Edge-Preserving Computed Tomography (CT) with Uncertain View Angles

Per Christian Hansen

DTU Compute, Technical University of Denmark

Joint work with

Johnathan M. Bardsley – Univ. of Montana, USA Yiqiu Dong & Nicolai A. B. Riis – DTU, Denmark Felipe Uribe – LUT Univ., Finland

F. Uribe, J.M. Bardsley, Y. Dong, P.C. Hansen, & N.A.B. Riis, A hybrid Gibbs sampler for edge-preserving tomographic reconstruction with uncertain angles, SIAM/ASA J. UQ, 10 (2022), pp. 1293–1320, doi 10.1137/21M1412268.

sites.dtu.dk/cuqi — cuqi-dtu.github.io/CUQIpy





This work is part of the project Computational Uncertainty Quantification for Inverse problems, which is funded by The Villum Foundation.

- A collaborative effort to develop a mathematical, statistical and computational framework for UQ.
- We released the first version of our software package:



- Some applications
 - X-ray computed tomography: industrial inspection, materials science.
 - Electrical impedance tomography (EIT) and hybrid EIT.
 - Inverse problems in tokamak plasma physics.
 - Dynamical models in drug kinetics.

Overview of This Talk

Prelude

- X-ray CT model
- Uncertain view angles

Fugue

- The joint problem of image reconstruction and view angle estimation
- A Bayesian framework
- A hybrid Gibbs sampler
- Some implementation details
- Numerical results

Coda

Conclusions

Applications of X-Ray Computed Tomography (CT)



Lab scanner



Medical scanner





Synchrotron

Industrial inspection

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The Principles of X-Ray CT

The Principle

Send X-rays through the object at different *view angles*, and measure their attenuation.



Lambert-Beer law \rightarrow attenuation of an X-ray through the object fis a line integral:

$$b_i = \int_{\operatorname{ray}_i} f(x,y) \, d\ell \; ,$$

f =attenuation coef.

A discrete version:

A x = b

 $m{A} \sim$ measurement geometry, $m{x} \sim$ reconstruction, $m{b} \sim$ data.



Uncertain View Angles



Each position of the X-ray source is defined by a corresponding view angle θ_i .

The true view angles θ_i^{tru} may differ from the assumed **nominal view an**gles θ_i^{nom} .

- The model for the measured data is $\boldsymbol{b} = \boldsymbol{A}(\theta^{\text{tru}})\boldsymbol{x} + \boldsymbol{e}$, where \boldsymbol{e} is the measurement noise, \boldsymbol{x} represents the image, and $\boldsymbol{A}(\theta^{\text{tru}})$ is the forward model defined for the *unknown* true angles.
- A "naive" (and potentially inferior) reconstruction uses the matrix $A(\theta^{\text{nom}})$ based on the nominal angles.

The Need for Handling Uncertain Angles

A simple example generated with the <u>AIR Tools II</u> MATLAB package:

```
N = 200;
theta_nom = 3:3:180;
theta_true = theta_nom + 0.1*randn(size(theta_nom));
A_nom = paralleltomo(N,theta_nom);
A_true = paralleltomo(N,theta_true);
X = phantomgallery('threephases',N); x = X(:); b = A_true*x;
options.lbound = 0; options.ubound = 1;
x_nom = kaczmarz(A_nom, b,200,[],options);
x_true = kaczmarz(A_true,b,200,[],options);
```

Reconstr. with true angles



Reconstr. with nominal angles



Dealing with Uncertain Angles, No UQ (references in our papers)

Two-stage methods – first estimate the angles ("angle recovery," "alignment reconstitution"), then reconstruct with potential error propagation.

- Cross-correlation of projections of simple objects/phantoms, e.g., with few particles or spheres.
- Obtain information about the object's apparent movement through the use of markers.
- Use methods from computer vision.

Joint methods – estimate the true angles and the reconstruction via a single non-convex optimization problem.

- Solve the joint problem via an alternating variable-projection scheme.
- Solve the joint optimization problem in a Bayesian setting.
- Use a Bayesian approach based on a mixture framework.

