Spectral and Diffraction Tomography

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UCL Inverse Probs 2013

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This is the 'wild west' frontier of applied inverse problems.
These examples come from experimental literature and talking to experimentalists where they have done some experiments and numerics but not yet formulated the mathematical problems clearly.

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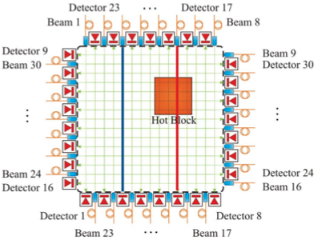
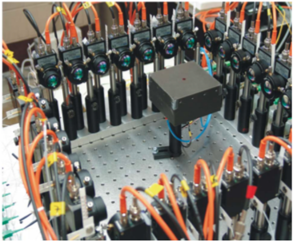
Infrared absorption tomography

- This work derives mainly from studies of combustion where tomography of the distribution of **chemcal species** and temperature is probed using collimated beams from a tuneable infra red laser.
- Relatively small numbers of line integrals are measured as the sources and detectors are fixed, scan rates (including scanning wavelengths) are relatively fast.
- The experimental apparatus from Wisconsin group is shown on the next slide. My interest in this work is thanks to a MIRAN workshop on Chemical Species Tomography at Manchester last year and especially I would like to thanks Scott Sanders for helpful discussions.

Wisconsin Apparatus





From An *et al*, Validation of temperature imaging by H_2O absorption spectroscopy using hyperspectral tomography in controlled experiments, Applied Optics, 50, A29-A37, 2011.

Simplified model

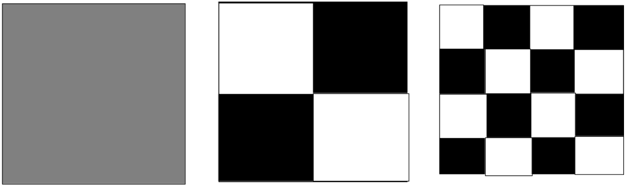
The attenuation S of the infrared light at wave length λ depends in a known but non-linear way on the temperature f, assuming the mole-fraction of the chemical species and pressure is constant. We define the spectral ray transform, for a unit vector ξ and point $x \in \mathbb{R}^3$ by

$$K_S f(x, \xi, \lambda) = \int S(f(x + s\xi), \lambda)\xi \, ds = XS(f, \lambda)(x, \xi)$$

and clearly for a fixed wavelength this is equivalent to the X-ray transform. The hope of the experimentalists is that by measuring a a range of wavelengths they can reduce the number of projections. Specifically in An *et al*'s paper two projections are used.
In discussions they agreed that there must be a null space for two projections as their regularized least squares reconstructions yielded plausible results they assumed it was not important.

Discrete case

At least when explaining to experimentalists it is useful to consider the two dimensional discrete case of a square a array of $N \times N$ pixels and two orthogonal projections. Of course there is a well known null space for the discrete Radon transform with two orthogonal projections consisting of 'checkered images'.



Two projections

Let f_{ij} be the pixel value on an $N \times N$ square grid x_{ij}. We take only two projections in the coordinate directions at $\lambda = \lambda_k$, $k = 1...L$ so that the data are

$$K_{1mk} = \sum_{j=1}^{N} S(f_{mj}, \lambda_k),\ K_{2mk} = \sum_{j=1}^{N} S(f_{jm}, \lambda_k).$$

- What we can deduce from just K_{1mk}, $m = 1...N$, $k = 1...L = N$? This is a system of N equations for N variables $(f_{mj})_{j=1}^{N}$.

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- Fixing a row of the image m the Jacobian matrix $(\partial K_{1mk}/\partial f_{mj})_{j,k=1}^{N}$. If this is invertible so the inverse function theorem guarantees that where a solution exists in is unique within a neighbourhood of that solution. (For example $S(f, \lambda) = f\lambda$ is no good but $S(f, \lambda) = f^{\lambda}$ is fine.)

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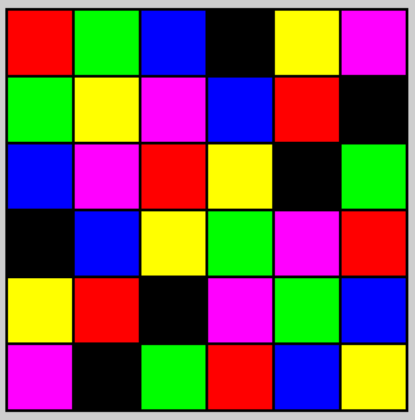
  so under generic conditions if the values of f_{mj} are different the columns of the Jacobian will be independent vectors.
- However that K_{1mk} is invariant under permutation of the values in the vector $(f_{m,j})_{j=1}^{N}$.

