Compressed Sensing for Electron Tomography

Matthew Guay

University of Maryland, College Park Department of Mathematics



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Radon transforms and compressed sensing



Sparsity across application domains



Experimental results

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Introduction

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- Tomography Producing a 3D reconstruction of an object by measuring changes in penetrating waves (or particles) which are sent through it. Many modalities, depending on wave type:
 - CT X-rays MRI Radio waves
 - ET Electrons PET Electron-positron annihilation
- Electron tomography (ET) 3D imaging using electron beams via a transmission electron microscope (TEM) or scanning transmission electron microscope (STEM).

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Our ET data

- Our NIH collaborators have provided STEM images of heavy metal-stained sections of cells, rotated incrementally about a fixed axis.
- Each image is a projection of the rotated object, a sequence of images indexed by rotation angle is a tilt series.
- Bright field STEM imaging: detectors measure electron beam attenuation through the object.
- Projections show intensity amplitude contrast due to the scattering of electrons by dense regions within the object.

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From tomography to Radon transforms

- A beam of n_0 electrons travels along line L through the object at each detector location, which counts the n electrons passing through undeviated.
- The ratio $\frac{n}{n_0}$ can be related to line integrals of an electron density function $f(x) : \mathbb{R}^3 \to \mathbb{R}$ via the Beer-Lambert law:

$$\log\left(\frac{n}{n_0}\right) \propto \int_L f(\boldsymbol{x}) \left| d\boldsymbol{x} \right| \tag{1}$$

• The function *f* forms the tomogram recovered from the projection data.

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From tomography to Radon transforms

• Radon transform - for $f : \mathbb{R}^2 \to \mathbb{R}$ and any line $L \subseteq \mathbb{R}^2$,

$$Rf(L) = \int_{L} f(\boldsymbol{x}) |d\boldsymbol{x}|.$$
 (2)

 This space of lines can be parametrized by a normal angle θ and a distance coordinate s:

$$Rf(\theta, s) = \int_{-\infty}^{\infty} f((t\sin\theta + s\cos\theta), (-t\cos\theta + s\sin\theta)) dt.$$

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From tomography to Radon transforms

- Parallel beam tomography used in ET decomposes 3D reconstruction into multiple independent 2D reconstruction problems.
- For each plane normal to the rotation axis, tomographic measurements provide samples {Rf(θ_i, s_j)}_{i∈I,j∈J} for some finite sets I, J.
- Measurement limitations make tomogram recovery an ill-posed operator inversion problem, either of *R* or the 2D Fourier transform due to the Fourier-slice theorem.

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The Fourier-slice theorem

- Fixing θ , the 1D Fourier transform of $Rf(\theta, s)$ in s can be related to the 2D Fourier transform of f.
- Fourier-slice theorem:

$$[Rf]^{\hat{}}(\theta,\gamma) = \hat{f}(\gamma\cos\theta,\gamma\sin\theta).$$

- ET Radon data can be numerically transformed into 2D Fourier samples on a polar grid. From a computational perspective, these are non-uniform discrete Fourier transform (NDFT) samples.
- Treating projections as NDFT data has been used in recent CS-ET work. Our approach uses non-transformed Radon domain data.



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Compressed sensing background

- Compressed sensing: Assume a signal (vector) $f : \mathbb{R}^D \to \mathbb{R}$, a set of M measurement vectors $\{\varphi_m\} \subseteq \mathbb{R}^D$, and a representation frame $\{\psi_n\}_{n=1}^N \subseteq \mathbb{R}^D$.
- Stack measurements in columns as measurement matrix $\Phi \in \mathbb{R}^{D \times M}$ and frame elements as representation matrix $\Psi \in \mathbb{R}^{D \times N}$.
- A priori signal assumption: f is s-sparse in Ψ: ||Ψ^Tf||₀ ≤ s. (Analytic sparsity)
- Most existing CS results focus on orthonormal basis or tight frame Ψ for which $f = \Psi \Psi^T f$.

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Compressed sensing background

• Goal: Given measurements $b = \Phi^T f$, efficiently recover f even if M < N as:

$$f^* = \underset{g \in \mathbb{R}^D}{\operatorname{arg\,min}} ||\Psi^T g||_1 \text{ such that } b = \Phi^T g.$$
(3)

• The feasibility of this approach depends on the structure of $\Theta \triangleq \Phi^T \Psi$.

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Restricted isometry property

• Isometry constant δ_k : k = 1, 2, ... The smallest nonnegative number such that

$$(1 - \delta_k)||x||_2^2 \le ||\Theta x||_2^2 \le (1 + \delta_k)||x||_2^2$$

for all k-sparse $x \in \mathbb{R}^N$.

- Theorem (Candes): If $\delta_{2s} < \sqrt{2} 1$ given the previous hypotheses, (3) recovers f exactly.
- RIP bounds are difficult to verify directly. Estimates can be made by analyzing off-diagonal entries of Θ^TΘ.

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CS for tomography

- Each sample $Rf(\theta_i, s_j)$ corresponds to a measurement vector $\varphi_{ij} \in \mathbb{R}^D$ stacked in measurement matrix Φ .
- Common choices of Ψ: Identity matrix, wavelet synthesis matrix, discrete cosine transform synthesis matrix.
- In ET, also common to let $\Psi^T = TV$ the total variation operator.
- For a 2D discrete image f,

$$TVf \triangleq \sqrt{\Delta_x^+ f + \Delta_y^+ f}$$

for forward finite x- and y-differences Δ^+ .