Our method uses a Bayesian approach that solves the joint problem and *provides* UQ for both the reconstruction and the view angles.

Formulation of the Joint Problem

Notation:

- The vector **b** holds the measured data.
- The vectors $m{x}$ and $m{ heta}$ hold the image pixels and the view angles.
- The matrix $A(\theta)$ represents the CT forward model for view angles θ .

The inverse problem is linear in \boldsymbol{x} and nonlinar in $\boldsymbol{\theta}$:

find
$$(\pmb{x}, \pmb{ heta})$$
 such that $\pmb{b} = \pmb{A}(\pmb{ heta})\,\pmb{x} + \pmb{e}$

Here \boldsymbol{e} represents additive measurement noise. The noise is log-Poisson; we approximate it with a Gaussian

$$m{e} \sim \mathcal{N}(m{0}, \lambda m{I})$$
 .

We want to be able to reconstruct edges in the image, since edges often carry the most important information, e.g., about defects or tumors.

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The Bayesian Inverse Problem

We formulate a Bayesian inverse problem with a likelihood that involves both \boldsymbol{x} and $\boldsymbol{\theta}$:

$$\pi_{\mathsf{pos}}({\pmb{x}},{\pmb{ heta}}) \; \propto \; \pi_{\mathsf{lik}}({\pmb{b}} \,| \, {\pmb{x}},{\pmb{ heta}}) \; \pi_{\mathsf{pri}}({\pmb{x}}) \; \pi_{\mathsf{pri}}({\pmb{ heta}}) \; .$$

- As mentioned, $\pi_{\mathsf{lik}}(\boldsymbol{b}|\boldsymbol{x}, \boldsymbol{ heta})$ is a Gaussian.
- For π_{pri}(x) we use a Laplace distribution of the differences of neighbour pixels. This enables the desired sharp edges in the image; it has connections to total variation (TV) regularization.
- For $\pi_{pri}(\theta)$ we use the von Mises distribution, i.e., a *periodic* normal distribution $\propto \exp(\kappa \cos(x))$.

Hyperparameters ("uninformative"):

- λ in the Gaussian likelihood,
- δ in the Laplace-difference prior for \pmb{x} ,
- κ in the von Mises prior for θ ,
- exponential distributions $\pi_{\text{hyp}}(\cdot) = \beta \exp(-\beta \cdot)$ with $\beta = 10^{-4}$.



The Posterior

$$\begin{split} \pi_{\mathsf{pos}}(\pmb{x},\pmb{\theta},\lambda,\delta,\kappa) & \propto & \pi_{\mathsf{lik}}(\pmb{b}\,|\,\pmb{x},\pmb{\theta},\lambda)\times\pi_{\mathsf{pri}}(\pmb{x}\,|\delta)\times\pi_{\mathsf{pri}}(\pmb{\theta}\,|\,\kappa) \\ & \times & \pi_{\mathsf{hyp}}(\lambda)\times\pi_{\mathsf{hyp}}(\delta)\times\pi_{\mathsf{hyp}}(\kappa) \end{split}$$

with $oldsymbol{b} \in \mathbb{R}^m$, $oldsymbol{x} \in \mathbb{R}^n$, $oldsymbol{ heta} \in \mathbb{R}^p$ and

in which I = identity matrix and D = bidiag(-1, 1).

Conditional Densities for the Posterior

$$\pi_{pos}(\boldsymbol{x}, \boldsymbol{\theta}, \lambda, \delta, \kappa) = \lambda^{m/2} \, \delta^n \, l_0(\kappa)^{-p} \exp\left(-\frac{\lambda}{2} \|\boldsymbol{A}(\boldsymbol{\theta})\boldsymbol{x} - \boldsymbol{b}\|_2^2 -\delta\left(\|(\boldsymbol{I} \otimes \boldsymbol{D})\boldsymbol{x}\|_1 + \|(\boldsymbol{D} \otimes \boldsymbol{I})\boldsymbol{x}\|_1\right) + \kappa \sum_{i=1}^p \cos(\theta_i - \theta_i^{\text{nom}}) - \beta\lambda - \beta\delta - \beta\kappa\right)$$

