Westfälische Wilhelms-Universität Münster

Variational Methods and PDEs on Graphs with Applications in Data Processing and Machine Learning

Talk at the FAU, Erlangen

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April 26th, 2018

Outline

Introduction

- Motivation
- Related work

Methods

- Finite weighted graphs
- Graph construction
- Discrete differential operators on graphs
- Translating variational methods and PDEs to graphs

Applications

- Diffusion-based problems
- Interpolation-based problems

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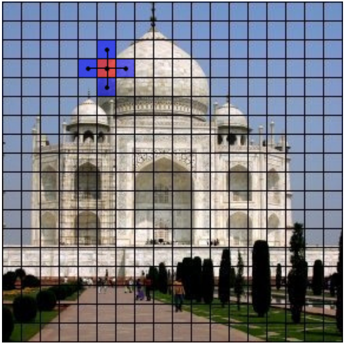
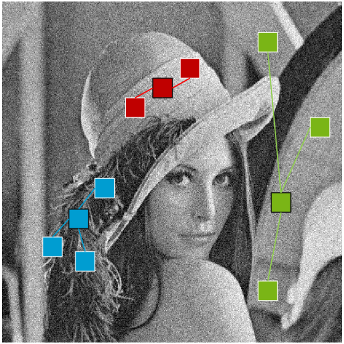
Discrete data modeling using finite graphs

Question: How can we apply graphs for image processing?



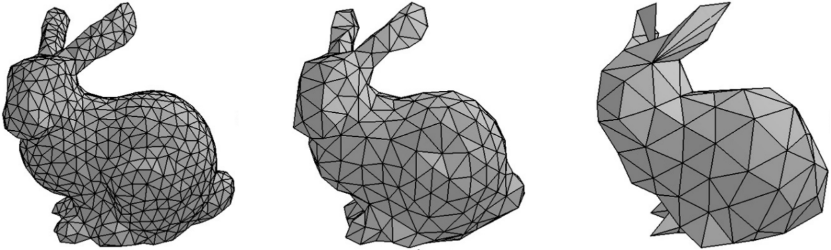
Local neighborhood of a pixel



Nonlocal neighborhood of a pixel

Discrete data modeling using finite graphs

Question: How can we apply graphs for polygon mesh processing?

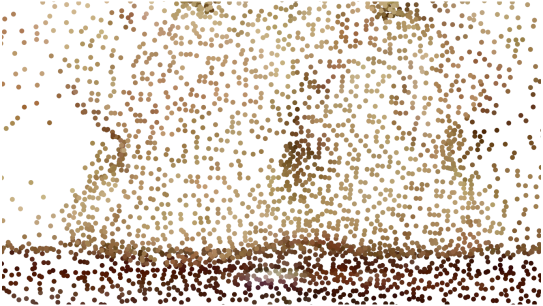


Polygon mesh approximation of a 3D surface.

Image courtesy: Gabriel Peyré

Discrete data modeling using finite graphs

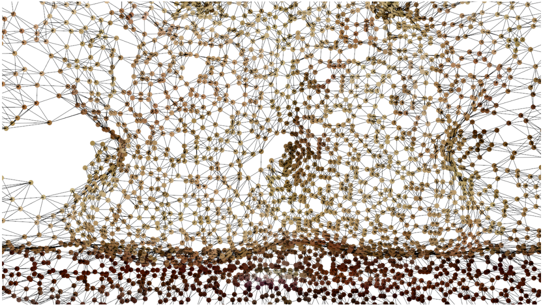
Question: How can we apply graphs for point cloud processing?



Colored 3D point cloud data of a scanned chair

Discrete data modeling using finite graphs

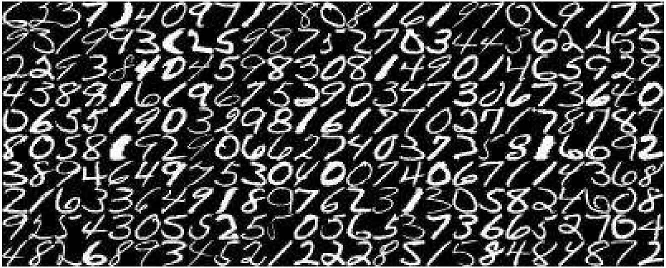
Question: How can we apply graphs for point cloud processing?



Graph construction on a 3D point cloud

Discrete data modeling using finite graphs

Question: How can we apply graphs for machine learning?

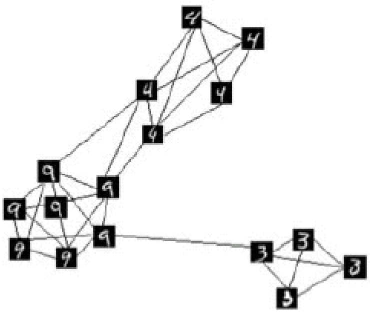


Subset of handwritten digits from MNIST database [1]

[1] Y. LeCun, C. Cortes, C. Burges: *The MNIST database of handwritten digits*

Discrete data modeling using finite graphs

Question: How can we apply graphs for machine learning?



Graph construction using suitable similarity features

Related work

Finite weighted graphs:

- A. Elmoataz, O. Lézoray, S. Bougleux: *Nonlocal Discrete Regularization on Weighted Graphs: a Framework for Image and Manifold Processing*. IEEE TIP 17 (2008)
- T. Bühler, M. Hein: *Spectral Clustering based on the Graph p-Laplacian*, Proc. of ICML (2009)
- F. Lozes, A. Elmoataz, O. Lezoray: *Partial Difference Operators on Weighted Graphs for Image Processing on Surfaces and Point Clouds*. IEEE TIP 23 (2014)
- Y. van Gennip, N. Guillen, B. Osting, A.L. Bertozzi: *Mean Curvature, Threshold Dynamics, and Phase Field Theory on Finite Graphs*. Milan Journal of Mathematics 82 (2014)
- B. Osting, C. White, E. Oudet: *Minimal Dirichlet Energy Partitions for Graphs*. SIAM J. Sci. Comput. 36 (2014)
- C. Garcia-Cardona, E. Merkurjev, A. Bertozzi, A. Flenner, A.G. Percus: *Multiclass Data Segmentation using Diffuse Interface Methods on Graphs*. IEEE Trans. PAMI. 36 (2014)
- S.H. Kang, B. Shafei, and G. Steidl: *Supervised and transductive multi-class segmentation using p-Laplacians and RKHS methods*. Journal of Visual Communication and Image Representation 25 (2014)
- E. Merkurjev, E. Bae, A.L. Bertozzi, X.C. Tai: *Global Binary Data Optimization on Graphs for Data Segmentation*. J. Math. Imag. Vis. 52 (2015)
- Z. Shi, S. Osher, and W. Zhu: *Weighted Nonlocal Laplacian on Point Cloud*. UCLA CAM Reports: cam16-88 (2016)

Related work

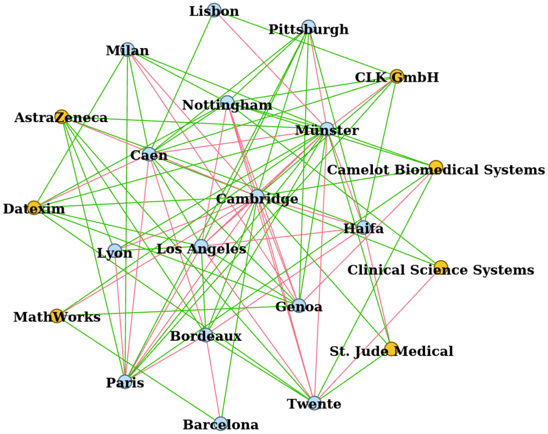
Nonlocal operators and variational models:

