L-Infinity Variational Problems on Graphs: Applications and Continuum Limits

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IMA Workshop, Theory and Algorithms of Graph-Based Learning
Applied Mathematics, Friedrich–Alexander University Erlangen–Nürnberg
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Outline

Motivation

$L$-Infinity Variational Problems
   Analysis of the Continuum Functional
   Analysis of the Graph Functional
   Applications

Continuum Limit
   Related Works
   Continuum Limit of Lipschitz Learning
   Application to Ground States
1 Motivation
Semi-supervised learning

Given a set of points \( \{x_1, \ldots, x_n\} \subset \Omega \subset \mathbb{R}^d \) with labels \( g(x_1), \ldots, g(x_N), N \ll n \), find a function \( u : \{x_1, \ldots, x_n\} \to \mathbb{R} \) such that \( u(x_i) = g(x_i) \) for \( i = 1, \ldots, N \).
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Graph \( p \)-Laplacian learning

Design a weighted graph \( G = (V, w) \) with vertices \( V = \{x_1, \ldots, x_n\} \) and find \( u : V \to \mathbb{R} \) such that
\[
    u \in \arg \min \sum_{x,y \in V} w_{xy}^p |u(y) - u(x)|^p
\]
and \( u(x_i) = g(x_i), i = 1, \ldots, N \).

\( p \)-Laplacian learning

Find \( u \in W^{1,p}(\Omega) \) such that
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    u \in \arg \min \int_\Omega |\nabla u|^p dx,
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continuum limit \( n \to \infty \) via \( \Gamma \)-convergence [GS15; ST19]
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Problem: well-posedness of pointwise contraints only for \( p > d \).

\( \implies \) In the limit of high-dimensional data \( d \to \infty \) one is forced to consider the case \( p = \infty \) (Lipschitz learning).
Lipschitz learning

Graph Lipschitz learning

Find $u : V \to \mathbb{R}$ such that

$$u \in \arg \min \max_{x,y \in V} w_{xy} |u(y) - u(x)|,$$

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Find $u \in W^{1,\infty}(\Omega)$ such that

$$u \in \arg \min \operatorname{ess sup}_{x \in \Omega} |\nabla u(x)|,$$

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Both problems lack uniqueness $\leadsto$ infinity harmonics (absolute minimizers):
Lipschitz learning

**Graph $\infty$-Laplacian Lipschitz learning**

Find $u : V \rightarrow \mathbb{R}$ such that

$$\Delta^G_\infty u(x_i) = 0$$

for $i = n + 1, \ldots, n + \text{constraints}$.

$$\Delta^G_\infty u(x) = \max_{y \in V} w_{xy}(u(y) - u(x)) + \min_{y \in V} w_{xy}(u(y) - u(x))$$

is the graph $\infty$-Laplacian.

**$\infty$-Laplacian Lipschitz learning**

Find $u \in W^{1,\infty}(\Omega)$ such that

$$\Delta_\infty u(x) = 0$$

for $x \in \Omega \setminus \{x_1, \ldots, x_N\} + \text{constraints}$.

$$\Delta_\infty u(x) = \sum_{i,j=1}^{d} \partial_i u(x) \partial_{ij} u(x) \partial_j u(x)$$

is the $\infty$-Laplacian.
## Lipschitz learning

### Graph $\infty$-Laplacian Lipschitz learning

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Continuum limit $n \rightarrow \infty$ via viscosity solutions [Cal19]
**Lipschitz learning**

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continuum limit $n \to \infty$ via $\Gamma$-convergence [Roi20] (second part!)
**L-Infity eigenvalue problems**

The functional \( u \mapsto \|\nabla u\|_\infty \) also appears in nonlinear eigenvalue problems:

\[
\min \frac{\|\nabla u\|_p}{\|u\|_p} \iff \lambda_p |u|^{p-2}u = -\Delta_p u
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p \to \infty
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\infty\text{-Laplacian eigenfunctions: } [\text{JL05; JLM99a; JLM99b}]

Continuum limit via viscosity solutions: [BBT20]
\textbf{\(L\)-Infinity eigenvalue problems}

The functional \( u \mapsto \| \nabla u \|_\infty \) also appears in nonlinear eigenvalue problems:

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\[
p \to \infty \quad \downarrow
\]

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$p \to \infty$

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$p/\infty$-harmonic potentials and asymptotics in $p$: [EP16]
\textbf{L}-Infinity eigenvalue problems

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\begin{align*}
\min \frac{\| \nabla u \|_p}{\| u \|_p} & \iff \lambda_p |u|^{p-2} u = -\Delta_p u \\
\min \frac{\| \nabla u \|_\infty}{\| u \|_p} & \iff \lambda_{\infty,p} |u|^{p-2} u \in \partial \| \nabla u \|_\infty
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p \to \infty \quad \iff \quad \min \frac{\|\nabla u\|_{\infty}}{\|u\|_p} \quad \iff \quad \lambda_{\infty,p} |u|^{p-2} u \in \partial \|\nabla u\|_{\infty}
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Relation to distance functions: [BKB20] (first part!)
Our set-up (for the first part)

We let $\Omega \subset \mathbb{R}^d$ be an open domain, $\mathcal{O} \subset \overline{\Omega}$ be a closed set, and define

$$
\mathcal{E} : L^2(\Omega) \rightarrow \mathbb{R}, \quad u \mapsto \begin{cases} 
\|\nabla u\|_{\infty}, & u \in W^{1,\infty}_\mathcal{O}(\Omega), \\
+\infty, & \text{else},
\end{cases}
$$

where $W^{1,\infty}_\mathcal{O}(\Omega) = \{ u \in W^{1,\infty}(\Omega) : u = 0 \text{ on } \mathcal{O} \}$. 

