Approximating the partition function of the ferromagnetic Ising model

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Counting, Inference and Optimization on Graphs
Princeton, 2nd-5th November 2011

The Ising model

Let $G = (V, E)$ be a graph, with indeterminates $\gamma = (\gamma_e : e \in E)$ associated to the edges.

Definition

The Ising partition function is

$$Z_{\mathrm{Ising}}(G;\gamma) = \sum_{\sigma : V \to \{0,1\}} \prod_{e \in E} \left(1 + \gamma_e \delta_e(\sigma)\right),$$

where $\delta_e(\sigma)$ is 1 if σ assigns the same value to the two endpoints of e, and 0 otherwise.

We are interested in computing the partition function in the *ferromagnetic* case, which corresponds to evaluating the polynomial $Z_{\mathrm{Ising}}(G;\gamma)$ in the positive orthant, $\gamma \geq 0$.

Some remarks

- In the q-state Potts model, a configuration is a function $V \to \{0, 1, \ldots, q-1\}$. The Ising model is the special case $q = 2$. Leslie Goldberg will consider the general Potts model later. For the time being, we stick to the 2-spin situation.

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- It is #P-hard to compute $Z_{\mathrm{Ising}}(G; \gamma)$ exactly, given G and an assignment to γ.
- It is NP-hard even to approximate $Z_{\mathrm{Ising}}(G; \gamma)$ in the non-ferromagnetic case, corresponding to $\gamma \geq -1$.

Approximate computation: FPRAS

Definition

An *FPRAS* is a randomised algorithm that produces a result that is correct to within relative error $1 \pm \varepsilon$ with high probability. It must run in time $\mathrm{poly}(n, \varepsilon^{-1})$, where n is the input size.

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Theorem (Jerrum & Sinclair 1990)

There is an FPRAS for $Z_{\mathrm{Ising}}(G; \gamma)$ in the ferromagnetic region $(\gamma \geq 0)$.

(Alternatively: there is an FPRAS for the Tutte polynomial along the positive branch of the hyperbola defined by $q = 2$.)

Attempt 1: direct simulation

The FPRAS for the ferromagnetic Ising partition function is an example of the Markov chain Monte Carlo (MCMC) method, but a direct application, based on single-site updates clearly fails. The following simulation illustrates the point:

Demo

(Acknowledgements to Bernd Nottelmann and Peter Young.)

We can say that the Markov chain is not “rapidly mixing”.

Attempt 2: expansion in terms of even subgraphs

Call an edge subset A *even* if every vertex in (V, A) has even degree.

Then we have the following alternative "high temperature" expansion of the partition function:

$$Z_{\text{Ising}}(G;\gamma) = 2^{|V|} \prod_{e \in E} w'_e \sum_{\substack{A \subseteq E \\ A \text{ even}}} \prod_{e \in A} w_e$$

where $w'_e = (\gamma_e + 2)/2$ and $w_e = \gamma_e/(\gamma_e + 2)$.

The Markov chain based on single-edge updates of even subsets (and defective even subsets) *is* rapidly mixing... yielding an FPRAS.

Extension to "consistent" external field

Now suppose there is a multiplicative weight $1 + \mu_v \sigma(v)$ at each vertex v. There is again a high-temperature expansion:

$$Z_{\text{Ising}}(G; \gamma, \boldsymbol{\mu}) = 2^{|V|} \cdots \sum_{A \subseteq E} \prod_{e \in A} w_e \prod_{\substack{v \in V \\ \deg_A(v) \text{ odd}}} z_v$$

where $z_v = \mu_v / (\mu_v + 2)$ and w_e is as before. (An easily computable product of weights has been omitted.)

A slight modification of the earlier Markov chain with single-edge updates works here also, provided $\mu_v \geq 0$ (or $\mu_v \leq 0$) for all $v \in V$.

But what if the field is *inconsistent*, i.e., μ_v takes negative values as well as positive?

