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Graph Ginzburg–Landau: discrete dynamics, continuum limits, and applications. An overview

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1 Introduction

In [BF12, BF16] the graph Ginzburg–Landau functional,

$$F_\varepsilon(u) := \frac{\varepsilon}{2} \sum_{i,j \in V} \omega_{ij}(u_i - u_j)^2 + \frac{1}{\varepsilon} \sum_{i \in V} W(u_i), \tag{1}$$

was introduced. Here u is a real-valued function on the node set V of a simple[1], undirected graph (with u_i its value at node i), $\omega_{ij} \geq 0$ are edge weights which are assumed to be positive on all edges in the graph and zero between non-neighbouring nodes i and j, ε is a positive parameter, and W is a double well potential with wells of equal depth. A typical choice is the quartic polynomial $W(x) = x^2(x-1)^2$ which has wells of depth 0 at $x = 0$ and $x = 1$, but we will encounter some situations where other choices are useful or even necessary.

This introduction of this graph-based functional was inspired by its continuum counterpart,

$$\mathcal{F}_\varepsilon(u) := \varepsilon \int_\Omega |\nabla u|^2 \, dx + \frac{1}{\varepsilon} \int_\Omega W(u) \, dx, \tag{2}$$

which was introduced into the materials science literature to model phase separation (such as the separation of oil and water) [CH58], but has since been extensively used in the image processing literature as well, because of its intimate connection to the total variation functional, which we will explore further below. In $\mathcal{F}_\varepsilon(u)$ above, u is a real-valued function on a domain $\Omega \subset \mathbb{R}^n$ and ε and W are as before. For small positive values of ε, minimization of $\mathcal{F}_\varepsilon$ will lead to functions u which take values close to the wells of W (say 0 and 1) while keeping the L^2 norm of the gradient small. Minimizers of $\mathcal{F}_\varepsilon$[2] tend to have regions where $u \approx 0$ and regions where $u \approx 1$, with transition regions in between whose length is (approximately) minimal and whose thickness is of order ε.

The study of a graph-based version of the Ginzburg–Landau functional in [BF12] was motivated by the translation of the phase separating behaviour of its continuum counterpart $\mathcal{F}_\varepsilon$ into node clustering behaviour on a graph. Forcing the double well potential term to have a small value has the same effect as before: It drives u to take values close to 0 or 1. The term $\sum_{i,j} \omega_{ij}(u_i - u_j)^2$ encourages u to take similar values on those nodes which are connected by a highly weighted edge. These two effects together result in a function u which can be interpreted as a labelling function which indicates which of two clusters a node in the graph belongs to, based on the (weighted) structure of the graph. Combined with either an additional fidelity term in the functional, which weakly enforces compatibility of the final result with a priori known

[1] We call a graph simple if it has no self-loops and at most one edge between each pair of nodes.

[2] Careful readers will have noted that minimizers of $\mathcal{F}_\varepsilon$ are given by constant functions which take value 0 everywhere or value 1 everywhere. In practice $\mathcal{F}_\varepsilon$ is always minimized with some additional term or constraint present as we will see shortly.

data, or a hard mass constraint (if the desired cluster sizes are known), the graph Ginzburg–Landau functional was sucessfully used in [BF12] for various data clustering and classification[3] and image segmentation[4] tasks.

The method used in [BF12] to minimize the graph Ginzburg–Landau functional again took its inspiration from a practice which is common in the world of continuum variational methods[5]: using a gradient flow. This approach consists of introducing an artificial time parameter and computing a solution to $u_t = -\text{grad}\, F_\varepsilon$. For the graph Ginzburg–Landau functional, this leads to the graph Allen–Cahn equation,

$$\frac{d}{dt} u_i = -\varepsilon(\Delta u)_i - \frac{1}{\varepsilon} W'(u_i) \tag{3}$$

which earns its name due to its great similarity to the (continuum) Allen–Cahn equation[6], which is the L^2 gradient flow of $\mathcal{F}_\varepsilon$ [AC79]. In the equation above we have used the suggestive notation

$$(\Delta u)_i := \sum_j \omega_{ij}(u_i - u_j). \tag{4}$$

In fact, the object in (4) has been extensively studied by the field of spectral graph theory [Chu97] and is known as the (combinatorial) graph Laplacian.