Applications: Lipschitz learning, $\infty$-Laplacian equations, minimal Lipschitz extensions, etc.

We want to understand

▶ its ground states
▶ its gradient flow
▶ its discretization on graphs

We don't want to approximate with finite $p$.

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(\|\nabla u\|_{\infty} = \lim_{p \to \infty} \|\nabla u\|_p)
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2 \( L \)-Infinity Variational Problems
Outline

Motivation

$L$-Infinity Variational Problems
Analysis of the Continuum Functional
Analysis of the Graph Functional
Applications

Continuum Limit
Related Works
Continuum Limit of Lipschitz Learning
Application to Ground States
Ground states are distance functions

We are interested in ground states of $\mathcal{E}$, i.e.,

$$u^* \in \arg \min_{u \in W^{1,\infty}_0(\Omega)} \frac{\|\nabla u\|_{\infty}}{||u||_p}, \quad p \in [1, \infty).$$  \hfill (2)
Ground states are distance functions

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(2)

**Theorem [BKB20]**

The unique non-negative minimizer of (2) with $\| \nabla u \|_{\infty} = 1$ is given by

$$\text{dist}(x, \mathcal{O}) = \min_{y \in \mathcal{O}} d_\Omega(x, y),$$

where $d_\Omega(\cdot, \cdot)$ is the geodesic distance in $\Omega$.

If $\mathcal{O} = \partial \Omega$ or $\Omega$ is convex, then $d_\Omega(x, y)$ can be replaced by $|x - y|$.
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N.B.: for $p = \infty$ other minimizers can exists
Uniqueness of non-negative eigenfunctions

Many numerical schemes for eigenfunctions rely on non-negativity of the first eigenfunction (cf. Perron-Frobenius theory).

Are there other non-negative eigenfunctions than the distance function?
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**Proposition [BKB20]**

Any non-negative function \( u \in L^2(\Omega) \) meeting \( \lambda u \in \partial E(u) \) coincides with a multiple of the distance function.
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Proposition [BKB20]

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Corollary

Using the results from [BB20]: For any non-negative datum \( f \in L^2(\Omega) \), the solution of the gradient flow

\[
    u'(t) + \partial E(u(t)) \ni 0, \quad u(0) = f,
\]

meets

\[
    \frac{u(t, x)}{E(u(t))} \to \text{dist}(x, \mathcal{O}) \quad \text{as } t \to \infty.
\]
An explicit solution for the gradient flow

For better understanding we let \( \mathcal{O} = \partial \Omega \) and define \( d(x) = \text{dist}(x, \partial \Omega) \).

\[
\begin{align*}
    r &:= \max_{x \in \Omega} d(x), & \text{in-radius of } \Omega, \\
    \Omega_\tau &:= \{ x \in \Omega : d(x) \geq \tau \}, & \text{inner parallel set, } 0 \leq \tau \leq r.
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Theorem [BKB20]

Let $f(x) \equiv r$ for all $x \in \Omega$.

Then there exists $g : [0, t_\ast] \rightarrow [0, 1]$ with $g(0) = 0$ and $g(t_\ast) = 1$ such that

$$u(t, x) = \min \left\{ \frac{1}{g(t)}d(x), r \right\}$$

solves the gradient flow $u'(t) + \partial E(u(t)) \ni 0$, $u(0) = f$, for $0 \leq t \leq t_\ast$. 

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![Graph of the solution](image-url)
An explicit solution for the gradient flow

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Underlying ODE

Function $g(t)$ has to be chosen as solution to

$$\begin{cases} g'(t) &= \frac{g(t)^2}{I(rg(t))}, \\
g(0) &= 0, \end{cases} \quad (3)$$

where

$$I(\tau) = \int_{\Omega \setminus \Omega_{\tau}} d(x)^2 \, dx.$$
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where

\[
I(\tau) = \int_{\Omega \setminus \Omega_\tau} d(x)^2 dx.
\]

For convex sets one can show

\[
I(\tau) \simeq \tau^3, \quad \tau \ll 1, \quad \Rightarrow \quad g(t) \simeq \sqrt{t}, \quad t \ll 1.
\]

In general,

\[
I(\tau) \gtrsim \tau^3, \quad \tau \ll 1, \quad \Rightarrow \quad g(t) \lesssim \sqrt{t}, \quad t \ll 1.
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Application to Ground States
Definitions

Given a finite weighted graph $G = (\Omega, w)$ (cf. [ETT15]) and a subset of vertices $\mathcal{O} \subset \Omega$, we define

$$E(u) = \max_{x,y \in \Omega} w(x, y) |u(y) - u(x)|, \quad u \in \mathcal{H}_\mathcal{O}(\Omega),$$

