# Nonlinear PDE continuum limits in data science and machine learning

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# Outline

Nondominated sorting



3 Semi-supervised learning



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- 2 Convex hull peeling
- 3 Semi-supervised learning



Motivating example: Google Goggles

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#### Figure: Query image

# Motivating example: Google Goggles



Figure: Query image

Figure: Retrieved images

# Multi-query image retrieval

Problem: Find images in a dataset S that are similar to multiple query images.

Pareto method: "Solve" the multi-objective optimization problem

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#### Pareto points:



How do we solve the multi-objective optimization problem

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Basic approach:

**(**) Choose some weights  $\alpha_i \in [0, 1]$  with  $\sum_{i=1}^d \alpha_i = 1$  and define

$$f_{\alpha}(I) = \alpha_1 f_1(I) + \alpha_2 f_2(I) + \cdots + \alpha_d f_d(I).$$

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Solve the scalarized optimization problem

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Problems:

Difficult to choose weights

2 Ignores relevant solutions



















































# Multi-query image retrieval

#### First Pareto front:



Hsiao, K.-J., Calder, J., and Hero III, A. O. (2015). Pareto-depth for multiple-query image retrieval. *IEEE Transactions on Image Processing*, 24(2):583–594.

#### Nondominated sorting

Let  $X_1, \ldots, X_n$  be points in  $\mathbb{R}^d$  and set  $S = \{X_1, \ldots, X_n\}$ .

Define the partial order

$$x \leq y \iff x_i \leq y_i \text{ for all } i \in \{1, \ldots, d\}.$$

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#### Definition

Nondominated sorting is the process of arranging S into layers  $\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, \ldots$ , defined by

 $\mathcal{F}_1 = \text{Minimal elements of } S,$ 

 $\mathcal{F}_k$  = Minimal elements of  $S \setminus (\mathcal{F}_1 \cup \cdots \cup \mathcal{F}_{k-1})$ .

# Applications

#### Multi-objective optimization

- Genetic algorithms [Deb et al., 2002]
- Gene selection and ranking [Hero, 2003]
- Database systems [Papadias et al., 2005]
- Anomaly detection [Hsiao et al., 2012]
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#### **Combinatorics and probability**

- Longest monotone subsequences [Ulam, 1961]
- Longest chain in Euclidean space [Hammersley, 1972]
- Patience sorting [Aldous and Diaconis, 1999]
- Young Tableaux [Viennot, 1984]
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#### Other applications

- Molecular biology [Pevzner, 2000]
- Integrated circuit design [Adhar, 2007]

### Demo: 50 Random samples





 $n=10^2 \; {\rm points}$ 



 $n=10^3 \text{ points}$ 



 $n=10^4 \ {\rm points}$ 



 $n=10^5 \; {\rm points}$ 



 $n=10^6 \ {\rm points}$ 

# Demo: Gaussian distribution



 $n=10^2 \text{ points}$


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## A PDE continuum limit for nondominated sorting

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Let  $U_n : \mathbb{R}^d \to \mathbb{N}_0$  be the function that 'counts' the layers  $\mathcal{F}_1, \mathcal{F}_2, \dots$ 



#### Theorem (Calder, Esedoglu, Hero, 2014)

There exists a universal constant  $c_d > 0$  such that with probability one

 $n^{-\frac{1}{d}} U_n \longrightarrow c_d u$  locally uniformly as  $n \to \infty$ 

where  $u \in C^{0,\frac{1}{d}}([0,\infty)^d)$  is the unique nondecreasing  $(u_{x_i} \ge 0)$  viscosity solution of

(P) 
$$\begin{cases} u_{x_1} \cdots u_{x_d} = f & \text{in } \mathbb{R}^d_+ := (0, \infty)^d \\ u = 0 & \text{on } \partial \mathbb{R}^d_+. \end{cases}$$

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Calder, J., Esedoğlu, S., and Hero, A. O. (2014). A Hamilton-Jacobi equation for the continuum limit of non-dominated sorting. *SIAM Journal on Mathematical Analysis*, 46(1):603–638.