In [MKB13] a second method was devised for (approximately) minimizing the graph Ginzburg–Landau functional: the graph Merriman–Bence–Osher (MBO) scheme. Also this method took its inspiration from an existing continuum method. The MBO scheme (or threshold dynamics scheme) was originally introduced as a method for approximating flow by mean curvature [MBO92, MBO93]. It consists of alternatively diffusing the indicator function of a set and thresholding the diffused result back to an indicator function. On a graph, this gives rise to the following iterative scheme:

$$\begin{aligned}
u_i^0 = (\chi_S)_i &:= \begin{cases} 1, & \text{if } i \in S, \\ 0, & \text{if } i \in S^c, \end{cases} \\
u^{n+\frac{1}{2}} &\text{ solves} \\
&\begin{cases} u(0) = u^n, \\ \frac{d}{dt} u_i = -(\Delta u)_i, & \text{on } (0, \tau], \end{cases} \\
u^{n+1} &= \begin{cases} 1, & \text{if } u^{n+\frac{1}{2}}(\tau) \geq \frac{1}{2}, \\ 0, & \text{if } u^{n+\frac{1}{2}}(\tau) < \frac{1}{2}. \end{cases}
\end{aligned} \tag{5}$$

On an intuitive level, one can think of the thresholding step (going from $u^{n+\frac{1}{2}}$ to u^n) as (approximately) mimicking the effect of the nonlinear term $-\frac{1}{\varepsilon} W'(u_i)$ in the Allen–Cahn equation. The MBO scheme is usually easier to implement than the nonlinear Allen–Cahn equation.

Both the Allen–Cahn and MBO approach have been used successfully for various applications in later papers, e.g. [HLPB13, MKB13, GCMB⁺14, HSB15, CvGS⁺17, MBC18], and for the former convergence has been proven [LB17]. At the end of this overview paper we will

[3]Data clustering refers to the process of grouping data points together without a priori knowledge of the classes —except perhaps class size– while data classification refers to that process using such prior knowlwedge.

[4]Image segmentation is the process of extracting specific structures from an image. For a digital image this can be interpreted to mean clustering or classification of the image's pixels.

[5]Variational methods broadly refer to the practice of modelling a system as the minimizer of a given function(al).

[6]Note that the minus sign in the Laplacian term is not a mistake: Different from the continuum Laplacian, the graph Laplacian is positive semi-definite.

discuss some of these applications, but first we will dive deeper into the theoretical understanding of the Ginzburg–Landau functional and its related dynamics that has been built since the functional's introduction in [BF12]. These theoretical studies can roughly be divided into two categories: those that are concerned with the functional or the dynamics on the discrete graph level and those that try to bridge the gap between the discrete and continuum worlds. In Section 2 we take a look at the former and in Section 3 we discuss the latter. In Section 4 we give an overview of some applications of these methods.

2 Discrete dynamics

The graph Laplacian which we discussed above is an important operator when studying discrete dynamics on graphs. As is well known from spectral graph theory [Chu97], the spectral properties of the graph Laplacian tell us important information about the properties of the underlying graph (such as its number of connected components). Conversely, any graph dynamics driven by the graph Laplacian will be highly dependent on the graph structure.

It is somewhat misleading to talk about *the* graph Laplacian, as there are different versions of the discrete Laplacian that appear in the literature. To understand their differences, we need to consider the node degree

$$d_i := \sum_{j\in V} \omega_{ij}.$$

The three most commonly encountered graph Laplacians are the combinatorial graph Laplacian defined above, the random walk graph Laplacian, which has an additional factor d_i^{-1} on the right hand side compared to the combinatorial graph Laplacian in (4), and the symmetrically normalised graph Laplacian $d_i^{-1/2}\sum_j \omega_{ij}\left(d_i^{-1/2}u_i - d_j^{-1/2}u_j\right)$.

Where we encountered the combinatorial graph Laplacian in the dynamics above, we can also consider versions which use the random walk or symmetrically normalised graph Laplacian. In fact, by introducing the parameter r, we can capture both the combinatorial ($r = 0$) and random walk Laplacians ($r = 1$) in the same definition:

$$(\Delta u)_i := d_i^{-r} \sum_j \omega_{ij}(u_i - u_j). \tag{6}$$

Taking the gradient flow of the graph Ginzburg–Landau functional with respect to the topology generated by the inner product

$$\langle u, v\rangle_{\mathcal{V}} := \sum_{i\in V} u_i v_i d_i^r$$

on the space of real-valued node functions $\mathcal{V} := \{u : V \to \mathbb{R}\}$, naturally leads to an Allen–Cahn equation which uses the generalised definition of the graph Laplacian from (6)[7]. The symmetrically normalised Laplacian cannot be incorporated in this framework and we will not consider it further here.