(4)
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where

- $\Omega$ is the vertex set, $w : \Omega \times \Omega \to \mathbb{R}_{\geq 0}$ are edge weights,

- $\mathcal{H}_\mathcal{O}(\Omega)$ is the space of graph functions vanishing on $\mathcal{O}$, equipped with inner product

$$\langle u, v \rangle = \sum_{x \in \Omega} u(x) v(x).$$
Definitions

Given a finite weighted graph $G = (\Omega, w)$ (cf. [ETT15]) and a subset of vertices $\mathcal{O} \subset \Omega$, we define

$$E(u) = \max_{x,y \in \Omega} w(x, y) |u(y) - u(x)|, \quad u \in \mathcal{H}_\mathcal{O}(\Omega),$$

(4)

where

- $\Omega$ is the vertex set, $w : \Omega \times \Omega \to \mathbb{R}_{\geq 0}$ are edge weights,

- $\mathcal{H}_\mathcal{O}(\Omega) = \{u : \Omega \to \mathbb{R} : u|_\mathcal{O} = 0\}$ is the space of graph functions vanishing on $\mathcal{O}$, equipped with inner product $\langle u, v \rangle = \sum_{x \in \Omega} u(x)v(x)$. 
Distance functions as ground states

We consider

$$\min_{u \in \mathcal{H}_0(\Omega)} \frac{E(u)}{\|u\|_p}, \quad p \in [1, \infty)$$  \hspace{1cm} (5)$$

**Theorem [BKB20]:**

The unique minimizer of (5) with $E(u) = 1$ is given by

$$\text{dist}_w(x, \Omega) = \min_{y \in \Omega} d_w(x, y),$$  \hspace{1cm} (6)$$

where

$$d_w(x, y) = \min \left\{ \sum_{i=1}^{n} \frac{1}{w(x_{i-1}, x_i)} : n \in \mathbb{N}, x_0 \sim \cdots \sim x_n, x_0 = x, x_n = y \right\}.$$
Distance functions as ground states

Furthermore, the gradient flow

\[ u'(t) + \partial E(u(t)) \ni 0, \quad u(0) = r > 0 \]

meets

\[ u(t, x) = \min \left\{ \frac{1}{g(t)} \text{dist}_w(x, \mathcal{O}), r \right\}, \]

where \( g : (0, \infty) \to \mathbb{R} \) solves

\[
\begin{cases}
  g'(t) &= \frac{g(t)^2}{I(\tau g(t))}, \\
  g(0) &= 0,
\end{cases} \quad I(\tau) = \sum_{x \in \Omega \setminus \mathcal{O}, \text{dist}_w(x, \mathcal{O}) < \tau} \text{dist}_w(x, \Gamma)^2.
\]
Outline

Motivation

$L$-Infinity Variational Problems
- Analysis of the Continuum Functional
- Analysis of the Graph Functional
- Applications

Continuum Limit
- Related Works
- Continuum Limit of Lipschitz Learning
- Application to Ground States
Distance to boundary of a grid graph
Distance function with respect to nonlocal patch distance
Distance function with respect to nonlocal patch distance
Distance to point on a discretized manifold
Distance to point on a discretized manifold
Distance to point on a discretized manifold
Distance to point on a discretized manifold
Distance to point on a discretized manifold
3 Continuum Limit
Graph setting

Consider a sequence of points \((x_i)_{i \in \mathbb{N}} \subseteq \Omega\).
Graph setting

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- The first \(N\) vertices
  \[
  \mathcal{O} := \{x_1, \ldots, x_N\},
  \]
  correspond to the labeled vertices.
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- For \(n \geq N\) the discrete sets
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  \[ \Omega_n := \{x_1, \ldots, x_n\}, \]
  correspond to the unlabeled vertices.

Behaviour of graph functionals/operators for \(n \to \infty\)?
Weights and Scaling

The weights are given by a kernel function \( \eta : \mathbb{R} \rightarrow \mathbb{R}^+_0 \),

\[
w_n(x, y) := \eta_{s_n}(|x - y|) := \eta(|x - y| / s_n)
\]

where \( s_n > 0 \) is the so-called scaling parameter.
Weights and Scaling

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where \( s_n > 0 \) is the so-called scaling parameter.

Assumptions on the kernel

(K1) \( \eta \) is positive and continuous at 0;
(K2) \( \eta \) is monotonously decreasing;
(K3) \( \text{supp}(\eta) \subset B_{r_\eta} \) for some \( r_\eta > 0 \).
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The scaling is introduced to give significant weight to vertices that are close together,
Weights and Scaling

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(K1) $\eta$ is positive and continuous at 0;
(K2) $\eta$ is monotonously decreasing;
(K3) supp($\eta$) $\subset B_{r_\eta}$ for some $r_\eta > 0$.

- The scaling is introduced to give significant weight to vertices that are close together,
- we assume that $s_n \xrightarrow{n \to \infty} 0$. 
Weights and Scaling

Leon Bungert, Tim Roith · AM · L-Infinity Variational Problems on Graphs

September 17, 2020 26/54
We control the scaling parameter $s_n$ via the value $r_n := \sup_{x \in \Omega} \text{dist}(x, \Omega)$. 

