Polychromatic sparse image reconstruction and mass attenuation spectrum estimation via B-spline basis function expansion†

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Terminology and Notation

- $\|\cdot\|_p$ denotes the ℓ_p norm,
- "$\succeq$" is the elementwise version of "$\geq$",
- I and $\mathbf{0}$ represent an identity matrix and a zero vector,
- B1 spline means B-spline of order 1,
- $I_+(\boldsymbol{\alpha})$ is an indicator function defined as

$$I_+(\boldsymbol{\alpha}) \triangleq \begin{cases} 0, & \boldsymbol{\alpha} \succeq \mathbf{0} \\ +\infty, & \text{otherwise} \end{cases}$$

- $\iota^{\mathsf{L}}(s)$ is the *Laplace transform* of $\iota(\kappa)$:

$$\iota^{\mathsf{L}}(s) \triangleq \int \iota(\kappa) \mathrm{e}^{-s\kappa} \, \mathrm{d}\kappa$$

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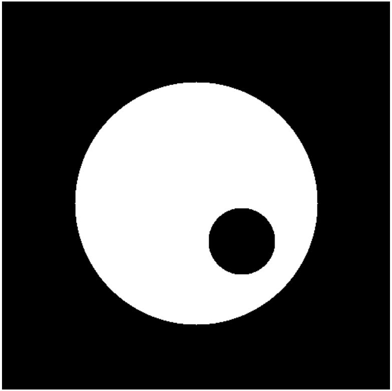
Numerical Examples

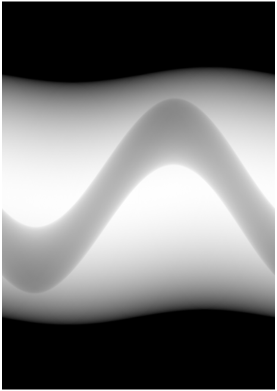
Conclusion

Introduction to CT Imaging

An X-ray computed tomography (CT) scan consists of hundreds of projections with the beam intensity measured by thousands of detectors for each projection.



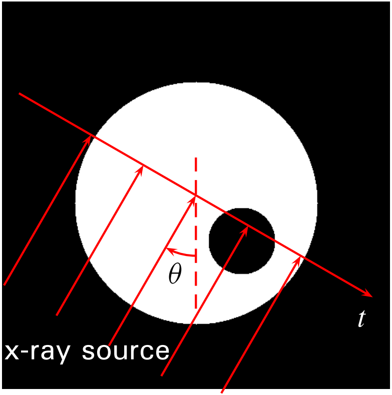
Image



sinogram

Introduction to CT Imaging (Parallel Beam)

A detector array is deployed parallel to the t axis and rotates against the X-ray source collecting projections. Sinogram is the set of collected projections as a function of angle at which they are taken.



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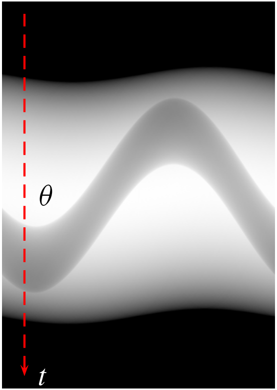

sinogram

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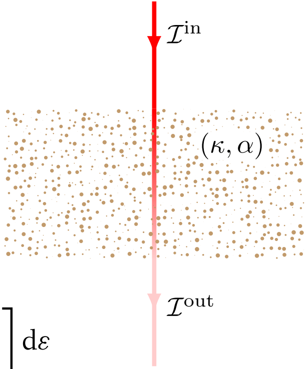
Polychromatic X-ray CT Model

- Incident energy $\mathcal{I}^{\text{in}}$ spreads along photon energy ε with density $\iota(\varepsilon)$:

$$\int \iota(\varepsilon)\,\mathrm{d}\varepsilon = \mathcal{I}^{\text{in}}.$$



- Noiseless energy measurement obtained upon traversing a straight line $\ell = \ell(x, y)$ through an object composed of a single material:

$$\mathcal{I}^{\text{out}} = \int \iota(\varepsilon) \exp\left[-\kappa(\varepsilon) \int_{\ell} \alpha(x, y)\,\mathrm{d}\ell\right] \mathrm{d}\varepsilon$$

where $\kappa(\varepsilon)$ is object's mass attenuation function.