The two main discrete dynamics that are studied in the context of the graph Ginzburg–Landau functional are those generated by the graph Allen–Cahn equation and the graph MBO scheme which are explained in the previous section. For both of their continuum counterparts it is known that they approximate flow by mean curvature in a sense that can be made precise in the form of various limiting arguments. In its geometric formulation, (continuum) flow by

[7] Using this inner product, the Allen–Cahn gradient flow also picks up a factor d_i^{-r} in the $\frac{1}{\varepsilon}W'(u_i)$ term. Alternatively, we can redefine the double well potential term in F_ε to be $\frac{1}{\varepsilon}\langle W \circ u, \chi_V\rangle_{\mathcal{V}}$, in which case the gradient flow remains unchanged as in (3). Both choices appear in the literature.

mean curvature of a Euclidean subset is obtained by letting its boundary evolve with a normal velocity at each point proportional to the boundary's curvature at that point [Bra78, AC79]. The possibility of singularity formation during this process has given rise to different formulations of continuum flow by mean curvature, such as the level set description [CGG91, ES91, ES92a, ES92b, ES95]. In [BK91] and [ESS92] it was proven that solutions of the continuum Allen–Cahn equation converge (when $\varepsilon \to 0$) to solutions of the continuum flow by mean curvature. The first paper does this in the radial case (where flow by mean curvature is well understood), while the second shows that the Allen–Cahn solutions converge to viscosity solutions of the level set equation for continuum flow by mean curvature. Also solutions of the continuum MBO scheme converge to solutions of the continuum flow by mean curvature (in some appropriate senses) when $\tau \to 0$ [Eva93, BG95].

It is therefore reasonable to ask if similar connections can be found between the various discrete dynamics. In particular the following questions have been considered: (a) Are the graph Allen–Cahn equation and MBO scheme related and if so, how? (b) Can a graph-based flow by mean curvature be defined in a way that preserves important properties of its continuum counterpart? Specifically, (c) are the graph Allen–Cahn equation and MBO scheme approximations of graph based flow by mean curvature in any rigorous sense?

In [vGGOB14] these questions were first asked and, in the case of question (b), partly answered. In [vGGOB14] (and its sequel [vG19]) a graph-based version of the variational formulation for flow by mean curvature, which was originally given by [ATW93, LS95] in the continuum, was introduced[8]: Given an initial node set S_0, a discrete time step ($\Delta t > 0$) sequence of node sets evolving by graph-based mean curvature flow is defined by

$$S_n \in \underset{S \subset V}{\operatorname{argmin}} \, \mathrm{TV}(\chi_S) + \frac{1}{\Delta t} \langle \chi_S, \mathrm{sd}_{n-1} \rangle_{\mathcal{V}}. \tag{7}$$

Here sd_{n-1} is a signed distance to the set S_{n-1} from the previous iteration and the graph total variation is defined as

$$\mathrm{TV}(u) := \frac{1}{2} \sum_{i,j \in V} \omega_{ij} |u_i - u_j|.$$

In particular, we note that

$$\mathrm{TV}(\chi_S) = \sum_{\substack{i \in S \\ j \in S^c}} \omega_{ij} \tag{8}$$

is the graph cut between the node subset S and its complement (a concept known from graph theory).

Above we have been a bit vague in defining the signed distance sd_{n-1}. This was done on purpose, as it is still a topic of ongoing research what influence the choice of distance has on the resulting flow. In [vGGOB14] the signed distance was taken to the boundary of the set S_{n-1}, which was defined to be the union of the set of nodes in S which have a neighbour in S^c and the set of nodes in S^c which have a neighbour in S. While this definition gives rise to a well-defined flow on a given graph and is an obvious discretisation of the continuum distance used in [ATW93, LS95], it is unstable with respect to small perturbations in the graph structure. Consider 'completing' a given graph by adding an edge with a very small positive

[8]In the same paper, also a graph-based (mean) curvature,

$$(\kappa_S)_i := d_i^{-r} \begin{cases} \sum_{j \in S^c} \omega_{ij}, & \text{if } i \in S, \\ -\sum_{j \in S} \omega_{ij}, & \text{if } i \in S^c, \end{cases}$$

was introduced, with the property that $\mathrm{TV}(\chi_S) = \langle \kappa_S, \chi_S \rangle_{\mathcal{V}}$.

weight between every pair of non-neighbouring nodes. If we expect flow by mean curvature to resemble a diffusion generated process, as per our question (c) above, such a small perturbation of the edge weights should not have a large impact on the resulting flow. This perturbation however, does have a major impact on the boundaries of node subsets: For any nonempty proper subset of V, every node in the graph is now in its boundary. This suggests that to be able to answer question (c) positively, a different notion of distance needs to be employed in the definition of graph flow by mean curvature. This is a subject of current research by the author and coauthors.