Leon Bungert, Tim Roith · AM · L-Infinity Variational Problems on Graphs September 17, 2020 26/54
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Leon Bungert, Tim Roith · AM · L-Infinity Variational Problems on Graphs September 17, 2020 26/54
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$L$-Infinity Variational Problems
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Analysis of the Graph Functional
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Consistency of Lipschitz Learning with Infinite Unlabeled Data and Finite Labeled Data

Jeff Calder

Abstract. We study the consistency of Lipschitz learning on graphs in the limit of infinite unlabeled data and finite labeled data. Previous work has conjectured that Lipschitz learning is well-posed in this limit, but is insensitive to the distribution of the unlabeled data, which is undesirable for semi-supervised learning. We first prove that this conjecture is true in the special case of a random geometric graph model with kernel-based weights. Then we go on to show that on a random geometric graph with self-tuning weights, Lipschitz learning is in fact highly sensitive to the distribution of the unlabeled data, and we show how the degree of sensitivity can be adjusted by tuning the weights. In both cases, our results follow from showing that the sequence of learned functions converges to the viscosity solution of an $\infty$-Laplace-type equation and studying the structure of the limiting equation.

Figure: J. Calder. “Consistency of Lipschitz learning with infinite unlabeled data and finite labeled data”. In: SIAM Journal on Mathematics of Data Science 1.4 (2019), pp. 780–812
Graph Infinity Laplacian

- Consider a sequence \((x_i)_{i \in \mathbb{N}} \subset T = \mathbb{R}^d / \mathbb{Z}^d\).
Graph Infinity Laplacian

- Consider a sequence $(x_i)_{i \in \mathbb{N}} \subset \mathbb{T} = \mathbb{R}^d / \mathbb{Z}^d$.
- Graph infinity Laplacian:

$$
\Delta^G_{\infty} u_n(x) = \max_{y \in \Omega_n} \eta(|x - y|)(u_n(y) - u_n(x)) + \min_{y \in \Omega_n} \eta(|x - y|)(u_n(y) - u_n(x)).
$$
Graph Infinity Laplacian

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  \]
- Infinity Laplacian:
  \[
  \Delta_{\infty} u(x) = \sum_{i,j=1}^{d} \partial_i u(x) \partial_j u(x) \partial_{ij} u(x).
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Graph Infinity Laplacian

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- Infinity Laplacian:

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\Delta_{\infty} u(x) = \sum_{i,j=1}^{d} \partial_i u(x) \partial_j u(x) \partial_{ij} u(x).
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Graph \(\infty\)-Laplacian Lipschitz learning

Find \(u_n : \Omega_n \to \mathbb{R}\) such that

\[
\Delta^G_{\infty} u_n = 0 \text{ in } \Omega_n \setminus \mathcal{O},
\]

\[
u_n = g \text{ on } \mathcal{O}.
\]

\(\infty\)-Laplacian Lipschitz learning

Find \(u \in W^{1,\infty}(T)\) such that

\[
\Delta_{\infty} u = 0 \text{ in } T \setminus \mathcal{O},
\]

\[
u = g \text{ on } \mathcal{O}.
\]

continuum limit \(n \to \infty\) via viscosity solutions [Cal19]
Graph Infinity Laplacian

[Cal19, Thm. 2.1]

For a null sequence $s_n$ such that

$$\frac{r_n^2}{s_n^3} \to 0$$

then we have that $u_n \to u$ uniformly, where $u \in C^{0,1}(\mathbb{T})$ is the unique viscosity solution of the infinity Laplace equation on $\mathbb{T}$, i.e.,

$$\lim_{n \to \infty} \max_{x \in \Omega_n} |u_n(x) - u(x)| = 0.$$
Analysis of $p$-Laplacian Regularization in Semi-Supervised Learning

Dejan Slepčev$^1$ and Matthew Thorpe$^2$

$^1$Department of Mathematical Sciences, Carnegie Mellon University, Pittsburgh, PA 15213, USA

$^2$Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge, CB3 0WA, UK

October 2017

Abstract

We investigate a family of regression problems in a semi-supervised setting. The task is to assign real-valued labels to a set of $n$ sample points, provided a small training subset of $N$ labeled points. A goal of semi-supervised learning is to take advantage of the (geometric) structure provided by the large number of unlabeled data when assigning labels. We consider random geometric graphs, with connection radius $\varepsilon(n)$, to represent the geometry of the data set. Functionals which model the task reward the regularity of the estimator function and impose or reward the agreement with the training data. Here we consider the discrete $p$-Laplacian regularization.

We investigate asymptotic behavior when the number of unlabeled points increases, while the number of training points remains fixed. We uncover a delicate interplay between the regularizing nature of the functionals considered and the nonlocality inherent to the graph constructions. We rigorously obtain almost optimal ranges on the scaling of $\varepsilon(n)$ for the asymptotic consistency to hold. We prove that the minimizers of the discrete functionals in random setting converge uniformly to the desired continuum limit. Furthermore we discover that for the standard model used there is a restrictive upper bound on how quickly $\varepsilon(n)$ must converge to zero as $n \to \infty$. We introduce a new model which is as simple as the original model, but overcomes this restriction.

