Loop corrections in spin models through density consistency

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Computing marginal distributions of discrete or semi-discrete Markov Random Fields (MRF) is a fundamental, generally intractable, problem with a vast number of applications on virtually all fields of science. We present a new family of computational schemes to calculate approximately marginals of discrete MRFs. This method shares some desirable properties with Belief Propagation, in particular providing exact marginals on acyclic graphs; but at difference with it, it includes some loop corrections, i.e. it takes into account correlations coming from all cycles in the factor graph. It is also similar to Adaptive TAP, but at difference with it, the consistency is not on the first two moments of the distribution but rather on the value of its density on a subset of values. Results on random connectivity and finite dimensional Ising and Edward-Anderson models show a significant improvement with respect to the Bethe-Peierls (tree) approximation in all cases, and with respect to Plaquette Cluster Variational Method approximation in many cases. In particular, for the critical inverse temperature $\beta_c$ of the homogeneous hypercubic lattice, the expansion of $(d\beta_c)^{-1}$ around $d = \infty$ of the proposed scheme is exact up to the $d^{-2}$ order, whereas the two latter are exact only up to the $d^{-1}$ order.

Introduction. Markov random fields (MRF) are indirect probabilistic graphical models in which random variables satisfy a conditional independence property, so that the joint probability measure can be expressed in a factorized form, each factor involving a possibly different subset of variables [1]. Computing marginal distributions of discrete or semi-discrete Markov Random Fields is a fundamental step in most approximate inference methods and high-dimensional estimation problems [2], such as the evaluation of equilibrium observables in statistical mechanics models. The exact calculation of marginal distributions is however intractable in general, and it is common to resort to stochastic sampling algorithms, such as Monte-Carlo Markov Chain, to obtain unbiased estimates of the relevant quantities. On the other hand, it is also useful to derive approximations of the true probability distribution, for which marginal quantities can be deterministically computed. An important family of approximations is the one of mean-field (MF) schemes. The simplest is naive mean-field (nMF), that neglects all correlations between random variables. An improved MF approximation [3], called Thouless-Anderson-Palmer (TAP) equations, works well for models with weak dependencies but it is usually unsuitable for MRFs on diluted models. Here, a considerable improvement is provided by the Bethe-Peierls approximation or Belief Propagation (BP), that is exact for probabilistic models defined on graphs without loops [4]. It is a matter of fact that BP has been successfully employed even in on loopy probabilistic models both in physics and in applications (see e.g. Berrou et al. [5]), yet the lack of analytical control on the effect of loops calls for novel approaches that could systematically improve with respect to BP. A traditional way to account for the effect of short loops is by means of Cluster Variational Methods (CVM), that treat exactly correlations generated between variables within a finite region $\mathcal{R}$ [6–8]. The main limitation of CVM resides in its algorithmic complexity, that grows exponentially with the size of the region $\mathcal{R}$. A completely different path to systematically improve BP is represented by loop series expansions [9–12] in which BP is obtained as a saddle-point in a corresponding effective field theory. Loop corrections to BP equations can be alternatively introduced in terms of local equations for correlation functions, as first suggested for pairwise models [13] and later extended to arbitrary factor graphs [14–16]. This method consists in considering deformed local marginal probabilities on a “cavity graph”, obtained removing a factor node (i.e. interaction), and imposing a consistency condition on single-node marginals. On trees, BP equations are recovered, whereas on loopy graphs the obtained set of equations is strongly under-determined and requires additional constraints. Linear-response relations were exploited to this purpose in [13], even though other moment closure methods are possible [14].

A different approach to approximate inference exploits the properties of multivariate Gaussian distributions, that have the advantage of retaining information on correlations albeit allowing for explicit calculations. In particular, Expectation Propagation (EP), which can be thought as an adaptive variant of TAP) is a very successful algorithmic technique in which a tractable approximate distribution is obtained as the outcome of an iterative process in which the parameters of a multivariate Gaussian are optimized by means of local moment matching conditions [17, 18]. EP has been applied to problems involving discrete random variables by employing atomic measures [19]. In the present work, we put forward a new family of computational schemes to calculate approximate marginals of discrete MRFs. We exploit the flexibility of multivariate Gaussian approximation methods but, unlike EC and inspired by beliefs marginalization condition in BP, we impose that marginals on discrete variables are locally consistent, a condition...
that we call \textit{density consistency}. When the underlying graph is a tree, the set of equations produced is equivalent to BP. As for Ref.[13], the density consistency condition leaves an under-determined system of equations on loopy graphs, that can be solved once supplemented with a further set of closure conditions. As a result of employing Gaussian distributions, higher order correlation functions between neighbors of a given variable are, at least partially, taken into account.

