

## Uncertainty Quantification for Markov Random Fields\*

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**Abstract.** We present an information-based uncertainty quantification method for general Markov random fields (MRFs). MRFs are structured, probabilistic graphical models over undirected graphs and provide a fundamental unifying modeling tool for statistical mechanics, probabilistic machine learning, and artificial intelligence. Typically, MRFs are complex and high-dimensional with nodes and edges (connections) built in a modular fashion from simpler, low-dimensional probabilistic models and their local connections; in turn, this modularity allows one to incorporate available data to MRFs and efficiently simulate them by leveraging their graph-theoretic structure. Learning graphical models from data and/or constructing them from physical modeling and constraints necessarily involves uncertainties inherited from data, modeling choices, or numerical approximations. These uncertainties in the MRF can be manifested either in the graph structure or the probability distribution functions and necessarily will propagate in predictions for quantities of interest. Here we quantify such uncertainties using tight, information-based bounds on the predictions of quantities of interest; these bounds take advantage of the graphical structure of MRFs and are capable of handling the inherent high dimensionality of such graphical models. We demonstrate our methods in MRFs for medical diagnostics and statistical mechanics models. In the latter, we develop uncertainty quantification bounds for finite-size effects and phase diagrams, which constitute two of the typical prediction goals of statistical mechanics modeling.

**Key words.** Markov random fields, uncertainty quantification, information theory, probabilistic inequalities, long range interactions

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**1. Introduction.** Probabilistic graphical models (PGMs) constitute one of the fundamental tools for probabilistic machine learning (ML) and artificial intelligence (AI), allowing for systematic and scalable modeling of uncertainty, causality, domain knowledge, and data assimilation [38, 49, 35]. The main idea behind PGMs is to represent complex models and associated learning processes using random variables and their interdependence through a graph. We achieve it by constructing structured, high-dimensional probabilistic models, involving many parameters, nodes, and edges, from simpler ones with few parameters, nodes, and edges, thus allowing for distributed probability computations, and by incorporating avail-

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able data, exploiting graph-theoretic model representations. PGMs are generally classified into Markov random fields (MRFs) defined over undirected graphs and Bayesian networks defined over directed acyclical graphs [49] that represent conditional independencies between random variables, as well as mixtures of those two classes [35]. Furthermore, the modeling flexibility of PGMs also allows one to combine dynamics, data, and deep learning in hidden Markov models [38, 50, 47], as well as in recent work brings together multiscale modeling, physical constraints, and neural networks [69, 41, 30].

Although the term random field may also refer to continuously indexed processes (e.g., Gaussian random fields), in this paper MRFs refer to structured probabilistic models defined on undirected graphs; such PGMs are also referred to as Markov networks. MRFs arise in statistical mechanics where interactions between particles are usually bidirectional, or when there may be no inherent evidence for causality (directionality) and thus undirected graphs are the appropriate structure for such probabilistic models [38, 49, 70]. Other applications of MRFs include image segmentation, image denoising [49, sect. 4.2], text processing [64, 56], bioinformatics [61], computer vision [45], Markov logic networks [21], Gaussian Markov networks [49, sect. 7.3], artificial intelligence [35], and statistical mechanics [55, sect. 19.4]. Overall, MRFs provide a fundamental unifying modeling tool for statistical mechanics, probabilistic ML, and AI [3, 38].

Learning MRFs can be based on available data; e.g., for learning the graph, we refer the reader to [49, 32, 43] for score-based methods and [55, 44] for independence tests on the graph, while maximum likelihood or Bayesian methods can be used for parameter identification [49]. On the other hand, MRFs in statistical mechanics can be constructed from physical modeling and related constraints [68, 55]. Therefore, the learning stage of MRFs necessarily involves uncertainties inherited from data, modeling choices, compromises on model complexity, or numerical approximations. These uncertainties in the MRF can be manifested either in the graph structure or the probability distribution functions, and necessarily will propagate through the graph structure and the corresponding structured probabilistic model in the predictions for quantities of interest (QoIs). To understand and quantify the impact of such uncertainties on model predictions, in this paper we present an information-based uncertainty quantification (UQ) method for general MRFs.

**Model uncertainty in probabilistic models.** In general probabilistic models, uncertainties arising just from the fluctuations of the QoIs, associated with a given probabilistic model  $p$ , are referred to as aleatoric and occur when sampling  $p$  [15]. They are handled by well-known tools, e.g., central limit theorems, concentration inequalities, Bayesian posteriors, MCMC, generalized polynomial chaos, etc. In contrast to this more standard type of UQ, in MRFs, due to the learning process described earlier, we have *model* uncertainties (also known as epistemic), both in the structure (graph) and the probabilistic model itself—including parametric ones.

Next, we briefly describe the information-theoretic formulation of model uncertainty for general probabilistic models, without assuming any graphical model structures; see [39] for more details. To practically address model uncertainty, we typically compromise by constructing a surrogate or approximation or baseline model  $p$ . We construct families  $\mathcal{Q}$  of (nonparametric) *alternative models*  $\tilde{p}$  to compare to  $p$ , while the “true” model  $p^*$ , which may be intractable or partly unknown, should belong to  $\mathcal{Q}$ ; for this reason, we can refer to  $\mathcal{Q}$  as the

ambiguity set, typically defined as a neighborhood of alternative models around the baseline  $p$ :

$$(1.1) \quad \mathcal{Q} = \mathcal{Q}^\eta = \{\tilde{p} : d(\tilde{p}, p) \leq \eta\},$$

where  $\eta > 0$  corresponds to the size of the ambiguity set and  $d = d(\tilde{p}, p)$  denotes a probability metric or divergence. The next natural mathematical goal is to assess the baseline model “compromise” and understand the resulting biases for the QoI  $f$  when we use  $p$  for predictions instead of the real model  $p^* \in \mathcal{Q}$ . We define the predictive uncertainty (or bias) for the QoI  $f$  when we use the baseline model  $p$  instead of any alternative model  $\tilde{p} \in \mathcal{Q}$  (including the real one  $p^*$ ) as the two worst case scenarios:

$$(1.2) \quad \sup_{\tilde{p} \in \mathcal{Q}^\eta} / \inf_{\tilde{p} \in \mathcal{Q}^\eta} \{E_{\tilde{p}}f - E_p f\},$$

where  $E_{\tilde{p}}f$  denotes the expected value of the QoI  $f$ . Therefore, (1.2) provides a robust performance guarantee for the predictions of the baseline model  $p$  for  $f$  within the ambiguity set  $\mathcal{Q}^\eta$ . This robust perspective for general probabilistic models  $p$  is known in operations research as *distributionally robust optimization* (DRO); see, e.g., [36, 37]. While the definition (1.2) is rather natural and intuitive, it is not obvious that it is practically computable since the neighborhood  $\mathcal{Q}^\eta$  is infinite-dimensional. However, it becomes tractable if we use for metric  $d$  in (1.1) the Kullback–Leibler (KL) divergence  $R(\tilde{p}||p)$ . Accordingly,  $\eta$  is a measure of the confidence in KL we put in the baseline model  $p$ . In recent work [15, 23, 39], it has been demonstrated that (1.2) (an infinite-dimensional optimization problem) is directly computable using the variational formula (following directly from the Donsker–Varadhan variational principle [23]):

$$(1.3) \quad \sup_{\tilde{p} \in \mathcal{Q}^\eta} / \inf_{\tilde{p} \in \mathcal{Q}^\eta} \{E_{\tilde{p}}f - E_p f\} = \pm \inf_{c>0} \left[ \frac{1}{c} \log \int e^{\pm c(f - E_p f)} p(dx) + \frac{\eta}{c} \right].$$

In this formula, we recognize two main ingredients:  $\eta$  is model uncertainty from (1.1), while the moment generating function (MGF)  $\int e^{\pm cf} p(dx)$  encodes the QoI  $f$  at the baseline model  $p$ . In [23, 39], the authors have developed techniques to compute (exactly or approximately via asymptotics [23]) as well as to provide explicitly upper and lower bounds on (1.2) in terms of concentration inequalities [39]. Tightness, i.e., when the sup and inf in (1.2) are attained by an appropriate measure  $\tilde{p}$ , has also been studied in [39]. Finally, related UQ bounds have been derived for Markov processes using variational principles and functional inequalities [8] and in rare events [2, 24].

**Main results.** The main thrust of our results here is to build on the aforementioned perspective for information-based UQ, in order to develop UQ methods for MRFs and to address their specific UQ challenges. In particular, here we address both structure (graph) and probabilistic uncertainties—including parametric ones—using tight, information-based bounds on the predictions of QoIs; although these new UQ bounds rely on (1.2), they specifically (a) take advantage of the graphical structure of MRFs, and (b) are capable of handling the inherent high dimensionality of such graphical models; i.e. there is a necessity for scalable UQ in the

size of the system, namely the number of nodes in MRFs such as in the thermodynamic limit of statistical mechanics models.

Regarding the scalability issue, in [46] the authors tested various model uncertainty metrics in defining  $d(\tilde{p}, p)$  in (1.1) such as the Hellinger distance and  $\chi^2$  divergence and inequalities such as the Csiszar–Kullback–Pinsker and Hammersley–Chapman–Robbins inequalities [67], in order to bound the model bias with respect to a QoI in the spirit of (1.3). It was shown that among these bounds the only one that scales with the dimension of the model  $p$  is (1.3) and  $d(\tilde{p}, p)$  should be the KL divergence.

Once we have settled on the use of the KL divergence for the aforementioned scalability reasons, we turn our attention to the baseline MRF  $p$ , the ambiguity set (1.1), and the corresponding alternative MRFs  $\tilde{p}$ . Based on the earlier discussion on model uncertainty for MRFs arising from statistical learning of graph models or physical modeling, we introduce a unifying perspective of three general types of alternative models  $\tilde{p}$ , based on their relative structure to the baseline  $p$ : Type I MRFs, where the graph structures (nodes and edges) are identical to the baseline  $p$  and the parameters of probability distributions are different; Type II, where the nodes are the same but the edges and parameters are different; and Type III, where the nodes, structures, and parameters are all different.

In general, MRFs satisfy the specific conditional independence properties discussed in subsection 2.2. Contrary to Bayesian networks, their distributions cannot always be factorized by a product of local conditional distributions or local functions over the graph. The celebrated *Hammersley–Clifford theorem*, also known as the *fundamental theorem of random fields* [49, 42, 55], guarantees such a factorization along maximal cliques of the graph under the assumption that  $p > 0$ . Here we make such an assumption for both baseline and Types I–III MRFs. Consequently, the KL divergence is finite without requiring absolute continuity with respect to  $p$ .

We take advantage of all the above, and we study UQ problems by developing a unified strategy for Types I–II MRFs, while Type III is not covered here as explained in section 3. We focus on the two primary ingredients of (1.2), namely the KL divergence and the MGF and how they manifest themselves on MRFs. In KL divergence, the factorization discussed earlier is a crucial tool for its simplification and numerical calculation. It allows us to compare local discrepancies in parameters and structures between the baseline  $p$  and alternative models. We call these discrepancies *excess factors of Types I–II* given  $p$ . We develop a unifying method for computing the excess factors by interrelating the maximal cliques of alternative MRFs and the baseline MRF  $p$ . As for the MGF, the choice of QoIs is determinant. We focus on two different QoIs: those that are involved in the models (e.g., sufficient statistics) as well as characteristic functions defined on events of interest.

Regarding the tightness of UQ bounds discussed earlier, we find specific distributions for which the derived UQ bounds for MRFs are attainable. In addition, we go beyond that and pose the following question: *Given a QoI and a baseline MRF  $p$ , what are the possible associated undirected graphs such that the conditional independence properties implied by the graphs are satisfied by the distributions?* Such a question introduces the concept of *tightness at a graph level*. There are cases where we can explicitly determine the associated graphs and others (when the structure is different from the baseline) that depend on the QoI. In the latter case, we give an example that points out a unifying method to construct the right graph or

at least a set of possible graphs.

**Demonstration of UQ for MRFs.** We first demonstrate all of the above concepts and UQ methods in a fairly simple and low-dimensional MRF example from medical diagnostics. Subsequently, we implement our approach on several high-dimensional statistical mechanics models, as they are fundamental in ML [3, 38]. We develop UQ bounds for finite-size effects and phase diagrams, which constitute two of the typical prediction goals of statistical mechanics modeling, and both require scalable UQ methods.

Specifically, we consider as a baseline model  $p$  an Ising-spin system with Kac-type interactions; see [57]. Such a model combines sufficient complexity—since it is not a mean field model—but it is still analytically fairly tractable to serve as a good benchmark problem for a high-dimensional MRF. Alternative models  $\tilde{p}$  considered here are (1) Ising models with perturbed interaction potentials with respect to the baseline, (2) models with truncated interactions to facilitate computational implementations [68], and (3) perturbations by a long range interaction (even longer than a Kac interaction). As we discuss in section 6, these systems are typically defined in bounded domains with boundary conditions being a given configuration outside of the domain. To have a graph description of these systems, MRFs need to be modified to account for conditioning a Gibbs distribution on an eliminated set of nodes identified as a configuration defined outside of the domain by using reduced Markov random fields (rMRFs) (see [49]). Typical questions we address in these examples include the following: (i) how to capture the phase diagram of a perturbed model through its comparison with the baseline phase diagram by bounding the model bias, and (ii) how to truncate an interaction so that the phase diagram of the baseline model and the truncated one are close within a prescribed tolerance. Note that an extensive analysis on the intersection between other concepts and methods from statistical mechanics—also including nonequilibrium statistical mechanics—and deep learning have been reviewed in [3].

**Related methods.** We note that existing general-purpose UQ and sensitivity analysis methods, e.g., gradient and ANOVA-based methods [63, 60, 29], cannot handle UQ with model uncertainties, due to their inherently parametric nature, while it is not clear how they can take advantage of the graphical, causal structure in MRFs. Furthermore, there is earlier work on model uncertainty that represents missing physics with a stochastic noise but without the detailed structure of a graphical model [51, 65]. In our work, there is a natural structure embedded in the model uncertainty, arising through the graph structure of the MRFs.

Sensitivity analysis also has a long history in statistical mechanics, known as linear and nonlinear response theory [59, 4], addressing the impact of small and larger parametric perturbations, respectively. These types of methods are covered by our approach, as models with perturbed weights are clearly of Type I.

Furthermore, in contrast to these results, a key point in our work here, also immediately clear from (1.3), is that the model perturbations we can consider are not necessarily small. For instance, the parameter  $\eta$  in (1.3) does not need to be small, allowing for global and nonparametric sensitivity analysis, the latter since the KL divergence allows us to consider models outside a specific parametric family, e.g., comparing statistical mechanics models with different potentials. Similarly, we explicitly compute the UQ bounds for large perturbations in a medical diagnostics example.

Sensitivity analysis in MRFs has also been studied in [14]. The authors tackle fundamental



questions such as bounding belief change between Markov networks with the same structure but different parameter values. They propose a distance measure and bound the relative change in probability queries by the relative change in parameters (Type I). Global sensitivity in parameters has been studied in [17]. In particular, the authors developed an algorithm that checks the robustness of a MAP configuration, i.e., the most likely configuration, in discrete probabilistic graphical models under global perturbations. The present work goes beyond local or global parametric sensitivity analysis that allows us to consider perturbations in both parameters and edges of the graph of the MRF and examines their impact on the prediction of specific QoIs. Special cases of our results for mean field and nearest neighbor Ising models were considered earlier in [46]. Finally, we note that parametric sensitivity analysis for the other class of (directed) probabilistic graphical models, namely Bayesian networks, was developed in [16] using tools similar to those in [14]. Parametric sensitivity analysis based on mutual information for multiscale partial differential equations and neural networks informed by Bayesian network priors was developed in [69, 66]. Model UQ based on information theory inequalities in the spirit of (1.3) was recently introduced for Bayesian networks arising in chemical sciences [30].

This article is organized as follows: We start with some concepts from graph theory to fix notation, and then we give a brief background of MRFs/rMRFs (section 2). Supplementary background behind rMRFs is provided in Appendix A. We formally introduce the idea of graph interconnections, the impact on distributions, and alternative models in section 3. The main results are presented in section 4 and provide UQ bounds for rMRFs, preparing the ground for applications to statistical mechanics models. In section 5, we present a simple example from medical diagnostics. Section 6 is devoted to UQ for finite-size effects, scalability, and finally UQ for phase diagrams for generic interactions and the Ising–Kac model. In the remaining sections of the appendix, we further discuss the Ising–Kac model, we provide the technical background required for the UQ analysis of section 6 (e.g., the Lebowitz–Penrose (LP) limit), and we include the proofs of the main results and explicit calculations of the UQ for medical diagnostics example and statistical mechanics.

## 2. Preliminaries.

**2.1. Definitions from graph theory.** We start with some notation and terminology from graph theory. A *graph* is a data structure  $\mathcal{G}$  consisting of a set of *nodes*  $\mathcal{V} = \{1, 2, \dots, N\}$  and a set of *edges*  $\mathcal{E}$ , i.e., all pairs of nodes  $i, j \in \mathcal{V}$  which are connected by an edge, denoted by  $(i, j)$ . An edge can be directed, denoted by  $i \rightarrow j$ , or undirected, denoted by  $i - j$ . A graph is *directed* (resp., *undirected*) if all the edges are directed (resp., undirected). The nodes  $i, j \in \mathcal{V}$  are *adjacent* if and only if  $(i, j) \in \mathcal{E}$ . The *neighborhood* of node  $i$ , denoted by  $\mathcal{N}_i$ , is the set of nodes to which  $i$  is adjacent. For sets of nodes  $A, B$ , and  $C$ ,  $C$  *separates*  $A$  from  $B$ , denoted by  $\{i \in A\} \perp_{\mathcal{G}} \{j \in B\} \mid \{k : k \in C\}$ , if and only if when we remove all the nodes in  $C$  there is no path connecting any node in  $A$  to any node in  $B$ . Last, if  $\mathcal{M} \subset \mathcal{V}$ , the *induced subgraph* of  $\mathcal{G}$  is defined as  $\mathcal{G}[\mathcal{M}] = (\mathcal{M}, \mathcal{E}')$ , where  $\mathcal{E}'$  includes all the edges  $(i, j) \in \mathcal{E}$  such that  $i, j \in \mathcal{M}$ .

**2.2. Conditional independence properties and MRFs.** In this subsection, we define three conditional independence properties that are necessary for MRFs.

Let  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ , and let  $\mathbf{Y} = \{Y_i\}_{i=1}^{|\mathcal{V}|}$  be a set of random variables such that each one is

attached to a node and  $|\mathcal{V}|$  denotes the cardinality of  $\mathcal{V}$ .

• **Pairwise Markov property (P):** Any two nonadjacent variables are conditionally independent (CI) given the rest; i.e., a conditional joint can be written as a product of conditional marginals; CI is denoted by  $Y_i \perp Y_j \mid \{Y_k : k \neq i, j\}$ .

• **Local Markov property (L):** Any variable  $Y_i$  is conditionally independent of all the others, given its neighbors, that is,  $Y_i \perp \{Y_k : k \notin \mathcal{N}_i\} \mid \{Y_k : k \in \mathcal{N}_i\}$ .

• **Global Markov property (G):** If  $A, B, C$  are sets of nodes, then any two sets of variables,  $\mathbf{Y}_A = \{Y_i : i \in A\}$  and  $\mathbf{Y}_B = \{Y_i : i \in B\}$ , are conditionally independent, given a separating set of variables  $\mathbf{Y}_C = \{Y_i : i \in C\}$ , that is,  $\mathbf{Y}_A \perp \mathbf{Y}_B \mid \mathbf{Y}_C$ .

It is obvious that (G) implies (L), which implies (P).

**Definition 2.1.** Let  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$  be an undirected graph where  $\mathcal{V} = \{1, 2, \dots, N\}$  is the set of nodes and  $\mathcal{E}$  is the set of edges. Let us also consider a set of random variables  $\mathbf{Y} = (Y_i)_{i \in \mathcal{V}}$  indexed by  $\mathcal{V}$  where each  $Y_i$  takes values on a finite set  $\mathcal{S}$ . Their joint probability distribution is denoted by  $p$ . We say that  $(\mathbf{Y}, p)$  is an MRF if and only if (G) is satisfied.