Figure: D. Slepcev and M. Thorpe. “Analysis of $p$-Laplacian regularization in semisupervised learning”. In: SIAM Journal on Mathematical Analysis 51.3 (2019), pp. 2085–2120
Graph Functional

The graph functional in [ST19] has the form

\[ E_n^{(p)}(u) = \frac{1}{s_n^{p+d}} \frac{1}{n^2} \sum_{x_i, x_j \in \Omega_n} \eta_{s_n}(x_i - x_j) |u(x_i) - u(x_j)|^p. \]
Graph Functional

- The graph functional in [ST19] has the form

\[ E_n^{(p)}(u) = \frac{1}{s_n^{p+d} n^2} \sum_{x_i, x_j \in \Omega_n} \eta_{s_n}(x_i - x_j) |u(x_i) - u(x_j)|^p. \]

- The constraints on \( \mathcal{O} \) can be incorporated in the functional

\[ E_{n,\text{cons}}^{(p)}(u) = \begin{cases} E_n^{(p)}(u) & \text{if } u(x) = g(x) \quad \forall x \in \mathcal{O}, \\ \infty & \text{else}. \end{cases} \]
Graph Functional

- The graph functional in [ST19] has the form

\[
E^{(p)}_n(u) = \frac{1}{s_n^{p+d} n^2} \sum_{x_i, x_j \in \Omega_n} \eta_{s_n} (x_i - x_j) |u(x_i) - u(x_j)|^p .
\]

- The constraints on \( O \) can be incorporated in the functional

\[
E^{(p)}_{n, \text{cons}}(u) = \begin{cases} 
E^{(p)}_n(u) & \text{if } u(x) = g(x) \quad \forall x \in O, \\
\infty & \text{else}.
\end{cases}
\]

- The points \((x_i)_{i \in \mathbb{N}} \subset \Omega\) are assumed to be i.i.d. w.r.t. to a probability measure \( \mu \in \mathcal{P}(\overline{\Omega}) \) with density \( \rho : \Omega \to \mathbb{R}_0^+ \).
Continuum Functional

For $u \in W^{1,p}(\Omega)$ the respective continuum functional has the form

$$E^{(p)}(u) = \int_{\Omega} |\nabla u|^p \rho^2(x) \, dx.$$
Continuum Functional

- For \( u \in W^{1,p}(\Omega) \) the respective continuum functional has the form
  \[
  E^{(p)}(u) = \int_{\Omega} |\nabla u|^p \rho^2(x) \, dx.
  \]

- A point-wise constraint on \( \mathcal{O} \) makes sense if \( p > d \) because of the embedding
  \[
  W^{1,p}(\Omega) \hookrightarrow C^{0,1-d/p}(\Omega).
  \]
For $d \geq 3$ the scaling parameter is controlled by the assumption

$$s_n \gg \left(\frac{\log(n)}{n}\right)^{1/d}.$$
For $d \geq 3$ the scaling parameter is controlled by the assumption

$$s_n \gg \left(\frac{\log(n)}{n}\right)^{1/d}.$$ 

Additionally the scaling has to converge sufficiently fast to zero,

$$ns_n^p \to 0,$$

otherwise the constraints are lost in the limit.
Convergence result of [ST19]

Let $u_n$ be a sequence of minimizers of $E_{n,\text{cons}}^{(p)}$, then almost surely it converges along a subsequence locally uniformly towards a minimizer $u \in W^{1,p}(\Omega)$ of $\mathcal{E}_{\text{cons}}^{(p)}$, i.e., for any subset $\Omega' \subset \subset \Omega$ we have that

$$\lim_{k \to \infty} \max_{x \in \Omega_n \cap \Omega'} |u_n(x) - u(x)| = 0.$$
### Convergence result of [ST19]

Let $u_n$ be a sequence of minimizers of $E_{n,\text{cons}}^{(p)}$, then almost surely it converges along a subsequence locally uniformly towards a minimizer $u \in W^{1,p}(\Omega)$ of $E_{\text{cons}}^{(p)}$, i.e., for any subset $\Omega' \subset \subset \Omega$ we have that

$$\lim_{k \to \infty} \max_{x \in \Omega_{n_k} \cap \Omega'} |u_{n_k}(x) - u(x)| = 0.$$  

- The proof employs $\Gamma$-convergence.
Convergence result of [ST19]

Let $u_n$ be a sequence of minimizers of $E_{n,\text{cons}}^{(p)}$, then almost surely it converges along a subsequence locally uniformly towards a minimizer $u \in W^{1,p}(\Omega)$ of $E_{\text{cons}}^{(p)}$, i.e., for any subset $\Omega' \subset \subset \Omega$ we have that

$$\lim_{k \to \infty} \max_{x \in \Omega_n \cap \Omega'} |u_{n_k}(x) - u(x)| = 0.$$ 

- The proof employs $\Gamma$-convergence.
- Uses optimal transport theory.
Continuum Limit of Total Variation on Point Clouds