Problem Formulation and Goal

Assume that

- both
  - the incident spectrum $\iota(\varepsilon)$ of X-ray source and
  - mass attenuation function $\kappa(\varepsilon)$ of the object

  are unknown.

Goal

- Estimate the density map $\alpha(x, y)$.

Polychromatic X-ray CT Model via Mass Attenuation

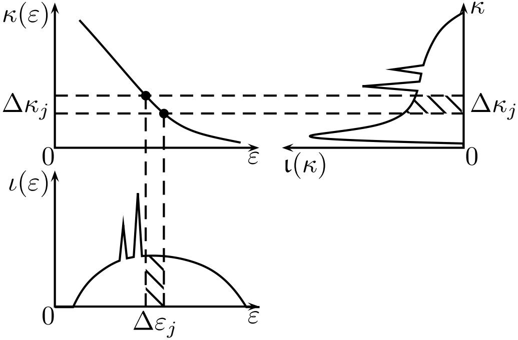


Figure 1: Relation between mass attenuation κ, incident spectrum ι, photon energy ε, and mass attenuation spectrum $\iota(\kappa)$.

Polychromatic X-ray CT Model via Mass Attenuation

We propose a polychromatic X-ray model via mass attenuation:

$$\mathcal{I}^{\text{in}} = \iota^{\mathsf{L}}(0), \qquad \mathcal{I}^{\text{out}} = \iota^{\mathsf{L}}\left(\int_{\ell} \alpha(x, y)\, \mathrm{d}\ell\right)$$

where

$$\iota^{\mathsf{L}}(s) \triangleq \int \iota(\kappa) \mathrm{e}^{-\kappa s}\, \mathrm{d}\kappa$$

is the *Laplace transform* of $\iota(\kappa)$,[2] see also [GD13a].
We need to estimate one function, $\iota(\kappa)$, rather than two, $\iota(\varepsilon)$ and $\kappa(\varepsilon)$!

▸ more

[2] Here, $s > 0$, in contrast with the traditional Laplace transform where s is generally complex.

Assumptions and Parameter Constraints

- Object's shadow covered by the receiver array;
- Known upper bound $\mathcal{I}^{\text{in}}_{\text{MAX}}$ on incident energy $\mathcal{I}^{\text{in}}$:

$$\mathcal{I}^{\text{in}} \leq \mathcal{I}^{\text{in}}_{\text{MAX}} \qquad \text{(total input energy constraint);}$$

- $\iota(\kappa)$ and $\alpha(x,y)$ are nonnegative for all κ, x and y:

$$\iota(\kappa) \geq 0, \qquad \alpha(x,y) \geq 0;$$

- Discretized density map $\alpha(x,y)$ is sparse in the discrete wavelet transform (DWT) domain.

Basis-function expansion of $\iota(\kappa)$

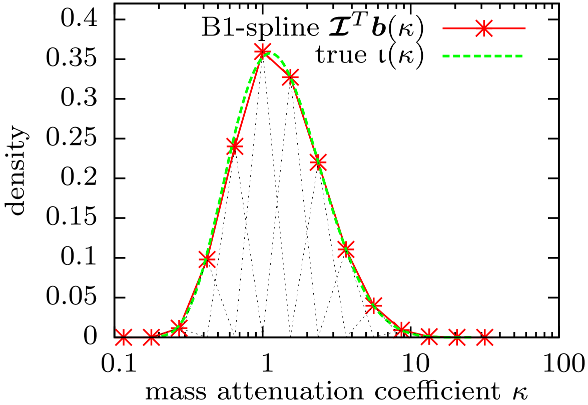


Figure 2: B1-spline approximation of $\iota(\kappa)$

Basis-function expansion of $\iota(\kappa)$

Express $\iota(\kappa)$ as a linear combination of J basis functions $\iota(\kappa) = \boldsymbol{\mathcal{I}}^T \boldsymbol{b}(\kappa)$ and discretize over space:

$$\mathcal{I}^{\text{in}} = \boldsymbol{\mathcal{I}}^T \boldsymbol{b}^{\mathsf{L}}(0), \qquad \mathcal{I}^{\text{out}} = \boldsymbol{\mathcal{I}}^T \boldsymbol{b}^{\mathsf{L}}(\boldsymbol{\phi}^T \boldsymbol{\alpha}) \tag{1}$$

where $\boldsymbol{b}^{\mathsf{L}}(s)$ is the Laplace transform of $\boldsymbol{b}(\kappa)$,

- $\boldsymbol{\mathcal{I}}$ is the $J \times 1$ vector of corresponding basis function coefficients,
- $\boldsymbol{\alpha}$ is a $p \times 1$ column vector representing the 2-D image $\alpha(x, y)$ that we wish to reconstruct,
- $\boldsymbol{\phi}$ is a $p \times 1$ vector of weights quantifying how much each element of $\boldsymbol{\alpha}$ contributes to the X-ray attenuation on the straight-line path ℓ.

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Noise Model

Assume noisy energy measurements $\{\mathcal{E}_i\}_{i=1}^{N}$ corrupted by lognormal noise, which yields

$$\mathcal{L}(\Phi\boldsymbol{\alpha},\mathcal{I}) = \left\| \begin{bmatrix} -\ln \mathcal{E}_1 \\ \vdots \\ -\ln \mathcal{E}_N \end{bmatrix} - \begin{bmatrix} -\ln\left[\boldsymbol{\mathcal{I}}^T \boldsymbol{b}^{\mathsf{L}}([\Phi\boldsymbol{\alpha}]_1)\right] \\ \vdots \\ -\ln\left[\boldsymbol{\mathcal{I}}^T \boldsymbol{b}^{\mathsf{L}}([\Phi\boldsymbol{\alpha}]_N)\right] \end{bmatrix} \right\|_2^2$$

where

- $\mathcal{L}(\Phi\boldsymbol{\alpha},\mathcal{I})$ is the negative log likelihood determined by the underlying noise model, and
- $\Phi = [\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \ldots, \boldsymbol{\phi}_N]^T$ is the $N \times p$ Radon transform matrix.

Constrained Penalized Optimization

$$\min_{\substack{\boldsymbol{\alpha},\mathcal{I} \\ C\mathcal{I}\succeq\boldsymbol{c}}} \mathcal{L}(\Phi\boldsymbol{\alpha},\mathcal{I}) + u\Big[\underbrace{\|\Psi^T\boldsymbol{\alpha}\|_1 + I_+(\boldsymbol{\alpha})}_{\triangleq r(\boldsymbol{\alpha})}\Big]$$

where

- $u > 0$ is a scalar tuning constant and
- Ψ^T is the sparsifying transform (DWT) matrix.

Goal: Estimate the image and incident energy density parameters

$$(\boldsymbol{\alpha},\mathcal{I}).$$

Alternating Descent Algorithm (NPG-AS)

Descend the objective $\mathcal{L}(\Phi\boldsymbol{\alpha}, \mathcal{I}) + u\,r(\boldsymbol{\alpha})$ by alternating between ❶ and ❷, where Iteration $i+1$ proceeds as follows:

1. *Nesterov's proximal-gradient (NPG) step* [Nes13] for $\boldsymbol{\alpha}$ with fixed $\mathcal{I} = \mathcal{I}^{(i)}$, yielding $\boldsymbol{\alpha}^{(i+1)}$, and
2. the *active-set (AS)* [GMW81, Ch. 5] step for $\mathcal{I}$ with fixed $\boldsymbol{\alpha} = \boldsymbol{\alpha}^{(i+1)}$, yielding $\mathcal{I}^{(i+1)}$

and i denotes the iteration index.

