How to Approximate a Blob with a Curve

An Overview of a Gradient-based Numerical Algorithm

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Based on joint work with Jonathan Hayase (UW) and Young-Heon Kim (UBC)

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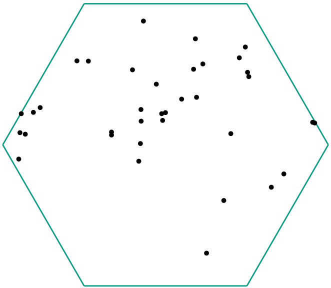
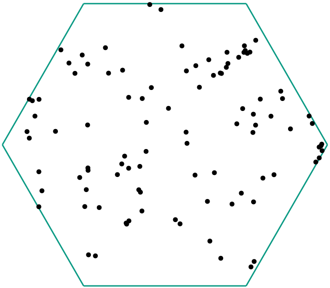
Summary

- Goal: Efficiently approximate n-d measures via m-dimensional sets $(m < n)$
  - "Approximate" in what sense?
  - "Efficient" in what sense?
- Outline:
  - Motivating examples
  - Define problem
  - Gradient structure
  - Algorithm
  - Regularization in Generative ML

Ex. 1: Learning noisily-embedded manifolds



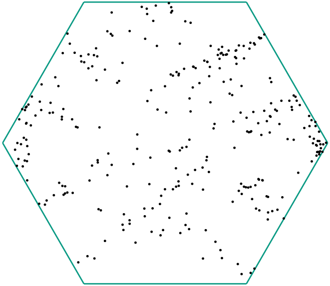
(a) A few data points...



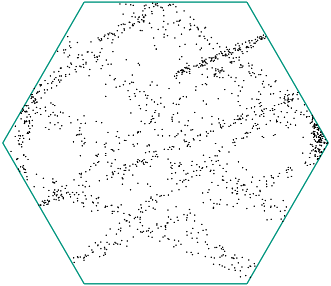
(b) ...and a few more.

Figure 1: Seemingly-unstructured data in a hexagon.

Ex. 1 (cont.): Learning noisily-embedded manifolds



(a) More...



(b) ...and more...

Figure 1: With more points, a picture begins to emerge.

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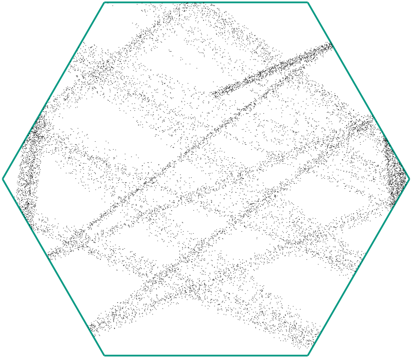

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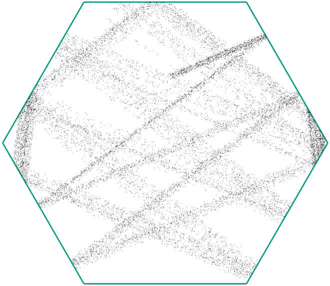
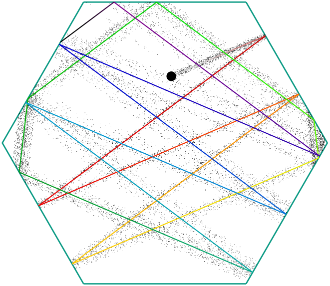


(a) The data.



(b) Extracted structure.

Figure 1: Recover a time-ordering!

Ex. 2: Approximating a properly-higher-dim. ρ

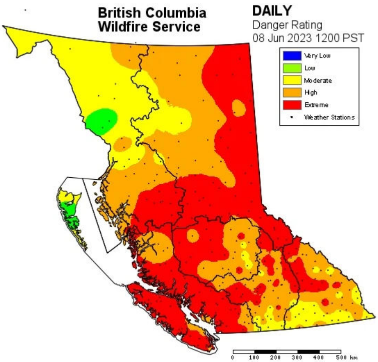
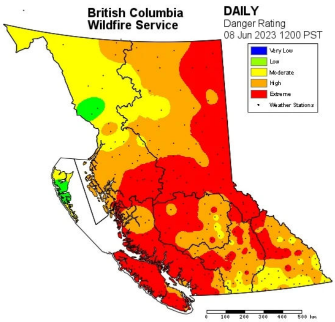


Figure 2: Wildfire danger map

Ex. 2: Approximating a properly-higher-dim. ρ



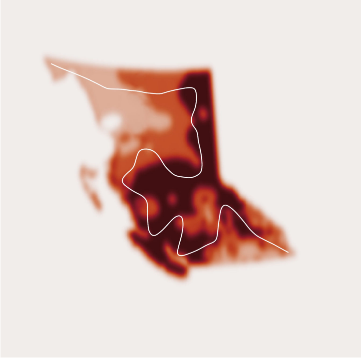


Figure 2: Example trajectory. (Is it "good?")

Summary of some applications

- $m = 1$, $n \in \{2, 3\}$: Routing problems (wildfire drone, package delivery routes, "continuous" TSP)
- $m = 1$, $n \geq 2$: Trajectory inference (e.g. cryo-EM, scRNA-seq)
- $m = 2$, $n = 3$: Catalytic surface design
- $1 \leq m \ll n$: Certain generative learning problems

Setting up the Problem

- Source:
  - $X \subseteq \mathbb{R}^m$ (compact)
- Target:
  - $\mu \in \mathcal{P}_{\text{cpt}}(\mathbb{R}^n)$
- Optimization variable:
  - $f : X \to \mathbb{R}^n$ (cont.)