Conditional densities:

$$\pi_1(\boldsymbol{x} | \boldsymbol{\theta}, \lambda, \delta) \propto \exp\left(-\frac{\lambda}{2} \|\boldsymbol{A}(\boldsymbol{\theta}) \, \boldsymbol{x} - \boldsymbol{b}\|_2^2 - \delta\left(\|(\boldsymbol{I} \otimes \boldsymbol{D}) \, \boldsymbol{x}\|_1 + \|(\boldsymbol{D} \otimes \boldsymbol{I}) \, \boldsymbol{x}\|_1\right)\right)$$

$$\pi_{2}(\boldsymbol{\theta} | \boldsymbol{x}, \lambda, \kappa) \propto \exp\left(-\frac{\lambda}{2} \|\boldsymbol{A}(\boldsymbol{\theta}) \, \boldsymbol{x} - \boldsymbol{b}\|_{2}^{2} + \kappa \sum_{i=1}^{p} \cos(\theta_{i} - \theta_{i}^{\text{nom}})\right)$$
$$\pi_{3}(\lambda | \boldsymbol{x}, \boldsymbol{\theta}) \propto \lambda^{m/2} \exp\left(-\lambda \left(\frac{1}{2} \|\boldsymbol{A}(\boldsymbol{\theta}) \, \boldsymbol{x} - \boldsymbol{b}\|_{2}^{2} + \beta\right)\right)$$
$$\pi_{4}(\delta | \boldsymbol{x}) \propto \delta^{n} \exp\left(-\delta \left(\|(\boldsymbol{I} \otimes \boldsymbol{D}) \, \boldsymbol{x}\|_{1} + \|(\boldsymbol{D} \otimes \boldsymbol{I}) \, \boldsymbol{x}\|_{1} + \beta\right)\right)$$
$$\pi_{5}(\kappa | \boldsymbol{\theta}) \propto l_{0}(\kappa)^{-p} \exp\left(-\kappa \left(\sum_{i=1}^{p} \cos(\theta_{i} - \theta_{i}^{\text{nom}}) + \beta\right)\right)$$

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$Hybrid\ Gibbs\ Sampler\ \rightarrow\ {\tt Different}\ {\tt Samplers}\ {\tt for}\ {\tt Each}\ {\tt Conditional}$

Initial states $\mathbf{x}^{(0)}, \boldsymbol{\theta}^{(0)}, \lambda^{(0)}, \delta^{(0)}, \kappa^{(0)}$

For $j = 1, 2, \ldots, N_{\mathsf{samp}}$

Sample image pixels

$$\boldsymbol{x}^{(j)} \sim \boldsymbol{\pi}_1(\cdot | \boldsymbol{\theta}^{(j-1)}, \lambda^{(j-1)}, \delta^{(j-1)})$$

Sample view angles

$$\boldsymbol{\theta}^{(j)} \sim \boldsymbol{\pi}_{2} \big(\cdot \, | \, \boldsymbol{x}^{(j)}, \boldsymbol{\lambda}^{(j-1)}, \boldsymbol{\kappa}^{(j-1)} \big)$$

Sample hyperparameters

$$\begin{split} \lambda^{(j)} &\sim \pi_3\left(\cdot \,|\, \boldsymbol{x}^{(j)}, \boldsymbol{\theta}^{(j)} \right. \\ \delta^{(j)} &\sim \pi_4\left(\cdot \,|\, \boldsymbol{x}^{(j)}\right) \\ \kappa^{(j)} &\sim \pi_5\left(\cdot \,|\, \boldsymbol{\theta}^{(j)}\right) \end{split}$$

End

Our implementation draws on several existing methods – our contribution is to bring them together and make them work.