As MRFs are defined on an undirected graph, it does not allow one to use the chain rule of conditional probabilities and further describe the probability distribution  $p(\mathbf{y})$ . A factorization rule for MRFs (i.e., for undirected graphs and the conditional independencies) is important and is provided by Hammersley and Clifford in their unpublished work [42, 40]. To state their result, we need a few more definitions. Let  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$  be a graph, and let  $c \subset \mathcal{V}$ :

- (i)  $c$  is called *clique* if any pair of nodes in  $c$  is connected by some edge.
- (ii)  $c$  is called *maximal clique* if any superset  $c'$  of  $c$  (i.e.,  $c' \supset c$ ) is no longer a clique. The set of all maximal cliques of graph  $\mathcal{G}$  is denoted by  $\mathcal{C}_{\mathcal{G}}$ .

**Hammersley–Clifford theorem.** A positive distribution  $p(\mathbf{y}) > 0$  satisfies one of (P), (L), and (G) of an undirected graph  $G$  if and only if  $p$  parametrized by some parameters  $\mathbf{w} = \{\mathbf{w}_c\}_{c \in \mathcal{C}_{\mathcal{G}}}$  can be represented as a product of clique potentials, i.e.,

$$(2.1) \quad P_{\Psi}^{\mathbf{w}}(\mathbf{y}) \equiv p(\mathbf{y} \mid \mathbf{w}) = \frac{1}{Z(\mathbf{w})} \prod_{c \in \mathcal{C}_{\mathcal{G}}} \Psi_c(\mathbf{y}_c \mid \mathbf{w}_c),$$

where  $\Psi_c(\mathbf{y}_c \mid \mathbf{w}_c)$  is a positive function defined on the random variables in clique  $c$  and parametrized by some parameters  $\mathbf{w}_c$  and is called a *clique potential*. Also,  $Z(\mathbf{w})$  is the *partition function* given by

$$(2.2) \quad Z(\mathbf{w}) = \sum_{\mathbf{y}} \prod_{c \in \mathcal{C}_{\mathcal{G}}} \Psi_c(\mathbf{y}_c \mid \mathbf{w}_c).$$

The theorem states that the set of all joint distributions on an undirected graph  $\mathcal{G}$  that can be factorized as in (2.1) is identical to the set of joint distributions that satisfy the conditional independence properties, under the restriction of strictly positive distributions.

**Remark 2.2.** Without the assumption of strict positiveness of the joint distribution  $p$ , the theorem is not valid. A counterexample has been obtained in [54].

**Remark 2.3.** The KL divergence or any other  $f$ -divergences between a baseline MRF that is assumed nonnegative and alternative MRFs of Types II–III (different structures; see

the introduction) could be infinite due to the loss of absolute continuity. In that case, the Wasserstein metric or the  $\Gamma$ -divergence [25] could potentially be good alternatives for the KL divergence in defining (1.1). The implementation of the Wasserstein metric or the  $\Gamma$ -divergence is still unexplored in the context of such MRFs. For this purpose, the development of new methods constitutes an important step towards comparing MRFs with different structures and nonnegative distributions. In this article, we restrict our attention to the Hammersley–Clifford theorem and we assume strictly positive probability distributions.

Given an MRF  $(\mathbf{Y}, p)$ , an rMRF is obtained by conditioning  $p$  on some observation  $\mathbf{U} = \mathbf{u}$  with  $\mathbf{U} \subset \mathbf{Y}$ . Hence, the distribution of the resulting rMRF has a reduced number of clique potentials. As we discuss in section 6, rMRFs are appropriate for formulating statistical mechanics models defined on bounded domains with a given configuration outside of the domain in a graph language. Next, we formally introduce rMRFs.

**2.2.1. Reduced Markov random fields (rMRFs).** Let  $\mathbf{Y} = \{Y_i\}_{i \in \mathcal{V}}$  be a collection of random variables indexed by a set of nodes  $\mathcal{V}$  of a graph  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ , taking values in some space  $\mathcal{Y}^{\mathcal{V}} = \otimes_{i=1}^{\mathcal{V}} \mathcal{Y}_i$ . Let  $p \equiv p(\cdot | \mathbf{w})$  be a strictly positive joint probability distribution of  $\mathbf{Y}$  parametrized by  $\mathbf{w}$  such that  $(\mathbf{Y}, p(\cdot | \mathbf{w}))$  is an MRF.

Let  $\mathbf{u}$  be a context, and let  $\mathcal{M} \subset \mathcal{V}$ . If  $\mathbf{U} = \{Y_i\}_{i \in \mathcal{M}}$  with  $\mathbf{U} = \mathbf{u}$ , we construct the corresponding rMRF as follows: let  $\mathbf{Z} = \{Y_i\}_{i \in \mathcal{V} \setminus \mathcal{M}}$ , and let  $q(\mathbf{z} | \mathbf{w})$  be the probability distribution factorized according to Proposition A.2 (the analogue of the Hammersley–Clifford theorem for rMRFs):  $q(\mathbf{z}) \equiv q(\mathbf{z} | \mathbf{w}) = \frac{1}{Z_{\mathbf{u}}(\mathbf{w})} \prod_{c \in \mathcal{C}_{\mathcal{G}}} \Psi_c[\mathbf{u}](\mathbf{z}_c | \mathbf{w}_c)$ . More details on rMRFs are given in Appendix A.

The next two sections are presented for rMRFs, as we can then recall formulas and the main results directly in the UQ analysis of statistical mechanics models in section 6. Their formulation and analysis hold for MRFs, and, when required, we will be providing more details for their implementation to MRFs.

**3. Mathematical formulation of UQ on MRFs/rMRFs.** Let  $q$  be an rMRF constructed by learning from available data or from physical modeling and related constraints. Constructing such a model involves uncertainties either in the graph structure or the probability distribution functions and necessarily will propagate through the graph structure and the corresponding structured probabilistic model in the predictions for QoIs. We quantify the impact of such uncertainties on model predictions by constructing ambiguity sets such as (1.1) consisting of alternative rMRFs given by

$$(3.1) \quad \mathcal{Q}^{\eta} = \{\text{rMRFs } \tilde{q} : R(\tilde{q} \| q) \leq \eta\},$$

where  $\eta > 0$  corresponds to the size of the ambiguity set. The alternative models  $\tilde{q}$  in (3.1) can be classified into Type I MRFs, where the graph structures (nodes and edges) are identical to the baseline  $q$  and the parameters of probability distributions are different; Type II, where the nodes are the same but the edges and parameters are different; and Type III, where the nodes, structures, and parameters are all different. Next, we mathematically formulate the alternative models.

**3.1. Alternative models.** Let  $(\mathcal{G}, \mathbf{w}, p)$  and  $(\tilde{\mathcal{G}}, \tilde{\mathbf{w}}, \tilde{p})$  be two MRFs with  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$  and  $\tilde{\mathcal{G}} = (\tilde{\mathcal{V}}, \tilde{\mathcal{E}})$  being the associated graphs, where  $\mathcal{V}$  and  $\tilde{\mathcal{V}}$  are the sets of nodes and  $\mathcal{E}$  and  $\tilde{\mathcal{E}}$  are



the sets of edges.

**Definition 3.1.**  $(\tilde{\mathcal{G}}, \tilde{\mathbf{w}}, \tilde{p})$  and  $(\mathcal{G}, \mathbf{w}, p)$  can have one of the following interconnections:

Type I:  $\tilde{\mathcal{V}} = \mathcal{V}$ ,  $\tilde{\mathcal{E}} = \mathcal{E}$ , and  $\tilde{\mathbf{w}} \neq \mathbf{w}$ ; or

Type II:  $\tilde{\mathcal{V}} = \mathcal{V}$ ,  $\mathcal{E} \subset \tilde{\mathcal{E}}$ , and  $\tilde{\mathbf{w}} \neq \mathbf{w}$ ; or

Type III:  $\tilde{\mathcal{V}} \neq \mathcal{V}$ ,  $\mathcal{E} \neq \tilde{\mathcal{E}}$ , and  $\tilde{\mathbf{w}} \neq \mathbf{w}$ .

From now on, we refer to the baseline model when we use the notation  $(\mathcal{G}, \mathbf{w}, p)$  and without loss of generality we assume  $\mathcal{E} \subset \tilde{\mathcal{E}}$ . This assumption simplifies the presentation of our approach, but intuitively speaking, the fewer edges an rMRF has, the more information it provides since in a sparser graph, there are more conditional independencies specified.

Based on that, we interrelate the maximal cliques of Types I–II models with those of  $p$ . In particular, for Type I there is a one-to-one correspondence between maximal cliques. Changes on the set of edges of a Type II model lead to different sets of maximal cliques, and one needs to examine the nature of the new edges and their impact on the maximal cliques of  $p$ . Finally, the new set of nodes of a Type III model leads to a drastically new structure that makes such interrelation of maximal cliques hard to achieve. Therefore, this case is not examined here.

Let  $\mathbf{u}$  be a context, and let  $\mathcal{M} \subset \mathcal{V} \cap \tilde{\mathcal{V}}$ . For  $\mathbf{U} = \{Y_i\}_{i \in \mathcal{M}}$  with  $\mathbf{U} = \mathbf{u}$ , we construct the corresponding rMRFs  $(\mathbf{Z}, q(\cdot | \mathbf{w}))$  and  $(\tilde{\mathbf{Z}}, \tilde{q}(\cdot | \tilde{\mathbf{w}}))$  parametrized by  $\mathbf{w}$  and  $\tilde{\mathbf{w}}$ , respectively. Based on the structural classification Types I–III, the probability distributions of  $\tilde{q}$  are treated as follows.

**Type I.** Let  $\mathcal{B} \subset \mathcal{C}_{\mathcal{G}}$  be the set of maximal cliques whose weights differ; i.e., for each  $c \in \mathcal{B}$ ,  $\tilde{\mathbf{w}}_c \neq \mathbf{w}_c$ . The clique potentials of  $\tilde{q}(\cdot | \tilde{\mathbf{w}})$  can be rewritten as

$$(3.2) \quad \tilde{\Psi}_c[\mathbf{u}](\mathbf{z}_c | \tilde{\mathbf{w}}_c) = \begin{cases} \Psi_c[\mathbf{u}](\mathbf{z}_c | \mathbf{w}_c) \Phi_c[\mathbf{u}](\mathbf{z}_c | \mathbf{w}_c, \tilde{\mathbf{w}}_c) & \text{if } c \in \mathcal{B}, \\ \Psi_c[\mathbf{u}](\mathbf{z}_c | \mathbf{w}_c) & \text{otherwise.} \end{cases}$$

We call  $\Phi_c[\mathbf{u}](\cdot | \tilde{\mathbf{w}}_c, \mathbf{w}_c) > 0$  a  $\tilde{q}$ -excess factor of Type I relative to  $q$  on  $c$  defined on variables  $\mathbf{z}_c$  in clique  $c \in \mathcal{B}$ . Cliques where no change on weights has occurred remain the same.

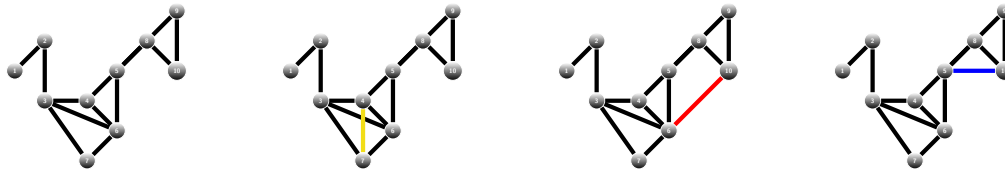
**Type II.** In this type, the class of maximal cliques  $\mathcal{C}_{\tilde{\mathcal{G}}}$  is different. The analysis becomes more complicated, and clique potentials need to be carefully considered. We look into the nature of one or more new edges by categorizing it as one of the following types: a new edge (i) can create a totally new maximal clique (see Figure 1, third graph), (ii) can connect two or more already existing maximal cliques (see Figure 1, second graph), and (iii) can enlarge an already existing maximal clique (see Figure 1, fourth graph).

By adding more than one new edge, the new maximal cliques of  $\tilde{\mathcal{G}}$  can be obtained by a combination of (i), (ii), and (iii). We introduce the following sets:

$$(3.3) \quad \mathcal{B}_{\cup} = \{\tilde{c} \in \mathcal{C}_{\tilde{\mathcal{G}}} \setminus \mathcal{C}_{\mathcal{G}} : \tilde{c} = \cup_i c_i \text{ for } c_i \in \mathcal{C}_{\mathcal{G}}\},$$

$$(3.4) \quad \mathcal{B}_{\subseteq} = \{\tilde{c} \in \mathcal{C}_{\tilde{\mathcal{G}}} \setminus \mathcal{C}_{\mathcal{G}} : \text{there exists } c \in \mathcal{C}_{\mathcal{G}} \text{ s.t. } c \subseteq \tilde{c}\},$$

$$(3.5) \quad \mathcal{B}_{\text{new}} = (\mathcal{C}_{\mathcal{G}} \cup \mathcal{B}_{\cup} \cup \mathcal{B}_{\subseteq})^c.$$



**Figure 1.** (First) Baseline MRF model  $p$  demonstrated by graph  $\mathcal{G}$ . (Second) Alternative model  $\tilde{p}$  with the associated graph obtained by adding the yellow edge (4–7) and connecting two maximal cliques of the  $p$  model,  $\{3, 4, 6\}$  and  $\{3, 6, 7\}$ ; thus,  $\tilde{p}$  has a new maximal clique  $\{3, 4, 6, 7\}$ . (Third) Alternative model  $\tilde{p}$  with the associated graph obtained by adding the red edge (6–10); thus,  $\tilde{p}$  has a totally new maximal clique  $\{6, 10\}$ . (Fourth) Alternative model  $\tilde{p}$  with the associated graph obtained by adding the blue edge (5–10) and enlarging the already existing clique,  $\{5, 8\}$ , to  $\{5, 8, 10\}$ .

Then the clique potentials of  $\tilde{q}$  can be rewritten as

$$(3.6) \quad \tilde{\Psi}_{\tilde{c}}[\mathbf{u}](\mathbf{z}_{\tilde{c}} | \tilde{\mathbf{w}}_{\tilde{c}}) = \begin{cases} \prod_{c_i} \Psi_{c_i}[\mathbf{u}](\mathbf{z}_{c_i} | \mathbf{w}_{c_i}) \Phi_{\tilde{c}}^{(ii)}[\mathbf{u}](\mathbf{z}_{\tilde{c}} | \mathbf{w}_c, \tilde{\mathbf{w}}_c) & \text{if } \tilde{c} \in \mathcal{B}_{\cup}, \\ \Psi_c[\mathbf{u}](\mathbf{z}_c | \mathbf{w}_c) \Phi_{\tilde{c}}^{(iii)}[\mathbf{u}](\mathbf{z}_{\tilde{c}} | \mathbf{w}_c, \tilde{\mathbf{w}}_c) & \text{if } \tilde{c} \in \mathcal{B}_{\subseteq}, \\ \tilde{\Psi}_{\tilde{c}}[\mathbf{u}](\mathbf{z}_{\tilde{c}} | \tilde{\mathbf{w}}_{\tilde{c}}) & \text{if } \tilde{c} \in \mathcal{B}_{\text{new}}, \\ \Psi_c[\mathbf{u}](\mathbf{z}_c | \mathbf{w}_c) & \text{if } \tilde{c} \in \mathcal{C}_{\tilde{\mathcal{G}}}. \end{cases}$$

We call  $\Phi_{\tilde{c}}^{(ii)}, \Phi_{\tilde{c}}^{(iii)} > 0$   $\tilde{q}$ -excess factors of Type II relative to  $q$  on  $\tilde{c}$  defined on the variables of  $\tilde{c}$ . In fact, the two functions play the role of the discrepancy at a distribution level when new maximal clique  $\tilde{c}$  has been created by connecting existing maximal cliques  $c_i$  and by enlarging an existing maximal clique. When  $\tilde{c} \in \mathcal{B}_{\text{new}}$ , there is no need to express the clique potential through the potentials of  $q(\cdot | \mathbf{w})$ . For simplicity, we assume that clique potentials on common maximal cliques between  $\mathcal{G}$  and  $\tilde{\mathcal{G}}$  do not change. However, one can consider different potentials, and in that case, a term  $\Phi$  should be introduced similar to (ii) and (iii). For convenience, we establish one last unifying terminology. We call

$$(3.7) \quad \Phi_{\mathbf{u}}^{\text{I}}(\mathbf{Z}) := \prod_{c \in \mathcal{B}} \Phi_c[\mathbf{u}](\mathbf{Z}_c),$$

$$(3.8) \quad \Phi_{\mathbf{u}}^{\text{II}}(\mathbf{Z}) := \prod_{\tilde{c} \in \mathcal{B}_{\text{new}}} \tilde{\Psi}_{\tilde{c}}[\mathbf{u}](\mathbf{Z}_{\tilde{c}} | \tilde{\mathbf{w}}_{\tilde{c}}) \prod_{\tilde{c} \in \mathcal{B}_{\cup}} \Phi_{\tilde{c}}^{(ii)}[\mathbf{u}](\mathbf{Z}_{\tilde{c}}) \prod_{\tilde{c} \in \mathcal{B}_{\subseteq}} \Phi_{\tilde{c}}^{(iii)}[\mathbf{u}](\mathbf{Z}_{\tilde{c}} | \tilde{\mathbf{w}}_{\tilde{c}})$$

total  $\tilde{q}$ -excess factors of Types I and II relative to  $q$ , respectively. The total  $\tilde{q}$ -excess factor of Type I relative to  $q$  captures all the parameter changes, while the total  $\tilde{q}$ -excess factor of Type II relative to  $q$  captures all the structural discrepancies. In the case of an MRF, we drop the context  $\mathbf{u}$  from (3.7) and (3.8) and  $\mathbf{Z}$  is replaced by  $\mathbf{Y}$ . Equations (3.3)–(3.8) are explicitly specified in the medical diagnostics application in section 5 and its detailed analysis in Appendix D, as well as in statistical mechanics; see section 6. In Type III, there exists the total  $\tilde{q}$ -excess factor of Type III relative to  $q$ . However, due to the high degree of discrepancies, we cannot interrelate maximal cliques of Type III model with  $q$ , and by extension each  $\tilde{q}$ -excess factor cannot be determined. The next results are straightforward but essential in our calculations. To avoid heavy notation, we remind the reader that  $q(\cdot) = q(\cdot | \mathbf{w})$  and  $\tilde{q}(\cdot) = \tilde{q}(\cdot | \tilde{\mathbf{w}})$ .

**Partition function of alternative models.** Based on the above description of alternative models, the partition function of  $\tilde{q}$  is given in the next lemma.

**Lemma 3.2.** *Let  $(\mathbf{Z}, q)$  be an rMRF. Then for any alternative rMRF  $(\mathbf{Z}, \tilde{q})$  of type  $i$  with  $i = \text{I}, \text{II}$ , its partition function is expressed as*

$$(3.9) \quad \tilde{Z}_{\mathbf{u}}(\tilde{\mathbf{w}}) = E_q[\Phi_{\mathbf{u}}^i] Z_{\mathbf{u}}(\mathbf{w}),$$

where  $\Phi_{\mathbf{u}}^i$  is given by (3.7) and (3.8).

**Proof.** The proof is based on the method of interrelating the distribution  $q$  and  $\tilde{q}$ , utilizing the total  $\tilde{q}$ -excess factors relative to  $q$  given by (3.7) and (3.8). The explicit computation is provided in Appendix B.1. ■

**Likelihood ratio.** The following lemma provides the likelihood ratio between  $\tilde{q}$  and  $q$  and constitutes the key ingredient for the simplification of (4.2) and the UQ bounds provided in (4.1).

**Lemma 3.3.** *Let  $(\mathbf{Z}, q)$  be an rMRF. Then for any alternative rMRF  $(\mathbf{Z}, \tilde{q})$  of type  $i$  with  $i = \text{I}, \text{II}$ , the corresponding likelihood ratio satisfies*

$$(3.10) \quad \frac{d\tilde{q}}{dq} = \frac{\Phi_{\mathbf{u}}^i}{E_q[\Phi_{\mathbf{u}}^i]},$$

where  $\Phi_{\mathbf{u}}^i$  is given by (3.7) and (3.8).

The proof is omitted, as the lemma is a direct consequence of the method of interrelating two distributions discussed above and Lemma 3.2. Note that both results hold for MRFs denoted by  $(\mathbf{Y}, p)$  and  $(\mathbf{Y}, \tilde{p})$ , dropping the context  $\mathbf{u}$  from  $\Phi_{\mathbf{u}}^i$  in (3.10).