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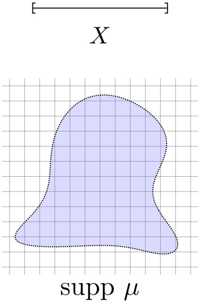

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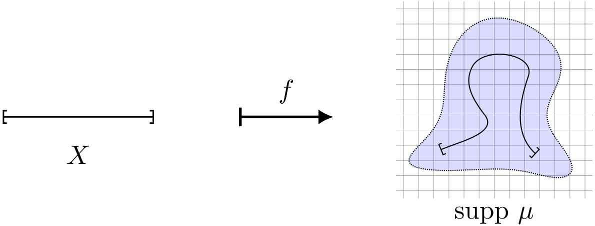


How "close" is $f(X)$ to μ?

- Want OT cost, but $f(X)$ a set
- Idea:

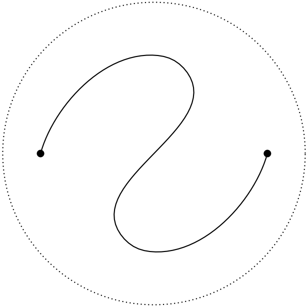
$$\mathcal{J}_p(f;\mu) = \inf_{\nu \in \mathcal{P}(f(X))} \mathbb{W}_p^p(\mu, \nu)$$

- Equivalently [**K.**, Hayase, Kim '24; Prop. 2.7]:

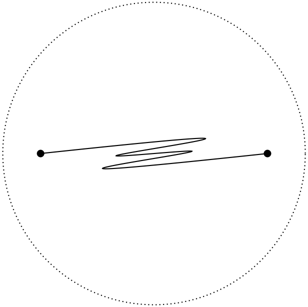
$$\begin{aligned} \mathcal{J}_p(f;\mu) &= \int_{\mathbb{R}^n} d^p(\omega, f(X)) \; d\mu(\omega) \\ &= \mathbb{E}_\mu[d^p(\omega, f(X))] \end{aligned}$$

Visualization

Q: Which shape better "fills" unit disk?



(a) One candidate



(b) ...And another

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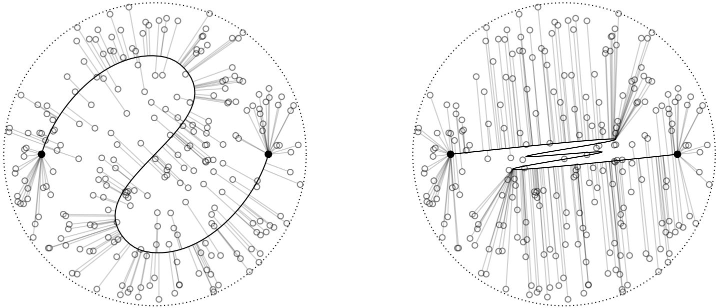

(a) A “good” filling (b) A “bad” filling

Quantifying complexity of f

- No complexity constraint → degeneracy; efficiency meaningless

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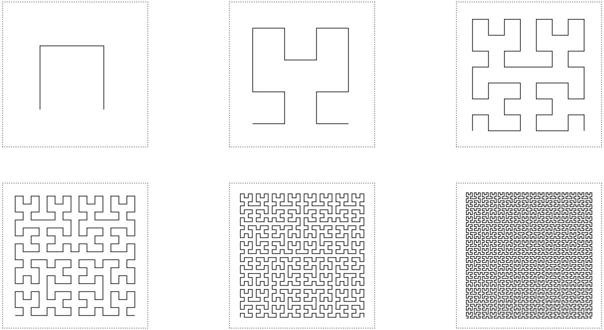

Quantifying complexity of f

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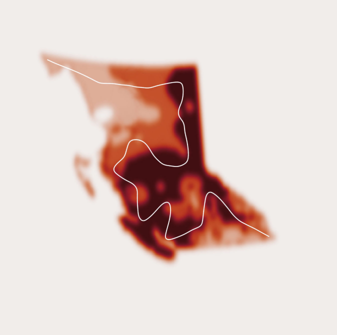


(a) Efficient trajectory

(b) Inefficient trajectory

Quantifying complexity of f

- No complexity constraint $\to$ degeneracy
- We use:

$$\begin{aligned}\mathcal{C}(f) &:= \|f\|_{W^{k,q}(X,\mathbb{R}^n)} \\ &= \left(\sum_{j=1}^{n}\sum_{|\alpha|\le k}\|D^\alpha f_j\|_{L^q}^q\right)^{1/q}.\end{aligned}$$

- Examples:

(a) Cheap f

(b) Expensive f

(c) Expensive f

The “best” f

- For $\lambda > 0$, minimize

$$\boxed{\mathscr{J}_\lambda(f;\mu) \coloneqq \mathscr{J}_p(f;\mu) + \lambda\mathscr{C}(f).}$$

- Computing global solutions:
  - “Probably” NP-Hard
  - For $k, q = 1$ & discrete μ, get TSP as $\lambda \to 0$.
- How about local improvements?

Improving an f

Theorem (Informal)

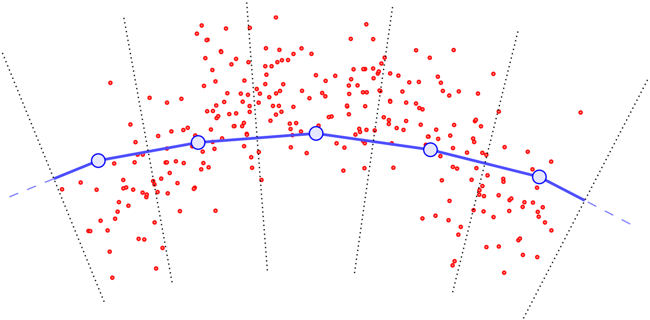
With technical hypotheses, get a vector field F and measure ν s.t. for all continuous ξ,

$$\lim_{\varepsilon \to 0} \frac{\mathcal{J}_p(f + \varepsilon\xi; \rho) - \mathcal{J}_p(f; \rho)}{\varepsilon} = \int -\langle F, \xi \rangle \, d\nu.$$

- Some details swept under rug ("what's domain of integration?")
- F like (negative) "gradient" (sans regularity issues)
- $-\langle F, \xi \rangle_{L^2(\nu)}$ like directional derivative
- ν very simple; F more complicated

What is F?

