Applications of continuous and discrete Mathematical Programming to Transmission Electron Microscopy.

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Reunión de conclusión del proyecto MTM2016 y seguimiento de BBVA

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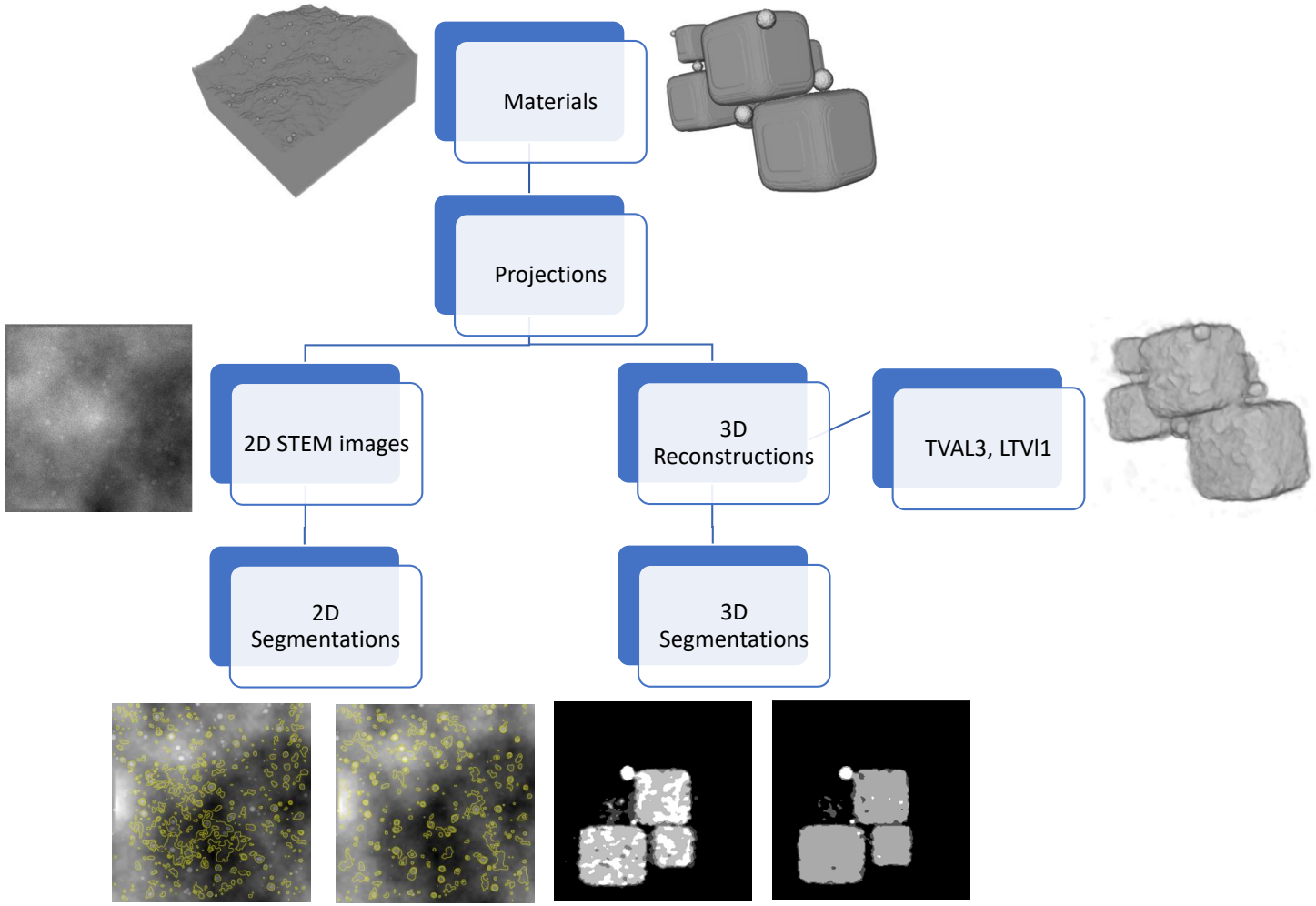
Using the ℓ_1-norm for Image-based Tomographic Reconstruction. *Expert Systems with Applications.*

J.J. Calvino, M. López-Haro, J.M. Muñoz-Ocaña, J. Puerto, A.M. Rodríguez-Chía. (2021)
Segmentation of Scanning-Transmission Electron Microscopy Images using Ordered Median Problem. *European Journal of Operational Research.*

Electron Tomography and STEM images



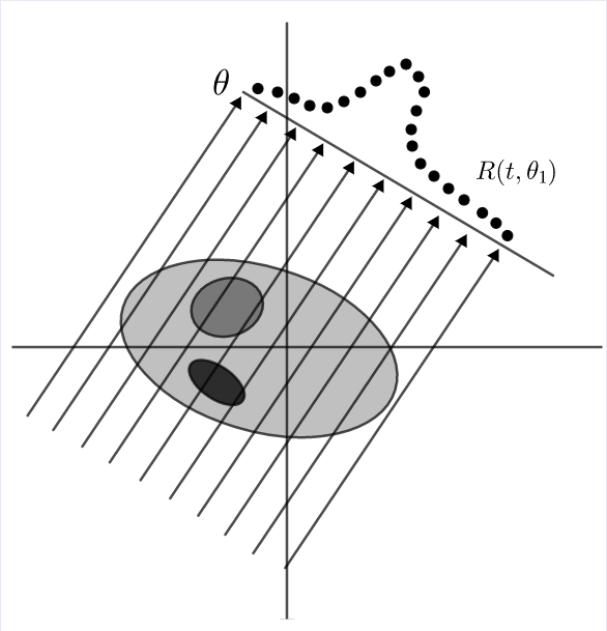
Basic concepts

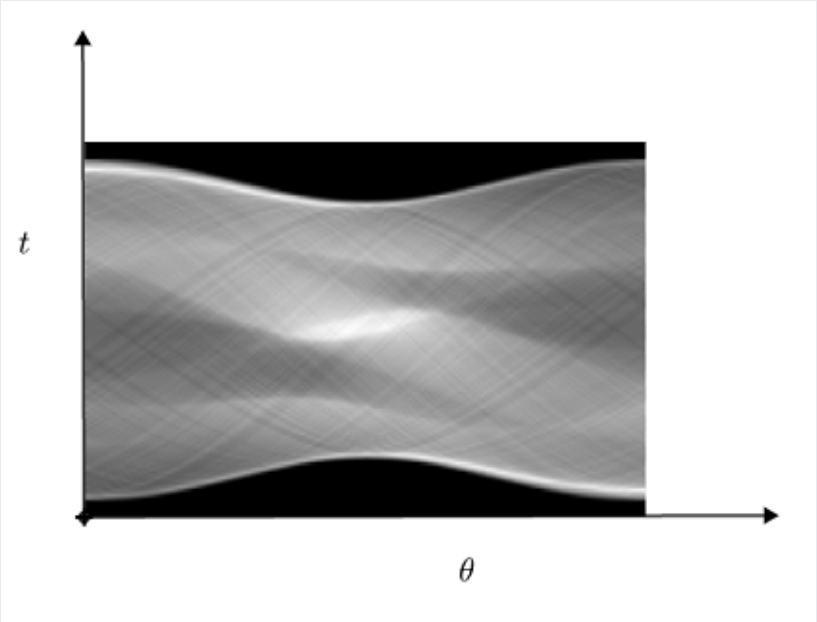
- We will work with images (2D) and volumes (3D) which are made of pixels or voxels.
- $f(x, y) \in [0, 1]$ contains the information about the intensity of each pixel x.
- A gray scale is used to show the pixel intensities in a visual way.

- Projections.

