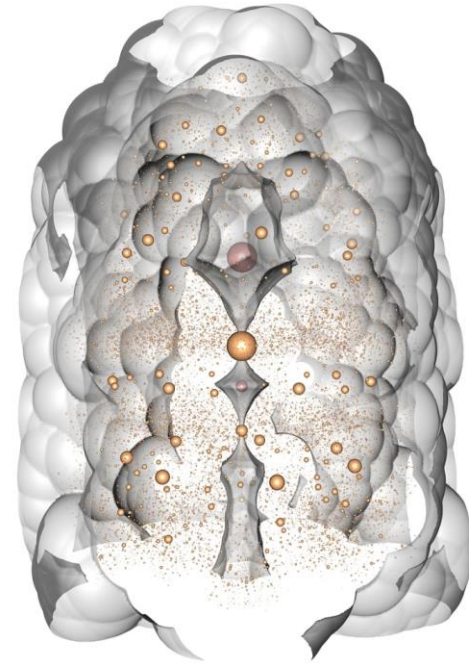
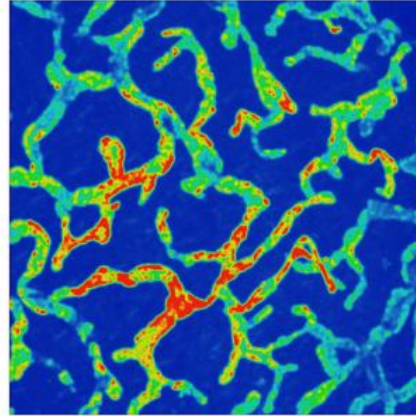


# Algorithms & Software for Topological Data Analysis

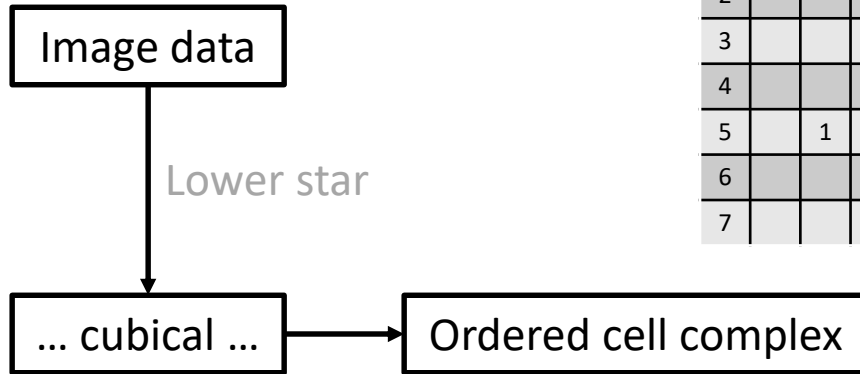
*Jan Reininghaus*  
*(Siemens Industry Software)*

# Roadmap

Image data

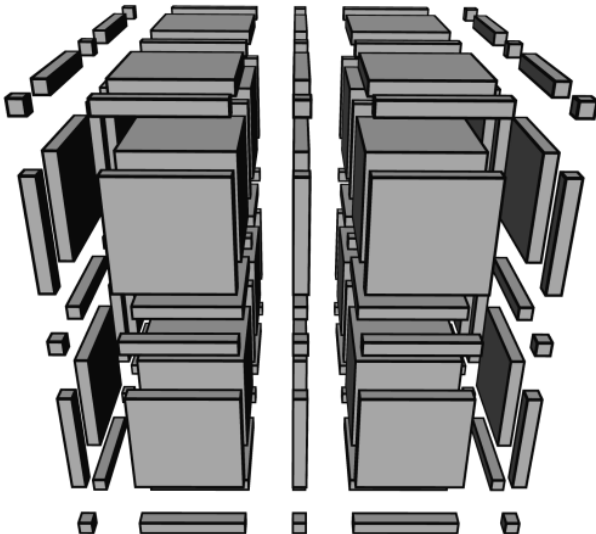


# Roadmap

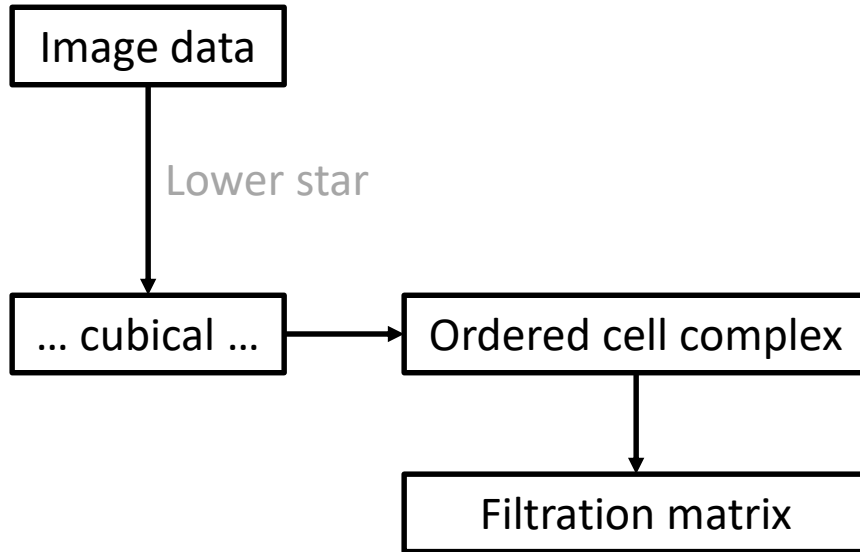


	1	2	3	4	5	6	7
1		1		1			
2						1	
3					1		
4						1	
5		1					
6					1		
7							

1.3
3.2
2.8
6.1
9.1
8.3
5.9

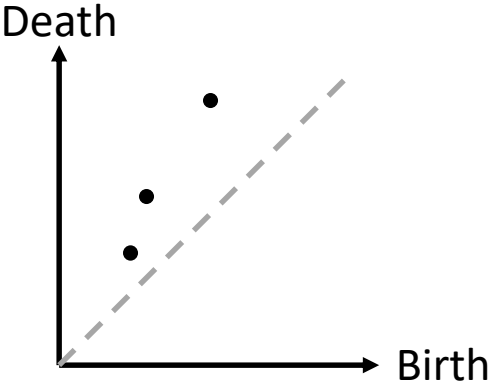
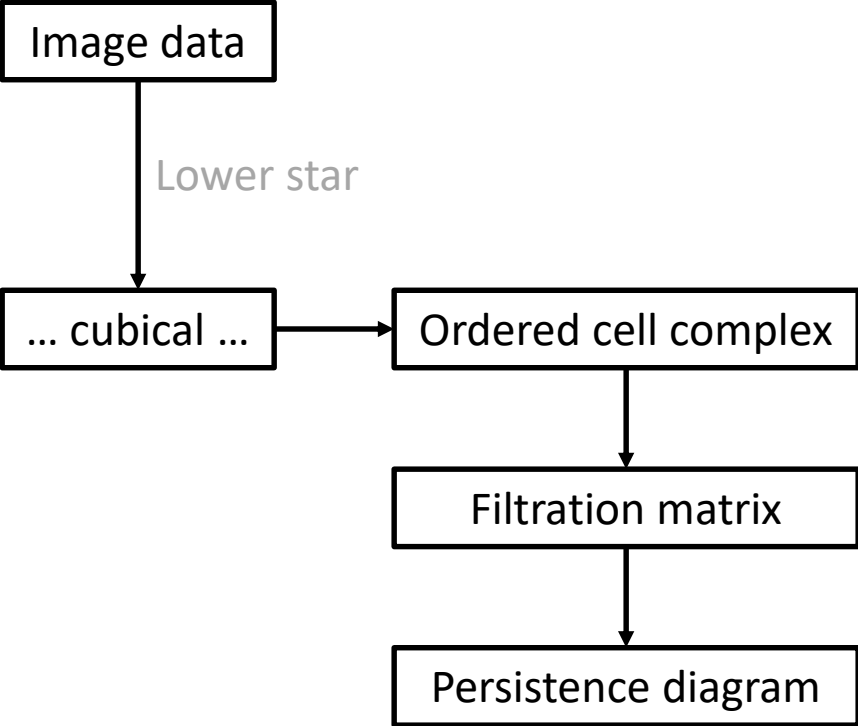


# Roadmap

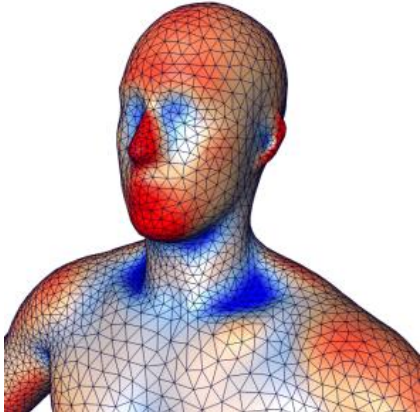
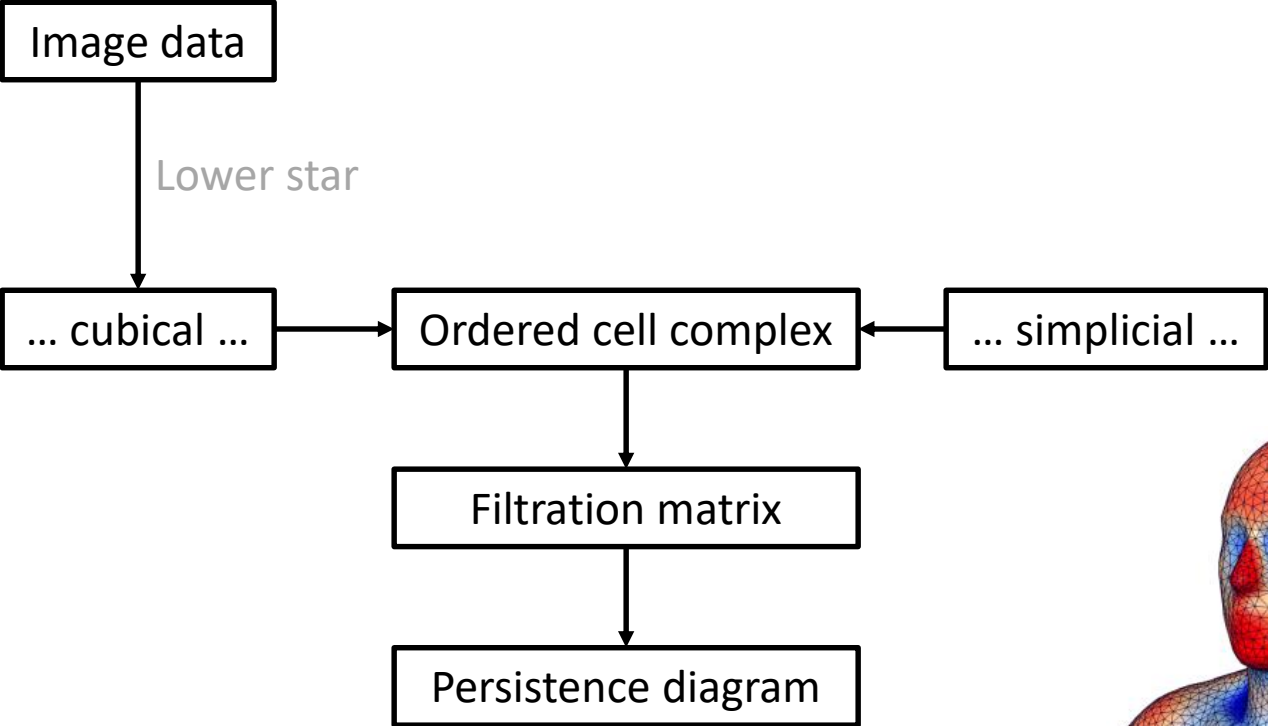


	1	2	3	4	5	6	7
1	1		1		1		
2		1				1	
3			1				1
4				1	1		
5					1		1
6						1	
7							1

# Roadmap



# Roadmap



# Roadmap

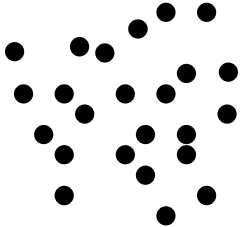


Image data

Point data

Lower star

Alpha shape

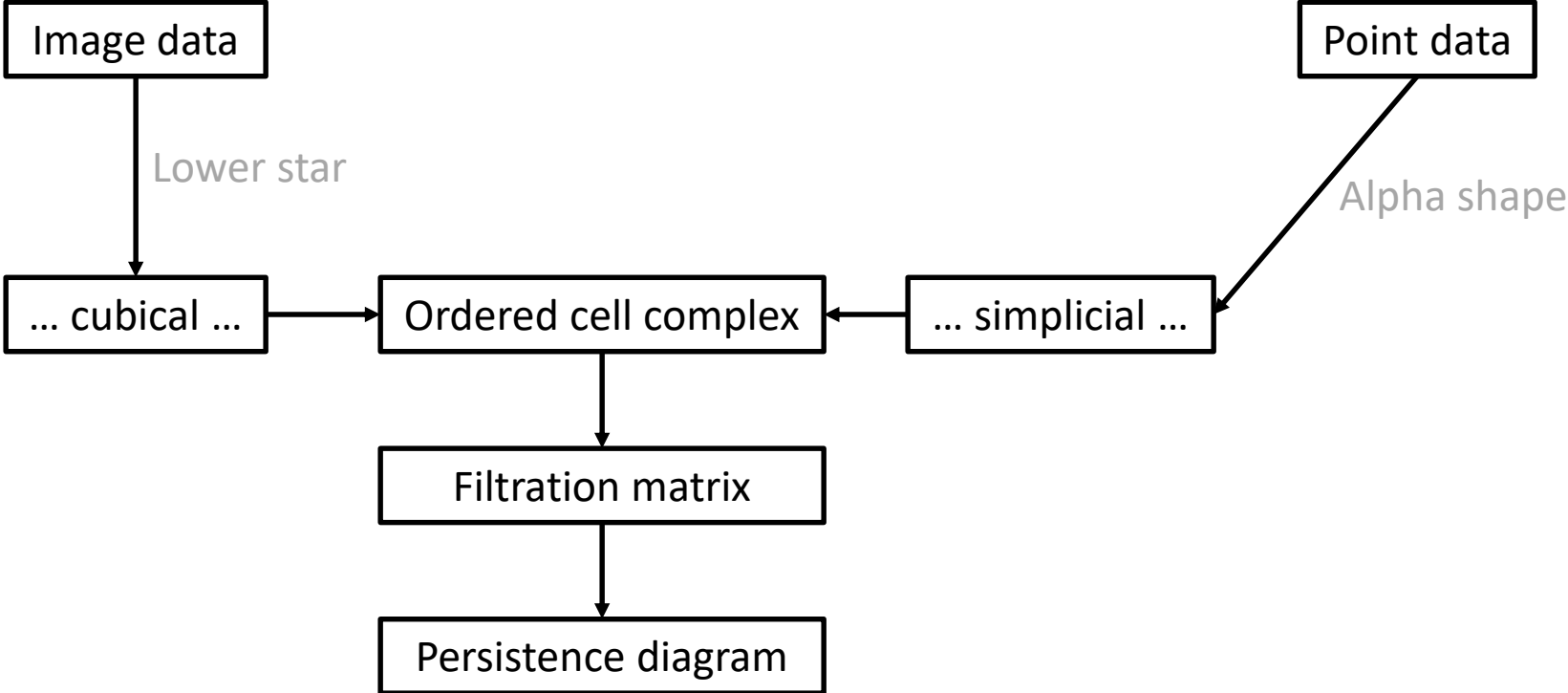
... cubical ...

Ordered cell complex

... simplicial ...

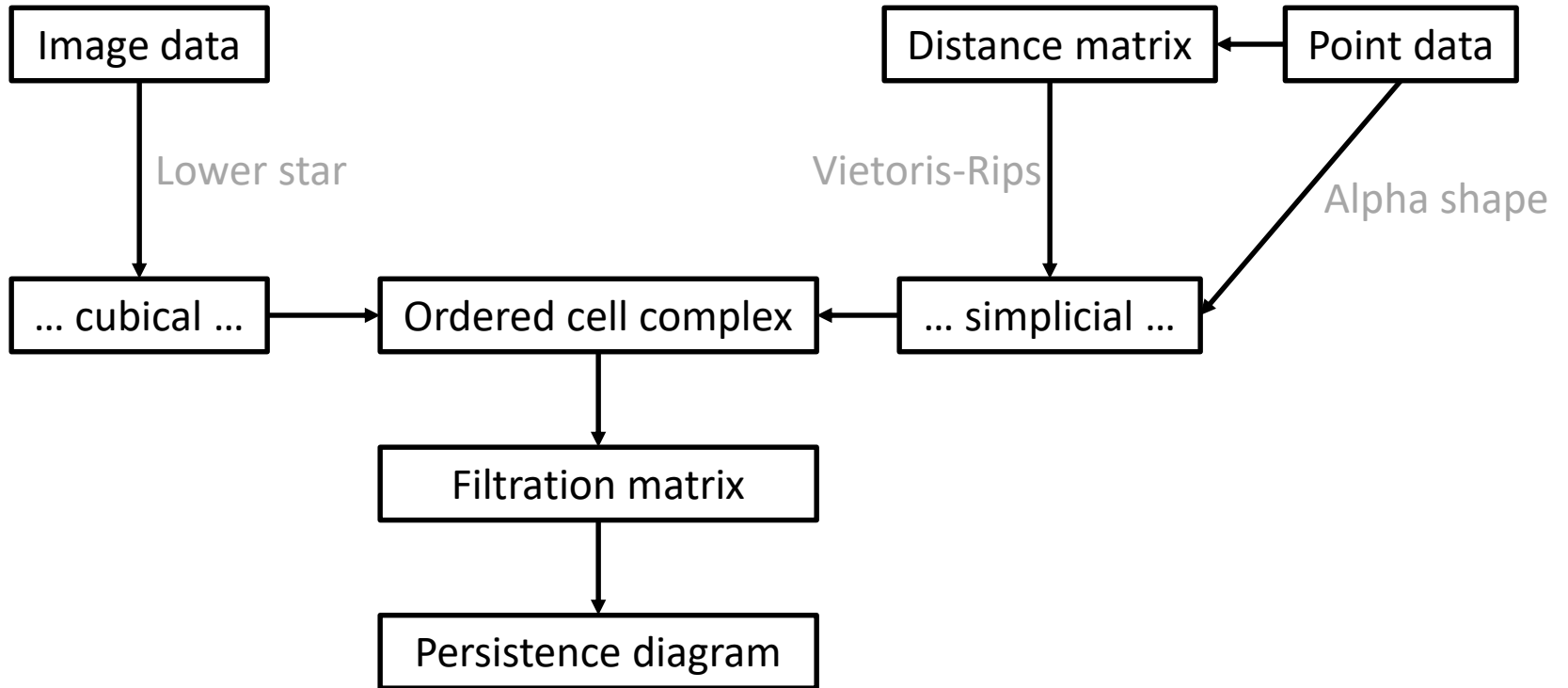
Filtration matrix

Persistence diagram



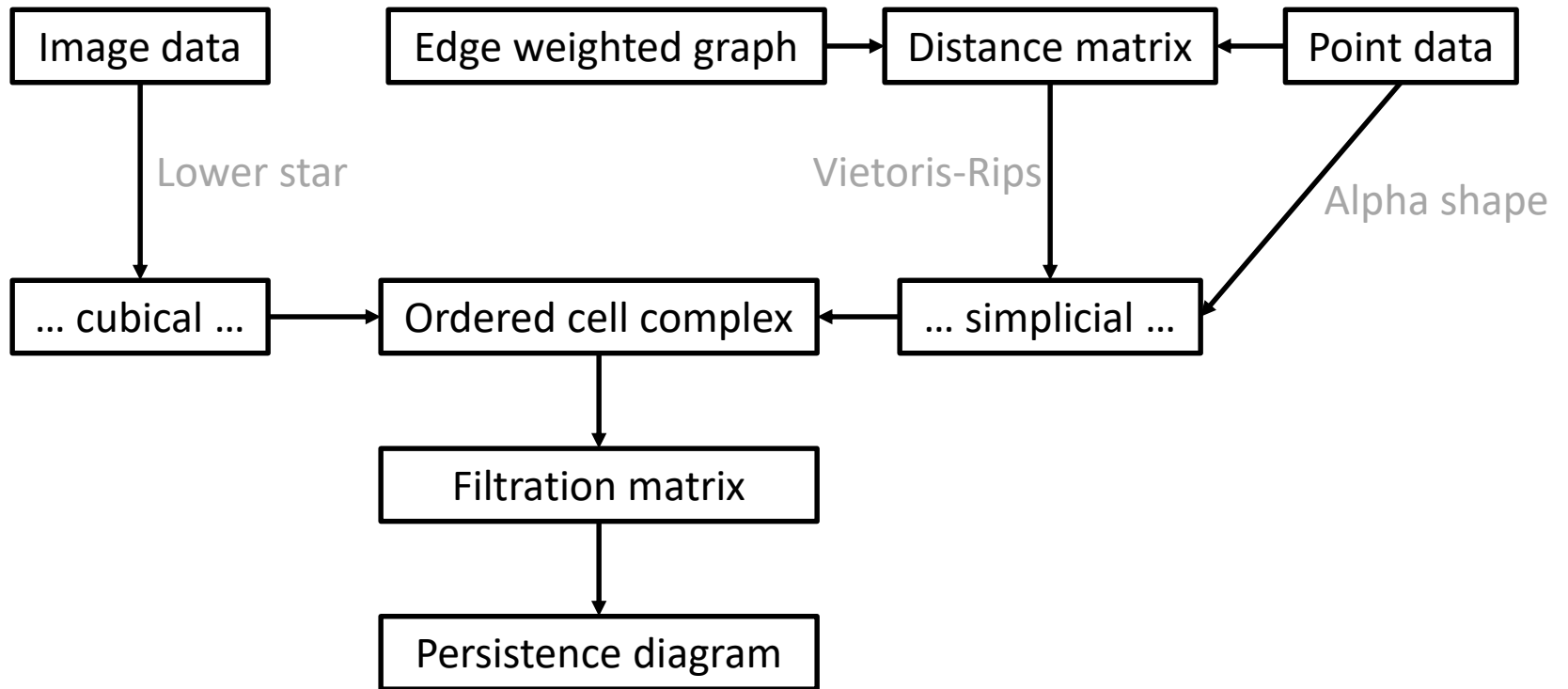
# Roadmap

1	3	78	65	3	46	12	1
7	6	23	78	65	3	46	23
5	34	61	2	78	65	3	46
2	6	2	10	2	1	1	51
78	65	3	46	6	1	4	35
1	6	78	65	3	46	24	32
6	6	6	5	78	65	3	46
1	78	65	3	46	2	15	12

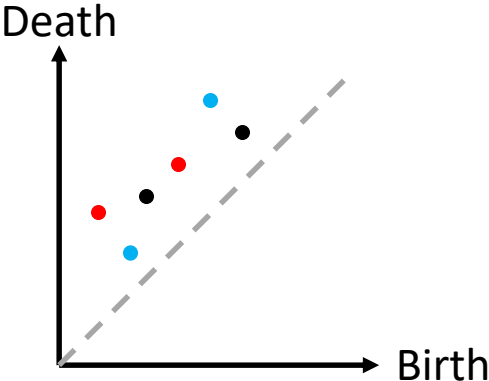
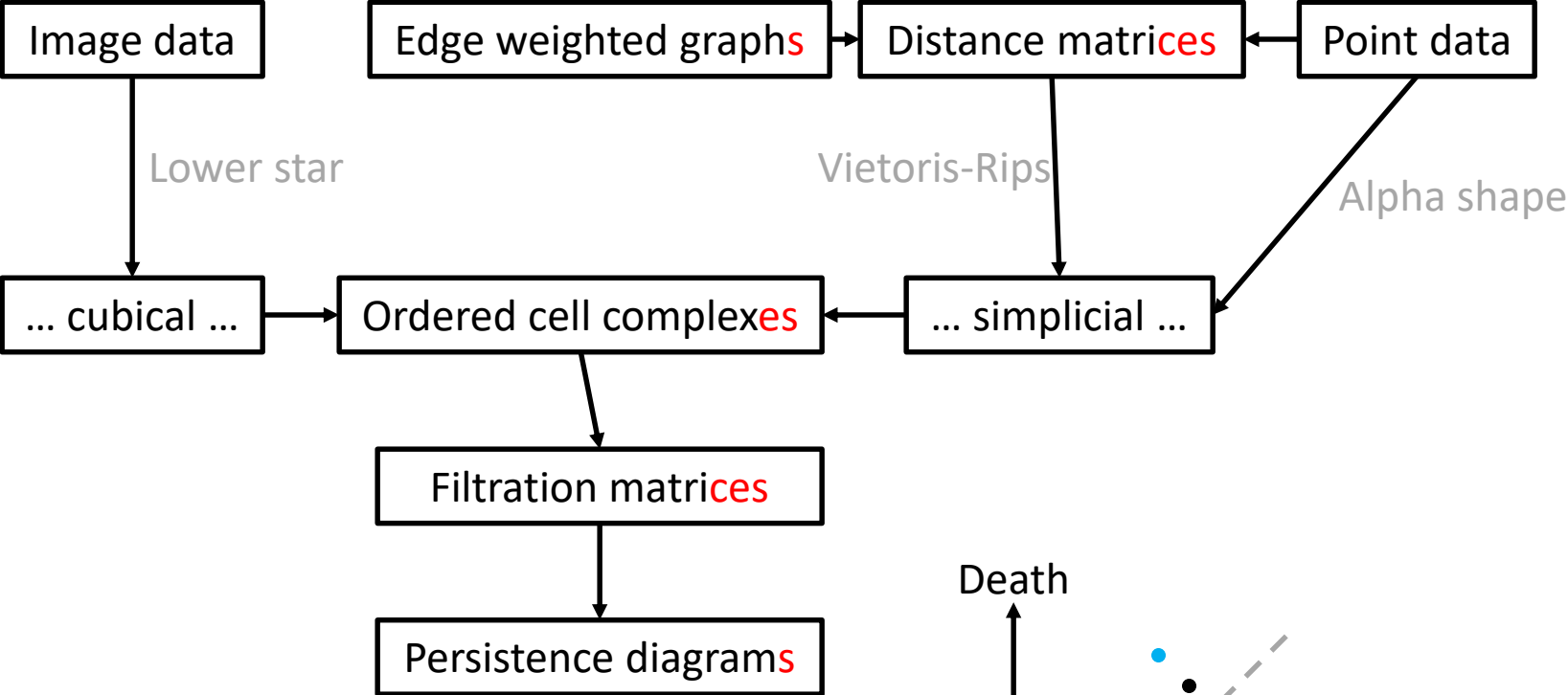