**3.2. KL divergence.** As we see in section 4, our UQ methods rely on the KL divergence as a means to measure “distance” between baseline and alternative MRFs. The fact that it scales correctly with the dimension of the baseline model [23] as well as the commonalities in parameters and structures between baseline and alternative models combined with the Hammersley–Clifford theorem allows the KL divergence to be expressed in a simplified and informative form. In particular, we show that KL divergence (which is finite due to the positive probabilities  $q$  and  $\tilde{q}$ ) depends only on the total  $\tilde{q}$ -excess factor relative to  $q$  given by (3.7) and (3.8). To simplify the notation, we omit the dependence of  $\mathbf{Z}$  from  $\kappa_i, f$ , and  $\Phi_{\mathbf{u}}^i$ .

**Lemma 3.4.** *Let  $(\mathbf{Y}, p^{\mathbf{w}})$ ,  $(\mathbf{Y}, \tilde{p}^{\tilde{\mathbf{w}}})$  be two MRFs defined over graphs  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$  and  $\tilde{\mathcal{G}} = (\mathcal{V}, \tilde{\mathcal{E}})$ , respectively. Let  $\mathbf{u}$  be a context, and let  $\mathcal{M} \subset \mathcal{V}$ . We consider the corresponding rMRFs  $(\mathbf{Z}, q), (\mathbf{Z}, \tilde{q})$ :*

(a) *If  $\tilde{q}$  is type  $i$ , with  $i = \text{I}$  or  $\text{II}$ , then the KL divergence is given by*

$$(3.11) \quad \begin{aligned} R(\tilde{q}||q) &= E_{\tilde{q}} \left[ \log \frac{\tilde{q}}{q} \right] = E_q \left[ \frac{\tilde{q}}{q} \log \frac{\tilde{q}}{q} \right] \\ &= E_{\tilde{q}}[\log \Phi_{\mathbf{u}}^i] - \log E_q[\Phi_{\mathbf{u}}^i] = \frac{1}{E_q[\Phi_{\mathbf{u}}^i]} E_q [\Phi_{\mathbf{u}}^i \log \Phi_{\mathbf{u}}^i] - \log E_q[\Phi_{\mathbf{u}}^i], \end{aligned}$$

where  $\Phi_{\mathbf{u}}^i$  is defined in (3.7) and (3.8) accordingly.

(b) If  $\tilde{q}$  is type i, with  $i = \text{I or II}$ , then for any  $f$  satisfying (4.3), the KL divergence is given by

$$(3.12) \quad \mathcal{R}(\tilde{q}||q) = C_i E_{\tilde{q}}[f] + \frac{E_q[\kappa_i \Phi_{\mathbf{u}}^i]}{E_q[\Phi_{\mathbf{u}}^i]} - \log E_q[\Phi_{\mathbf{u}}^i], \quad \Phi_{\mathbf{u}}^i(\mathbf{Z}) = e^{C_i f(\mathbf{Z}) + \kappa_i(\mathbf{Z})}.$$

*Proof.* (a) We express the KL divergence as follows:

$$R(\tilde{q}||q) = E_{\tilde{q}} \left[ \log \frac{\tilde{q}}{q} \right] = E_q \left[ \frac{\tilde{q}}{q} \log \frac{\tilde{q}}{q} \right].$$

Then we use Lemma 3.3 and we obtain (3.11). For (b), we additionally recall (4.3).  $\blacksquare$

**Remark 3.5.** As mentioned in Lemma 3.3, the result holds for MRFs denoted by  $(\mathbf{Y}, p)$  and  $(\mathbf{Y}, \tilde{p})$ , dropping the context  $\mathbf{u}$  from  $\Phi_{\mathbf{u}}^i$ .

**4. Main results.** In this section, we present an information-based UQ method on the predictions for QoIs for general MRFs/rMRFs by quantifying the model uncertainty for MRFs/rMRFs arising from statistical learning of graph models or from physical modeling. Our starting point is the Donsker–Varadhan variational principle [22], which in turn implies the *Gibbs variational principle* for the KL divergence (see [15, 23]):

$$(4.1) \quad \sup_{\lambda > 0} \left\{ \frac{-\Lambda_p^f(-\lambda) - R(\tilde{q}||q)}{\lambda} \right\} \leq E_{\tilde{q}}[f] \leq \inf_{\lambda > 0} \left\{ \frac{\Lambda_q^f(\lambda) + R(\tilde{q}||q)}{\lambda} \right\}.$$

As mentioned earlier, we focus on KL divergence, as it scales correctly with the dimension of the baseline model [23]. In the above inequality,  $q$  is the baseline rMRF and  $\tilde{q}$  is an alternative model in the ambiguity set defined in (3.1). We note that at an MRF point of view, (4.1) holds as well. Moreover,  $\Lambda_q^f(\lambda)$  is the cumulant generating function (CGF) computed with respect to  $p$  given by

$$(4.2) \quad \Lambda_q^f(\lambda) := \log E_q[e^{\lambda f}],$$

while  $f$  is a QoI. The class of QoIs that we examine here is discussed in the next subsection.

We take advantage of the total  $\tilde{q}$ -excess factors relative to  $q$ , the likelihood ratio, and an explicit formula for KL divergence on MRFs/rMRFs (see Lemma 3.4) in section 3, as well as of the handling of the inherent high dimensionality of such graphical models, and we obtain tight and scalable, information-based bounds on the predictions for QoIs. Finally, we prove the tightness of the UQ bounds; i.e., we prove that the bounds are attainable by MRFs/rMRFs, we compute their probability distributions, and we develop a strategy to determine their associated graph structures.

**4.1. Quantities of interest.** We primarily consider two classes of QoIs  $f(\mathbf{Z})$ . The first has QoIs that are expressed as a characteristic function on events of interest such as (5.1) in the medical diagnostics example presented in section 5. The second class consists of QoIs that are sufficient statistics for the models  $q$  and  $\tilde{q}$  and are also present in the total  $\tilde{q}$ -excess factor of Types I and II relative to  $q$ ; i.e., we consider  $f(\mathbf{Z})$ , which satisfies

$$(4.3) \quad f(\mathbf{Z}) = \frac{1}{C_i} (\log \Phi_{\mathbf{u}}^i(\mathbf{Z}) + \kappa_i(\mathbf{Z})), \quad i = \text{I, II},$$

for some nonzero constant  $C_i \equiv C_i(\mathbf{w}, \tilde{\mathbf{w}}, \mathbf{u}) < 1$  and a function  $\kappa_i(\cdot) \equiv \kappa_i(\cdot \mid \mathbf{w}, \tilde{\mathbf{w}}, \mathbf{u})$  that may depend on  $\mathbf{w}, \tilde{\mathbf{w}}, \mathbf{u}$ ; see also (3.12). Such a class covers observables involved in finite-size effects and phase diagrams for the statistical mechanics models examined later (e.g., averages of spins given by (6.12)). The CGF given by (4.2) is computable for QoIs in both classes.

**4.2. UQ bounds.** The next theorem is a UQ result on rMRFs that is obtained by consolidating the total  $\tilde{q}$ -excess factors relative to  $q$ , likelihood ratio, KL divergence, and QoIs. Part (a) provides the UQ bounds for a general QoI, and hence we use such bounds for QoIs examined in the medical diagnostics application in section 5. Part (b) is particularly applicable for QoIs that satisfy (4.3), so they are exploited in the statistical mechanics section.

**Theorem 4.1.** *Let  $(\mathbf{Y}, p)$ ,  $(\mathbf{Y}, \tilde{p})$  be two MRFs defined over graphs  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$  and  $\tilde{\mathcal{G}} = (\mathcal{V}, \tilde{\mathcal{E}})$ , respectively. Let  $\mathbf{u}$  be a context, and let  $\mathcal{M} \subset \mathcal{V}$ . We consider the corresponding rMRFs  $(\mathbf{Z}, q)$ ,  $(\mathbf{Z}, \tilde{q})$ . If  $\tilde{q}$  is of type  $i$ , with  $i = \text{I or II}$ , then we have the following:*

(a) *For any QoI  $f(\mathbf{Z})$ , the following bounds hold:*

$$(4.4) \quad \pm E_{\tilde{q}}[f] \leq \inf_{\lambda > 0} \frac{1}{\lambda} \left\{ \log E_q[e^{\pm \lambda f}] + \frac{1}{E_q[\Phi_{\mathbf{u}}^i]} E_q[\Phi_{\mathbf{u}}^i \log \Phi_{\mathbf{u}}^i] - \log E_q[\Phi_{\mathbf{u}}^i] \right\}.$$

(b) *For any QoI  $f(\mathbf{Z})$  that satisfies (4.3), the following bounds hold:*

$$(4.5) \quad \pm E_{\tilde{q}}[f] \leq \frac{1}{1 - C_i} \inf_{\lambda > 0} \frac{1}{\lambda} \left\{ \log E_q[e^{\pm \lambda f}] - \log E_q[\Phi_{\mathbf{u}}^i] + \frac{E_q[\kappa_i \Phi_{\mathbf{u}}^i]}{E_q[\Phi_{\mathbf{u}}^i]} \right\},$$

where  $\Phi_{\mathbf{u}}^i$  is the total  $\tilde{q}$ -excess factor relative to  $q$  given by (3.7) and (3.8), and  $\kappa_i$  and  $C_i$  are defined in (4.3). Note that when  $\tilde{q}$  is of Type I,  $\tilde{Z}_{\mathbf{u}}(\tilde{\mathbf{w}}) = Z_{\mathbf{u}}(\tilde{\mathbf{w}})$ .

The proof given in Appendix B.2 is based on Lemma 3.4 and the characterization of the exponential integrals. An application to a single parameter exponential family is given in Appendix B.2.

**4.3. Tightness of UQ bounds for MRFs/rMRFs.** Here we prove that the inequalities (4.4) and (4.5) are tight, i.e., they become an equality for a suitable model  $\tilde{q} \in \mathcal{Q}^n$  given by (3.1) standing for the worst case scenarios. The practical interpretation of the tightness of UQ bounds is that these distributions are reasonable, as they belong to the ambiguity set in (3.1).

**Theorem 4.2.** *Let  $(\mathbf{Z}, q)$  be an rMRF defined in subsection 2.2.1 and  $f(\mathbf{Z})$  be a QoI with a finite MGF  $E_q[e^{\lambda f(\mathbf{Z})}]$  in a neighborhood of the origin. Then there exist  $0 < \eta_{\pm} \leq \infty$  such that for any  $\eta \leq \eta_{\pm}$  there exist probability measures  $q^{\pm} = q^{\pm}(\eta) \in \mathcal{Q}_{\eta}$ , where  $\mathcal{Q}_{\eta}$  is given in (3.1), such that (4.4) and (4.5) become an equality. Furthermore,  $q^{\pm} = q^{\lambda_{\pm}}$ , with*

$$(4.6) \quad dq^{\lambda_{\pm}} = \frac{e^{\lambda_{\pm} f}}{E_q[e^{\lambda_{\pm} f}]} dq$$

and  $\lambda_{\pm}$  being the unique solutions of  $R(q^{\lambda_{\pm}} \| q) = \eta$ . In particular, the total  $q^{\pm}$ -excess factor relative to  $q$ , denoted by  $\Phi_{\mathbf{u}}^{\pm}$ , satisfies

$$\Phi_{\mathbf{u}}^{\pm} = e^{\lambda_{\pm} f} \quad \text{and} \quad C_i = \lambda_{\pm}, \quad \kappa_i = 0, \quad \text{respectively.}$$



*Proof.* See Appendix B.3. ■

The result holds also for MRFs. The corresponding quantities involved in the theorem are denoted by  $p, p^{\lambda^\pm}$ , and  $\Phi^\pm$ .

**Remark 4.3.** For convenience, we use its MRF version. Given a baseline MRF  $(\mathbf{Y}, p)$ , its associated graph  $\mathcal{G}$ , and a QoI  $f$ , Theorem 4.2 guarantees the existence of probability distributions  $p^{\lambda^\pm}$  such that (4.4) and (4.5) become an equality (this is not an unlikely extreme case) and also specifies the distributions explicitly. However, it does not imply how different the associated graphs of  $p^\pm$  are, compared to the graph associated to  $p$ , or, grossly speaking, if they are Type I or II. Depending on  $f$ , there are cases where this can be determined. In fact, by recalling the Hammersley–Clifford theorem, we express

$$(4.7) \quad dp^{\lambda^\pm} = \frac{e^{\lambda^\pm f}}{E_p[e^{\lambda^\pm f}]} \frac{1}{Z(\mathbf{w})} \prod_{c \in \mathcal{C}_{\mathcal{G}}} \Psi_c(\mathbf{y}_c | \mathbf{w}_c) = \frac{1}{Z^\pm(\lambda^\pm, \mathbf{w})} \prod_{c \in \mathcal{C}_{\mathcal{G}}} e^{\lambda^\pm f} \Psi_c(\mathbf{y}_c | \mathbf{w}_c),$$

where  $Z^\pm(\lambda^\pm, \mathbf{w}) = E_p[e^{\lambda^\pm f}] Z(\mathbf{w})$  is the partition function of  $p^{\lambda^\pm}$ .

We turn our attention to the product in (4.7). Each factor is defined on a maximal clique of  $\mathcal{G}$  apart from  $e^{\lambda^\pm f}$ . We focus on  $f$ . Suppose that  $f$  is a QoI with domain  $\text{Dom}(f)$  and cannot be written as a sum of more than two functions, e.g., sample average. If there is a maximal clique  $c_0$  such that  $\text{Dom}(f) \subseteq c_0$ , then it turns out that all clique potentials of  $p^{\lambda^\pm}$  and  $p$  are equal except  $\tilde{\Psi}_{c_0} = e^{\lambda^\pm f} \Psi_{c_0}$ , and hence

$$(4.8) \quad dp^{\lambda^\pm} = \frac{1}{E_p[e^{\lambda^\pm f}] Z(\mathbf{w})} \underbrace{e^{\lambda^\pm f} \Psi_{c_0}}_{\tilde{\Psi}_{c_0}} \prod_{c \neq c_0} \Psi_c(\mathbf{y}_c | \mathbf{w}_c).$$

The associated graphs of  $p^{\lambda^\pm}$  are apparently of Type I, as no change on maximal cliques occurs. If  $\text{Dom}(f) \cap c \neq \emptyset$  for more than two maximal cliques  $c$ , then the graphs associated to  $p^{\lambda^\pm}$  have been changed and thus are Type II. An example is discussed in subsection 5.1. On the other hand, if  $f$  can be expressed as a sum of some functions  $f = \sum_i f_i$ , then we may have more than one candidate graph associated to  $p^{\lambda^\pm}$  that is either Type I or II. In fact, the exponential can be factorized further (e.g.,  $e^{\lambda^\pm f} = \prod_i e^{\lambda^\pm f_i}$ ), giving rise to more than one way of matching the clique potentials in the sense of (4.8).

**Remark 4.4.** The parameter  $\eta$  in Theorem 4.2 is also called the *misspecification parameter*, and it can be thought of as a *nonparametric “stress test”* for the rMRF and can be tuned by hand so one can explore how the level of uncertainty affects QoIs. Alternatively,  $\eta$  can be computed as the KL divergence from the available data (e.g., data used to construct the baseline model in medical diagnostics; see section 5) in the form of a histogram or a KDE and thus subs for the distance of the baseline model from the unknown true model [30].

**5. UQ for medical diagnostics.** Let us introduce a simple example from medical diagnostics. We exploit its simplicity and low dimensionality to demonstrate MRF modeling with parameters and structures learned from data as well as the types of uncertainties that arise naturally in MRF modeling.

**Setup.** Consider the problem of investigating interdependence (structure) and its strength (parameters) between smoking (S), asthma (A), lung cancer (L), and cough (C) [20]. It is assumed there are prior expert knowledge and data encoded by a probabilistic model (distribution)  $p^*$  defined on  $\{S, C, L, A\}$ . Due to limitations in expert knowledge and data, the true distribution  $p^*$  itself may be altogether unknown. This, in turn, forces us to build a surrogate baseline model  $p$ , which therefore is uncertain in ways we will specify next.

**Baseline MRF.** Let  $\mathcal{D} = \{\mathbf{d}[1], \dots, \mathbf{d}[N]\}$  be a large collection of patient records sampled from  $p^*$ . Using a structure-learning algorithm on the data  $\mathcal{D}$  (for instance, a greedy score-based structure search algorithm for log-linear models [49, 38]), a model with the structure of  $\mathcal{G}$  illustrated in Figure 2(left) is built [20]. We assume that the graph is undirected, as the directionality associated with the variable dependencies is not known (or is not expected). Subsequently, by parameter learning (for instance, using maximum likelihood estimation [49]) the weights  $\mathbf{w}$  become specified from the available data. From now on the resulting model  $(\mathcal{G}, \mathbf{w}, p)$  is called the baseline model.



**Figure 2.** (Left) MRF structure  $(\mathbf{Y}, p) = (\{S, C, L, A\}, p)$  over  $\mathcal{G}$  with joint probability distribution  $p$ .  $S \in \{s_0, s_1\}$ ,  $L \in \{l_0, l_1\}$ ,  $A \in \{a_0, a_1\}$ , and  $C \in \{c_0, c_1\}$ . For example, the values  $s_0$  and  $s_1$  can be thought as smoking and nonsmoking, respectively, and so forth. The random variables  $\mathbf{Y} = \{Y_1, Y_2, Y_3, Y_4\} = \{S, L, A, C\}$  are accordingly attached to the nodes in  $\mathcal{V} = \{1, \dots, 4\}$  with edges in  $\mathcal{E} = \{1-2, 2-3, 2-4, 3-4\}$ . The class of maximal cliques is  $\mathcal{C}_{\mathcal{G}} = \{\{1, 2\}, \{2, 3, 4\}\}$ . (Right) A Type II model  $(\tilde{\mathcal{G}}, \tilde{\mathbf{w}}, \tilde{p})$  over  $\mathbf{Y} = \{S, C, L, A\}$  with joint probability distribution  $\tilde{p}$ . The associated graph is demonstrated by  $\tilde{\mathcal{G}} = (\mathcal{V}, \tilde{\mathcal{E}})$  with  $\tilde{\mathcal{E}} = \mathcal{E} \cup \{1-4\}$ . The new edge is shown in red.

As in [20], the joint probability distribution could be a log-linear model (see [49, section 4.4]) and thanks to the Hammersley–Clifford theorem is factorized over the maximal cliques with clique potentials  $\Psi_c(\mathbf{y}_c \mid \mathbf{w}_c) = e^{w_c f_c(\mathbf{y}_c)}$ ,  $\mathbf{w} = \{\mathbf{w}_c\}_{c \in \mathcal{C}_{\mathcal{G}}}$ , where  $f_c$  is often called a *feature*.

**Alternative models.** Both learning steps can induce uncertainties in structure and/or parameters on the baseline. Next, we model and quantify such uncertainties by considering alternative models to the baseline of Types I and II: we focus on graphical models that may have been obtained by learning structure and parameters from either a different data set  $\tilde{\mathcal{D}} = \{\tilde{\mathbf{d}}[1], \dots, \tilde{\mathbf{d}}[\tilde{N}]\}$  or the same data set  $\mathcal{D}$  but with different prior (expert) knowledge. We denote the corresponding alternative models  $(\tilde{\mathcal{G}}, \tilde{\mathbf{w}}, \tilde{p})$  and assume they can also be represented by an MRF with  $\tilde{p} > 0$  in the class of log-linear models with clique potentials being given by  $\tilde{\Psi}_c(\mathbf{y}_c) = e^{\tilde{w}_c \tilde{f}_c(\mathbf{y}_c)}$ . We consider the following QoIs defined as

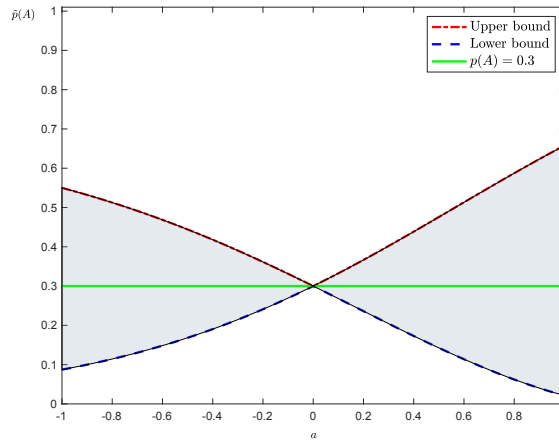
$$(5.1) \quad g(\mathbf{Y}) = \mathbf{1}_A \quad \text{for any event of interest } A \subset \Omega.$$

For instance,  $A = \{\text{patient is smoker with asthma}\} = \{\omega = (\omega_1, \omega_2, \omega_3, \omega_4) : \omega_1 = s_0, \omega_3 = a_0\}$ .