Projections

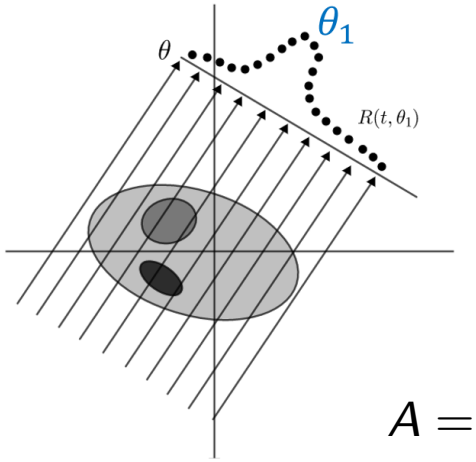
Sinogram





Projection Matrix

We suppose we have an image which is made of N pixels, k projections recover with p electron beams each one.

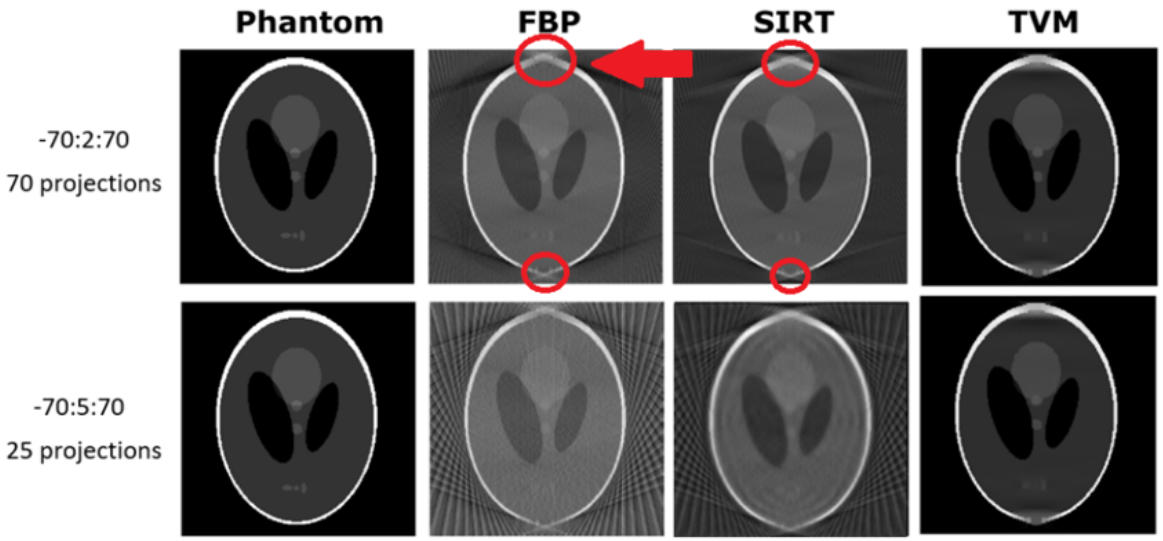


$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,N} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p,1} & a_{p,2} & \cdots & a_{p,N} \\ a_{p+1,1} & a_{p+1,2} & \cdots & a_{p+1,N} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p+p,1} & a_{p+p,2} & \cdots & a_{p+p,N} \\ \vdots & \vdots & \ddots & \vdots \\ a_{(k-1)p+1,1} & a_{(k-1)p+1,2} & \cdots & a_{(k-1)p+1,N} \\ \vdots & \vdots & \ddots & \vdots \\ a_{kp,1} & a_{kp,2} & \cdots & a_{kp,N} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix} = \begin{bmatrix} b_{\theta_1 1} \\ b_{\theta_1 2} \\ \vdots \\ b_{\theta_1 p} \\ \vdots \\ b_{\theta_2 1} \\ \vdots \\ b_{\theta_2 p} \\ \vdots \\ b_{\theta_k 1} \\ \vdots \\ b_{\theta_k p} \end{bmatrix}$$

Models

Reconstruction models

- Analytical models (Fourier Transform)(Filtered Back Projection).
- Algebraic models (ART, SIRT, Cimmino).
- Compressed sensing models (Total Variation).



Total Variation model

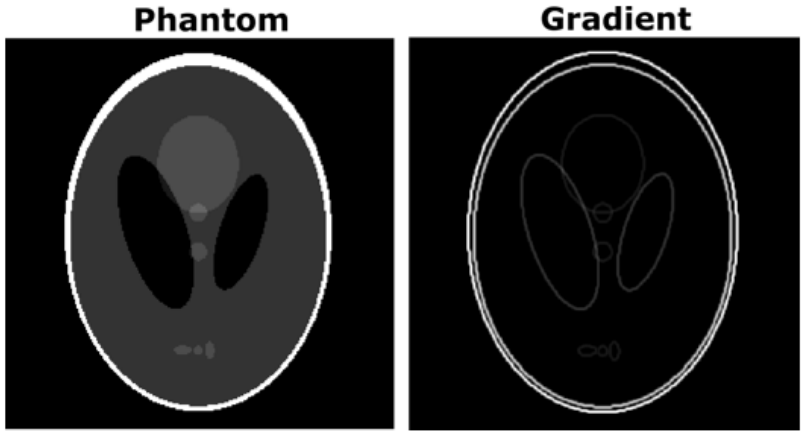
Total Variation model, which minimizes the gradient of the image, can be written as

$$\min_x \sum_i ||D_i x||_2, \quad s.t. \quad Ax = b,$$

where

- x is the image we are reconstructing.
- b is the original sinogram.
- D_i calculates the gradient of x at pixel i which is obtained as follow:

$$(x_i - x_{i+1}, x_i - x_{n+i}).$$



ℓ_1-norm minimization

$$(\mathrm{LTV}_{\ell_1}) \quad \min_x \sum_i (||D_i x||_1) + \frac{\mu}{2}||Ax - b||_1$$

ℓ_1-norm minimization

$$(\mathrm{LTV}_{\ell_1}) \quad \min_x \sum_i (||D_i x||_1) + \frac{\mu}{2}||Ax - b||_1$$

Resolution procedure

- Linearization of the model
  Variables: 3206471 $(x, z^+, z^-, h^+, h^-, v^+, v^-)$
  Constraints: 2116607 for 1024×1024 pixels and 8 projections.

ℓ_1-norm minimization

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- Complementary slackness conditions $\Rightarrow$ Fixing variables.

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- Complementary slackness conditions ⇒ Fixing variables.
- Lagrangian dual to obtain primal and dual variables.
  Subgradient and Volume (Barahona and Anbil, 2000)

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Resolution procedure

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- Complementary slackness conditions $\Rightarrow$ Fixing variables.
- Lagrangian dual to obtain primal and dual variables.
  Subgradient and Volume (Barahona and Anbil, 2000)
- Reduced formulation R-LTV_{ℓ_1}.

Linearization of the model

$$
\begin{array}{llll}
(\mathrm{LTV}_{\ell_1}) & \min & \mu \sum_{\theta} (z_\theta^+ + z_\theta^-) + \beta \sum_i (h_i^+ + h_i^- + v_i^+ + v_i^-) & \\
& \text{s.t.} & A_\theta x - b_\theta = z_\theta^+ - z_\theta^-, & \theta = 1, \ldots, p \cdot n \\
& & x_i - x_{i+1} = h_i^+ - h_i^-, & i = 1, \ldots, n^2 \\
& & x_i - x_{i+n} = v_i^+ - v_i^-, & i = 1, \ldots, n^2 \\
& & z_\theta \geq 0, & \theta = 1, \ldots, p \cdot n \\
& & 0 \leq x_i, h_i^+, h_i^-, v_i^+, v_i^- \leq 1, & i = 1, \ldots, n^2
\end{array}
$$