It should also be noted that the variational approach to flow by mean curvature on graphs is different from the 'partial difference equation on graphs' approach in [ECED14].

Most progress has been made on question (a): How are the graph MBO scheme and Allen–Cahn equation related? The answer, as given in [BvGcpa], is that MBO corresponds to a specific time discretisation of Allen–Cahn, with some important caveats which we will address below.

First we will redefine the graph Allen–Cahn equation slightly:

$$\frac{d}{dt}u = -\Delta u - \frac{1}{\varepsilon}W' \circ u.$$

Comparing this with (3) we see that ε is lacking from the Laplacian term. The ε has been removed with an eye to the limiting behaviour for $\varepsilon \to 0$ which we will discuss in more detail below. From the point of view of the discrete dynamics, we can simply interpret this as a rescaling of time.

We partly discretise the Allen–Cahn equation above with a time step τ: We treat the diffusion term continuously in time, while using an implicit Euler discretisation for the potential term:

$$u^{k+1} = e^{-\tau\Delta}u^k - \frac{\tau}{\varepsilon}W' \circ u^{k+1}. \tag{9}$$

We note that $e^{-\tau\Delta}u_k$ is the solution at time τ of the graph diffusion equation $\frac{d}{dt}u = -\Delta u$ with initial condition u^k. This time discretisation addresses one obvious difference between the Allen–Cahn equation and MBO scheme: The former is continuous in time, while each iteration of the latter generates outputs at discrete times. The second immediately noticeable discrepancy between these two dynamics, is that MBO produces binary ($\{0,1\}$-valued) results at a given node in each iteration, while solutions of the Allen–Cahn equation a priori can have any real value at a node. To deal with this, we change the (discretised) Allen–Cahn equation further: Instead of using a continuous function W as double well potential, such as the quartic polynomial given above, we use the double obstacle potential:

$$W(x) := \begin{cases} \frac{1}{2}x(1-x), & \text{if } x \in [0,1], \\ +\infty, & \text{otherwise.} \end{cases}$$

The non-smoothness of this potential requires us to interpret W' in a subdifferential way. This is done rigorously in [BvGcpa], where it is concluded that for $\lambda := \frac{\tau}{\varepsilon} = 1$, the iterates of (9) are the same as the iterates of the graph MBO scheme (5). Moreover, every sequence $\tau_n \to 0$ has a subsequence whose corresponding sequence of solutions to (9) converges pointwise to a solution of the graph Allen–Cahn equation (3). If $0 < \lambda < 1$ the iterates of (9) correspond to an MBO-like scheme with a relaxed thresholding step, in which the hard thresholding step function is replaced by a piecewise linear continuous approximation. This allows the semi-discrete scheme to avoid pinning[9] in certain situations, which can be of practical interest.

[9]In this context, pinning describes the trivial dynamics which can occur in the MBO scheme when τ is so small that at every node the value of $u^{n+\frac{1}{2}}$ is on the same side of $\frac{1}{2}$ as in u^n and thus $u^{n+1} = u^n$ and no more changes occur. For more information, see [vGGOB14, vG19].

In [BvGepb] the above procedure, which relates the graph Allen–Cahn equation to the graph MBO scheme, is applied to a version of the Allen–Cahn equation with an additional term which assures that mass is conserved along iterates (where the mass of a node function is defined to be $\mathcal{M}(u) := \sum_{i\in V} d_i^r u_i$). The resulting mass preserving MBO scheme corresponds to a version of the one introduced in [vG18] for (approximately) minimizing the pattern forming Ohta–Kawasaki functional on graphs.

We close this section with a quick return to question (c). Even though the search for an explicit relationship between the graph Allen–Cahn equation and MBO scheme on the one hand and graph flow by mean curvature on the other is still open, there are some preliminary results worth mentioning in this context. These results are also of interest in their own right and are formulated in the language of Γ-convergence.