- G. Gilboa, S. Osher: *Nonlocal Operators with Applications to Image Processing*. Multiscale Model. Simul. 7 (2008)
- P. Arias, V. Caselles, G. Sapiro: *A Variational Framework for Non-Local Image Inpainting*. Energy Minimization Methods in Computer Vision and Pattern Recognition (2009)
- X. Zhang, M. Burger, X. Bresson, S. Osher: *Bregmanized Nonlocal Regularization for Deconvolution and Sparse Reconstruction*. SIAM Journal on Imaging Sciences 3 (2010)
- J.F. Aujol, G. Gilboa, N. Papadakis: *Nonlocal Total Variation Spectral Framework*. SSMV (2015)
- A. Chambolle, M. Morini, M. Ponsiglione: *Nonlocal Curvature Flows*. Arch Rat Mech Anal (2015)
- J. Lellmann, K. Papafitsoros, C.-B. Schönlieb, D. Spector: *Analysis and Application of a Nonlocal Hessian*. SIAM Journal on Imaging Sciences 8 (2015)

Transition from discrete to continuous mathematics:

- M. Belkin, P. Niyogi: *Towards a Theoretical Foundation for Laplacian-Based Manifold Methods*. J. Comput. System Sci. 74 (2008)
- U. von Luxburg, M. Belkin, O. Bousquet: *Consistency of Spectral Clustering*. The Annals of Statistics 36 (2008)
- N. Garcia Trillos, D. Slepcev: *Continuum Limit of Total Variation on Point Clouds*. Archive of Rational Mechanics and Analysis 1 (2016)
- N. Garcia Trillos, D. Slepcev, J. von Brecht, T. Laurent, and X. Bresson: *Consistency of Cheeger and ratio graph cuts*. Journal of Machine Learning Research 17 (2016)

Related work



Visualization of existing and newly established cooperations within the H2020 RISE project *“Nonlocal Methods for Arbitrary Data Sources (NoMADS)”*

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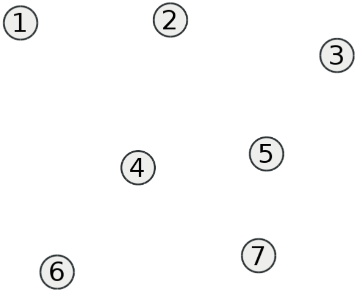

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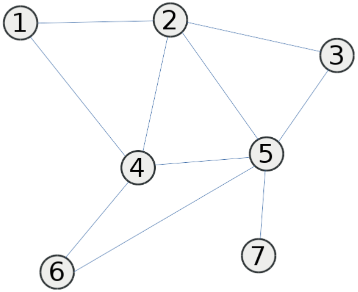

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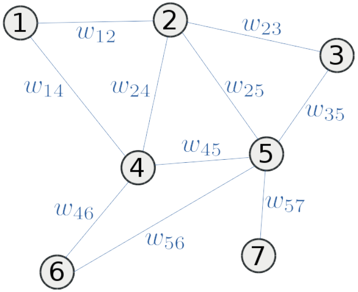
- a weight function $w \colon E \rightarrow [0, 1]$ with: $w(u, v) > 0 \Leftrightarrow (u, v) \in E$



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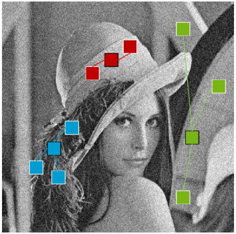
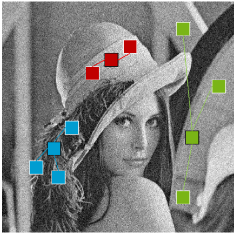
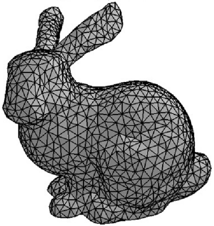


Finite weighted graphs

Application data is represented by a vertex function $f\colon V \to \mathbb{R}^m$, e.g.,

- Grayscale values or RGB colors
- 3D coordinates

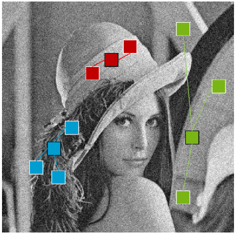


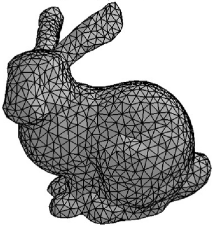


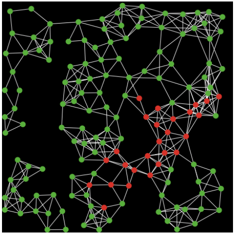
Finite weighted graphs

Application data is represented by a vertex function $f: V \to \mathbb{R}^m$, e.g.,

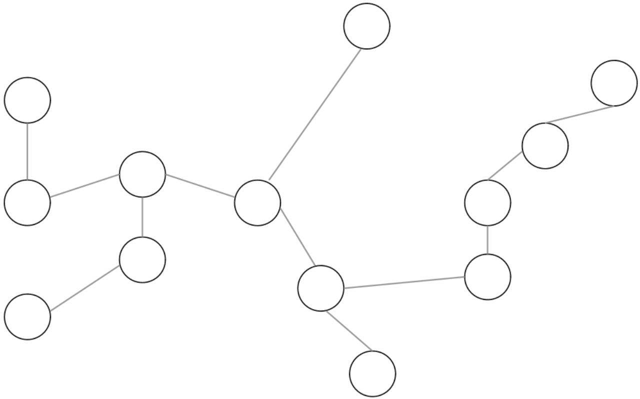
- Grayscale values or RGB colors
- 3D coordinates
- Labels