The Model. Consider a factorized distribution of binary variables \(x_1, \ldots, x_n \in X = \{-1, 1\}\) for arbitrary positive factors \(\psi_a : X_a \to \mathbb{R}_+\), each depending on a sub-vector \(x_a = \{x_i\}_{i \in \partial a} \in X_a\)

\[
p(x) = \frac{1}{Z} \prod_{a \in A} \psi_a (x_a). \tag{1}
\]

The bipartite graph \(G = (V, E)\) with \(V = I \cup A\) the disjoint union of variable indices \(I = \{1, \ldots, n\}\) and factor indices \(E = \{(ia) : i \in \partial a\}\), is called the factor graph of the factorization (1), and as we will see some of its topological features are crucial to devise good approximations. Particular important cases of (1) include e.g. Ising spin models, many neural network models and the uniform distribution of solutions of \(k\)-SAT formulas. Computing marginal distributions from \(p\) is in general NP-Hard (i.e. computationally intractable).

\textbf{Density Consistency.} Following Gaussian Expectation Propagation (otherwise called adaptive TAP or Expectation Consistency) [17, 18], we will approximate an intractable \(p(x)\) by a Normal distribution \(g(x)\). To do so, we will replace each \(\psi_a (x_a)\) by an appropriately defined multivariate normal distribution \(\phi_a (x_a) = N (x_a; \mu^a, \Sigma^a)\). Parameters \(\mu^a, \Sigma^a\) will be selected as follows. First define

\[
g(x) = \frac{1}{Z_g} \prod_{a \in A} \phi_a (x_a) = \frac{1}{Z} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)}.
\]

Defining auxiliary distributions \(g^{(a)}(x) = \frac{1}{Z_g} g(x) \sum_{x_a \in X_a} \delta (x_a - x_a) \frac{\phi_a (x_a)}{\phi_a (x_a)}\) and \(g^{(i)}(x) = \frac{1}{Z_i} g(x) \sum_{\hat{x}_i \in X} \delta (x_i - \hat{x}_i)\), matching between marginals \(g^{(i)}(x_i)\) and \(g^{(a)}(x_a)\) results in

\[
\frac{\mu_i}{\Sigma_{ii}} = \text{atanh} (\langle x_i \rangle_{g^{(a)}}) \tag{2}
\]

\(\forall i \in \partial a, a \in A\), giving \(\sum_a |\partial a|\) equations. As we will see, (2) is chosen because it ensures exactness on acyclic graphs. We call \textit{Density Consistency} (DC) any scheme that enforces Eq. (2). We propose to complement Equation (2) with matching of first moments and Pearson correlation coefficients \(\text{corr} \; (x, y) = \langle xy \rangle_Q - \langle x \rangle_Q \langle y \rangle_Q / (\langle x^2 \rangle_Q - \langle x \rangle_Q^2)^{-\frac{1}{2}} (\langle y^2 \rangle_Q - \langle y \rangle_Q^2)^{-\frac{1}{2}}\) (although other closures are possible, see A4)

\[
\mu_i = \langle x_i \rangle_{g^{(a)}} , \quad \frac{\Sigma_{ij}}{\sqrt{\Sigma_{ii} \Sigma_{jj}}} \Rightarrow \rho_{\text{corr}} ^{g^{(a)}} (x_i, x_j) \tag{3}
\]

for \(i \neq j\) where \(\rho \in [0, 1]\) is an interpolating parameter that is fixed to 1 for the time being. Relations (2)-(3) give a system of \(\sum_a |\partial a| (|\partial a| + 3)\) equations and unknowns, that can be solved iteratively to provide an approximation for the first \(\langle x_i \rangle_Q\) and second moments \(\langle x_i x_j \rangle_Q\) of the original distribution. In a parallel update scheme (in which all factors parameters are update simultaneously) the computational cost of each iteration is \(O (N^3)\), dominated by the calculation of \(\Sigma\).

On acyclic factor graphs, the method converges in a finite number of iterations and is exact, i.e. on a fixed point, \(\langle x_i \rangle_Q\) equals to the magnetization \(\langle x_i \rangle_P\). Therefore, as both the DC scheme and BP are exact on acyclic graphs, their estimation of marginals must coincide. However, a deeper connection can be pointed out. If a DC scheme applies zero covariances (e.g. by setting \(\rho = 0\) in (3)), on a DC fixed point on any factor graph the quantities \(m_{ai} = \text{tanh} (\mu^a_i / \Sigma_{ii})\) satisfy the Belief Propagation (BP) equations. Moreover, DC follows dynamically a BP update. In particular, when equations converge, magnetizations \(m_i = \text{tanh} (\mu_i / \Sigma_{ii})\) are equal to the corresponding belief magnetizations (Proof in A1).