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Theoretical challenges

- There is little theory in place for recovering *f* from (3) given nonlinear sparsifying transforms (e.g. *TV*).
- ET measurement matrices Φ are deterministic, do not satisfy RIP for useful (k,δ_k) values.
- Simple measurement variation: choose measurement angles $\{\theta_i\}$ randomly in some range.
- Still not RIP, empirically this performs worse than uniformly-spaced angle choices.

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Radon RIP, random vs. uniform sampling images.

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- Nevertheless, empirical results are good.
- Question: Why does this work with non-RIP measurements? An open, practical problem for applying CS to many physical measurement situations.
- Thought: Are there additional *a priori* assumptions about signal structure that can be exploited for physical imaging?
- e.g. if Θ is (k, δ_k) RIP for some nice subset of k-sparse signals?

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Additional challenges

• Equation (3) can be related to the regularized least-squares problem

$$f^* = \underset{g \in \mathbb{R}^D}{\operatorname{arg\,min}} ||\Phi^T g - b||_2^2 + \lambda ||\Psi^T g||_1,$$

for some weight parameter λ .

- This formulation allows for the use of multiple regularizers simultaneously; useful in practice but on shaky ground in CS theory.
- $\bullet\,$ We used identity, DB8 wavelet and TV regularizers with three weight parameters
- Difficult to get good a priori estimates of optimal weight values.



Radon transforms and compressed sensing

Sparsity across application domains



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Image complexity across applications

- Sparse signal models rely on accurate prior knowledge about object structure.
- The statistical image properties which influence the choice of sparsity model correlate with imaging application domain.



Figure: (a) Iron oxide nanoparticles, (Saghi et al., 2011). (b) Gallium-palladium nanoparticles, (Leary et al., 2013). (c) Renal cell section. (d) Retinal cell section.

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Image complexity across applications

- Nanoparticle images high-contrast features, piecewise-constant ("cartoon-like") intensities.
- Feature spatial scale may be large compared to the image's smallest-resolved spatial scale.
- Biological images Features at varying contrasts and multiple spatial scales.
- Textural content due to noise, variations in embedding media, and structural features at or near highest resolution.

Image complexity across applications

- Image "complexity" is difficult to fully characterize but reflected in the sparsity/compressibility of the data.
- Nanoparticle images may be highly sparse in common sparsity models identity sparsity, TV sparsity, wavelet sparsity.
- Biological images may be less sparse in all of these domains, hindering the efficacy of undersampled recovery.
- These observations are consistent with results in our work and the work of other groups on CS-ET in materials and biological sciences.

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Compressibility image

Image complexity across applications

- The advantages of CS reconstruction come at the price of data-dependence.
- This fact and its implications bear careful explanation for non-mathematical practitioners.
- A comprehensive understanding of which sparsity models are appropriate for different image types would require an enormous organizational effort by the microscopy community.

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Numerical techniques

• The full equation our CS-ET algorithm minimizes is

$$f^* = \underset{g \in \mathbb{R}^D}{\arg\min} ||\Phi^T g - b||_2^2 + \lambda_1 ||g||_1 + \lambda_2 ||TVg||_1 + \lambda_3 ||Wg||_1$$

for each 2D slice of the tomogram, for some choice of regularization weights λ_i .

- 1024 2D slices, each 1024×256 (maybe thinner).
- This remains difficult to solve quickly on modern computational hardware.

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(4)

The split-Bregman algorithm

- The split-Bregman algorithm for convex optimization solves problems with multiple ℓ^1 and ℓ^2 norm terms efficiently.
- Two-step iterative scheme that decouples the ℓ^1 and ℓ^2 minimizations in (4).
- ℓ^2 minimization can be solved by conjugate gradients (or better when possible), ℓ^1 by a fast shrinkage routine.
- This and naive parallelization (MATLAB's parfor routine) drops CS-ET reconstruction time on the new NWC workstation to under 30 minutes for the pancreatic cell tomogram.

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split-Bregman phantom animation.

Experimental results

- For phantoms with the nanoparticle statistical properties, CS-ET recovery is markedly better than alternative methods.
- For biological tomograms, CS-ET matches or exceeds alternative methods, but by a smaller margin.
- Still demonstrates the feasibility of undersampled recovery, which is evidently of interest for some tomography applications.

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Phantom + bio reconstruction comparison images

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Future work - CS-ET

- The application of CS recovery algorithms to deterministic, non-RIP sensing problems suggests the need for new theoretical developments.
- Practically, there remain challenges for packaging CS-ET techniques for non-mathematical practitioners.
- Nontrivial choices for sparsity models, regularization parameters, number of Bregman iterations which may be data-dependent.
- Collaboration with NIBIB is ongoing for optimized numerical implementations for greater speed/use on their computing clusters.

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Future work - Sparse inpainting

- Additionally for tomography, these results could be combined with sparse inpainting techniques to alleviate missing wedge artifacts.
- Missing wedge Mechanical limitations force the range of $\{\theta_i\}$ samples to be smaller than $[-90^\circ, 90^\circ]$. Causes characteristic artifacts.
- Ariel and Ben are working with Wojtek to solve this problem.

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Works cited

- R Leary, Z Saghi, P Midgley, and D Holland. Compressed sensing electron tomography. Ultramicroscopy, 2013.
- Z Saghi, D Holland, R Leary, A Falqui, G Bertoni, A Sederman, L Gladden, and P Midgley. Three-dimensional morphology of iron oxide nanoparticles with reactive concave surfaces. a compressed sensing-electron tomography (cs-et) approach. Nano letters, 11(11):4666–4673, 2011.

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