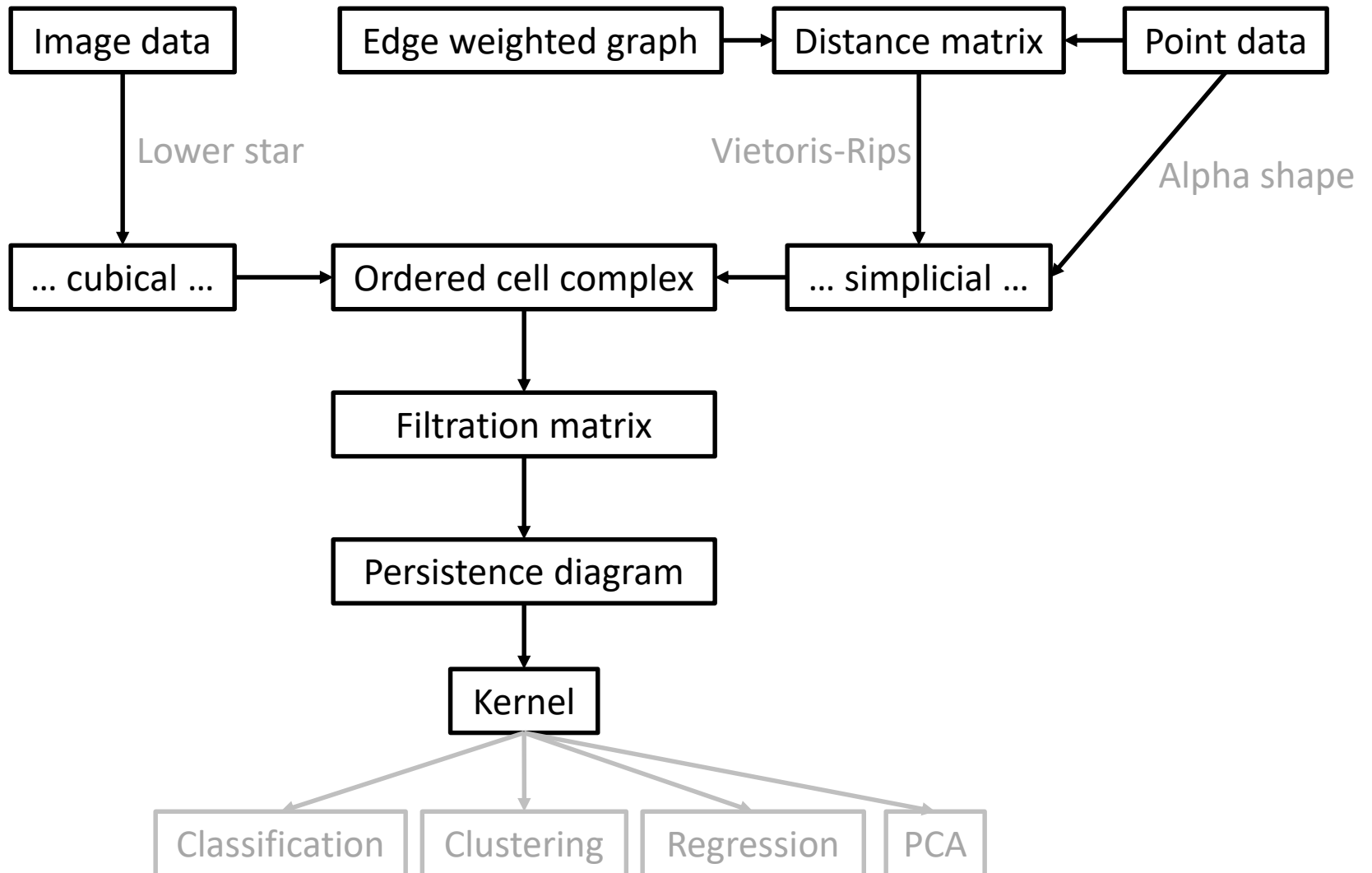
# Roadmap



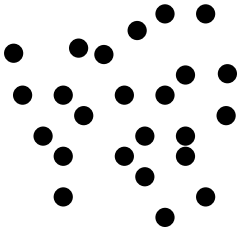
# Roadmap



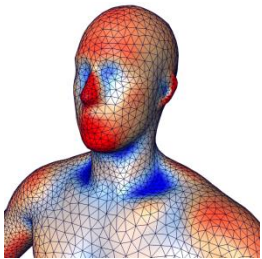
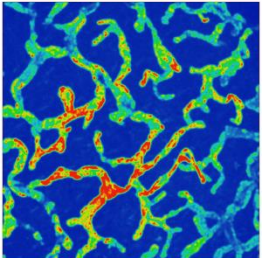
# Roadmap



# Computational Pipeline

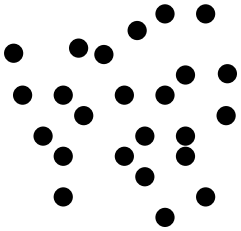


1	3	78	65	3	46	12	1
7	6	23	78	65	3	46	23
5	34	61	2	78	65	3	46
2	6	2	10	2	1	1	51
78	65	3	46	6	1	4	35
1	6	78	65	3	46	24	32
6	6	6	5	78	65	3	46
1	78	65	3	46	2	15	12

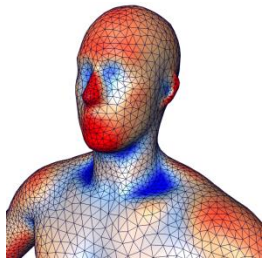
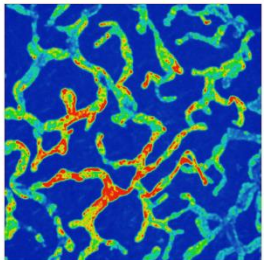


Input data

# Computational Pipeline



1	3	78	65	3	46	12	1
7	6	23	78	65	3	46	23
5	34	61	2	78	65	3	46
2	6	2	10	2	1	1	51
78	65	3	46	6	1	4	35
1	6	78	65	3	46	24	32
6	6	6	5	78	65	3	46
1	78	65	3	46	2	15	12



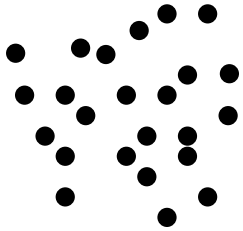
Input data

1.3
3.2
2.8
6.1
9.1
8.3
5.9

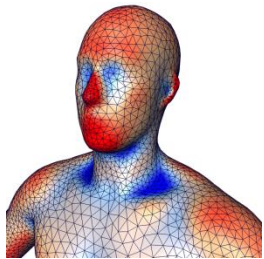
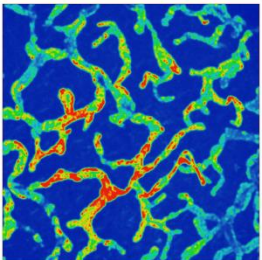
	1	2	3	4	5	6	7
1		1		1			
2						1	
3					1		
4						1	
5		1					
6					1		
7							

Boundary matrix  
+ weights

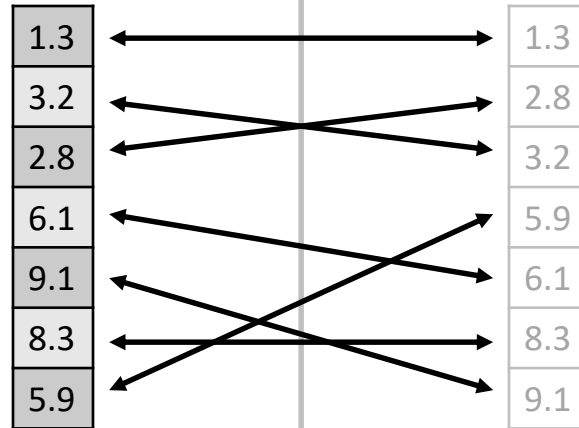
# Computational Pipeline



1	3	78	65	3	46	12	1
7	6	23	78	65	3	46	23
5	34	61	2	78	65	3	46
2	6	2	10	2	1	1	51
78	65	3	46	6	1	4	35
1	6	78	65	3	46	24	32
6	6	6	5	78	65	3	46
1	78	65	3	46	2	15	12



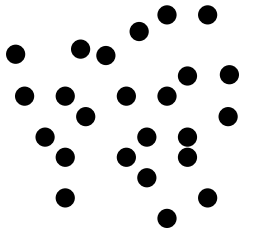
Input data



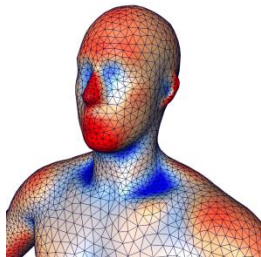
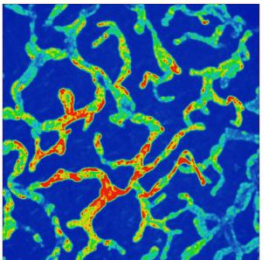
	1	2	3	4	5	6	7
1		1		1			
2						1	
3					1		
4						1	
5		1					
6					1		
7							

Boundary matrix  
+ weights

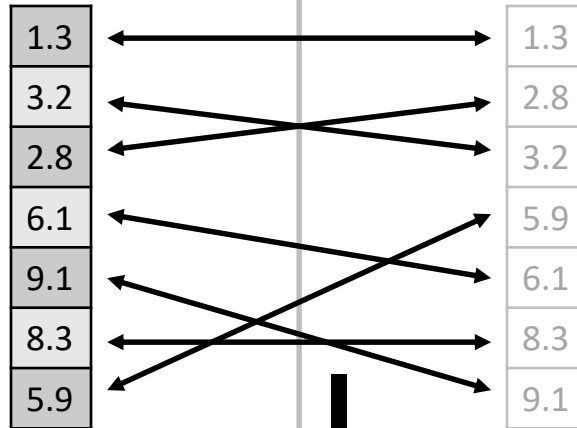
# Computational Pipeline



1	3	78	65	3	46	12	1
7	6	23	78	65	3	46	23
5	34	61	2	78	65	3	46
2	6	2	10	2	1	1	51
78	65	3	46	6	1	4	35
1	6	78	65	3	46	24	32
6	6	6	5	78	65	3	46
1	78	65	3	46	2	15	12



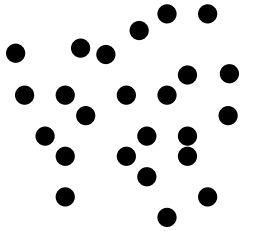
Input data



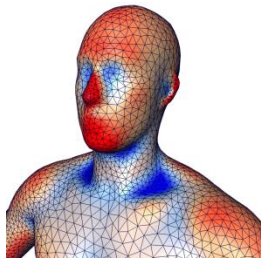
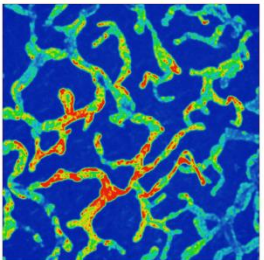
	1	2	3	4	5	6	7
1		1		1			
2						1	
3					1		
4						1	
5		1					
6					1		
7							

Boundary matrix  
+ weights

# Computational Pipeline



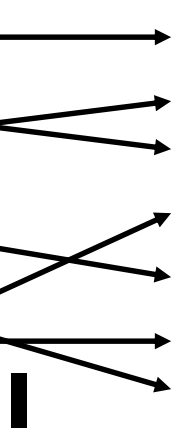
1	3	78	65	3	46	12	1
7	6	23	78	65	3	46	23
5	34	61	2	78	65	3	46
2	6	2	10	2	1	1	51
78	65	3	46	6	1	4	35
1	6	78	65	3	46	24	32
6	6	6	5	78	65	3	46
1	78	65	3	46	2	15	12



Input data

1.3
3.2
2.8
6.1
9.1
8.3
5.9

1.3
2.8
3.2
5.9
6.1
8.3
9.1



1	3	2	5	7	6	4
1	3	2	7	4	6	5

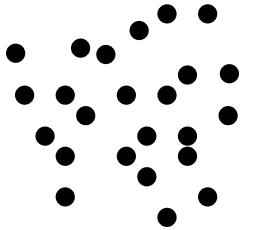
	1	2	3	4	5	6	7
1		1		1			
2						1	
3					1		
4						1	
5		1					
6					1		
7							

Boundary matrix  
+ weights

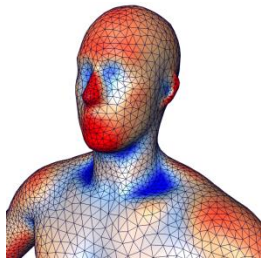
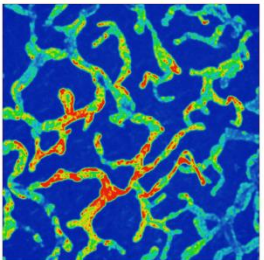
	1	2	3	4	5	6	7
1		1		1			
2		1				1	
3					1		
4				1		1	
5					1		
6						1	
7							



# Computational Pipeline



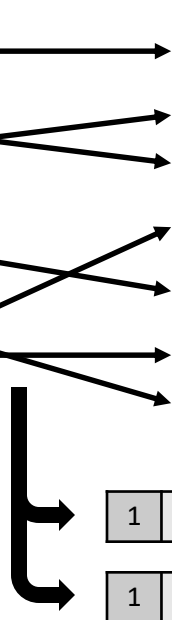
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7	6	23	78	65	3	46	23
5	34	61	2	78	65	3	46
2	6	2	10	2	1	1	51
78	65	3	46	6	1	4	35
1	6	78	65	3	46	24	32
6	6	6	5	78	65	3	46
1	78	65	3	46	2	15	12



Input data

1.3
3.2
2.8
6.1
9.1
8.3
5.9

1.3
2.8
3.2
5.9
6.1
8.3
9.1



1	3	2	5	7	6	4
---	---	---	---	---	---	---

1	3	2	7	4	6	5
---	---	---	---	---	---	---

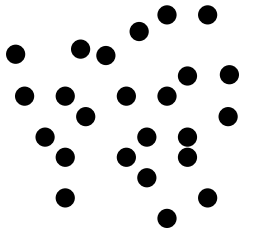
	1	2	3	4	5	6	7
1		1		1			
2						1	
3					1		
4						1	
5		1					
6				1			
7							

Boundary matrix  
+ weights

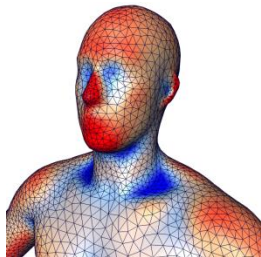
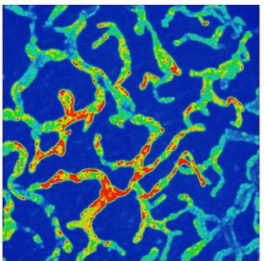
	1	2	3	4	5	6	7
1	1		1		1		
2		1				1	
3			1				1
4				1	1		
5					1		1
6						1	
7							1

Filtration matrix  
+ permutation maps

# Computational Pipeline



1	3	78	65	3	46	12	1
7	6	23	78	65	3	46	23
5	34	61	2	78	65	3	46
2	6	2	10	2	1	1	51
78	65	3	46	6	1	4	35
1	6	78	65	3	46	24	32
6	6	6	5	78	65	3	46
1	78	65	3	46	2	15	12



Input data

1.3
3.2
2.8
6.1
9.1
8.3
5.9

1.3
2.8
3.2
5.9
6.1
8.3
9.1

1	3	2	5	7	6	4
1	3	2	7	4	6	5

	1	2	3	4	5	6	7
1		1		1			
2						1	
3					1		
4						1	
5		1					
6					1		
7							

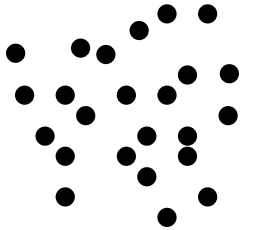
Boundary matrix  
+ weights

	1	2	3	4	5	6	7
1			1		1		
2			1			1	
3							1
4					1	1	
5							1
6							1
7							

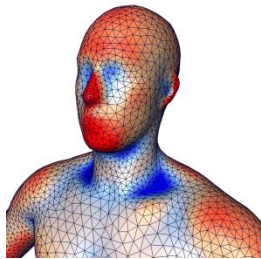
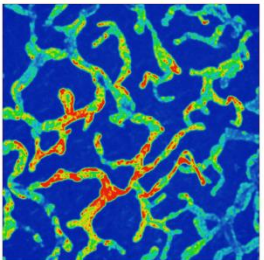
Filtration matrix  
+ permutation maps

	1	2	3	4	5	6	7
1			1		1		
2			1			1	
3							1
4					1	1	
5							1
6							1
7							

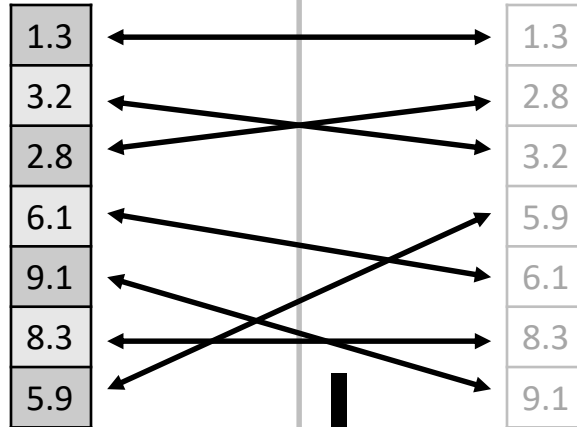
# Computational Pipeline



1	3	78	65	3	46	12	1
7	6	23	78	65	3	46	23
5	34	61	2	78	65	3	46
2	6	2	10	2	1	1	51
78	65	3	46	6	1	4	35
1	6	78	65	3	46	24	32
6	6	6	5	78	65	3	46
1	78	65	3	46	2	15	12



Input data



	1	2	3	4	5	6	7
1		1		1			
2						1	
3					1		
4						1	
5		1					
6					1		
7							

Boundary matrix  
+ weights

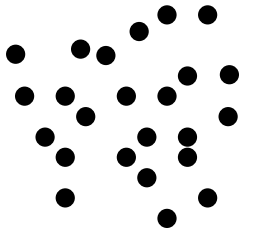
	1	2	3	4	5	6	7
1	1		1		1		
2		1				1	
3			1				1
4				1	1		
5					1		1
6						1	
7							1

Filtration matrix  
+ permutation maps

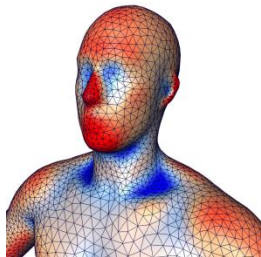
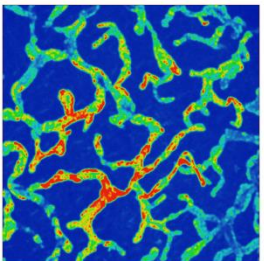
	1	2	3	4	5	6	7
1	1		1		1		
2		1					
3			1				1
4				1			
5					1		1
6						1	
7							1

Reduced matrix

# Computational Pipeline



1	3	78	65	3	46	12	1
7	6	23	78	65	3	46	23
5	34	61	2	78	65	3	46
2	6	2	10	2	1	1	51
78	65	3	46	6	1	4	35
1	6	78	65	3	46	24	32
6	6	6	5	78	65	3	46
1	78	65	3	46	2	15	12