Complementary slackness conditions

$$z^+_{\theta,k}(\frac{\mu}{2} + \tau_{\theta,k}) = 0, \qquad \theta \in \Theta,\ k \in K,$$

$$z^-_{\theta,k}(\frac{\mu}{2} - \tau_{\theta,k}) = 0, \qquad \theta \in \Theta,\ k \in K,$$

$$h^+_i(1 - \alpha_i) = 0, \qquad i \in I^h,$$

$$h^-_i(1 + \alpha_i) = 0, \qquad i \in I^h,$$

$$v^+_i(1 - \delta_i) = 0, \qquad i \in I^v,$$

$$v^-_i(1 + \delta_i) = 0, \qquad i \in I^v.$$

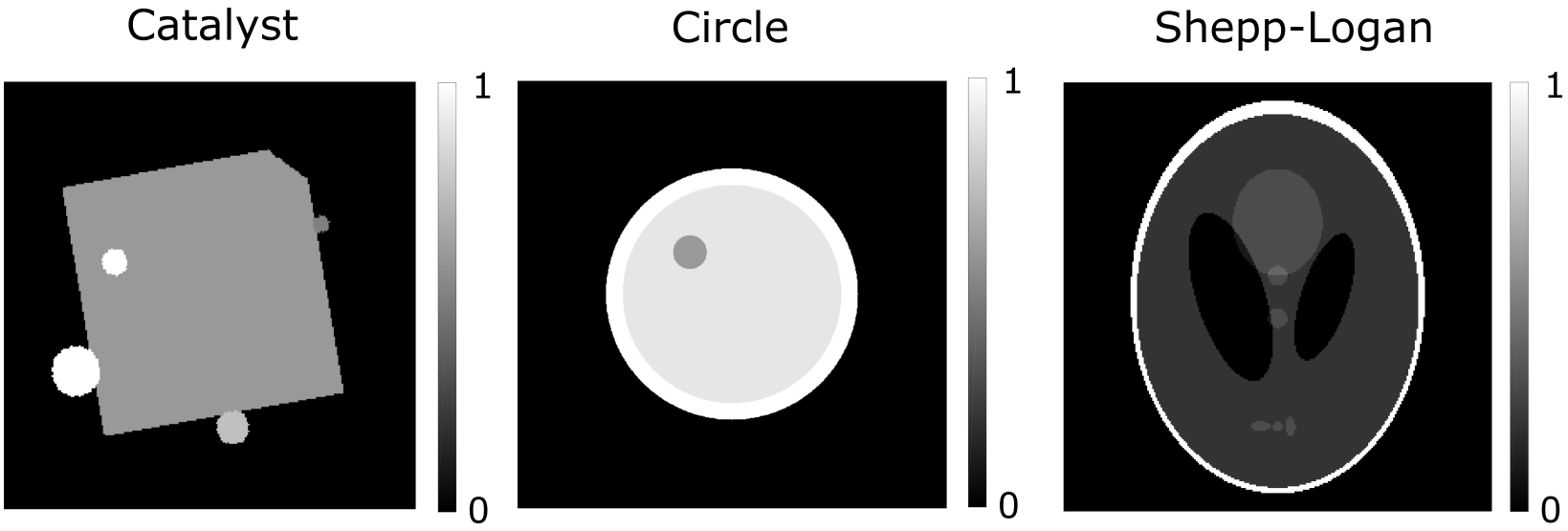
$$\tau_{\theta,k}(A_{\theta,k}x - z^+_{\theta,k} + z^-_{\theta,k} - b_{\theta,k}) = 0, \qquad \theta \in \Theta,\ k \in K,$$

$$\alpha_i(x_i - x_{i+1} - h^+_i + h^-_i) = 0, \qquad i \in I^h,$$

$$\delta_i(x_i - x_{i+n} - v^+_i + v^-_i) = 0, \qquad i \in I^v.$$

- $|1 - \alpha_i| > \varepsilon$ y $|1 + \alpha_i| > \varepsilon \Rightarrow h^+_i = h^-_i = 0$, i.e., $x_i = x_{i+1}$.
- $|1 - \delta_i| > \varepsilon$ y $|1 + \delta_i| > \varepsilon \Rightarrow v^+_i = v^-_i = 0$, i.e., $x_i = x_{i+n}$.

Phantoms

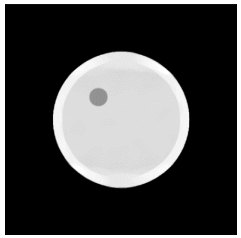
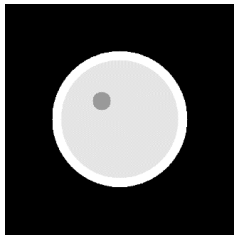
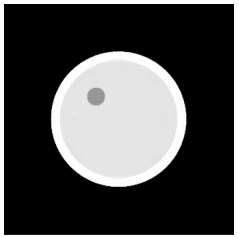
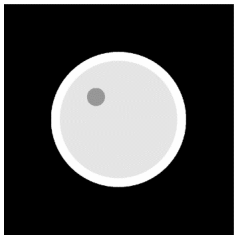


	Size		TVM_{ROF}	LTV_{ℓ_1}		R-LTV_{ℓ_1}			
						$\varepsilon = 0.625$		$\varepsilon = 0.9375$	
		μ	Error	Error	Time (s)	Error	Time (s)	Error	Time (s)
Catalyst 20°	512×512	2^7	2.9506	0.0026	208.4	3.9048	61.6	0.6765	99.0
		2^{10}	2.4749	0.0759	178.3	4.1199	68.9	0.1278	97.8
	1024×1024	2^2	9.1736	0.0103	1412.4	6.1456	293.5	1.3925	838.9
		2^9	4.2832	0.0167	1704.5	8.9550	338.3	2.1799	1021.8
Circle 20°	512×512	2^4	10.1022	0.0026	138.1	2.4378	43.0	1.5052	60.8
		2^8	8.5764	0.0102	156.9	2.4050	43.8	0.4105	62.9
	1024×1024	2^3	22.9713	0.0161	1179.5	4.0110	192.1	1.1360	346.1
		2^9	15.3521	2.0638	2230.9	8.9013	179.5	2.1711	648.7
Shepp-Logan 20°	512×512	2^{11}	42.0587	33.5665	305.2	37.1811	99.0	34.0079	184.0
		2^7	38.7823	33.9012	380.6	37.1757	78.3	34.0633	156.4
	1024×1024	2^8	77.1798	67.8608	1928.9	83.2911	620.6	68.9473	1074.3
		2^6	76.9172	67.9078	1920.4	77.3609	757.3	69.0492	1490.1
3D particle 20°	512×512	2^{13}	997.3568	941.2781	50583.8	948.3910	46019.5	946.2156	48042.3
		2^9	958.1982	946.4871	72610.3	946.5640	30570.4	948.7411	43261.3

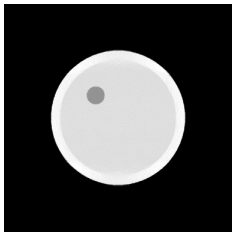
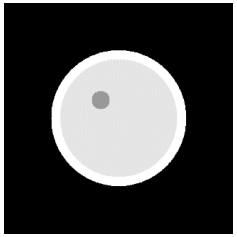
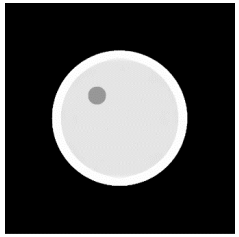
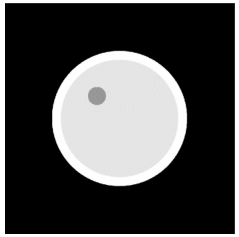
Table: Best computational results obtained with different values of parameter μ. Projections recorded from $-70°$ to $70°$ every $20°$.

