Stochastic Optimisation for Large-Scale Inverse Problems

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6 September, 2024

Main Aim and Outline

$$x^\sharp \in \arg\min_x \left\{ \sum_{i=1}^n f_i(A_i x) + g(x) \right\}$$

- proper, convex and lower semi-continuous
- n large and/or $A_i x$ expensive

Outline:

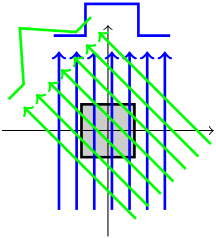
1) **Why?** Inverse Problems and Optimization
2) **How?** Randomized Algorithms for Convex Optimization
3) **So what?** Applications: PET, CT, ...

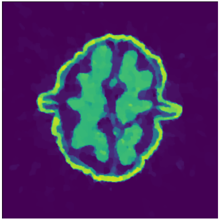
CT Reconstruction with TV

Total variation (TV)

Rudin, Osher, Fatemi '92

$$\mathcal{R}(x) = \|Dx\|_1$$





$$\min_x \left\{ \sum_{j=1}^{s} \|K_j x - b_j\|^2 + \lambda \|Dx\|_1 + \imath_+(x) \right\}$$

$$\min_x \left\{ \sum_{i=1}^{n} f_i(A_i x) + g(x) \right\}$$

$n = s$
$f_i(y) = \|y - b_i\|^2 \quad i \in [n]$
$A_i = K_i \quad i \in [n]$
$g(x) = \lambda \|Dx\|_1 + \imath_+(x)$

Motion corrected CT reconstruction

$$\min_x \left\{ \sum_{i=1}^{s} \|K M_i x - b_i\|^2 + \mathcal{R}(x) \right\}$$

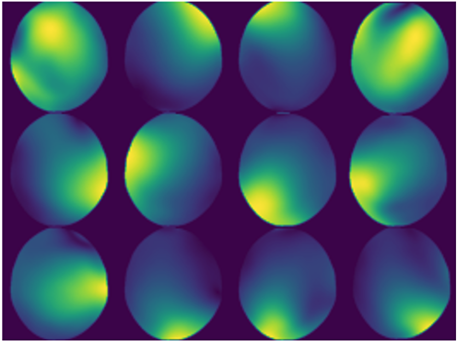
- M_i motion transformation
- here $s = 10$ motion gates; computations are a bottleneck
- No motion correction: $M_i = I$

e.g. Delplancke, Thielemans, Ehrhardt '21

Parallel MRI

$$\min_x \left\{ \sum_{i=1}^{s} \|SF C_i x - b_i\|^2 + \mathcal{R}(x) \right\}$$

- C_i sensitivity map for ith MR coil, $s = 12$



Pruessmann et al. '99

Stochastic Optimisation Algorithms

Building blocks for Convex Optimisation

Template:

$$\min_x \{f(Ax) + g(x) = F(x) + g(x)\}$$

- Ingredient 1 (gradient descent)

$$x^+ = x - \tau \nabla F(x)$$

- Ingredient 2 (proximal point algorithm)

$$x^+ = \mathrm{prox}_{\tau g}(x) = \arg\min_z \left\{ \frac{1}{2}\|z - x\|^2 + \tau g(z) \right\}$$

- Ingredient 3 (conjugation)
  if f is prox-friendly, but $f \circ A$ is not: split f and A
  $f(Ax) = f^{**}(Ax) = \sup_y \{\langle Ax, y\rangle - f^*(x)\}$

  Dual: $\min_y \{f^*(y) + g^*(-A^*y)\}$
  Primal-Dual: $\min_x \max_y \{\langle Ax, y\rangle - f^*(y) + g(x)\}$

Building Algorithms

Template: $\min_x \{f(Ax) + g(x) = F(x) + g(x)\}$

New algorithms are designed by mix-and-match:

Proximal Gradient Descent: Combettes and Wajs '05

$$x^+ = \mathrm{prox}_{\tau g}(x - \tau \nabla F(x))$$

Primal-Dual Hybrid Gradient Chambolle and Pock '11

$$x^+ = \mathrm{prox}_{\tau g}(x - \tau A^* y)$$

$$\overline{x} = x + \theta(x^+ - x)$$

$$y^+ = \mathrm{prox}_{\sigma f^*}(y + \sigma A\overline{x})$$

Revisiting Gradient Descent: SGD and its variants ($g = 0$)