Calder, J. (2016). A direct verification argument for the Hamilton-Jacobi equation continuum limit of nondominated sorting. Nonlinear Analysis Series A: Methods, Theory & Applications, 141:88–108

Current work: Rate of convergence (Brendan Cook)



# Demo: Multimodal f



Let  $X_1, \ldots, X_n$  be *i.i.d.* random variables in  $[0, \infty)^d$  with continuous density f.

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$$\langle Du,v\rangle \approx u(x+v)-u(x)$$



Let's suppose that  $n^{-\alpha}U_n \longrightarrow u \in C^1$  as  $n \to \infty$  for some  $\alpha \in [0, 1]$ .



 $\begin{array}{lll} \langle Du,v\rangle &\approx & u(x+v)-u(x)\\ &\approx & (\# \text{ fronts in } A)n^{-\alpha}\\ &\approx & (\# \text{ samples in } A)^{\alpha}n^{-\alpha} \end{array}$ 

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If  $\alpha d = 1$ , or  $\alpha = 1/d$ , then

$$u_{x_1}\cdots u_{x_d}=f$$

### Ordering within each front

Let  $X_1, \ldots, X_n$  be i.i.d. random variables with density f on  $[0, 1]^2$ . Define

 $V_n(X_i) =$ Index of  $X_i$  within its Pareto front.



## Demo: Uniform distribution on $[0,1]^2$

$$(\mathsf{T}) \begin{cases} \langle Dv, D^{\perp}u \rangle = f & \text{in } (0,1)^2, \\ v = 0 & \text{on } (0,1) \times \{x_2 = 1\}. \end{cases}$$
$$(\mathsf{T}') \begin{cases} \langle Dw, vD^{\perp}u \rangle = wf & \text{in } (0,1)^2, \\ w = 1 & \text{on } \{x_1 = 1\} \times (0,1) \end{cases}$$





Algorithm (PDE-based Ranking)

**(**) Select k points from  $X_1, \ldots, X_n$  at random. Call them  $Y_1, \ldots, Y_k$ .  $(k \ll n)$ 

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$$\hat{f}(x) = \frac{1}{kh^d} \cdot \# \Big\{ Y_i : Y_i \in [x, x + h\mathbf{1}] \Big\}.$$

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#### Notes:

- Total complexity is  $O(k + h^{-d} + n)$ .
- If we fix k and h, independent of n, then Steps 1-3 have O(1) complexity.

Calder, J., Esedoğlu, S., and Hero, A. O. (2015). A PDE-based approach to nondominated sorting. *SIAM Journal on Numerical Analysis*, 53(1):82–104.

# CPU Time (C/C++)



- # Subsamples =  $k = 10^7$ , Grid for solving PDE =  $250 \times 250$ .
- $O(n \log n)$  non-dominated sorting of [Felsner and Wernisch, 1999].

## Application in anomaly detection



Abbasi, B., Calder, J., and Oberman, A.M. Anomaly detection and classification for streaming data using PDEs *SIAM Journal on Applied Mathematics*, 78(2), 921–941, 2018.
#### Results

Anomaly detection with PDE-based ranking: Reduces complexity from  $O(n^2)$  to O(n).



Abbasi, B., Calder, J., and Oberman, A.M. Anomaly detection and classification for streaming data using PDEs SIAM Journal on Applied Mathematics, 78(2), 921–941, 2018.

#### Results

Anomaly detection for streaming data:



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### Examples of detected anomalies...

with classifications using the new transport equations.



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Calder (UofM)

PDE continuum limits

### Outline

1 Nondominated sorting



3 Semi-supervised learning



**Question:** How to define 'median' in dimensions  $d \ge 2$ ?

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Barnett [Barnett, 1976]: Convex hull peeling



Convex hull peeling median := Centroid of final layer

## MNIST handwritten digit dataset

6 5

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#### Definition

Convex hull peeling is the process of arranging S into convex layers  $C_1, C_2, C_3, \ldots$ , defined by

 $C_1 =$ Vertices of convex hull of S,

 $C_k$  = Vertices of convex hull of  $S \setminus (C_1 \cup \cdots \cup C_{k-1})$ .

#### Applications:

- Robust statistics, machine learning, etc.
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- Fingerprint matching [Poulos et al., 2005].