The notion of Γ-convergence is specifically tailored to minimization problems. Its precise definition can be found in any of the standard works on the topic [Bra02, DM93] and we will not repeat it here. For our present purposes it is enough to remember the main result which makes this a worthwhile concept: If a sequence of function(al)s (f_n) Γ-converges to a limit function f_∞ and (x_n) is a sequence such that x_n minimizes f_n, then every limit point of (x_n) is a minimizer of f_∞.

In [vGB12] it was proven that the graph Ginzburg–Landau functionals $\frac{1}{\sqrt{\varepsilon}}F_{\sqrt{\varepsilon}}$[10] Γ-converge (when $\varepsilon \to 0$) to a limit functional that takes the value $\mathrm{TV}(u)$ when $u = \chi_S$ for some node set S and $+\infty$ otherwise. This mirrors a well-known result from [MM77, Mod87] which states that in the continuum the functionals $\mathcal{F}_\varepsilon$ Γ-converge (when $\varepsilon \to 0$) to a limit functional that is equal to the total variation on indicator functions and $+\infty$ otherwise.

Because flow by mean curvature is defined in (7) via (approximate) minimization of total variation (and because the first variation of total variation is graph curvature in the sense of footnote 8), this limiting result which connects the functional which generates the Allen–Cahn equation as a gradient flow to the total variation teases a connection between Allen–Cahn and flow by mean curvature on graphs.

A similarly promising Γ-convergence result is formulated for the graph MBO scheme in [vG18]. To understand this result, we need to consider the Lyapunov functional for the graph MBO scheme, introduced in [vGGOB14] (following the introduction of a similar functional for the continuum MBO scheme in [EO15]):

$$J_\tau(u) := \langle 1-u, e^{\tau\Delta}u\rangle_{\mathcal{V}}.$$

This is a Lyapunov functional for the graph MBO scheme, in the sense that $k \mapsto J(u^k)$ is non-increasing if (u^k) is a sequence of iterates generated by the graph MBO scheme in (5). Moreover, these iterates can also be obtained as minimizers of the first variation of J_τ:

$$u^{k+1} \in \operatorname*{argmin}_v dJ_\tau(v;u^k), \quad \text{where} \quad dJ_\tau(v;u^k) = \langle 1-2e^{-\tau\Delta u^k}, v\rangle_{\mathcal{V}}.$$

The minimization is over $[0,1]$-valued node functions v. We thus see that, at nodes where $1-2^{-\tau\Delta u^k} < 0$, minimization of $dJ_\tau(v;u^{k+1})$ forces v to take the value 1 at that node. Similarly, at nodes where $1-2^{-\tau\Delta u^k} > 0$ the function v will take value 0. Hence, we recover the MBO scheme (up to the underdetermined value at nodes where $1-2^{-\tau\Delta u^k} = 0$).

In [vG18] it was proven that $\frac{1}{\tau}J_\tau$ Γ-converges to the same limit functional we encountered as Γ-limit of $\frac{1}{\sqrt{\varepsilon}}F_{\sqrt{\varepsilon}}$ (when $\varepsilon \to 0$), i.e. the functional which is equal to $\mathrm{TV}(u)$ when $u = \chi_S$ for some node set S and $+\infty$ otherwise. For the same reasons as above, this is a promising sign that also the graph MBO scheme has links to flow by mean curvature.

[10]The rescaling $\frac{1}{\sqrt{\varepsilon}}F_{\sqrt{\varepsilon}}$ amounts to removing the ε prefactor from the first term in (1). The reason for this is that, contrary to the corresponding term in the continuum functional $\mathcal{F}_\varepsilon$, this discrete gradient term is finite even for binary functions u and so no rescaling with ε is needed to keep this term finite in the limit $\varepsilon \to 0$.

3 Continuum limits

In the previous section we discussed dynamics and some Γ-convergence results at a discrete level: All the dynamics and convergence results happened against the fixed background of a given finite graph. We can also consider the question what happens if we let the graphs change in such a way that we can reasonably talk about continuum limits.

We will discuss here three different ways to consider graph limits: Γ-convergence along a sequence of graphs generated through mesh refinements; Γ-convergence along a sequence of graphs generated through sampling; and graphon limits. The results and papers discussed in this section typically consider W to be a smooth double well potential, such as the quartic polynomial given in Section 1[11].

