



Joint Reconstruction in Multi-Spectral Electron Tomography

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1 Electron Tomography

2 Reconstruction Approach



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2 Reconstruction Approach





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1 Electron Tomography

2 Reconstruction Approach



Electron tomography

- Scanning Transmission Electron Microscopy
 - Creates 2D projections of thin samples.
 - Depicts density distribution.
 - Atomic resolution, magnification to resolution of 0.1 nm.
 - Analyse small samples in various fields.





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- Elemental mappings
 - Determine chemical makeup of a sample.
 - Energy dispersion X-ray spectroscopy (EDS).
 - Technical limitations.





Electron tomography

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 - Atomic resolution, magnification to resolution of 0.1 nm.
 - Analyse small samples in various fields.
- Elemental mappings
 - Determine chemical makeup of a sample.
 - Energy dispersion X-ray spectroscopy (EDS).
 - Technical limitations.
- Tomography reconstruction
 - 3D distributions allows more insight.
 - Projections from various angles.
 - Tomography reconstruction required.







HAADF

Silicon



Aluminium





HAADF

Silicon



Aluminium





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Aluminium





HAADF

Silicon



Aluminium







Aluminium







Forward model

All possible line integrals.






- All possible line integrals.
- Radon transform
 - $\mathcal{R}\colon L^1(\Omega_R)\to L^1(\Omega_S).$







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- Radon transform $\mathcal{R} \colon L^1(\Omega_R) \to L^1(\Omega_S).$
- Reconstruction via solving

$$\mathcal{R}u_1 = f_1^{\dagger}, \quad \ldots \quad \mathcal{R}u_n = f_n^{\dagger}.$$





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- $\mathcal{R}u = f$ is ill-posed problem.
- Poisson distributed noise.
- Kullback-Leibler divergence $D_{KL}: L^1(\Omega_S) \times L^1(\Omega_S) \to [0, \infty]:$

$$D_{\mathcal{KL}}(v,f) = \begin{cases} \int_{\Omega_S} v - f - f \ln\left(\frac{v}{f}\right) dx & v \ge 0, \ f \ge 0 \ a.e. \\ \infty & \text{otherwise} \end{cases}$$





Outline



1 Electron Tomography

2 Reconstruction Approach

3 Implementation and Numerical Results





$$\min_{u=(u_1,\ldots,u_n)} R(u) + \sum_{i=1}^n \lambda_i D_{KL}(\mathcal{R}u_i, f_i^{\dagger})$$





$$\min_{\boldsymbol{u}=(u_1,\ldots,u_n)} \boldsymbol{R}(\boldsymbol{u}) + \sum_{i=1}^n \lambda_i D_{KL}(\mathcal{R}\boldsymbol{u}_i,\boldsymbol{f}_i^{\dagger})$$

Suitable regularization?





$$\min_{u=(u_1,\ldots,u_n)} R(u) + \sum_{i=1}^n \lambda_i D_{KL}(\mathcal{R}u_i, f_i^{\dagger})$$

- Suitable regularization?
- Incorporate a priori information or expectations.



Sirt reconstruction of a slice



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- Local correlation.



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- Complementing information:



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 - Common features,



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- Suitable regularization?
- Incorporate a priori information or expectations.
- Local correlation.
- Complementing information:
 - Common features,
 - Diffusion and mixing.



Sirt reconstruction of a slice





TGV for scalar valued images

1

For $u \in L^1(\Omega, \mathbb{R})$,

$$\mathsf{TV}(u) = \sup \bigg\{ \int_{\Omega} u \operatorname{div} \phi \quad \bigg| \ \phi \in \mathcal{C}^{\infty}_{c}(\Omega, \ \mathbb{R}^{d}), \ \||\phi|_{2}\|_{\infty} \leq 1 \bigg\}.$$

ī.





