Applying PDE methods on graphs to find approximate solutions to the Max-Cut and Max-K-Cut problems.

Blaine Keetch, Yves van Gennip

University of Nottingham

Blaine.Keetch@nottingham.ac.uk, y.vangennip@nottingham.ac.uk

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The Idea

- Define differentiable graph functionals with a variable ε, which as $\varepsilon \to 0$ the functionals Γ-converge to NP-hard objective functionals.
- If the functionals Γ-converge and satisfy an equi-coercive property, then as $\varepsilon \to 0$ minimizers of the differentiable graph functional will converge to minimizers of the objective functional.
- Use methods from PDE theory to find in practice minimizers of the differentiable functions which (hopefully) approximate minimizers of the objective functional.

Preliminaries

- Let $G = (V, E, \omega)$, then we define the weight on an edge $(i, j) \in E$ by ω_{ij} and the degree of a node by $d_i := \sum_{j \in V} \omega_{ij}$.
- A graph $G \in \mathcal{G}$ if G is simple (for all $i \in V, \omega_{ii} = 0$), undirected (for all $(i, j) \in E$, $\omega_{ij} = \omega_{ji}$), no isolated nodes (for all $i \in V$, $d_i > 0$), and V is finite.
- We define $\mathcal{V}$ to be the set consisting of all node functions $u : V \to \mathbb{R}$, and $\mathcal{V}^K$ by $U : V \to \mathbb{R}^K$.
- For $r \in [0, 1]$ we define the inner products $\langle u, v \rangle_{\mathcal{V}} := \sum_{i \in V} u_i v_i d_i^r$ and

$$\langle U, V \rangle_{\mathcal{V}^K} := \sum_{i \in V} \sum_{k \in \{1,\ldots,K\}} u_{ik} v_{ik} d_i^r .$$

Max-Cut

Definition

Let $G \in \mathcal{G}$ and let V_1 and V_{-1} be two disjoint subsets of V. The size of the cut $C = V_{-1}|V_1$ is

$$s(C) := \sum_{\substack{i \in V_{-1} \\ j \in V_1}} \omega_{ij}.$$

Let $\mathcal{C}$ be the space of all possible partitions of V into two disjoint subsets.

Definition

A maximum cut of G is a cut $C^* \in \mathcal{C}$ such that, for all cuts $C \in \mathcal{C}$, $s(C) \leq s(C^*)$.

Max-K-Cut

Definition

Let $G \in \mathcal{G}$. Let $X = V_1 | \dots | V_K$ be a node partition of V into K disjoint non-empty subsets. Then we call X a K-cut of G, and the value of the K-cut is defined by

$$S(X) = \sum_{\substack{k,l \in \{1,\dots,K\} \\ k<l}} \sum_{i \in V_k, j \in V_l} \omega_{ij}$$

Max-K-Cut

We call $\mathcal{X}$ as the space of all possible node partitions of V into K disjoint non-empty subsets.

Definition

A maximum K-cut of $\mathcal{G}$ is a K-cut X^* such that, for all $X \in \mathcal{X}$, $S(X) \leq S(X^*)$.

Signless Graph Ginzburg-Landau functional

Let $r \in [0, 1]$ and let $u \in \mathcal{V}$. We define the signless Laplacian operator by

$$(\Delta_r^+ u)_i := \frac{1}{d_i^r} \sum_{j \in V} \omega_{ij}(u_i + u_j).$$

Let $G \in \mathcal{G}$, $\varepsilon > 0$, and $u \in \mathcal{V}$. Then the signless graph Ginzburg-Landau functional is defined by

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

where $W(x) = (x^2 - 1)^2$.

This functional can be expressed by

$$f_\varepsilon^+(u) = \langle u, \Delta_r^+ u \rangle_{\mathcal{V}} + \frac{1}{\varepsilon} \sum_{i \in V} W(u_i).$$

Max-Cut objective functional

Let $\mathcal{V}^b := \{u \in \mathcal{V} : \forall\, i \in V, u_i \in \{-1, 1\}\}$ be the space of binary node functions and let $G \in \mathcal{G}$. For every $u \in \mathcal{V}^b$, let $C_u \in \mathcal{C}$ be the cut induced by u, then for all $u \in \mathcal{V}$ we define the functional f_0^+ by

$$f_0^+(u) := \begin{cases} 2\sum_{i,j\in V} \omega_{ij} - 4s(C_u), & \text{if } u \in \mathcal{V}^b, \\ +\infty, & \text{if } u \in \mathcal{V} \setminus \mathcal{V}^b. \end{cases}$$

By proving that as $\varepsilon \to 0$, $f_\varepsilon^+ \xrightarrow{\Gamma} f_0^+$, and that the functionals satisfy an equi-coercive property, we have that minimizers of f_ε^+ will converge to minimizers of f_0^+.