Input data

1.3
3.2
2.8
6.1
9.1
8.3
5.9

1.3
2.8
3.2
5.9
6.1
8.3
9.1

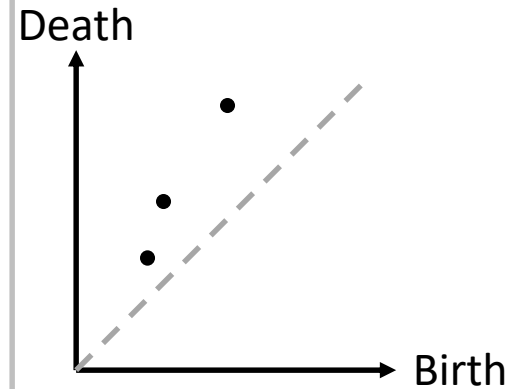
1	3	2	5	7	6	4
1	3	2	7	4	6	5

	1	2	3	4	5	6	7
1		1		1			
2						1	
3					1		
4						1	
5		1					
6					1		
7							

Boundary matrix  
+ weights

	1	2	3	4	5	6	7
1			1		1		
2			1			1	
3							1
4					1	1	
5							1
6							1
7							

Filtration matrix  
+ permutation maps

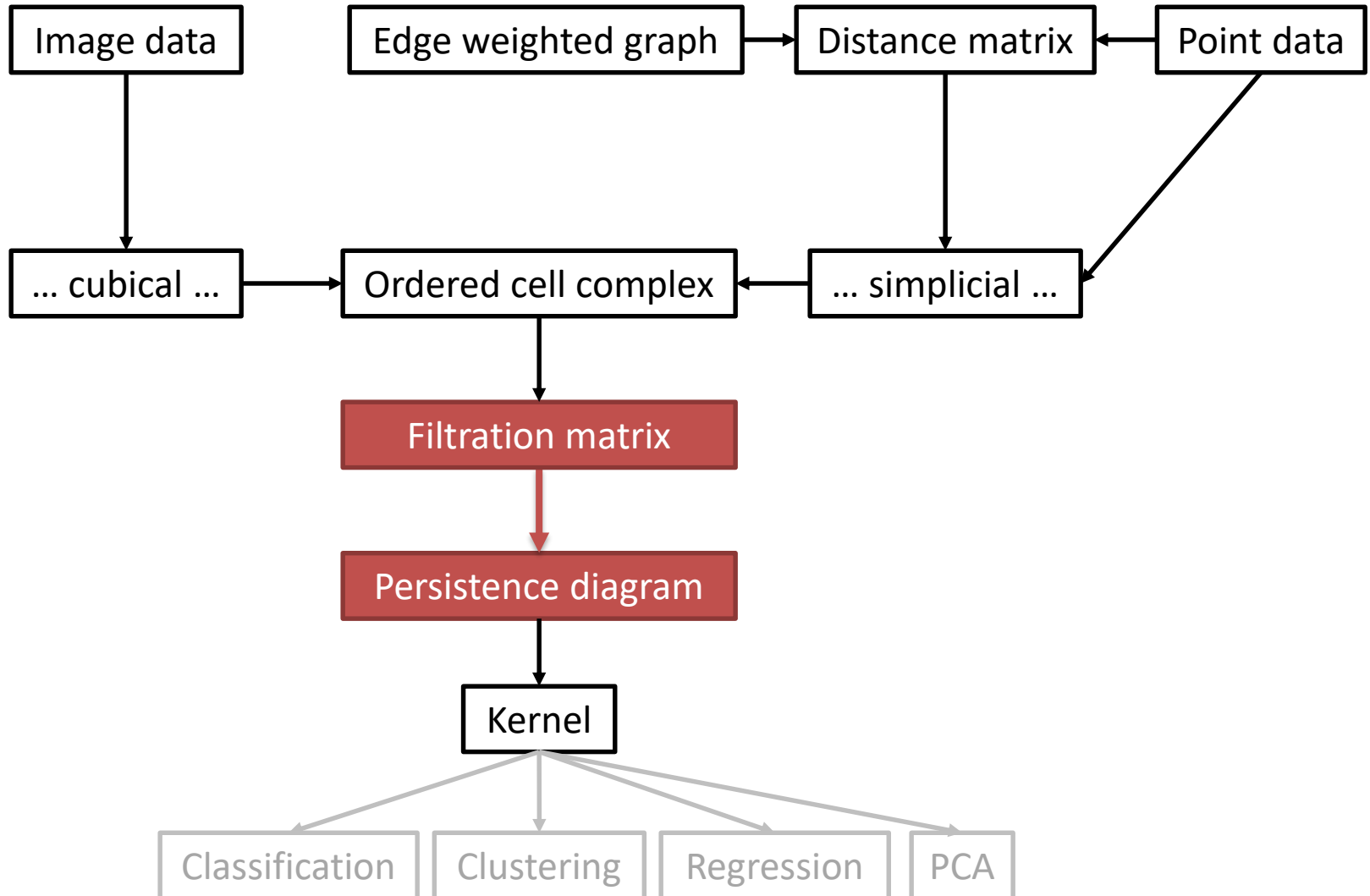


	1	2	3	4	5	6	7
1			1		1		
2			1				
3							1
4					1		
5							1
6							1
7							

Reduced matrix  
→ diagram

# Part 1: Phat - [bitbucket.org/phat-code/phat](http://bitbucket.org/phat-code/phat)

Joint work with: U. Bauer, M. Kerber, H. Wagner



# Classic Matrix Reduction

	1	2	3	4	5	6	7
1	1		1		1		
2			1			1	
3							1
4					1	1	
5							1
6							1
7							


Pivot-to-Column Map

# Classic Matrix Reduction

	1	2	3	4	5	6	7
1	1		1		1		
2			1			1	
3							1
4					1	1	
5							1
6							1
7							

3

Pivot-to-Column Map

# Classic Matrix Reduction

	1	2	3	4	5	6	7
1	1		1		1		
2			1			1	
3							1
4					1	1	
5							1
6							1
7							

3
5

Pivot-to-Column Map



# Classic Matrix Reduction

	1	2	3	4	5	6	7
1	1		1		1	1	
2			1			1	
3							1
4					1		
5							1
6							1
7							

3
5

Pivot-to-Column Map

# Classic Matrix Reduction

	1	2	3	4	5	6	7
1	1		1		1		
2			1				
3							1
4					1		
5							1
6							1
7							

3
5

Pivot-to-Column Map

# Classic Matrix Reduction

	1	2	3	4	5	6	7
1	1		1		1		
2			1				
3							1
4					1		
5							1
6							1
7							

3
5
7

Pivot-to-Column Map

# Phat features

- Algorithms:
  - Standard
  - Row
  - Twist (best sequential performance/complexity ratio)
  - Chunk (parallel)
  - Spectral sequence (best parallel performance/complexity ratio)
  - Dualized versions of all above
- Column data structures:
  - vector\_vector
  - vector\_heap (best performance/complexity ratio)
  - vector\_set
  - vector\_list (purely educational)
  - sparse\_pivot\_column
  - heap\_pivot\_column
  - full\_pivot\_column
  - bit\_tree\_pivot\_column (fastest, requires N memory)

# Phat performance

	List	Vector	Set	Heap	A-Heap	A-Set	A-Full	<b>A-Bit-Tree</b>
standard	17.1	2.8	7.5	5.9	5.6	8.6	2.3	1.62
standard*	2580.0	168.0	17.3	13.5	14.6	16.0	3.9	0.57
twist	16.3	2.7	7.0	5.7	5.4	6.5	2.2	1.59
<b>twist*</b>	0.23	0.03	0.04	0.02	0.03	0.03	0.02	<b>0.02</b>
row	39.9	4.3	20.3	7.2	21.4	37.9	15.5	13.8
row*	0.25	0.06	0.06	0.05	0.08	0.09	0.05	0.05
chunk	0.63	0.19	0.6	0.50	0.35	0.5	0.24	0.24
chunk*	2.9	0.42	0.1	0.11	0.17	0.14	0.07	0.04
spectral	10.7	1.8	4.03	3.3	3.4	4.3	2.1	1.2
<b>spectral*</b>	0.35	0.03	0.05	0.04	0.04	0.04	0.02	<b>0.01</b>

Dataset: 3-skeleton of the Vietoris–Rips filtration  
of 64 points on a 2-sphere (7e5 columns)

	List	Vector	Set	Heap	A-Heap	A-Set	A-Full	<b>A-Bit-Tree</b>
<b>twist*</b>	2635.4	339.9	4.9	2.0	2.5	6.1	2.1	<b>1.0</b>
<b>spectral*</b>	2644.8	349.2	5.2	1.9	3.3	6.6	3.1	<b>1.0</b>

Dataset: 3-skeleton of the Vietoris–Rips filtration  
of 192 points on a 2-sphere (6e7 columns)

# Phat performance

	List	Vector	Set	Heap	A-Heap	A-Set	A-Full	<b>A-Bit-Tree</b>
standard	141.1	16.1	23.9	17.5	19.4	21.5	10.8	10.7
standard*	460.2	39.6	27.5	18.8	20.8	22.8	14.0	9.8
<b>twist</b>	9.8	0.54	0.30	0.11	0.13	0.13	0.09	<b>0.07</b>
twist*	337.1	18.6	0.99	0.52	0.52	0.72	0.24	0.11
row	9.9	1.5	0.50	0.48	1.5	2.1	1.2	0.78
row*	350	43.8	1.0	0.93	24.5	44.0	15.5	7.0
chunk	1.8	0.19	0.19	0.12	0.09	0.09	0.08	0.08
chunk*	5.7	0.53	0.27	0.22	0.19	0.17	0.13	0.14
<b>spectral</b>	8.4	0.78	0.19	0.11	0.11	0.11	0.08	<b>0.06</b>
spectral*	339.2	21.9	0.90	0.65	0.74	0.74	0.35	0.12

Dataset:  $64^3$  image dat set (2e6 columns)

	List	Vector	Set	Heap	A-Heap	A-Set	A-Full	<b>A-Bit-Tree</b>
<b>twist</b>	2080.2	101.7	26.4	11.3	11.1	12.3	10.4	<b>8.8</b>
<b>chunk</b>	894.5	156.1	9.8	6.5	6.3	6.2	5.6	<b>4.7</b>
spectral	1197.7	261.7	11.9	8.5	8.5	8.4	7.1	6.1

Dataset:  $256^3$  image dat set (1e8 columns)

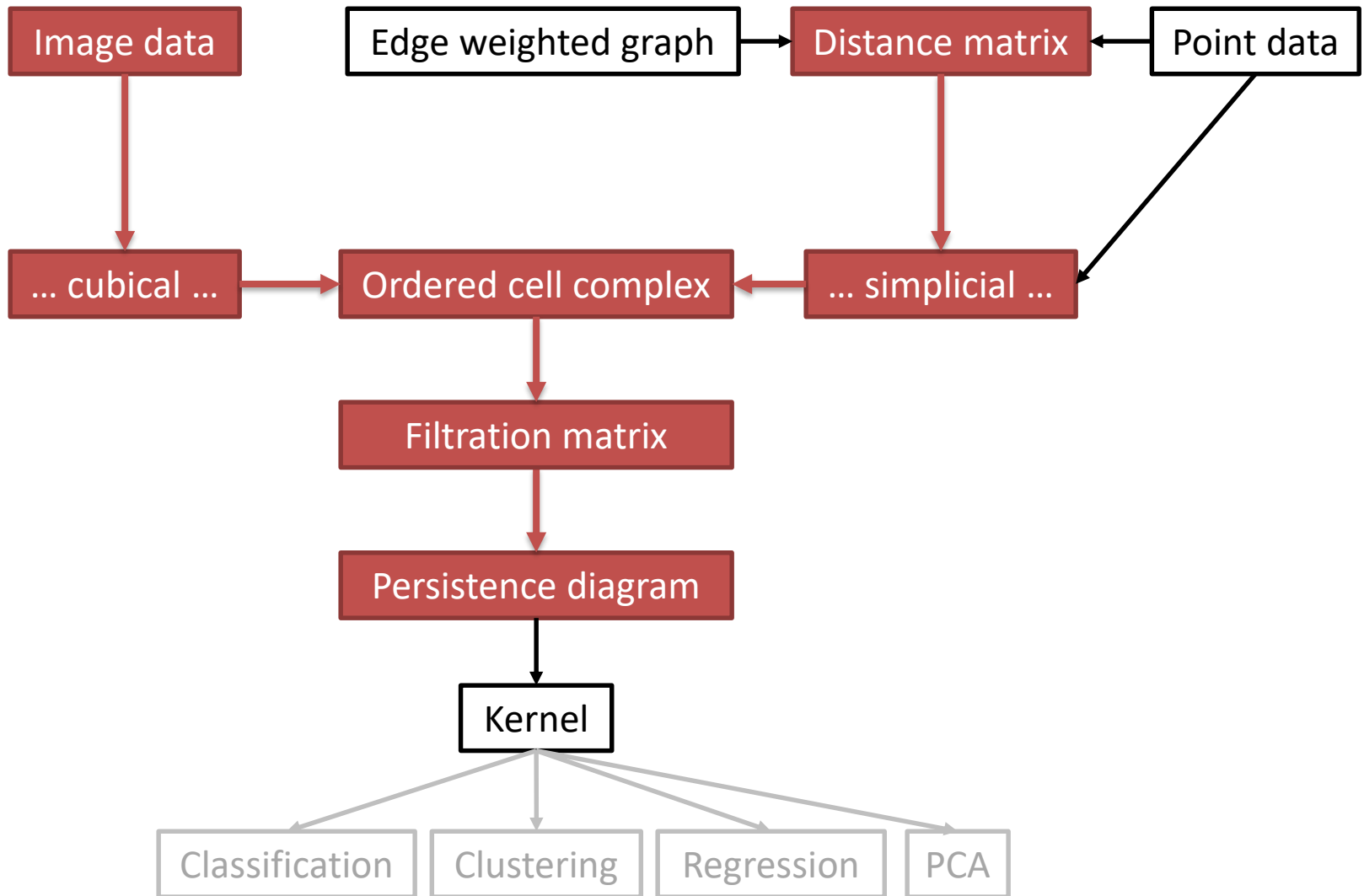
# Phat comparison

	Dionysus	JavaPlex	Perseus	Gudhi	Phat (simple)	Phat (opt)
Rips 64	2.6	4.4	18.0	0.15	0.02	0.01
Rips 192	359	465	(m)	9.8	2.0	1.0
Image 64 <sup>3</sup>		163	11 139		0.11	0.06
Image 256 <sup>3</sup>		(m)	(m)		11.3	4.7

	Dionysus	JavaPlex	Perseus	Gudhi	Phat (simple)	Phat (opt)
Rips 64	60 MB	270 MB	718 MB	44 MB	53 MB	61 MB
Rips 192	4.9 GB	12.3 GB	(m)	3.1 GB	3.6 GB	3.8 GB
Image 64 <sup>3</sup>		2.04 GB	1.5 GB		0.16 GB	0.16 GB
Image 256 <sup>3</sup>		(m)	(m)		10.2 GB	10.3 GB

# Part 2: Dipha - [github.com/DIPHA/dipha](https://github.com/DIPHA/dipha)

Joint work with: Ulrich Bauer, M. Kerber





# Why Distributed?

- Fast algorithms and data structures: Twist + Bit-tree + Dualization
  - Can process millions of simplices per second
  - Bottlenecked by memory consumption
- Memory efficient approaches only for special cases

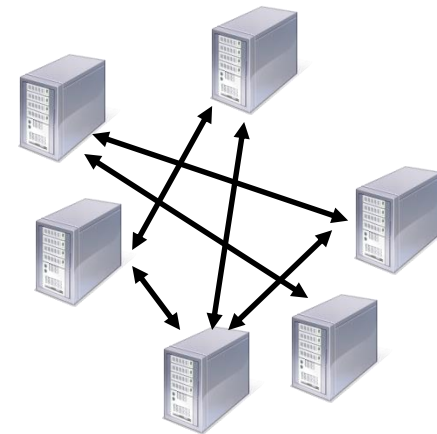
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IST Austria: 256 GB

vs.



50 x 64 GB = 3.2 TB

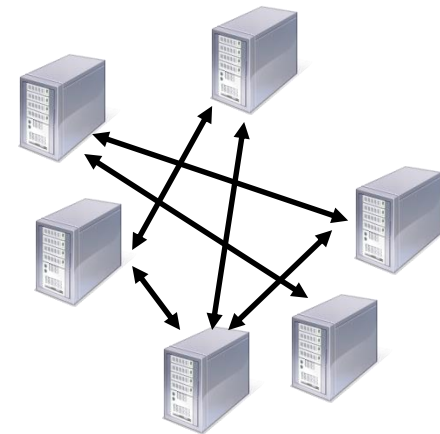
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IST Austria: 256 GB

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50 x 64 GB = 3.2 TB

Challenge: High latency (> 1000x)

# Spectral Sequence Matrix Reduction

	1	2	3	4	5	6	7
1	1		1		1		
2			1			1	
3							1
4				1	1		
5					1		1
6						1	
7							1



Pivot-to-Column Map

# Spectral Sequence Matrix Reduction

	1	2	3	4	5	6	7
1	1		1		1		
2			1			1	
3							1
4				1	1		
5					1		1
6						1	
7							1

3

Pivot-to-Column Map

# Spectral Sequence Matrix Reduction

	1	2	3	4	5	6	7
1	1		1		1		
2		1	1			1	
3							1
4				1	1		
5					1		1
6						1	
7							1

3
5

Pivot-to-Column Map

# Spectral Sequence Matrix Reduction

	1	2	3	4	5	6	7
1	1		1		1	1	
2		1	1			1	
3			1				1
4				1			
5					1		1
6						1	
7							1

3
5

Pivot-to-Column Map

# Spectral Sequence Matrix Reduction

	1	2	3	4	5	6	7
1	1		1	1	1	1	
2		1	1	1	1	1	
3			1	1	1	1	1
4				1	1	1	
5					1	1	1
6						1	1
7							1

3
5
7

Pivot-to-Column Map



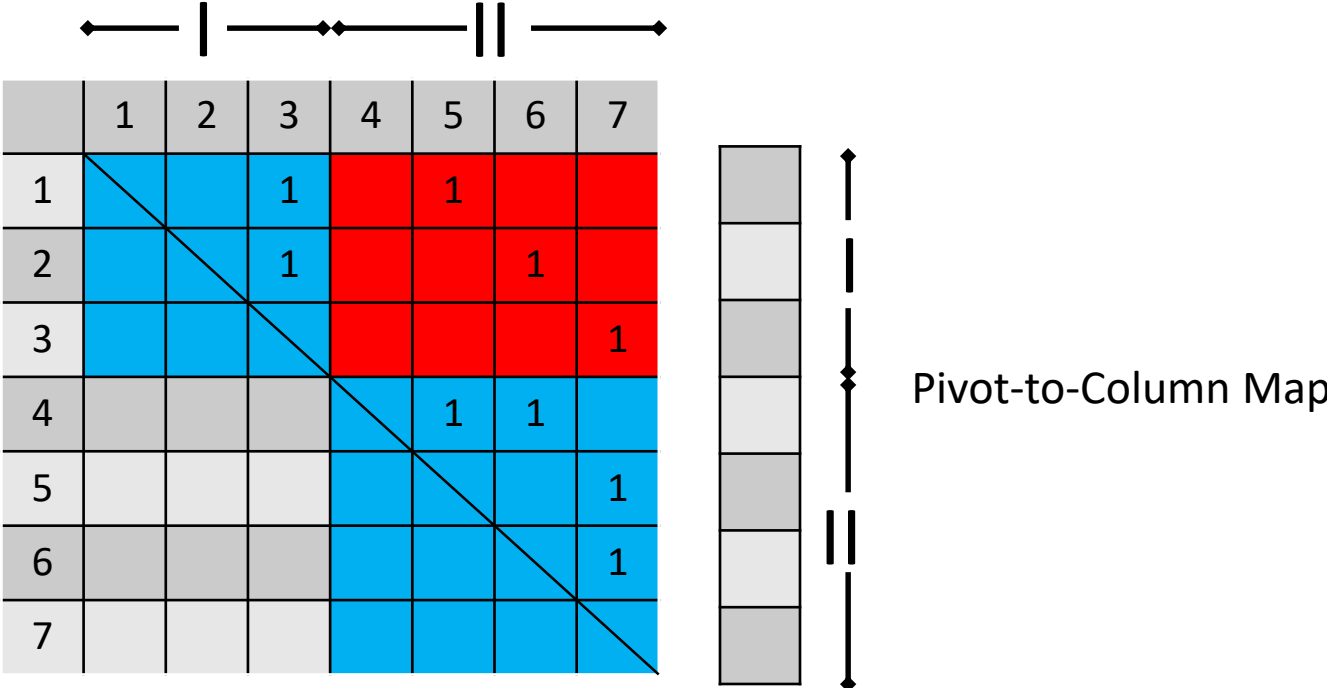
# Spectral Sequence Matrix Reduction

	1	2	3	4	5	6	7
1	1		1		1		
2		1	1				
3			1				1
4				1			
5					1		1
6						1	
7							1

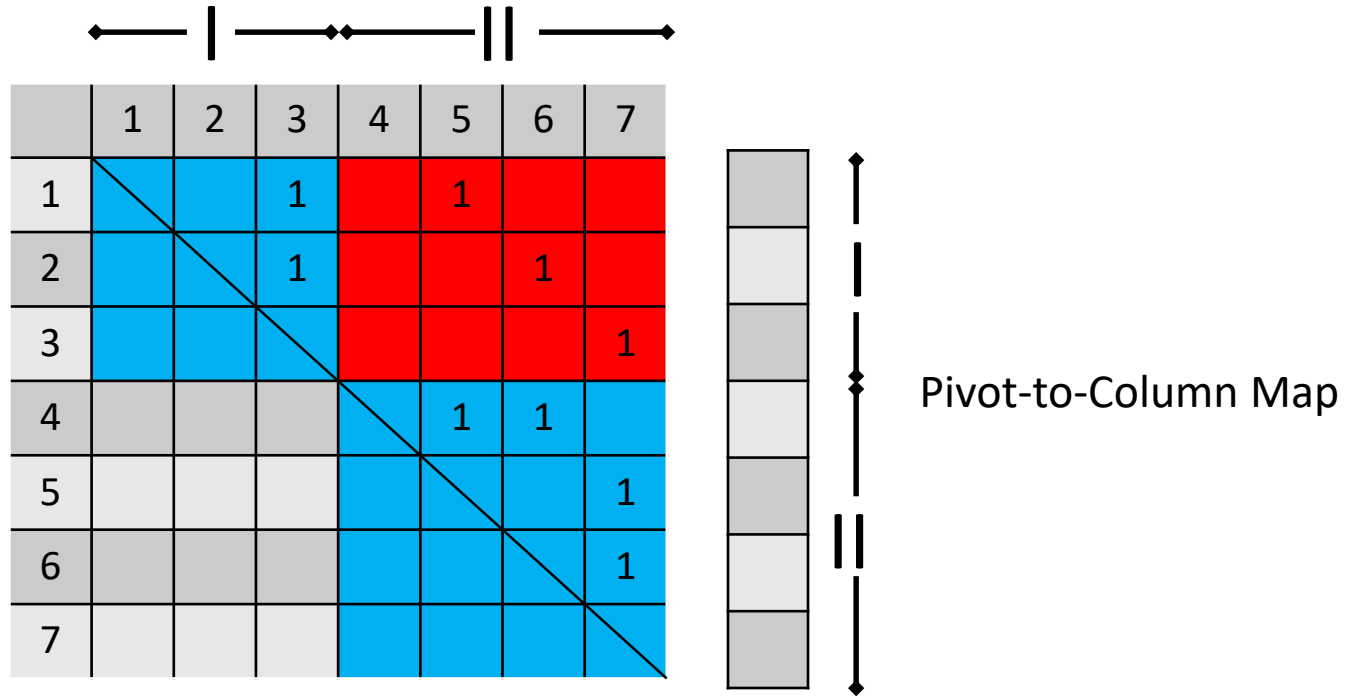
3
5
7

Pivot-to-Column Map

# Inefficient Distributed Matrix Reduction

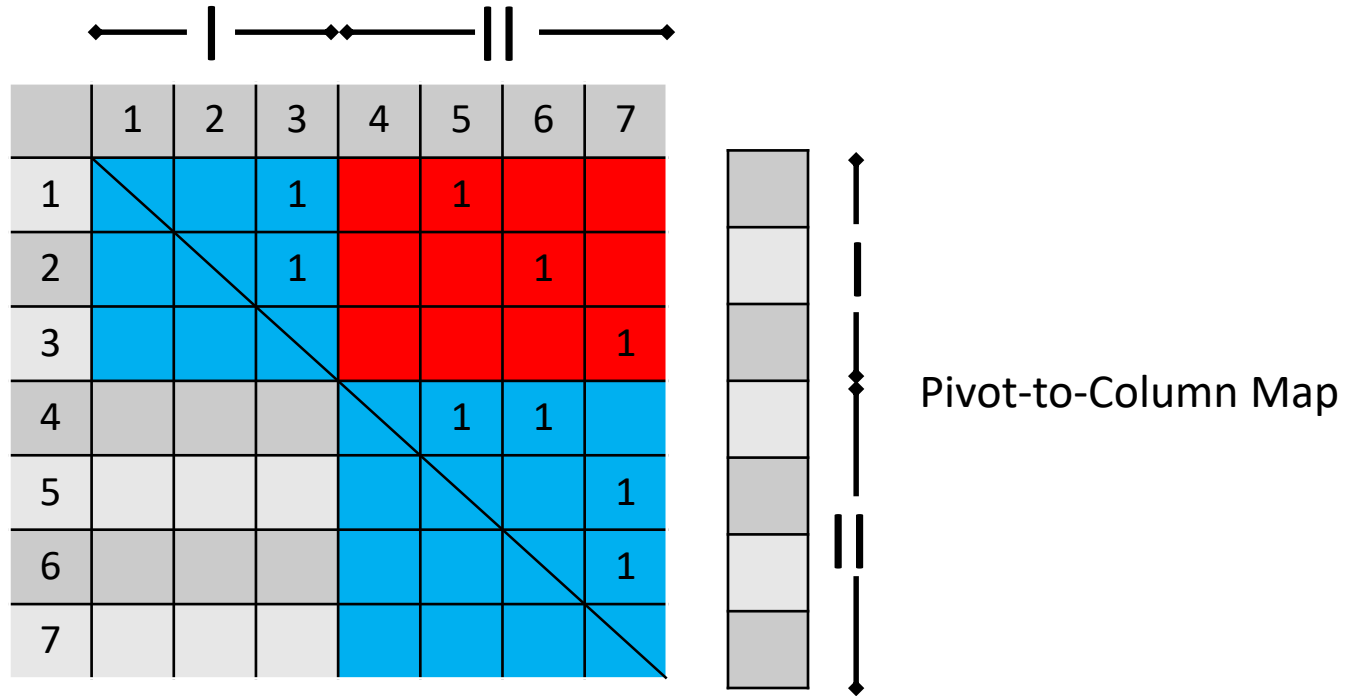


# Inefficient Distributed Matrix Reduction



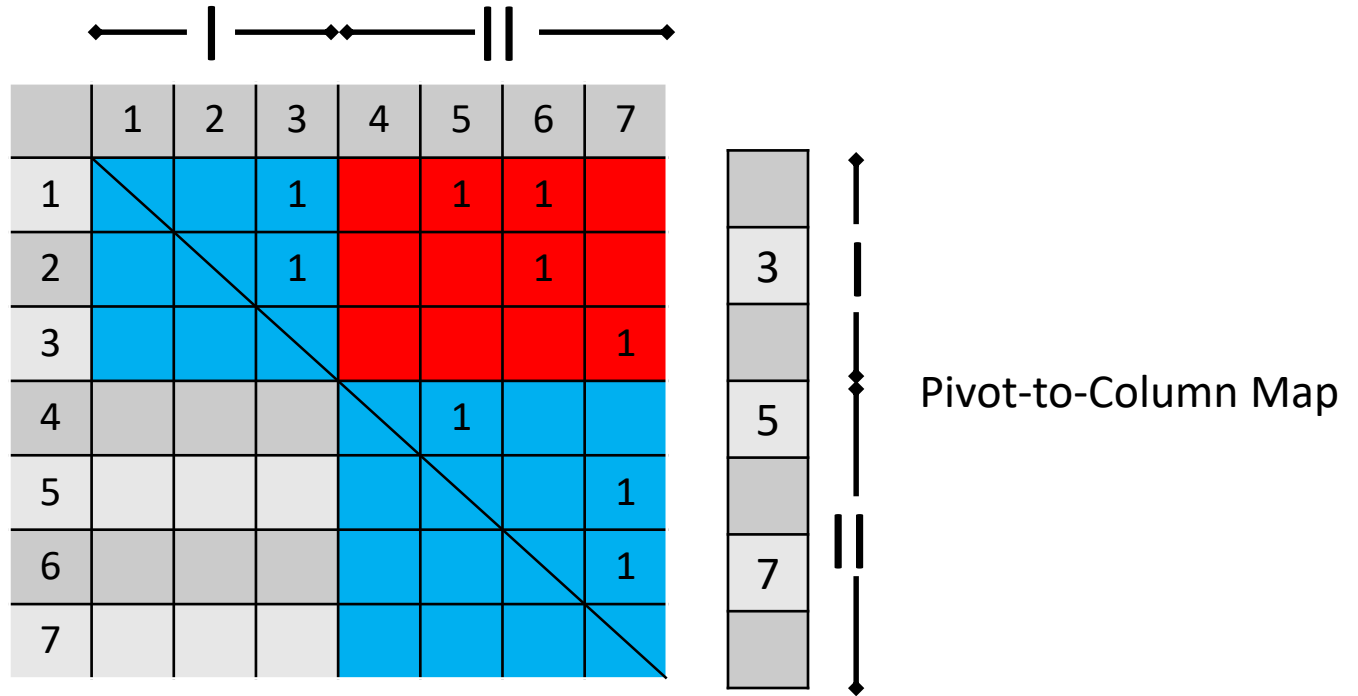
Step 1	
I	Load cols 1-3
II	Load cols 4-7