In [vGB12] a sequence of 4-regular graphs is generated by refining a regular mesh on the flat torus. Identifying the torus with $[0,1]^2$ (with periodic boundary conditions) it can be discretised by a square grid with horizontal and vertical spacing $\frac{1}{N}$, such that the resulting graph will have N^2 points. Choosing the edge weights $\omega_{ij} = \frac{1}{N}$ on all edges of this square grid, we denote the resulting graph Ginzburg–Landau functional (obtained from $\frac{1}{\sqrt{\varepsilon}} F_{\sqrt{\varepsilon}}$ in (1); see footnote 10) by $F_{\varepsilon,N}$. By choosing $\varepsilon = N^{-\alpha}$ for $\alpha > 0$ large enough (depending on the growth rate of W near its wells) and letting $N \to \infty$, $F_{\varepsilon,N}$ is shown to Γ-converge to a functional which is equal to the anistropic total variation for $\{0,1\}$-valued functions of bounded variation (and $+\infty$ otherwise), with the anisotropies aligned with the horizontal and vertical directions of the grid: $\int |u_x| + |u_y| \, dx$.

The paper [vGB12] also considers a second sequence of discrete Ginzburg–Landau functionals generated by directly discretising the continuum Ginzburg–Landau functional in (2) using forward finite differences for the gradient and equidistant Riemann sums for the integrals. This leads to a different scaling in the discrete functional: The gradient term has a factor ε (where this was N^{-1} in $F_{\varepsilon,N}$) and the potential term a factor $\varepsilon^{-1}N^{-2}$ (which was ε^{-1} in $F_{\varepsilon,N}$). Again setting $\varepsilon = N^{-\alpha}$, but this time with $\alpha > 0$ small enough (depending on the polynomial growth of W') a different Γ-limit is recovered: a functional which is proportional[12] to the standard isotropic total variation $\int |\nabla u| \, dx$ for $\{0,1\}$-valued functions of bounded variation (and $+\infty$ otherwise). We see that the graph functional $F_{\varepsilon,N}$ retains information about the structure of the graph (the horizontal and vertical directions of its grid) even in the limit, while the discrete functional which is obtained using standard discretisation techniques from numerical analysis does not retain this information (as one would want for consistency of a numerical method).

An important step in deriving the discrete-to-continuum results in [vGB12] discussed above is the identification of the graph-based functions with continuum-based functions, as the setup of Γ-convergence requires the domain of the functionals along the sequence, $F_{\varepsilon,N}$, to agree with the domain of the limit functional. This is done by identifying the graph-based functions with their piecewise constant extensions, which is possible because the grid structure of the graph gives a tesselation of $[0,1]^2$. The next type of discrete-to-continuum Γ-convergence results we discuss here use a different technique which can be used in less regularly structured situations.

In [GTS16], the authors consider a sequence of graphs constructed by sampling ever more points X_i (which serve as the graphs' vertices) from $D \subset \mathbb{R}^d$ according to some measure ν and constructing an edge structure via the weights $\omega_{ij} := \varepsilon^{-d}\eta(|X_i - X_j|/\varepsilon)$, where η is some given kernel (which can be taken to have compact support if complete graphs are to be avoided). The identification of functions defined on such graphs with functions defined on D is accomplished using ideas from optimal transport theory. The key idea is not to consider graph-based functions

[11]Which is not to say these result could not be generalised to include non-smooth potentials such as the double obstacle potential considered in Section 2.

[12]With proportionality factor depending on the explicit form of W.

u_n and continuum-based functions u by themselves, but look at function-measure pairs (μ_n, u_n), (μ, u), with $u_n \in L^p(D, \mu_n)$ and $u \in L^p(D, \mu)$ and express convergence using a transportation distance between such pairs:

$$d_{TL^p}((\mu_n, u_n), (\mu, u))^p := \inf_{\pi \in \Gamma(\mu_n, \mu)} \int_D \int_D (|x-y|^p + |u_n(x) - u(y)|^p)\, d\pi(x,y),$$

where $\Gamma(\mu_n, \mu)$ denotes the set of all Borel measures on $D \times D$ whose marginal on the first variable is μ_n and whose marginal on the second variable is μ. By letting $\mu_n := \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$, the empirical measure supported at the sampled points, this provides the discrete-to-continuum identification needed to make sense of Γ-convergence statements.