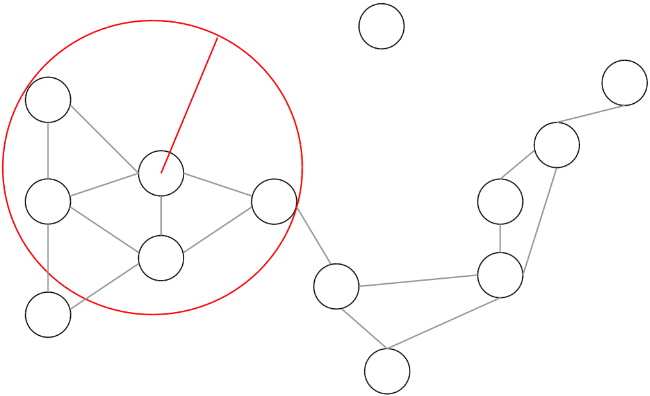


General graph construction



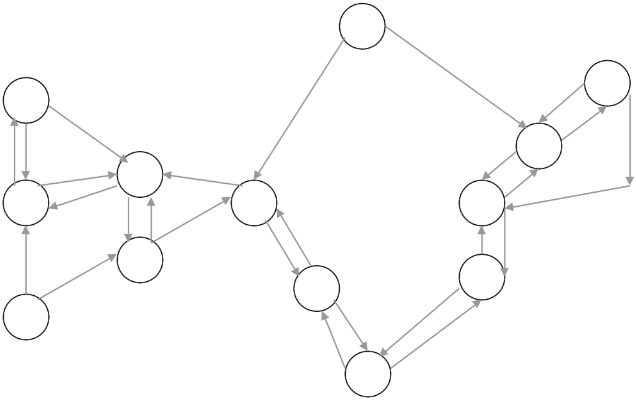
Minimum spanning tree

General graph construction



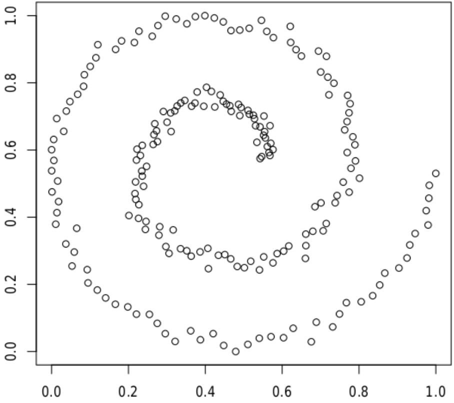
ϵ-ball graph

General graph construction



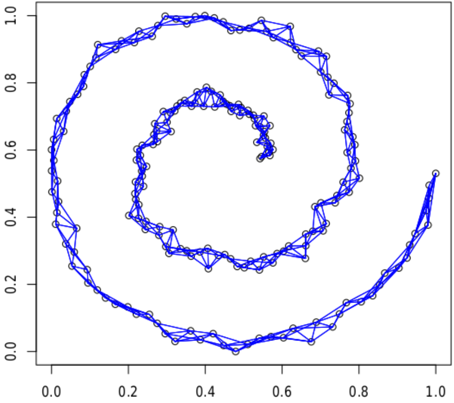
k-nearest-neighbor graph (k=2)

General graph construction



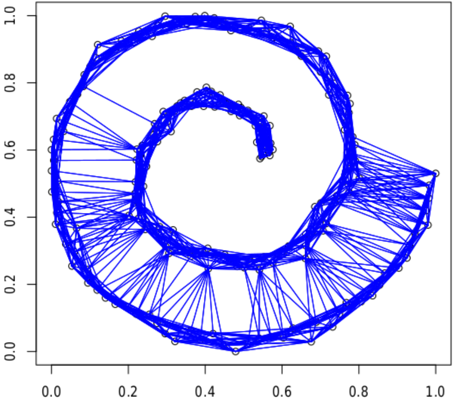
Distribution of 2D points

General graph construction



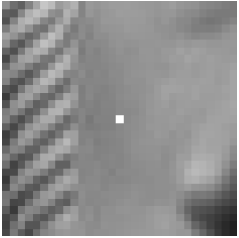
k-NN graph for k=3

General graph construction



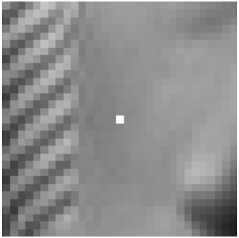
k-NN graph for k=15

Patches in nonlocal image processing



Pixel of interest

Patches in nonlocal image processing



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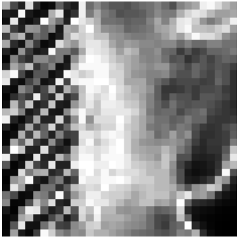
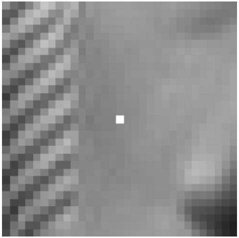


Intensity-based distance

Patches in nonlocal image processing



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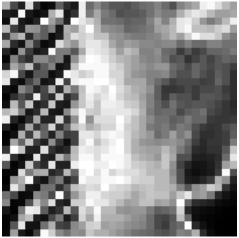

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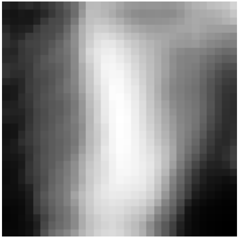
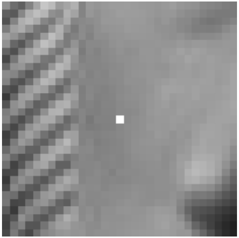


Patch-based distance [2]

[2] A. Buades: *A Nonlocal Algorithm for Image Denoising*. CVPR (2005)

Patches in nonlocal image processing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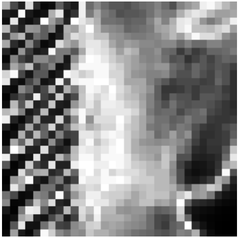
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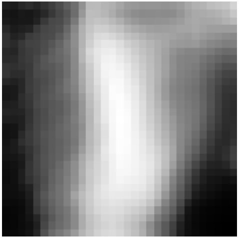

Patch-based distance [2]

Question:
How to construct patches for regularity on 3D point cloud data?

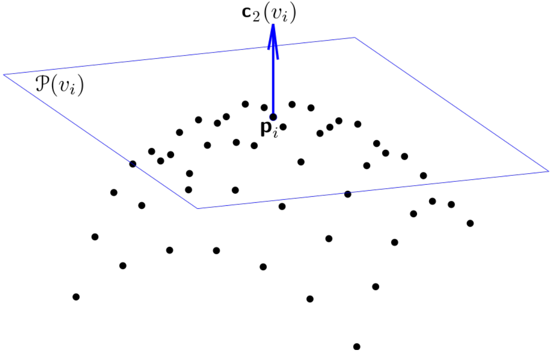
[2] A. Buades: *A Nonlocal Algorithm for Image Denoising*. CVPR (2005)

Patch construction for 3D point clouds

3D point cloud data of a curved surface

[3] F. Lozes, A. Elmoataz, O. Lezoray: *Partial Difference Operators on Weighted Graphs for Image Processing on Surfaces and Point Clouds*. IEEE TIP 23 (2014)

Patch construction for 3D point clouds



Estimated tangential plane with outer normal

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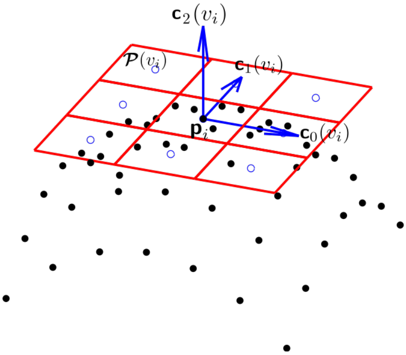

Construction of oriented patch in tangential plane

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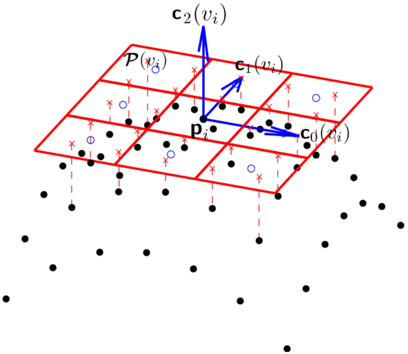

Projection of local neighborhood values onto patch

[3] F. Lozes, A. Elmoataz, O. Lezoray: *Partial Difference Operators on Weighted Graphs for Image Processing on Surfaces and Point Clouds*. IEEE TIP 23 (2014)