**Type I.** We consider the class of log-linear models  $\tilde{p}$  over  $\mathcal{G}$  with weight change in one maximal clique after learning weights from  $\tilde{\mathcal{D}}$ . Let  $c$  be the maximal clique that a weight change occurred. If  $p_I \equiv p(B_c)$  and  $a \in [-1, 1]$  (depending on  $\tilde{p}$ ), then for any event of interest  $A$ , the following holds:

$$(5.2) \quad \pm \tilde{p}(A) \leq \inf_{\lambda > 0} \frac{1}{\lambda} \left\{ \log \left( \frac{p(A)e^{\pm\lambda} + 1 - p(A)}{e^{aw_c p_I} + 1 - p_I} \right) - \frac{aw_c e^{aw_c p_I}}{e^{aw_c p_I} + 1 - p_I} \right\},$$

where  $a \in [-1, 1]$  stands for the model uncertainty of alternative models of Type I and  $w_c$  is the weight on  $c$  of  $p$ . The derivation of the UQ bounds in (5.2) is given in Appendix D, while their demonstration as functions of the uncertainty parameter  $a$  for any event of interest  $A$  with  $p(A) = 0.3$  and when  $p_I = 0.2$  is given in Figure 3.

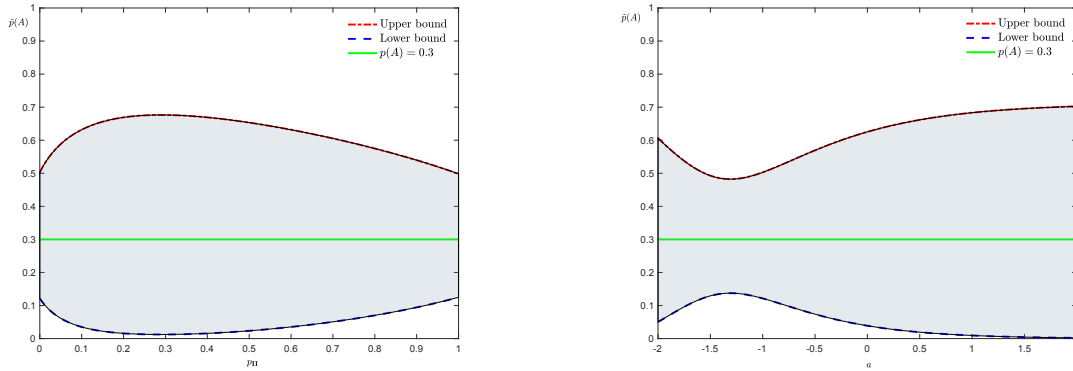


**Figure 3.** For any event of interest,  $A$  with  $p(A) = 0.3$ , the red dashed-dot and the blue dashed curve are the upper bound and lower bounds for  $\tilde{p}(A)$  provided in (5.2), computed as functions of the weight change  $a$ .

**Type II.** We consider the class of log-linear models  $\tilde{p}$  over  $\tilde{\mathcal{G}}$  with  $\tilde{\mathcal{V}} = \mathcal{V}$ ,  $\tilde{\mathcal{E}} = \mathcal{E} \cup e$ , where the new edge  $e$  (see, e.g., Figure 2(right)) enlarges an already existing maximal clique  $\tilde{c}$  in the sense of the analysis in subsection 3.1 after structure learning from  $\tilde{\mathcal{D}}$ . The model uncertainties lie in the binary function  $\tilde{f}_{\tilde{c}}$  defined on  $\tilde{c}$  and the new weight  $\tilde{\mathbf{w}}_{\tilde{c}}$ . The binary function  $\tilde{f}_{\tilde{c}}$  induces a set  $B_{\tilde{c}} = \{(\omega_1, \omega_2, \omega_3, \omega_4) : \tilde{f}_{\tilde{c}}(\omega_{\tilde{c}}) = 1\}$ . The set  $B_{\tilde{c}}$  satisfies one of the following:  $B_{\tilde{c}} \cap B_c = \emptyset$  or  $B_{\tilde{c}} \cap B_c \neq \emptyset$ . For  $B_{\tilde{c}} \cap B_c = \emptyset$ , if  $p_I \equiv p(B_c)$ ,  $p_{II} \equiv p(B_{\tilde{c}})$ , and  $a \in \mathbb{R}$ , then for any event of interest  $A$ , the following holds:

$$(5.3) \quad \pm \tilde{p}(A) \leq \inf_{\lambda > 0} \frac{1}{\lambda} \left\{ \log \left( \frac{p(A)e^{\pm\lambda} + 1 - p(A)}{1 - (1 - e^{(1+a)w_c})p_{II} - (1 - e^{-w_c})p_I} \right) - \frac{w_c e^{-w_c} p_I - (1+a)w_c e^{(1+a)w_c} p_{II}}{1 - (1 - e^{(1+a)w_c})p_{II} - (1 - e^{-w_c})p_I} \right\}.$$

The derivation of the UQ bounds in (5.3) is given in Appendix D, while their demonstration for any event  $A$  with  $p(A) = 0.3$  as functions of the uncertainty parameters  $a$  (when  $p_I = 0.2$ ,  $w_c = 1.5$ , and  $p_{II} = 0.7$ ) and  $p_{II}$  (when  $p_I = 0.2$ ,  $w_c = 1.5$ , and  $a = -0.2$ ) is given in Figure 4. Note that the case where  $B_{\bar{c}} \cap B_c \neq \emptyset$  is more complicated. However, the KL divergence is still explicitly computable (see Remark D.1).

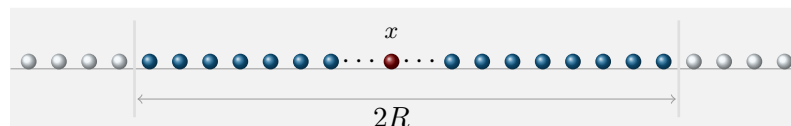


**Figure 4.**  $A$  is an event of interest with  $p(A) = 0.3$ . (Left) For  $p_I = 0.2$ ,  $w_c = 1.5$ , and  $a = -0.2$ , the red dash-dot and the blue dashed curves are the upper bound and lower bounds for  $\tilde{p}(A)$  provided in (5.3), computed as functions of  $p_{II}$ . (Right) For  $p_I = 0.2$ ,  $w_c = 1.5$ , and  $p_{II} = 0.7$ , the red curve and the blue are the upper bound and lower bounds for  $\tilde{p}(A)$ , computed as functions of the weight change  $a \in [-2, 2]$ .

**5.1. Tightness.** Let  $g$  be the QoI given by (5.1). By applying Theorem 4.2, there exist probability measures  $p^\pm = p^\pm(\eta) \in \mathcal{Q}^\eta$ , where  $\mathcal{Q}^\eta$  is given in (3.1), such that (4.4) becomes an equality and  $p^\pm = p^{\lambda^\pm}$  are given by  $dp^{\lambda^\pm} = \frac{e^{\lambda^\pm \mathbf{1}_A}}{p(A)e^{\lambda^\pm} + 1 - p(A)} dp$ , with  $\lambda_\pm$  being the unique solution of  $R(p^{\lambda^\pm} \| p) = \eta$ . Depending on the event of interest  $A$ , we can determine the graph associated with  $p^{\lambda^\pm}$ . Specifically, if  $A = \cap_i A_i$ , where all  $A_i$  are defined on the same maximal clique of  $\mathcal{G}$  given in Figure 2, then the graph associated with  $p^{\lambda^\pm}$  is  $\mathcal{G}$ , and hence both models are Type I. If at least two  $A_i, A_j$  are defined on different maximal cliques, the associated graphs are different from  $\mathcal{G}$ ; e.g., let  $A = \{\text{patient is smoker with asthma}\} = \{\omega = (\omega_1, \omega_2, \omega_3, \omega_4) : \omega_1 = s_0, \omega_3 = a_0\} = \{\omega : \omega_1 = s_0\} \cap \{\omega : \omega_3 = a_0\}$ . Since the total  $p^\pm$ -excess factor relative to  $p$   $\Phi^\pm = e^{\lambda^\pm \mathbf{1}_A}$  cannot be further factorized, the new graph has the same set of nodes with an extra edge  $1 - 3$ , that is,  $\tilde{\mathcal{E}} = \mathcal{E} \cup \{1 - 3\}$ . In that case, both models are Type II.

**6. UQ for statistical mechanics.** Large-scale physical systems of interacting particles, such as gases, liquids, and solids, are at the core of statistical mechanics and in particular of equilibrium statistical mechanics. The macroscopic properties of a system can be understood through its underlying microscopic description, which fundamentally requires the microscopic states and an interaction between microscopic constituents. Statistical mechanics models such as the Ising model are fundamental in ML, especially energy-based probabilistic models (generally defined as (6.6)) such as Boltzmann machines [38]. Furthermore, methods from equilibrium statistical mechanics combined with information theory can provide first insights into profound cornerstones of deep learning. For example, although we use the KL divergence

defined in Lemma 3.4 for UQ, KL between an energy-based model and available data equals the difference between Gibbs and Helmholtz free energy and is a natural “distance” to use for statistical learning. Note that both UQ and statistical learning can be considered as dual concepts [7]. A more extensive analysis of these ideas and generally on the intersection between statistical mechanics—also including nonequilibrium statistical mechanics—and deep learning have been reviewed in [3].



**Figure 5.** One-dimensional Ising-spin lattice on  $\Delta$  (light grey area with blue, red, and white particles). The spin located at  $x \in \Delta$  (red particle) interacts only with spins located at  $y$  in  $B_x(R)$  (blue particles) with strength of interaction  $J(x, y)$ . The red spin does not interact with the white ones, as they are located at distance greater than  $R$  from  $x$ .

**6.1. Ising model.** An illustrative example is the Ising model, where the space of all microstates is the collection of all spin configurations on a bounded region  $\Delta \subseteq \mathbb{Z}^d$ :

$$\Omega := \{\pm 1\}^\Delta = \left\{ \sigma_\Delta = \{\sigma_\Delta(x)\}_{x \in \Delta} : \sigma_\Delta(x) \in \{+1, -1\} \right\}$$

as in Figure 5; see [57, 49]. An interaction between spins can be short, long range, or a combination (such as the Lennard-Jones potential [58]), positive (ferromagnetism), etc; see [57, 31, 34]. Here we consider a  $d$ -dimensional Ising-spin system on  $\Delta$  with a generic interaction  $\mathbf{J} = \{J(x, y) : x, y \in \Delta\}$  satisfying three properties: for all  $x, y \in \Delta$  and  $z \in \mathbb{R}^d$ ,

$$(6.1) \quad J(x+z, y+z) = J(x, y) \quad (\text{translational invariance}),$$

$$(6.2) \quad J(x, y) = J(y, x) \quad (\text{symmetry}),$$

$$(6.3) \quad \sum_{x \neq 0} |J(0, x)| < \infty \quad (\text{summability}),$$

and for an external field,  $h \in \mathbb{R}$ . Let  $R > 0$  be the length of the range of interaction. For  $x \in \mathbb{Z}^d$ ,  $B_x(R) = \{y \in \mathbb{Z}^d : \|x - y\|_d \leq R\}$  is the set of all spins that the spin located at  $x$  interacts with and  $\|x - y\|_d := \sqrt{\sum_{i=1}^d |x_i - y_i|^2}$ . For convenience, we denote  $B_{x,R}^\neq := B_x(R) \setminus x$ .

**6.1.1. Boundary conditions.** Boundary conditions are a fundamental concept in statistical mechanics [62]. For simplicity, let us assume that  $\Delta$  is a hypercube. We consider a system where particles not only interact with particles in  $\Delta$  but also with particles “outside” of  $\Delta$ . Let  $\bar{\sigma}_{\Delta^c}$  be a given fixed configuration of spins on the complement of  $\Delta$  denoted by  $\Delta^c$ ; see Figure 10. The Hamiltonian energy of the system is given by

$$(6.4) \quad H^{\mathbf{J},h}(\sigma_\Delta | \bar{\sigma}_{\Delta^c}) = H^{\mathbf{J},h}(\sigma_\Delta) - \sum_{x \in \Delta} \sum_{y \in \Delta^c} J(x, y) \sigma_\Delta(x) \sigma_\Delta(y),$$



where

$$(6.5) \quad H^{\mathbf{J},h}(\sigma_\Delta) = -\frac{1}{2} \sum_{x \in \Delta} \sum_{y \in \Delta} J(x,y) \sigma_\Delta(x) \sigma_\Delta(y) - h \sum_{x \in \Delta} \sigma_\Delta(x).$$

The Gibbs measure with boundary condition  $\bar{\sigma}_{\Delta^c}$  is defined as

$$(6.6) \quad \mu_{\mathbf{J},\beta,h}^\Delta(\sigma_\Delta \mid \bar{\sigma}_{\Delta^c}) = \frac{1}{Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J},\beta,h)} e^{-\beta H^{\mathbf{J},h}(\sigma_\Delta \mid \bar{\sigma}_{\Delta^c})},$$

where  $Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J},\beta,h) = \sum_{\sigma_\Delta} e^{-\beta H^{\mathbf{J},h}(\sigma_\Delta \mid \bar{\sigma}_{\Delta^c})}$  is the partition function.

**6.1.2. rMRF formulation.** A system with configuration as boundary conditions does not admit an MRF description. So, we describe the system using rMRFs. The set of nodes is  $\mathbb{Z}^d$ , the set of edges can be constructed by looking at all  $(x,y)$  such that  $\|x-y\|_d \leq R$ , and the context is  $\mathbf{u} = \bar{\sigma}_{\Delta^c}$ , which corresponds to a fixed boundary condition.  $(\sigma_\Delta, \mu_{\mathbf{J},\beta,h}^\Delta(\cdot \mid \bar{\sigma}_{\Delta^c}))$  is then an rMRF with maximal cliques  $c_x = \{y \in \Delta : y \in B_{x,R}^\neq\}$  (spins in  $c_x$  interact with all spins in  $c_x$ ). Let  $\mathbf{w} = \{\mathbf{w}_{c_x}\}_{x \in \Delta}$  with  $\mathbf{w}_{c_x} = (\mathbf{J}_{c_x}, \beta, h)$  and  $\mathbf{J}_{c_x} = \{J(x,y) : y \in c_x\}$ . We express each clique potential as

$$(6.7) \quad \Psi_{c_x} = \exp \left\{ \beta \sigma_\Delta(x) \left( h + \frac{1}{2} \sum_{\substack{y \in \Delta \\ y \in B_{x,R}^\neq}} J(x,y) \sigma_\Delta(y) + \sum_{\substack{y \in \Delta^c \\ y \in B_{x,R}^\neq}} J(x,y) \bar{\sigma}_{\Delta^c}(y) \right) \right\}.$$

Note that we may resume the full notation when needed, that is,  $\Psi_{c_x} \equiv \Psi_{c_x}[\bar{\sigma}_{\Delta^c}](\sigma_{c_x} \mid \mathbf{w}_{c_x})$ , where  $\sigma_{c_x}$  is the Ising-spin configuration defined on all  $y \in c_x$ .

## 6.2. UQ formulation.

**6.2.1. Alternative models.** We consider models on a lattice with perturbed interaction in the strength (Type I) and/or range (Type II) such as truncated or long range interaction. Given  $\mathbf{J}$  as in subsection 6.1, an interaction  $F(x,y)$  satisfying (6.1)–(6.3) with length of range  $R_F$ , we say that  $\tilde{\mathbf{J}}^F = \{\tilde{J}^F(x,y) : x,y \in \mathbb{Z}^d\}$  is a perturbed interaction if

$$(6.8) \quad \tilde{J}^F(x,y) = J(x,y) \mathbf{1}_{\|x-y\|_d \leq R} + F(x,y) \mathbf{1}_{\|x-y\|_d \leq R_F} + F(x,y) \mathbf{1}_{\|x-y\|_d > R_F}.$$

We say that a perturbed interaction is Type I if and only if

$$(6.9) \quad R = R_F \text{ and } \text{supp}(F) = \{(x,y) : \|x-y\|_d \leq R_F\}.$$

We say that a perturbed interaction is Type II if and only if

$$(6.10) \quad R = R_F \text{ and } \text{supp}(F) = \{(x,y) : \|x-y\|_d > R_F\}.$$

The rMRF formulation of the system with  $\tilde{\mathbf{J}}^F$  goes similarly as in subsection 6.1.2. Note that the graph representation simplifies a possible complexity of  $J$ ,  $F$ , and  $\tilde{J}^F$  as we connect nodes  $x,y$  according to the range of  $J$ ,  $F$ , and  $\tilde{J}^F$  and assign the corresponding strengths  $J(x,y)$ ,  $F(x,y)$ , and  $\tilde{J}^F(x,y)$ .

### 6.2.2. Total $\tilde{q}_\Delta$ -excess factor relative to $q_\Delta$ .

**Lemma 6.1.** Let  $\tilde{\mathbf{J}}^{\mathbf{F}}$  be defined in subsection 6.2.1 with support given by (6.9) or (6.10), and let  $q_\Delta(\cdot) := \mu_{\mathbf{J},\beta,h}^\Delta(\cdot \mid \bar{\sigma}_{\Delta^c})$ ,  $\tilde{q}_\Delta(\cdot) := \mu_{\tilde{\mathbf{J}}^{\mathbf{F}},\beta,\tilde{h}}^\Delta(\cdot \mid \bar{\sigma}_{\Delta^c})$  be the corresponding Gibbs measures defined in (6.6). The total  $q_\Delta$ -excess factor for  $i = \text{I, II}$  is given by

$$(6.11) \quad \Phi_{\bar{\sigma}_{\Delta^c}}^i(\sigma_\Delta) = \exp \left\{ \beta \sum_{x \in \Delta} \sigma_\Delta(x) \left( (\tilde{h} - h) + \frac{1}{2} \sum_{y \in A_x^i \cap \Delta} F(x, y) \sigma_\Delta(y) \right. \right. \\ \left. \left. + \sum_{y \in A_x^i \cap \Delta^c} F(x, y) \bar{\sigma}_{\Delta^c}(y) \right) \right\},$$

where for each  $x \in \Delta$ ,  $A_x^{\text{I}} = B_x(R)$  and  $A_x^{\text{II}} = B_x(R)^c$ , with  $B_x(R)^c$  being the complement of  $B_x(R)$ .

The proof is straightforward (see Appendix E.2). Both  $(\tilde{h} - h)$  and  $F(x, y)$  in the total  $\tilde{q}_\Delta$ -excess factor relative to  $q_\Delta$  point out how different the external fields and interactions are, respectively, as the latter satisfies  $F(x, y) = \tilde{J}^{\mathbf{F}}(x, y) - J(x, y)$ .

**6.2.3. Quantities of interest.** The use of phase diagrams is central in physics and material science. A phase diagram is defined as a graphical representation of equilibrium states under different thermodynamic parameters, such as external field  $h$ , temperature  $T$ , and pressure  $P$ . It is typically computed in the thermodynamic limit (i.e., a limiting process with  $\Delta \nearrow \mathbb{Z}^d$  such that the ratio between interatomic distances and macroscopic lengths vanishes) [57]. Equilibrium states are characterized by order parameters such as magnetization. For that, we consider the following observable:

$$(6.12) \quad m(\sigma_\Delta) := \frac{1}{|\Delta|} \sum_{x \in \Delta} \sigma_\Delta(x),$$

where  $|\Delta|$  stands for the volume of a hypercube  $\Delta \subset \mathbb{Z}^d$ . As  $\Delta$  invades the whole  $\mathbb{Z}^d$ , the expectation of  $m(\sigma_\Delta)$  yields the magnetization. Other QoIs could also be considered, e.g., correlation functions  $v(\sigma_\Delta) = \frac{1}{|\Delta|^2} \sum_{x \in \Delta} \sum_{y \in \Delta} \sigma_\Delta(x) \sigma_\Delta(y)$ .