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The Main Challenge: How to Work With π_1

$$\pi_1(\mathbf{x}, \mathbf{\theta}, \lambda, \delta, \kappa) \propto \exp\left(-rac{\lambda}{2} \|\mathbf{A}(\mathbf{ heta}) \, \mathbf{x} - \mathbf{b}\|_2^2 - \delta\left(\|(\mathbf{I} \otimes \mathbf{D}) \, \mathbf{x}\|_1 + \|(\mathbf{D} \otimes \mathbf{I}) \, \mathbf{x}\|_1
ight)
ight)$$

Linear and large-scale in x

• Use an iterative solver: CGLS (conjugate gradients for least squares problems)

Non-differentiable due to $\|\cdot\|_1$

 Introduce the usual smoothing (known from, say, TV) →

Nonlinear in $oldsymbol{ heta}$.

• Wikipedia: Laplace's approximation fits an un-normalised Gaussian approximation to a (twice differentiable) un-normalised target density.



More About Laplace's Approximation

Approximate $\pi_1(\mathbf{x})$ by a *Gaussian* density $\pi_G(\mathbf{x}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{H}^{-1})$ with $\boldsymbol{\mu} = \text{MAP}$ estimator of π_1 and $\boldsymbol{H} = \text{approximate Hessian of } -\log \pi_1$:

$$\mu(\mathbf{x}) = \lambda \mathbf{H}^{-1}(\mathbf{x}) \mathbf{A}(\mathbf{\theta})^{\top} \mathbf{b}$$

$$\mathbf{H}(\mathbf{x}) = \lambda \mathbf{A}(\mathbf{\theta})^{\top} \mathbf{A}(\mathbf{\theta}) + \delta \left((\mathbf{I} \otimes \mathbf{D})^{\top} \mathbf{W}_{1}(\mathbf{x}) (\mathbf{I} \otimes \mathbf{D}) + (\mathbf{D} \otimes \mathbf{I})^{\top} \mathbf{W}_{2}(\mathbf{x}) (\mathbf{D} \otimes \mathbf{I}) \right)$$

$$\mathbf{W}_{1}(\mathbf{x}) = \operatorname{diag} \left[\left\{ ((\mathbf{I} \otimes \mathbf{D})\mathbf{x})^{2} + \varepsilon^{2} \right\}^{-1/2} \right]$$

$$\mathbf{W}_{2}(\mathbf{x}) = \operatorname{diag} \left[\left\{ ((\mathbf{D} \otimes \mathbf{I})\mathbf{x})^{2} + \varepsilon^{2} \right\}^{-1/2} \right]$$

For details see, e.g., (Bardsley, 2018, §4.3.1).

Much easier to work with – but the Gaussian approximation $\pi_{G}(x)$ misses the heavy tails of $\pi_{1}(x)$ and hence our uncertainties are imprecise.

We now develop a so-called *horseshoe prior* (Uribe, Dong, H, 2023), also based on a Gaussian approximation, that can better handle heavy tails.

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How To Sample From π_G ?

In principle we can use Metropolis-Hastings to sample from π_G ; but we only produce one proposal which is always accepted. This is conceptually identical to the unadjusted Langevin algorithm (ULA).

We thus obtain $x^{(j)}$ by solving the following linear least squares problem with a random perturbation of the right-hand side:

$$\min_{\mathbf{x}} \left\| \begin{bmatrix} \sqrt{\lambda} \mathbf{A}(\boldsymbol{\theta}^{(j-1)}) \\ \sqrt{\delta} \mathbf{W}_1(\mathbf{x}^{(j-1)})^{1/2} (\mathbf{I} \otimes \mathbf{D}) \\ \sqrt{\delta} \mathbf{W}_2(\mathbf{x}^{j-1})^{1/2} (\mathbf{D} \otimes \mathbf{I}) \end{bmatrix} \mathbf{x} - \begin{bmatrix} \sqrt{\lambda} \mathbf{b} + \boldsymbol{\xi}_0 \\ \boldsymbol{\xi}_1 \\ \boldsymbol{\xi}_2 \end{bmatrix} \right\|_2$$

where $\boldsymbol{\xi}_i \sim \mathcal{N}(0, \boldsymbol{I})$ for i = 0, 1, 2.