# Inefficient Distributed Matrix Reduction



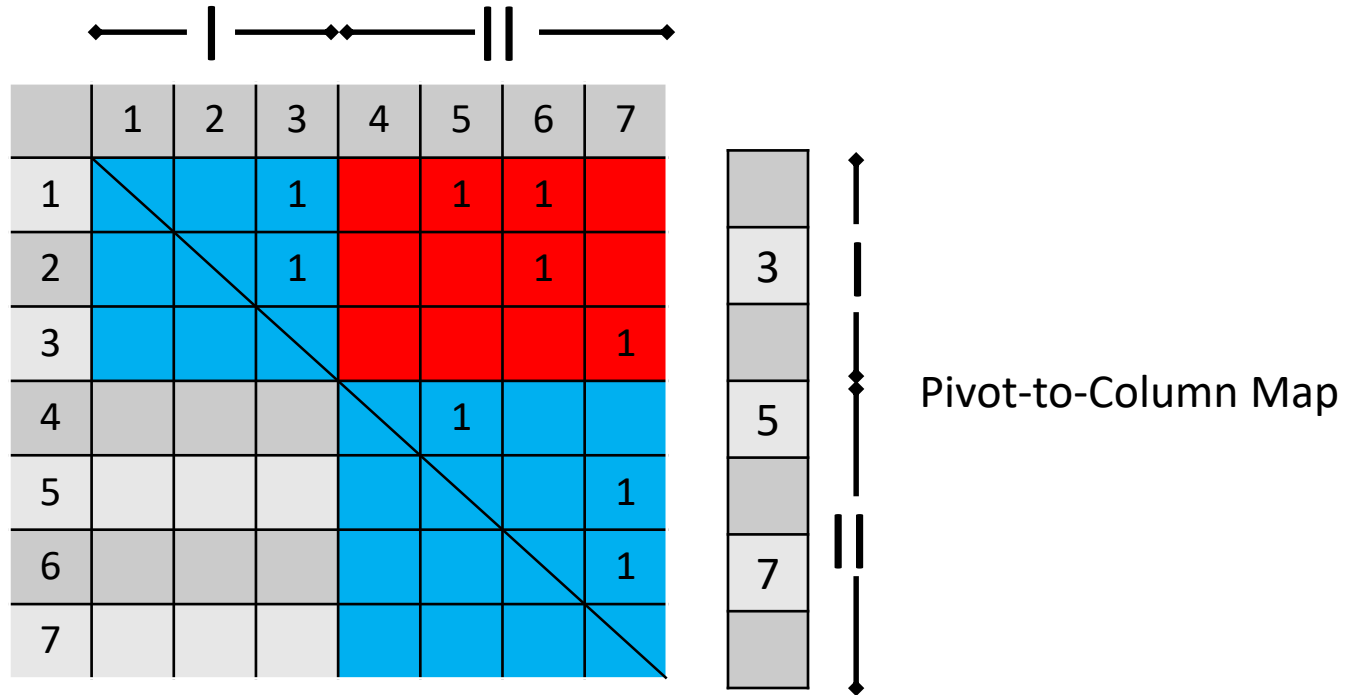
	Step 1	Step 2
I	Load cols 1-3	Reduce to idx 1
II	Load cols 4-7	Reduce to idx 4

# Inefficient Distributed Matrix Reduction



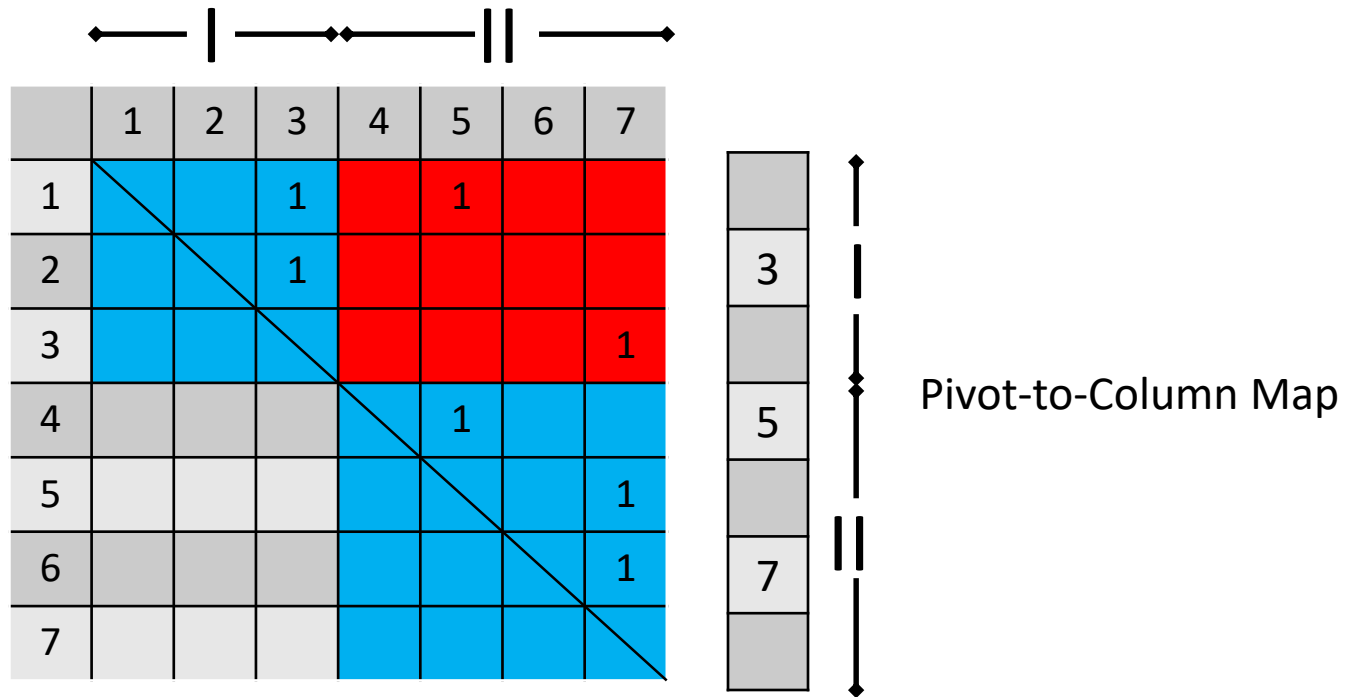
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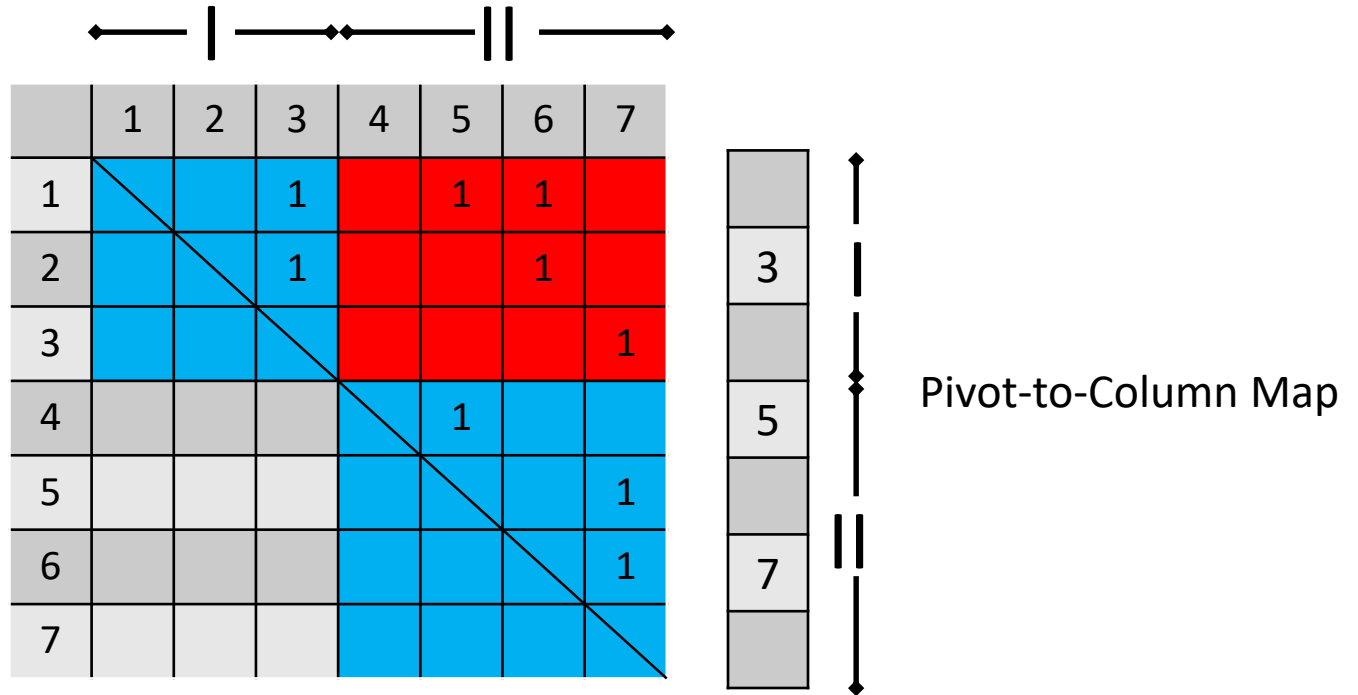
	Step 1	Step 2	Step 3
I	Load cols 1-3	Reduce to idx 1	idle
II	Load cols 4-7	Reduce to idx 4	Reduce to idx 1

# Inefficient Distributed Matrix Reduction



	Step 1	Step 2	Step 3
I	Load cols 1-3	Reduce to idx 1	idle
II	Load cols 4-7	Reduce to idx 4	Reduce to idx 1

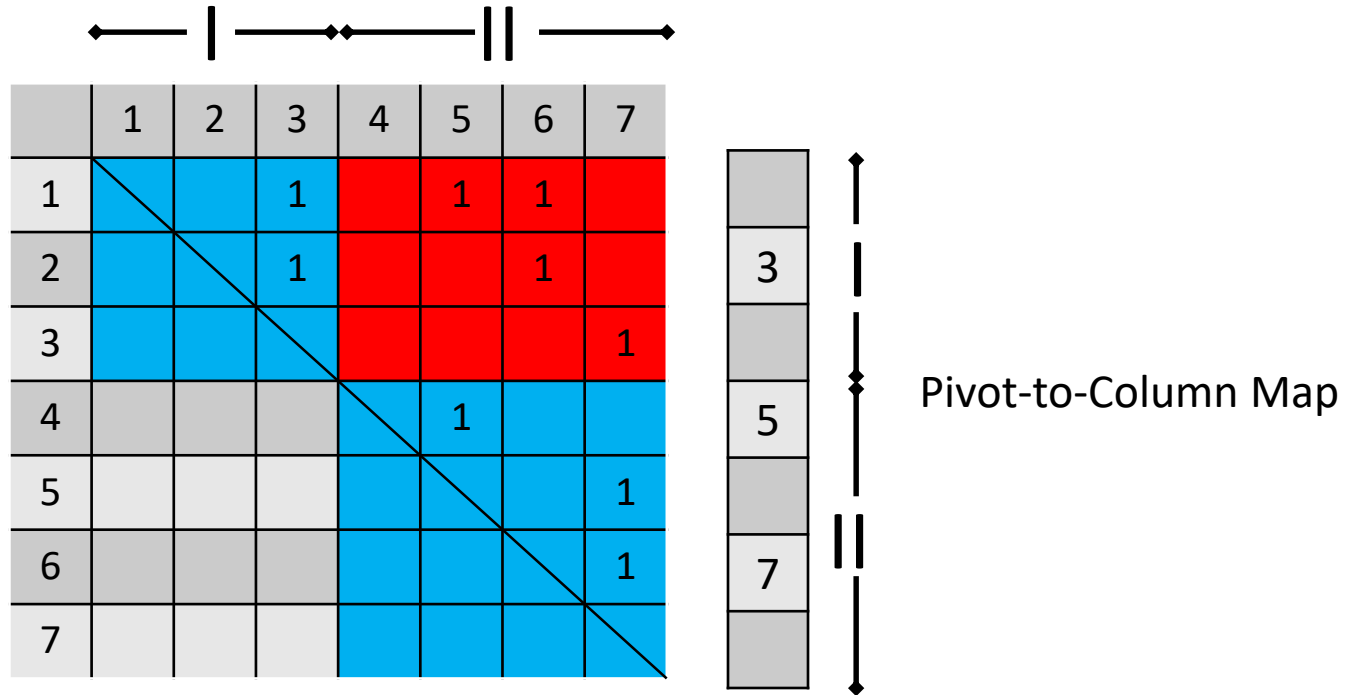
# Efficient Distributed Matrix Reduction



	Step 1	Step 2
I	Load cols 1-3	Reduce to idx 1
II	Load cols 4-7	Reduce to idx 4

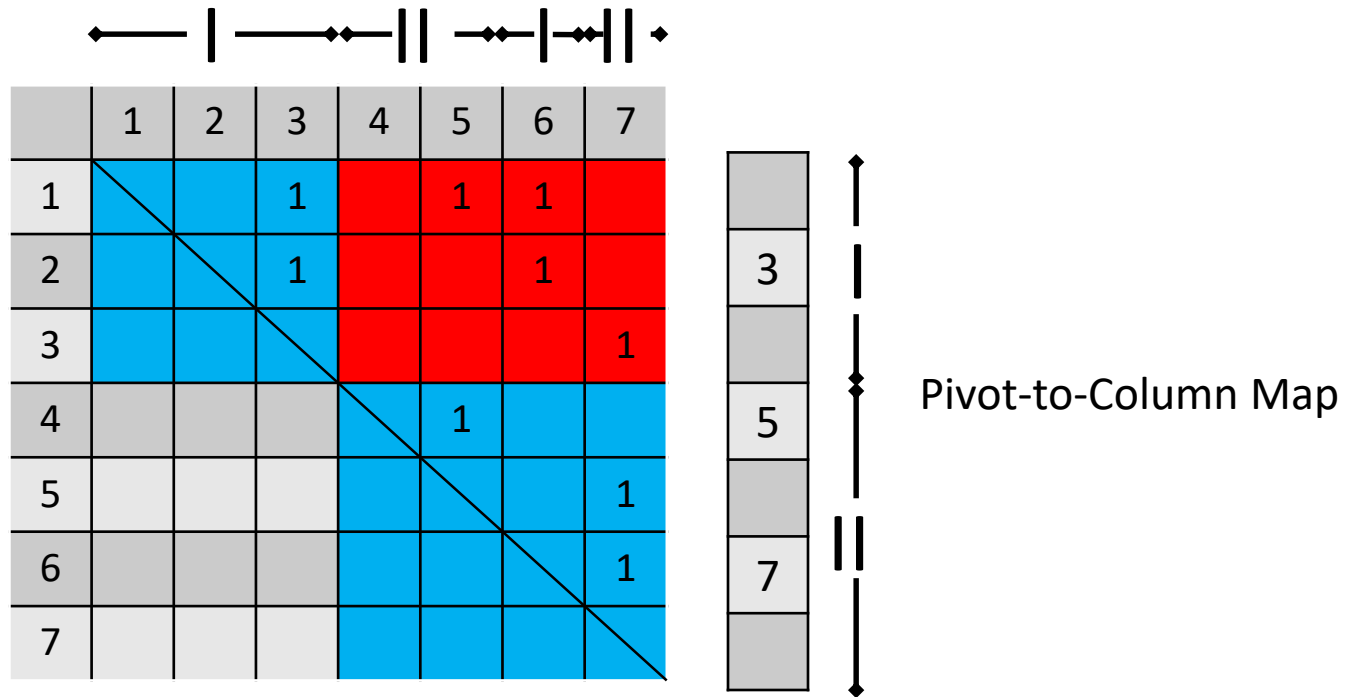


# Efficient Distributed Matrix Reduction



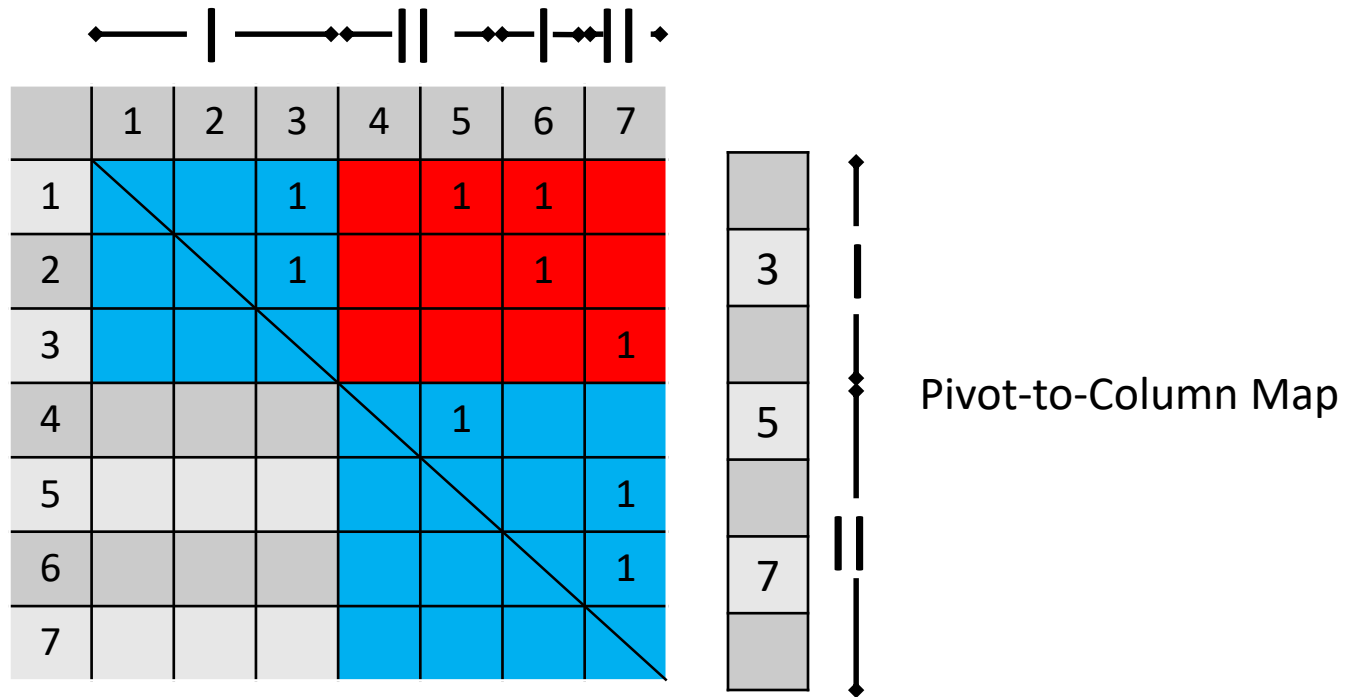
	Step 1	Step 2	Step 3
I	Load cols 1-3	Reduce to idx 1	Recv. unreduced cols from II
II	Load cols 4-7	Reduce to idx 4	Send. unreduced cols to I

# Efficient Distributed Matrix Reduction



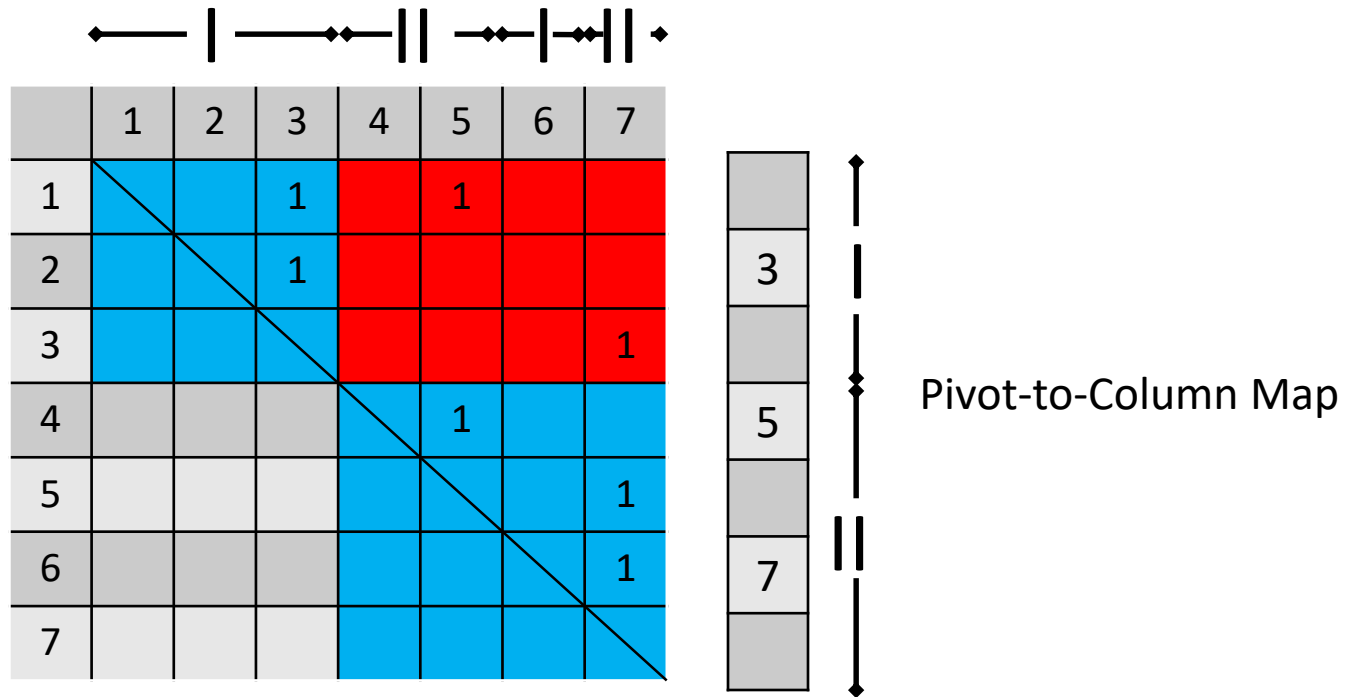
	Step 1	Step 2	Step 3
I	Load cols 1-3	Reduce to idx 1	Recv. unreduced cols from II
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# Efficient Distributed Matrix Reduction



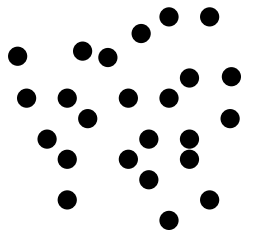
	Step 1	Step 2	Step 3	Step 4
I	Load cols 1-3	Reduce to idx 1	Recv. unreduced cols from II	Reduce to idx 1
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# Efficient Distributed Matrix Reduction