Gradient flow of f_ε^+

Let $u_0 \in \mathcal{V}$. The gradient flow equation of f_ε^+ in $\mathcal{V}$ is

$$\begin{cases} \frac{du_i}{dt} = -(\Delta_r^+ u)_i - \frac{1}{\varepsilon} d_i^{-r} W'(u_i), & \text{for } t > 0, \\ u_i = (u_0)_i, & \text{for } t = 0. \end{cases}$$

Since f_ε^+ is not convex, as $t \to \infty$ the solution of the $\mathcal{V}$-gradient flow is not guaranteed to converge to a global minimum, and can get stuck in local minimizers.

MBO Scheme

The MBO scheme on a graph describes the evolution of a node subset $S_0 \subseteq V$ as follows:
Inputs: Initial node set $S_0 \subseteq V$, and a time step dt.
Output: A node set $S_n \subseteq V$, the MBO evolution of S_0.
For $j = 1$: (convergence) do the following:
Signless Diffusion Step: Let $u = e^{-\Delta_r^+ \tau}(\chi_{S_{j-1}} - \chi_{S_{j-1}^c})$ denote the solution at time τ of the initial value problem

$$\frac{du_i}{dt} = -(\Delta_r^+ u)_i, \quad u(0) = \chi_{S_{j-1}} - \chi_{S_{j-1}^c}.$$

Threshold Step: Define the set $S_j \subseteq V$ to be

$$S_j = \{i \in V : u_i > 0\}.$$

Multiclass Signless Graph Ginzburg-Landau functional

Let $G \in \mathcal{G}$, $\varepsilon > 0$, $K \in \mathbb{N}$, and $U \in \mathcal{V}^K$. Then the multiclass signless graph Ginzburg-Landau functional is defined by

$$F^+_{\varepsilon,K}(U) := \frac{1}{2} \sum_{k\in\{1,\dots,K\}} \sum_{i,j\in V} \omega_{ij}(u_{ik} + u_{jk}) + \frac{1}{\varepsilon} \sum_{i\in V} (\prod_{k\in\{1,\dots,K\}} |(U)_{i,:} - E_k|^2_1).$$

where

$$(E_k)_i := \begin{cases} 1 & \text{if } i = k, \\ -1 & \text{if } i \neq k. \end{cases}$$

This functional can be expressed by

$$F^+_{\varepsilon,K}(U) = \langle U, \Delta^+ U \rangle_{\mathcal{V}^K} + \frac{1}{\varepsilon} \sum_{i\in V} (\prod_{k\in\{1,\dots,K\}} |(U)_{i,:} - E_k|^2_1).$$

Max-K-Cut objective functional

We define the following space of matrices in $\mathcal{V}^K$,

$$\Omega_K := \{U \in \mathcal{V}^K : \forall i \in V, j \in \{1, \dots, K\},$$

$$(U)_{ij} \in \{-1, 1\}, \sum_{k \in \{1,\dots,K\}} u_{ik} = -(K-2)\}.$$

Let $G \in \mathcal{G}$. For all $j \in \{1, \dots, K\}$ let V_j be the node subset induced by $(U)_{:,j}$. Then, for all $U \in \mathcal{V}^K$ we define F_0 by,

$$F^+_{0,K}(U) := \begin{cases} 2(K-2)\sum_{i,j \in V} \omega_{ij} + 4\sum_{k \in \{1,\dots,K\}} \sum_{i,j \in V_k} \omega_{ij} & \text{if } U \in \Omega_K, \\ +\infty & \text{otherwise.} \end{cases}$$

Convex Splitting Scheme

Using the well known convex splitting scheme [A.L Yuille, A. Rangarajan: 2002], we can decompose the functional $F^+_{\varepsilon,K}$ into a convex part and a concave part.

- $F^+_{convex} = \langle U, \Delta^+ U\rangle_{\mathcal{V}^K} + C\langle U, U\rangle_{\mathcal{V}^K}$,
- $F^+_{concave} = \frac{1}{\varepsilon}\sum_{i\in V}(\prod_{k\in\{1,\dots,K\}} |(U)_{i,:} - E_k|_1^2) - C\langle U, U\rangle_{\mathcal{V}^K}$.

The functional $F^+_{\varepsilon,K}$ is then minimized by the scheme

$$U^{n+1}_{ik} + dt\frac{\delta F^+_{convex}}{\delta U_{ik}}(U^{n+1}_{ik}) = U^n_{ik} - dt\frac{\delta F^+_{concave}}{\delta U_{ik}}(U^n_{ik}).$$

The convex splitting scheme applied on a functional is proven to find local minimizers.

Did it work?

In [B.Keetch, Y.v.Gennip,2018 (to appear)] we show that in practice using the MBO Scheme to minimize f_ε^+ produces good approximations to the solution of the Max-Cut problem on a variety of graphs.

The results of applying the convex splitting scheme to minimize $F_{\varepsilon,K}^+$ seem to be promising. The Max-K-cut approximations produced in this way are in practice larger than the expected value produced if the K-cuts were produced at random. These tests have been performed on a variety of graphs and we are currently writing up the results.

Further plans

We are interested in other computationally demanding problems which can be approximated by applying PDE methods on graphs. We have functionals that Γ-converge to min/max bisection objective functionals, and I'm currently working on using ODE methods to detect graph isomorphisms.

We are also interested in finding ways to obtain performance guarantees for our minimization algorithms.

Thanks for your attention!