Example: Color patches on 3D point clouds

Color patch construction on 3D point cloud of a scanned woman

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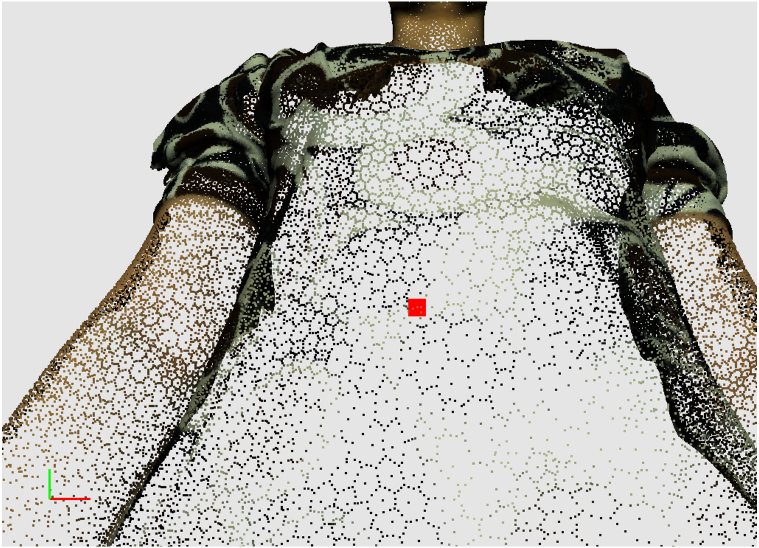

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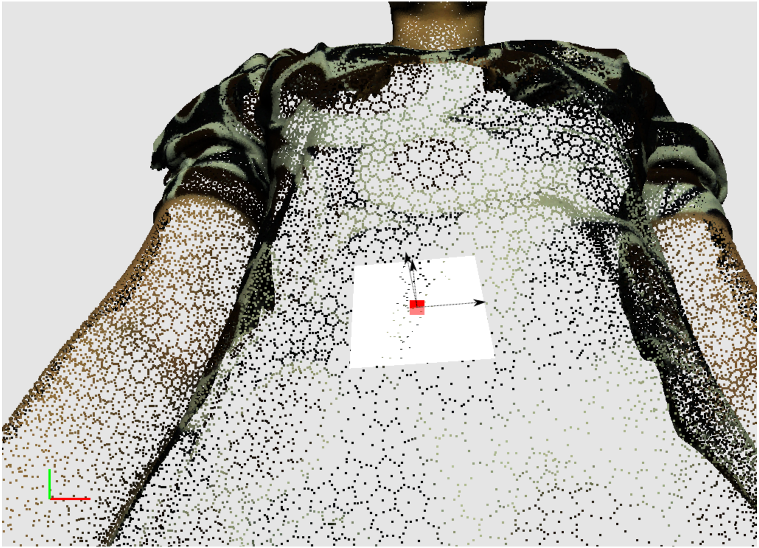

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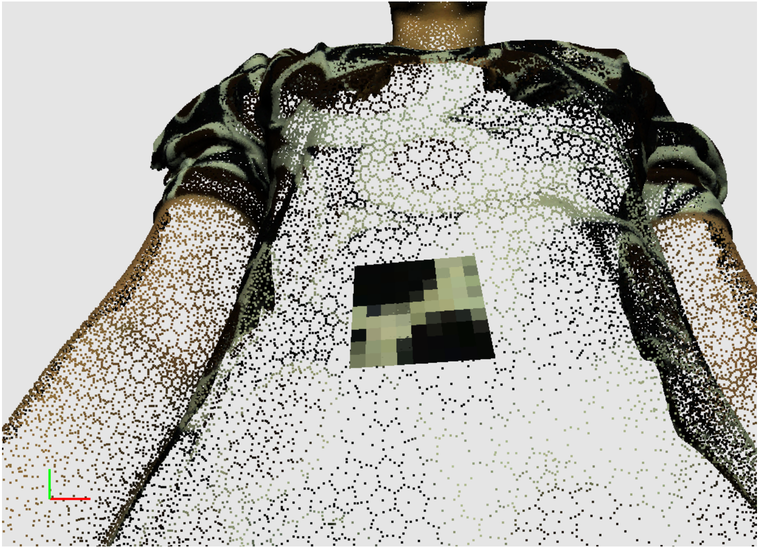

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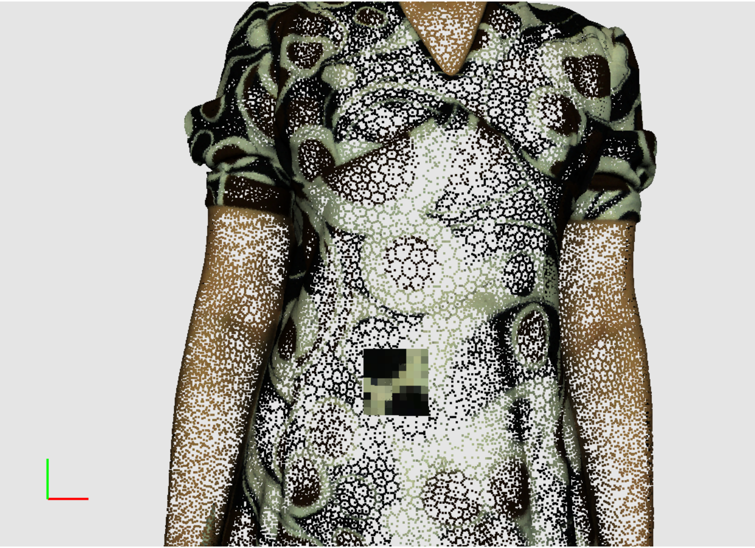

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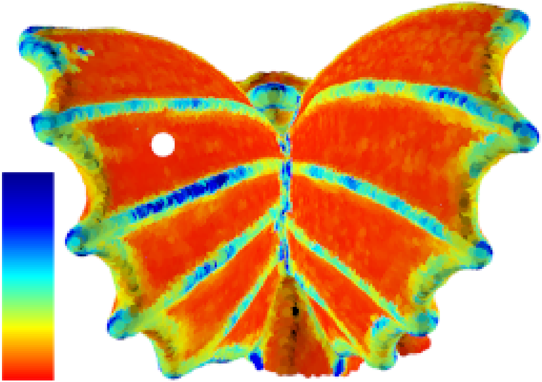
Example: Color patches on 3D point clouds

Color patch construction on 3D point cloud of a scanned woman

Example: Height patches on 3D point clouds

Height patch on 3D point cloud of a scanned gargoyle statue

Example: Height patches on 3D point clouds



Visualization of Euclidean distance between current height patch (white) to all other patches

Weighted finite differences

Let (V, E, w) be a weighted graph and let $f\colon V \to \mathbb{R}^m$ be a vertex function. The weighted finite difference $d_w\colon H(V) \to H(E)$ of $f \in H(V)$ along an edge $(u, v) \in E$ is given as:

$$d_w f(u, v) = \sqrt{w(u, v)}(f(v) - f(u)) \quad (1)$$

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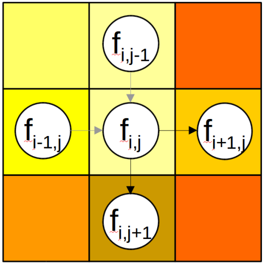
Then the weighted gradient of f in a vertex $u \in V$ is given as:

$$\nabla_w f(u) = (\partial_v f(u))_{v \in V} \quad \text{with} \quad \partial_v f(u) = d_w f(u, v) \quad (2)$$

Special case: local image processing

Let $G = (V, E, w)$ be a directed 2-neighbour grid graph with:

$$\partial_v f(u) = \sqrt{w(u,v)}(f(v) - f(u)) \quad \text{and} \quad w(u,v) = \begin{cases} \frac{1}{h^2}, & \text{if } u \sim v \\ 0, & \text{else} \end{cases}$$



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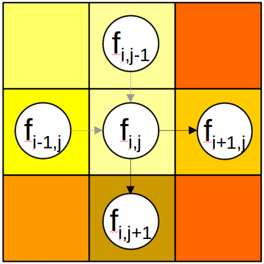

$\rightarrow$ Weighted finite differences correspond to forward differences!