Circle

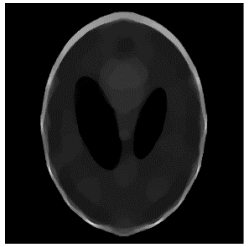
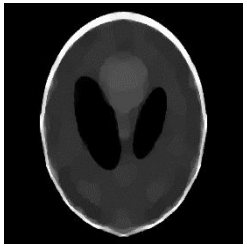
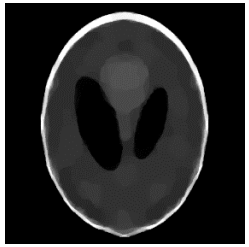
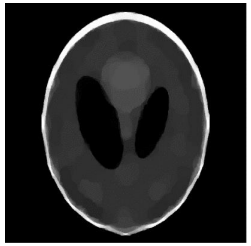
$\mu_{\mathrm{LTV}_{\ell_1}} = 2^3$

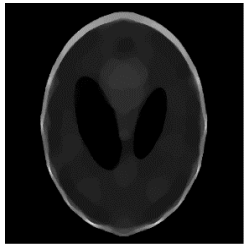
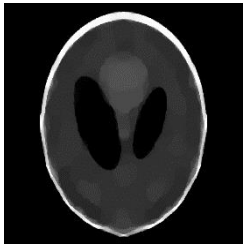
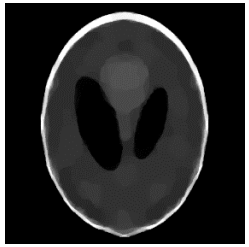
TVM_{ROF}	LTV_{ℓ_1}	$\mathrm{R\text{-}LTV}_{\ell_1}$-3	
			
||Rec-P||=22.9713	||Rec-P||=0.0161	||Rec-P||=4.0110	||Rec-P||=1.1360
		ε=0.625	ε=0.9375
1179.5 s	1179.5 s	98.3+97.6 s	98.3+247.8 s

$\mu_{TVM_{ROF}} = 2^9$

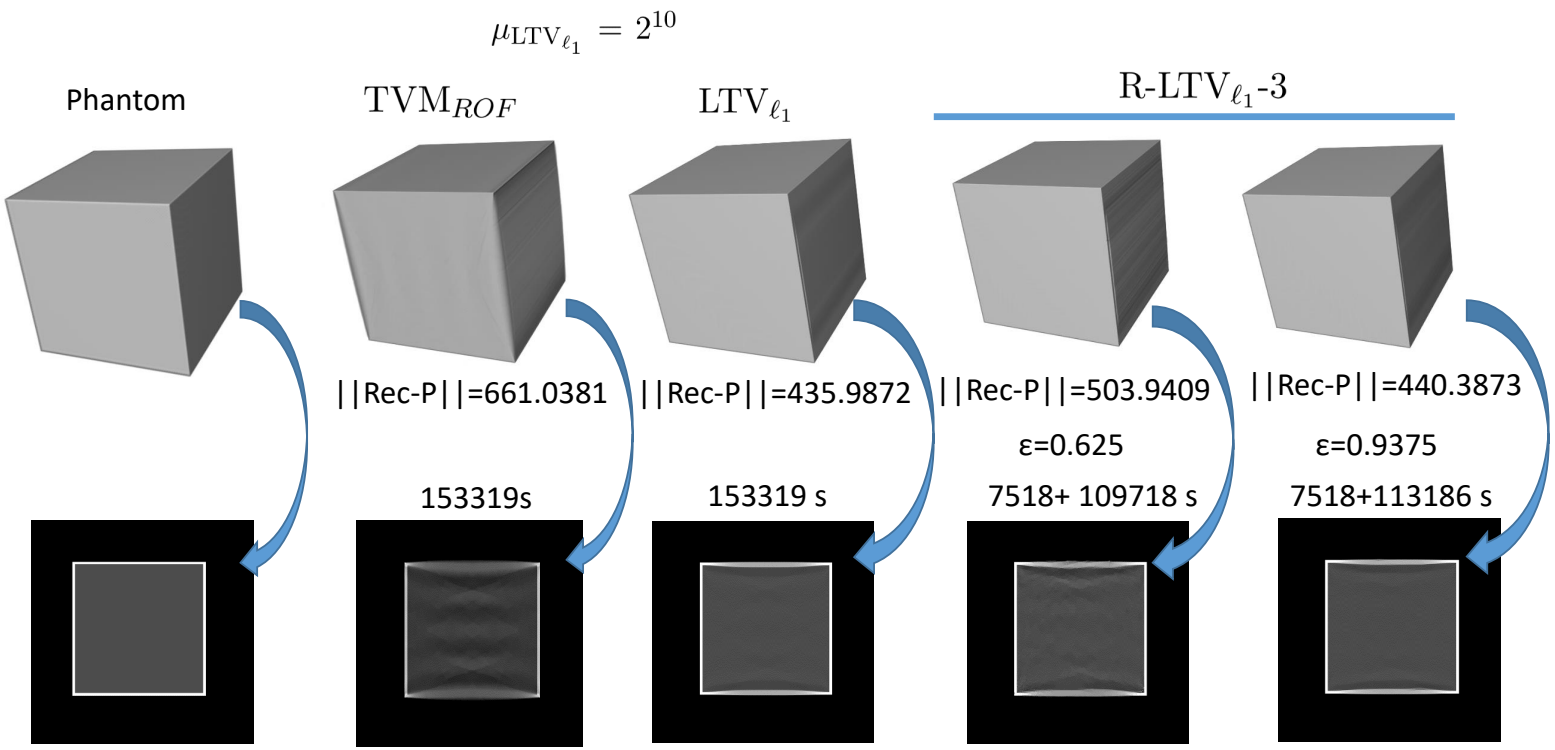
TVM_{ROF}	LTV_{ℓ_1}	$\mathrm{R\text{-}LTV}_{\ell_1}$-3	
			
||Rec-P||=15.3521	||Rec-P||=2.0638	||Rec-P||=8.9013	||Rec-P||=2.1711
		ε=0.625	ε=0.9375
2230.9 s	2230.9 s	100.5+79 s	100.5+548 s

Shepp-Logan

	TVM_{ROF}	LTV_{ℓ_1}	$\mathrm{R\text{-}LTV}_{\ell_1}$-3	
$\mu_{\mathrm{LTV}_{\ell_1}} = 2^8$				
	‖Rec-P‖=77.1798	‖Rec-P‖=67.8608	‖Rec-P‖=83.2911	‖Rec-P‖=68.9473
			ε=0.625	ε=0.9375
	1928.9 s	1928.9 s	99.4+512.2 s	99.4 + 974.9 s

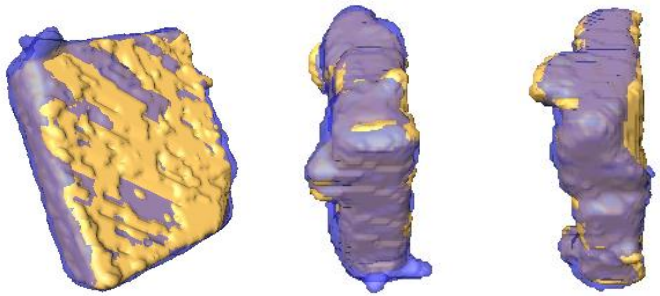
	TVM_{ROF}	LTV_{ℓ_1}	$\mathrm{R\text{-}LTV}_{\ell_1}$-3	
$\mu_{TVM_{ROF}} = 2^6$				
	‖Rec-P‖=76.9172	‖Rec-P‖=67.9078	‖Rec-P‖=77.3609	‖Rec-P‖=69.0492
			ε=0.625	ε=0.9375
	1920.4 s	1920.2 s	97.2+660.1 s	97.2 + 1392.1 s

Cube

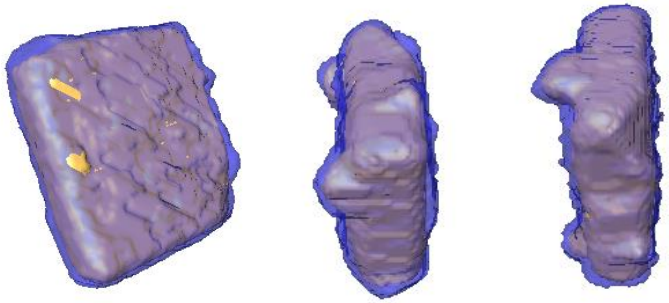

$\mu_{\mathrm{LTV}_{\ell_1}} = 2^{10}$
Phantom
TVM_{ROF}
LTV_{ℓ_1}
R-LTV_{ℓ_1}-3
||Rec-P||=661.0381
||Rec-P||=435.9872
||Rec-P||=503.9409
||Rec-P||=440.3873
ε=0.625
ε=0.9375
153319s
153319 s
7518+ 109718 s
7518+113186 s