Interlude: an interesting class of counting problems

Denote by #BIS the problem of counting independent sets in a bipartite graph.

Fact (Dyer, Goldberg, Greenhill & Jerrum, 2000)

#BIS is inter-reducible — in an approximation-preserving sense — with several other counting problems (e.g., downsets in a partial order, stable matchings, Widom-Rowlinson model in statistical physics).

A class of sampling problems of intermediate computational complexity or an illusion?

A logically defined complexity class

The complexity class, $\#\mathrm{RH}\Pi_1$, containing "Bipartite Independent Set" and its peers is characterised by syntactically restricted sentences in first order logic. In fact, #BIS is complete for this class with respect to approximation-preserving reducibility. (C.f. "restricted Krom SNP" / "Linear Datalog".)

E.g., the set of downsets in a partial order $(A, \prec)$ may be expressed as

$$\big\{D : \forall x, y \in A.\ \neg D(x) \vee \neg(y \prec x) \vee D(y)\big\}.$$

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$$\big(\equiv \neg\big(D(x) \wedge (y \prec x) \wedge \neg D(y)\big)\big)$$

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First order universal quantification.

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CNF. (Only one clause in this instance!)

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$$\bigl\{D : \forall x, y \in A.\ \neg D(x) \vee \neg(y \prec x) \vee D(y)\bigr\}.$$

Each clause has at most one unnegated relation symbol and at most one negated relation symbol.

Some restrictions of the Ising model

- Zero external field: $\mu_v = 0$, for all $v \in V$.
- Consistent external field: $\mu_v \geq 0$, for all v (or $\mu_v \leq 0$, for all v).
- Ferromagnetic: $\gamma_e \geq 0$, for all $e \in E$.

Computational complexity of some variants

Ising partition function	Exact	Approximate
Zero field, planar	FP[1]	-
Ferromagnetic, consistent field	#P-hard	FPRAS[2]
Ferromagnetic, general field	#P-hard	?
Antiferromagnetic/spinglass	#P-hard	NP-hard[3]

Notes

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Notes

[1]Reduction to dimer coverings (perfect matchings) [Fisher].

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Notes

[2] We saw this earlier.

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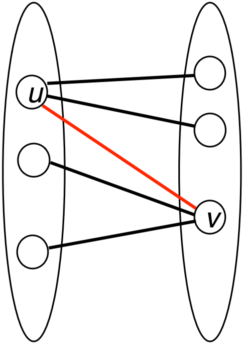
Notes

[3] Essentially Max Cut.

General external field: idea for a reduction

It is possible to encode an instance of #BIS as an instance of the ferromagnetic Ising model with general field:

- 1 means "OUT";
- 0 means "IN";
- $1 + \mu_u = (1+\gamma)^{\deg(u)}$.



$$\gamma_e = \gamma > 0$$

- 1 means "IN";
- 0 means "OUT";
- $1 + \mu_v = (1+\gamma)^{-\deg(v)}$.

Calculation

$\sigma(u) - \sigma(v)$	Contribution	Equals
IN – IN	$1 \times 1 \times (1+\gamma)^{-1}$	$(1+\gamma)^{-1}$
IN – OUT	$1 \times (1+\gamma) \times 1$	$1+\gamma$
OUT – IN	$(1+\gamma) \times (1+\gamma) \times (1+\gamma)^{-1}$	$1+\gamma$
OUT – OUT	$(1+\gamma) \times 1 \times 1$	$1+\gamma$

Fleshing out the details (and also doing the reduction in the other direction) yields:

Theorem (Goldberg and Jerrum, 2007)

Computing the partition function of a ferromagnetic Ising model with a general fields is equivalent to #BIS *under approximation-preserving reductions.*

Complexity of some variants (reprise)

Ising partition function	Exact	Approximate
Zero field, planar	FP	-
Ferromagnetic, consistent field	#P-hard	FPRAS
Ferromagnetic, general field	#P-hard	#BIS-equivalent
Antiferromagnetic/spinglass	#P-hard	NP-hard