Discrete case easier to visualize:



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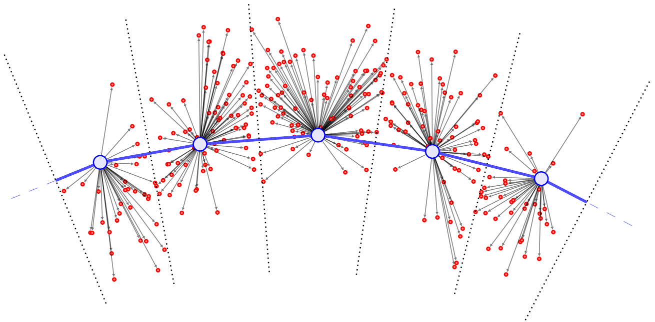
Discrete case easier to visualize: Compute $(p-1)$ barycenter



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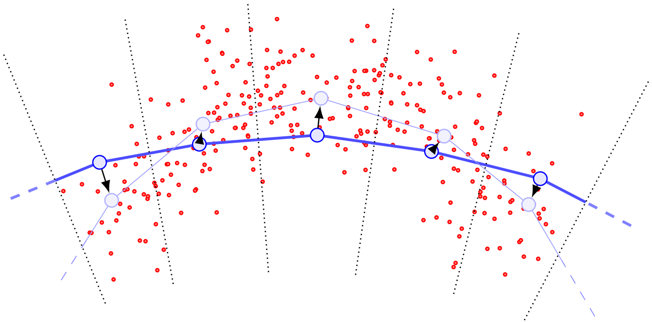

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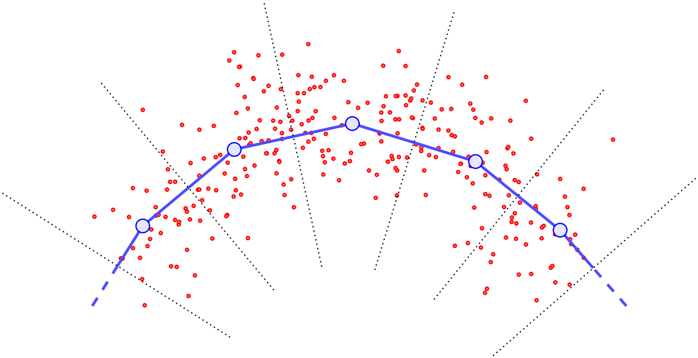


Visualizing F in cont. case

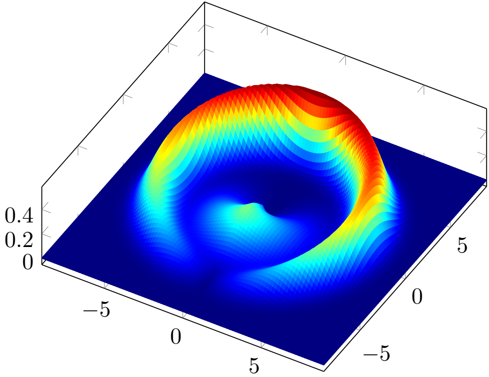


Figure 5: An example μ

Visualizing F in cont. case

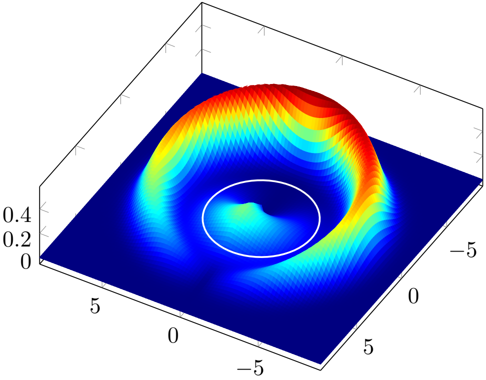


Figure 5: An example f approximating μ

Visualizing F in cont. case

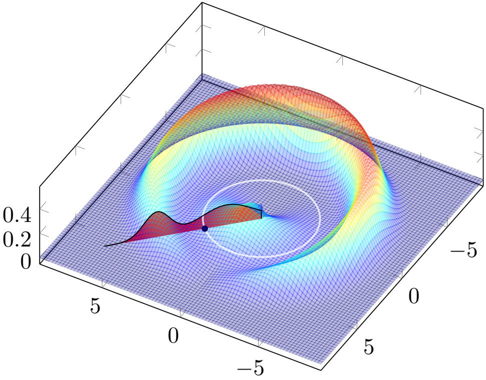


Figure 5: Slicing

Overview

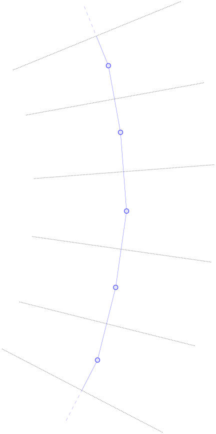
- Big picture:
  - Discretize f
  - Compute F $(= -\nabla \mathcal{J}_p)$ and $-\nabla \mathcal{C}$
  - Optimize to get step size η
  - $f \leftarrow f + \eta(F - \lambda \nabla \mathcal{C})$
- Challenges:

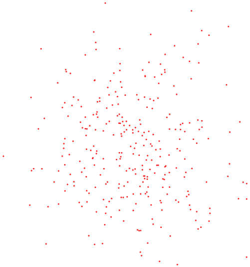
C1. Discretization of f is delicate

C2. Efficient Voronoi cell assignments for F

C3. How to compute $-\nabla \mathcal{C}$?