This done by means of the CGLS iterative method.

- Each iteration involves one matrix-vector multiplication with $A(\theta^{(j-1)})$ and one with its transpose.
- We found experimentally that 10 iterations are sufficient.

How to Sample π_2 ?

We introduce a partitioning of the matrix and the rhs, where each block $\boldsymbol{A}(\theta_i)$ and $\boldsymbol{b}(\theta_i)$ correspond to the *i*th view angle.

We use a single-component Metropolis algorithm with componentwise updates applied to

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{A}(\theta_1) \\ \boldsymbol{A}(\theta_2) \\ \vdots \\ \boldsymbol{A}(\theta_p) \end{bmatrix} \quad \boldsymbol{b} = \begin{bmatrix} \boldsymbol{b}(\theta_1) \\ \boldsymbol{b}(\theta_2) \\ \vdots \\ \boldsymbol{b}(\theta_p) \end{bmatrix}$$

$$\pi_2(\boldsymbol{\theta} \,|\, \boldsymbol{x}, \lambda, \kappa) \propto \prod_{i=1}^{p} \exp\left(-\frac{\lambda}{2} \|\boldsymbol{A}(\theta_i) \,\boldsymbol{x} - \boldsymbol{b}(\theta_i)\|_2^2 + \kappa \cos(\theta_i - \theta_i^{\mathsf{nom}})\right).$$

Given $\theta^{[0]} = \theta^{(j-1)}$ from the Gibbs sampler, we perform 20 burn-in cycles:

$$\begin{split} \theta_1^{[k+1]} &\sim \pi_2 \left(\boldsymbol{\theta} \,|\, \boldsymbol{x}, \lambda, \kappa, \left[\theta_2^{[k]}, \theta_3^{[k]}, \dots, \theta_p^{[k]} \right] \right), \\ \theta_2^{[k+1]} &\sim \pi_2 \left(\boldsymbol{\theta} \,|\, \boldsymbol{x}, \lambda, \kappa, \left[\theta_1^{[k+1]}, \theta_3^{[k]}, \dots, \theta_p^{[k]} \right] \right), \\ &\vdots \\ \theta_p^{[k+1]} &\sim \pi_2 \left(\boldsymbol{\theta} \,|\, \boldsymbol{x}, \lambda, \kappa, \left[\theta_1^{[k+1]}, \theta_2^{[k+1]}, \dots, \theta_{p-1}^{[k+1]} \right] \right). \end{split}$$

This produces the next sample $\boldsymbol{\theta}^{(j)} = \boldsymbol{\theta}^{[20]}$ in our hybrid Gibbs sampler.

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Illustration of Working with π_2



Left: von Mises prior with the respective component densities.

Right: zoom-in on selected component densities; the true angles are shown as solid green lines.

In this example, the values of $\pmb{x}, \ \lambda$ and κ are assumed known.

Sampling the Hyperpriors

 \vartriangleright The conditional density π_3 can be written in closed form

$$\pi_{3}(\lambda | \mathbf{x}, \boldsymbol{\theta}) = \frac{\omega^{\tau}}{\Gamma(\tau)} \, \lambda^{\tau-1} \exp(-\omega \, \lambda).$$

with $\tau = \frac{m}{2} + 1$ and $\omega = \frac{1}{2} \|\boldsymbol{A}(\boldsymbol{\theta}) \boldsymbol{x} - \boldsymbol{b}\|_2^2 + \beta$

 \vartriangleright We approximate the conditional density π_4 by a distribution written in closed form

$$\tilde{\pi}_{4}(\delta | \mathbf{x}) \approx \frac{\varpi^{\nu}}{\Gamma(\nu)} \, \delta^{\nu-1} \exp(-\varpi \, \delta)$$

with $\nu = n + 1$ and $\varpi = \mathbf{x}^{\top} ((\mathbf{I} \otimes \mathbf{D})^{\top} \mathbf{W}_1(\mathbf{x}) (\mathbf{I} \otimes \mathbf{D}) + (\mathbf{D} \otimes \mathbf{I})^{\top} \mathbf{W}_2(\mathbf{x}) (\mathbf{D} \otimes \mathbf{I})) \mathbf{x} + \beta.$

 \triangleright Sampling of the conditional density $\pi_5(\kappa | \theta)$ is done by a standard random-walk Metropolis algorithm.