Iteration Step ❶ for Estimating $\boldsymbol{\alpha}$ (NPG)

❶ aims at minimizing $\underbrace{\mathcal{L}(\Phi\boldsymbol{\alpha}, \mathcal{I}^{(i)})}_{\triangleq l(\boldsymbol{\alpha})} + u r(\boldsymbol{\alpha})$.

Nesterov's proximal-gradient step for $\boldsymbol{\alpha}$ in Iteration $i+1$:

$$\theta^{(i+1)} = \frac{1}{2}\left[1 + \sqrt{1 + 4\left(\theta^{(i)}\right)^2}\right]$$

$$\bar{\boldsymbol{\alpha}}^{(i+1)} = \boldsymbol{\alpha}^{(i)} + \frac{\theta^{(i)} - 1}{\theta^{(i+1)}}\left(\boldsymbol{\alpha}^{(i)} - \boldsymbol{\alpha}^{(i-1)}\right) \qquad \text{Nesterov acceleration}$$

$$\boldsymbol{\alpha}^{(i+1)} = \operatorname{prox}_{\beta u r}\left(\bar{\boldsymbol{\alpha}}^{(i+1)} - \beta \nabla l\left(\bar{\boldsymbol{\alpha}}^{(i+1)}\right)\right) \qquad \text{proximal gradient}$$

where $\beta > 0$ is a step size and $\frac{\theta^{(i)}-1}{\theta^{(i+1)}}$ is extrapolation weight [XY13].

▸ ADMM ▸ Step Size

Iteration Step ❷ for Estimating $\mathcal{I}$ (AS)

❷ aims at minimizing $\mathcal{L}(\Phi\boldsymbol{\alpha}^{(i+1)}, \mathcal{I})$ under the linear constraints:

$$C\mathcal{I} \succeq \boldsymbol{c}$$

where

$$C \triangleq \begin{bmatrix} I \\ -\frac{[\boldsymbol{b}^{\mathsf{L}}(0)]^T}{\|\boldsymbol{b}^{\mathsf{L}}(0)\|_2} \end{bmatrix} \qquad \boldsymbol{c} \triangleq \begin{bmatrix} \mathbf{0} \\ -\frac{\mathcal{I}^{\mathsf{in}}_{\mathsf{MAX}}}{\|\boldsymbol{b}^{\mathsf{L}}(0)\|_2} \end{bmatrix}.$$

The active-set method uses gradient-projection to search for active constraints and simultaneously approximate the quadratic steepest descent step for the simplified problem under these equality constraints, see [GD13b] for details.

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Simulation Example I

- The inspected object, assumed to be made of iron, contains irregularly shaped inclusions.

Figure 3: The ‘ground truth’ 1024×1024 image.

Simulation Example II

- Mass-attenuation function $\kappa(\varepsilon)$ for iron extracted from the NIST database [HS95].
- Polychromatic sinogram simulated using photon-energy discretization with 130 equi-spaced discretization points over the range 20 keV to 150 keV that approximates well the support of $\iota(\varepsilon)$.

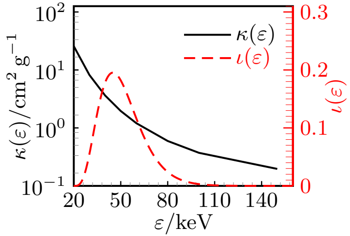

Figure 4: Simulated mass attenuation and incident X-ray spectrum as functions of the photon energy ε.