Even if we can find the values of the pixels along that row, we have no hope of finding the order in which they occur from one projection.
In general for given data K_{1mk} the solution $(f_{mj})_{j=1}^{N}$ will be unique up to a permutation $j \to \sigma(j)$ giving $N!$ solutions for that row. For this one projection we can apply any permutation on any row of the image giving $N \cdot N!$ solutions.

A Latin square



Each colour (label) appear exactly once in each row and column.

Two orthogonal projections - Latin Squares

- Assuming we have been able to identify the values $\{f_{mj}\}_{j=1}^{N}$ for each m but not the ordering from one projection, and similarly $\{f_{jm}\}_{j=1}^{N}$ from the other projection, in the special case in which no value appears in two different rows the solution is unique.

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- By consider the case where f_{ij} takes only N distinct values and these occur in each row and column.
- In this case $K_{pmk}, p = 1, 2$ depends only on k. Any $N \times N$ Latin square where the values of the f_{ij} are the labels for the squares gives a solution. There are $L(N)$ $N \times N$ Latin squares where

$$\prod_{k=1}^{N} (k!)^{N/k} \geq L(N) \geq \frac{(N!)^{2N}}{N^{N^2}}$$

with for example $L(10)$ approximately 9.98×10^{36}.

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One might expect some of the values in any given image to be the same within the precision to which we can work.
We can expect a large number of solutions that fit the data from two projections and without additional information the imaging problem is not possible to solve.

An et al's results

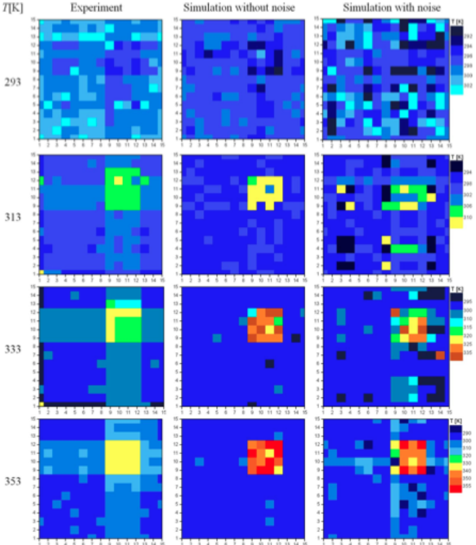

Fig. 5. (Color online) Four temperature reconstruction results for experimental data (first column), simulated noise-free data (second column), and simulated data with noise ($\sigma = 0.0002$, third column). Temperature at left indicates the temperature of the block. The ambient gas surrounding the block is at 297 K.

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- The transverse case does not have such a null space - indeed it can be inverted using limited data.

A tale of two strain tomographies

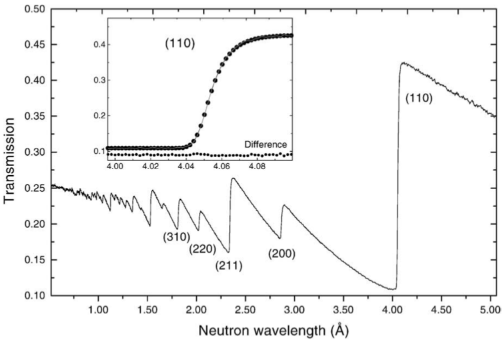
- Both x-rays and neutrons are *diffracted* by crystals, this is widely used for crystallography
- Metals are *polychrstaline*, that is they consist of small randomly oriented crystals.
- For polycrystalline materials the diffraction pattern is averaged over the action of the rotation group $SO(3)$.
- If the metal is subjected to linear elastic strain the crystals are deformed changing their diffraction pattern.
- Using a narrow collimated beam of x-rays or neutrons we might hope to get some kind of average strain along the beam.
- While this has not yet been done experimentally there has been some feasibility studies for two possible methods.

Bragg edge tomography

From Santiseban *et al*, 'Strain imaging by Bragg edge neutron transmission', Nuclear Instruments and Methods in Physics Research A, 481,765768,2002.

> *The transmission spectrum of thermal neutrons through a polycrystalline sample displays sudden, well-defined increases in intensity as a function of neutron wavelength (Fig. 1). These Bragg edges occur because for a given {h,l,k} reflection, the Bragg angle increases as the wavelength increases until 2θ is equal to 180°. At wavelengths greater than this critical value, no scattering by this particular {h,l,k} lattice spacing can occur, and there is a sharp increase in the transmitted intensity.*

766 J.R. Santisteban et al. / Nuclear Instruments and Methods in Physics Research A 481 (2002) 765–768



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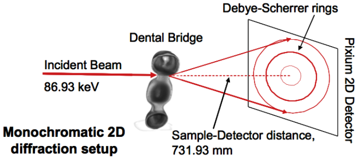
- Using this approach we believe what they have estimated is the *Longitudinal* ray transform of the strain.
- As linear strain is the symmetric derivative of the deformation vector this technique measures just.... the change in thickness!