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**Players:** Paul and Carol **State space:**  $\mathcal{X} := \{X_1, \dots, X_n\}$ 

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Paul's goal: Reach vertex of convex hull Carol's goal: Obstruct Paul
















Paul's optimal choice: Any halfspace supporting current convex layer Carol's optimal choice: Any point on the previous convex layer



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Value function =  $U_n(x^0)$  = Convex depth function.

Calder (UofM)



n = 50 points





 $n=10^5 \; {\rm points}$ 

Calder (UofM)

# A PDE continuum limit for convex hull peeling

Let  $X_1, \ldots, X_n$  be i.i.d. with a continuous density f on a convex set  $\Omega \subset \mathbb{R}^d$ .

Let  $U_n$  be the function that 'counts' the associated convex layers  $C_1, C_2, \ldots$ 



# Partial differential equation (PDE) continuum limit

#### Theorem (Joint with C. Smart)

There exists a universal constant  $\alpha_d$  such that with probability one

 $n^{-\frac{2}{d+1}}U_n \longrightarrow \alpha_d u$  uniformly on  $\Omega$ ,

where  $u \in C(\overline{\Omega})$  is the unique viscosity solution of

$$\nabla u \cdot \operatorname{cof}(-\nabla^2 u) \nabla u = f^2 \quad \text{in } \Omega$$
  
 
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This is just motion by a power of Gauss curvature

$$\frac{dS}{dt} = f^{-2/(d+1)} \kappa_G^{1/(d+1)} \mathbf{n}.$$

(1)

# A PDE continuum limit for convex hull peeling



Figure: Convex layers vs continuum limit for  $n = 5 \times 10^3$ .

# A nonconvex example



Figure: Convex layers corresponding to disjoint clusters.

# A nonconvex example



Figure: Two different solutions continuum PDE.

# The halfmoon



Figure: Convex layers corresponding to the halfmoon distribution.

# The halfmoon



Figure: Solution of PDE for the halfmoon example.

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**Fully supervised:** In fully supervised learning, we are given training data  $(x_i, y_i)$  for i = 1, ..., n, where  $x_i \in \mathcal{X}$  are the data points and  $y_i \in \mathcal{Y}$  are the known labels.

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Classification when  $\mathcal{Y}$  finite – Regression when  $\mathcal{Y} = \mathbb{R}^d$ .

Example: Automated image captioning

# Example: Automated image captioning



A woman is throwing a frisbee in a park.



A dog is standing on a hardwood floor.



A stop sign is on a road with a mountain in the background



A little girl sitting on a bed with a teddy bear.



A group of people sitting on a boat in the water.



A giraffe standing in a forest with trees in the background.

[Yann LeCun, Yoshua Bengio, Geoffrey Hinton. Deep learning. Nature, 2015.]

# Example: Automated image captioning fail



(-11.269838) a woman holding a baby giraffe in a zoo

[Andrej Karpathy's NeuralTalk]

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Brief list of example applications:

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- Inferring protein structure from sequencing
### Applications

Why is semi-supervised learning useful?

It is expensive to label data, and we have an abundance of unlabeled data.

#### Brief list of example applications:

- Speech recognition
- 2 Webpage classification
- Inferring protein structure from sequencing

A great introductory book [Chapelle et al., 2006].

#### Model:



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**1** Data (labeled and unlabeled) is a graph  $(\mathcal{X}, \mathcal{W})$ .

- $\mathcal{X} \subset \mathbb{R}^d$  are the vertices and
- $\mathcal{W} = (w_{xy})_{x,y \in \mathcal{X}}$  are the nonnegative edge weights.
- $w_{xy} \approx 1$  if x, y similar, and  $w_{xy} \approx 0$  when dissimilar.

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#### Semi-supervised smoothness assumption

Similar points  $x, y \in \mathcal{X}$  in high density regions of the graph should have similar labels.

### Laplacian regularization

$$\min_{u:\mathcal{X}\to\mathbb{R}}\sum_{x,y\in\mathcal{X}}w_{xy}^2(u(x)-u(y))^2 \text{ subject to } u(x)=g(x) \text{ for all } x\in\mathcal{O}.$$

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The minimizer  $u:\mathcal{X}\rightarrow\mathbb{R}$  satisfies the linear system

$$\sum_{y \in \mathcal{X}} w_{xy}^2(u(x) - u(y)) = 0$$
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**References:** 

- Original work [Zhu et al., 2003]
- Learning [Zhou et al., 2005][Ando and Zhang, 2007]
- Manifold ranking [He et al., 2006] [Wang et al., 2013] [Yang et al., 2013] [Zhou et al., 2011] [Xu et al., 2011]

### Ill-posed with small amount of labeled data



### Ill-posed with small amount of labeled data



• Graph is  $n = 10^5$  i.i.d. random variables uniformly drawn from  $[0, 1]^2$ .