Simulation Example III

- 1024-element measurement array;
- Radon transform matrix Φ constructed directly on GPU (multi-thread version on CPU is also available) with full circular mask [DGQ11];
- Our performance metric is the relative square error (RSE) of an estimate $\widehat{\boldsymbol{\alpha}}$ of the signal coefficient vector:

$$\mathrm{RSE}\{\widehat{\boldsymbol{\alpha}}\} = 1 - \left(\frac{\widehat{\boldsymbol{\alpha}}^T \boldsymbol{\alpha}}{\|\widehat{\boldsymbol{\alpha}}\|_2 \|\boldsymbol{\alpha}\|_2} \right)^2.$$

Compared Methods

- the traditional filtered backprojection (FBP) method w/wo linearization,[3]
- the FPC_{AS} method [Wen + 10] w/wo linearization
- our constrained penalized least-squares (CPLS) method [GD14],
- our
  - NPG-AS alterating descent method and
  - NPG for known mass attenuation spectrum $\iota(\kappa)$.
- the PG-AS method (without Nesterov's acceleration strategy).

Maximum number of iterations is $M = 2000$ for all iterative methods.
We normalize the energy measurements by their largest value and set $\mathcal{I}^{\text{in}}_{\text{MAX}} = 1$.

more

[3] linearization requires knowing the spectrum and mass attenuation (material) exactly

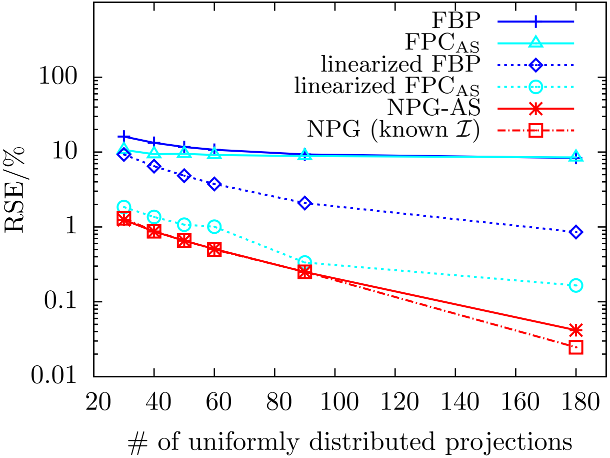

Figure 5: RSE versus the number of equally spaced projections for different reconstruction methods.

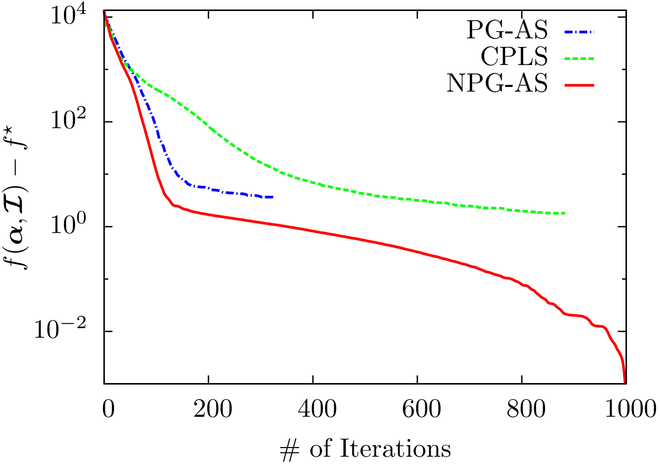

Figure 6: Centered objective $f - f^\star$ versus # of iterations for reconstructions from 180 parallel projections.[4]

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[4] $f(\boldsymbol{\alpha}, \boldsymbol{\mathcal{I}}) = \mathcal{L}(\Phi\boldsymbol{\alpha}, \boldsymbol{\mathcal{I}}) + ur(\boldsymbol{\alpha})$ and $f^\star$ is it optimal value.