Adjoint operator and divergence

Let $f \in H(V)$ be a vertex function and let $G \in H(E)$ be an edge function.

One can deduce the adjoint operator $d_w^* : H(E) \to H(V)$ of $d_w : H(V) \to H(E)$ by the following property:

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Then the divergence $\text{div}_w : H(E) \to H(V)$ of G in a vertex $u \in V$ is given as:

$$\text{div}_w G(u) = -d_w^* G(u) = \sum_{v \sim u} \sqrt{w(u,v)} (G(u,v) - G(v,u)) \tag{4}$$

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One can deduce the adjoint operator $d_w^* : H(E) \to H(V)$ of $d_w : H(V) \to H(E)$ by the following property:

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Then the divergence $\text{div}_w : H(E) \to H(V)$ of G in a vertex $u \in V$ is given as:

$$\text{div}_w G(u) = -d_w^* G(u) = \sum_{v \sim u} \sqrt{w(u,v)} (G(u,v) - G(v,u)) \tag{4}$$

We have in particular the following conservation law:

$$\sum_{u \in V} \text{div}_w G(u) = 0 \tag{5}$$

Translating variational problems to graphs

Example: A general variational denoising model

Translating variational problems to graphs

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Find a minimizer $f \colon V \to \mathbb{R}^m$ of the energy functional

$$E(f) \ = \ \lambda ||f - f_0||^2 + ||\nabla f||_{p,q}^p \ , \qquad \lambda > 0$$

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with $$||\nabla f||_{p,q} \;=\; \left(\frac{1}{p}\sum_{u\in V}\left(\sum_{v\sim u}|\nabla f(u,v)|^q\right)^{\frac{p}{q}}\right)^{\frac{1}{p}}, \quad 1 \leq p, q < \infty.$$

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Special cases:

p=q=1 : (Anisotropic) total variation regularization

p=q=2 : Tikhonov regularization

Graph p-Laplacian operators

Observation:

Deriving optimality conditions leads to the graph p-Laplace operator [4].

[4] A. Elmoataz, M. Toutain, D. Tenbrinck: *On the p-Laplacian and infinity-Laplacian on Graphs with Applications in Image and Data Processing*. SIAM Journal on Imaging Sciences 8 (2016)

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Isotropic graph p-Laplacian:

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Translating PDEs to weighted graphs

Example: Heat equation

Let $S \subset \mathbb{R}^n$ be a smooth compact manifold and $f : S \times [0, T] \to \mathbb{R}$ twice differentiable on S be a vertex function. One important partial differential equation (PDE) is a surface diffusion process of the form:

$$\begin{cases} \frac{\partial f(x,t)}{\partial t} & = \Delta^S f(x,t) \,, \\ f(x, t = 0) & = f_0(x) \,, \end{cases} \tag{6}$$

for which $f_0 : S \to \mathbb{R}$ is the initial value of f at time $t = 0$.

Translating PDEs to weighted graphs

Example: Heat equation

Let $G(V, E, w)$ be a weighted graph and let $f : V \times [0, T] \to \mathbb{R}$ be a vertex function. One important partial difference equation (PdE) is a graph diffusion process of the form:

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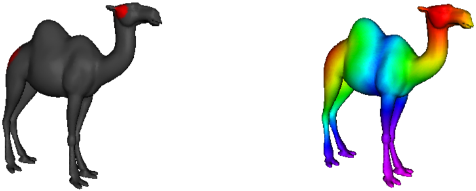

Connection to discretization schemes

Choosing the right graph construction and weight function we recover:

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Discretization schemes for gradient operators:

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Outline

Introduction

- Motivation
- Related work

Methods

- Finite weighted graphs
- Graph construction
- Discrete differential operators on graphs
- Translating variational methods and PDEs to graphs

Applications

- Diffusion-based problems
- Interpolation-based problems

Diffusion-based problems on graphs

The initial value problem for graph p-Laplacian diffusion is given as:

$$\begin{cases} \frac{\partial f(u,t)}{\partial t} & = \Delta_{w,p}^{a} f(u,t) \\ f(u, t = 0) & = f_0(u) \end{cases}$$

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Applying forward Euler time discretization leads to an iterative scheme:

$$f^{n+1}(u) \;=\; f^{n}(u) + \Delta t \sum_{v \sim u} (w(u,v)^{p/2} |f(v) - f(u)|^{p-2} (f(v) - f(u))$$

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l^∞-norm stability can be guaranteed under the following CFL condition:

$$1 \; \geq \; \Delta t \sum_{v \sim u} (w(u,v)^{p/2} |f(v) - f(u)|^{p-2}$$

Image denoising

Perturbed grayscale image

Image denoising

Comparison of different reconstruction results

Color denoising on 3D point clouds

Noisy data

[16] D. Tenbrinck, F. Lozes, A. Elmoataz: *Solving Minimal Surface Problems on Surfaces and Point Clouds*. SSVM (2015)

Color denoising on 3D point clouds

Noisy data

Result (local)
600 iterations

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Color denoising on 3D point clouds

Noisy data

Result (local)
1200 iterations

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Color denoising on 3D point clouds

Noisy data

Result (local)
1200 iterations

Result (nonlocal)
1200 iterations

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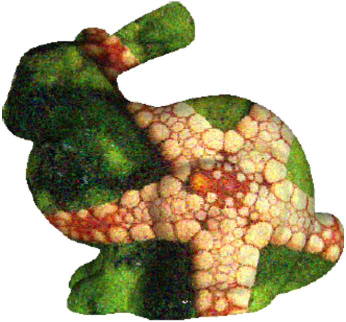
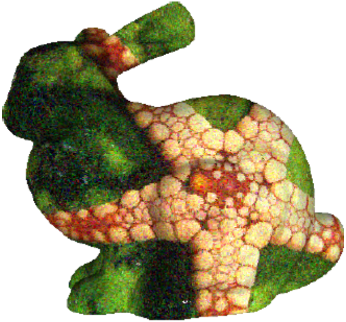
Color denoising on 3D point clouds



Colored 3D point cloud corrupted by RGB noise

Color denoising on 3D point clouds



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Reconstructed point cloud for $p = 1$ (local)

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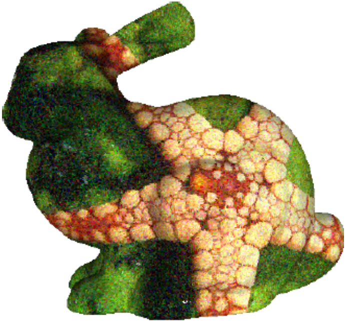