• 
$$w_{xy} = 1$$
 if  $|x - y| < 0.01$  and  $w_{xy} = 0$  otherwise.

• Over 95% of labels in [0.4975, 0.5025].

[Nadler et al., 2009][El Alaoui et al., 2016]

## $\ell_p$ -based Laplacian regularization

For any  $p < \infty$ :

$$\min_{u:\mathcal{X}\to\mathbb{R}}\sum_{x,y\in\mathcal{X}}w_{xy}^p|u(x)-u(y)|^p \quad \text{subject to } u(x)=g(x) \text{ for all } x\in\mathcal{O}. \tag{3}$$

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# $\ell_p$ -based Laplacian regularization

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#### **References:**

- Finite p: [Bridle and Zhu, 2013][Alamgir and Luxburg, 2011]
- $p = \infty$ : [Kyng et al., 2015] [Luxburg and Bousquet, 2004]
- Absolutely minimal Lipschitz extensions: [Aronsson et al., 2004]

*p*-Laplacian learning:  $n = 10^5$  points,  $h = 10^{-2}$ 



p=2 Simulations are the work of Mauricio Flores (co-supervised by Gilad Lerman).

Calder (UofM)

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*p*-Laplacian learning:  $n = 10^5$  points,  $h = 10^{-2}$ 

p = 3

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$$w_{xy} = \Phi\left(rac{|x-y|}{h}
ight),$$

where h > 0, and  $\Phi : [0, \infty) \to [0, \infty)$ .

For  $p < \infty$  we write

$$J_p(u):=\sum_{x,y\in\mathcal{X}_n}w_{xy}^p|u(x)-u(y)|^p,$$

and for  $p = \infty$  we write

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$$J_\infty(u) \coloneqq \max_{x,y\in\mathcal{X}_n} \{w_{xy}|u(x)-u(y)|\}.$$

For  $n \geq 1$ , let  $u_n : \mathcal{X}_n \to \mathbb{R}$  be the solution of

$$\min_{u:\mathcal{X}_n\to\mathbb{R}}J_p(u) \quad \text{subject to } u(x)=g(x) \text{ for all } x\in\mathcal{O}.$$

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**Question:** What can we say about  $u_n$  as  $n \to \infty$ ?

$$r_n = \sup \left\{ s > 0 \, | \, B(x,s) \cap \mathcal{X}_n = \emptyset \text{ for some } x \in U \right\}.$$
(5)

Theorem ( $p = \infty$  [Calder, 2017a] )

Suppose that  $h_n \to 0$  such that

$$\lim_{n \to \infty} \frac{r_n^2}{h_n^3} = 0.$$
(6)

Then  $u_n \longrightarrow u$  uniformly as  $n \to \infty$ ,

where  $u \in C(\mathbb{T}^d)$  is the unique viscosity solution of the  $\infty$ -Laplace equation

n

$$\begin{cases} \Delta_{\infty} u = 0 & \text{in } \mathbb{T}^d \setminus \mathcal{O} \\ u = g & \text{on } \mathcal{O} \end{cases}$$
(8)

Note that (6) holds almost surely when

$$\lim_{n \to \infty} \frac{n h_n^{3d/2}}{\log(n)} = \infty.$$
(9)

(7)

#### Theorem (Finite p [Calder, 2017b])

Let  $d , and suppose that <math>h_n \rightarrow 0$  such that

$$\lim_{n \to \infty} n h_n^p = 0 \quad \text{and} \quad \lim_{n \to \infty} \frac{n h_n^{d+4}}{\log(n)} = \infty.$$
(10)

Then with probability one

$$u_n \longrightarrow u$$
 uniformly as  $n \to \infty$ , (11)

where  $u \in C(\mathbb{T}^d)$  is the unique viscosity solution of the weighted *p*-Laplace equation

$$\begin{cases} \operatorname{div} \left( f^2 |\nabla u|^{p-2} \nabla u \right) = 0 & \text{in } \mathbb{T}^d \setminus \mathcal{O} \\ u = g & \text{on } \mathcal{O} \end{cases}$$
(12)

A very similar result appeared recently in [Slepčev and Thorpe, 2017].