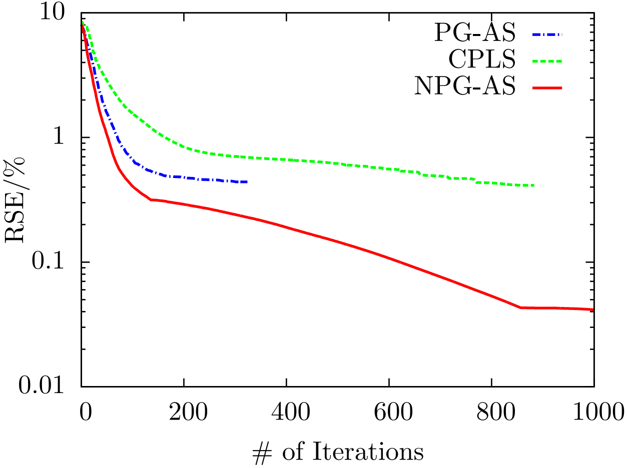
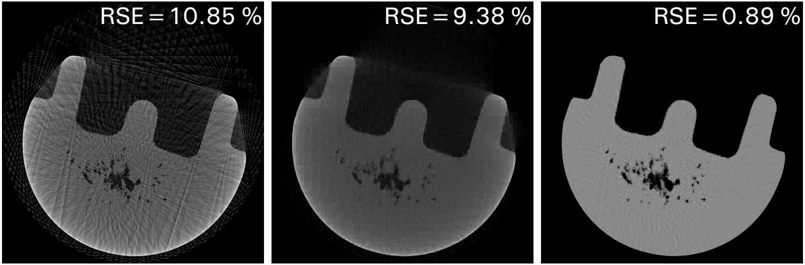


Figure 7: RSE versus # of iterations for reconstructions from 180 parallel projections.



(a) FBP (b) $\mathrm{FPC}_{\mathrm{AS}}$ (c) NPG-AS

Figure 8: Reconstructions from 40 parallel projections.

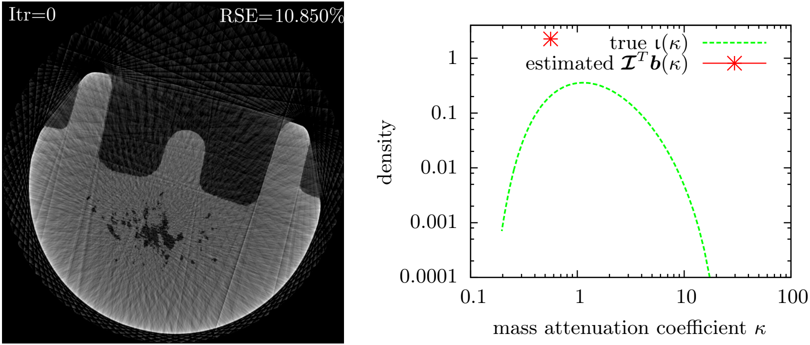
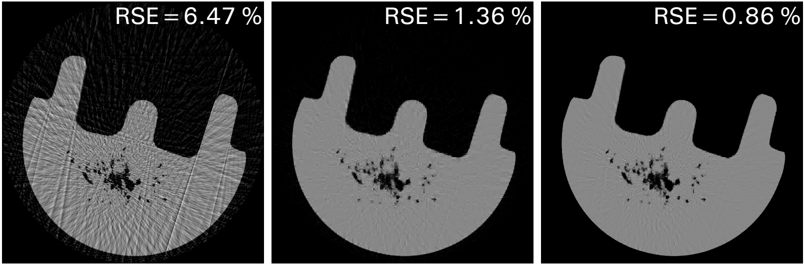


Figure 9: Estimated $\boldsymbol{\alpha}$ and $\mathcal{I}^T\boldsymbol{b}(\kappa)$ from 40 parallel projections.



(a) linearized FBP (b) linearized $\mathrm{FPC}_{\mathrm{AS}}$ (c) NPG

Figure 10: Reconstructions from 40 parallel projections with prior knowledge of the X-ray spectrum and the inspected material.

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Future Work

- Apply other noise models
  - e.g., Poisson,

  and penalty functions,
  - e.g., total variation.
- Generalize our polychromatic signal model to handle multiple materials and develop corresponding reconstruction schemes for this scenario.