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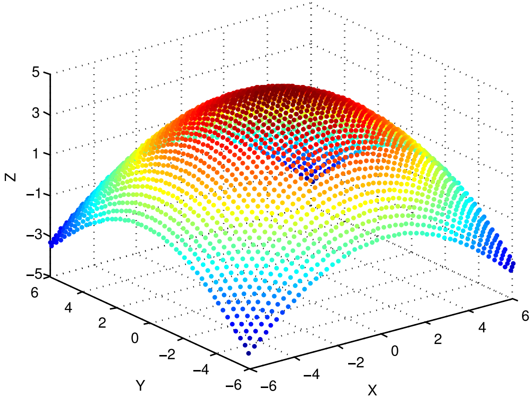

Unperturbed 3D point cloud

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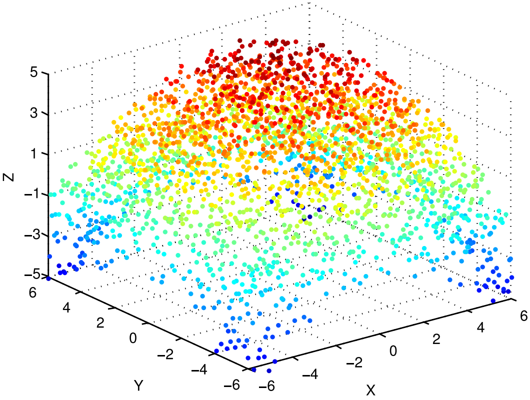

Perturbed 3D point cloud

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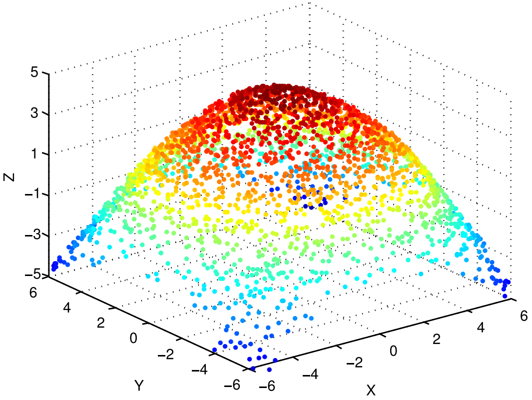

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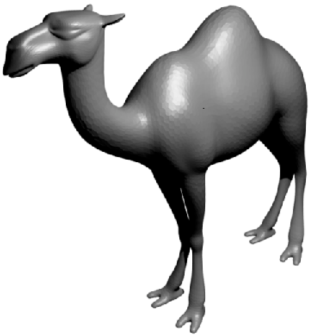

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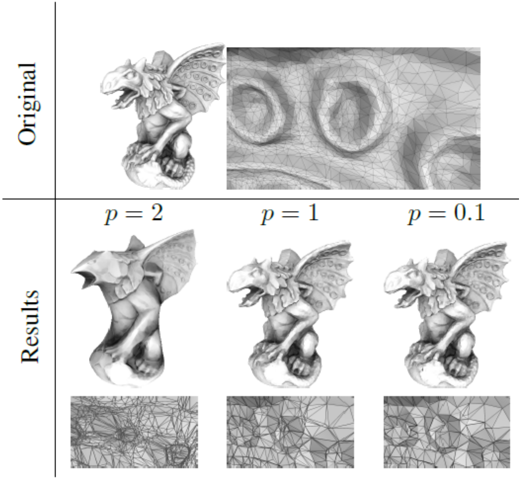

Interpolation-based problems on graphs

Another class of PdEs on graphs are interpolation problems of the form:

$$\begin{cases} 0 = \Delta_{w,p}^{a} f(u)\,, & \text{for } u \in A, \\ f(u) = g(u)\,, & \text{for } u \in \partial A, \end{cases}$$

for which $A \subset V$ is a subset of vertices and $\partial A = V \setminus A$ and the given information g are application dependent.

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Solving this Dirichlet problem amounts in finding the stationary solution of a diffusion process with fixed boundary conditions.

$$\begin{cases} \frac{\partial f(u,t)}{\partial t} = \Delta_{w,p}^{a} f(u,t)\ , & \text{for } u \in A, \\ f(u) = g(u)\ , & \text{for } u \in \partial A. \end{cases} \quad (7)$$

Interpolation problems

1. Use the same numerical scheme as for diffusion processes:

$$f^{n+1}(u) \ = \ f^n(u) + \Delta t \sum_{v \sim u} (w(u,v)^{p/2} |f(v) - f(u)|^{p-2} (f(v) - f(u))$$

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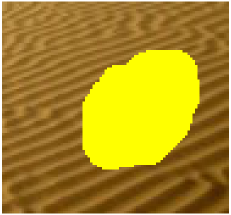

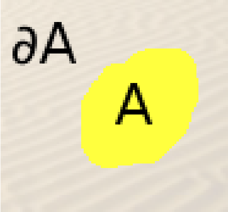

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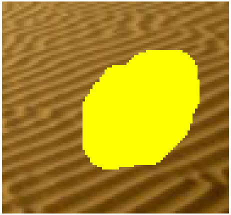

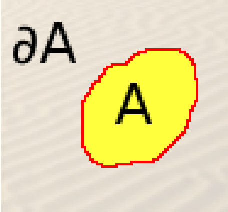

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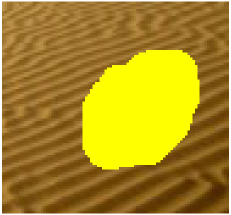

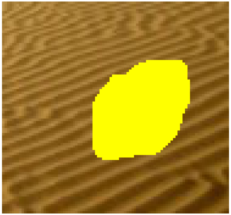

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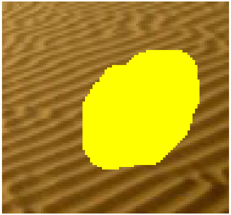

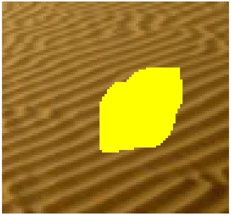

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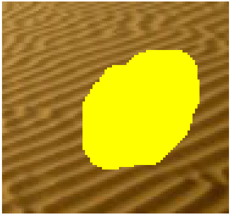

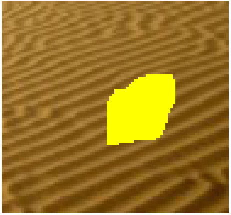

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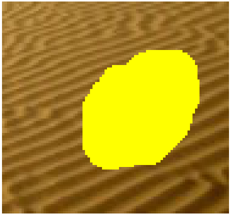

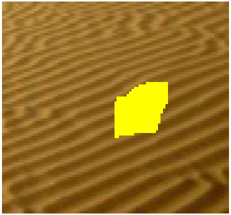

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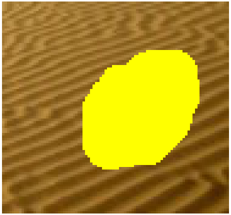

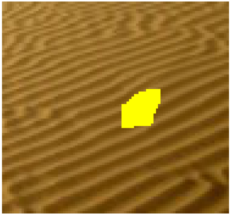

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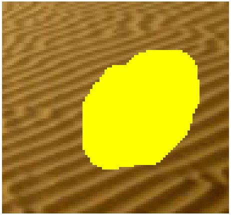

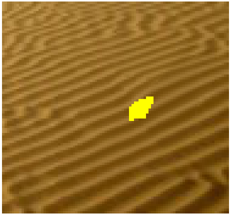

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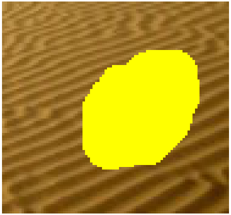
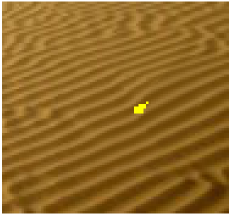
$$f^{n+1}(u) \; = \; f^n(u) + \Delta t \sum_{v \sim u} (w(u,v)^{p/2} |f(v) - f(u)|^{p-2} (f(v) - f(u))$$