Interestingly, the DC scheme can be thought of as a Gaussian pairwise EP scheme with a modified consistency condition. The latter can be obtained by keeping (3) and replacing atanh \((x)\) in the RHS of (2) by the qualitatively similar \(\frac{e^{x}}{e^{x} + 1}\). This of course renders the method inexact on acyclic graphs and turns out to give generally a much worse approximation in many cases (See A4). In addition, as it also happens with the EP method, Gaussian densities in factors \(\psi_a\) can be moved freely between factors (sharing the same variables) without altering the approximation (details in A3).
Figure 1. Comparison of DC, BP and LC on single-instances of disordered systems. (a) Magnetizations of AntiFerromagnetic Ising Model on a triangular lattice with $N = 100, |E| = 6N$, $J = -1$, $\beta = 0.52$ and random binary fields of $|h_i| = 0.2$. (b) Magnetization of Ferromagnetic Ising Model on a Random Regular (RR) Graph, $N = 300$, degree 4, $\beta = 0.35$, $J = 1$ and random binary fields of $|h_i| = 0.3$. (c) Correlations of (heterogeneous) Ising Model on Barabasi-Albert graph, $N = 100$, $n_0 = k = 2$ without external fields (the solution is found by using $\rho^* = 0.95$ and it is divergent for $\rho > \rho^*$). (d) Magnetizations of a random 4–SAT instance at $\alpha = \frac{M}{N} = 4$ at $\beta \rightarrow \infty$. (e) Correlations of (heterogeneous) Ferromagnetic Ising Model on a Random Regular (RR) Graph, $N = 300$, degree 4 and $\beta = 0.3$. (f) Correlations on a 3D hypercubic toroidal lattice ferromagnetic (heterogeneous) Ising Model, $N = 6^3$ and $\beta = 0.21$ and no external fields. In heterogeneous ferromagnetic models, couplings are drawn from a uniform distribution in (0.5, 1.5).

Numerical results We tested the method on the Ising model on many different scenarios on heterogeneous systems, with a selection of results given in Figure 1. True values for magnetization and correlations were computed with a damping parameter around 0.95 to improve convergence. The DC method provides a substantial correction to BP magnetizations and correlations in almost all cases; it also improves single-node marginal estimates w.r.t. Loop Corrected Belief Propagation [14] in several cases: correlations were not accessible through the code provided in [20]. We underline that, despite the computational cost per iteration of LCBP on bounded-degree graphs being approximately with long Monte-Carlo runs ($\sim 10^5$ Monte-Carlo Gibbs-sampling steps) for Ising models and with the exact (exponential) trace for up to $N = 28$ in the case of $k$–SAT. All simulations have been performed with a damping parameter around 0.95 to improve convergence. The DC method provides a substantial correction to BP magnetizations and correlations in almost all cases; it also improves single-node marginal estimates w.r.t. Loop Corrected Belief Propagation [14] in several cases: correlations were not accessible through the code provided in [20].

Homogeneous Ising model Consider a homogeneous ferromagnetic Ising Model with coupling constant $J$ and external field $h$ on on a $d$-dimensional lattice with periodic (toroidal) boundary condition: because of the translational invariance, all Gaussian factors $\phi_0$ are identical and the covariance matrix admits an analytic diagonalization. Therefore it is possible to estimate equilibrium observables through an analytical DC scheme also in the thermodynamic limit. After some calculations, at a given temperature the DC solution is found by solving the following system of 3 fixed point equations $\sigma_0 = \frac{\alpha m}{\beta + \sigma_0}$, $\sigma_1 = \sigma_0^\gamma $, and $y = m (\gamma_0 + \gamma_1)$ in the Gaussian parameters $\gamma_0, \gamma_1$ where $m = \langle x_i \rangle_{\sigma_0}$, $c = \langle x_i x_j \rangle_{\sigma_0}$ are the moments computed under the ‘tilted’ distribution $g^{(\alpha)}$, and $\sigma_0, \sigma_1, \gamma_0, \gamma_1$ equal respectively $\Sigma_{ii}, \Sigma_{ij}, (2d)^{-1} (\Sigma^{-1})_{ii}, (\Sigma^{-1})_{ij}$ for $i, j$ two first lattice neighbors. Defining $R_d(r) = \frac{1}{2} \int_0^{\infty} dte^{-dt^2} I_0^{(d)} (rt)$, where $I_0$ is the modified Bessel function of the first kind of order 0, and after some straightforward algebraic manipulations, we finally obtain the following equations (here $h = 0$ for simplicity) for variable $\beta, m, r = \gamma_1 \gamma_0^{-1}$:
The maximum value of $\beta$ for which a paramagnetic solution exists can be analytically derived by substituting $m = 0$ and taking $\sup_{-1 < r \leq 0} \beta(r)$ from (4). For $d \geq 3$ the maximum is realized at $r = -1$, obtaining:

$$\beta_p = \tanh \left( 1 - \frac{1}{x_d} \right) = \frac{x_d (x_d - 1)}{2 x_d - 1} + \frac{x_d}{2 d}$$  \hspace{1cm} (6)$$

where $x_d = 2 d R_d (-1)$. Values of $\beta_p$ for various dimensions $d$ are reported in Table I. The paramagnetic solution is stable in the full range $0 \leq \beta < \beta_p$ for $d \geq 3$.