Nicolás García Trillos & Dejan Slepčev

Communicated by F. Otto

Abstract

We consider point clouds obtained as random samples of a measure on a Euclidean domain. A graph representing the point cloud is obtained by assigning weights to edges based on the distance between the points they connect. Our goal is to develop mathematical tools needed to study the consistency, as the number of available data points increases, of graph-based machine learning algorithms for tasks such as clustering. In particular, we study when the cut capacity, and more generally total variation, on these graphs is a good approximation of the perimeter (total variation) in the continuum setting. We address this question in the setting of $\Gamma$-convergence. We obtain almost optimal conditions on the scaling, as the number of points increases, of the size of the neighborhood over which the points are connected by an edge for the $\Gamma$-convergence to hold. Taking of the limit is enabled by a transportation based metric which allows us to suitably compare functionals defined on different point clouds.
Outline

Motivation

$L$-Infinity Variational Problems
Analysis of the Continuum Functional
Analysis of the Graph Functional
Applications

Continuum Limit
Related Works
Continuum Limit of Lipschitz Learning
Application to Ground States
The graph functional now has the form

\[
E_n^{(\infty)}(u) = \frac{1}{s_n} \max_{x_i, x_j \in \Omega_n} \eta_{s_n}(x_i - x_j) |u(x_i) - u(x_j)|.
\]
The graph functional now has the form

\[ E_n^{(\infty)}(u) = \frac{1}{s_n} \max_{x_i, x_j \in \Omega_n} \eta_{s_n}(x_i - x_j) |u(x_i) - u(x_j)|. \]

The respective continuum functional for \( u \in W^{1,\infty}(\Omega) \) reads

\[ \mathcal{E}^{(\infty)}(u) := \text{ess sup} \sup_{x \in \Omega} |\nabla u(x)|. \]
The graph functional now has the form
\[
E_n^{(\infty)}(u) = \frac{1}{s_n} \max_{x_i, x_j \in \Omega_n} \eta_{s_n}(x_i - x_j) |u(x_i) - u(x_j)|.
\]

The respective continuum functional for \( u \in W^{1, \infty}(\Omega) \) reads
\[
\mathcal{E}^{(\infty)}(u) := \ ess \sup_{x \in \Omega} |\nabla u(x)|.
\]

We want to establish a \( \Gamma \)-convergence result to obtain a similar result for a sequence of minimizers.
Gamma Convergence

For a metric space \((X, d_X)\) a sequence of functionals \(F_n : X \to [0, \infty]\) \(\Gamma\)-converges to \(F : X \to [0, \infty]\) if the following two conditions hold:
Gamma Convergence

For a metric space \((X, d_X)\) a sequence of functionals \(F_n : X \to [0, \infty]\) \(\Gamma\)-converges to \(F : X \to [0, \infty]\) if the following two conditions hold:

- For each sequence \((x_n)_{n \in \mathbb{N}} \subset X\) with \(x_n \to x\)

\[
F(x) \leq \lim \inf F_n(x_n);
\]
Gamma Convergence

For a metric space \((X, d_X)\) a sequence of functionals \(F_n : X \rightarrow [0, \infty]\) \(\Gamma\)-converges to \(F : X \rightarrow [0, \infty]\) if the following two conditions hold:

- For each sequence \((x_n)_{n \in \mathbb{N}} \subset X\) with \(x_n \rightarrow x\)
  \[F(x) \leq \lim \inf F_n(x_n);\]

- For every \(x \in X\) and there exists a sequence \((x_n)_{n \in \mathbb{N}} \subset X\) with \(x_n \rightarrow x\) such that
  \[F(x) \geq \lim \sup F_n(x_n).\]
Non-Local Auxiliary Functional

Similar to the proof in [GS15] it is convenient to first establish a convergence result for a non-local continuum functional.
Non-Local Auxiliary Functional

Similar to the proof in [GS15] it is convenient to first establish a convergence result for a non-local continuum functional.

Non-Local to Local Convergence

Let $\Omega$ be convex. For $u \in L^\infty(\Omega)$ and $s > 0$ we define

$$E_s^{(\infty)}(u) := \frac{1}{s} \text{ess sup}_{x,y \in \Omega} \{ \eta_s(x - y) |u(x) - u(y)| \}.$$

For a null sequence $s_n$ we have that

$$E_{s_n}^{(\infty)} \overset{\Gamma}{\rightarrow} \sigma_\eta E^{(\infty)}.$$
Non-Local Auxiliary Functional

Similar to the proof in [GS15] it is convenient to first establish a convergence result for a non-local continuum functional.

Non-Local to Local Convergence

Let $\Omega$ be convex. For $u \in L^\infty(\Omega)$ and $s > 0$ we define

$$\mathcal{E}_s^{(\infty)}(u) := \frac{1}{s} \text{ess sup}_{x,y \in \Omega} \{ \eta_s(x - y) |u(x) - u(y)| \}.$$

For a null sequence $s_n$ we have that

$$\mathcal{E}_{s_n}^{(\infty)} \xrightarrow{\Gamma} \sigma_\eta \mathcal{E}^{(\infty)}.$$

- The value $\sigma_\eta$ is defined as

$$\sigma_\eta := \text{ess sup}_{x \in \mathbb{R}^d} \{ \eta(x) |x| \}.$$
**limsup Inequality**