**6.2.4. CGF.** Let  $\Delta$  be a hypercube in  $\mathbb{Z}^d$ . Given a configuration  $\bar{\sigma}_{\Delta^c}$ , the baseline model is an Ising model with interaction  $\mathbf{J}$  defined in subsection 6.1. We compute the CGF defined by (4.2) with respect to the baseline model  $q_\Delta$  (the computation is given in (E.3)):

$$(6.13) \quad \Lambda_{q_\Delta; |\Delta| m(\sigma_\Delta)}(\pm \lambda) = \beta |\Delta| \left( P_{h \pm \frac{\lambda}{\beta}, \beta, \mathbf{J}}^\Delta(\bar{\sigma}_{\Delta^c}) - P_{h, \beta, \mathbf{J}}^\Delta(\bar{\sigma}_{\Delta^c}) \right),$$

where  $P_{h, \beta, \mathbf{J}}^\Delta$  stands for the thermodynamic pressure [57], defined as

$$P_{h, \beta, \mathbf{J}}^\Delta(\bar{\sigma}_{\Delta^c}) := \frac{Z(\mathbf{J}, \beta, h, \bar{\sigma}_{\Delta^c})}{\beta |\Delta|}.$$

**6.2.5. KL divergence.** Here we utilize Lemma 3.4 and specify the KL divergence in terms of  $\kappa_i$  and  $\Phi_u$  as involved in (3.12) when the alternative models are Ising models with a perturbed interaction  $\tilde{\mathbf{J}}^F$  defined in subsection 6.2.1. Then we bound it by using Lemma 6.3. Before that, we use a well-established tool in statistical mechanics referred to as norm- $\|\cdot\|_1$  [62] to alternatively bound the KL divergence. After all, we conclude that our UQ approach gives a narrower area (i.e., the area between the upper and lower UQ bound) provided by Theorem 4.1 and thus has less uncertainty; see Figure 6.

Norm- $\|\cdot\|_1$ : Let  $\Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}}(\sigma_X)$  be the following quantity:

$$(6.14) \quad \Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}}(\sigma_X) = \begin{cases} -\frac{1}{2}\beta J(x, y)\sigma_{\Delta}(x)\sigma_{\Delta}(y), & X = \{x, y\}, x \neq y, \\ -\beta\sigma_{\Delta}(x)(h + \sum_{y \in B_{x,R}^{\neq} \cap \Delta^c} J(x, y)\bar{\sigma}_{\Delta^c}(y)), & X = \{x\}, \\ 0 & \text{otherwise,} \end{cases}$$

and similarly we define  $\Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{\tilde{h}, \beta, \tilde{\mathbf{J}}^F}(\sigma_X)$ . Then

$$(6.15) \quad \beta H^{\mathbf{J}, h}(\sigma_{\Delta} | \bar{\sigma}_{\Delta^c}) = \sum_{X: X \cap \Delta \neq \emptyset} \Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}}(\sigma_X).$$

Also,  $\beta H^{\tilde{\mathbf{J}}^F, \tilde{h}}(\sigma_{\Delta} | \bar{\sigma}_{\Delta^c})$  is defined similarly. Then the norm- $\|\cdot\|_1$  of  $\Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}} - \Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{\tilde{h}, \beta, \tilde{\mathbf{J}}^F}$  is defined as

$$(6.16) \quad \|\Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}} - \Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{\tilde{h}, \beta, \tilde{\mathbf{J}}^F}\|_1 = \sum_{0 \ni X} \|\Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}} - \Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{\tilde{h}, \beta, \tilde{\mathbf{J}}^F}\|_{\infty},$$

where  $\|\Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}} - \Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{\tilde{h}, \beta, \tilde{\mathbf{J}}^F}\|_{\infty} = \sup_{\sigma_X} |\Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}}(\sigma_X) - \Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{\tilde{h}, \beta, \tilde{\mathbf{J}}^F}(\sigma_X)|$  for  $X \subset \mathbb{Z}^d$ .

**Lemma 6.2.** Let  $F$  be an interaction satisfying (6.1)–(6.3) with support given by (6.9) or (6.10); then

$$R(\tilde{q}_{\Delta} \| q_{\Delta}) \leq 2|\Delta| \|\Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}} - \Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{\tilde{h}, \beta, \tilde{\mathbf{J}}^F}\|_1 \leq 2\beta|\Delta| \left( |\tilde{h} - h| + \sum_{x \neq 0} |F(0, x)| \right).$$

*Proof.* See Appendix E.1. ■

Let us turn to our approach developed in section 4. We recall the total  $\tilde{q}_{\Delta}$ -excess factor relative to  $q_{\Delta}$  from subsection 6.2.2 as well as the quantities from section 4.1, and we express  $\log \Phi_{\bar{\sigma}_{\Delta^c}}^i(\sigma_{\Delta}) = C_I |\Delta| m(\sigma_{\Delta}) + \kappa_I(\sigma_{\Delta})$ , with

$$(6.17) \quad C_I = \beta(\tilde{h} - h) < 1, \quad \kappa_I(\sigma_{\Delta}) = \beta \sum_{x \in \Delta} \sigma_{\Delta}(x) \left( \frac{1}{2} \sum_{y \in A_x^i \cap \Delta} F(x, y) \sigma_{\Delta}(y) \right) + \beta F(\Delta | \bar{\sigma}_{\Delta^c}),$$

where  $F(\Delta | \bar{\sigma}_{\Delta^c}) = \sum_{x \in \Delta} \sum_{y \in A_x^i \cap \Delta^c} F(x, y) \bar{\sigma}_{\Delta^c}(y)$ . We bound  $\kappa_I(\sigma_{\Delta})$  as

$$(6.18) \quad 0 \leq \kappa_I(\sigma_{\Delta}) \leq \beta|\Delta| \left( \frac{1}{2} + 2R \frac{|\partial \Delta|}{|\Delta|} \right) \sum_{x \neq 0} |F(x, y)|,$$

where we use the next lemma.

**Lemma 6.3.** Let  $L$  and  $\partial\Delta$  be the side and the boundary of the hypercube  $\Delta$ , respectively, with  $L \gg R_F$ . Then, for any interaction  $\mathbf{F} = \{F(x, y) : x, y \in \mathbb{Z}^d\}$  satisfying (6.1)–(6.3) and range  $R_F$ , the following hold:

(i) If the support of  $F$  is given by (6.9), then

$$\sum_{x \in \Delta} \sum_{\substack{y \in \Delta^c \\ y \in B_{x, R_F}^{\neq}}} F(x, y) \leq R_F |\partial\Delta| \sum_{x \neq 0} |F(0, x)|.$$

(ii) If the support of  $F$  is given by (6.10), then

$$\sum_{x \in \Delta} \sum_{y \in \Delta^c} F(x, y) \leq R_F |\Delta| \sum_{x \neq 0} |F(0, x)|.$$

*Proof.* The bounds are straightforward once we split the sum as follows:

$$\sum_{x \in \Delta} \sum_{\substack{y \in \Delta^c \\ y \in B_{x, R_F}^{\neq}}} F(x, y) = \sum_{\substack{x \in \Delta \\ \text{dist}(x, \Delta^c) \leq R_F}} \sum_{\substack{y \in \Delta^c \\ y \in B_{x, R_F}^{\neq}}} F(x, y) + \sum_{\substack{x \in \Delta \\ \text{dist}(x, \Delta^c) > R_F}} \sum_{y \in \Delta^c} F(x, y) \leq R_F |\Delta|,$$

where  $\text{dist}(x, \Delta^c) = \inf\{\|x - y\| : y \in \Delta^c\}$ . Note that when  $L \ll R_F$ , both (i) and (ii) are bounded by  $R_F |\Delta| \sum_{x \neq 0} |F(0, x)|$ . ■

**6.3. UQ for finite-size effects and boundary conditions.** Having computed all the ingredients needed for the analysis of subsections 3.2, 4.1, and 4.2 under the above statistical mechanics formulation through rMRFs, we capture the behavior of  $m(\sigma_\Delta)$  given in (6.12) with respect to the perturbed model  $\tilde{q}_\Delta$ . The analysis from now on refers to models of Type I. Although Type II models can be worked on similarly, one example of Type II is discussed in Appendix F. To get the UQ bounds for  $E_{\tilde{q}_\Delta}[m(\sigma_\Delta)]$ , for  $f(\mathbf{Z}) = |\Delta| m(\sigma_\Delta)$  we can either apply (4.1) using the crude bound in Lemma 6.2,

$$(6.19) \quad \pm E_{\tilde{q}_\Delta}[m(\sigma_\Delta)] \leq \inf_{\lambda > 0} \left\{ \frac{P_{h \pm \frac{\lambda}{\beta}, \beta, \mathbf{J}}^\Delta - P_{h, \beta, \mathbf{J}}^\Delta}{\lambda/\beta} + 2 \frac{\beta}{\lambda} (|\tilde{h} - h| + \mathcal{F}) \right\},$$

or Theorem 4.1:

$$(6.20) \quad \pm E_{\tilde{q}_\Delta}[m(\sigma_\Delta)] \leq \frac{1}{1 - \beta(\tilde{h} - h)} \inf_{\lambda > 0} \left\{ \frac{P_{h \pm \frac{\lambda}{\beta}, \beta, \mathbf{J}}^\Delta - P_{h, \beta, \mathbf{J}}^\Delta}{\lambda/\beta} + \frac{\beta}{\lambda} \mathcal{F} \left( 1 + R_F \frac{|\partial\Delta|}{|\Delta|} \right) \right\},$$

with  $\partial\Delta$  being the boundary of the hypercube  $\Delta$  and  $\mathcal{F} := \sum_{x \neq 0} |F(0, x)|$ , which is bounded due to the property (6.3) and  $R_F = R$ .

Furthermore, inequality (6.20) implies a new UQ formula for systems with a fixed configuration outside of the domain that here is considered as a Dirichlet-type boundary condition. In particular, it allows us to quantify the effect of the boundary conditions on  $\partial\Delta$  on the QoIs, as can be seen more clearly when  $\tilde{h} = h$ . Note that the term  $\frac{|\partial\Delta|}{|\Delta|}$  in (6.20) comes from a more careful bound on the KL divergence using Lemma 6.3, while this term has been eliminated in (6.19) due to the relative crudeness of the bound of KL in Lemma 6.2; see also Figure 6.

**6.4. UQ for phase diagrams.** Here we capture the phase diagram of the perturbed model  $\tilde{q}_\Delta$  looking at the magnetization defined in subsection 6.2.3. We study the limit of the bounds obtained in subsection 6.3. The high dimensionality of statistical mechanics models requires *scalable bounds* at the thermodynamic limit. In fact, the MGF and the KL divergence scale correctly with the size of the system  $|\Delta|$  (all are multiplied by  $|\Delta|$ ; see (6.13), Lemma 6.2, and (6.18)). Let  $M(\tilde{\mathbf{J}}^F, \tilde{\beta}, \tilde{h})$  be the limit as  $\Delta \nearrow \mathbb{Z}^d$  of  $E_{\tilde{q}_\Delta}[m(\sigma_\Delta)]$ . Then the limit  $\Delta \nearrow \mathbb{Z}^d$  of (6.20) is

$$(6.21) \quad \pm M(\tilde{\mathbf{J}}^F, \beta, \tilde{h}) \leq \frac{1}{1 - \beta(\tilde{h} - h)} \inf_{\lambda > 0} \left\{ \frac{(P_{h \pm \frac{\lambda}{\beta}, \beta, \mathbf{J}} - P_{h, \beta, \mathbf{J}})}{\lambda/\beta} + \frac{\beta}{\lambda} \mathcal{F} \right\},$$

with  $\lim_{\Delta \nearrow \mathbb{Z}^d} P_{h, \beta, \mathbf{J}}^\Delta = P_{h, \beta, \mathbf{J}}$  by Theorem 2.3.3.1 in [57] and  $\lim_{\Delta \nearrow \mathbb{Z}^d} \frac{|\partial \Delta|}{|\Delta|} = 0$ , while in the limit of (6.19) the thermodynamic pressure is only replaced by its limit  $P_{h, \beta, \mathbf{J}}$ . The bounds for the  $\tilde{\beta} \neq \beta$  can be adjusted similarly.

**6.5. Ising–Kac model.** Here we consider an Ising-spin model with a Kac-type interaction as a baseline model. Such a model combines sufficient complexity since it is not a mean field model –but is still analytically fairly tractable to serve as a good benchmark problem for a high-dimensional rMRF. We illustrate the uncertainty area of the phase diagram for both (6.21) and the limit of (6.19) when the alternative models are a Kac perturbation and a truncated Kac interaction.

An Ising-spin model with a Kac-type interaction behaves like a mean field (or Van der Waals model in a gas lattice) in the limit with the convexity of free energy emerging naturally in the limit, contrary to mean field or Curie–Weiss models where Maxwell’s equal area law is required to refine the nonconvex free energy (double well shape) [57]. Such a discrepancy comes from the fact that each spin interacts with all particles in the same way and independently. The idea of Kac was to keep such a picture on large regions but relatively small compared to the range of interaction. Then the thermodynamic incorrectness of the free energy (i.e., the nonconvex free energy) on these large regions looks refined at the scale of interaction. Therefore, the system contains a two-scale behavior that was carried out by introducing a small parameter  $\gamma > 0$  known as *Kac scaling*. As we suppose that an Ising-spin model is endowed by such an interaction, the model overall has three scales: the lattice spacing is 1, the range of interaction is  $\gamma^{-1}$ , and the size of the system is much larger than  $\gamma^{-1}$ , and all are well-separated, contrary to the mean field model where the range of interaction is the same as the size of the system. Next, we formally introduce the model.

**6.6. Mathematical background of Ising–Kac model.** A Kac-type interaction is defined as

$$(6.22) \quad J_\gamma(x, y) = \gamma^d J(\gamma x, \gamma y), \quad x, y \in \mathbb{Z}^d,$$

where  $\gamma$  is a positive parameter sufficiently small and  $J$  is a nonnegative (ferromagnetic interaction), even, symmetric function (i.e.,  $J(r, r') = J(r', r)$  for every  $r, r' \in \mathbb{R}^d$ ) and a translational invariant (i.e.,  $J(r, r') = J(r' + a, r + a)$  for every  $r, r' \in \mathbb{R}^d$  and  $a \in \mathbb{R}^d$ ) function such that  $J(r) = 0$  for all  $|r| > 1$ ,  $\int_{\mathbb{R}^d} J(r) dr = \mathcal{J}$ , and  $J \in C^2(\mathbb{R}^d)$ . The use of  $\mathbf{J}_\gamma$  stands



for the collection of  $J_\gamma(x, y)$ , that is,  $\mathbf{J}_\gamma = \{J_\gamma(x, y)\}_{\mathbb{Z}^d \times \mathbb{Z}^d}$ . As  $\gamma$  becomes smaller, more particles are included in a spin neighborhood with  $\gamma^{-1}$  diameter and while the strength of the interactions becomes weaker.

Let  $\Delta$  be a bounded,  $\mathcal{P}_{\mathbb{R}^d}^{(l)}$ -measurable region, with  $L \gg \gamma^{-1}$  (see Appendix C.1),  $\beta > 0$  be the inverse temperature,  $h \in \mathbb{R}$  be the external magnetic field, and  $\bar{\sigma}_{\Delta^c}$  be a given configuration on its complement (see Figure 5 with  $R = \gamma^{-1}$ ).

**Hamiltonian energy.** The Hamiltonian energy of a spin configuration  $\sigma_\Delta$  given  $\bar{\sigma}_{\Delta^c}$  is

$$(6.23) \quad \begin{aligned} H_\gamma^{\mathbf{J}, h}(\sigma_\Delta \mid \bar{\sigma}_{\Delta^c}) = & -\frac{1}{2} \sum_{x \neq y \in \Delta} J_\gamma(x, y) \sigma_\Delta(x) \sigma_\Delta(y) - \sum_{\substack{x \in \Delta, \\ y \in \Delta^c}} J_\gamma(x, y) \sigma_\Delta(x) \bar{\sigma}_{\Delta^c}(y) \\ & - h \sum_{x \in \Delta} \sigma_\Delta(x) \quad (\text{Hamiltonian energy}). \end{aligned}$$

**Finite volume Gibbs measure.** The Gibbs measure given a fixed boundary condition  $\bar{\sigma}_{\Delta^c}$  is defined as follows:

$$(6.24) \quad \mu_{\mathbf{J}, \beta, h}^{\Delta, \gamma}(\cdot \mid \bar{\sigma}_{\Delta^c}) = \frac{1}{Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J}, \beta, h)} e^{-\beta H_\gamma^{\mathbf{J}, h}(\sigma_\Delta; \bar{\sigma}_{\Delta^c})} \quad (\text{finite volume Gibbs measure}),$$

where  $Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J}, \beta, h)$  is the normalization (partition function). To simplify the notation, we shall often drop  $\gamma$  and the given configuration in the complement of  $\Delta$  from the Gibbs measure, resuming the full notation when needed, and therefore we write  $\mu_{\beta, \Delta}^{J, h} \equiv \mu_{\beta, \Delta, \gamma}^{\bar{\sigma}_{\Delta^c}, J, h}$ .

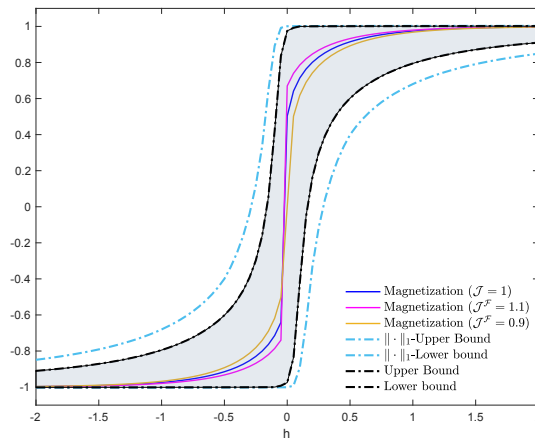
**Thermodynamic pressure.** The thermodynamic pressure for the Ising–Kac model denoted by  $P_{\mathbf{J}, \beta, h}^{\Delta, \gamma}$  is defined as

$$(6.25) \quad P_{\mathbf{J}, \beta, h}^{\Delta, \gamma}(\bar{\sigma}_{\Delta^c}) := \frac{\log Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J}, \beta, h)}{\beta |\Delta|}.$$

Its Lebowitz–Penrose (LP) limit (i.e.,  $\lim_{\gamma \rightarrow 0} \lim_{\Delta \nearrow \mathbb{Z}^d} p_{\mathbf{J}, \beta, h}$ ) is given by

$$(6.26) \quad p_{\mathbf{J}, \beta, h} := - \inf_{m \in [-1, 1]} \{-hm + \phi_{\mathbf{J}, \beta, 0}(m)\}, \quad \phi_{\mathbf{J}, \beta, h}(m) := \left\{ -\frac{\mathcal{J}}{2} m^2 - hm \right\} - \frac{1}{\beta} I(m)$$

(see also Appendix C.4 for further discussion). The rMRF formulation of such a model and its perturbations considered next is structured analogously to the ones in subsection 6.1.2, and for that reason we omit it.



**Figure 6.** The curves in blue, magenta, and dark yellow are the magnetizations of the Ising model with Kac interaction at inverse temperatures  $\beta = \tilde{\beta} = 1.1$ ,  $h = h$  and total strengths  $\mathcal{J} = 1$ ,  $\tilde{\mathcal{J}}^F = 1.1$  ( $a = 0.1$ ), and  $0.9$  ( $a = -0.1$ ) (validation), respectively. The black dashed-dot curves are the UQ upper and lower bounds provided by Corollary 6.5 and viewed as functions of  $h \in [-2, 2]$ . The grey area depicts the size of the uncertainty region. The light blue dashed-dot curves are the UQ upper and lower bounds obtained using norm- $\|\cdot\|_1$ . The uncertainty area of the phase diagram in grey is significantly better than the uncertainty area between the light blue dashed-dot curves. This comes from the fact that the difference between the limit of (6.19) and (6.21) lies on the term  $\frac{\beta}{\lambda}\mathcal{F}$  which is multiplied by 2.