C1: Need evenly-spaced samples of f





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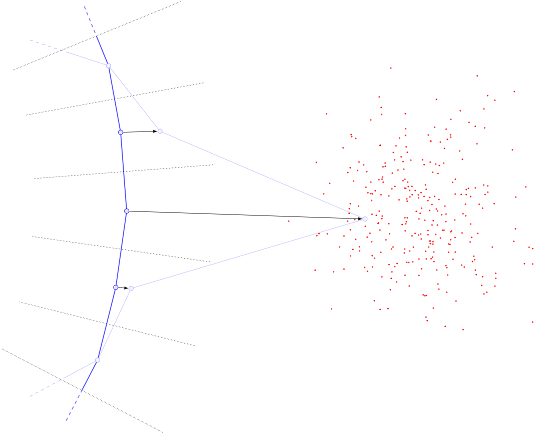

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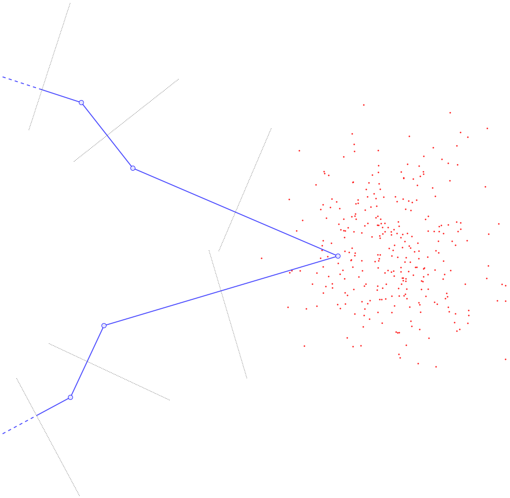


C1: Evenly-spaced samples of f—our method

- After each iteration:
  - Fit cubic spline f to samples
  - Define: Arclength functional

$$L(\mathsf{f}; a, b) = \int_a^b \sqrt{\sum_{j=1}^{n} (\dot{\mathsf{f}}_j)^2}\ dt$$

  - Compute total length ℓ
  - Get evenly-spaced values l_i on $[0, \ell]$
  - For given l_i, want t_i such that $L(\mathsf{f}; 0, t_i) \approx l_i$...
  - Binary search then polish w/ Newton's method

C1: Evenly-spaced samples of f, cont.

- Need: Efficient query method for arclength $L(\mathsf{f}; 0, t)$
  - Quadrature a bit slow
  - [5] reduces $L(\mathsf{f}; 0, t)$ to an elliptic integral explicitly solved in [3]
  - Reduction: need factorization into real quadratics

$$\sum_{j=1} (\dot{\mathsf{f}}_j)^2 = Q_1(t) Q_2(t),$$

    (exists if $\dot{\mathsf{f}} \neq 0$; use fast root-finding algorithms)
  - When $n = 2$: Get a stable, analytic formula via trick $q_1^2 + q_2^2 = (q_1 - iq_2)(q_1 + iq_2)$
- End result: Fast resampling of f

C2: Quickly computing F

- Continuous data: Special case μ uniform, $\operatorname{supp}\mu$ PL
  1. Explicitly compute Voronoi diagram
  2. Fast triangular decomposition of $\operatorname{supp}\mu$
  3. Triangles: F has analytic formula in terms of hypergeometric function
  4. Sum results
- Discrete data: Need faster Voronoi assignments
  - CPU-method: spatial-acceleration datastructures
  - GPU-method: brute-force

C2: CPU method, acceleration datastructures

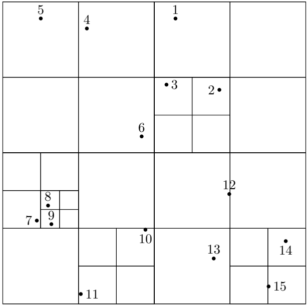


Figure 6: Example orthant subdivision for $\mathsf{M} = 15$ samples of $\mathrm{Unif}([0,1]^2)$.

C2: CPU method, acceleration datastructures

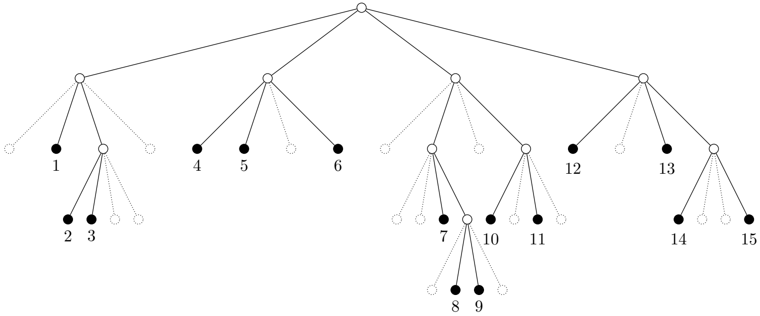


Figure 6: The tree datastructure encoding the quadrants shown previously.

