Automatic alignment for Tomographic reconstruction

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Mathematical formulation & approach



Express the reconstruction problem as an optimization problem:

$$\min_{\mathbf{x}} \|W\mathbf{x} - \mathbf{p}\|_2^2,$$

where

- $\mathbf{x} \in \mathbb{R}^n$ image
- $\mathbf{p} \in \mathbb{R}^{lm}$ projection data
- $W \in \mathbb{R}^{lm imes n}$ projection matrix
- *n* number of pixels (voxels)
- I number of angles
- *m* number of detector pixels



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For example, in a 2D parallel beam geometry, **a** consists of an angle and offset perturbation for each projection angle.



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Bi-level optimization problem

$$\min_{\mathbf{x},\mathbf{a}} \|W(\mathbf{a})\mathbf{x} - \mathbf{p}\|_2^2,$$



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$$\min_{\mathbf{x},\mathbf{a}}\sum_{i=1}^{l}\|W_i(\mathbf{a}_i)\mathbf{x}-\mathbf{p}_i\|_2^2,$$

- W_i projection matrix for the ith angle
- \mathbf{a}_i alignment parameters for the i^{th} angle,
- \mathbf{p}_i projection data for the *i*th angle.



Can we retrieve both \mathbf{x} and \mathbf{a} ?



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- If W has full row-rank, we can fit the data for any **a**
- How well we can retrieve a depends on x
- Solution is at best unique up to global shifts and rotations



How do we solve the bi-level optimization problem?

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Exploit structure:

• quadratic in x, non-linear in a



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$$\min_{\mathbf{x},\mathbf{a}}\sum_{i=1}^{l}\|W_i(\mathbf{a}_i)\mathbf{x}-\mathbf{p}_i\|_2^2,$$

Exploit structure:

- quadratic in x, non-linear in a
- for fixed x, separates in l independent low-dimensional problems for a_i



Intermezzo: Variable projection



Intermezzo: Variable projection [Golub & Pereyra, 1973]

 $\min_{\mathbf{x},\mathbf{y}} \|A(\mathbf{y})\mathbf{x} - \mathbf{b}\|_2^2,$

- eliminate **x** explicitly as $\mathbf{x} = A(\mathbf{y})^{\dagger}\mathbf{b}$,
- formulate a non-linear least-squares problem:

$$\min_{\mathbf{y}} \left\| \left(A(\mathbf{y})A(\mathbf{y})^{\dagger} - I \right) \mathbf{b} \right\|_{2}^{2}$$

• this approach is superior to solving the joint problem with a GN method.



This idea can be generalized to solve problems of the form

 $\min_{\mathbf{x},\mathbf{y}} f(\mathbf{x},\mathbf{y}),$

by solving for $\overline{\mathbf{x}}$ s.t. $\nabla_{\mathbf{x}} f(\overline{\mathbf{x}}, \mathbf{y}) = 0$ and substituting this back:

 $\min_{y} \overline{f}(\mathbf{y}),$

with $\overline{f}(\mathbf{y}) = f(\overline{\mathbf{x}}(\mathbf{y}), \mathbf{y})$.



Theorem [Aravkin & van Leeuwen, 2012]

Given a twice-differentiable function $f(\mathbf{x}, \mathbf{y})$, define $\overline{f}(\mathbf{y}) = f(\overline{\mathbf{x}}, \mathbf{y})$ with $\nabla_{\mathbf{x}} f(\overline{\mathbf{x}}, \mathbf{y}) = 0$ then

$$\nabla \overline{f}(\mathbf{y}) = \nabla_{\mathbf{y}} f(\overline{\mathbf{x}}, \mathbf{y}),$$

and

$$\nabla^2 \overline{f} = \nabla_{\mathbf{y}}^2 f - \nabla_{\mathbf{x},\mathbf{y}} f^{\mathsf{T}} \left(\nabla_{\mathbf{x}}^2 f \right)^{-1} \nabla_{\mathbf{x},\mathbf{y}} f.$$



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Corollary

If, in addition, we require that $\nabla_{\mathbf{x}}^2 f(\overline{\mathbf{x}}, \mathbf{y}) \succeq 0$, then a local minimum $\overline{\mathbf{y}}$ of \overline{f} , together with the corresponding $\overline{\mathbf{x}}$ is a local minimum of f.