**6.6.1. Phase diagram of perturbed Kac model.** Let us define a perturbation of a Kac potential.

**Definition 6.4.** Let  $F_\gamma$  be an even function satisfying (6.1)–(6.3) and (6.22) with length of range  $\gamma^{-1}$  and  $\mathcal{F} := \int_{\mathbb{R}^d} F(r)dr$ . We define

$$(6.27) \quad \tilde{J}_\gamma^F(x, y) = J_\gamma(x, y) + F_\gamma(x, y), \text{ such that } \mathcal{F} = a\mathcal{J}, \quad a \in [-1, 1].$$

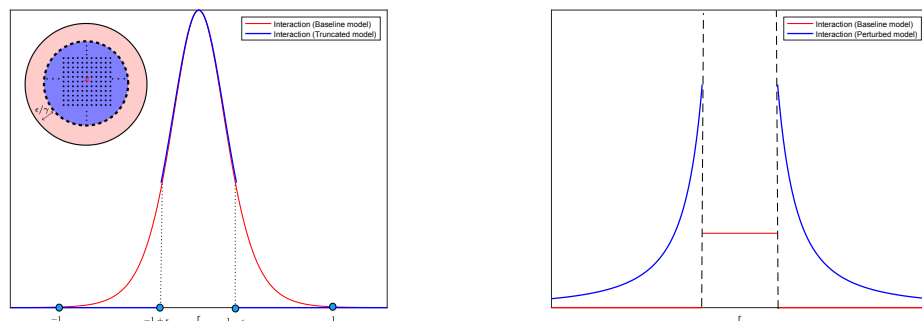
The parameter  $a$  represents the percentage of increase or decrease of the total strength of interaction  $\tilde{\mathcal{J}}^F := \int_{\mathbb{R}^d} \tilde{J}_\gamma^F(r)dr = (1 + a)\mathcal{J}$ .

**Corollary 6.5.** Let  $\tilde{J}^F$  be the interaction given in Definition 6.4. Then, for  $\gamma > 0$  small enough, the UQ bounds (6.19) and (6.20) hold for  $R_F = R = \gamma^{-1}$  and  $\mathcal{F} = |a|\mathcal{J}$ . The thermodynamic pressure  $P_{\mathbf{J}, \beta, h}^{\Delta, \gamma}$  is given in (6.25). Let  $M(\tilde{\mathbf{J}}^F, \beta, \tilde{h})$  be the LP limit of  $E_{\tilde{q}_\Delta}[m(\sigma_\Delta)]$ . Then the UQ bounds (6.21) and LP limit of (6.19) hold with the LP limit of  $P_{\mathbf{J}, \beta, h}^{\Delta, \gamma}$  being  $p_{\mathbf{J}, \beta, h}$  given in (6.26).

**Remark 6.6.** Inequality (6.19) represents crude bounds, as norm- $\|\cdot\|_1$  (subsection 6.2.5) has been used, while (6.20) obtained by Theorem 4.1 includes more details. The difference is illustrated in Figure 6. Furthermore, even if there is a  $\gamma^{-1}$  in the term  $2\gamma^{-1}\frac{|\partial\Delta|}{|\Delta|}$  in (6.19), the order of the LP limit makes it vanish as  $L \rightarrow \infty$ .

**Validation.** Given  $\beta$ ,  $h$ ,  $\mathcal{J}$ , and a tolerance  $\eta > 0$ , we can construct with the use of norm- $\|\cdot\|_1$  and Lemma 6.2 a class of models such that  $\mathcal{Q}_\eta^I := \{\tilde{q}_\Delta : 2\beta a\mathcal{J} \leq \eta\}$ . This is the

subclass of  $\mathcal{Q}^\eta$  defined in (1.1) with the KL divergence in place of  $d$ . In Figure 6,  $\beta = 1.1$  and  $\mathcal{J} = 1$ , while the external field  $h$  varies from  $-2$  and  $2$ . The positive parameter  $\eta = 0.1$  and the perturbed model with 10% decrease ( $a = -0.1$ ) of the total strength (magnetization in magenta) is in  $\mathcal{Q}_{0.1}^I$  as demonstrated in dark yellow.



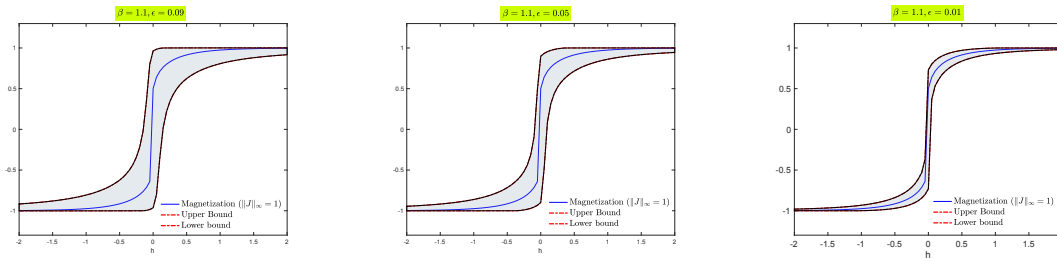
**Figure 7.** (Left) The red curve is a Kac interaction, and the blue curve is a truncation of it. The two curves coincide at all  $r$  with  $|r| \leq 1 - \epsilon$ . The embedded picture demonstrates the two interactions at the microscopic level. The red particle located at the site  $x \in \Delta \subset \mathbb{Z}^2$  interacts with the particles in the blue and the light red through  $J_\gamma$ . The particle interacts only with the particles in the blue area through  $\tilde{J}_\gamma^{-J}$  with range  $\gamma^{-1}(1 - \epsilon)$ . (Right) The red curve is an example of Kac interaction (piecewise constant) with  $J(r) = \mathbf{1}_{|r| \leq \frac{1}{2}}(r)$ , and the blue curve is a perturbation given by  $G(r) = \frac{a}{r^2} \mathbf{1}_{|r| > \frac{1}{2}}(r)$  for some  $a > 0$ .

**6.6.2. Phase diagram of truncated potential.** From a computational point of view, macroscopic properties of high-dimensional systems can be studied through simulation models where one can consider an appropriate truncated interaction which can reduce the computational overhead associated with the interaction [68, Chapter 3]. In our context, a truncated interaction can be thought of as follows: The support of the interaction  $J$  is  $[-1, 1]$  as in Figure 7.  $J$  is cut off at  $1 - \epsilon$  and  $-1 + \epsilon$  for some parameter  $\epsilon \in [-1, 1]$ . Then the resulting interaction is called the truncated interaction of  $J$  and its support is  $[-1 + \epsilon, 1 - \epsilon]$  of length  $2\epsilon$ . The introduced parameter  $\epsilon$  quantifies the impact of the truncation of the interaction  $J$ . Moreover, Figure 8 quantifies how the uncertainty area becomes smaller as  $\epsilon$  becomes smaller (and hence the truncated interaction tends to be the original  $J$ ). We mathematically define such an interaction as follows.

**Definition 6.7.** Let  $0 < \epsilon < 1$ . We define the truncated interaction as

$$(6.28) \quad \tilde{J}^{-J}(0, r) = \begin{cases} J(0, r), & |r| \leq 1 - \epsilon, \\ 0 & \text{otherwise.} \end{cases}$$

The truncated model can be viewed as Type II. However, to be consistent with the assumption  $\mathcal{E} \subset \tilde{\mathcal{E}}$  in Definition 3.1, we view it as perturbed interaction of Type I arising from the subtraction of  $J$  (also explains the notation  $\tilde{J}^{-J}$  in (6.28)) on regions of radius greater than  $1 - \epsilon$  as illustrated in Figure 7.



**Figure 8.** The three graphs demonstrate the uncertainty area in grey for different values of  $\epsilon$ . In all graphs, the blue solid line is the magnetization of the d-sing model with Kac interaction at inverse temperatures  $\beta = 1.1$ ,  $\|J\|_\infty = 1$ , and  $\tilde{h} = h$ . The black dashed-dot curves are the upper and lower bounds of magnetization of the truncated interaction  $\tilde{J}^{-J}$ , viewed as functions of  $h$ . (Left)  $\epsilon = 0.09$ . (Center)  $\epsilon = 0.05$ . (Right)  $\epsilon = 0.01$ .

**Corollary 6.8.** Let  $\tilde{J}^{-J}$  be the interaction given in Definition 6.7. Then, for  $0 < \epsilon < 1$  and  $\gamma > 0$  small enough, the UQ bounds (6.19) and (6.20) hold for  $R_{-J} = \gamma^{-1}$  and  $\mathcal{F} \leq \epsilon \|J\|_\infty$ . The thermodynamic pressure  $P_{\mathbf{J},\beta,h}^{\Delta,\gamma}$  is given in (6.25). Let  $M(\tilde{\mathbf{J}}^F, \beta, \tilde{h})$  be the LP limit of  $E_{\tilde{q}_\Delta}[m(\sigma_\Delta)]$ . Then the UQ bounds (6.21) and LP limit of (6.19) hold with the limit of  $P_{\mathbf{J},\beta,h}^{\Delta,\gamma}$  being  $p_{\mathbf{J},\beta,h}$  given by (6.26).

**Remark 6.9.** Given  $\beta, \|J\|_\infty$ , we can choose  $\epsilon \equiv \epsilon(\beta, \|J\|_\infty)$  sufficiently small. Consequently, the phase diagrams of the two models are close to each other, as the uncertainty area is very small (Figure 8). The parameter  $\epsilon$  quantifies the length of the area that one cuts off the initial interaction.

The same methods are applicable to other perturbations, e.g., the very long range in Appendix F and perturbations in “contexts”/configuration as boundary conditions.

**Conclusion and future work.** In this article, we developed an information-based UQ method for MRs/rMRFs. We considered a surrogate (baseline) MRF/rMRF constructed by physical modeling or by learning structure and parameters from data, and we quantified uncertainties inherited from data, modeling choices, or numerical approximations that are also propagated in predictions for QoIs. Our UQ method quantifies uncertainties not only in parameters but also in structures as well as is capable in handling the inherent high dimensionality of systems that admit an MRF/rMRF formulation. This was achieved by obtaining tight and scalable, information-based bounds on the predictions for QoIs.

We demonstrated our UQ method in an example from medical diagnostics as well as several high-dimensional equilibrium statistical mechanics models defined on bounded domains with suitable boundary conditions. We aim to extend the developed approach to nonequilibrium statistical mechanics systems [58] also arising in ML [3]. Furthermore, motivated by [30] we plan to develop robust UQ for Bayesian networks defined on directed acyclical graphs.

**Appendix A. Reduced Markov random fields (rMRFs).** Let  $\mathbf{Y} = \{Y_i\}_{i \in \mathcal{V}}$  be an MRF indexed by a set of nodes  $\mathcal{V}$  (finite or infinite) of a graph  $\mathcal{G}$ . Let us consider  $\mathcal{M} \subset \mathcal{V}$ . Let also  $\mathbf{U} = \{Y_i\}_{i \in \mathcal{M}}$ , and let  $\mathbf{u}$  be an assignment to them, namely  $\mathbf{U} = \mathbf{u}$ . If  $\mathbf{Z} := \{Y_i\}_{i \in \mathcal{V} \setminus \mathcal{M}}$ , what does the underlying graph corresponding to  $\mathbf{Z} \mid \mathbf{U} = \mathbf{u}$  look like? Can the conditional probability  $p(\mathbf{z} \mid \mathbf{U} = \mathbf{u})$  still keep a product structure/factorization as the joint distribution

given in (2.1)? To answer the questions, we need a special class of MRFs which are called *reduced Markov random fields* (rMRFs).

**Definition A.1.** Let  $\mathbf{Y} = \{Y_i\}_{i \in \mathcal{V}}$  be a collection of random variables indexed by a set of nodes  $\mathcal{V}$  (finite or infinite) of a graph  $\mathcal{G}$ . If  $(\mathbf{Y}, p)$  is an MRF,  $\mathbf{u}$  a context,  $\mathcal{M} \subset \mathcal{V}$ , and  $\mathbf{U} = \{Y_i\}_{i \in \mathcal{M}}$ , we define as an rMRF an MRF  $\mathbf{Z} = \{Y_i\}_{i \in \mathcal{V} \setminus \mathcal{M}}$  indexed by the set of nodes  $\mathcal{V} \setminus \mathcal{M}$  of the subgraph  $\mathcal{G}[\mathcal{V} \setminus \mathcal{M}]$  with joint distribution  $\mathbb{Q}$  such that

$$(A.1) \quad q(\mathbf{z}) \equiv \mathbb{Q}(\mathbf{Z} = \mathbf{z}) := p(\mathbf{z} \mid \mathbf{U} = \mathbf{u}).$$

Therefore,  $\mathbf{Z} \mid \mathbf{U} = \mathbf{u}$  could be thought as an induced subgraph of  $\mathcal{G}$  with set of nodes  $\mathcal{V} \setminus \mathcal{M}$ , that is, eliminating any node corresponding to random variables  $\mathbf{U}$  and any edge adjacent to them. Furthermore, according to Definition A.1,  $\mathbf{Z}$  is clearly an MRF and therefore the conditional probability  $p(\mathbf{z} \mid \mathbf{U} = \mathbf{u})$  is expected to have a product structure. All of the above are summarized in the following proposition.

**Proposition A.2.** Let  $\mathbf{Y}$  be an MRF with probability distribution  $p > 0$  parametrized by some parameters  $\mathbf{w} = \{\mathbf{w}_c\}_{c \in \mathcal{C}_\mathcal{G}}$  given in (2.1), and let  $\mathbf{U}, \mathbf{Z}$  be defined in the beginning of the subsection. Then  $q$  parametrized by  $\mathbf{w}$  is expressed as

$$(A.2) \quad q^{\mathbf{w}}(\mathbf{z}) \equiv p(\mathbf{z} \mid \mathbf{U} = \mathbf{u}, \mathbf{w}) = \frac{1}{Z_{\mathbf{u}}(\mathbf{w})} \prod_{c \in \mathcal{C}_\mathcal{G}} \Psi_c[\mathbf{u}](\mathbf{z}_c \mid \mathbf{w}_c),$$

where for every  $c \in \mathcal{C}_\mathcal{G}$

$$(A.3) \quad \Psi_c[\mathbf{u}](\mathbf{z}_c \mid \mathbf{w}_c) := \Psi_c(\mathbf{z}_c, \mathbf{u}_c \mid \mathbf{w}_c).$$

Moreover,  $Z_{\mathbf{u}}(\mathbf{w})$  is given by

$$(A.4) \quad Z_{\mathbf{u}}(\mathbf{w}) = \sum_{\mathbf{Y}} \prod_{c \in \mathcal{C}_\mathcal{G}} \Psi_c[\mathbf{u}](\mathbf{z}_c \mid \mathbf{w}_c).$$

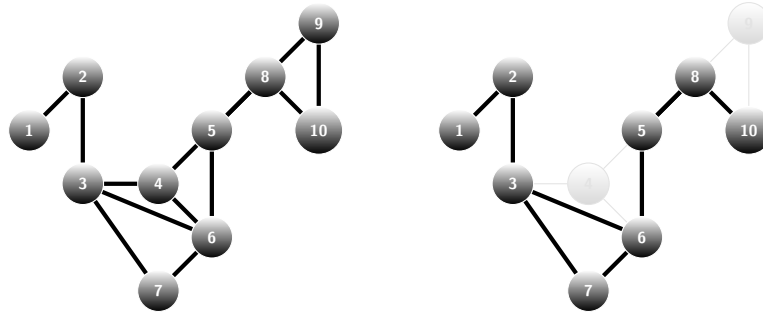
We refer the reader to [49, 55] for further discussion about MRFs, rMRFs, and the proofs of the Hammersley–Clifford theorem and Proposition A.2.

**A.1. Partition of the class of maximal cliques.** We further investigate the structure of the class of all maximal cliques. Precisely, we collect  $c \in \mathcal{C}_\mathcal{G}$  such that  $\mathbf{U} \cap \mathbf{Y}_c \neq \emptyset$ . This leads to a partition of the set of maximal cliques  $\mathcal{C}_\mathcal{G} = \mathcal{C}_{\mathbf{U}} \sqcup \mathcal{C}_\emptyset$ , with

$$(A.5) \quad \mathcal{C}_{\mathbf{U}} = \{c : \mathbf{U} \cap \mathbf{Y}_c \neq \emptyset\} \quad \text{and} \quad \mathcal{C}_\emptyset = \{c : \mathbf{U} \cap \mathbf{Y}_c = \emptyset\}$$

(see the example shown in Figure 9). On top of that, the partition of  $\mathcal{C}_\mathcal{G}$  makes the joint distributions  $q$  take the form

$$(A.6) \quad q(\mathbf{z}) = P_{\Psi}^{\mathbf{w}}[\mathbf{u}](\mathbf{z}) = \frac{1}{Z_{\mathbf{u}}(\mathbf{w})} \prod_{c \in \mathcal{C}_\emptyset} \Psi_c(\mathbf{y}_c \mid \mathbf{w}_c) \prod_{c \in \mathcal{C}_{\mathbf{U}}} \Psi_c[\mathbf{u}](\mathbf{z}_c \mid \mathbf{w}_c).$$



**Figure 9.** The set of nodes is  $\mathcal{V} = \{1, \dots, 10\}$  and  $\mathcal{M} = \{4, 9\}$ . Left:  $\mathbf{Y} = \{Y_i\}_{i=1}^{10}$  with joint distribution  $p$  is an MRF over  $\mathcal{G}$ . The set of maximal cliques is given by  $\mathcal{C}_{\mathcal{G}} = \{\{1, 2\}, \{2, 3\}, \{3, 4, 6\}, \{3, 6, 7\}, \{4, 5, 6\}, \{5, 8\}, \{8, 9, 10\}\}$ . Right:  $\mathbf{Z} = \{Y_i\}_{i \in \mathcal{V} \setminus \mathcal{M}}$  with joint distribution  $q$  is the corresponding rMRF over  $\mathcal{G}'$  with  $\mathbf{U} = \{Y_4, Y_9\}$  and  $\mathbf{u} = \{u_4, u_9\}$ . The rMRF is demonstrated by removing nodes 4 and 9 (faded nodes) from the graph  $\mathcal{G}$ .  $\mathcal{C}_{\mathbf{U}} = \{\{3, 4, 6, 7\}, \{4, 5, 6\}, \{8, 9, 10\}\}$ , while  $\mathcal{C}_{\emptyset} = \{\{1, 2\}, \{2, 3\}, \{5, 8\}\}$ .

## Appendix B. Proofs of the main results.

**B.1. Proof of Lemma 3.2.** In the following computation, we use either (3.2) for Type I or (3.6) for Type II:

$$\begin{aligned}
 \tilde{Z}_{\mathbf{u}}(\tilde{\mathbf{w}}) &= \sum_{\mathbf{z}} \prod_{\tilde{c}} \tilde{\Psi}_{\tilde{c}}[\mathbf{u}](\mathbf{z}_{\tilde{c}} \mid \tilde{\mathbf{w}}_{\tilde{c}}) \\
 &= \sum_{\mathbf{z}} \prod_c \Psi_c[\mathbf{u}](\mathbf{z}_c \mid \mathbf{w}_c) \Phi_{\mathbf{u}}^i(\mathbf{z}) \\
 &= \sum_{\mathbf{z}} \Phi_{\mathbf{u}}^i(\mathbf{z}) \prod_c \Psi_c[\mathbf{u}](\mathbf{z}_c \mid \mathbf{w}_c) \\
 &= Z_{\mathbf{u}}(\mathbf{w}) \sum_{\mathbf{z}} \Phi_{\mathbf{u}}^i(\mathbf{z}) \prod_c \Psi_c[\mathbf{u}](\mathbf{z}_c \mid \mathbf{w}_c) \frac{1}{Z_{\mathbf{u}}(\mathbf{w})} \\
 &= Z_{\mathbf{u}}(\mathbf{w}) E_q[\Phi_{\mathbf{u}}^i(\mathbf{z})].
 \end{aligned}$$

**B.2. Proof of Theorem 4.1.** This is mostly based on the proof of the characterization of the exponential integrals (see, e.g., [22]). Let the probability measure  $R$  be defined by

$$dR/dq = e^{f(\mathbf{Z})}/E_q[f(\mathbf{Z})].$$

Note that  $\mathcal{R}(\tilde{q}||q) < \infty$  since  $q, \tilde{q} > 0$ . Thus,

$$(B.1) \quad -\mathcal{R}(\tilde{q}||q) + E_{\tilde{q}}[f(\mathbf{Z})] = -\mathcal{R}(\tilde{q}||R) + \log E_q[e^{f(\mathbf{Z})}] \leq \log E_q[e^{f(\mathbf{Z})}],$$

where for the last inequality we use that  $\mathcal{R}(\tilde{q}||R) \geq 0$  and  $\mathcal{R}(\tilde{q}||R) = 0$  if and only if  $\tilde{q} = R$  [22, Lemma 1.4.1]. For part (a), we combine (3.11) of Lemma 3.4 and (B.1) and get

$$E_{\tilde{q}}[f(\mathbf{Z})] \leq \log E_q[e^{f(\mathbf{Z})}] + \frac{1}{E_q[\Phi_{\mathbf{u}}^i]} E_q[\Phi_{\mathbf{u}}^i \log \Phi_{\mathbf{u}}^i] - \log E_q[\Phi_{\mathbf{u}}^i].$$



By replacing  $f(\mathbf{Z})$  to  $\pm\lambda f(\mathbf{Z})$ , we obtain

$$\pm E_{\tilde{q}}[f(\mathbf{Z})] \leq \frac{1}{\lambda} \left\{ \log E_q[e^{\pm\lambda f(\mathbf{Z})}] + \frac{1}{E_q[\Phi_{\mathbf{u}}^i]} E_q[\Phi_{\mathbf{u}}^i \log \Phi_{\mathbf{u}}^i] - \log E_q[\Phi_{\mathbf{u}}^i] \right\}.$$

By optimizing over  $\lambda > 0$  (see [15, 53]), the following tight estimates are obtained:

$$\pm E_{\tilde{q}}[f(\mathbf{Z})] \leq \inf_{\lambda > 0} \frac{1}{\lambda} \left\{ \log E_q[e^{\pm\lambda f(\mathbf{Z})}] + \frac{1}{E_q[\Phi_{\mathbf{u}}^i]} E_q[\Phi_{\mathbf{u}}^i \log \Phi_{\mathbf{u}}^i] - \log E_q[\Phi_{\mathbf{u}}^i] \right\}.$$

Part (b) is proved similarly, utilizing (3.12) instead of (3.11).