Expanding (6) in powers of $d^{-1}$ we get

$$\frac{\beta_p - 1}{2 d} = 1 - \frac{1}{2} d^{-1} - \frac{1}{3} d^{-2} - \frac{17}{24} d^{-3} - \frac{799}{720} d^{-4} - \frac{2039}{720} d^{-5} + O(d^{-6})$$

which is exact up to the $d^{-4}$ order (the correct coefficient of $d^{-5}$ is $-\frac{2039}{720}$) [22]. For comparison, nMF is exact up to the $d^0$ order, BP is exact up to the $d^{-1}$ order, and Loop Corrected Bethe (LCB) and Plaquette CVM (PCVM, [21]) are exact up to the $d^{-2}$ order.

The minimum value of $\beta$ for which a magnetized solution exists can be also computed by seeking a point with $d \beta_p = 0$ with the complication that $\beta$ is defined implicitly by (4)-(5) (details in B2). The resulting equation has a single solution that has been numerically computed and shown in Table (I) as $\beta_m$. It turns out to be smaller but always very close to $\beta_p$ and coincident up to numerical precision for $d \geq 5$. Note that for inverse temperatures in the (albeit small) range $\beta_m < \beta < \beta_p$, the DC approximation has both magnetized and a paramagnetic stable solutions, suggesting a phase coexistence that should be absent in the real system [23].

**Discussion** We proposed a general approximation scheme for distributions of discrete variables that show interesting properties, including being exact on acyclic factor graphs and providing a form of loop corrections on graphs with cycles. The method can be in part solved analytically on homogeneous systems such as finite dimensional hypercubic lattices with periodic conditions. Analytical predictions from the model show a number of interesting features that are not shared by other mean-field approaches: the method provides finite size corrections which are in close agreement with numerical simulations; the paramagnetic solution exists only for $\beta < \beta_p$ (in PCVM and BP, the paramagnetic solution exists for all $\beta \geq 0$, although it stops being stable at a finite value of $\beta$); it can capture some types of heterogeneity where the Bethe-Peierls approximation can not (such as in RR graphs). Numerical simulations are in good agreement on different models, including random-field Ising with various topologies and random $k$–SAT. On lattices, the method could in principle be rendered more accurate by taking into account small loops explicitly. This will be object of future research.

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1 $R_d (-1)$ is divergent and the maximum for $d = 2$ is located in $-1 < r^* < 0$. The solution for $d = 2$ is thus qualitatively different, see B.3.
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Appendix A: General properties of DC scheme

1. Relation with the Bethe approximation (BP)

On acyclic graphs, both the DC scheme and BP are exact and thus they must coincide on their computation of
marginals. However, a deeper connection can be pointed out. BP fixed point equations are

\[ m_{ai}(x_i) \propto \sum_{x_a} \psi_a(x_a) \prod_{j \in a \setminus i} m_{ja}(x_j) \]  
(A1)

\[ m_{ia}(x_i) \propto \prod_{b \in i \setminus a} m_{bi}(x_i) \]  
(A2)

\[ m_i(x_i) \propto \prod_{b \in i} m_{bi}(x_i) \]  
(A3)

Theorem 1. If (H1) the DC scheme applies zero covariances or (H2) the factor graph is acyclic, \( m_{ai}(x_i) \propto g^{a}(x_i) \) satisfies (A1)-(A2). Moreover, the updates follow dynamically BP updates. In particular, if equations converge, approximate marginals \( g(x_i) \) are proportional to belief magnetizations (A3).

Proof. In the either hypothesis (H1 or H2) , \( g^{a}(x_a) \propto \prod_{j \in \partial a} m_{ja}(x_j) \). Define \( m_{ai}(x_i) \propto \frac{g^{a}(x_i)}{m_{ai}(x_i)} \). We obtain

\[ m_{ai}(x_i) \propto \frac{1}{m_{ia}(x_i)} \int dx_{a\setminus i} g(x_a) \]

\[ \propto \int dx_{a\setminus i} \prod_{j \in \partial a \setminus i} m_{ja}(x_j) \phi_a(x_a) \]  
(A4)

Thanks to (2), \( g(x_i) \propto g^{a}(x_i) \) when \( x_i \in \{-1, 1\} \) (and this is precisely the purpose of (2)). In particular, for \( x_i \in \{-1, 1\} \) we get also

\[ m_{ai}(x_i) \propto \frac{1}{m_{ia}(x_i)} g^{a}(x_i) \]

\[ = \frac{1}{m_{ia}(x_i)} \sum_{x_a\setminus i} g^{a}(x_a) \psi_a(x_a) \]

\[ = \sum_{x_a\setminus i} \prod_{j \in \partial a \setminus i} m_{ja}(x_j) \psi_a(x_a) \]  
(A5)

which is Eq. (A1). Eq. (A2) is also verified in either hypothesis:

1. Factorized case: if \( \phi_a(x_a) = \prod_{i \in \partial a} \phi_a(x_i) \), then clearly \( m_{ai}(x_i) \propto \phi_a(x_i) \) and \( m_{ia}(x_i) \propto \prod_{b \in \partial \setminus a} m_{bi}(x_i) \)
2. Acyclic case: if $T_b$ denotes the set of factors in the connected component of $b$ once $i$ is removed, we get

$$m_{ia} (x_i) \propto g^{-a} (x_i)$$

\[
\propto \int dx_{-i} \prod_{b \in \partial \setminus a} \phi_b (x_b) \prod_{c \in T_b \setminus b} \phi_c (x_c) \\
\propto \prod_{b \in \partial \setminus a} \int dx_{b \setminus i} \phi_b (x_b) \prod_{j \in \partial \setminus i} g^{-b} (x_j) \\
\propto \prod_{b \in \partial \setminus a} \int dx_{b \setminus i} \phi_b (x_b) \prod_{j \in \partial \setminus i} m_{bj} (x_j) \\
\propto \prod_{b \in \partial \setminus a} m_{bi} (x_i)
\]  

(A6)

where the last line follows from (A4).

\[\Box\]

2. Relation with EP

The DC scheme can be thought of a modified Gaussian EP scheme for factors.

$$\hat{\psi}_{ij} (x_i, x_j) = \psi_{ij} (x_i, x_j) \delta (x_i + 1) + \delta (x_i - 1) \delta (x_i + 1) + \delta (x_i - 1)$$

Classic EP equations in this context can be obtained by replacing $\text{atanh} (x_i)_{g(a)}$ in the RHS of (2) by the qualitatively similar function $\frac{(x_i)_{g(a)}}{1 - (x_i)_{g(a)}}$, but this of course invalidates Theorems 1-2 and turns out to give a much worse approximation in general.

3. Weight gauge

One interesting property common to both DC and EP scheme concerns the possibility to move freely gaussian densities in and out the exact factors $\psi_a (x_a)$. Let $\rho_a (x_a)$ be Gaussian densities;

$$p (x) \propto g (x) \prod_a \psi_a (x_a)$$

$$q (x) \propto g (x) \prod_a \phi_a (x_a)$$

and $q$ a Gaussian EP or DC approximation. We have

$$p^{(a)} (x_a) \propto \psi_a (x_a) \int dx_{-a} \frac{g (x) \prod_b \phi_b (x_b)}{\phi_a (x_a)} \prod_{b \setminus a} \phi_b (x_b) / \phi_a (x_a)$$

(A7)

$$q (x_a) = \int dx_{-a} g (x) \prod_b \phi_b (x_b)$$

(A9)

$$= \int dx_{-a} \left[ g (x) \prod_b \rho_b (x_b) \right] \prod_b \phi_b (x_b) / \rho_b (x_b)
\]  

(A10)

\[\text{2 With the apparent ambiguity of the appearance of } \delta^k \text{ terms in } p (x), \text{ which is actually really not as problematic as it may seem as the distribution is defined up to a normalization factor; more precisely consider}

$$p (x) = \lim_{\sigma \to 0} \frac{1}{Z_o} \prod_{a \setminus x} \hat{\psi}_{a,x} (x_i, x_j)
\]  

for factors $\hat{\psi}_{a,x} (x_i, x_j) = \psi_{ij} (x_i, x_j) (N (x_i; 1, \sigma) + N (x_i; -1, \sigma)) (N (x_j; 1, \sigma) + N (x_j; -1, \sigma))$.}
As DC and EP algorithms impose constraints between $p^a(x)$ and $q(x)$, any approximating family $\{\phi_a\}$ for $(g, \{\psi_a\})$ leads to an equivalent family $\{\phi_a/\rho_a\}$ for $(g' = g \prod b \rho_b, \{\psi'_a = \psi_a/\rho_a\})$ for arbitrary factors $\rho_a$.

4. Other closure equations

Eq. 2 is the only condition needed to make the approximation scheme exact on tree-graphs. In principle one could complement it with any other condition in order to obtain a well-determined system of equations and unknowns in the factor parameters. In this work we tried other complementary closure equations (including matching of covariance matrix, constrained Kullback-Leiber Divergence minimization, matching of off-diagonal covariances, in addition to 2). However, we found out that 3 were experimentally performing uniformly better on all the cases we analyzed.

Appendix B: Homogeneous Ising Model

In a homogeneous ferromagnetic Ising Model with Hamiltonian $H = -J \sum_{i,j} x_i x_j - h \sum_i x_i$ defined on a $d$-dimensional hypercubic lattice with periodic (toroidal) boundary condition, all Gaussian factors $\phi_a$ are identical and the DC equations (32) at a given inverse temperature $\beta$ read:

\[ \begin{align*}
\sigma_0 &= -\frac{m}{\text{atanhm}} \\
\sigma_1 &= \frac{\epsilon - m^2}{1 - m^2} \sigma_0 \\
y &= m(\gamma_0 + \gamma_1)
\end{align*} \tag{B1} \]