A different approach

A different approach is suggested by Korsunsky *et al* in Strain tomography of polycrystalline zirconia dental prostheses by synchrotron x-ray diffraction, Acta Materialia, 59, 2501 2513, 2011. They notice that the diffraction pattern for a narrow beam of monochromatic x-rays through a polycrystalline material on a distant screen forms concentric circular Debye-Scherrer rings.



Korsunsky *et al* Fig 3

If the material in the beam was subjected to a uniform linear elastic strain the rings would become concentric ellipses, and the matrix defining each ellipse is proportional to the *strain tensor projected in the direction normal to the beam*. They presume without proof that for a non-uniform strain fitting an ellipse to the diffraction pattern results in an average of this transverse strain.

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- Let us consider a line parallel to the x_3 axis each value of the transverse strain ϵ_{ij}, $1 \leq i, j \leq 2$ results in a contribution to the intensity on the screen equally distributed on the ellipse

$$\epsilon_{11} q_1^2 + 2\epsilon_{12} q_1 q_2 + \epsilon_{22} q_2^2 = 1$$

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- let $\phi(\epsilon)$ be the density of strain values on along the line. The intensity at q is then

$$\mathcal{I}(q) = \int_{\epsilon : \epsilon_{11} q_1^2 + 2\epsilon_{12} q_1 q_2 + \epsilon_{22} q_2^2 = 1} \phi(\epsilon) d\epsilon_{11} d\epsilon_{12} d\epsilon_{22}$$

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$$\epsilon_{11} q_1^2 + 2\epsilon_{12} q_1 q_2 + \epsilon_{22} q_2^2 = 1$$

  in normalized screen coordinates $q = (q_1, q_2)$.
- let $\phi(\epsilon)$ be the density of strain values on along the line. The intensity at q is then

$$\mathcal{I}(q) = \int_{\epsilon : \epsilon_{11} q_1^2 + 2\epsilon_{12} q_1 q_2 + \epsilon_{22} q_2^2 = 1} \phi(\epsilon) d\epsilon_{11} d\epsilon_{12} d\epsilon_{22}$$

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- This is an integral over a *two parameter* family of planes in *three dimensional* ϵ space. A restricted Radon plane transform.
- No unique solution ϕ with out *a priori information*.

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We can reduce the data from each ray (which also makes it practically manageable) and then reconstruct as a tensor ray transform.

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  $$\int r\mathcal{I}(r^{-1/2}q)\, dr = q \cdot J\epsilon(x, \xi) \cdot q$$

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- From the polarization identity we can now find $J\epsilon(x,\xi)$

We hope to test this at the Diamond Light Source

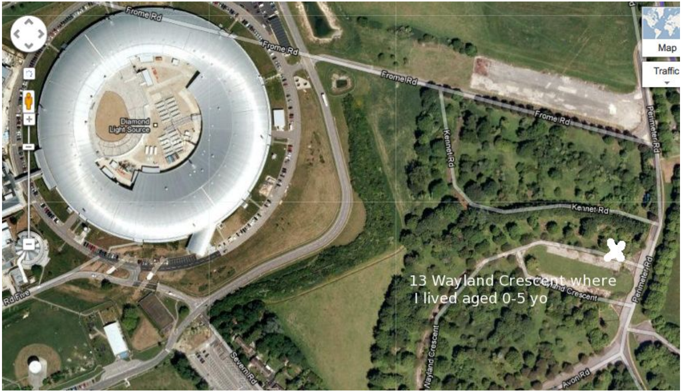

Photo: Google Earth

This synchrotron at Harwell provides a monochromatic collimated x-ray source. Manchester has its own beam and lab at Harwell as part of Manchester X-ray Imaging Facility.

Inverting the transverse ray transform

Consider a fixed unit vector η then for all ξ normal to η

$$\eta \cdot JF(x, \xi)\eta = \int \eta \cdot \Pi_\xi \cdot F(x + s\xi)\Pi_\xi \eta \, ds = X(\eta \cdot F\eta)(x, \xi)$$

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Which η do we use?

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We have the equations $\eta_i \cdot F\eta_i = d_i$, for $i = 1, ..., 6$ for the six unknowns $F_{i,j}$.

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Any five distinct points on the projective plane (unit vectors in $\mathbb{R}^3$) determine a projective conic

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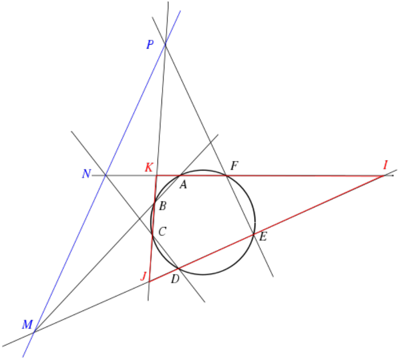

Conclusions

Rich tomography opens up a wide vista of new inverse problems for both theoretical and practical study.

Picture by Sam Lionheart, sunrise in Morocco