**Example B.1 (single-parameter exponential families).** This is a straightforward example and a simple illustration of the ideas in the proof of part (b) of Theorem 4.1, giving us insights into how well the ideas work together with a *rearranging argument*. The simplicity of this example arises from the fact that the exponential family is single parametric, and therefore the structural part is not present. The probability density function of a random variable  $X$ , with range  $R(X)$ , is given by

$$p^\theta(x) = P^\theta(X = x) = e^{\theta\phi(x) - F(\theta)}$$

taken with respect to some measure  $d\nu$  where  $F(\theta) = \log \int_x e^{\theta\phi(x)} \nu(dx)$  and  $\phi(x)$  is a real-valued function also known as a sufficient statistic. Suppose a second probability density function of the same single-parameter exponential family associated with  $\phi$ :

$$p^{\theta+\zeta}(x) = P^{\theta+\zeta}(X = x) = e^{(\theta+\zeta)\phi(x) - F(\theta+\zeta)}$$

for some  $\zeta < 1$ . One may want to investigate how sensitive the model is to such a change in  $\theta$  by  $\zeta$  with respect to  $\phi(X)$  as a means to bound  $E_{P^{\theta+\zeta}}[\phi(X)]$  or to find the error in replacing the first distribution by the “perturbed” one and being phrased as bound  $E_{P^{\theta+\zeta}}[\phi(X)] - E_{P^\theta}[\phi(X)]$ . The second exponential family is apparently a perturbation on parameters by  $\zeta$ , so we can think of the model as Type I. In addition, after employing UQ bounds, the CGF and KL divergence are the two main ingredients to compute: for any  $\lambda > 0$ ,

$$\begin{aligned} \Lambda_{P^\theta}^\phi(\lambda) &= \log E_{P^\theta}[e^{\lambda\phi(X)}] = F(\theta + \lambda) - F(\theta), \\ R(P^{\theta+\zeta} \| P^\theta) &= \zeta E_{P^{\theta+\zeta}}[\phi(X)] - \log E_{P^\theta}[e^{\zeta\phi(X)}]. \end{aligned}$$

The above expression for KL divergence comes from the calculation of expressing  $F(\theta + \lambda)$  in terms of  $F(\theta)$  and that every term is computed with respect to  $P^\theta$ . By substituting the quantities to the UQ bounds and by doing a delicate rearrangement of terms that is feasible because the QoI is a sufficient statistic for the model, we get

$$\pm E_{P^{\theta+\zeta}}[\phi(X)] \leq \frac{1}{1-\zeta} \inf_{\lambda > 0} \left\{ \frac{F(\theta + \lambda) - F(\theta)}{\lambda} + \frac{1}{\lambda} \log E_{P^\theta}[e^{\zeta\phi(X)}] \right\}.$$

**B.3. Proof of Theorem 4.2.** The existence and the explicit form of the distribution  $q^\pm$  relies on [39, Theorem 2]. Consequently, given a QoI  $f$ , we identify the total  $\tilde{q}$ -excess factor relative to  $q$  explicitly, that is,  $\Phi_u^\pm = e^{\lambda_\pm f}$ . However, the new element is that by utilizing the Hammersley–Clifford theorem,  $q^\pm$  defined on  $\mathbf{Z}$  are rMRFs, they lie in the class  $\mathcal{Q}_P^\eta$ , and the total  $\tilde{q}$ -excess factor relative to  $q$  is explicitly determined.

### Appendix C. Coarse-graining, Kac, and Hamiltonian estimates.



**Figure 10.** One-dimensional Ising-spin lattice on  $\Delta$  (white spins) with configuration boundary conditions on the complement of  $\Delta$  denoted as  $\bar{\sigma}_{\Delta^c}$  (black spins).

**C.1. Coarse-graining.** We divide  $\mathbb{R}^d$  into cubes of size  $l = \gamma^{-1/2}$ . We denote by  $\mathcal{P}_{\mathbb{R}^d}^{(l)}$  the partition of  $\mathbb{R}^d$ . Namely, for every  $i \in l\mathbb{Z}^d$  we set

$$(C.1) \quad I_{\gamma,i} = \{r \in \mathbb{R}^d : i_k \leq r_k \leq i_k + l, k = 1, \dots, d\}$$

( $r_k$  and  $i_k$  being the  $k$ th coordinates of  $r$  and  $i$ ). Then we call

$$(C.2) \quad \mathcal{P}_{\mathbb{R}^d}^{(l)} = \{I_{\gamma,i} : i \in l\mathbb{Z}^d\}$$

the collection of all the above cubes.

**Definition C.1** (see [57]). (1) A function  $f(r)$  is  $\mathcal{P}_{\mathbb{R}^d}^{(l)}$ -measurable if it is constant in each cube  $I_{\gamma,i}$ ,  $i \in l\mathbb{Z}^d$ .

(2) A region  $\Delta \subset \mathbb{R}^d$  is  $\mathcal{P}_{\mathbb{R}^d}^{(l)}$ -measurable if it can be written as a union of cubes of  $\mathcal{P}_{\mathbb{R}^d}^{(l)}$  (or its characteristic is  $\mathcal{P}_{\mathbb{R}^d}^{(l)}$ -measurable).

(3) Any  $\Delta \subset \mathbb{Z}^d$  can be identified as a union of cubes with length 1.

(4) The size of each cube is given by

$$(C.3) \quad |I_{\gamma,i}| = |I| = l^d = \gamma^{-d/2}$$

for every  $i \in l\mathbb{Z}^d$ . For notational simplicity, we drop  $\gamma$  from  $I_{\gamma,i}$ .

For any bounded region  $\Delta$   $\mathcal{P}_{\mathbb{R}^d}^{(l)}$ -measurable, we denote  $\mathbf{\Delta} := \Delta \cap \mathbb{Z}^d$ . Hence,  $\mathbf{I}_i = I_i \cap \mathbb{Z}^d$ .

**C.2. Coarse-grained interaction.** We introduce a new interaction  $\bar{J}_\gamma$  which describes the interaction between cubes. More precisely, for every  $i, j \in l\mathbb{Z}^d$  with  $i \neq j$ , we consider

$$(C.4) \quad \bar{J}_\gamma(i, j) = \frac{1}{|I|^2} \sum_{x \in \mathbf{I}_i} \sum_{y \in \mathbf{I}_j} J_\gamma(x, y),$$

and for  $i = j$ , we define

$$(C.5) \quad \bar{J}_\gamma(i, i) = \frac{1}{|I|(|I| - 1)} \sum_{x \in \mathbf{I}_i} \sum_{\substack{y \in \mathbf{I}_i \\ y \neq x}} J_\gamma(x, y).$$

**Lemma C.2.** For fixed and small  $\gamma > 0$ , for any  $x \in \mathbf{I}_i$  and any  $y \in \mathbf{I}_j$ ,  $i, j \in \mathbb{Z}^d$  with  $i \neq j$ , we have

$$(C.6) \quad |J_\gamma(x, y) - \bar{J}_\gamma(i, j)| \leq \gamma^{d+\frac{1}{2}} \|DJ\|_\infty \mathbf{1}_{|x-y| \leq 2\gamma^{-1}}.$$

Also, for any  $i \in \mathbb{Z}^d$  and any  $x, y \in \mathbf{I}_i$ , we have

$$(C.7) \quad |J_\gamma(x, y) - \bar{J}_\gamma(i, i)| \leq \gamma^d \|J\|_\infty.$$

*Proof.* Let  $x \in \mathbf{I}_i$ , and for any  $y \in \mathbf{I}_j$ ,  $i, j \in \mathbb{Z}^d$ , with  $i \neq j$ , we have

$$\begin{aligned} |J_\gamma(x, y) - \tilde{J}_\gamma(x, y)| &= |J_\gamma(x, y) - \frac{1}{|I|^2} \sum_{z \in \mathbf{I}_i} \sum_{w \in \mathbf{I}_j} J_\gamma(z, w)| \\ &\leq \frac{1}{|I|^2} \sum_{z \in \mathbf{I}_i} \sum_{w \in \mathbf{I}_j} |J_\gamma(x, y) - J_\gamma(z, w)| \\ &\leq \frac{1}{|I|^2} \sum_{z \in \mathbf{I}_i} \sum_{w \in \mathbf{I}_j} \gamma^d \|DJ\|_\infty \gamma |x - y - z + w| \mathbf{1}_{|x-y| \leq \gamma^{-1}} \\ &\leq \frac{1}{|I|^2} |I|^2 \gamma^d \|DJ\|_\infty \gamma \gamma^{-1/2} \mathbf{1}_{|x-y| \leq \gamma^{-1}} \\ &= \gamma^{d+\frac{1}{2}} \|DJ\|_\infty \mathbf{1}_{|x-y| \leq \gamma^{-1}}. \end{aligned}$$

We prove (C.7) similarly. ■

**C.3. Coarse-grained Hamiltonian energy.** In this section, we analyze the Hamiltonian energy by using the new interaction defined in (C.4) and the estimates in Lemma C.2. We start by introducing some notation: for any  $r \in \mathbb{R}^d$ , we define the following quantity as a *block spin configuration*:

$$(C.8) \quad \sigma^{(\gamma^{-1/2})}(r) := \frac{1}{|I|} \sum_{x \in \mathbf{I}_r} \sigma_{I_i}(x)$$

so that

$$\sigma^{(\gamma^{-1/2})}(r) = \frac{1}{|I|} \int_{I_r} \sigma^{(1)}(r') dr'.$$

Let  $\Delta \subset \mathbb{R}^d$  be a  $\mathcal{P}_{\mathbb{R}^d}^{(l)}$ -measurable region. We denote by  $\mathcal{M}_\Delta^{(\gamma^{-1/2})}$  all  $\mathcal{P}_{\mathbb{R}^d}^{(l)}$ -measurable functions on  $\Delta$  with values in

$$(C.9) \quad M^{(\gamma^{-1/2})} := \left\{ -1, -1 + \frac{1}{\gamma^{-d/2}}, \dots, 1 - \frac{1}{\gamma^{-d/2}}, 1 \right\}.$$

For any bounded  $\mathcal{P}_{\mathbb{R}^d}^{(l)}$ -measurable region  $\Delta$  and  $m_\Delta \in \mathcal{M}_\Delta^{(\gamma^{-1/2})}$ , we define as a *coarse-grained Hamiltonian energy*

$$\begin{aligned} \bar{H}_{\gamma,h}^{\mathbf{J}}(m_\Delta; m_{\Delta^c}) &:= \int_\Delta \phi_{\beta,h}(m_\Delta(r))dr + \frac{1}{4} \int_\Delta \int_\Delta J_\gamma(r, r') [m_\Delta(r) - m_\Delta(r')]^2 dr dr' \\ &\quad + \frac{1}{2} \int_\Delta \int_{\Delta^c} J_\gamma(r, r') [m_\Delta(r) - m_{\Delta^c}(r')]^2 dr dr' \\ &\quad - \frac{1}{2} \int_\Delta \int_{\Delta^c} J_\gamma(r, r') m_{\Delta^c}(r')^2 dr dr' \\ &\quad + \frac{1}{\beta} \int_\Delta I(m_\Delta(r))dr, \end{aligned} \quad (\text{C.10})$$

where

$$I(m) := -\frac{1-m}{2} \log \frac{1-m}{2} - \frac{1+m}{2} \log \frac{1+m}{2}, \quad (\text{C.11})$$

with  $\phi_{\mathbf{J},\beta,h}(m)$  being given in (6.26). We recall that  $\mathcal{J} = \int_{\mathbb{R}^d} J(r)dr$ .

**Lemma C.3.** *Let  $\Delta$  be any bounded  $\mathcal{P}_{\mathbb{R}^d}^{(l)}$ -measurable region  $\Delta$ ; then there exists a constant  $C > 0$  such that the following estimate holds:*

$$\left| H_{\gamma,h}^{\mathbf{J}}(\sigma_\Delta; \bar{\sigma}_{\Delta^c}) - \bar{H}_{\gamma,h}^{\mathbf{J}}(\sigma_\Delta^{(\gamma^{-1/2})}; \bar{\sigma}_{\Delta^c}^{(\gamma^{-1/2})}) \right| \leq C|\Delta|\gamma^{1/2}, \quad (\text{C.12})$$

where  $\sigma_\Delta^{(\gamma^{-1/2})}$  and  $\bar{\sigma}_{\Delta^c}^{(\gamma^{-1/2})}$  are defined in (C.8).

**C.4. Estimates for the thermodynamic pressure of an Ising–Kac model.** We recall that

$$P_{\mathbf{J},\beta,h}^{\Delta,\gamma}(\bar{\sigma}_{\Delta^c}) := \frac{\log Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J}, \beta, h)}{\beta|\Delta|}$$

and

$$p_{\mathbf{J},\beta,h} := -\inf_{m \in [-1,1]} \{-hm + \phi_{\mathbf{J},\beta,0}(m)\}.$$

If  $\epsilon(\gamma) = \gamma^{1/2} + \gamma^{d/2} \log \gamma^{-1}$ , then the following bounds hold: there exist constants  $c, c' > 0$  such that

$$P_{\mathbf{J},\beta,h}^{\Delta,\gamma}(\bar{\sigma}_{\Delta^c}) \leq p_{\mathbf{J},\beta,h} + \left( c \frac{\gamma^{-1}}{L} + c\epsilon(\gamma) \right) \quad (\text{upper bound}). \quad (\text{C.13})$$

Let  $m^*$  be the minimizer of  $\phi_{\mathbf{J},\beta,h}$ , then  $p_{\mathbf{J},\beta,h} = -\phi_{\mathbf{J},\beta,h}(m^*)$ , and then

$$P_{\mathbf{J},\beta,h}^{\Delta,\gamma}(\bar{\sigma}_{\Delta^c}) \geq p_{\mathbf{J},\beta,h} - |\phi_{\mathbf{J},\beta,h}([m^*]_\gamma) - \phi_{\mathbf{J},\beta,h}(m^*)| - c\epsilon(\gamma) - c' \frac{\gamma^{-1}}{L} \quad (\text{lower bound}), \quad (\text{C.14})$$

where  $[m^*]_\gamma$  is the value in (C.9) closest to  $m^*$ .

**C.5. Limit as  $\Delta \nearrow \mathbb{Z}^d$  and then  $\gamma \rightarrow 0$ .** By using the estimates for the Hamiltonian energy given in (C.12), (C.13), and (C.14), we can prove that

$$(C.15) \quad \limsup_{\gamma \rightarrow 0} \lim_{\Delta \nearrow \mathbb{Z}^d} P_{\mathbf{J},\beta,h}^{\Delta,\gamma}(\bar{\sigma}_{\Delta^c}) \leq p_{\mathbf{J},\beta,h},$$

$$(C.16) \quad \liminf_{\gamma \rightarrow 0} \lim_{\Delta \nearrow \mathbb{Z}^d} P_{\mathbf{J},\beta,h}^{\Delta,\gamma}(\bar{\sigma}_{\Delta^c}) \geq p_{\mathbf{J},\beta,h},$$

and therefore, if  $P_{\mathbf{J},\beta,h}^\gamma := \lim_{\Delta \rightarrow \mathbb{Z}^d} P_{\mathbf{J},\beta,h}^{\Delta,\gamma}$ , then

$$(C.17) \quad \lim_{\gamma \rightarrow 0} P_{\mathbf{J},\beta,h}^\gamma = p_{\mathbf{J},\beta,h} = - \inf_{m \in [-1,1]} \{-hm + \phi_{\mathbf{J},\beta,0}(m)\}.$$

Hence, the thermodynamic pressure converges to the mean field pressure at the LP limit, namely

$$\lim_{\gamma \rightarrow 0} \lim_{\Delta \nearrow \mathbb{Z}^d} P_{\mathbf{J},\beta,h}^{\Delta,\gamma} = p_{\mathbf{J},\beta,h},$$

where  $p_{\mathbf{J},\beta,h}$  is defined in (6.26). The convexity properties are provided by the limit as  $\Delta \nearrow \mathbb{Z}^d$  and then preserved by  $\gamma \rightarrow 0$ .

**C.6. Thermodynamics of an Ising-spin model with a Kac potential.** It is shown that when  $\gamma > 0$  is sufficiently small, the phase diagram of an Ising-spin model with a Kac potential is close to the phase diagram of a mean field model. Precisely, in [13, 11] (see also [57]) it is proved that for  $d \geq 2$ , if  $h \neq 0$ , then there exists a unique DLR measure [58]. If  $h = 0$ , there exists a critical value of inverse temperature  $\beta_c(\gamma) > 0$  such that for any  $\beta < \beta_c(\gamma)$ , there exists one DLR measure, while for  $\beta > \beta_c(\gamma)$  there are at least two distinct DLR measures  $\mu_{\beta,\gamma}^\pm$ . Finally, there is an absence of phase transition when  $\gamma$  is kept small (for more details, see [57, 58] and references therein).

## Appendix D. Detailed analysis of medical diagnostics.

**D.1. Baseline model.** Let us consider the undirected graph in Figure 2 [20] denoted by  $\mathcal{G}$ . The class of maximal cliques is  $\mathcal{C}_{\mathcal{G}} = \{\{1, 2\}, \{2, 3, 4\}\}$ . The distribution defined over the graph is a log-linear model with clique potentials given by  $\Psi_c(\mathbf{y}_c | \mathbf{w}_c) = e^{w_c f_c(\mathbf{y}_c)}$ , where all the weights  $\mathbf{w}_c$  and the binary functions  $f_c$  are known. For example, for  $c = \{1, 2\}$ ,  $\mathbf{w}_{\{1,2\}} = 1.5$  and

$$f_{\{1,2\}}(\mathbf{y}_{\{1,2\}}) = \begin{cases} 1, & \mathbf{y}_{\{1,2\}} \in \{(s_1, l_1), (s_1, l_0), (s_0, l_0)\}, \\ 0, & \mathbf{y}_{\{1,2\}} \in \{(s_0, l_1)\}. \end{cases}$$

Each binary function  $f_c$  induces a set  $B_c = \{(\omega_1, \omega_2, \omega_3, \omega_4) : f_c(\omega_c) = 1\}$ . For example,  $B_{\{1,2\}} := \{\omega : \omega_{\{1,2\}} \in \{(s_1, l_1), (s_1, l_0), (s_0, l_0)\}\}$ . We compare predictions between the baseline and alternatives of Types I and II (see section D.2) for the following QoIs:

$$g(\mathbf{Y}) = \mathbf{1}_A \quad \text{for any event of interest } A \subset \Omega.$$

For instance,  $A = \{\text{patient is smoker with asthma}\} = \{\omega = (\omega_1, \omega_2, \omega_3, \omega_4) : \omega_1 = s_0, \omega_3 = a_0\}$ .