This tool was used in [GTS16] to prove that a rescaled graph total variation, $\varepsilon^{-1}n^{-2}\mathrm{TV}$, on such sampled graphs as described above, Γ-converges[13] to a constant (depending on η) times a weighted continuum total variation, with the weight depending on the sampling measure ρ:

$$\mathrm{TV}(u; \rho^2) := \sup\left\{ \int_D u \operatorname{div} \phi\, dx : \forall x \in D\ |\phi(x)| \le \rho^2(x), \phi \in C_c^\infty(D, \mathbb{R}^d) \right\}.$$

These discrete-to-continuum indentification methods have since been used in a series of papers to prove discrete-to-continuum Γ-convergence results for many different functionals, including the Ginzburg–Landau functional [TSVB+16, TKSSA17, TS18, ST19, TvG].

A third and final approach to discrete-to-continuum graph limits that should be mentioned here, is that of graphons [LS06, BCL+08, BCL+11, BCL+12, Gla15] (see [BCCL18] and references therein for recent generalisations), as applied in various recent papers [Med14, HFE18b, HFE18a]. A graphon is a measurable symmetric function K on $[0,1]^2$. By partitioning $[0,1]$ into n intervals of length $\frac{1}{n}$ and defining edge weights $w_{ij}^n := n^2 \int_{[\frac{i}{n}, \frac{i+1}{n}) \times [\frac{j}{n}, \frac{j+1}{n})} K(x,y)\, dx\, dy$, every graphon gives rise to a sequence of simple unweighted graphs. Conversely, any simple unweighted graph $G = (V(G), E(G))$ with $|V(G)| = n$ can be identified with a graphon by setting

$$K(x,y) := \begin{cases} 1, & \text{if } (i,j) \in E(G) \text{ and } (x,y) \in [\frac{i}{n}, \frac{i+1}{n}) \times [\frac{j}{n}, \frac{j+1}{n}), \\ 0, & \text{otherwise.} \end{cases}$$

A sequence of simple graphs (G_n) is called convergent if $t(F, G_n)$ is convergent for all simple graphs F, where

$$t(F, G_n) := \frac{\hom(F, G_n)}{|V(G_n)|^{|V(F)|}}$$

is the density of homomorphisms (i.e. adjacency preserving maps from $V(F)$, the vertex set of F, to $V(G_n)$, the vertex set of G_n). It is a fundamental result in the study of graphons that for each convergent sequence of simple graphs (G_n) there exists a graphon K such that, for all simple graphs F,

$$t(F, G_n) \to t(F, K) := \int_{[0,1]^{|V(F)|}} \prod_{(i,j) \in E(F)} K(x_i, x_j)\, dx.$$

In [HFE18a] convergence (with error estimates) of minimizers is proved for a discrete functional consisting of an ℓ^2 fidelity term plus the discrete gradient term from F_ε[14]. These minimizers are

[13] Where $\varepsilon \to 0$ slow enough as $n \to \infty$ for the sampled graphs to be connected with high probability.

[14] The paper considers the more general case where the gradient term has a power $p \in [1, \infty)$ instead of 2.

shown to converge to the minimizer of a continuum functional with a similar L^2 fidelity term and the L^2 norm[15] of the nonlocal gradient[16]

$$\nabla_K u(x,y) := K(x,y)^{1/2}(u(y) - u(x)),$$

where the kernel K is determined as graphon limit of the graphs determined by the edge weight matrices in the gradient term along the discrete sequence. To the best knowledge of the author, the graphon approach has not yet been applied to the graph Ginzburg–Landau functional.

4 Applications

The applications of PDE-inspired methods on graphs are numerous, even when we restrict ourselves to those which directly use (variants of) the graph Ginzburg–Landau functional. In this section we present a short selection of such applications.

One of the applications studied in [BF12, BF16] is image segmentation in the presence of some a priori information. A graph is constructed from a digital image in the following way: Each pixel in the image is represented by a node in the graph. A weighted edge structure is created via $\omega_{ij} := e^{\|z_i - z_j\|^2/\sigma^2}$, where z_i is a feature vector associated with pixel i. In simple cases, such a feature vector consists of the nine grey values of the pixels in the three by three window around the pixel (or the values from a larger window; or, in the case of colour images or hyperspectral images, the $9c$ intensity values, where c is the number of colour/spectral channels in the image), but it can also incorporate, say, texture filters. In principle such an edge weight is computed for each pair of pixels (i,j) in the graph, but since this is computationally unfeasible in practice, [BF12, BF16] proposes to use the Nyström matrix completion technique [Nys28, Nys29, BFCM02, FBCM04] which approximates the full weight matrix based on a sampled subset of pairs. The a priori known pixel assignments are incorporated into the functional via a fidelity term. The resulting Allen–Cahn equation with fidelity term is solved by combining a convex splitting method with a projection onto the top eigenvectors of the graph Laplacian (which in turn makes the Nyström method even more valuable, as it allows for a quick computation of the top eigenvectors and eigenvalues, without the need to compute the full weight matrix). In [BF12, BF16] the same method is also applied to other data classification and clustering methods, which each require their own context specific graph construction (and fidelity terms or mass constraints), but can all be tackled with the same general Allen–Cahn/Nyström approach. In [CvGS+17] this same method was incorporated into an image segmentation and measurement method developed to be employed in zoological research (specifically for the automated detection and measurement of the blaze (white spot) on a bird's head in pictures). It should also be mentioned here that image segmentation can be achieved through other PDE-inspired graph-based methods as well, see for example [ELT16] and references therein.