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Original

TV

TGV for scalar valued images

For $u \in L^1(\Omega, \mathbb{R})$,

$$\mathsf{TGV}_{\alpha}^{2}(u) = \sup \left\{ \int_{\Omega} u \mathsf{div}^{2} \phi \mid \phi \in \mathcal{C}_{c}^{\infty}(\Omega, \ \mathcal{S}^{d \times d}), \\ \| |\phi|_{2} \|_{\infty} \leq \alpha_{0}, \| |\operatorname{div} \phi|_{2} \|_{\infty} \leq \alpha_{1} \right\}.$$

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Equivalent representation:

 $\mathsf{TV}(u) = \||\mathrm{D}u|_2\|_{\mathcal{M}}$

TGV for scalar valued images

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$$\mathsf{TGV}_{\alpha}^{2}(u) = \min_{w \in \mathsf{BD}(\Omega, \mathbb{R}^{d})} \alpha_{1} \| |\mathrm{D}u - w|_{2} \|_{\mathcal{M}} + \alpha_{0} \| |\mathcal{E}w|_{2} \|_{\mathcal{M}}$$

TGV for vector valued images

For $u \in L^1(\Omega, \mathbb{R}^m)$,

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Frobenius norm: $|N|_{\rm fr} = \sqrt{\sum_{i,j} N_{i,j}^2}$

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Joint sparsity.

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Effect on reconstruction:

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Effectively reduces noise,

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Effect on reconstruction:

- Effectively reduces noise,
- Promotes piecewise linear functions,

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Joint sparsity.

Effect on reconstruction:

- Effectively reduces noise,
- Promotes piecewise linear functions,
- Promotes joint features in channels.

Reconstruct $u = (u_1, \ldots, u_n)$ from data $f^{\dagger} = (f_1^{\dagger}, \ldots, f_n^{\dagger})$:

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 from data $f^{\dagger} = (f_1^{\dagger}, ..., f_n^{\dagger})$:
For $\alpha = (\alpha_0, \alpha_1), \ \lambda \in (0, \infty)^n$,
(Tikh) $u^{\dagger} \in \underset{u \in L^1(\Omega_R, \mathbb{R}^n)}{\operatorname{argmin}} \operatorname{TGV}_{\alpha}^2(u) + \mathcal{I}_{\{\tilde{u} \ge 0\}}(u) + \sum_{i=1}^n \lambda_i D_{KL}(\mathcal{R}u_i, f_i^{\dagger})$

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- Indicator function ensure feasibility by introducing constraints.
- Weighted sum of Kullback-Leibler discrepancies to account for Poisson noise.

Analytical properties

$$(\mathsf{Tikh}) \qquad u^{\dagger} \in \operatorname*{argmin}_{u \in L^{1}(\Omega_{R})^{n}} \mathsf{TGV}_{\alpha}^{2}(u) + \mathcal{I}_{\{\tilde{u} \geq 0\}}(u) + \sum_{i=1}^{n} \lambda_{i} D_{\mathcal{KL}}(\mathcal{R}u_{i}, f_{i}^{\dagger})$$




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Proposition

Under suitable assumptions:





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Under suitable assumptions:

Solutions to (Tikh) exist.





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Under suitable assumptions:

- Solutions to (Tikh) exist.
- Are stable with respect to Poisson noise vanishing in D_{KL} .





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Proposition

Under suitable assumptions:

- Solutions to (Tikh) exist.
- Are stable with respect to Poisson noise vanishing in D_{KL}.
- For vanishing noise in all channels, a TGV²_α-minimal solution to *Ru* = f[†] can be retrieved using suitable parameter choices.





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M. Holler, R. Huber, F. Knoll: "Coupled regularization with multiple data discrepancies", Inverse Problems



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Primal-dual algorithm to find saddle point.





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- Primal-dual algorithm to find saddle point.
- Evaluation of Radon transfrom and backprojection at high computational cost.





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- Custom Radon transform implementation with exact adjoint.





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- Highly parallel implementation possible.