A gradient-based method for minimizing \overline{f} can be implemented as follows

Algorithm

$$\mathbf{x}^{(k+1)} = \operatorname{argmin}_{\mathbf{x}} f(\mathbf{x}, \mathbf{y}^{(k)})$$

$$\mathbf{y}^{(k+1)} = \mathbf{y}^{(k)} - \alpha_k \nabla_{\mathbf{y}} f(\mathbf{x}^{(k+1)}, \mathbf{y}^{(k)})$$



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We are completely free to choose the most appropriate method to solve the inner and outer optimization problems.



Algorithms



Bi-level optimization problem

$$\min_{\mathbf{x},\mathbf{a}} \|W(\mathbf{a})\mathbf{x} - \mathbf{p}_i\|_2^2,$$

There are two natural choices:

- project out a (Align-then-Reconstruct),
- project out x (Reconstruct-then-Align).





• Use favourite method to solve alignment problems (independently)





$$\begin{aligned} \mathbf{a}_i^{(k+1)} &= \operatorname*{argmin}_{\mathbf{a}_i} \| W_i(\mathbf{a}_i) \mathbf{x}^{(k)} - \mathbf{p}_i \|_2^2 \\ \mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + \Delta \mathbf{x}^{(k)} \end{aligned}$$

- Use favourite method to solve alignment problems (independently)
- Use GN method to compute $\Delta \mathbf{x}^{(k)}$:



Basic algorithm for A-R (modified)

$$\mathbf{a}_i^{(k+1)} = \underset{\mathbf{a}_i}{\operatorname{argmin}} \| W_i(\mathbf{a}_i) \mathbf{x}^{(k)} - \mathbf{p}_i \|_2^2$$
$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \Delta \mathbf{x}^{(k)}$$

- Use favourite method to solve alignment problems (independently)
- Use GN method to compute $\Delta \mathbf{x}^{(k)}$:

$$\Delta \mathbf{x}^{(k)} = W(\mathbf{a}^{(k+1)})^{\dagger} \left(\mathbf{p} - W(\mathbf{a}^{(k+1)}) \mathbf{x}^{(k)} \right)$$



Algorithm for R-A $\mathbf{x}^{(k+1)} = W(\mathbf{a}^{(k)})^{\dagger}\mathbf{p}$ $\mathbf{a}^{(k+1)} = \mathbf{a}^{(k)} + \Delta \mathbf{a}^{(k)},$

• Use standard iterative (Krylov) method to apply pseudo-inverse



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Take Δa^(k) to be the (scaled) negative gradient:



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 $\mathbf{a}^{(k+1)} = \mathbf{a}^{(k)} + \Delta \mathbf{a}^{(k)},$

- Use standard iterative (Krylov) method to apply pseudo-inverse
- Take $\Delta \mathbf{a}^{(k)}$ to be the (scaled) negative gradient:

$$\begin{split} \Delta \mathbf{a}^{(k)} \propto -J(\mathbf{x}^{(k+1)}, \mathbf{a}^{(k)})^T \left(W(\mathbf{a}^{(k)})\mathbf{x}^{(k+1)} - \mathbf{p} \right), \\ \text{where } J(\mathbf{x}, \mathbf{a}) = \left(\frac{\partial W(\mathbf{a})\mathbf{x}}{\partial \mathbf{a}} \right) \end{split}$$



Numerical examples



$$(W_{h,\Delta\theta}f)(r,\theta) = \int_{\Omega} \mathrm{d}s \, f(s)\delta(r+h-n(\theta+\Delta\theta)\cdot s),$$



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where $\Omega = [-1, 1]^2$, $r \in [-1, 1]$, $\theta \in [0, \pi)$, $n(\theta) = (\cos(\theta), \sin(\theta))^T$.

• Discretize domain using *n* pixels, use midpoint rule to approximate integral,



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Possible issues:

- Gradient w.r.t. **a** might not be available; use appropriate derivative-free method [Nocedal & Wright, 2006]
- Renegade null-space elements may cause problems in A-R approach



Conclusions



• Unified mathematical framework to derive algorithms for automatic alignment



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- Decouple alignment and reconstruction problems by *variational projection*



- Unified mathematical framework to derive algorithms for automatic alignment
- Decouple alignment and reconstruction problems by *variational projection*
- Regularization (e.g., TV) can be included
- Further analysis needed to understand exactly why R-A approach appears to work better



Thank you!



Bibliography



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