2. Iterate until no more changes in border zone
3. Add border nodes to ∂A and repeat with 1 until $A = \emptyset$.





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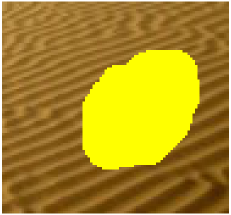

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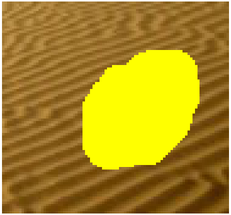


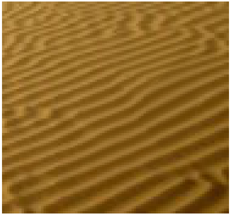
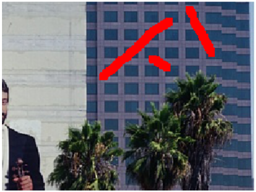


Image inpainting

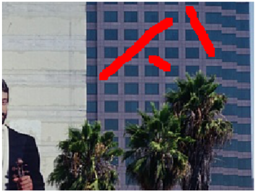
Original image



Masked areas

Image inpainting

Original image



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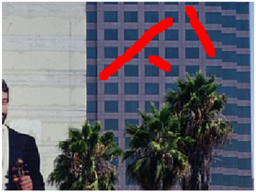


Masked areas

Reconstruction (local)

Reconstruction (nonlocal)

Color inpainting on 3D point clouds

3D point cloud of a scanned person

Color inpainting on 3D point clouds

3D point cloud of a scanned person

User-defined region for color inpainting

Color inpainting on 3D point clouds

3D point cloud of a scanned person

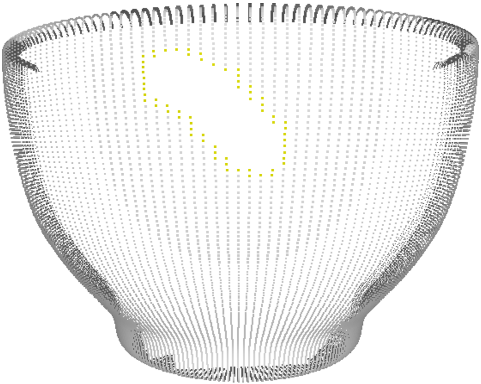
Result of color inpainting (local)

Color inpainting on 3D point clouds

3D point cloud of a scanned person

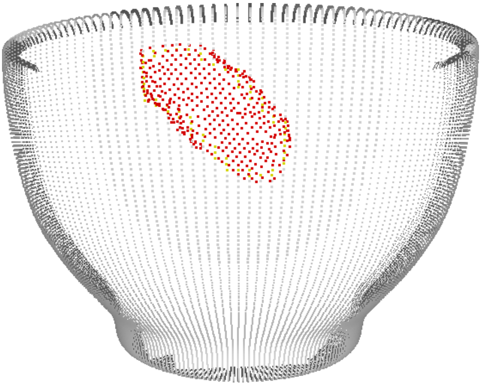
Result of color inpainting (nonlocal)

Geometric inpainting



3D point cloud of a scanned cup with artificial hole in wall

Geometric inpainting

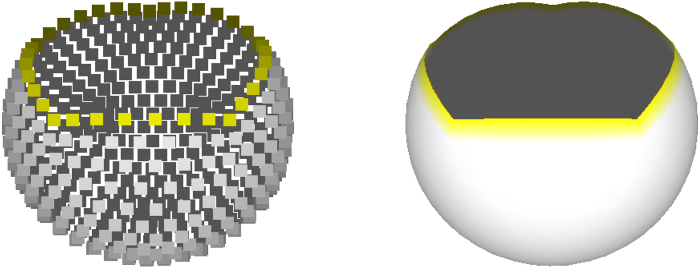


Filled in points (red) after geometric inpainting

Geometric inpainting

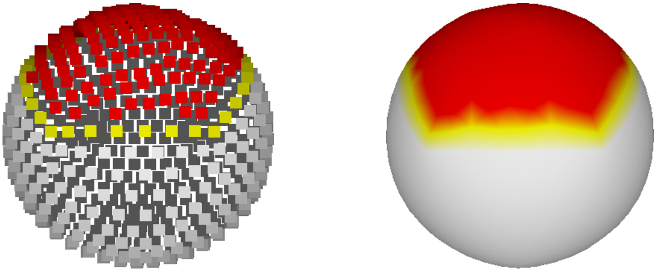
Rendering of inpainted cup

Geometric inpainting



3D point cloud of an incomplete sphere (left) and rendered visualization (right)

Geometric inpainting



3D point cloud of inpainted sphere (left) and rendered visualization (right)

Geometric inpainting

Scanned vase with hole

Geometric inpainting

Scanned vase with hole

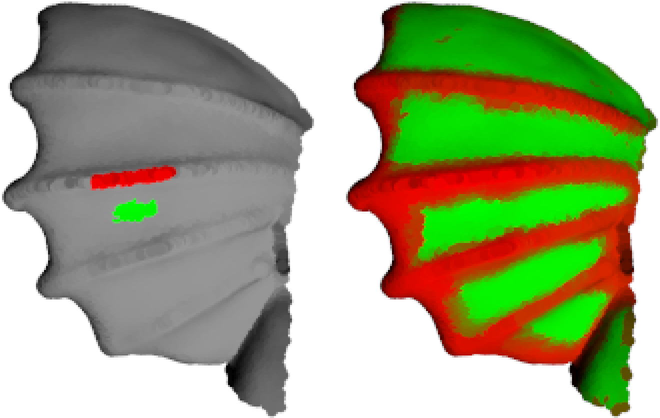
Geometric inpainting result

Geometric inpainting

Scanned vase with hole

Color inpainting result

Colorization

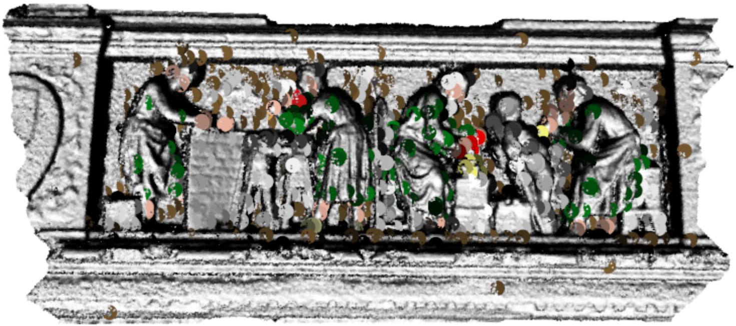


User-defined color scribbles on 3D point cloud (left) and colorization result (right)

Colorization

User-defined color scribbles on 3D point cloud (left) and colorization result (right)

Colorization



User-defined color scribbles on 3D point cloud

Colorization

Colorization result

Colorization

User-defined color scribbles on 3D point cloud (left) and colorization result (right)