The DC solution is found by solving the above system of 3 fixed-point equations in the Gaussian parameters $y, \gamma_0, \gamma_1$ where $\sigma_0, \sigma_1, \gamma_0, \gamma_1$ equal respectively $\Sigma_{ii}$, $\Sigma_{ij}$, $(2d)^{-1}(\Sigma^{-1})_{ii}$, $(\Sigma^{-1})_{ij}$ for $i, j$ two first lattice neighbors. Here $m = \langle x_i \rangle_{g(a)}$ and $c = \langle x_i x_j \rangle_{g(a)}$ are the moments computed under the distribution $g^{(a)}$:

\[ \begin{align*}
m &= \text{tanh} \left[ z + \text{atanh} (\text{tanh} \Gamma \text{tanh} z) \right] \\
c &= \text{tanh} \left[ \Gamma + \text{atanh} (\text{tanh}^2 z) \right]
\end{align*} \]

where

\[ \begin{align*}
z &= \frac{\beta h}{2d} \left( \frac{1}{\sigma_0 + \sigma_1} \frac{1}{\gamma_0 + \gamma_1} - 1 \right) y \\
\Gamma &= \beta J + \frac{\sigma_1}{\sigma_0^2 - \sigma_1^2} + \gamma_1
\end{align*} \]

The matrix $\Sigma$ is the gaussian covariance matrix whose inverse is parametrized as follows:

\[ \Sigma^{-1} = S^{(d)} = 2d^2 \gamma_0 I_L + \gamma_1 A^{(d)} \]

where $A^{(d)}$ is the lattice adjacency matrix in dimension $d$, whose diagonalization is discussed in the next section.

1. Diagonalization of $A^{(d)}$

The hypercubic lattice in $d$ dimensions can be regarded as the cartesian product of linear-chain graphs, one for each dimension. The adiacency matrix of the whole lattice can be thus expressed as function of the adiacency matrices of the single linear chains, by means of the Kronecker product (indicated by $\otimes$):

\[ A^{(d)} = A^{(1)} \otimes I_L \otimes \ldots \otimes I_L + I_L \otimes A^{(1)} \otimes I_L \otimes \ldots I_L + \ldots + I_L \otimes \ldots \otimes I_L \otimes A^{(1)} \]
where $A^{(1)}$ is the adjacency matrix of a (closed) linear chain of size $L$:

$$A^{(1)} = \begin{bmatrix}
0 & 1 & 0 & \cdots & 0 & 0 & 1 \\
1 & 0 & 1 & \cdots & 0 & 0 & 0 \\
0 & 1 & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & 1 & 0 \\
0 & 0 & 0 & \cdots & 1 & 0 & 1 \\
1 & 0 & 0 & \cdots & 0 & 1 & 0 \\
\end{bmatrix}$$

The above expression allows to compute the spectral decomposition of $A^{(d)}$ just by knowing the spectrum of the adjacency matrix of the linear chain. The matrix $A^{(1)}$ is a special kind of circulant matrix and therefore it can be diagonalized exactly [24]. Its eigenvalues and eigenvectors are shown below:

$$\lambda^{(1)}_x = 2 \cos \left( \frac{2 \pi}{L} x \right) \quad \nu^{(1)}_x = \frac{1}{\sqrt{L}} \left( 1, w_x, w_x^2, \ldots, w_x^{L-1} \right)$$

where $x \in \{0, ..., L - 1\}$ and $w_x = e^{i \frac{2 \pi}{L} x}$.

The spectral decomposition of $A^{(d)}$ reads:

$$\lambda^{(d)}_{x_1, \ldots, x_d} = \sum_{j=1}^{d} \lambda^{(1)}_{x_j} = 2 \sum_{j=1}^{d} \cos \left( \frac{2 \pi}{L} x_j \right)$$

$$\nu_{x_1, \ldots, x_d} = \otimes_{j=1}^{d} \nu^{(1)}_{x_j}$$

We recall now the expression of the eigenvalues of $S^{(d)}$:

$$\lambda_{x_1, \ldots, x_d} = 2d \gamma_0 + 2 \gamma_1 \sum_{j=1}^{d} \cos \left( \frac{2 \pi}{L} x_j \right)$$

The inverse matrix elements $\Sigma_{ii}, \Sigma_{ij}$ can be computed in a straightforward way. In particular, in the thermodynamic limit ($L \to \infty$) their expressions read:

$$\sigma_0 = \frac{1}{\gamma_0} R(r)$$

$$\sigma_1 = \frac{1}{\gamma_0 r} \left[ \frac{2d}{R^2} - R(r) \right]$$

where $r = \frac{2a}{\gamma_0}$ and $R_d(r) = \frac{1}{2} \int_0^\infty dt e^{-dr} [I_0 (rt)]^d$, where $I_0$ is the modified Bessel function of the first kind of order 0.