Experiment

TVM_{ROF}
$\mu_{\mathrm{TVM}_{ROF}} = 2^2$



LTV_{ℓ_1}
$\mu_{\mathrm{LTV}_{\ell_1}} = 0.5$



R-LTV_{ℓ_1}-3 $\mu_{\mathrm{LTV}_{\ell_1}} = 0.5$
$\varepsilon = 0.9375$

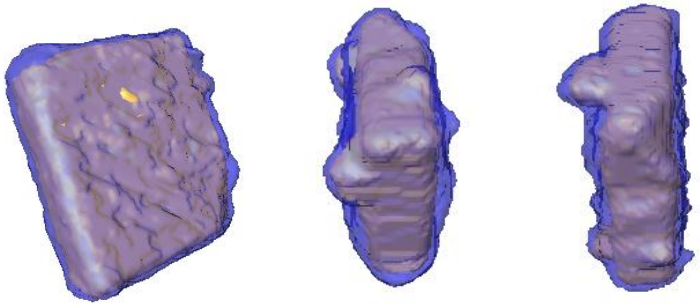


Image segmentation

Segmentation

Segmentation subdivides an image into its constituent regions or objects. The level to which the subdivision is carried depends on the problem being solved.

How are the images segmented?

Segmentation techniques are applied on **STEM images** (2D projections) and **electron tomography reconstructions** (3D projections) .

Segmentation of nontrivial images is one of the most difficult tasks in image processing.
Segmentation accuracy determines the eventual success or failure of computerized analysis procedures.

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Image segmentations

1	1	1	1	1	1	1	2	1	1
2	1	3	2	2	2	2	2	1	1
2	1	1	2	2	3	3	3	3	2
2	2	2	3	3	4	4	2	2	2
1	1	2	3	4	4	5	5	5	4
3	3	4	4	4	5	5	4	3	3
2	2	2	3	3	3	4	4	3	1
1	1	1	2	2	1	1	1	1	1

1	2	3	4	5
25	23	16	11	5
ω_1	ω_2	ω_3	ω_4	ω_5

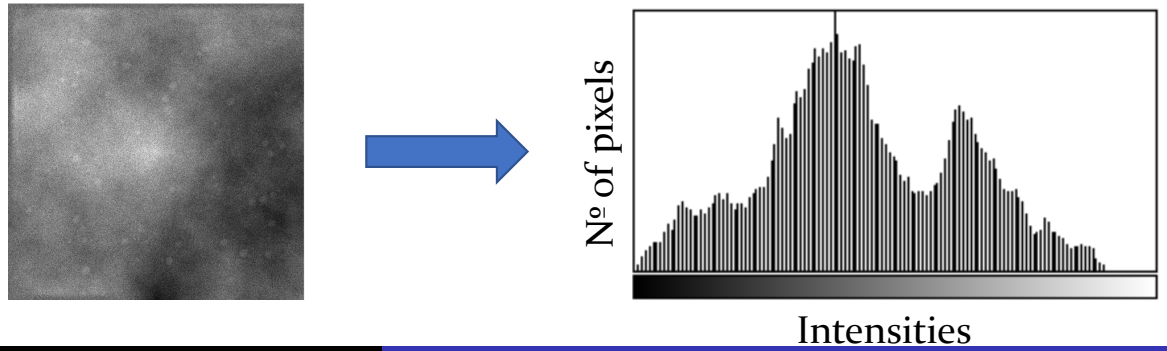


Image segmentations

1	1	1	1	1	1	1	2	1	1
2	1	3	2	2	2	2	2	1	1
2	1	1	2	2	3	3	3	3	2
2	2	2	3	3	4	4	2	2	2
1	1	2	3	4	4	5	5	5	4
3	3	4	4	4	5	5	4	3	3
2	2	2	3	3	3	4	4	3	1
1	1	1	2	2	1	1	1	1	1

1	2	3	4	5
25	23	16	11	5
ω_1	ω_2	ω_3	ω_4	ω_5

1. Selecting p intensities j which will be the representative of cluster at position j

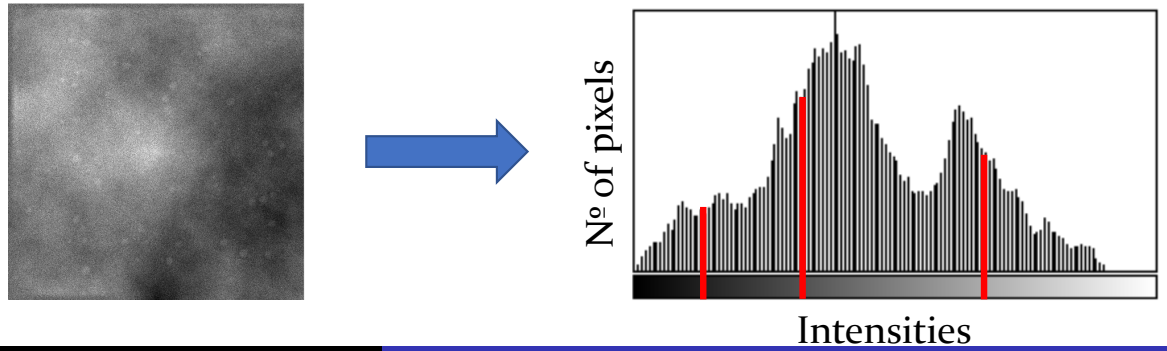


Image segmentations

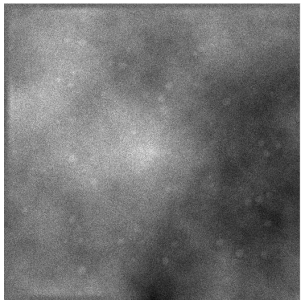
1	1	1	1	1	1	1	2	1	1
2	1	3	2	2	2	2	2	1	1
2	1	1	2	2	3	3	3	3	2
2	2	2	3	3	4	4	2	2	2
1	1	2	3	4	4	5	5	5	4
3	3	4	4	4	5	5	4	3	3
2	2	2	3	3	3	4	4	3	1
1	1	1	2	2	1	1	1	1	1

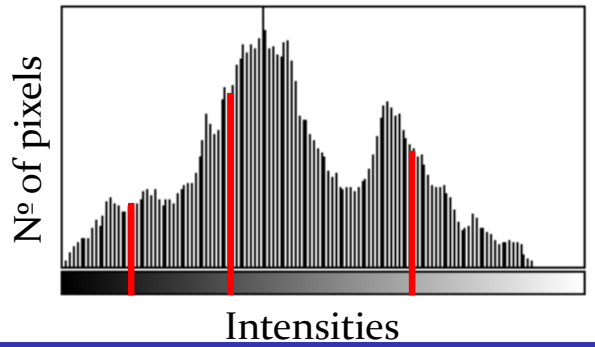
1	2	3	4	5
25	23	16	11	5
ω_1	ω_2	ω_3	ω_4	ω_5