The Ginzburg–Landau based method for image segmentation and data clustering and classification has been adapted and extended to allow for multiple phases [GCMB+13, GCFP13, MGCB+14, GCMB+14, GCFP15], high-dimensional data (such as hyperspectral images) [HLB12, HSB15, MMK17], and computation with the MBO scheme instead of the Allen–Cahn equation [MKB13]. It has also proven useful for clustering signed graphs, i.e. graphs in which the edge weights can have negative, as well as non-negative, values, with the (highly) negatively weighted edges connecting pairs of nodes that should not be clustered together [CPvG]. In this case the MBO scheme uses a signed graph Laplacian, which is the sum of a regular graph Laplacian on the graph induced by the positively weighted edges and a signless Laplacian (see (10) below) on the graph induced by the negatively weighted edges.

[15] Or L^p norm.

[16] Or $Ku(x,y) := K(x,y)^{1/p}(u(y) - u(x))$.

We end with an application which uses a variant of the graph Ginzburg–Landau functional: (approximate) computation of the maximum cut of a graph. A classic task in graph theory [Kar72, GJS74, PT95] (with some applications in physics and engineering [BGJR88, DL94a, DL94b, EJR03, MM06, GM19]) is to find the maximum value the graph cut from (8) can have, if we allow S to be any subset of the graph's vertex set. To tackle this task, in [KvG] the signless graph Ginzburg–Landau functional is introduced:

$$F_\varepsilon^+(u) := \frac{\varepsilon}{2}\sum_{i,j\in V}\omega_{ij}(u_i+u_j)^2 + \frac{1}{\varepsilon}\sum_{i\in V}W(u_i).$$

Note that the only apparent difference between F_ε^+ and F_ε is the plus sign instead of the minus sign in (what in F_ε was) the discrete gradient term of the functional. There is, however, a significant second difference: While in F_ε the specific placement of the two wells of W was not very important (we chose the well locations to be at 0 and 1 to make their connection to indicator functions of node sets more immediate), in F_ε^+ it is important that the wells are placed symmetrically with respect to the origin, e.g. $W(x) := (x-1)^2(x+1)^2$ with wells located at ± 1. The reason for this is that we want minimizers of F_ε^+ (without any further constraints imposed) to be (approximately) binary and not just constant functions equal to, say, 0.

Heuristically it quickly can be seen that in minimizing F_ε^+, the first term encourages u to take different values in strongly connected nodes, thereby leading to high graph cut values. While any hard guarantees of this kind (which are unlikely, given that accurately solving the maximum cut problem is NP-hard [TSSW00]) or even lower bound guarantees on the performance of the method (how close are minimizers to a maximum cut?) are lacking, in practice the method gives results that are competitive with those of the well-established Goemans–Williamson method [GW95].

The practical (approximate) minimization of F_ε^+ is achieved via a variant of the MBO scheme, which uses a signless graph Laplacian [DR94, HS04, CRS07, JC⁺10, BH11],

$$(\Delta^+ u)_i := d_i^{-r}\sum_j \omega_{ij}(u_i+u_j), \tag{10}$$

instead of one of the usual graph Laplacians. This method is faster and scales to much larger graphs than the Goeman–Williamsion method on the same hardware. An extension of these methods to mulitple phases is in development by the authors of [KvG].

5 Conclusions

In this overview article we have looked at multiple appearances of the graph Ginzburg–Landau functional (and related concepts) in both theoretical studies and applications in recent literature. It is a paradigmatic example of a variational method on graphs which is inspired by ideas, concepts, and results from the area of continuum variational methods, and which has been very successfully applied in various practical contexts, yet is also still a central object in an area of active study.

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