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 $^{^1 \}mbox{Graz}$ Application for Tomographic Reconstruction) software tool





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$$u^{\dagger} \in \operatorname*{argmin}_{u \in L^{1}(\Omega_{R})^{n}} \mathrm{TGV}_{\alpha}^{2}(u) + \mathcal{I}_{\{\tilde{u} \geq 0\}}(u) + \sum_{i=1}^{n} \lambda_{i} D_{KL}(\mathcal{R}u_{i}, f_{i}^{\dagger})$$

- Primal-dual algorithm to find saddle point.
- Evaluation of Radon transfrom and backprojection at high computational cost.
- Custom Radon transform implementation with exact adjoint.
- Highly parallel implementation possible¹.
- Time consumption: in average 5 seconds per slice. (300 × 300 with 4 channels)

¹Graptor (Graz Application for Tomographic Reconstruction) software tool





























Sirt reconstruction

Decoupled TGV reconstruction







Decoupled TGV reconstruction



Coupled TGV reconstruction









- Tikhonov approach for reconstruction in electron tomography:
 - Joint penalty via Total Generalised Variations.





- Joint penalty via Total Generalised Variations.
- Weighted sum of Kullback-Leibler discrepancies.





- Joint penalty via Total Generalised Variations.
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- Solutions exist and are stable.





- Joint penalty via Total Generalised Variations.
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- Solutions exist and are stable.
- Recover TGV-minimal solutions for vanishing noise.





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- Reconstruction quality:





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- Solutions exist and are stable.
- Recover TGV-minimal solutions for vanishing noise.
- Reconstruction quality:
 - Joint reconstruction of all channels.





- Joint penalty via Total Generalised Variations.
- Weighted sum of Kullback-Leibler discrepancies.
- Solutions exist and are stable.
- Recover TGV-minimal solutions for vanishing noise.
- Reconstruction quality:
 - Joint reconstruction of all channels.
 - Remove noise substantially.





- Joint penalty via Total Generalised Variations.
- Weighted sum of Kullback-Leibler discrepancies.
- Solutions exist and are stable.
- Recover TGV-minimal solutions for vanishing noise.
- Reconstruction quality:
 - Joint reconstruction of all channels.
 - Remove noise substantially.
 - Maintains features and details.





- Joint penalty via Total Generalised Variations.
- Weighted sum of Kullback-Leibler discrepancies.
- Solutions exist and are stable.
- Recover TGV-minimal solutions for vanishing noise.
- Reconstruction quality:
 - Joint reconstruction of all channels.
 - Remove noise substantially.
 - Maintains features and details.
 - Superior reconstructions.





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IGDK 1754: Optimization and Numerical Analysis for Partial Differential Equations with Nonsmooth Structures







Kristian Bredies Martin Holler Georg Haberfehlner





References

- R. Huber, G.Haberfehlner, M. Holler, G. Kothleitner and K. Bredies. "Total Generalized Variation regularization for multi-modal electron tomography", accepted in RSC Nanoscale February 2019.²
- M.Holler, R. Huber and F.Knoll. "Coupled regularization with multiple data discrepancies", Inverse Problems 34 084003, 2018.
- Kristian Bredies. Recovering piecewise smooth multichannel images by minimization of convex functionals with total generalised variation penalty. In Efficient Algorithms for Global Optimization Methods in Computer Vision.
- Kristian Bredies and Martin Holler. Regularization of linear inverse problems with total generalized variation. Journal of Inverse III-Posed Problems.
- F. Knoll, M. Holler, T. Koesters, R. Otazo, K. Bredies, and D. K. Sodickson. Joint MR-PET reconstruction using a multi-channel image regularizer. IEEE Transactions on Medical Imaging.
- R. K. Leary and P. A. Midgley. Analytical electron tomography. Advanced Tomography Techniques for Materials Applications.

²Graptor (Graz Application for Tomographic Reconstruction)