### 2. Simplified DC equations

It is possible to simplify the original system (B1) in order to get a fixed point equation for the magnetization $m$. By eliminating the variable $y$ and setting $J = 1$ we get

$$z = m \left( \frac{1}{\sigma_0 + \sigma_1} - (\gamma_0 + \gamma_1) \right) + \frac{\beta h}{2d}$$

$$= m \gamma_0 \left( \frac{1}{R_d(r) + \frac{1}{2} \left[ \frac{1}{2d} - R_d(r) \right]} - r - 1 \right) + \frac{\beta h}{2d}$$

$$\Gamma = \beta + \frac{\sigma_1}{\sigma_0 - \sigma_1} + r \gamma_0$$

$$= \beta + \gamma_0 \left( \frac{1}{R_d^2(r) - \frac{1}{2d} \left[ \frac{1}{2d} - R_d(r) \right]^2} + r \right)$$

(B6)

(B7)
Now, putting together Eq.(B1) with Eq.(B6)-(B7) and the definitions (B4)-(B5) we get the following system:

\[ \beta = \text{atanh} \left( \frac{1}{d} k_d(r) (1 - m^2) + m^2 \right) - g_d(r) \frac{\text{atanh} m}{m} - \text{atanh} \left( \tan^2 \left( f_d(r) \text{atanh} + \frac{\beta h}{2d} \right) \right) \]  
\[ m = \tanh \left[ f_d(r) \text{atanh} + \frac{\beta h}{2d} + \right. \]
\[ + \left. \text{atanh} \left( \tanh \left( \beta + g_d(r) \frac{\text{atanh} m}{m} \right) \right) \text{atanh} \left( f_d(r) \text{atanh} + \frac{\beta h}{2d} \right) \right] \]  

where \( k_d(r) = \frac{1-2dR_d(r)}{2d^2 R_d(r)} \), \( g_d(r) = \frac{k_d(r)}{1-k_d(r)^2} + rR_d(r) \), \( f_d(r) = \frac{1}{1+k_d(r)} - (r + 1)R_d(r) \). Such equations can be solved at fixed \( r \) in the variables \( \beta, m \). For \( h = 0 \) the system reduces to a single fixed point equation for \( m = M(m(r), r) \) while \( \beta \) is fixed by (B8).

**Computation of \( \beta_p \)**

For the paramagnetic solution \( m = 0 \) (with \( h = 0 \)) we get the following equation for \( \beta(r) \):

\[ \beta = \text{atanh} \left( \frac{1}{d} R_d(r) - 1 \right) \]  

For \( d \geq 3 \), the maximum value at which a paramagnetic solution exists corresponds to the point \( r = -1 \). Therefore, the value of the critical point \( \beta_p \) is computed by taking the \( r \to -1 \) limit of Eq.(B8):

\[ \beta_p = \text{atanh} \left( 1 - \frac{1}{2} \right) - z \left( \frac{z - 1}{2z - 1} \right) + \frac{z}{2d} \]  

with \( z = 2dR_d(-1) \).

**Computation of \( \beta_m \)**

Eqs. (B8)-(B9) implicitly define a function \( m(r) \) such that \( M(m(r), r) = m \), and thus also \( \beta(r) = \beta(m(r), r) \). We seek to find the point \( m^* = m(r^*) \) and \( \beta_m = \beta(m^*, r^*) \) such that \( \frac{d\beta}{dm}(m^*, r^*) = 0 \). Taking the total derivative of \( \beta(m(r), r) \) we get the equation to be solved

\[ 0 = \frac{d\beta}{dr} = \frac{\partial \beta}{\partial m} \frac{d m}{d r} + \frac{\partial \beta}{\partial m} \frac{d m}{d r} \]

To compute \( \frac{d m}{d r} \) we use its implicit definition,

\[ 0 = \frac{d}{dr} \{ M(m(r), r) - m(r) \} \]
\[ = \left( \frac{\partial M}{\partial m} (m(r), r) - 1 \right) \frac{d m}{d r} + \frac{\partial M}{\partial r} (m(r), r) \]
\[ \frac{d m}{d r} = -\frac{\frac{\partial M}{\partial m} (m(r), r)}{-\frac{\partial M}{\partial m} (m(r), r) - 1} \]

to get finally the \( 2 \times 2 \) system in variables \( m, r \):

\[ \frac{\partial \beta}{\partial r} (m, r) \left( \frac{\partial M}{\partial m} (m, r) - 1 \right) - \frac{\partial M}{\partial r} (m, r) \frac{\partial \beta}{\partial m} (m, r) = 0 \]  
\[ M(m, r) - m = 0 \]
Stability

The stability of a fixed point $m^* = m(r^*)$ can be analyzed by computing $\left. \frac{dM}{dm} \right|_{m^*}$. In particular, starting from the system (B8)-(B9) where $r$ is implicitly defined as $r = R(\beta, m)$, the instability occurs when $\left. \frac{dM}{dm} \right|_{m^*} = 1$. Writing the original system using the definition of $r$ we get $m = M(m, R(\beta, m))$ and $\beta = B(m, R(\beta, m))$. The equation we want to solve is

$$\frac{1}{\partial R/\partial m} = \frac{\partial M}{\partial m} + \frac{\partial M}{\partial r} \frac{\partial R}{\partial m}.$$

To compute $\frac{\partial R}{\partial m}$ we use again its implicit definition:

$$0 = \frac{\partial B}{\partial m} + \frac{\partial B}{\partial r} \frac{\partial R}{\partial m}.$$

The final system to solve is

$$M(m, r) - m = 0 \quad (B13)$$
$$\frac{\partial M}{\partial m} - \frac{\partial M}{\partial r} \frac{\partial B}{\partial m} = 1 \quad (B14)$$

For $d \geq 3$, the solution becomes unstable exactly at the point $(r_m, \beta_m)$ computed through B11-B12.