C2: CPU method, acceleration datastructures

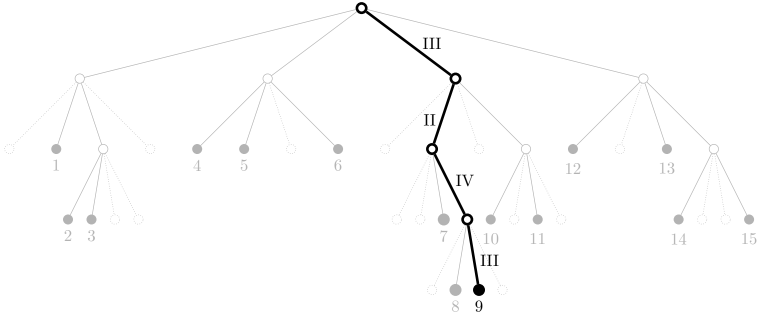


Figure 6: Associate lexicographic strings to each node, and permute input data array to be lex. sorted

C2: CPU method, acceleration datastructures

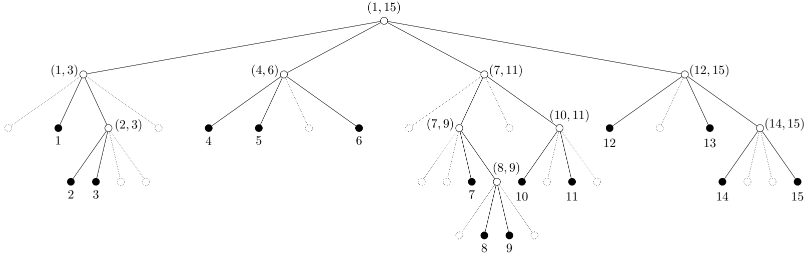


Figure 6: Annotate nodes of tree with range of descendants (also, diameter).

C2: CPU method, Performing the Voronoi Assignments

- With trees above, construct further k-d tree
- Core loop:
  1. Take data pt. v_i
  2. Query k-d tree for closest samples y_i^0, y_i^1 of f
  3. Let $r_i = \left| d(v_i, y_i^0) - d(v_i, y_i^1) \right|$ and compute
  $$j_i \coloneqq \lfloor \log_2 \left(r_i / \operatorname{diam}(\text{node for } v_i) \right) \rfloor$$
  4. Slice trailing j_i entries off `lex_code`(v_i); yields ancestor a_i
  5. Fact: All descendants $(v_i, \ldots, v_{i'})$ of a_i in same Voronoi cell as v_i
  6. Assign all $(v_i, \ldots, v_{i'})$; let $i = i' + 1$ and loop

C2: CPU method, Pictures

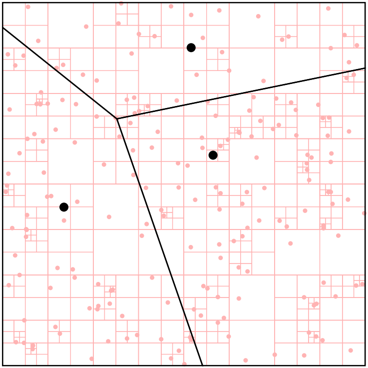


Figure 7: Starting configuration.

C2: CPU method, Pictures

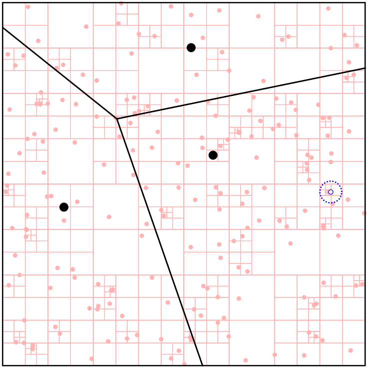


Figure 7: Select v_i.

C2: CPU method, Pictures

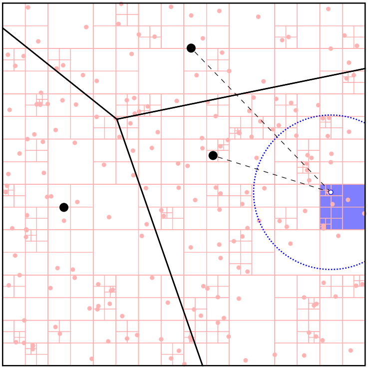


Figure 7: Compute ancestor $a_i \subseteq B_{r_i}(v_i)$

C2: CPU method, Benchmarking

M	Mean exec. time $\pm\,\sigma$ (ms)		Median (ms)		Mem. est. (MiB)		Allocs. est. (#)	
	Our alg.	k-d tree	Our alg.	k-d tree	Our alg.	k-d tree	Our alg.	k-d tree
$2.16 \cdot 10^5$	43 ± 4	45 ± 11	43	39	21.03	32.96	521697	864014
$5.12 \cdot 10^5$	76 ± 7	116 ± 25	76	107	36.70	78.13	879072	2048014
$8.00 \cdot 10^5$	102 ± 5	190 ± 35	103	184	48.83	122.07	1143060	3200014
$1.00 \cdot 10^6$	114 ± 6	242 ± 92	115	221	56.16	152.59	1297350	4000014
$1.20 \cdot 10^6$	126 ± 7	307 ± 148	127	281	62.81	181.11	1433556	4800014
$1.50 \cdot 10^6$	152 ± 13	398 ± 172	149	383	72.39	228.88	1627029	6000014
$1.80 \cdot 10^6$	161 ± 9	493 ± 273	164	461	81.83	274.66	1798515	7200014
$2.00 \cdot 10^6$	168 ± 10	550 ± 316	169	514	86.72	305.18	1906332	8000014
$2.50 \cdot 10^6$	196 ± 12	711 ± 477	198	619	99.70	381.47	2150112	10000014
$5.00 \cdot 10^6$	300 ± 23	1587 ± 1201	304	1304	155.41	762.94	3123312	20000014
$1.00 \cdot 10^7$	467 ± 30	3370 ± 2805	471	2838	245.37	1490	4500033	40000014

Table 1: Benchmarking for $\mu = \text{Unif}([0,1]^2)$. M: # input data pts. $N = 100$: # Voronoi cell roots (also uniform).

