# The CTMRG method

This still leaves us with the problem that  $A_l$  and  $F_l$  are twice as big as  $A$  and  $F$ ! We have to find some way to shrink them, while keeping them covering as much area as possible.

In technical terms, this means maximising the eigenvalues of  $A$ . To do this, we diagonalise  $A_l$  by applying the transformations

$$A_l(a) \rightarrow P^T(a)A_l(a)P(a), F_l(a, b) \rightarrow P^T(a)F_l(a, b)P(b)$$

where  $P(a)$  is an orthogonal matrix.

# The CTMRG method

By then removing the smaller eigenvalues of  $A_l$  to reduce it to the same size as  $A$ , and applying the same transformation to  $F$ , we have ‘expanded’ the area that the corner transfer matrix covers, while keeping it at the same dimension.

This procedure can then be repeated as many times as required, producing more and more accurate approximations each time.

It is also very easy to permanently increase the size of the matrices — simply keep more eigenvalues of  $A_l$ .

# The CTMRG method

- 1 Start with initial approximations for  $A(a)$  and  $F(a, b)$ .
- 2 Calculate  $A_I(a)$  and  $F_I(a, b)$ .
- 3 Diagonalize  $A_I(a)$ , i.e. find orthogonal matrices  $P_I(a)$  such that  $P_I^T(a)A_I(a)P_I(a)$  is diagonal, with diagonal entries in order from largest to smallest.
- 4 If we want to expand the matrices, set  $n = n + 1$ .
- 5 Let  $P(a)$  be the first  $n$  columns of  $P_I(a)$ .
- 6 Set  $A(a) = P^T(a)A_I(a)P(a)$  and  $F(a, b) = P^T(a)F_I(a, b)P(b)$ .
- 7 Return to step 2.

# The CTMRG method

We now calculate  $\kappa$  by

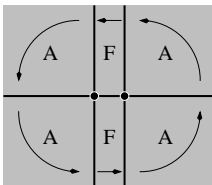
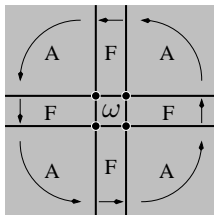
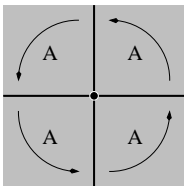
$$\kappa = \frac{Z_1 Z_3}{Z_2^2},$$

where the  $Z$ s are partition functions of the plane, but some with extra cells:

$$Z_1 = \text{Tr} \sum_a A^4(a), \quad Z_2 = \text{Tr} \sum_{a,b} A^2(a)F(a,b)A^2(b)F(b,a)$$

$$Z_3 = \text{Tr} \sum_{a,b,c,d} \omega \begin{pmatrix} a & b \\ c & d \end{pmatrix} A(a)F(a,c)A(c)F(c,d)A(d)F(d,b)A(b)F(b,a).$$

# The CTMRG method



# The CTMRG method

Nishino and Okunishi were able to use the CTMRG method to obtain very accurate numerical calculations, which they applied to a variety of models.

In more recent years Foster and Pinettes (2003) and Mangazeev *et al.* (2009) also applied the method to great success.

However, (as far as we know) no one has used this method for series expansions... so far!



# Series calculations with CTMRG

One of the reasons was quite obvious: how do you diagonalise a matrix of series (exactly in the first few terms)?

In this method, we need to diagonalise the matrices  $A_l(a)$ .

We experimented with a few methods and found that in easy cases, the tried and trusted power method works quite well.

# Series calculations with CTMRG

## Theorem

Let  $A$  be a matrix of power series where  $\lambda_1$  and  $\lambda_2$  have leading powers  $l_1$  and  $l_2$ . Suppose we have a (unit-norm) estimate  $\hat{\mathbf{x}}_1$  of  $\mathbf{x}_1$  which is accurate to  $m$  terms, i.e.

$$\hat{\mathbf{x}}_1 - \mathbf{x}_1 = O(z^m).$$

Then

$$\|A\hat{\mathbf{x}}_1\| - \lambda_1 = O(z^{l_1+m})$$

and

$$\frac{A\hat{\mathbf{x}}_1}{\|A\hat{\mathbf{x}}_1\|} - \mathbf{x}_1 = O(z^{m+l_2-l_1}).$$

In other words, the power method gives us  $l_2 - l_1$  extra correct terms for every iteration.