Numerical Experiments

Software: our Python package CUQIpy + <u>ASTRA</u> package for CT models.

We compare with the <u>CT-VAE</u> method (Riis et al., 2020) that computes the MAP estimate (no UQ) through

$$\min_{\mathbf{x}} \frac{1}{2} \| \boldsymbol{C}_{\boldsymbol{\nu}} (\boldsymbol{A}(\boldsymbol{\theta}) \, \boldsymbol{x} - \boldsymbol{b} + \boldsymbol{\mu}_{\boldsymbol{\nu}}) \|_{2}^{2} + \gamma \mathsf{TV}(\boldsymbol{x}),$$

where TV(x) denotes Total Variation regularization and γ = regularization parameter. In this model, ν = measurement noise + model discrepancy, with mean μ_{ν} and covariance matrix $(\boldsymbol{C}_{\nu}^{\top}\boldsymbol{C}_{\nu})^{-1}$.

We generate noisy data

$$\boldsymbol{b} = \boldsymbol{A}(\boldsymbol{\theta}^{ ext{tru}}) \, \boldsymbol{x}^{ ext{tru}} + \boldsymbol{e}, \qquad \boldsymbol{e} \sim \mathcal{N}(\boldsymbol{0}, \sigma^2 \boldsymbol{I})$$

with noise level $\sigma = 0.01 \| \boldsymbol{A}(\boldsymbol{\theta}^{\text{tru}}) \, \boldsymbol{x}^{\text{tru}} \|_2 / \sqrt{m}$.

The Fanbeam CT Problem

Image size $150 \times 150 \rightarrow n = 22500$ pixels. Detector with 225 pixels and p = 90 view angles $0^{\circ}, 4^{\circ}, 8^{\circ}, \dots, 356^{\circ} \rightarrow m = 20250$ measurements. Phantoms "grains" and "ppower" from AIR Tools II.



Estimated View Angles



Left: posterior mean and true view angles θ_i .

Right: zoom-in on component densities for selected θ_i . True angles are shown as solid green lines, posterior mean angles as dashed blue lines, and the angles estimated by the CT-VAE method are shown as dotted red lines.

Estimated Reconstruction of Phantom with 50 Grains



Left: MAP estimate from the CT-VAE method.

Middle: posterior mean and standard deviation from our method.

Right: ditto from hybrid Gibbs sampler with fixed nominal angles.

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Estimated Reconstruction of Phantom with 100 Grains



Left: MAP estimate from the CT-VAE method.

Middle: posterior mean and standard deviation from our method.

Right: ditto from hybrid Gibbs sampler with fixed nominal angles.

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Estimated Reconstruction of Sparse Phantom



Left: MAP estimate from the CT-VAE method.

Middle: posterior mean and standard deviation from our method.

Right: ditto from hybrid Gibbs sampler with fixed nominal angles.

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Posterior Hyperparameters – Sparse Phantom



Samples and estimated densities of λ (noise parameter), δ (Laplace-diff. parameter), and κ (von Mises parameter).

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Coda – Conclusions

In short

- In many CT problems we need to correct for uncertain view angles.
- The Bayesian framework allows us to solve the joint problem ...
- and perform UQ on both the reconstruction and the angles.
- Our numerical results confirm the applicability of our method.

Challenges

- Deriving an efficient sampler is challenging:
 - high dimension problem for the image x,
 - nonlinear problem for the view angles $oldsymbol{ heta}$.
- The Gaussian approximation misses the heavy tails of the posterior; our new *horseshoe prior* seeks to circumvent with this issue.
- A framework for other large-scale inverse problems with uncertain parameters what are good preconditioners for CGLS?
- How to incorporate the framework in our software package CUQIpy?