3. $D=2$

On a 2-dimensional square lattice, the DC solution is qualitatively different w.r.t. $d \geq 3$ because the function $R(r)$ is logarithmically divergent for $r \rightarrow -1$. In such case the maximum value at which the paramagnetic solution exists ($\beta_p = 0.37693$) corresponds to the point $r_p = -0.994843$. The ferromagnetic solution turns out to be stable for $r_m < r < 0$ with $r_m = -0.99405$, corresponding to $\beta_m = 0.388448$ (the point $(r_m, \beta_m)$ is found as a solution of Eq. B13-B14). Therefore there exists a temperature interval $\beta_p < \beta < \beta_m$ in which no stable DC solution can be found.

For finite size lattices the DC solution can still be found numerically, showing similar performances with respect to CVM on both ferromagnetic and spin glass models (Fig. 2). However, especially on ferromagnetic systems DC solution is numerically unstable close to the transition $\beta_p$. One way to reduce numerical instability in such region is to decrease the interpolation parameter $\rho$, typically fixed to 1 for DC. Nevertheless, the meaning of the DC($\rho$) approximation in this case is not clear.

One possible way to improve the DC approximation is to take into account small loops explicitly. In particular, we consider a gaussian family of approximating distribution factorized over plaquettes of $2^d$ spins ($d$ is the number of dimensions). Plaquettes are chosen in such a way that there is no overlap between links in the gaussian distribution. In this way, DC equation are exact on a plaquette tree with only site-overlaps. Results are shown in 2: plaquette-DC (pDC) is in general slightly better than standard DC and comparable to CVM.

4. Finite size corrections

In homogeneous models the gaussian covariance matrix can be diagonalized analytically even for a finite size lattice (of size $L$). Therefore we can compute finite size corrections to the DC solution at a fixed $\beta$, as shown in the following plot:

DC solution turns out to be in good agreement with MC results; on the other hand, BP does not take into account at all finite size corrections because of the local character of the approximation.
Figure 2. Left: distribution of non-overlapping plaquettes (in grey) on a 2-dimensional square lattice. Right: correlations on 2-dimensional Ising Model on square lattice of size $L = 10$ at $\beta = 0.36$, with 0 external field and couplings drawn from a uniform distribution in $(0.5, 1.5)$. Comparison of DC, pDC, BP and CVM

Figure 3. Finite size correction of equilibrium correlations at $\beta = 0.215$ on a 3-dimensional cubic lattice of size $L \in \{5, ..., 15\}$ with $h = 0, J = 1$. Comparison of BP and DC solutions with Monte-Carlo simulations.

5. Scaling of $\beta_c$ in the high dimensional limit

Starting from the expression of the critical inverse temperature $\beta_p$ it is possible to compute the $1/d$ expansion in the high-dimensional limit. We recall the expression of the critical temperature (B10):

$$\beta_p = \text{atanh} \left(1 - \frac{1}{z}\right) - z \left(\frac{z - 1}{2z - 1}\right) + \frac{z}{2d}$$

where $z = 2dR_d (-1)$. 
Defining \( x = 1/d \) and expanding around \( x = 0 \) we get:

\[
\frac{1}{2d\beta p} = 1 - \frac{1}{2} d^{-1} - \frac{1}{3} d^{-2} - \frac{13}{24} d^{-3} - \frac{979}{720} d^{-4} - \frac{2039}{480} d^{-5} + O(d^{-6}).
\]

This expansion is exact up to the \( d^{-4} \) order (the correct coefficient of \( d^{-5} \) is \( -\frac{2009}{480} \)) \([22]\). For comparison, Mean Field is exact up to the \( d^0 \) order, Bethe is exact up to the \( d^{-1} \) order, and Loop-Corrected Bethe and Plaquette-CVM are exact up to the \( d^{-2} \) order.

For the sake of completeness, we report the series expansion of \( R_d(-1) \) around \( x = 0 \):

\[
R_d(-1) = \frac{1}{2} d^{-1} + \frac{1}{4} d^{-2} + \frac{3}{8} d^{-3} + \frac{3}{4} d^{-4} + \frac{15}{8} d^{-5} + \frac{355}{64} d^{-6} + \frac{595}{32} d^{-7} + O(d^{-8}).
\]