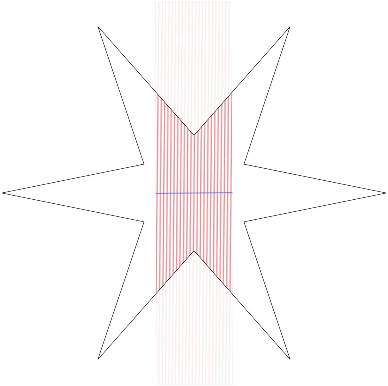
C3: Computing Sobolev gradient $-\nabla \mathcal{C}$

- In C1 we fit a cubic spline f
- In general: $\mathsf{f} \notin W^{k,q}(X; \mathbb{R}^n)$
- $\Rightarrow$ need new spline of order $k+2$.
- Approach:
  1. Get B-Spline basis; compute $C^k(X; \mathbb{R}^n)$ spline interpolating resampled f
  2. Derivatives of all orders linear in spline coefficients
  3. Spline coefficients linear in fitted points
  4. Linear relationships can be precomputed very quickly (inverse of $(k+2)$-width banded matrix) *once* per loop
  5. $\Rightarrow$ fast computation of derivatives of all orders

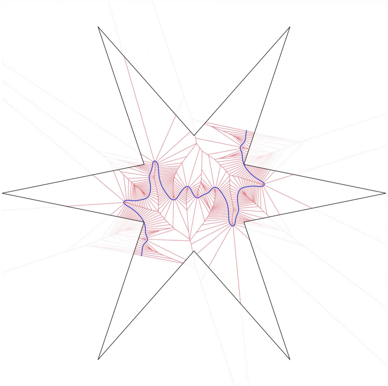
Bottom Line

- Runtime:
  - Resampling f evenly:
    - Fast for $n = 2$
    - Good for $n > 2$
  - Computing $F = -\nabla \mathcal{J}_p$:
    - Special continuous case: Very fast if $\operatorname{supp} \mu$ convex; decent otherwise
    - Discrete case: Acceptable on CPU; extremely fast on GPU
  - Approximating $-\nabla \mathcal{C}$:
    - *Very* fast
- Memory:
  - Lightweight except discrete CPU method for $F = -\nabla \mathcal{J}_p$

Example numerics



(a) $i = 1$



(b) $i = 150$

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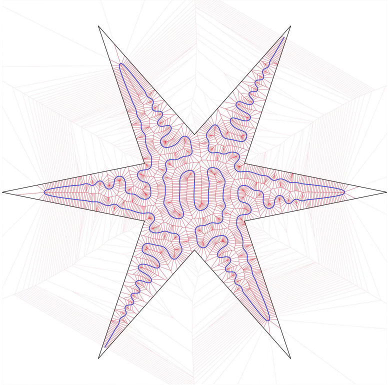
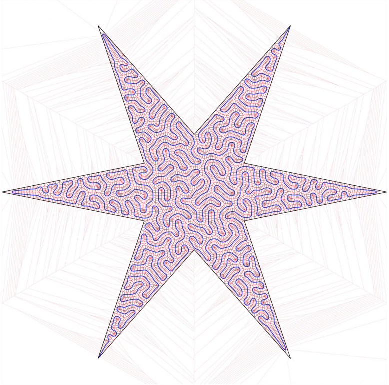
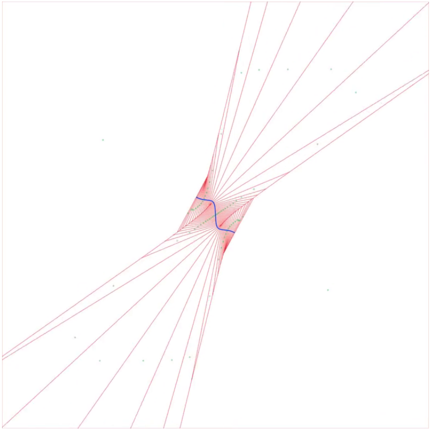


(a) $i = 300$



(b) $i = 1000$

More simulations



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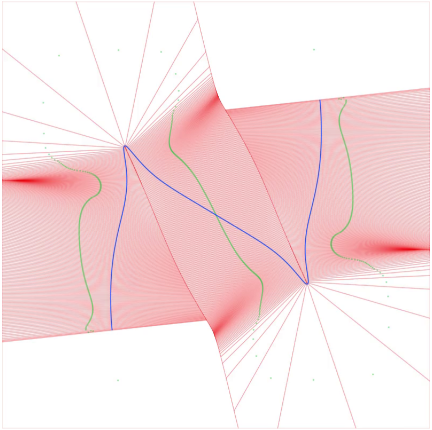

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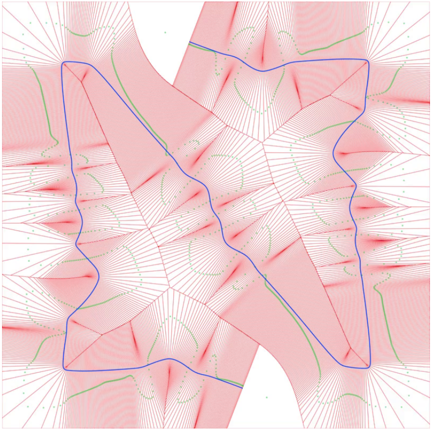