## Regularity in semi-supervised learning

The PDE-limit can be used to prove Hölder regularity.

#### Theorem

Assume p > d. For every  $\alpha < \frac{p-d}{p-1}$  there exists  $C, \delta$  such that

$$\mathbb{P}\left[orall x,y\in\mathcal{X}_n,\;|u_n(x)-u_n(y)|\leq C(|x-y|^lpha+n^{rac{1}{p}}h)
ight]\geq 1\!-\!\exp\left(-\delta nh^{d+4}+C\log(n)
ight)$$
$$\min_{u:\mathcal{X}_n\to\mathbb{R}}J_p(u)=\sum_{x,y\in\mathcal{X}_n}w_{xy}^p|u(x)-u(y)|^p\quad\text{subject to }u(x)=g(x)\text{ for }x\in\mathcal{O}\subset\mathcal{X}_n$$

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The minimizer  $u: \mathcal{X}_n \to \mathbb{R}$  satisfies

$$\begin{cases} \Delta_p^{\mathcal{X}_n} u = 0 & \text{ in } \mathcal{X}_n \setminus \mathcal{O}, \\ u = g & \text{ on } \mathcal{O}, \end{cases}$$

where  $\Delta_p^{\mathcal{X}_n} u: \mathcal{X} \to \mathbb{R}$  is the graph  $p ext{-Laplacian}$  defined by

$$\Delta_p^{\mathcal{X}_n} u(x) = \sum_{y \in \mathcal{X}_n} w_{xy}^p |u(y) - u(x)|^{p-2} (u(y) - u(x)).$$

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#### References on graph p-Laplacian:

 [Manfredi et al., 2015] [Zhou and Schölkopf, 2005] [Amghibech, 2003] [Bühler and Hein, 2009] [Luo et al., 2010]

# Graph Laplacian as $p \to \infty$

Note that solutions of

$$\Delta_p^{\mathcal{X}_n} u(x) = \sum_{y \in \mathcal{X}_n} w_{xy}^p |u(y) - u(x)|^{p-2} (u(y) - u(x)) = 0$$

satisfy

$$\left(\sum_{\substack{y \in \mathcal{X}_n \\ u(y) \ge u(x)}} w_{xy}^p |u(y) - u(x)|^{p-1}\right)^{1/p} = \left(\sum_{\substack{y \in \mathcal{X}_n \\ u(y) < u(x)}} w_{xy}^p |u(y) - u(x)|^{p-1}\right)^{1/p}.$$

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Send  $p \to \infty$  to get

$$\max_{y\in\mathcal{X}_n}w_{xy}(u(y)-u(x))=\max_{y\in\mathcal{X}_n}w_{xy}(u(x)-u(y)).$$

or

$$\Delta^{\mathcal{X}_n}_\infty u(x) := \max_{y\in\mathcal{X}_n} w_{xy}(u(y)-u(x)) + \min_{y\in\mathcal{X}_n} w_{xy}(u(y)-u(x)) = 0.$$

$$\min_{u:\mathcal{X}_n \to \mathbb{R}} J_\infty(u) = \max_{x,y \in \mathcal{X}_n} w_{xy} |u(x) - u(y)| \quad \text{subject to } u(x) = g(x) \text{ for } x \in \mathcal{O} \subset \mathcal{X}_n$$

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#### **Reference:**

[Kyng et al., 2015]

## Game theoretic *p*-Lapacian

We can also consider the game theoretic p-Laplacian for semi-supervised learning:

$$\begin{cases} \frac{1}{d_n} \Delta_2^{\mathcal{X}_n} u_n + \lambda (p-2) \Delta_{\infty}^{\mathcal{X}_n} u_n = 0 & \text{in } \mathcal{X}_n \setminus \mathcal{O} \\ u = g & \text{in } \mathcal{O}, \end{cases}$$

where  $d_n(x) = \sum_{y \in \mathcal{X}_n} w_{xy}^2$  and  $\lambda = \lambda(\Phi)$ .