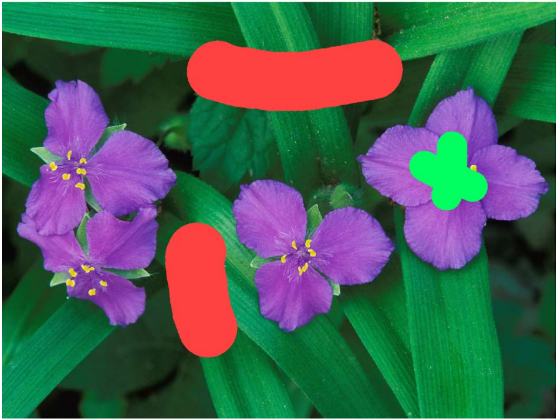
Semi-supervised image segmentation

User-defined segmentation labels

Semi-supervised image segmentation

Segmentation result

Semi-supervised image segmentation



User-defined segmentation labels

Semi-supervised image segmentation

Segmentation result

Semi-supervised segmentation

Original data

Semi-supervised segmentation

Original data

User-defined labels

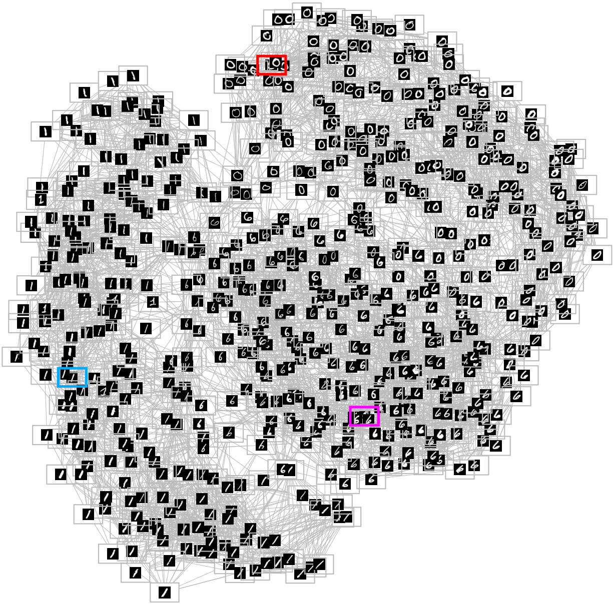
Semi-supervised segmentation


Original data

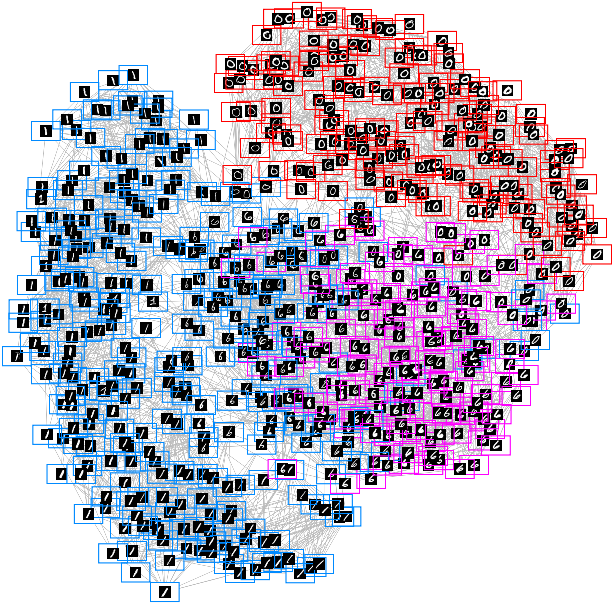

User-defined labels


Segmented data

Semi-supervised classification

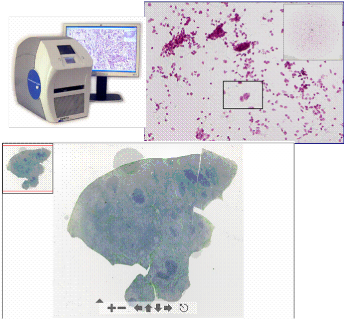


Semi-supervised classification



Cell classification in histology

Classify different cell types using very few expert interactions
→ especially: healthy and pathological cells for cervical cancer.



[17] Datexim. http://www.datexim.com/en/

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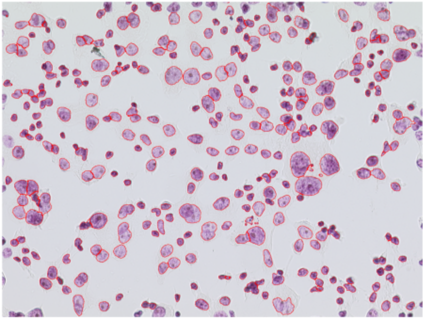

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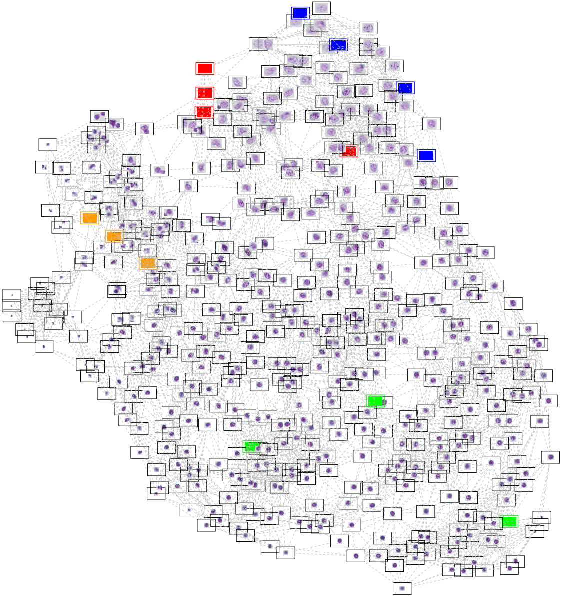

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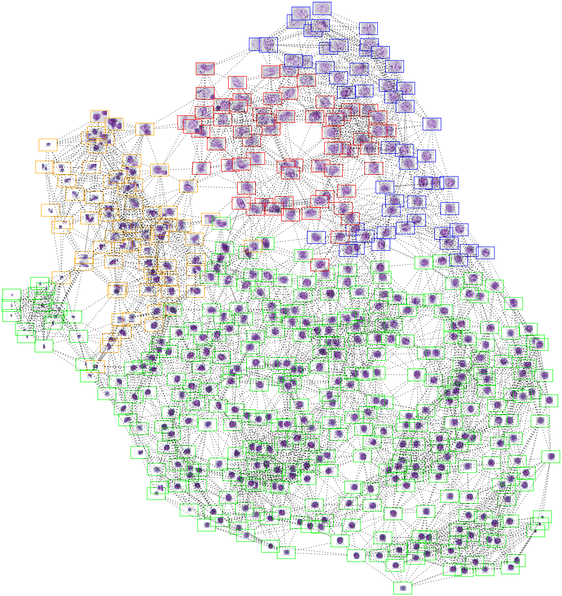

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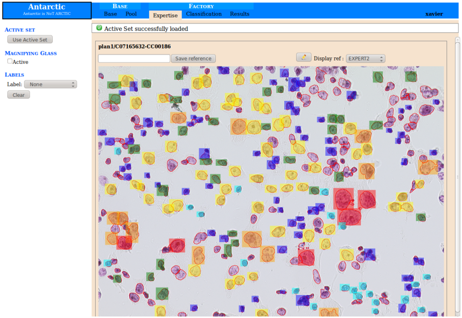

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Thank you for your attention!

Any questions?

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