1. Selecting p intensities j which will be the representative of cluster at position j
2. Allocating every intensity to one cluster by minimizing the allocation cost

$$d_{ij} = |i - j|$$

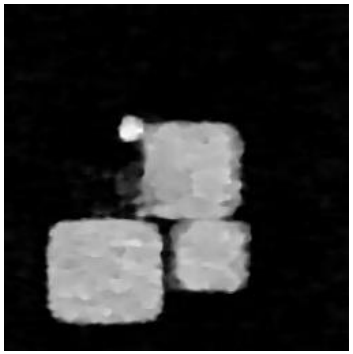
$$\omega_{ij} = d_{ij}\omega_i$$



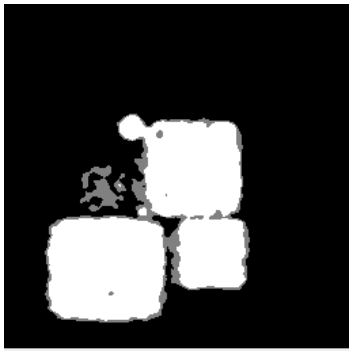


Segmentation models

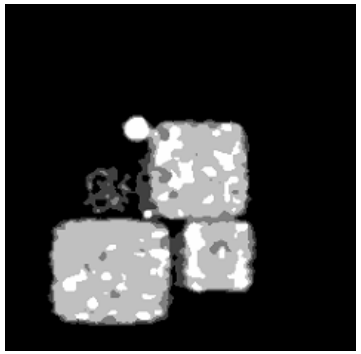
Electron Tomography reconstruction



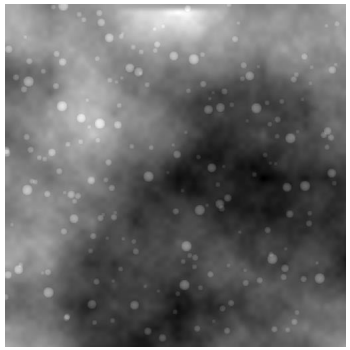
OTSU segmentation



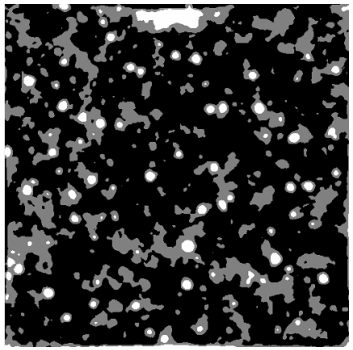
K-means segmentation



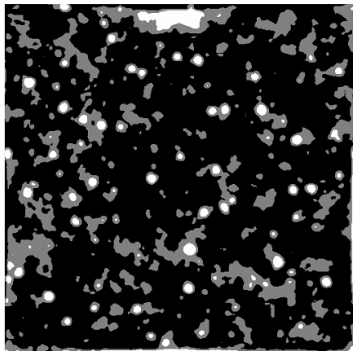
STEM image



OTSU segmentation



K-means segmentation



Ordered median Problem?

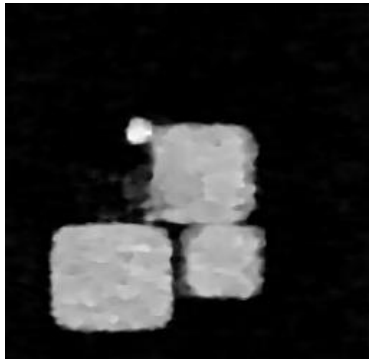
- Let assume that we have N different intensities and let $A = \{1, \ldots, N\}$.
- $d_{ij} = |i - j|$, distance between intensity i and intensity j (j is a representative of one cluster), with $i, j \in A$.
- $\omega_{ij} = \omega_i d_{ij}$, weight of allocating intensity i to representative j.

$$x_{ij}^k = \begin{cases} 1, & \text{if intensity } i \text{ is allocated in cluster represented by } j \\ & \quad \text{and } \omega_{ij} \text{ is the } k\text{-th smallest assignment cost,} \\ 0, & \text{otherwise.} \end{cases}$$

$$y_j = \begin{cases} 1, & \text{if a cluster is represented by intensity } j \\ 0, & \text{otherwise.} \end{cases}$$

$$\min \sum_{i,j,k} \lambda^k \omega_{ij} x_{ij}^k$$

λ-vector



Smallest elements

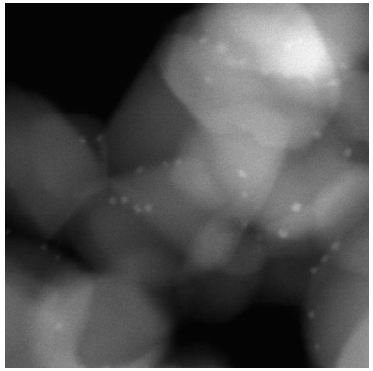
Anti-k-centrum

$\lambda = (1, \dots, 1, 0, \dots, 0)$

Largest elements

k-centrum

$\lambda = (0, \dots, 0, 1, \dots, 1)$



$(k_1\text{-}\ k_2)$-Antitrimmed mean

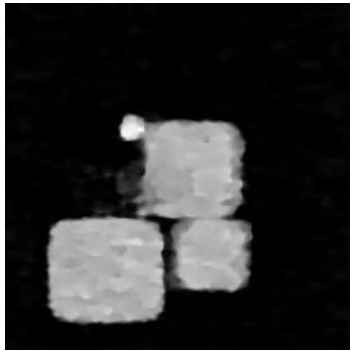
$\lambda = (1, \dots, 1, 0, \dots, 0, 1, \dots, 1)$

$(k_1\text{-}\ k_2)$-Trimmed mean

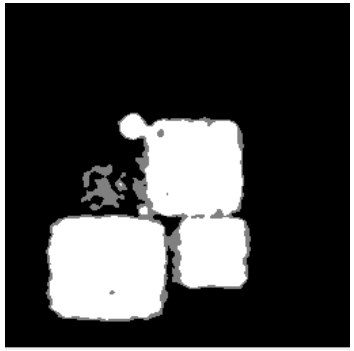
$\lambda = (0, \dots, 0, 1, \dots, 1, 0, \dots, 0)$