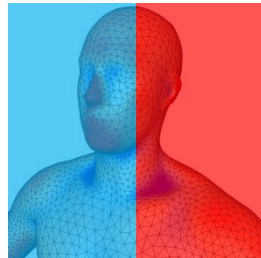
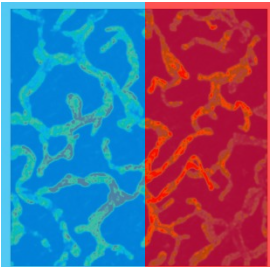


	Step 1	Step 2	Step 3	Step 4
I	Load cols 1-3	Reduce to idx 1	Recv. unreduced cols from II	Reduce to idx 1
II	Load cols 4-7	Reduce to idx 4	Send. unreduced cols to I	idle

# Distributed Computational Pipeline



1	3	78	65	3	46	12	1
7	6	23	78	65	3	46	23
5	34	61	2	78	65	3	46
2	6	2	10	2	1	1	51
78	65	3	46	6	1	4	35
1	6	78	65	3	46	24	32
6	6	6	5	78	65	3	46
1	78	65	3	46	2	15	12



Input data

1.3
3.2
2.8
6.1
9.1
8.3
5.9

1.3
2.8
3.2
5.9
6.1
8.3
9.1

1	3	2	5	7	6	4
---	---	---	---	---	---	---

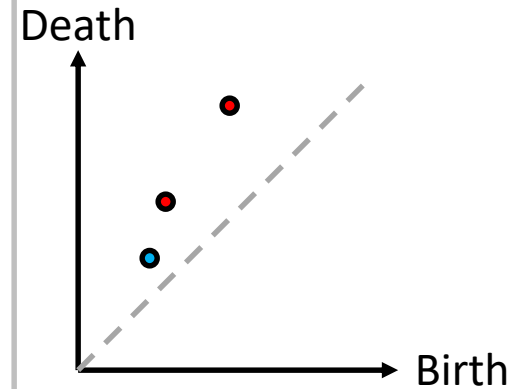
1	3	2	7	4	6	5
---	---	---	---	---	---	---

	1	2	3	4	5	6	7
1	1	1		1			
2		1				1	
3					1		
4				1		1	
5					1		
6					1		
7							

Boundary matrix  
+ weights

	1	2	3	4	5	6	7
1	1		1		1		
2		1	1			1	
3			1				1
4				1	1		
5					1		1
6						1	
7							1

Filtration matrix  
+ permutation maps



	1	2	3	4	5	6	7
1	1		1		1		
2		1	1			1	
3			1				1
4				1			
5					1		1
6						1	
7							1

Reduced matrix  
+ diagram

# Dipha summary

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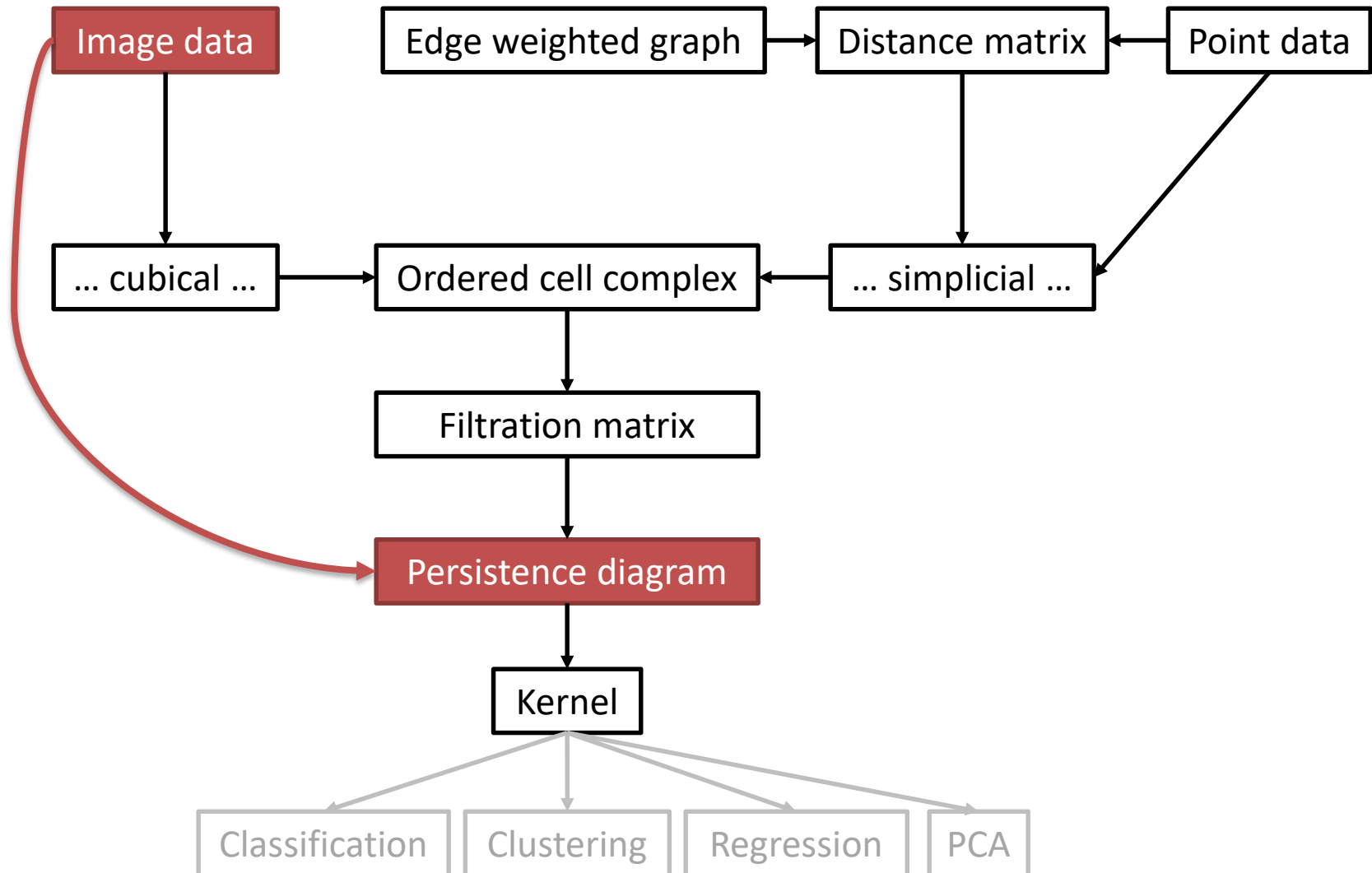
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5. Morse:  $1024^3$  noise image ( $\rightarrow$  8 billion columns) with 256 nodes:  
 $\rightarrow$  13 min, 3.2 GB Memory peak, 10 GB peak traffic per node pair  
(single machine would need  $\sim 640$  GB RAM)

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 $\rightarrow$  13 min, 3.2 GB Memory peak, 10 GB peak traffic per node pair  
(single machine would need  $\sim 640$  GB RAM)
6. Rips: 3000 points, dimension: 2 ( $\rightarrow$  5 billion columns), with 380 nodes:  
 $\rightarrow$  20 min, 4 GB Memory peak

# Part 3: Discrete Morse theory

Joint work with: D. Guenther, I. Hotz, H. Wagner

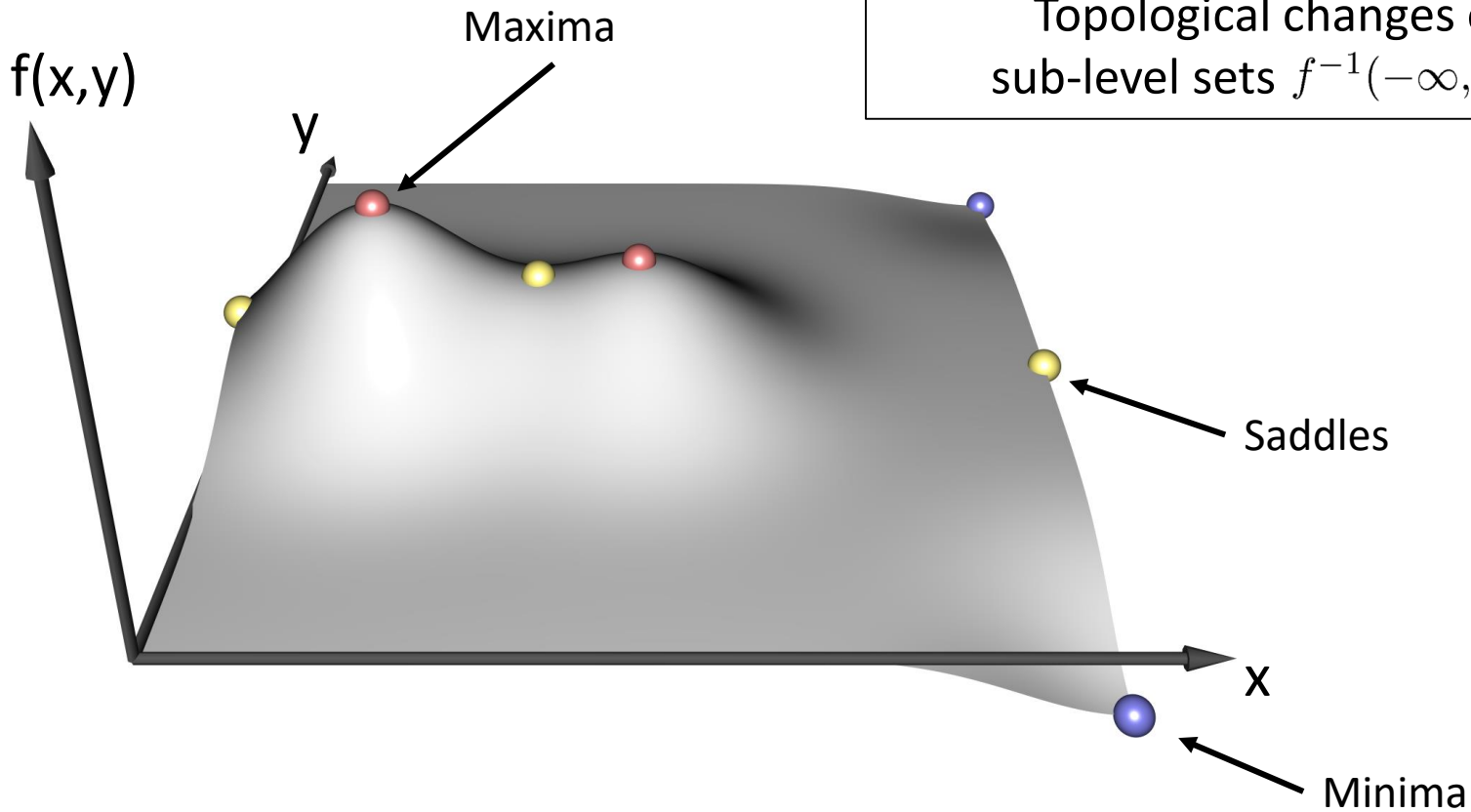


# What is ... Morse theory?

Critical points of  $f : \Omega \rightarrow \mathbb{R}$



Topological changes of  
sub-level sets  $f^{-1}(-\infty, t]$

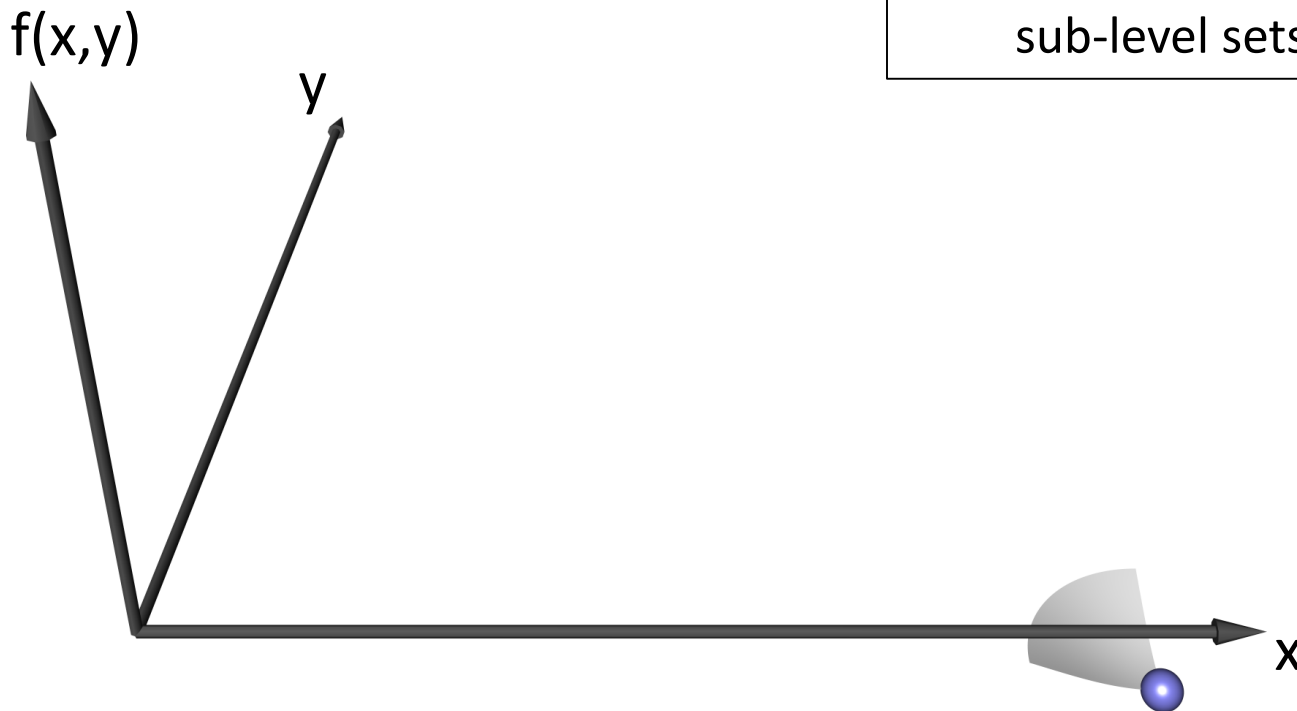


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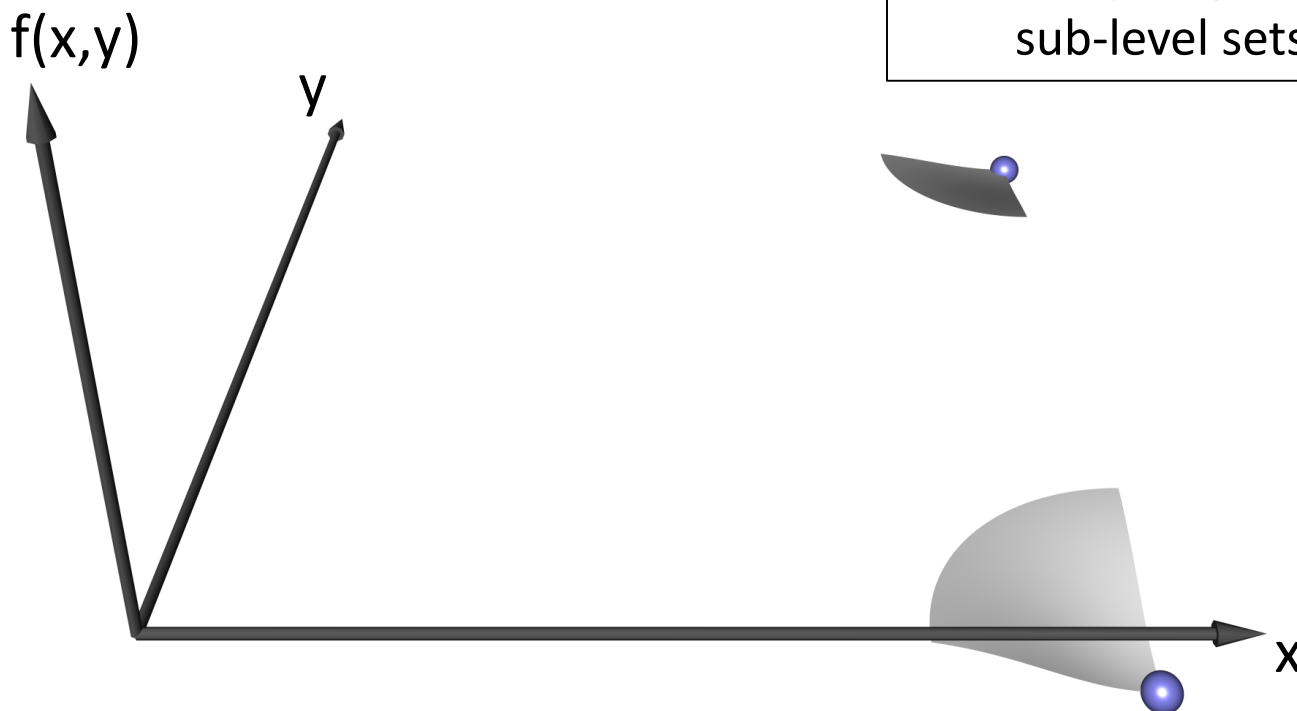


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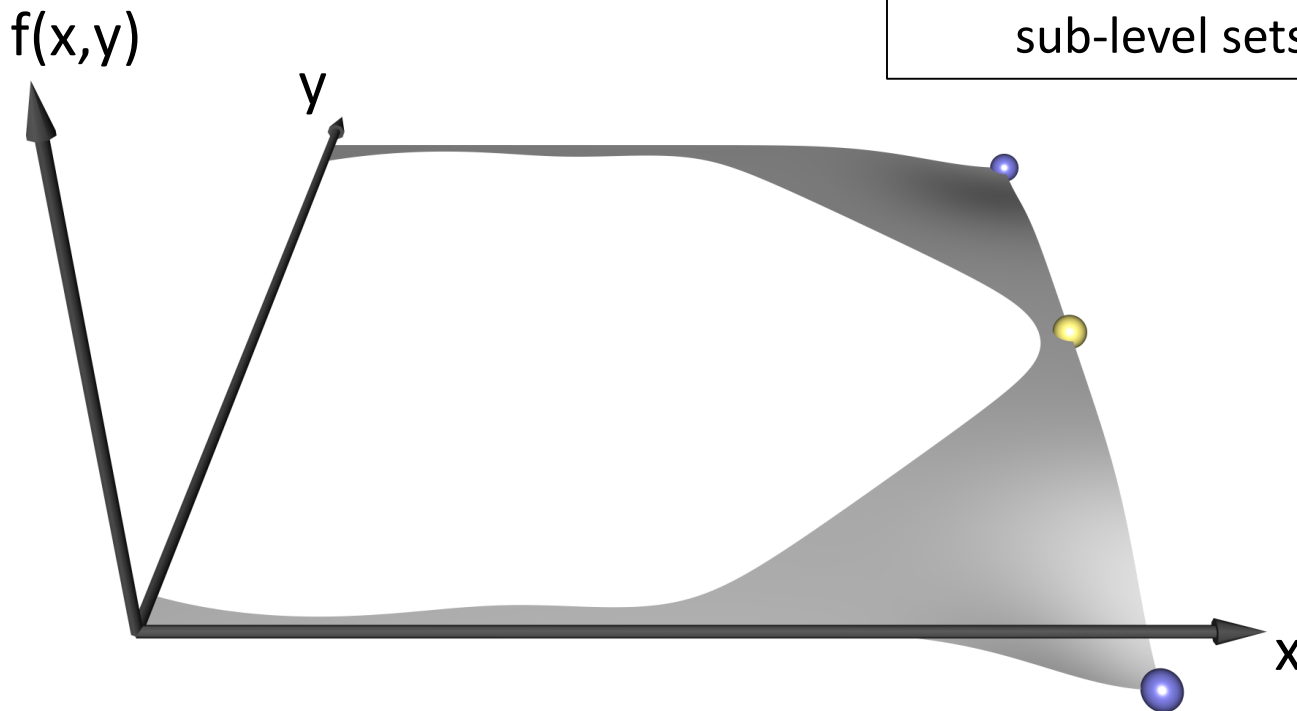


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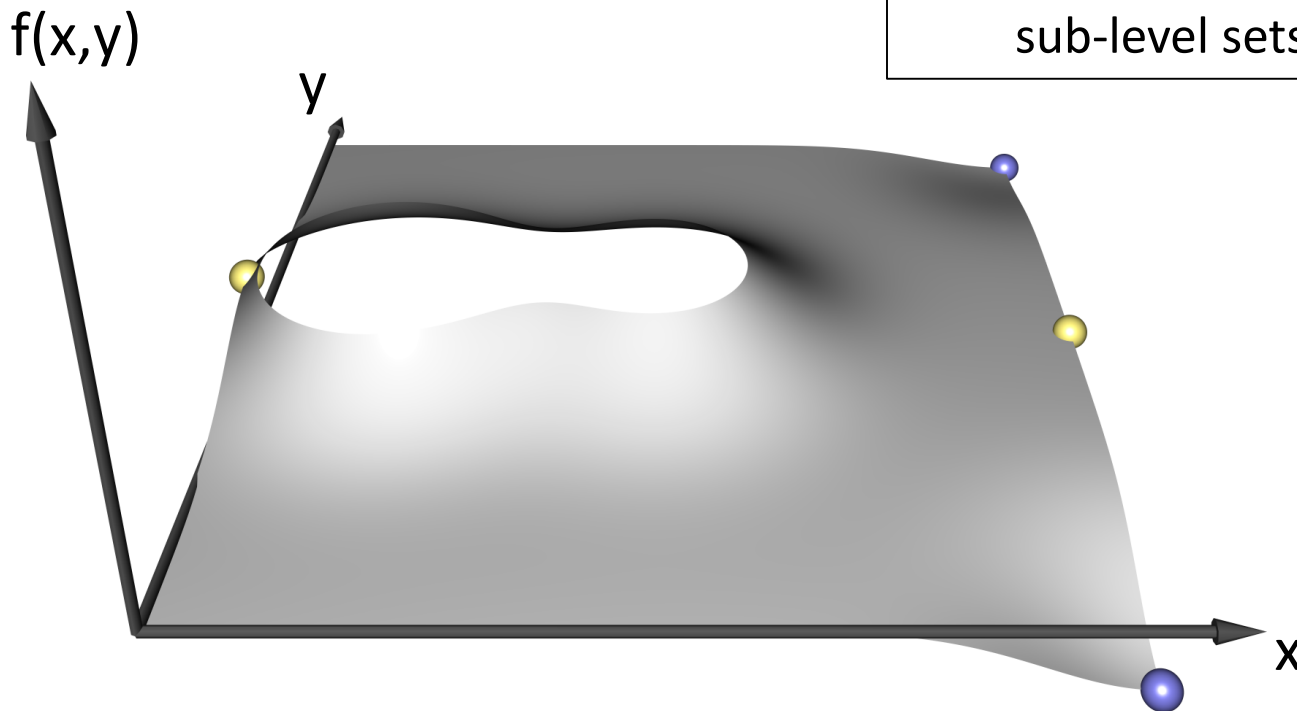


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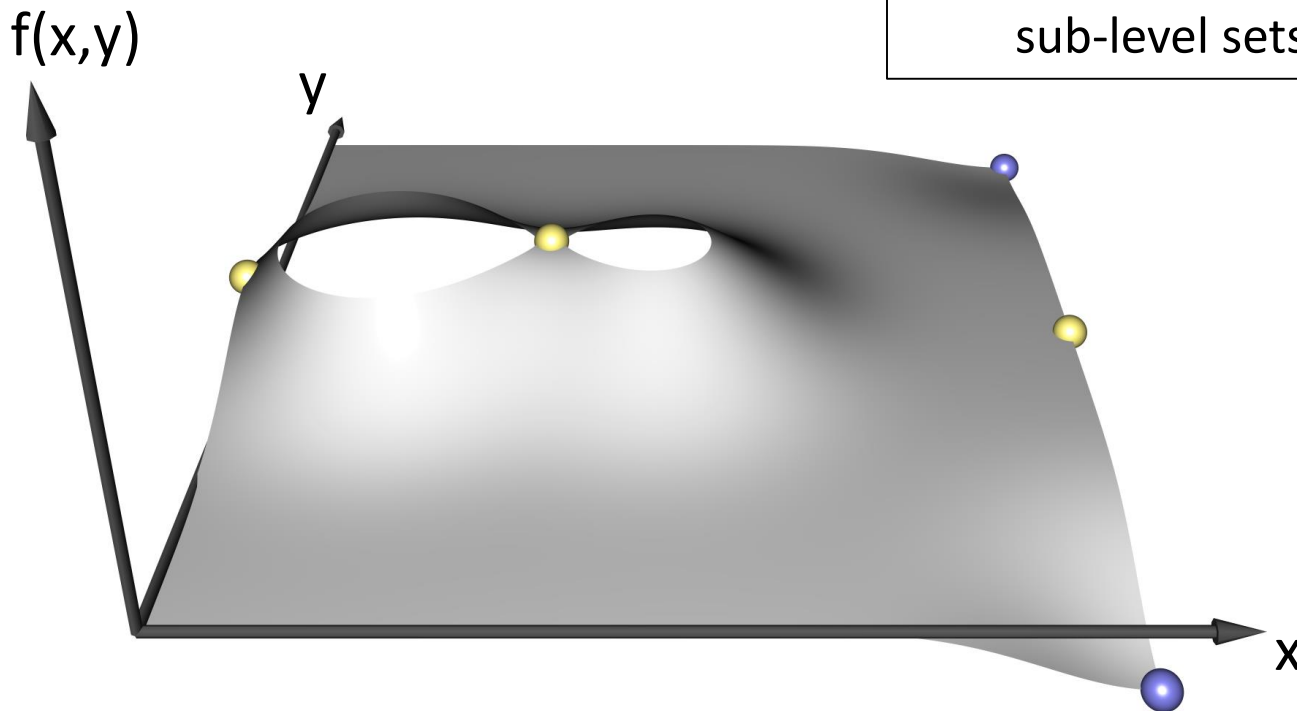