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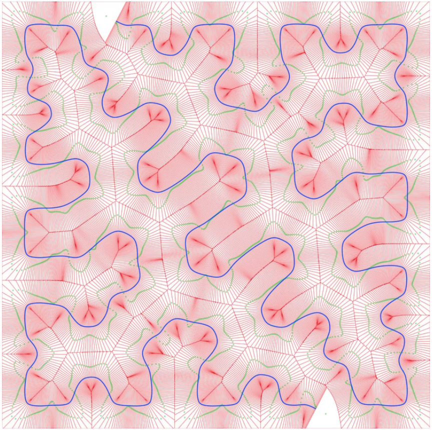
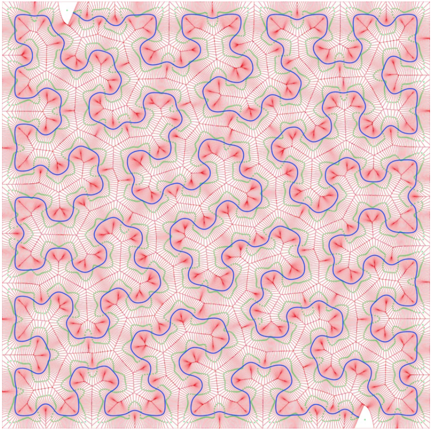
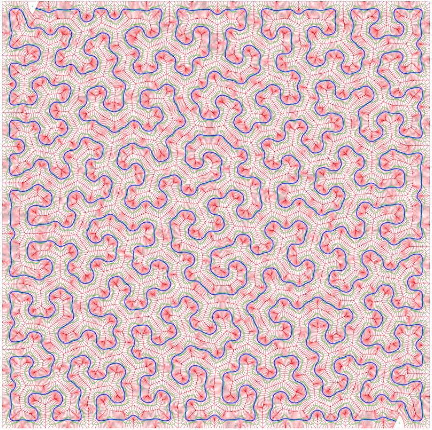


More simulations



More simulations



Transition: Numerics $\to$ gen. ML

Setting:

- μ "hidden;" only have $\hat{\mu}_N$
- Goal: Generate novel samples $\sim \mu$

Common assumption:

- μ concentrated on low-dim. set

Role of regularization:

- Classical: avoidance of overfitting
- New: Better expressability within model class

Recall: WGAN

Notation:

- Latent ρ, generator f_θ, critic D_w

Goal: Minimize

$$W_1(\mu, (f_\theta)_\# \rho) = \sup \left\{ \int D_w \; d(\mu - (f_\theta)_\# \rho) \;\middle|\; D_w \in \mathrm{Lip}_1 \right\}$$

Training:

- D_w: step (with reg.) along ∇_w
- f_θ: step along $-\nabla_\theta$

WGAN, cont.

Takeaway:

- Classical: reg. only *critic* D_w
- Generator f_θ: gradients from $D_w \implies$ implicit reg.?

Our proposal:

- "Factor" WGAN:
  1. m-to-n: Learn *set* $\mathrm{supp}((f_\theta)_\# \rho)$ w/o knowing f
  2. m-to-m: Learn param. f_θ
- Isolate "hard" m-to-n problem (learning *shape* of support) and regularize it
- Do "easy" m-to-m step second

New regularization interpretation

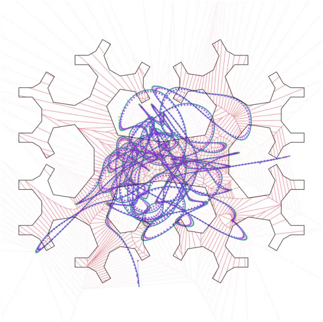
Role of explicit reg.

- f_θ avoids self-intersections
- fewer points outside $\text{supp}(\mu)$
- $\text{Lip}(f_\theta)$ small $\implies$ better preservation of locality

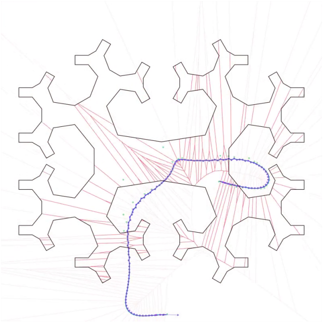
The point:

- Reparam. φ with $(f_\theta \circ \varphi)_\# \rho = (\pi_{f_\theta})_\# \mu$ less singular
- φ less singular $\implies$ better training
  - Low-regularity functions often difficult to express in model class
  - Slow convergence, training instability, ...

A regularized "generator"

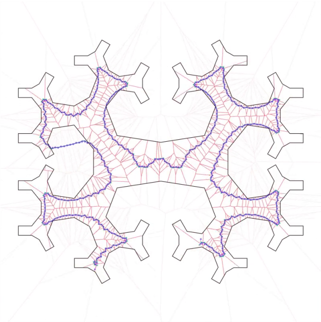


(a) $i = 1$

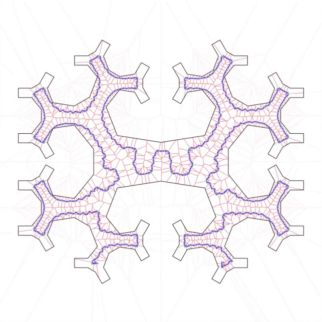


(b) $i = 110$

A regularized "generator"

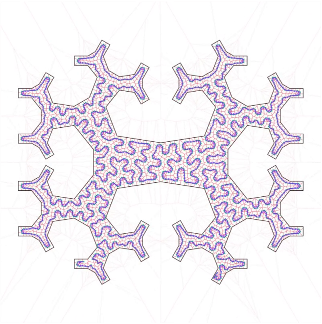


(a) $i = 800$



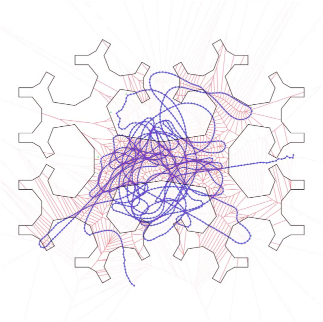
(b) $i = 1120$

A regularized "generator"