Comparing segmentation models

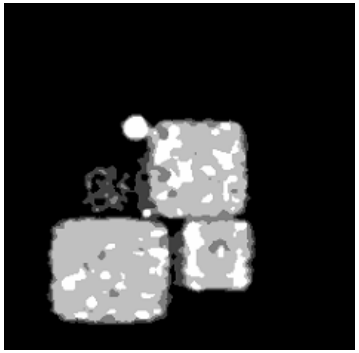
Electron Tomography reconstruction



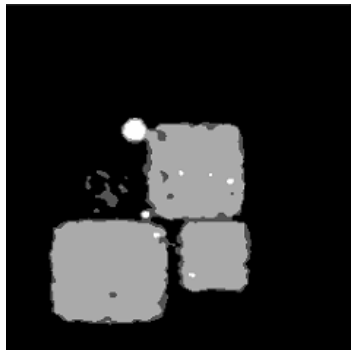
OTSU segmentation



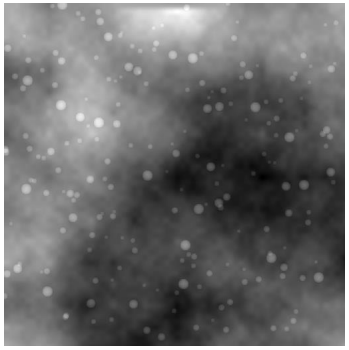
K-means segmentation



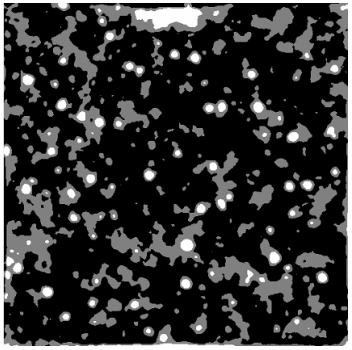
DOMP segmentation



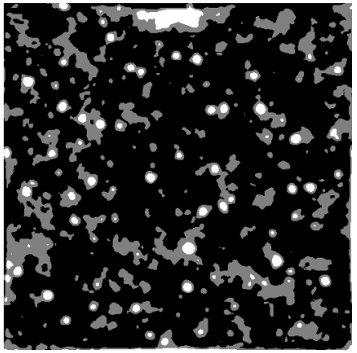
STEM image



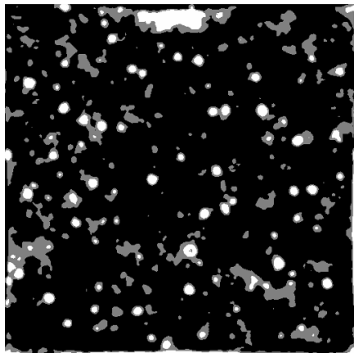
OTSU segmentation



K-means segmentation



DOMP segmentation



Anti k-centrum, $\lambda = (1, \ldots, 1, 0, \ldots, 0)$

$$\lambda = (\underbrace{1, \ldots, 1}_{x_{ij}}, 0, \ldots, 0)$$

ANTI-k-C

$$\begin{aligned}
\min \quad & \sum_{i,j \in A} \omega_{ij} x_{ij} \\
\text{s.t.} \quad & \sum_{j \in A} y_j = p, \\
& x_{ij} \leq y_j, && \forall i, j \in A, \\
& \sum_{j \in A} x_{ij} \leq 1, && \forall i \in A, \\
& \sum_{i,j \in A} x_{ij} = k, \\
& x_{ij}, y_j \in \{0, 1\}, && \forall i, j \in A
\end{aligned}$$

		DOMPG				Anti-k-C			
N	p	Time	Gap BB	Gap RL	Nodes	Time	Gap BB	Gap RL	Nodes
128	2	651.88	0	0.0011	0	0.43	0	0.0011	0
128	3	548.87	0	0	0	0.31	0	0	0
128	4	576.28	0	0.000575	0	0.33	0	0.000575	0
128	5	533.22	0	0	0	0.29	0	0	0
256	2	-	-	-	-	16.16	0	0.00095	0
256	3	-	-	-	-	17.39	0	0.0001	0
256	4	-	-	-	-	15.81	0	0.00005	0
256	5	-	-	-	-	13.41	0	0	0
512	2	-	-	-	-	110.77	0.000025	0.001075	0
512	3	-	-	-	-	109.64	0.00005	0.0001	0
512	4	-	-	-	-	99.02	0	0	0
512	5	-	-	-	-	101.52	0	0	0
1024	2	-	-	-	-	661.56	0.000025	0.00275	10
1024	3	-	-	-	-	669.84	0	0	0
1024	4	-	-	-	-	583.23	0	0	0
1024	5	-	-	-	-	564.76	0	0.000025	0

Formulations I

W. Ogryczak, A. Tamir. (2003)
Minimizing the sum of the k largest functions in linear time.

M. Labbé, D. Ponce, J. Puerto. (2017)
A comparative study of formulations and solution methods for the discrete ordered p-median problem.

A. Marín, D. Ponce, J. Puerto. (2020)
A fresh view on the Discrete Ordered Median Problem based on partial monotonicity.

I. Espejo, J. Puerto, A.M. Rodríguez-Chía. (2021)
A comparative study of different formulations for the capacitated discrete ordered median problem.

Ogryczak and Tamir (2003), $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$

$$
\begin{array}{llll}
\text{OT} & \min & \displaystyle\sum_{k\in A}(\lambda_{N-k+1}-\lambda_{N-k})(kt_k+\sum_{i\in A} d_{ik}) & \\
& \text{s.t.} & d_{ik}+t_k \geq \displaystyle\sum_{j\in A}\omega_{ij}x_{ij}, & \forall i,k\in A,\\
& & \displaystyle\sum_{j\in A} y_j = p, & \\
& & x_{ij}\leq y_j, & \forall i,j\in A,\\
& & \displaystyle\sum_{j=1}^{n} x_{ij}=1, & \forall i\in A,\\
& & x_{ij},y_j\in\{0,1\}, & \forall i,j\in A,\\
& & d_{ik}\geq 0, & \forall i,k\in A,\\
& & t_k\in\mathbb{R}, & \forall k\in A.
\end{array}
$$

$(k_1$-$k_2)$-Anti-Trimmed-mean (Ogryczak-Tamir)

$$\lambda = (\underbrace{1,\ldots,1}_{u_{ij}},0\ldots,0,1,\ldots,1) \Rightarrow \bar{\lambda} = (\underbrace{0,\ldots,0,0,\ldots,0,1,\ldots,1}_{x_{ij}})$$

$$
\begin{array}{llll}
(k_1\text{-}k_2)\text{-ANT-TM}_{OT} & \min & \displaystyle\sum_{j,k\in A} \omega_{jk} u_{jk} + kt + \sum_{i\in A} d_i & \\
& \text{s.t.} & d_i + t \geq \displaystyle\sum_{j\in A} \omega_{ij} x_{ij}, & \forall i \in A, \\
& & \displaystyle\sum_{j\in A} y_j = p, & \forall i,j \in A, \\
& & x_{ij} \leq y_j, & \forall i,j \in A, \\
& & \displaystyle\sum_{j\in A} x_{ij} = 1, & \forall i \in A,
\end{array}
$$

$(k_1$-$k_2)$-Anti-Trimmed-mean (Ogryczak-Tamir)

$$\lambda = (\underbrace{1,\ldots,1}_{u_{ij}},0\ldots,0,1,\ldots,1) \Rightarrow \bar{\lambda} = (\underbrace{0,\ldots,0,0,\ldots,0,1,\ldots,1}_{x_{ij}})$$

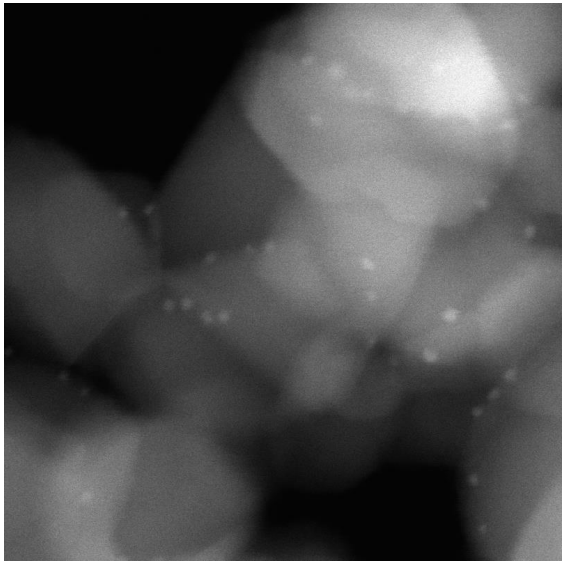
$$
\begin{array}{llll}
(k_1\text{-}k_2)\text{-ANT-TM}_{OT} & \min & \displaystyle\sum_{j,k\in A} \omega_{jk} u_{jk} + kt + \sum_{i\in A} d_i & \\
& \text{s.t.} & u_{ij} \leq x_{ij}, & \forall i,j \in A, \\
& & \displaystyle\sum_{i,j\in A} u_{ij} = k_1, & \\
& & \displaystyle\sum_{a:\omega_{ia}>\omega_{ij}} x_{ia} + y_j \leq 1, & \forall i,j \in A, \\
& & x_{ij}, u_{ij}, y_j \in \{0,1\}, & \forall i,j \in A, \\
& & d_i \geq 0, & \forall i \in A, \\
& & t \in \mathbb{R}. &
\end{array}
$$