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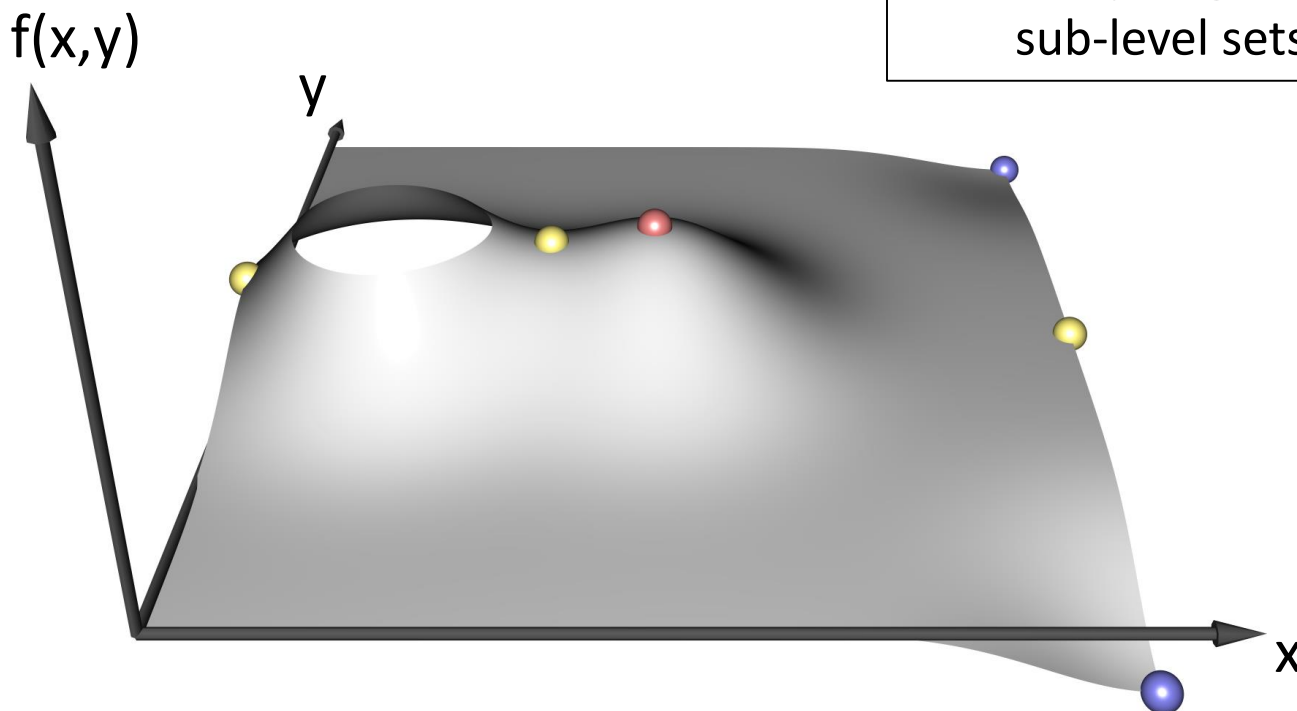


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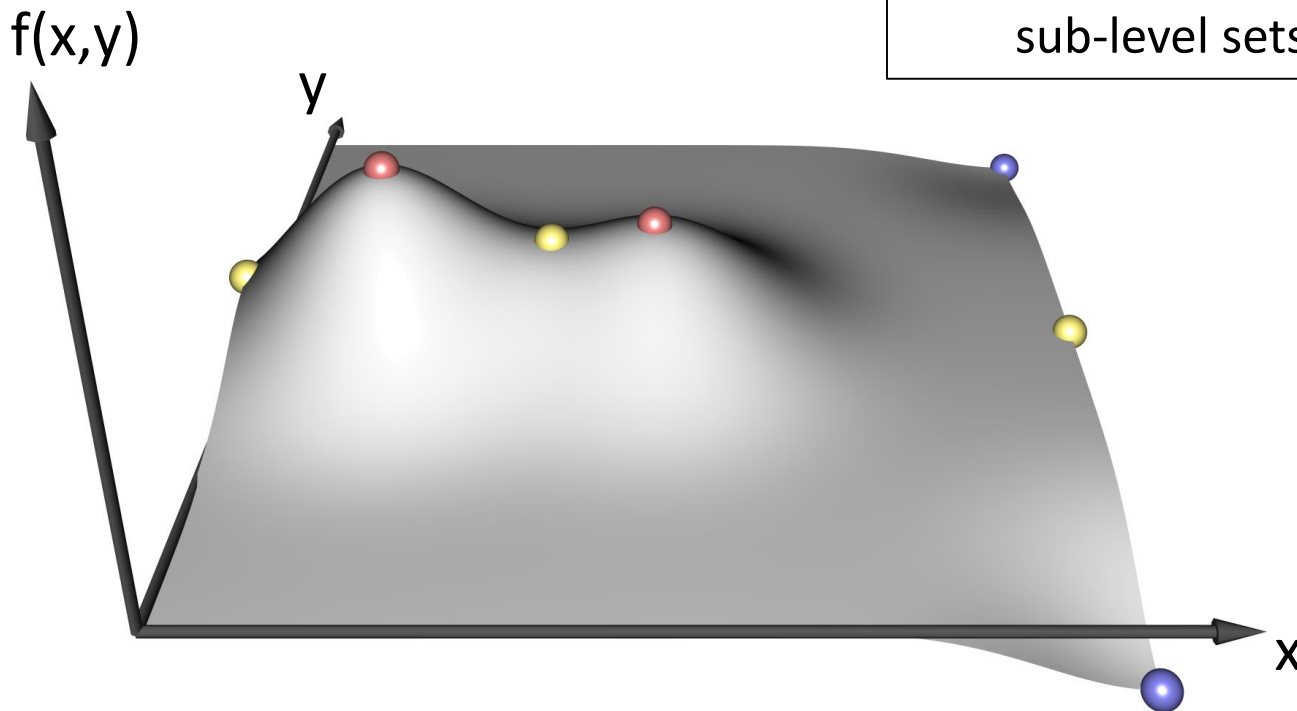


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Critical points of  $f : \Omega \rightarrow \mathbb{R}$



Topological changes of  
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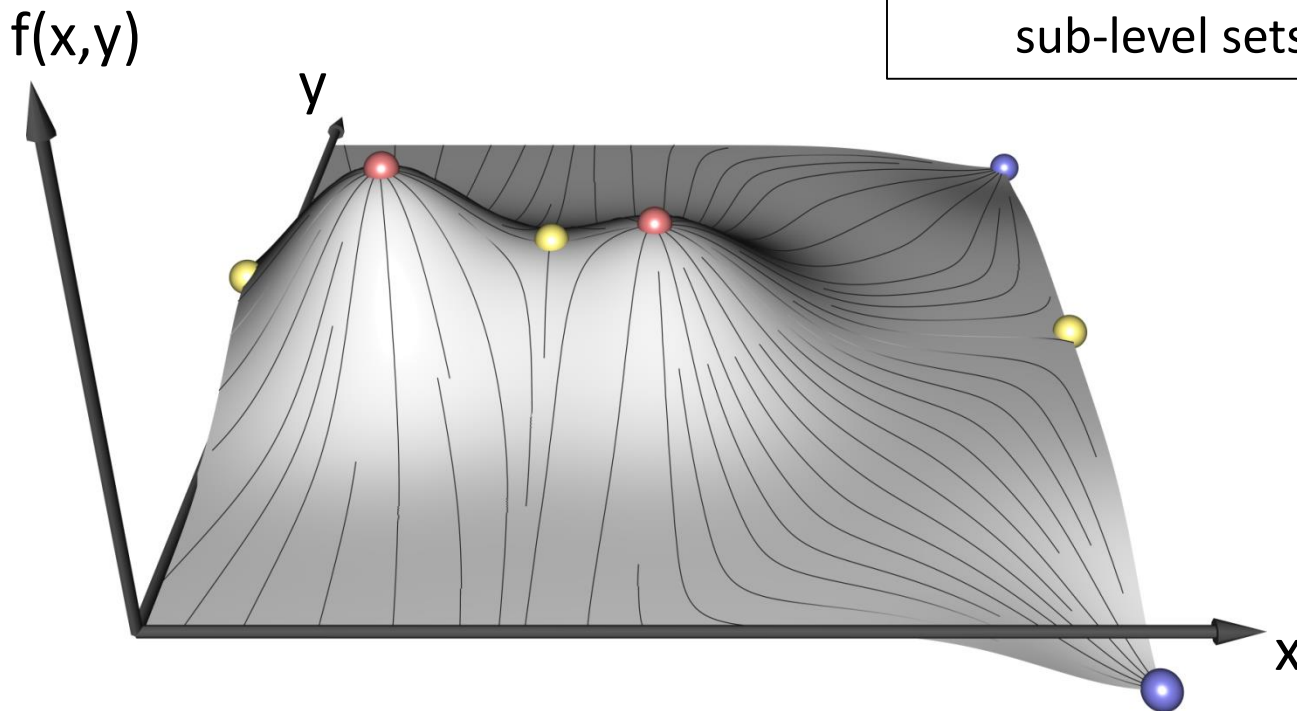


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Topological changes of  
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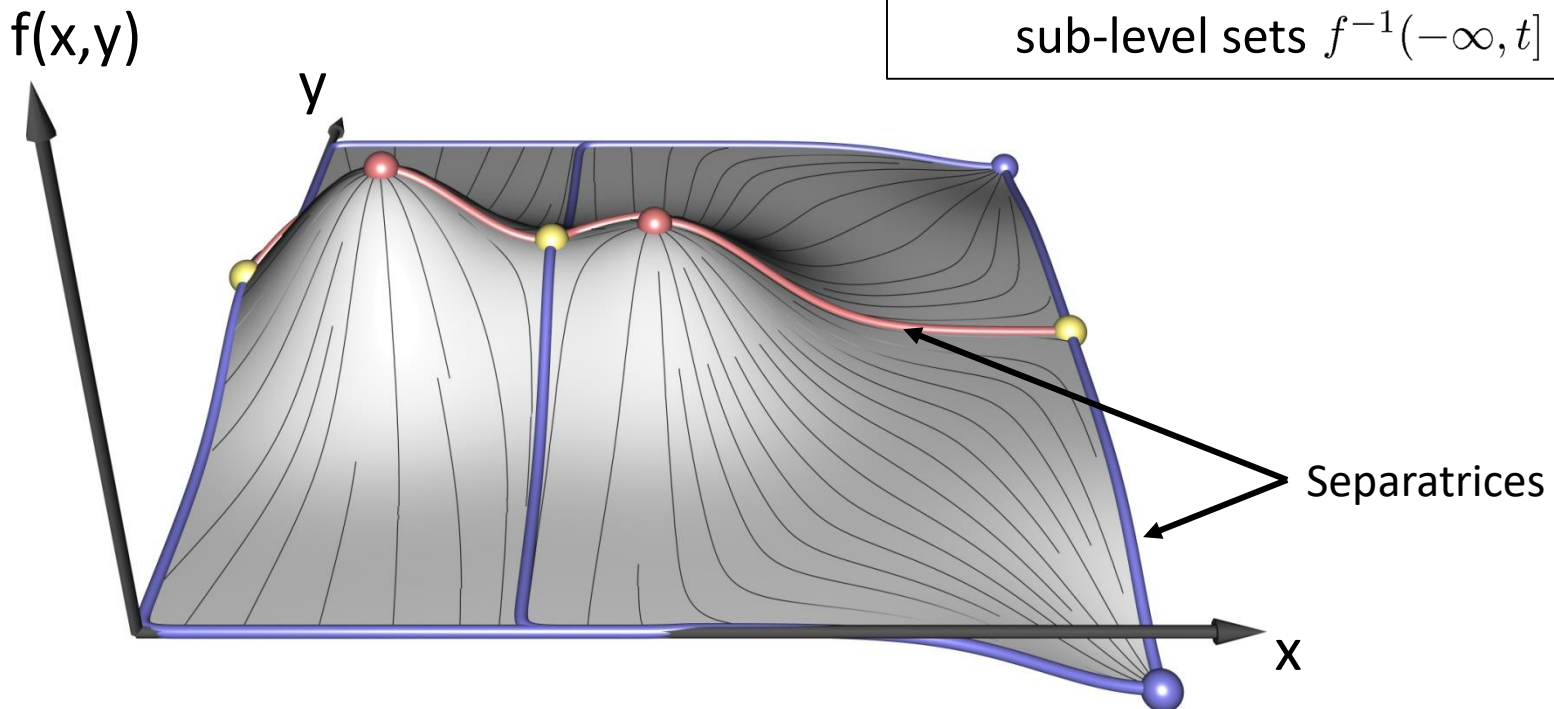


# What is ... Morse theory?

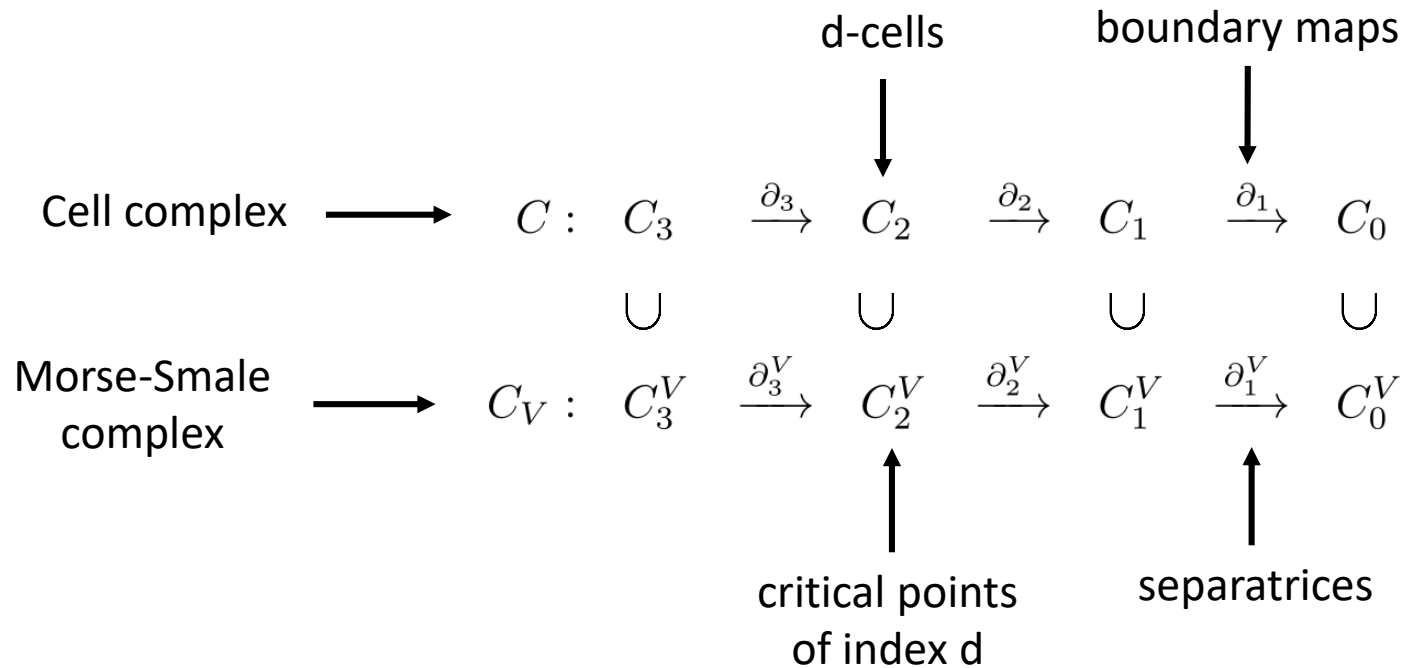
Critical points + **separatrices**



Topological changes of  
sub-level sets  $f^{-1}(-\infty, t]$



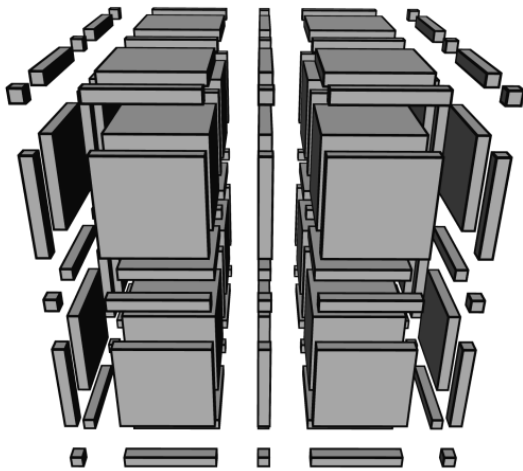
# Computing persistent homology using Morse theory



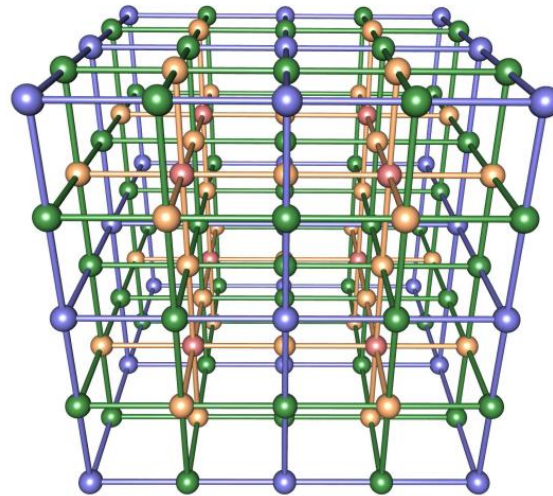
$Persistence(C, f) = Persistence(C_V, f)$
---

# Discrete Morse theory intuition

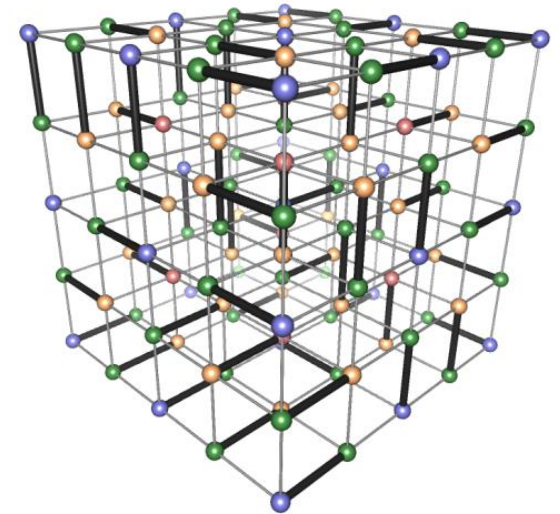
Combinatorial gradient field  $\Leftrightarrow$  *acyclic matching* of the cell graph



Cell complex



Cell graph



Acyclic matching

Critical points

–

unmatched nodes

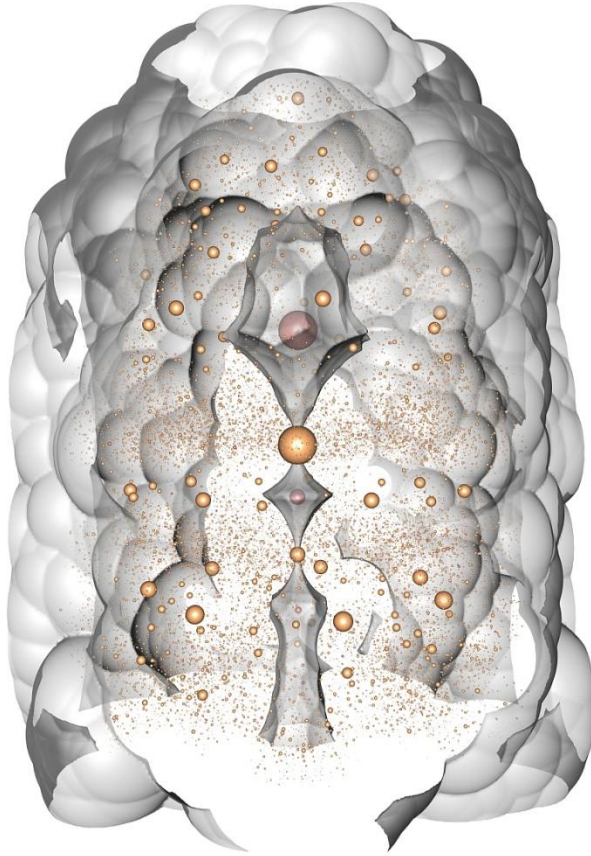
Separatrices

–

alternating paths



# Example



Data set size: 1120 x 1131 x 1552 (8 GB)

Total running time: ca. 5h

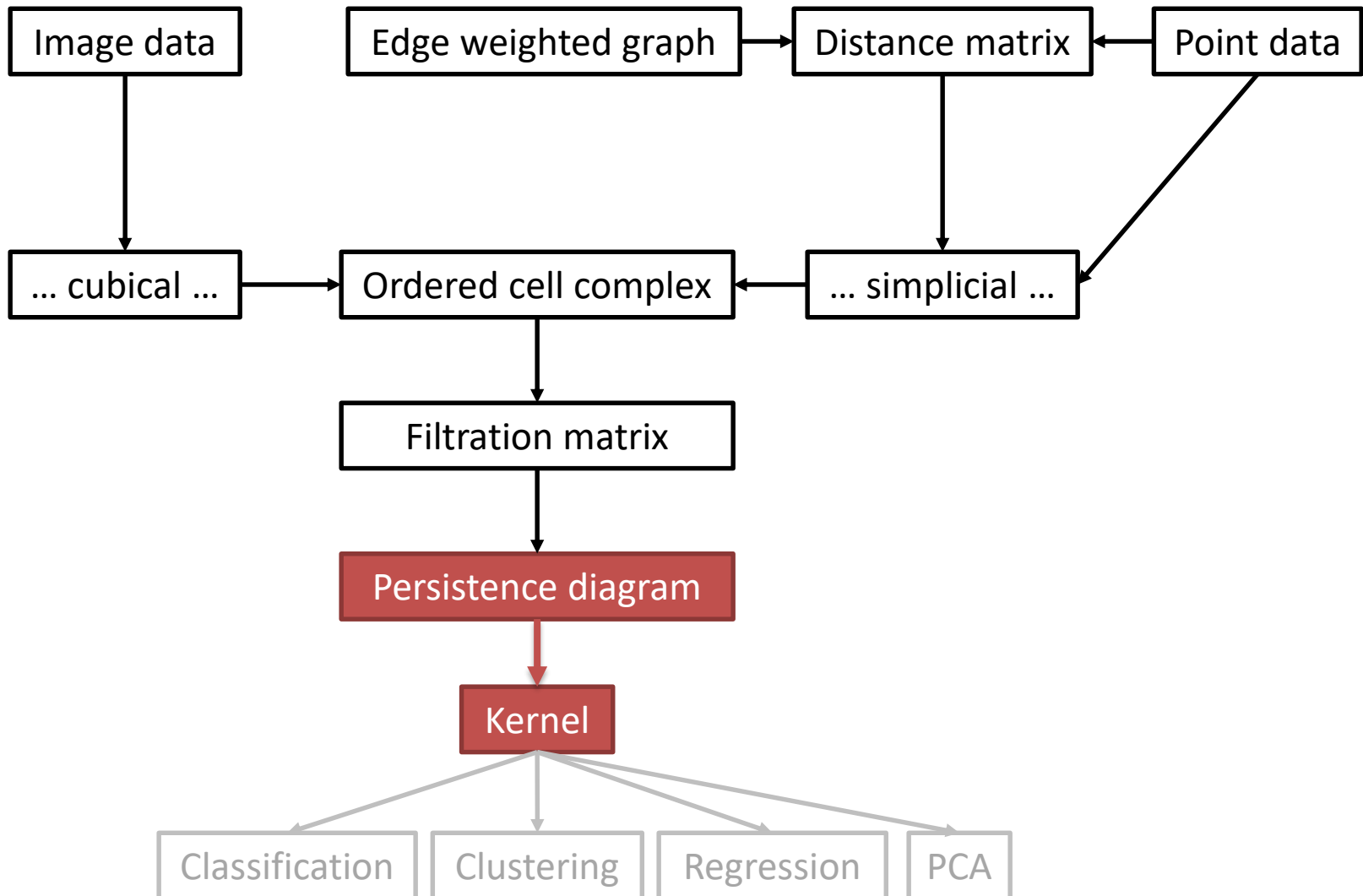
Memory requirement: 1.3 TB → 24 GB

Critical points scaled by persistence  
of a distance field of a molecular  
surface (data courtesy: D. Baum)