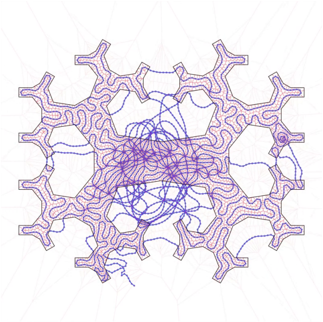


(a) $i = 1850$

(cont.): Unregularized Generator

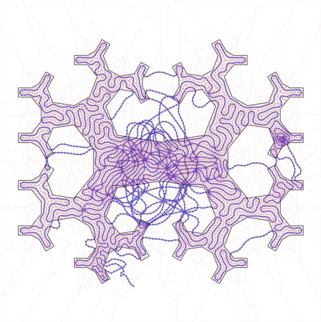


(a) $i = 110$

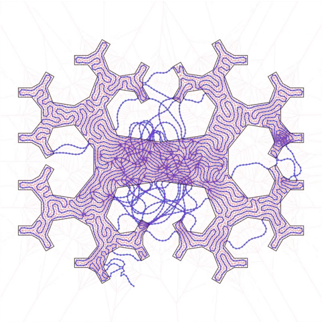


(b) $i = 800$

(cont.): Unregularized Generator

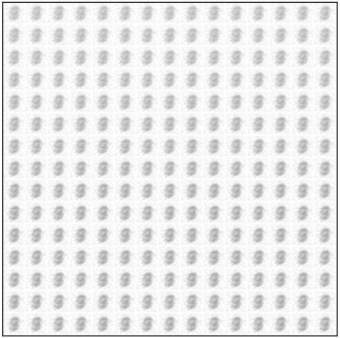


(a) $i = 1120$

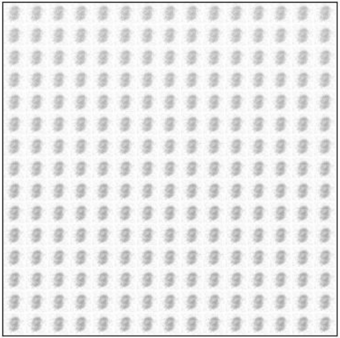


(b) $i = 1850$

Proof of concept: training on MNIST



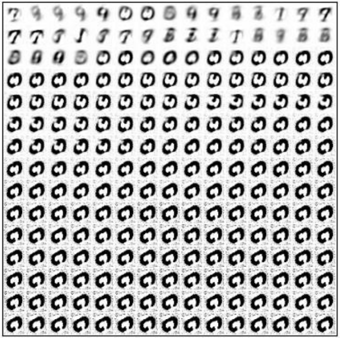
(a) 1 epoch (wd)



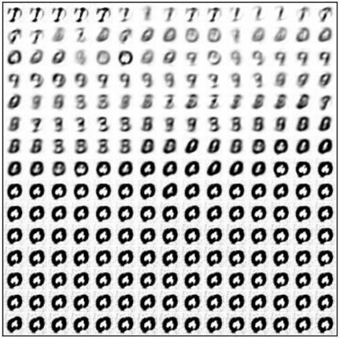
(b) 1 epoch (reg)

Figure 11: f sampled at 15^2 uniformly-spaced points on $[0, 1]$

Proof of concept: training on MNIST



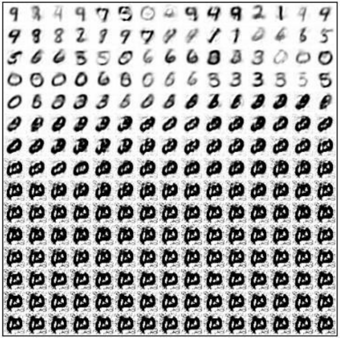
(a) 30 epochs (wd)



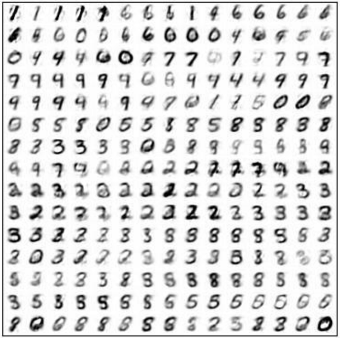
(b) 30 epochs (reg)

Figure 11: f sampled at 15^2 uniformly-spaced points on $[0, 1]$

Proof of concept: training on MNIST



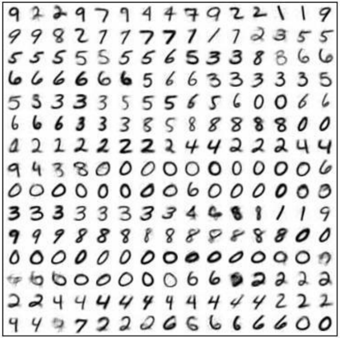
(a) 100 epoch (wd)



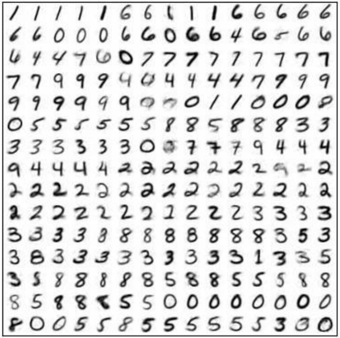
(b) 100 epoch (reg)

Figure 11: f sampled at 15^2 uniformly-spaced points on $[0, 1]$

Proof of concept: training on MNIST



(a) 1000 epochs (wd)



(b) 1000 epochs (reg)

Figure 11: f sampled at 15^2 uniformly-spaced points on $[0, 1]$

Thank you for your attention!

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