Take \( u \in W^{1,\infty}(\Omega) \), use **Rademacher’s theorem** and the inequality

\[
|u(x) - u(y)| \leq C |x - y|^\lambda \|\nabla u\|_{0,p},
\]

where \( 0 \leq \lambda \leq 1 - (d/p) \) to show that

\[
\lim_{n \to \infty} \mathcal{E}_{s_n}(u) = \sigma_\eta \operatorname{ess \ sup}_{x \in \Omega} (\nabla u(x)).
\]
Take a sequence \((u_n)_{n \in \mathbb{N}} \subset L^\infty(\Omega)\) such that \(u_n \overset{L^\infty}{\rightarrow} u\) and assume that
\[
\liminf_{n \to \infty} E_{s_n}^{(\infty)}(u_n) < \infty.
\]
**liminf Inequality**

- Take a sequence \((u_n)_{n \in \mathbb{N}} \subset L^\infty(\Omega)\) such that \(u_n \xrightarrow{L^\infty} u\) and assume that
  \[
  \liminf_{n \to \infty} E_{s_n}(u_n) < \infty.
  \]

- For each \(h \in \mathbb{R}^d\) the functions
  \[
  v_n^h(x) := \frac{u_n(x) - u_n(x + s_n h)}{s_n}
  \]
  converge weak* in \(L^\infty\) to \(\nabla u \cdot h\).
**liminf Inequality**

- Take a sequence \((u_n)_{n \in \mathbb{N}} \subset L^\infty(\Omega)\) such that \(u_n \xrightarrow{L^\infty} u\) and assume that
  \[
  \liminf_{n \to \infty} \mathcal{E}_{s_n}(\infty)(u_n) < \infty. 
  \]

- For each \(h \in \mathbb{R}^d\) the functions
  \[
  v_n^h(x) := \frac{u_n(x) - u_n(x + s_n h)}{s_n} 
  \]
  converge weak* in \(L^\infty\) to \(\nabla u \cdot h\).

- Using weak* lower semi-continuity of the norm \(\|\cdot\|_\infty\) yields the inequality.
How do we establish $\Gamma$-convergence for a sequence of discrete functions?
In our case we associate discrete functions with piecewise constant $L^\infty$ functions.
In our case we associate discrete functions with piecewise constant $L^\infty$ functions.

Consider a map $p_n : \Omega \to \Omega_n$ such that

$$p_n(x) \in \arg\min_{y \in \Omega_n} |x - y|.$$
In our case we associate discrete functions with piecewise constant $L^\infty$ functions.

Consider a map $p_n : \Omega \to \Omega_n$ such that
$$p_n(x) \in \arg \min_{y \in \Omega_n} |x - y|.$$ 

We extend the functional $E_n(\infty)$ onto $L^\infty$ using the set
$$A_n = \{ u \in L^\infty : u \text{ is constant on } p_n^{-1}(x_i), \ x_i \in \Omega_n \},$$

namely, for $u \in L^\infty$ we set
$$E_n(\infty)(u) := E_n(\infty)(u|_{\Omega_n}) + \chi A_n(u),$$

where
$$u|_{\Omega_n}(x_i) := \frac{1}{|p_n^{-1}(x_i)|} \int_{p_n^{-1}(x_i)} u(x) \, dx.$$
For $u_n \in A_n$ we have that

$$
E_n^{(\infty)}(u_n) = \frac{1}{s_n} \sup_{x,y \in \Omega} \eta_{s_n}(p_n(x) - p_n(y)) |u_n(x) - u_n(y)|.
$$
For $u_n \in A_n$ we have that
\[
E_n^{(\infty)}(u_n) = \frac{1}{s_n} \text{ess sup}_{x,y \in \Omega} \eta_{s_n}(p_n(x) - p_n(y)) |u_n(x) - u_n(y)|.
\]

We want to have an estimate
\[
\eta_{s_n}(p_n(x) - p_n(y)) \geq \eta_{s_n}(x - y).
\]
For \( u_n \in \mathcal{A}_n \) we have that
\[
E_n^{(\infty)}(u_n) = \frac{1}{s_n} \text{ess sup}_{x,y \in \Omega} \eta_{s_n}(p_n(x) - p_n(y))|u_n(x) - u_n(y)|.
\]

We want to have an estimate
\[
\eta_{s_n}(p_n(x) - p_n(y)) \geq \eta_{\tilde{s}_n}(x - y).
\]

If \(|p_n(x) - p_n(y)| > s_n\) it follows that
\[
|x - y| \geq |p_n(x) - p_n(y)| - 2\|Id - p_n\|_{\infty} > s_n - 2r_n =: \tilde{s}_n.
\]
For $u_n \in A_n$ we have that
\[ E_n^{(\infty)}(u_n) = \frac{1}{s_n} \text{ess sup}_{x,y \in \Omega} \eta_{s_n}(p_n(x) - p_n(y)) |u_n(x) - u_n(y)|. \]

We want to have an estimate
\[ \eta_{s_n}(p_n(x) - p_n(y)) \geq \eta_{\tilde{s}_n}(x - y). \]

If $|p_n(x) - p_n(y)| > s_n$ it follows that
\[ |x - y| \geq |p_n(x) - p_n(y)| - 2 \|Id - p_n\|_\infty \]
\[ > s_n - 2r_n =: \tilde{s}_n. \]