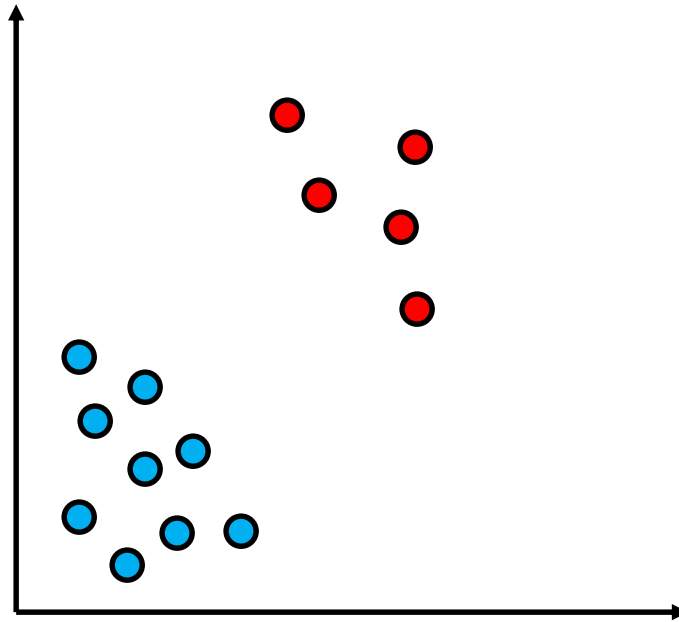
The full cell complex is never represented explicitly

# Part 4: Persistence-Scale-Space kernel

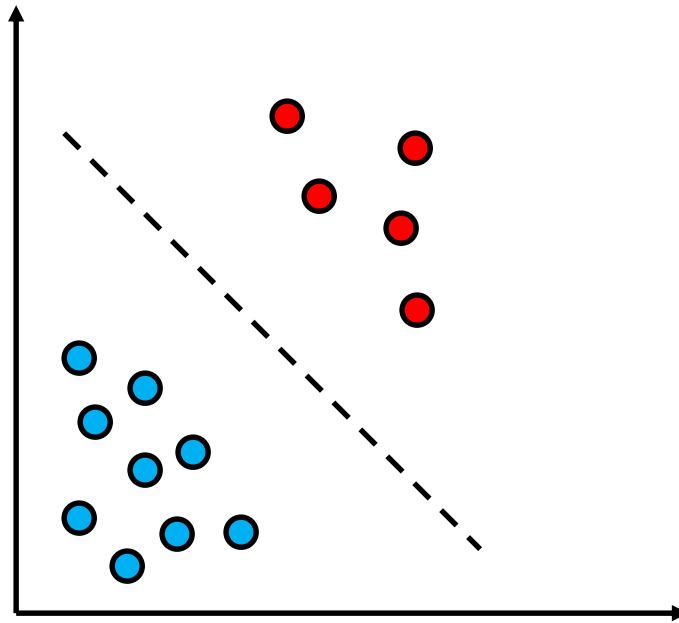
Joint work with: S. Huber, R. Kwitt, U. Bauer



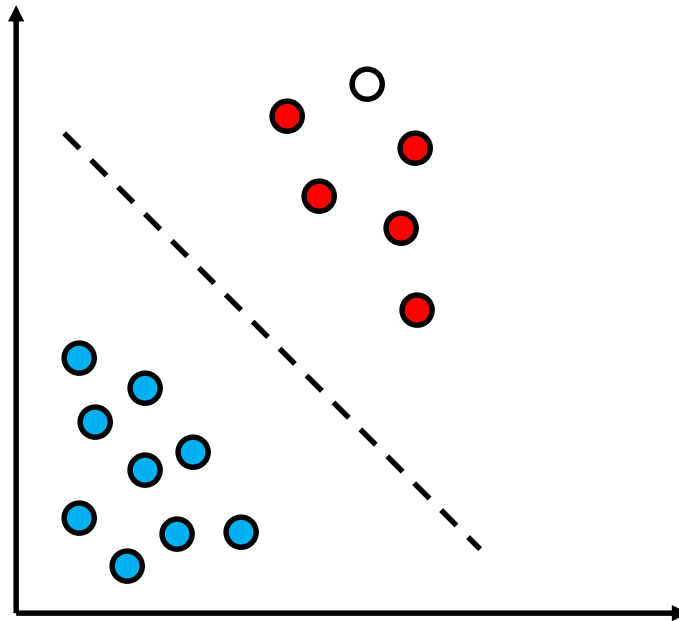
# Topological Machine Learning



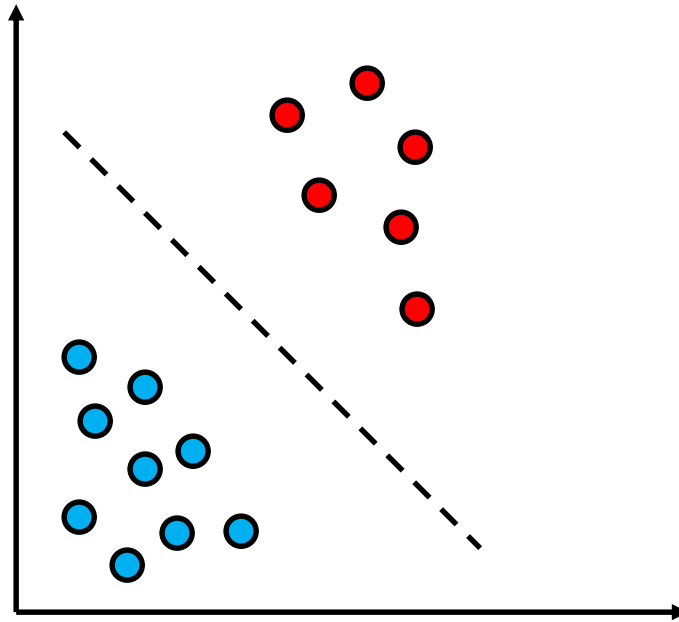
# Topological Machine Learning



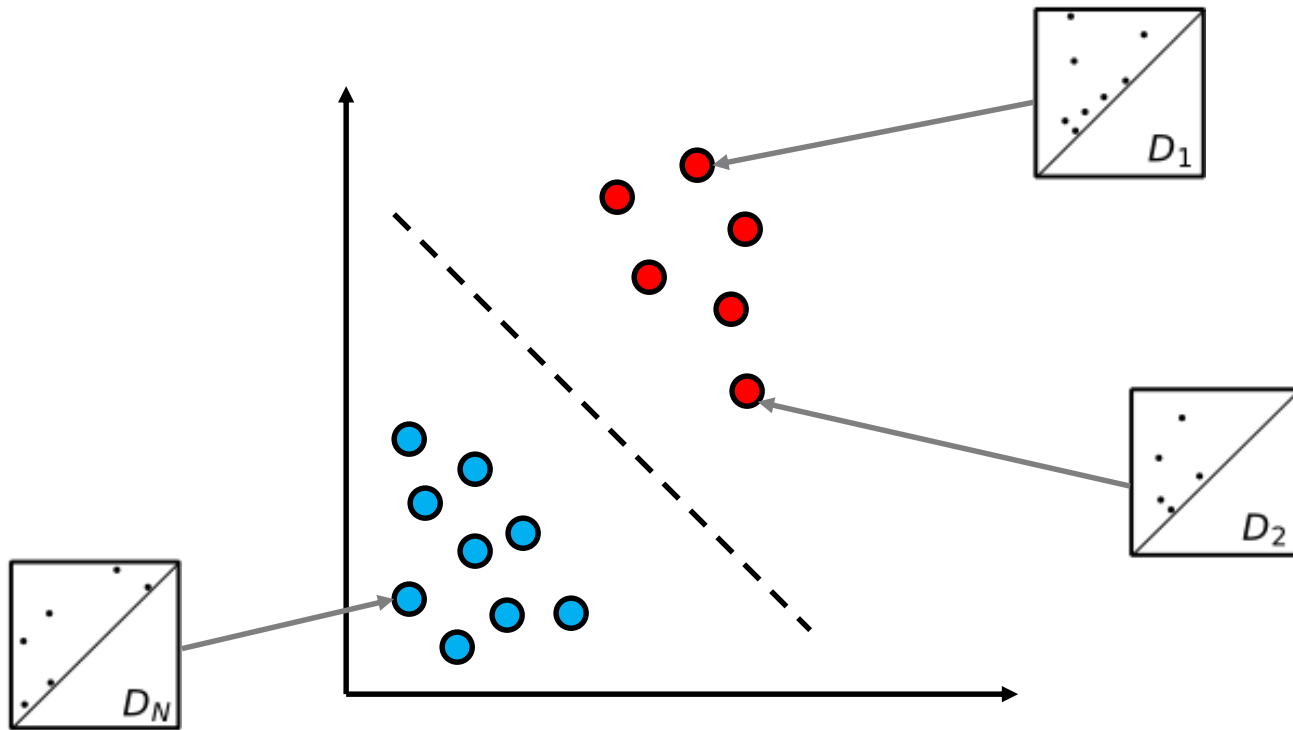
# Topological Machine Learning



# Topological Machine Learning



# Topological Machine Learning



# Kernels

## Definition

Given a set  $\mathcal{X}$ , a function  $k: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  is a **kernel** if there exists a Hilbert space  $\mathcal{H}$ , called **feature space**, and a map  $\Phi: \mathcal{X} \rightarrow \mathcal{H}$ , called **feature map**, such that  $k(x, y) = \langle \Phi(x), \Phi(y) \rangle_{\mathcal{H}}$  for all  $x, y \in \mathcal{X}$ .

(Equivalently:  $k$  is a kernel if it is symmetric and positive definite)



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Kernel induced pseudo-metric on  $\mathcal{X}$ :

$$d_k(x, y) = \sqrt{k(x, x) + k(y, y) - 2k(x, y)} = \|\Phi(x) - \Phi(y)\|_{\mathcal{H}}$$

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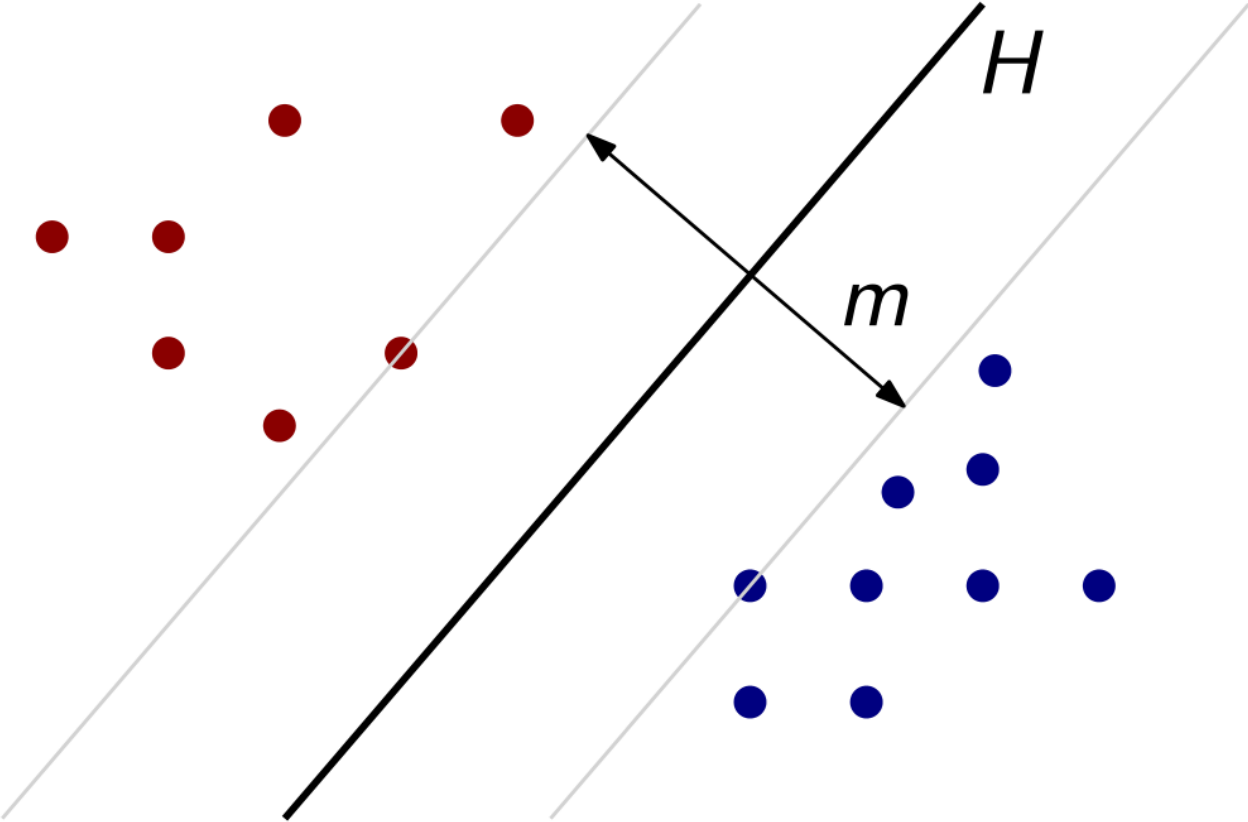
## Definition

We call  $k$  **stable** w.r.t. a metric  $d$  on  $\mathcal{X}$  if there is a constant  $C > 0$  such that

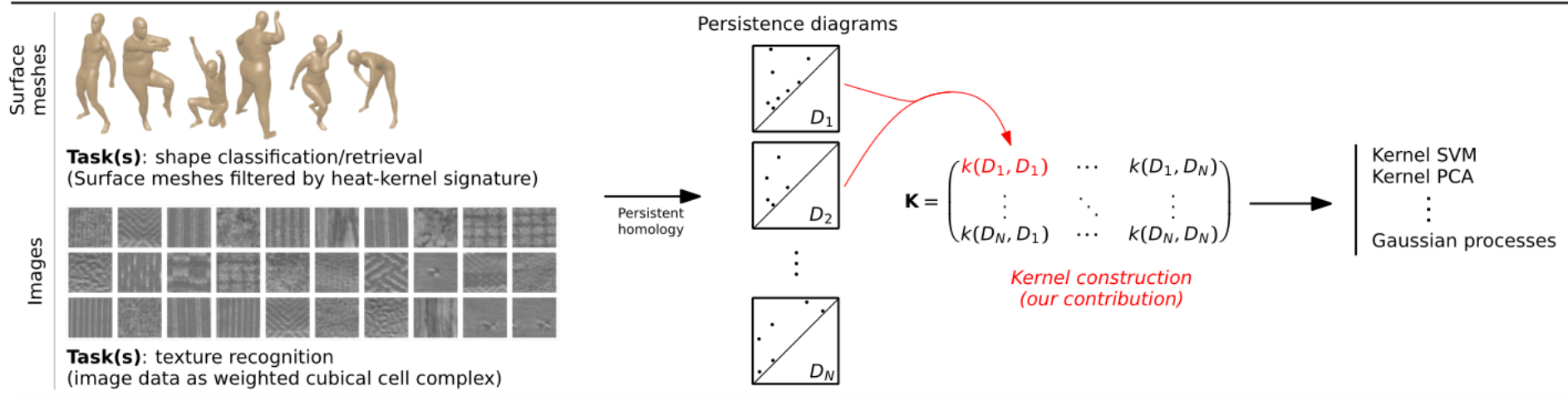
$$d_k(x, y) \leq C d(x, y)$$

(Equivalently:  $k$  is stable if  $\Phi$  is Lipschitz-continuous)

# Why Stability?



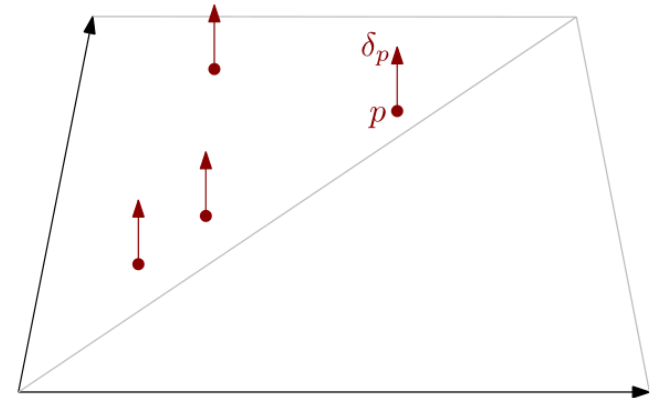
# Basic idea



# An Unstable Kernel

Persistence diagram  $\Leftrightarrow$  multi-set of points in  $\Omega = \{(x_1, x_2) \in \mathbb{R}^2 : x_2 \geq x_1\}$

- Feature map:  $\Phi : \mathcal{D} \rightarrow H^{-2}(\Omega) : D \mapsto \sum_{p \in D} \delta_p$

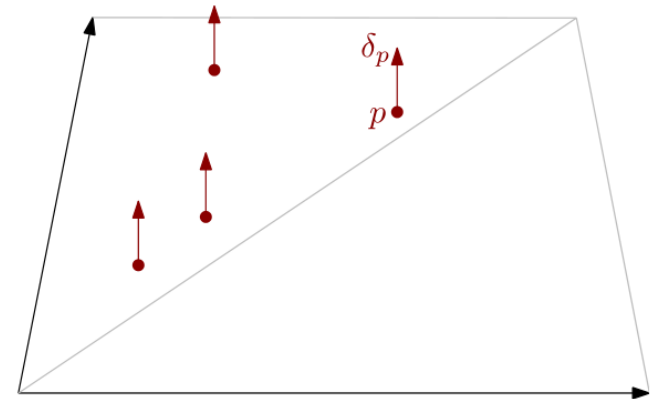


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- Corresponding kernel is not Wasserstein stable

$$d_{W,p}(F, G) = \left( \inf_{\gamma} \sum_{x \in F} \|x - \gamma(x)\|_{\infty}^p \right)^{\frac{1}{p}}$$

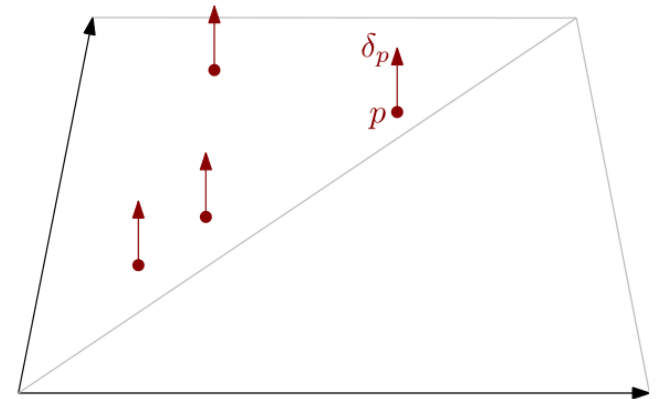


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- Use  $\sum_{p \in D} \delta_p$  as initial condition for diffusion process
- Dirichlet boundary condition  $\rightarrow$  stability

# A Stable Multi-Scale Kernel

## Definition

For a given persistence diagram  $D$ , we consider the solution  $u: \Omega \times \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}, (x, t) \mapsto u(x, t)$  of the partial differential equation

$$\Delta_x u = \partial_t u \quad \text{in } \Omega \times \mathbb{R}_{> 0}, \quad (1)$$

$$u = 0 \quad \text{on } \partial\Omega \times \mathbb{R}_{\geq 0}, \quad (2)$$

$$u = \sum_{p \in D} \delta_p \quad \text{on } \Omega \times \{0\}. \quad (3)$$

The feature map  $\Phi_\sigma: \mathcal{D} \rightarrow L_2(\Omega)$  at scale  $\sigma > 0$  is defined as

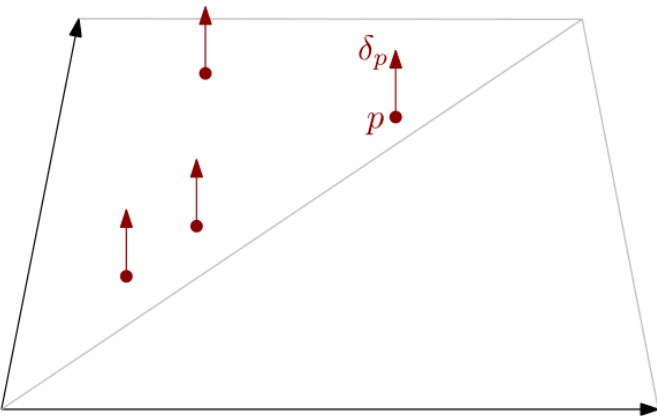
$$\Phi_\sigma(D) = u|_{t=\sigma} \quad (4)$$

This map yields the persistence scale space kernel  $k_\sigma$  on  $\mathcal{D}$  as

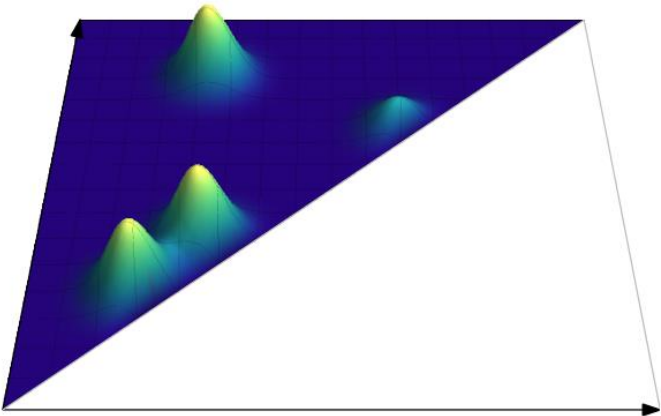
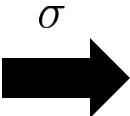
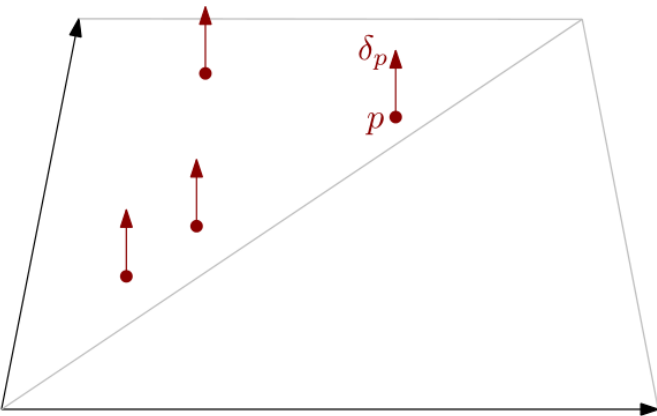
$$k_\sigma(F, G) = \langle \Phi_\sigma(F), \Phi_\sigma(G) \rangle_{L_2(\Omega)}. \quad (5)$$



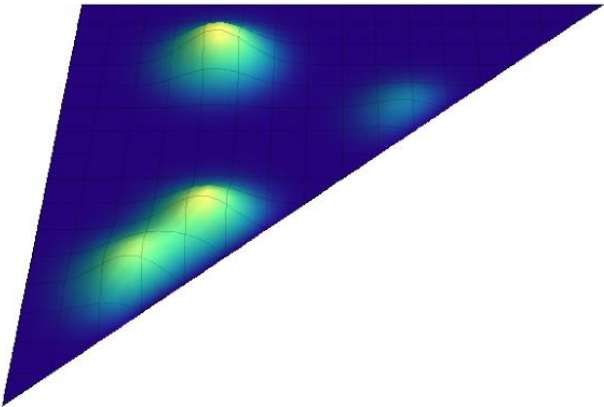
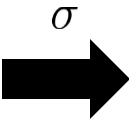
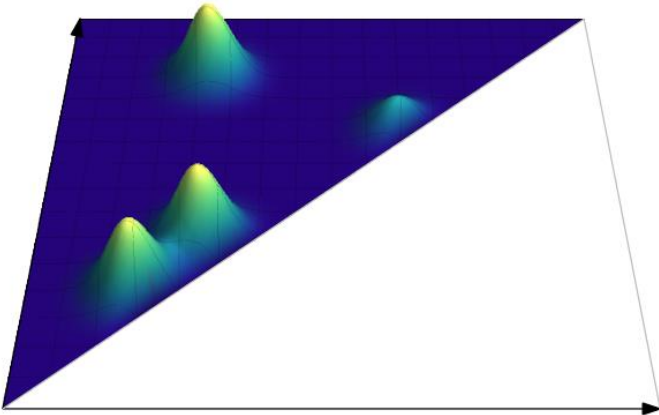
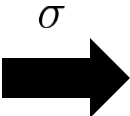
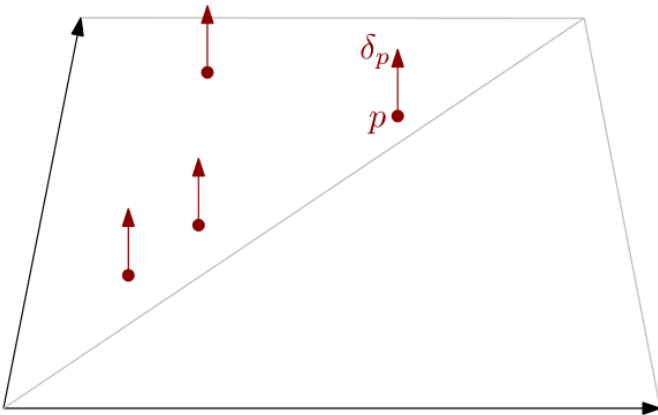
# Example