# Series calculations with CTMRG

Once we have the largest eigenvalue of  $A_l(a)$ , we can deflate it to

$$A_l(a) - \lambda_1 \mathbf{x}_1 \mathbf{x}_1^T$$

and apply the power method again, until we have all the eigenvalues/vectors.

This is good as long as the eigenvalues of  $A_l$  are non-degenerate. (In this case, we define 'degenerate' as having the same leading order.)

For our test case (hard squares), this actually does happen for small sizes (up to  $5 \times 5$ ). However, if we want to go farther, we need more sophisticated methods.

# Series calculations with CTMRG

If we have the first few terms of an eigenvalue (even a degenerate one), we can use the shifted inverse power method.

More precisely, if  $\lambda_0$  is equal to exactly one eigenvalue of  $A_I(a)$  up to order  $z^m$ , then  $(A_I(a) - \lambda_0 I)$  shifts the eigenvalues of  $A_I(a)$  so that all but one have leading order at most  $m$ , and the remaining one has leading order more than  $m$ .

In that case,  $(A_I(a) - \lambda_0 I)^{-1}$  has one eigenvalue with leading order less than  $-m$ , with the leading order of all other eigenvalues more than that.

The power method, applied to  $(A_I(a) - \lambda_0 I)^{-1}$ , will now identify this eigenvalue unambiguously.

# Series calculations with CTMRG

This still leaves us the problem of finding the first few terms of an eigenvalue exactly. There are several possibilities.

Often the eigenvalues of  $A_l(a)$  do not change much from iteration to iteration. In that case, we can use the eigenvalues of the previous  $A_l(a)$  to shift the current matrix. This is very efficient if we know many initial terms.

If we do not have a previous value for the eigenvalue, we can often still calculate the first few terms of an eigenvalue by looking at the block structure of  $A_l$ .

# Block diagonalization

If all else fails, we use block diagonalization. This involves applying a change-of-basis transformation to  $A_l(a)$  so that it takes a block-diagonal form, rather than strictly diagonal.

As long as we do not split up a block when we cut off rows and columns, this still works.

We have proved an equivalent to the earlier theorem for block diagonalization, which states that every iteration of a modified power method gives us  $l_{k+1} - l_k$  terms for  $k \times k$  blocks.

## Results for hard squares

With these modifications, the CTMRG can be made to work for series expansions.

Using matrices of size  $29 \times 29$ , we were able to generate 92 terms of the hard squares partition function. This took us 18 ( $\times 10$ ) hours of computer time without any serious attempt at programmatical optimization.

For comparison, Baxter and Tsang (1980) generated 43 series terms, and we know of no-one else who has generated more. (We believe the reasons for lack of progress in this method are more due to eigenvalue degeneracy, which we have overcome.)

# Arnoldi method

Recently we discovered that instead of diagonalizing  $A_I$ , we can use the Arnoldi method to transform it into a tridiagonal matrix and use that for  $A$ .

This is much faster than diagonalizing  $A_I$  and does not always have problems with degenerate eigenvalues (which are not truly degenerate in any case).

Though not as accurate numerically, it appears to yield the same number of series terms at each finite size as explicit diagonalization.

If we can eliminate all degeneracy problems, this is clearly the way to go.



# Potts model

We have modified the CTMRG to work for the Potts model in zero-field, theoretically for any specified  $q$ .

With matrices of size  $18 \times 18$ , we can get 56 terms of the partition function per site for  $q = 3$ .

The current record for  $q = 3$  is 72 terms by Jensen, using the finite lattice method.

# Self-avoiding polygons

We are also trying to enumerate self-avoiding polygons using this method. The main challenges for this are:

- Walks lie on the bonds of the lattice, whereas the CTMRG is used for models with spins at the sites.
- The self-avoiding constraint is non-local, but the model must be expressible in IRF format.

We believe we can solve both these obstacles, but have not yet managed to make it work!

# Conclusion

- The CTMRG is a very efficient method based on the CTM method by Baxter, and developed by Nishino and Okunishi.
- We have managed to get this method working for series expansions.
- Our method is quite general, and should be able to be applied efficiently to many spin models.
- A wider class of models, including vertex models and self-avoiding walks, may also be possible.
- We are on the lookout for more models to apply it to!

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