Therefore,
\[ E_n^{(\infty)}(u_n) \geq \frac{\tilde{s}_n}{s_n} \mathcal{E}_{\tilde{s}_n}^{(\infty)}(u_n). \]
For \( u_n \in \mathcal{A}_n \) we have that
\[
E_n^{(\infty)}(u_n) = \frac{1}{s_n} \text{ess sup}_{x,y \in \Omega} \eta_{s_n}(p_n(x) - p_n(y)) \left| u_n(x) - u_n(y) \right|.
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If \( |p_n(x) - p_n(y)| > s_n \) it follows that
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Therefore,
\[
E_n^{(\infty)}(u_n) \geq \frac{\tilde{s}_n}{s_n} \mathcal{E}_{\tilde{s}_n}^{(\infty)}(u_n).
\]

For \( r_n / s_n \to 0 \) we have that \( \frac{\tilde{s}_n}{s_n} \to 1 \).
Discrete to Continuum Convergence

Let $\Omega$ be convex. For any null sequence $s_n$ such that

$$\frac{r_n}{s_n} \to 0,$$

we have that

$$E^{(\infty)}_{n, \text{cons}} \rightharpoonup_{\Gamma} \sigma_\eta E^{(\infty)}_{\text{cons}}.$$
Discrete to Continuum Convergence

Let $\Omega$ be convex. For any null sequence $s_n$ such that

$$r_n \rightarrow 0,$$

we have that

$$E_{n,\text{cons}}(\infty) \rightharpoonup \sigma_\eta E_{\text{cons}}(\infty).$$

Convergence of minimizers?
A sequence of functionals $F_n : X \to \mathbb{R}$ is called **compact** if for any bounded sequence $x_n$ the property

$$\sup_{n \in \mathbb{N}} F_n(x_n) < \infty$$

implies that $(x_n)_{n \in \mathbb{N}}$ is relatively compact.
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$$
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**Compactness Result**

Let $s_n$ be a null sequence such that

$$
\frac{r_n}{s_n} \to 0
$$

then $E_{n,\text{cons}}^{(\infty)}$ is a compact sequence of functionals. Therefore, every sequence of minimizers for $E_{n,\text{cons}}^{(\infty)}$ has a cluster point which is a minimizer of $E_{\text{cons}}^{(\infty)}$. 

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### Compactness Result

Let \( s_n \) be a null sequence such that

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\frac{r_n}{s_n} \to 0
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then \( E_{n,\text{cons}}^{(\infty)} \) is a compact sequence of functionals. Therefore, every sequence of minimizers for \( E_{n,\text{cons}}^{(\infty)} \) has a cluster point which is a minimizer of \( E_{\text{cons}}^{(\infty)} \).

Let \( K \subset L^\infty(\Omega) \) be a bounded set such that for every \( \varepsilon > 0 \) there exists a finite partition \( \{V_i\}_{i=1}^n \) of \( \Omega \) with

\[
\text{ess sup}_{x,y \in V_i} |u(x) - u(y)| \leq \varepsilon \quad \forall u \in K, i = 1, \ldots, n,
\]

then \( K \) is relatively compact.
Outline

Motivation

$L$-Infinity Variational Problems
  Analysis of the Continuum Functional
  Analysis of the Graph Functional
  Applications

Continuum Limit
  Related Works
  Continuum Limit of Lipschitz Learning
  Application to Ground States
We consider

\[ u^* \in \arg \min_{u \in L^\infty(\Omega)} \frac{E_{n,\text{cons}}^{(\infty)}(u)}{\|u\|_p} \]
We consider

\[ u^* \in \text{arg min}_{u \in L^\infty(\Omega)} \frac{E^{(\infty)}_{n,\text{cons}}(u)}{\|u\|_p}. \]

The constraint is given by \( g \equiv 0 \), from which we have that the functionals are one-homogeneous.
Convergence of distance functions

Let $s_n$ be a null sequence such that

$$\frac{r_n}{s_n} \rightarrow 0,$$

then every sequence $u_n$ with

$$u_n \in \arg \min_{\|u\|_p=1} E^{(\infty)}_{n,\text{cons}}(u)$$

has a cluster point $u^* \in W^{1,\infty}$ with

$$u^* \in \arg \min_{\|u\|_p=1} \mathcal{E}^{(\infty)}_{\text{cons}}(u).$$
Ideas for the proof

- Observe that $u_n$ is bounded and $\sup_n E_n^{(\infty)}(u_n) < \infty$. 
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- Observe that $u_n$ is bounded and $\sup_n E_n(\infty)(u_n) < \infty$.
- Compactness property implies that $u_{n_k} \to u^*$ in $L^\infty$. 
Ideas for the proof

- Observe that $u_n$ is bounded and $\sup_n E_n(\infty)(u_n) < \infty$.
- Compactness property implies that $u_{n_k} \to u^*$ in $L^\infty$.
- Use liminf inequality to obtain that

$$u^* \in \arg \min_{\|u\|_p = 1} E_{\text{cons}}^{(\infty)}(u).$$
Thank you for your attention!

Questions?

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4 References