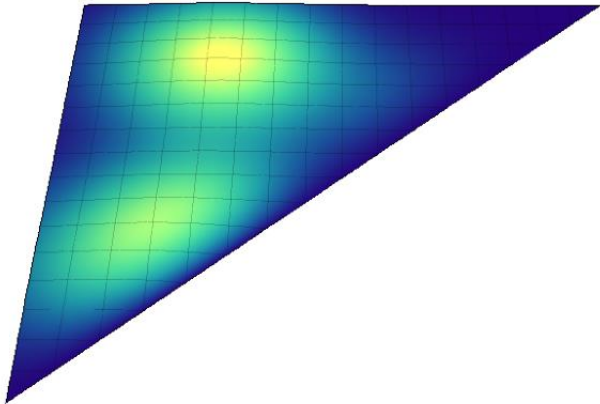
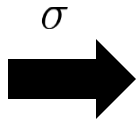
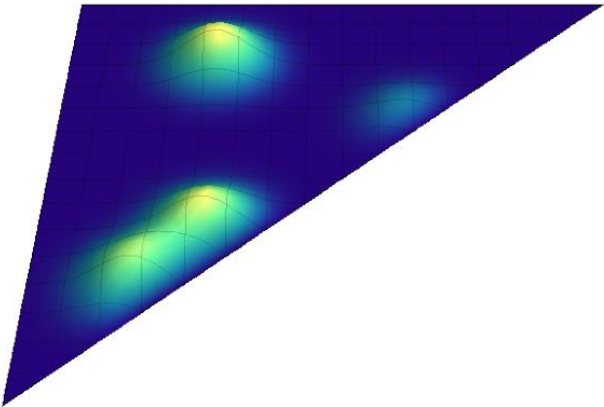
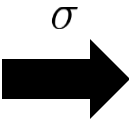
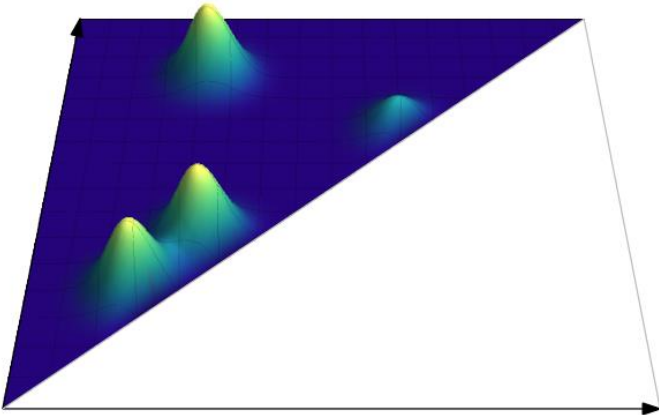
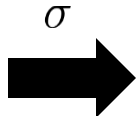
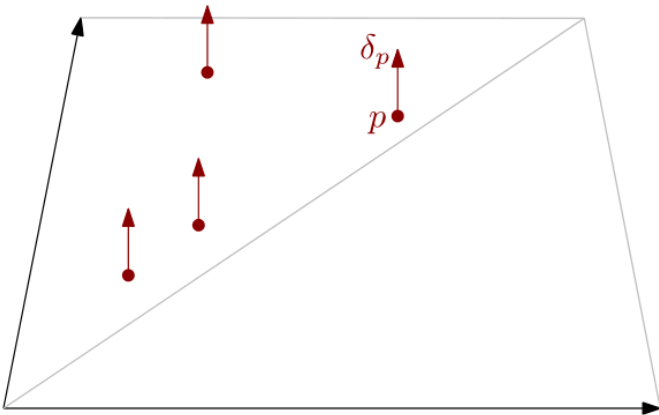
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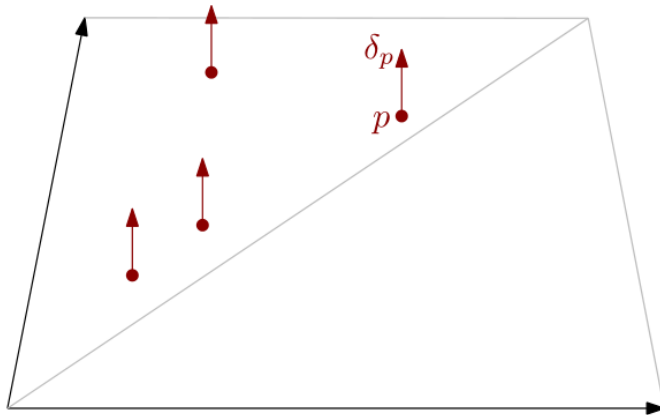
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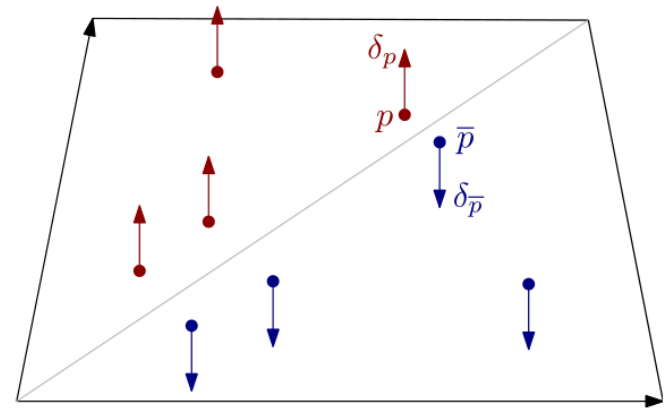
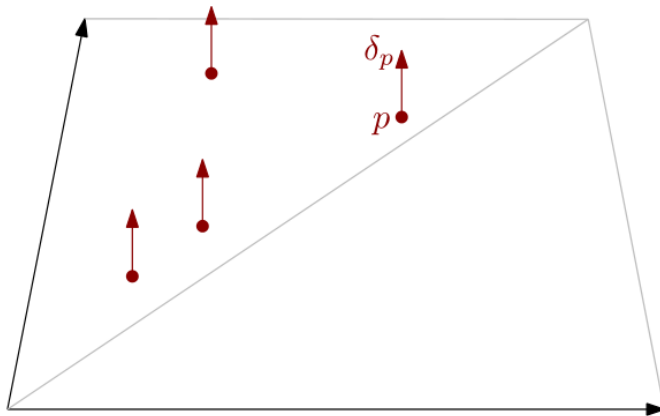
# Example



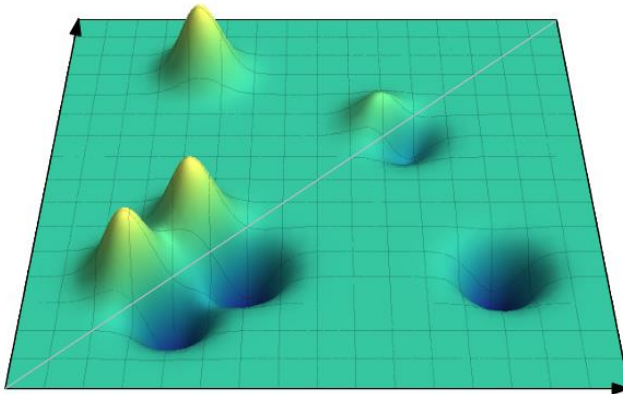
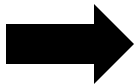
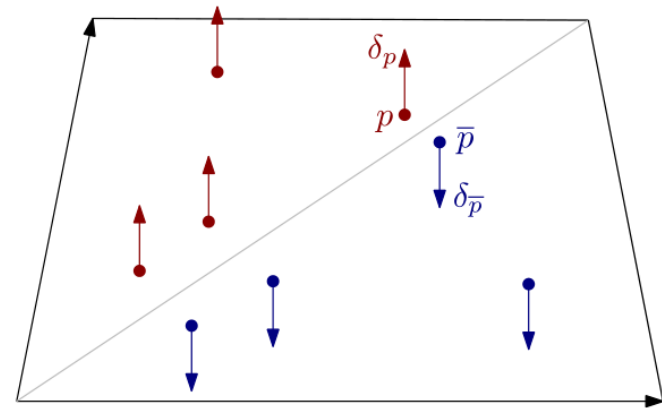
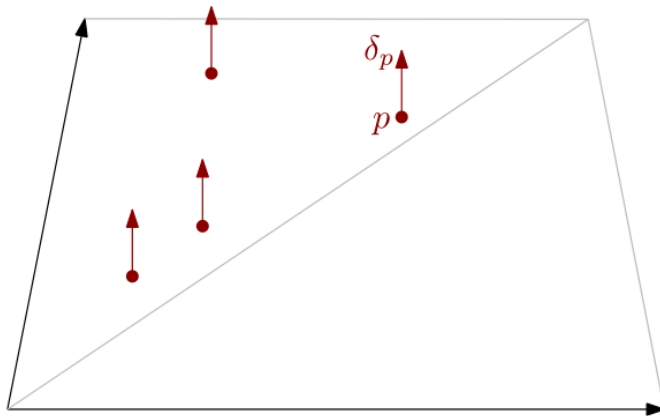
# Analytic Solution



# Analytic Solution

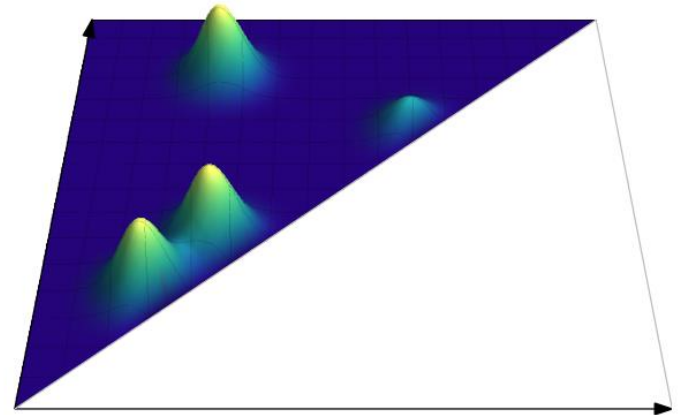
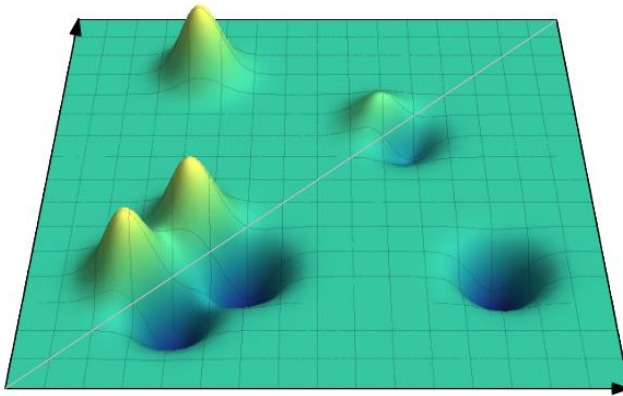
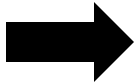
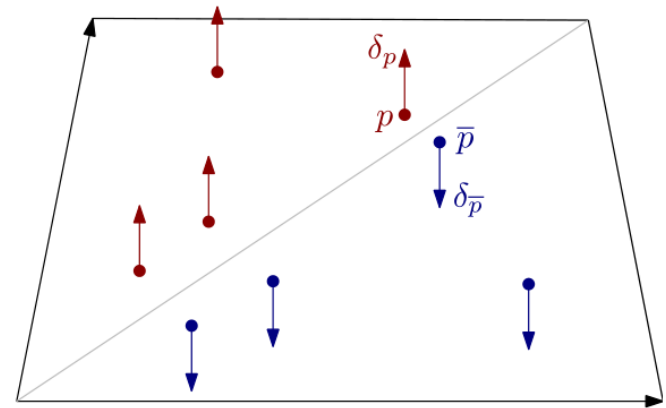
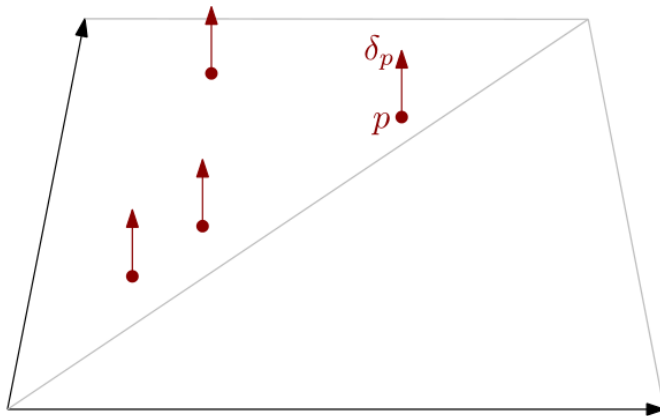


# Analytic Solution



$$u(x, t) = \frac{1}{4\pi t} \sum_{p \in D} e^{-\frac{\|x-p\|^2}{4t}} - e^{-\frac{\|x-\bar{p}\|^2}{4t}}$$

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# Kernel Evaluation

$$\Phi_\sigma(D): \Omega \rightarrow \mathbb{R}, \quad x \mapsto \frac{1}{4\pi\sigma} \sum_{p \in D} e^{-\frac{\|x-p\|^2}{4\sigma}} - e^{-\frac{\|x-\bar{p}\|^2}{4\sigma}} \quad (7)$$

$$\begin{aligned} k_\sigma(F, G) &= \int_{\Omega} \Phi_\sigma(F) \Phi_\sigma(G) dx \\ &= \frac{1}{2} \int_{\mathbb{R}^2} \Phi_\sigma(F) \Phi_\sigma(G) dx \\ &= \frac{1}{2} \frac{1}{(4\pi\sigma)^2} \sum_{\substack{p \in F \\ q \in G}} \int_{\mathbb{R}^2} \left( e^{-\frac{\|x-p\|^2}{4\sigma}} - e^{-\frac{\|x-\bar{p}\|^2}{4\sigma}} \right) \cdot \left( e^{-\frac{\|x-q\|^2}{4\sigma}} - e^{-\frac{\|x-\bar{q}\|^2}{4\sigma}} \right) dx \\ &= \frac{1}{8\pi\sigma} \sum_{\substack{p \in F \\ q \in G}} e^{-\frac{\|p-q\|^2}{8\sigma}} - e^{-\frac{\|p-\bar{q}\|^2}{8\sigma}}. \end{aligned}$$

# 1-Wasserstein Stability

## Theorem

*The kernel  $k_\sigma$  is 1-Wasserstein stable.*

Proof:

$$\begin{aligned} & \|\Phi_\sigma(F) - \Phi_\sigma(G)\|_{L_2(\Omega)} \\ & \leq \left\| \sum_{u \in F} (N_u - N_{\bar{u}}) - (N_{\gamma(u)} - N_{\overline{\gamma(u)}}) \right\|_{L_2(\mathbb{R}^2)} \\ & \leq 2 \sum_{u \in F} \|N_u - N_{\gamma(u)}\|_{L_2(\mathbb{R}^2)} \\ & \leq \frac{1}{\sigma\sqrt{8\pi}} \sum_{u \in F} \|u - \gamma(u)\|_2 \\ & \leq \frac{1}{2\sigma\sqrt{\pi}} \sum_{u \in F} \|u - \gamma(u)\|_\infty \\ & = \frac{1}{2\sigma\sqrt{\pi}} d_{W,1}(F, G) \end{aligned}$$

# p-Wasserstein Stability

- A kernel  $k$  is **additive** if  $k(E \cup F, G) = k(E, G) + k(F, G)$
- A kernel  $k$  is **non-trivial** if there exists  $F, G$  s.t.  $k(F, G) \neq 0$

## Theorem

*A non-trivial additive kernel  $k$  on  $\mathcal{D}$  is not stable w.r.t.  $d_{W,p}$  for any  $1 < p \leq \infty$ .*

Proof: Compare rates of growth:

$$d_{k_\sigma} \left( \bigcup_{i=1}^n F, \emptyset \right) = n \sqrt{k(F, F)}$$
$$d_{W,p} \left( \bigcup_{i=1}^n F, \emptyset \right) = d_{W,p}(F, \emptyset) \cdot \begin{cases} \sqrt[p]{n} & \text{if } p < \infty, \\ 1 & \text{if } p = \infty \end{cases}$$

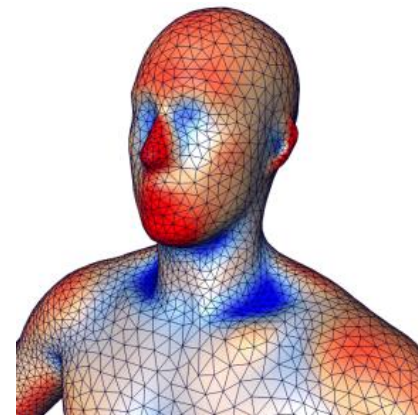
# Numerical Experiments – Shapes

SHREC 2014 real: 400 meshes from 40 humans in 10 different poses

Filtration: Heat Kernel Signature



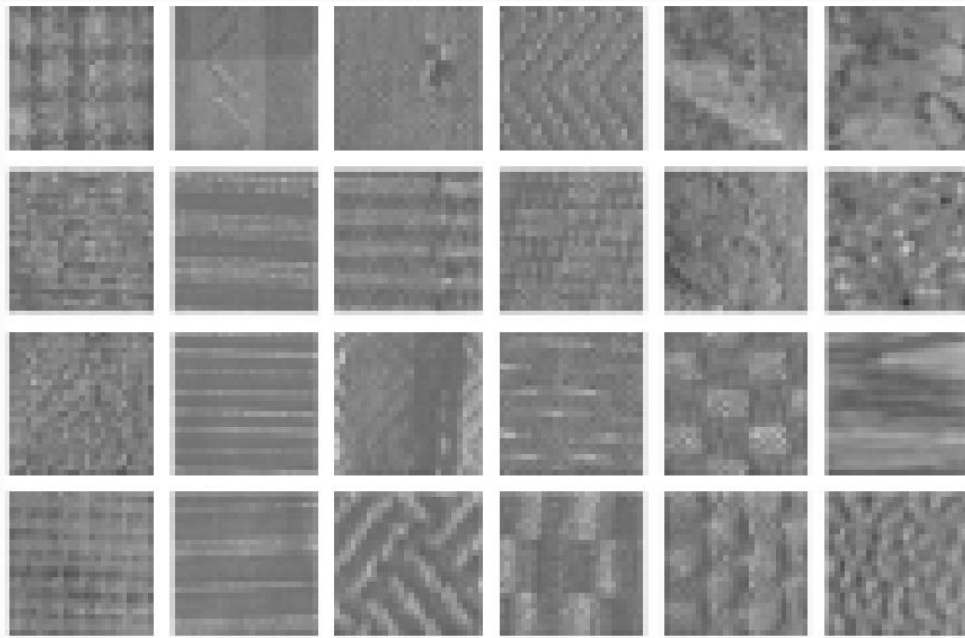
HKS $t_i$	$k^L$	$k_\sigma$	$\Delta$
$t_1$	$45.2 \pm 5.8$	$48.8 \pm 4.9$	+3.5
$t_2$	$31.0 \pm 4.8$	$46.5 \pm 5.3$	+15.5
$t_3$	$30.0 \pm 7.3$	$37.8 \pm 8.2$	+7.8
$t_4$	$41.2 \pm 2.2$	$50.2 \pm 5.4$	+9.0
$t_5$	$46.2 \pm 5.8$	$62.5 \pm 2.0$	+16.2
$t_6$	$33.2 \pm 4.1$	$58.0 \pm 4.0$	+24.7
$t_7$	$31.0 \pm 5.7$	<b><math>62.7 \pm 4.6</math></b>	+31.7
$t_8$	<b><math>51.7 \pm 2.9</math></b>	$57.5 \pm 4.2$	+5.8
$t_9$	$36.0 \pm 5.3$	$41.2 \pm 4.9$	+5.2
$t_{10}$	$2.8 \pm 0.6$	$27.8 \pm 5.8$	+25.0



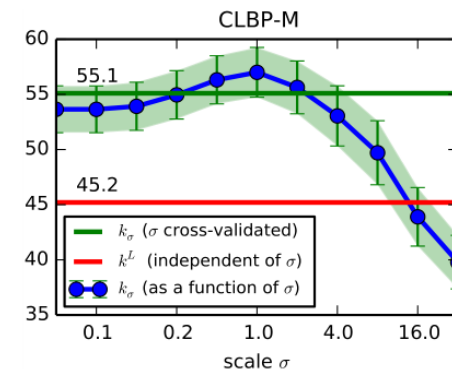
# Numerical Experiments – Textures

Outex-TC-00000: 240 textures (24 classes, 10 samples each)

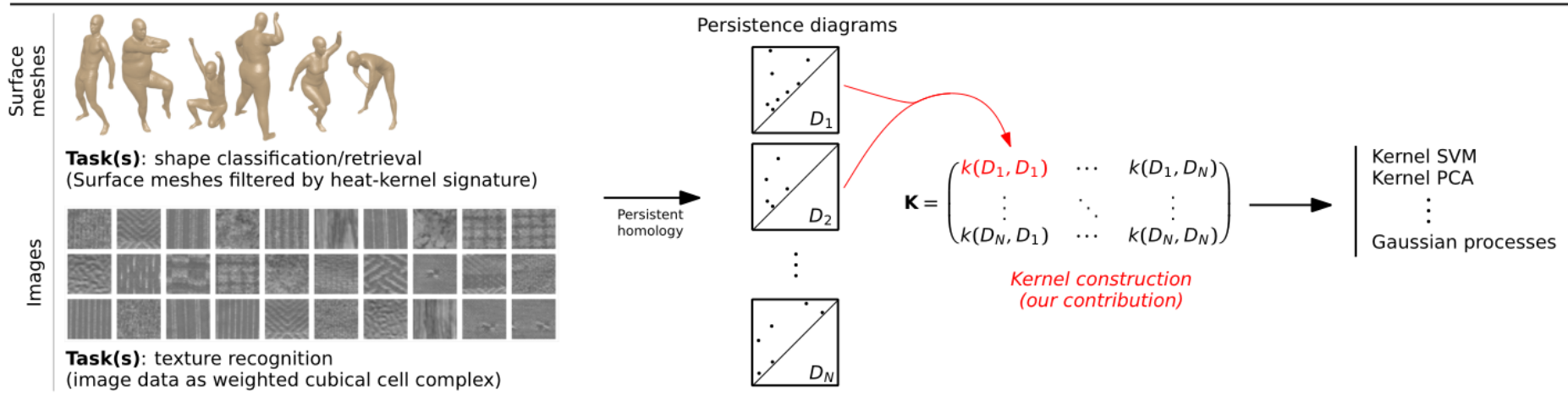
Filtration: Complete-Local-Binary-Pattern filter



CLBP Operator	$k^L$	$k_\sigma$	$\Delta$
CLBP-S	$58.0 \pm 2.3$	<b><math>69.2 \pm 2.7</math></b>	+11.2
CLBP-M	$45.2 \pm 2.5$	<b><math>55.1 \pm 2.5</math></b>	+9.9
CLBP-S (SVM- $\chi^2$ )		$76.1 \pm 2.2$	
CLBP-M (SVM- $\chi^2$ )		$76.7 \pm 1.8$	



# Part 4: Conclusion



$$k_\sigma(F, G) = \frac{1}{8\pi\sigma} \sum_{\substack{p \in F \\ q \in G}} e^{-\frac{\|p-q\|^2}{8\sigma}} - e^{-\frac{\|p-\bar{q}\|^2}{8\sigma}},$$

- Exact evaluation in  $O(n^2)$
- Approximate evaluation in  $O(n)$

# Summary

- Part 1: Phat – fast matrix reduction algorithms: [phat@github](#)
- Part 2: Dipha – distributed computation: [dipha@github](#)
- Part 3: Discrete Morse theory – large image data
- Part 4: A kernel for topological machine learning