		DOMP$_G$				OT$_\theta$ CAC				(k_1,k_2)-TM$_{OT}$			
N	p	Time	Gap BB	Gap RL	Nodes	Time	Gap BB	Gap RL	Nodes	Time	Gap BB	Gap RL	Nodes
128	2	7203.12$^{(4)}$	8.33	10.54	71701.25	18.20	0	0.70	13.25	1.22	0	0.91	0
128	3	7202.09$^{(4)}$	5.90	10.25	77007.25	17.19	0	0.42	0	1.50	0	0.76	1.5
128	4	7202.50$^{(4)}$	4.74	10.01	128057	15.40	0	0.14	0	1.14	0	0.45	2.5
128	5	7201.44$^{(4)}$	2.85	10.02	153064.75	16.06	0	0.23	0	0.96	0	0.59	0
256	2	-	-	-	-	154.74	0	0.24	42.75	13.86	0	1.11	0
256	3	-	-	-	-	182.61	0	0.16	49.25	15.39	0	1.36	605.75
256	4	-	-	-	-	187.47	0	0.16	0	12.90	0	0.93	158.5
256	5	-	-	-	-	208.75	0	0.28	290.5	12.46	0	1.14	587.75
512	2	-	-	-	-	2819.58	0	0.19	151	262.89	0	1.32	1991
512	3	-	-	-	-	4133.13	0	0.16	351.5	695.10	0	1.62	7973.5
512	4	-	-	-	-	3999.28	0	0.16	587	234.02	0	1.21	3969.25
512	5	-	-	-	-	5138.95	0	0.24	2073.25	381.47	0	1.40	7934.75
1024	2	-	-	-	-	-	-	-	-	7200.87$^{(4)}$	2.81	2.82	1081
1024	3	-	-	-	-	-	-	-	-	7200.43(1)$^{(4)}$	11.10	11.12	0
1024	4	-	-	-	-	-	-	-	-	7201.15$^{(4)}$	22.79	22.81	710.25
1024	5	-	-	-	-	-	-	-	-	6932.82$^{(3)}$	1.66	1.80	531.75

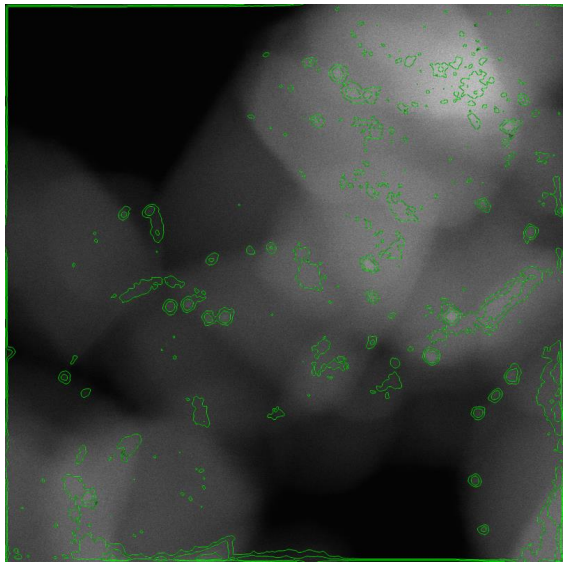
Table: Computational results for ET reconstructions. DOMP$_G$, OT$_\theta$, and (k_1,k_2)-TM$_{OT}$ mean formulations have been applied to solve the $(k_1$-$k_2)$-trimmed mean problem.

Results

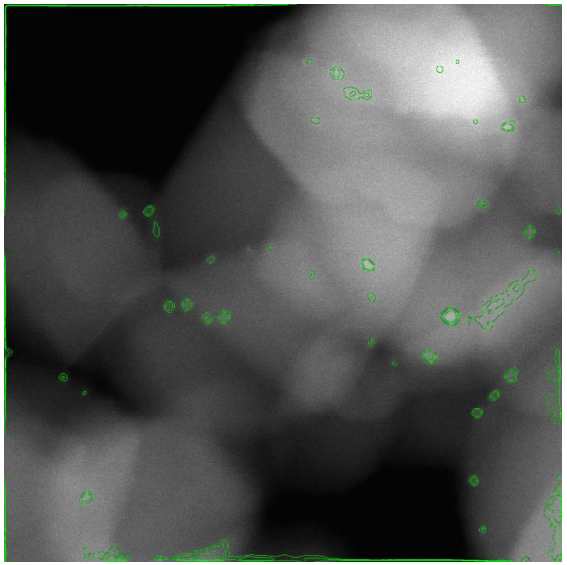
2D image



K-means, p=4

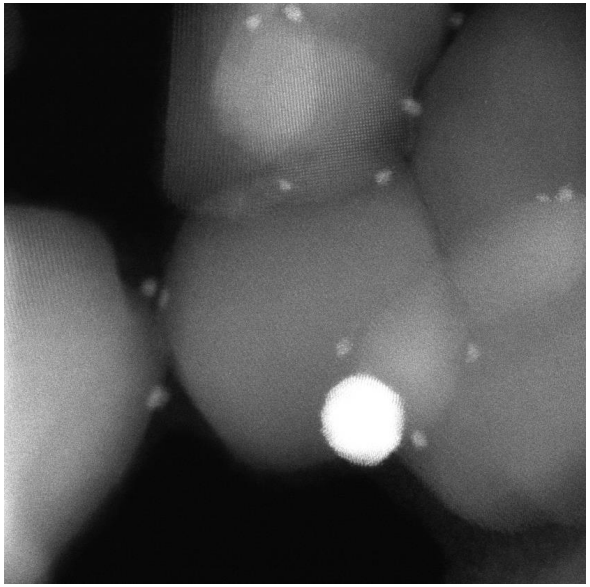


(k_1- k_2)-Trimmed mean p=4
k_1=10, k_2=10

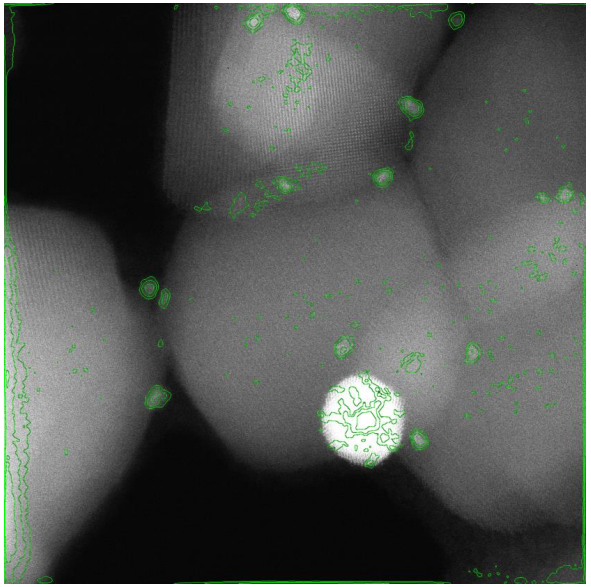


Results

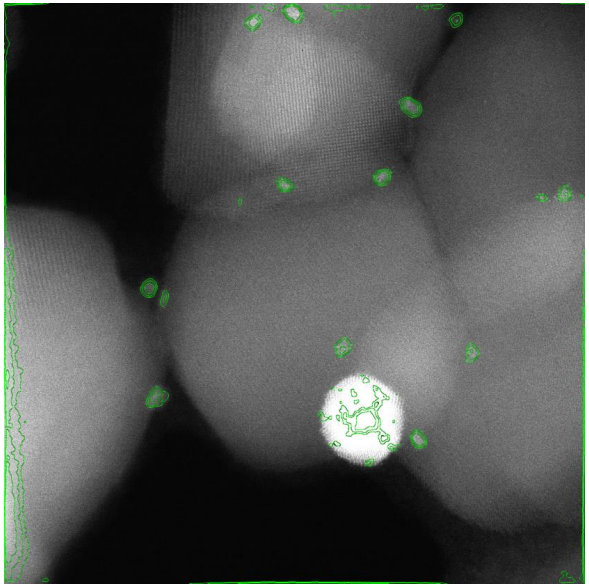
2D image



K-means, p=4



(k_1- k_2)-Trimmed mean p=4
k_1=10, k_2=10



Conclusions

- Mathematical Programming plays an important role in image processing.
- ℓ_1-norm minimization models have provided more accurate reconstructions.
- Ordered median problem provides high quality electron microscopy image segmentations.
- Computational time is reduced by taking advantage of λ-vector structure.

Thank you for your attention