## D.2. Alternative models.

**D.2.1. Type I.** First, we consider the class of log-linear models  $\tilde{p}$  over  $\mathcal{G}$  with weight change in one maximal clique. Let  $c$  be the maximal clique that a weight change occurred. Then the clique potential is given by

$$\tilde{\Psi}_c(\mathbf{y}_c) = e^{\tilde{w}_c f_c(\mathbf{y}_c)}.$$

The weight after increasing or decreasing by 100a% equals  $\tilde{w}_c = (1 + a)w_c$ , where  $a \in [-1, 1]$  stands for the model uncertainty of alternative models of Type I and  $w_c$  is the weight on  $c$  of the baseline model  $p$ . For example, for  $\{1, 2\}$ , the corresponding clique potential is expressed as

$$\begin{aligned}\tilde{\Psi}_{\{1,2\}}(\mathbf{y}_{\{1,2\}} \mid \tilde{\mathbf{w}}_{\{1,2\}}) &= e^{\tilde{w}_{\{1,2\}} \tilde{f}_{\{1,2\}}(\mathbf{y}_{\{1,2\}})} \\ &= \Psi_{\{1,2\}}(\mathbf{y}_{\{1,2\}} \mid \mathbf{w}_{\{1,2\}}) \Phi_{\{1,2\}}(\mathbf{y}_{\{1,2\}} \mid \tilde{\mathbf{w}}_{\{1,2\}}),\end{aligned}$$

with

$$\Phi_{\{1,2\}}(\mathbf{y}_{\{1,2\}} \mid \tilde{\mathbf{w}}_{\{1,2\}}) = e^{-0.2w_{\{1,2\}} f_{\{1,2\}}(\mathbf{y}_{\{1,2\}})}$$

since we consider the simplest case where  $\tilde{f}_{\{1,2\}}(\mathbf{y}_{\{1,2\}}) = f_{\{1,2\}}(\mathbf{y}_{\{1,2\}})$  as well as the fact that  $\tilde{w}_{\{1,2\}} - w_{\{1,2\}} = -0.2w_{\{1,2\}}$ . Note that  $\mathcal{B} = \{c\}$ , where  $\mathcal{B}$  is defined in subsection 3.1.

**Derivation of (5.2).** We compute all the quantities involved in (4.4) explicitly. Let us start with the CGF:

$$\begin{aligned}\Lambda_p^f(\lambda) &= \log E_p[e^{\lambda g}] = \log \left( \sum_{\mathbf{y} \in A} e^{\lambda g} p(\mathbf{y}) + \sum_{\mathbf{y} \notin A} e^{\lambda g} p(\mathbf{y}) \right) \\ &= \log \left( e^{\lambda} p(A) + 1 - p(A) \right).\end{aligned}$$

It is straightforward to see that

$$(D.1) \quad \frac{d\tilde{p}}{dp} = \frac{\Phi^I}{E_p[\Phi^I]} = \frac{e^{aw_c f_c}}{e^{aw_c} p_I + 1 - p_I},$$

and we now go through the computation of  $E_p[\Phi^I]$ :

$$\begin{aligned}E_p[\Phi^I] &= \sum_{\mathbf{y}} \Phi^I(\mathbf{y}) p(\mathbf{y}) = \sum_{\mathbf{y}} e^{aw_c f_c(\mathbf{y}_c)} p(\mathbf{y}_c) \\ &= \sum_{\mathbf{y} \in B_c} e^{aw_c f_c(\mathbf{y}_c)} p(\mathbf{y}) + \sum_{\mathbf{y} \notin B_c} e^{aw_c f_c(\mathbf{y}_c)} p(\mathbf{y}) \\ &= e^{aw_c} p_I + 1 - p_I.\end{aligned}$$

Similarly, we prove that

$$(D.2) \quad E_p[\Phi^I \log \Phi^I] = aw_c e^{aw_c} p_I.$$

Overall, by recalling (3.11) the KL divergence equals

$$R(\tilde{p} \| p) = \frac{aw_c e^{aw_c} p_I}{e^{aw_c} p_I + 1 - p_I} - \log(e^{aw_c} p_I + 1 - p_I).$$



**D.2.2. Type II.** We consider the class of log-linear models  $\tilde{p}$  over  $\tilde{\mathcal{G}}$  with  $\tilde{\mathcal{V}} = \mathcal{V}$ ,  $\tilde{\mathcal{E}} = \mathcal{E} \cup e$ , where  $e$  is a new edge (see, for example, Figure 2(right)). We assume that the edge  $e$  enlarges an already existing maximal clique in the sense of the analysis in subsection 3.1. The model uncertainties arising from structure learning from either a new data set  $\tilde{\mathcal{D}}$  and/or different prior knowledge (see, for example, Figure 2(right)) lie in the binary function  $\tilde{f}_{\tilde{c}}$  defined on  $\tilde{c}$  and the new weight  $\tilde{w}_{\tilde{c}}$ , where  $\tilde{c}$  is the enlargement of an existing maximal clique  $c$ . The weight  $\tilde{w}_{\tilde{c}}$  can also be expressed with respect to  $w_c$ :  $\tilde{w}_{\tilde{c}} = (1+a)w_c$ . This time  $a \in \mathbb{R}$ , not necessarily in  $[-1, 1]$  as before (e.g.,  $w_c = 1.5$  and  $\tilde{w}_{\tilde{c}} = 5$ ). Then the corresponding clique potential is given by

$$\tilde{\Psi}_{\tilde{c}}(\mathbf{y}_{\tilde{c}}) = e^{\tilde{w}_{\tilde{c}}\tilde{f}_{\tilde{c}}(\mathbf{y}_{\tilde{c}})} = e^{(1+a)w_c\tilde{f}_{\tilde{c}}(\mathbf{y}_{\tilde{c}})}.$$

The binary function  $\tilde{f}_{\tilde{c}}$  induces a set  $B_{\tilde{c}} = \{(\omega_1, \omega_2, \omega_3, \omega_4) : \tilde{f}_{\tilde{c}}(\omega_{\tilde{c}}) = 1\}$ . For example, let  $\tilde{\mathcal{G}} \neq \mathcal{G}$  (also  $\mathcal{C}_{\tilde{\mathcal{G}}} \neq \mathcal{C}_{\mathcal{G}}$ ) and  $\mathbf{w} \neq \tilde{\mathbf{w}}$ . Intuitively, a change on the set of edges can be thought of as structure learning from either a new data set  $\tilde{\mathcal{D}}$  and/or different prior knowledge; see, for example, Figure 2(right), where only one new edge has been added.

The set  $B_{\tilde{c}}$  satisfies one of the following:  $B_{\tilde{c}} \cap B_c = \emptyset$  or  $B_{\tilde{c}} \cap B_c \neq \emptyset$ . Note that  $\mathcal{B}_{\subseteq} = \{\tilde{c}\}$  and  $\mathcal{B}_{\cup} = \mathcal{B}_{new} = \emptyset$ , with  $\mathcal{B}_{\subseteq}$ ,  $\mathcal{B}_{\cup}$  and  $\mathcal{B}_{new}$  being defined in subsection 3.1.

**Derivation of (5.3).** The CGF is the same as in the derivation of (5.2). Let us compute the expected value of the total  $\tilde{p}$ -excess factor of Type II relative to  $p$  with respect to  $p$ :

$$\begin{aligned} E_p[\Phi^{\text{II}}] &= \sum_{\mathbf{y}} \Phi^{\text{II}}(\mathbf{y})p(\mathbf{y}) = \sum_{\mathbf{y}} e^{(1+a)w_c\tilde{f}_{\tilde{c}}-w_cf_c}p(\mathbf{y}) \\ &= \sum_{\mathbf{y} \in B_c} e^{aw_cf_c(\mathbf{y}_c)}p(\mathbf{y}) + \sum_{\mathbf{y} \in B_{\tilde{c}}} e^{(1+a)w_c\tilde{f}_{\tilde{c}}-w_cf_c}p(\mathbf{y}) + \sum_{\mathbf{y} \notin B_c \cup B_{\tilde{c}}} e^{(1+a)w_c\tilde{f}_{\tilde{c}}-w_cf_c}p(\mathbf{y}) \\ (D.3) \quad &= e^{(1+a)w_c}p_{\text{II}} + e^{-w_c}p_{\text{I}} + 1 - p_{\text{I}} - p_{\text{II}}. \end{aligned}$$

We split the sum into the three sums since  $B_c \cap B_{\tilde{c}} = \emptyset$ . Similarly, we prove that

$$(D.4) \quad E_p[\Phi^{\text{II}} \log \Phi^{\text{II}}] = -w_ce^{-w_c}p_{\text{I}} + (1+a)w_ce^{(1+a)w_c}p_{\text{II}}.$$

Overall, by recalling (3.11) the KL divergence equals

$$R(\tilde{p}||p) = \frac{-w_ce^{-w_c}p_{\text{I}} + (1+a)w_ce^{(1+a)w_c}p_{\text{II}}}{e^{(1+a)w_c}p_{\text{II}} + e^{-w_c}p_{\text{I}} + 1 - p_{\text{I}} - p_{\text{II}}} - \log \left( -w_ce^{-w_c}p_{\text{I}} + (1+a)w_ce^{(1+a)w_c}p_{\text{II}} \right).$$

**Remark D.1.** If  $B_c \cap B_{\tilde{c}} \neq \emptyset$ , then we need to split the sum of (D.3) as follows: Let  $U \equiv B_c \cap B_{\tilde{c}}$ ; then

$$\begin{aligned} E_p[\Phi^{\text{II}}] &= \sum_{\mathbf{y}} \Phi^{\text{II}}(\mathbf{y})p(\mathbf{y}) = \sum_{\mathbf{y}} e^{(1+a)w_c\tilde{f}_{\tilde{c}}-w_cf_c}p(\mathbf{y}) \\ &= \sum_{\mathbf{y} \in B_c \setminus U} e^{aw_cf_c(\mathbf{y}_c)}p(\mathbf{y}) + \sum_{\mathbf{y} \in B_{\tilde{c}} \setminus U} e^{(1+a)w_c\tilde{f}_{\tilde{c}}-w_cf_c}p(\mathbf{y}) + \sum_{\mathbf{y} \in U} e^{(1+a)w_c\tilde{f}_{\tilde{c}}-w_cf_c}p(\mathbf{y}) \\ &\quad + \sum_{\mathbf{y} \notin B_c \cup B_{\tilde{c}}} e^{(1+a)w_c\tilde{f}_{\tilde{c}}-w_cf_c}p(\mathbf{y}) \\ &= e^{(1+a)w_c}(p_{\text{II}} - p(U)) + e^{-w_c}(p_{\text{I}} - p(U)) + e^{aw_c}p(U) + 1 - p_{\text{I}} - p_{\text{II}} + p(U). \end{aligned}$$

Note that  $p_I, p_{II}$ , and  $p(U)$  are computable, as  $p$  is known.

### Appendix E. Analysis of UQ for statistical mechanics.

**E.1. Proof of Lemma 6.2.** It is not difficult to show (see also Proposition II.1.2 and Lemma II.2.2C in [62]) that

$$(E.1) \quad \begin{aligned} |\log Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J}, \beta, h) - \log Z_{\bar{\sigma}_{\Delta^c}}(\tilde{\mathbf{J}}^F, \beta, h)| &\leq \beta \|H^{\mathbf{J}, h}(\sigma_{\Delta} | \bar{\sigma}_{\Delta^c}) - H^{\tilde{\mathbf{J}}^F, h}(\sigma_{\Delta} | \bar{\sigma}_{\Delta^c})\|_{\infty} \\ &\leq |\Delta| \|\Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}} - \Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \tilde{\mathbf{J}}^F}\|_1, \end{aligned}$$

which in turn gives

$$(E.2) \quad R(\tilde{q}_{\Delta} \| q_{\Delta}) \leq 2|\Delta| \|\Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}} - \Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \tilde{\mathbf{J}}^F}\|_1$$

since

$$\begin{aligned} R(\tilde{q}_{\Delta} \| q_{\Delta}) &= \beta \left( E_{\tilde{q}_{\Delta}}[H^{\mathbf{J}, h}(\sigma_{\Delta} | \bar{\sigma}_{\Delta^c})] - E_{q_{\Delta}}[H^{\tilde{\mathbf{J}}^F, h}(\sigma_{\Delta} | \bar{\sigma}_{\Delta^c})] \right) \\ &\quad + \log Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J}, \beta, h) - \log Z_{\bar{\sigma}_{\Delta^c}}(\tilde{\mathbf{J}}^F, \beta, h). \end{aligned}$$

A straightforward bound yields that

$$\|\Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \mathbf{J}} - \Phi_{\Delta, \bar{\sigma}_{\Delta^c}}^{h, \beta, \tilde{\mathbf{J}}^F}\|_1 \leq \beta \left( |\tilde{h} - h| + \sum_{x \neq 0} |F(0, x)| \right).$$

**E.2. Proof of Lemma 6.1.** It is a straightforward computation after subtracting the Hamiltonian energies with interaction  $J$  and

$$\tilde{J}^F(x, y) = J(x, y) \mathbf{1}_{\|x-y\|_d \leq R} + F(x, y) \mathbf{1}_{\|x-y\|_d > R} \quad (\text{Type I})$$

and

$$\tilde{J}^F(x, y) = J(x, y) \mathbf{1}_{\|x-y\|_d \leq R} + F(x, y) \mathbf{1}_{\|x-y\|_d > R} \quad (\text{Type II}).$$

#### E.2.1. Cumulant generating function for $f(\mathbf{Z}) = |\Delta| m(\sigma_{\Delta})$ .

$$(E.3) \quad \begin{aligned} \Lambda_{q_{\Delta}; |\Delta| m(\sigma_{\Delta})}(\pm \lambda) &= \log E_{q_{\Delta}}[e^{\lambda |\Delta| \frac{1}{|\Delta|} \sum_{x \in \Delta} \sigma_{\Delta}(x)}] \\ &= \log \left( \frac{1}{Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J}, \beta, h)} \sum_{\sigma_{\Delta}} e^{\lambda \sum_{x \in \Delta} \sigma_{\Delta}(x)} e^{-\beta H^{\mathbf{J}, h}(\sigma_{\Delta} | \sigma_{\Delta^c})} \right) \\ &= \log \left( e^{\lambda \sum_{x \in \Delta} \sigma_{\Delta}(x) - \beta H^{\mathbf{J}, h}(\sigma_{\Delta} | \sigma_{\Delta^c})} \right) - \log Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J}, \beta, h) \\ &:= \log Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J}, \beta, h \pm \frac{\lambda}{\beta}) - \log Z_{\bar{\sigma}_{\Delta^c}}(\mathbf{J}, \beta, h). \end{aligned}$$

Then, by using the definition of the thermodynamic pressure in (6.25), we get

$$(E.4) \quad \frac{1}{|\Delta|} \Lambda_{q_{\Delta}; |\Delta| m(\sigma_{\Delta})}(\pm \lambda) = \beta \left( P_{h \pm \frac{\lambda}{\beta}, \beta, \mathbf{J}}^{\Delta, \gamma} - P_{h, \beta, \mathbf{J}}^{\Delta, \gamma} \right).$$

## Appendix F. Phase diagram of a long range perturbation.

### F.1. Thermodynamics of a long range perturbation of one-dimensional Kac model.

There are a significant number of works in the literature studying the phase diagram of a one-dimensional ferromagnetic Ising model with long range interactions of the form  $1/r^k$ , with  $k$  indicating the decay of interaction and  $k \leq 2$ . For  $k < 2$ , the occurrence of phase transition has been proved (see [26, 27, 28]). For  $k = 2$ , the existence of a spontaneous magnetization at a low temperature is proved in [33]. The establishment of the existence of phase transition, proving the discontinuity of the magnetization at a critical point, also known as the *Thouless effect*, was proved by Aizenman et al. in [1]. In [12], the authors study the phase diagram of the system with interaction defined in (F.1) with  $F$  given in Definition F.1 as illustrated in Figure 7(right). Precisely, they have shown that there is a critical value of the inverse temperature depending on  $a$  and  $\gamma$  sufficiently small such that the system exhibits phase transition.

**F.1.1. Phase diagram of a long range perturbation.** We consider a one-dimensional ferromagnetic Ising-spin system with interactions that correspond to a  $1/r^2$  long range perturbation of the usual Kac model; see Figure 7(right).

**Definition F.1.** Let  $J_\gamma^{\text{pwc}}(x, y) = \gamma^d \mathbf{1}_{|x-y| \leq \frac{\gamma^{-1}}{2}}$  (i.e., a special case of Kac-type interaction where in fact  $J_\gamma^{\text{pwc}}(x, y)$  is piecewise constant interaction). Then we define

$$(F.1) \quad \tilde{J}_\gamma^F(x, y) = \begin{cases} J_\gamma^{\text{pwc}}, & 0 \leq |x - y| \leq (2\gamma)^{-1}, \\ F(x, y), & |x - y| > (2\gamma)^{-1}, \end{cases}$$

with  $F(x, y) = \frac{a}{|x-y|^2}$  for some number  $a \in (0, \infty)$ ; see Figure 7(right).

The range of the perturbation  $F$  is clearly Type II. We derive the UQ bounds as follows:

$$(F.2) \quad \begin{aligned} \log \Phi_{\bar{\sigma}_{\Delta^c}}^i(\sigma_\Delta) &= \beta \sum_{x \in \Delta} \sigma_\Delta(x) \left( \tilde{h} - h + \frac{1}{2} \sum_{y \in A_x^{\text{II}} \cap \Delta} F(x, y) \sigma_\Delta(y) \right. \\ &\quad \left. + \sum_{y \in A_x^{\text{II}} \cap \Delta^c} F(x, y) \bar{\sigma}_{\Delta^c}(y) \right), \end{aligned}$$

then  $C^{\text{II}} := \beta(\tilde{h} - h)$ , and then

$$\kappa_{\text{II}} := \beta \sum_{x \in \Delta} \sigma_\Delta(x) \left( \frac{1}{2} \sum_{y \in A_x^{\text{II}} \cap \Delta} F(x, y) \sigma_\Delta(y) + \sum_{y \in A_x^{\text{II}} \cap \Delta^c} F(x, y) \bar{\sigma}_{\Delta^c}(y) \right).$$

We bound  $\kappa_{\text{II}}$  based on the following:

$$(F.3) \quad \begin{aligned} \sum_{x \in \Delta} \sum_{y \in A_x^{\text{II}} \cap \Delta} F(x, y) &\leq |\Delta| \sum_{y \in A_0^{\text{II}}} F(0, y) = |\Delta| \sum_{y \in A_0^{\text{II}}} \frac{a}{y^2} \\ &= \gamma |\Delta| \sum_{y \in A_0^{\text{II}}} \frac{\gamma a}{(\gamma y)^2} \leq C \gamma |\Delta| \end{aligned}$$

for some constant  $C$  arising from  $\sum_{y \in A_0^\Pi} \frac{a}{y^2} < \infty$ . Then  $\kappa_\Pi \leq 2C\gamma|\Delta|$  and the UQ bounds for long range perturbation with  $\beta(\tilde{h} - h) < 1$  are

$$(F.4) \quad \pm E_{\tilde{q}_\Delta}[m(\sigma_\Delta)] \leq \frac{1}{1 - \beta(\tilde{h} - h)} \inf_{\lambda > 0} \left\{ \frac{P_{h \pm \frac{\lambda}{\beta}, \beta, \mathbf{J}}^{\Delta, \gamma} - P_{h, \beta, \mathbf{J}}^{\Delta, \gamma}}{\lambda/\beta} + \frac{\beta}{\lambda} 2C\gamma \right\}.$$

In the LP limit, we get

$$(F.5) \quad \pm M(\tilde{\mathbf{J}}^F, \beta, \tilde{h}) \leq \frac{1}{1 - \beta(\tilde{h} - h)} \inf_{\lambda > 0} \left\{ \frac{p_{h \pm \frac{\lambda}{\beta}, \beta, \mathbf{J}} - p_{h, \beta, \mathbf{J}}}{\lambda/\beta} \right\}.$$

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