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Polychromatic X-ray CT Model via Mass Attenuation

For invertible $\kappa(\varepsilon)$[5], define its inverse as $\varepsilon(\kappa)$. Then,

$$\mathcal{I}^{\text{in}} = \int \iota(\kappa)\,\mathrm{d}\kappa, \qquad \mathcal{I}^{\text{out}} = \int \iota(\kappa) \exp\left[-\kappa \int_\ell \alpha(x, y)\,\mathrm{d}\ell\right] \mathrm{d}\kappa$$

where

$$\iota(\kappa) \triangleq \iota(\varepsilon(\kappa))|\varepsilon'(\kappa)|$$

is the mass attenuation spectrum and the function $\varepsilon(\kappa)$ is differentiable with derivative

$$\varepsilon'(\kappa) = \frac{\mathrm{d}\varepsilon(\kappa)}{\mathrm{d}\kappa}$$

back

[5] Assumed for simplicity, extends easily to arbitrary $\kappa(\varepsilon)$.

Linearization

Note: Since $\iota^{\mathsf{L}}(s)$ is an invertible function of s, we can pre-process the energy measurements as follows:

$$(\iota^{\mathsf{L}})^{-1}(\mathcal{E}_i)$$

which is referred to as *linearization*.
We can then apply linear reconstruction methods to the above linearized measurements.

back

Constrained Penalized Optimization

Compared with CPLS [GD13b; GD14], we

- impose the nonnegativity constraint on the density map $\boldsymbol{\alpha}$ *directly* and hence eliminate one tuning constant,
- use exact ℓ_1 norm instead of its approximation and hence eliminate another tuning constant and improve the reconstruction performance,
- introduce a more general log likelihood term to handle Poisson and other noise models, in addition to the lognormal noise nodel.

back

ADMM Subroutine for the Proximal Operation

$$\operatorname{prox}_{\lambda r}(\boldsymbol{a}) = \arg\min_{\boldsymbol{\alpha}} \frac{1}{2}\|\boldsymbol{\alpha} - \boldsymbol{a}\|_2^2 + \lambda\|\Psi^T\boldsymbol{\alpha}\|_1 + \mathbb{I}_{[0,+\infty)}(\boldsymbol{\alpha})$$

Alternating direction method of multipliers (ADMM) [PB13] solves the proximal problem with the j-th iteration:

$$\boldsymbol{z}^{(j+1)} = \Psi\mathcal{T}_{\lambda/\rho}\left[\Psi^T(\boldsymbol{\alpha}^{(j)} - \boldsymbol{v}^{(j)})\right] \tag{2a}$$

$$\boldsymbol{\alpha}^{(j+1)} = \frac{1}{1+\rho}\left(\boldsymbol{a} + \rho(\boldsymbol{z}^{(j+1)} + \boldsymbol{v}^{(j)})\right)_+ \tag{2b}$$

$$\boldsymbol{v}^{(j+1)} = \boldsymbol{v}^{(j)} + \boldsymbol{z}^{(j+1)} - \boldsymbol{\alpha}^{(j+1)} \tag{2c}$$

where $\rho > 0$ is quadratic penalty parameter, usually set to 1.

back

Step Size β Selection

The step size β is adjusted by the backtracking strategy, which sets

$$\beta \leftarrow \beta/2$$

whenever the majorization condition

$$l(\boldsymbol{\alpha}^{(i)}) \leq l(\overline{\boldsymbol{\alpha}}^{(i)}) + \left(\boldsymbol{\alpha}^{(i)} - \overline{\boldsymbol{\alpha}}^{(i)}\right)^T \nabla l\left(\overline{\boldsymbol{x}}^{(i)}\right) + \frac{1}{2\beta}\left\|\boldsymbol{\alpha}^{(i)} - \overline{\boldsymbol{\alpha}}^{(i)}\right\|_2^2 \quad (3)$$

is violated. Note that (3) ensures descent of the objective function.

In our numerical examples, β is initialized by the Barzilai-Borwein (BB) method:

$$\frac{\left(\nabla l(\boldsymbol{\alpha}^{(0)})\right)^T \nabla l\left(\boldsymbol{\alpha}^{(0)} + \delta \nabla l(\boldsymbol{\alpha}^{(0)})\right)}{\delta \left\|\nabla l(\boldsymbol{\alpha}^{(0)})\right\|_2^2}$$

back