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where  $d_n(x) = \sum_{y \in \mathcal{X}_n} w_{xy}^2$  and  $\lambda = \lambda(\Phi)$ .

This is likely better conditioned numerically when p is large.

## Game theoretic *p*-Laplacian

Theorem (Finite p [Calder, 2017b]) Let  $d , and suppose that <math>h \rightarrow 0$  such that

$$\lim_{n \to \infty} \frac{nh^q}{\log(n)} = \infty,$$
(13)

where  $q = \max\{d + 4, 3d/2\}$ . Then with probability one

$$u_n \longrightarrow u$$
 uniformly as  $n \to \infty$ , (14)

where  $u \in C(\mathbb{T}^d)$  is the unique viscosity solution of the weighted *p*-Laplace equation

$$\begin{cases} \operatorname{div} \left( f^2 |\nabla u|^{p-2} \nabla u \right) = 0 & \text{in } \mathbb{T}^d \setminus \mathcal{O} \\ u = g & \text{on } \mathcal{O} \end{cases}$$
(15)

Notice no upper bound on h (i.e., we don't require  $nh^p \rightarrow 0$ ).

All graph Laplacians are monotone schemes. We just need consistency and stability.

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we have

$$\mathbb{E}[\Delta_p^{\mathcal{X}_n}\varphi(x)] = nh^d \int_{\mathbb{R}^d} \Phi(|z|) |\varphi(x+zh) - \varphi(x)|^{p-2} (\varphi(x+zh) - \varphi(x)) f(x+zh) \, dz.$$

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Plug in Taylor expansions and plug away...

$$\mathbb{E}[\Delta_p^{\mathcal{X}_n}\varphi(x)] = \frac{1}{2}C_p f^{-1}\mathsf{div}(f^2|\nabla\varphi|^{p-2}\nabla\varphi)nh^{d+p} + R(x)nh^{d+p+1},$$

where

$$|R(x)| \leq C \|\varphi\|_{C^3(\mathbb{R}^d)}^{p-1}.$$

The maximum principle can be used to prove Hölder continuity when p > d:

$$\begin{cases} \Delta_p u := \operatorname{div}(|\nabla u|^{p-2}\nabla u) = 0 & \text{in } U\\ u = g & \text{on } \partial U, \end{cases}$$

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Let us define

$$v(x) = u(x_0) + C|x - x_0|^{lpha}$$
 for  $lpha = rac{p-d}{p-1}.$ 

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$$v(x) = u(x_0) + C|x - x_0|^{\alpha}$$
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If  $B(x_0,r)\subset U$  then for  $C=(\max g-\min g)r^{-lpha}$  we have

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It follows that

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2 Show that  $\Delta_p^{\mathcal{X}_n} v(x) \leq 0$  for  $|x - y| \geq ch$  with high probability.

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**2** For the game theoretic *p*-Laplacian, we use a different local barrier  $v(x) = |x - y|^{\alpha} + Mh_n^{\alpha} \sum_{k=1}^{\infty} \beta^k \mathbb{1}_{\{2|x-y| > (k-1)h_n\}}, \text{ where } \beta < 1.$ 

The local barrier

$$v(x) = |x - y|^{\alpha} + Mh_n^{\alpha} \sum_{k=1}^{\infty} \beta^k \mathbb{1}_{\{2|x-y| > (k-1)h_n\}}$$

exploits the form of the graph  $\infty\text{-Laplacian}$ 

$$\Delta^{\mathcal{X}_n}_\infty u(x) = \max_{y\in\mathcal{X}_n} w_{xy}(u(y)-u(x)) + \min_{y\in\mathcal{X}_n} w_{xy}(u(y)-u(x)).$$



Calder (UofM)

 Fast algorithms: Primal dual/Nesterov acceleration for pLaplacian learning (Mauricio Flores)

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**9** Soft constraint: Extend the results to the soft constraint

$$\min_{u:\mathcal{X}_n \to \mathbb{R}} J_p(u) + \lambda \sum_{y \in \mathcal{O}} |u(x) - g(x)|^q.$$

# Outline

1 Nondominated sorting

- 2 Convex hull peeling
- 3 Semi-supervised learning





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