GD

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$$x^+ = x - \tau \sum_{i=1}^{n} \nabla F_i(x)$$

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SGD and variants

Uniformly at random select j

$$x^+ = x - \tau \tilde{\nabla}^j F(x)$$

- SGD: randomly choose j,

$$\tilde{\nabla}^j F(x) = n \nabla F_j(x)$$

nonconvergence for fixed τ, "slow" convergence for carefully decreasing τ Robbins and Monro '51

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- SAGA/SVRG: randomly choose j,

$$\tilde{\nabla}^j F(x) = n(\nabla F_j(x) - G_j) + G$$

  G historic gradient, G_j historic stochastic gradient Defazio et al. '14, Johnsen and Zhang '13, SAGA converges for $\tau \leq 1/(3nL_{\max})$

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- Similar algorithms for proximal point Bianchi '16, Traore et al. '23

Revisiting PDHG

PDHG:

$$
\begin{aligned}
x^+ &= \mathrm{prox}_{\tau g}(x - \tau A^* y) \\
\overline{x} &= x^+ + \theta(x^+ - x) \\
y^+ &= \mathrm{prox}_{\sigma f^*}(y + \sigma A\overline{x})
\end{aligned}
$$

Revisiting PDHG

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$$y^+ = \text{prox}_{\sigma f^*}(y + \sigma A\bar{x})$$

PDHG (dual extrapolation):

$$y^+ = \text{prox}_{\sigma f^*}(y + \sigma A x)$$
$$\bar{y} = y^+ + \theta(y^+ - y)$$
$$x^+ = \text{prox}_{\tau g}(x - \tau A^* \bar{y})$$

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PDHG (dual extrapolation with $f = \sum_i f_i$):

$$y_i^+ = \mathrm{prox}_{\sigma f_i^*}(y_i + \sigma A_i x), \quad i = 1, \ldots, n$$
$$\overline{y}_i = y_i^+ + \theta(y_i^+ - y_i), \quad i = 1, \ldots, n$$
$$x^+ = \mathrm{prox}_{\tau g}\left(x - \tau \sum_{i=1}^n A_i^* \overline{y}_i\right)$$

From PDHG to SPDHG

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Stochastic PDHG (SPDHG): Chambolle, Ehrhardt, Richtárik, Schönlieb '18

Uniform at randomly select j

$$y_i^+ = \text{prox}_{\sigma f_i^*}(y_i + \sigma A_i x), \quad i = j$$

$$\overline{y}_i = y_i^+ + \theta n(y_i^+ - y_i), \quad i = j; \quad \overline{y}_i = y_i \text{ else}$$

$$x^+ = \text{prox}_{\tau g}(x - \tau \textstyle\sum_{i=1}^n A_i^* \overline{y}_i)$$

- convergence for $\sigma\tau < 1/(n \max_i \|A_i\|^2)$, $\theta = 1$
  Chambolle, Ehrhardt, Richtárik, Schönlieb '18, Gutiérrez, Delplancke, Ehrhardt '21, Alacaoglu, Fercoq, Cevher '22

SPDHG as SAGA

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SPDHG as SAGA (new):

Uniform at randomly select j

$$y_i^+ = \mathrm{prox}_{\sigma f_i^*}(y_i + \sigma A_i x), \quad i = j$$

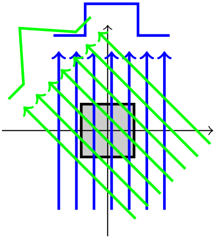
$$\tilde{\nabla}^j = (1 + \theta n) A_j^*(y_j^+ - y_j) + \textstyle\sum_{i=1}^n A_i^* y_i$$

$$x^+ = \mathrm{prox}_{\tau g}(x - \tau \tilde{\nabla}^j)$$

- essentially SAGA version of SPDHG
- for $\sigma = 1$, step size bound $\tau < 1/(n \max_i \|A_i\|^2)$ 3× larger

Numerical Results

Subsets / minibatching



Forward Operator: $K : X \to \mathbb{R}^s$

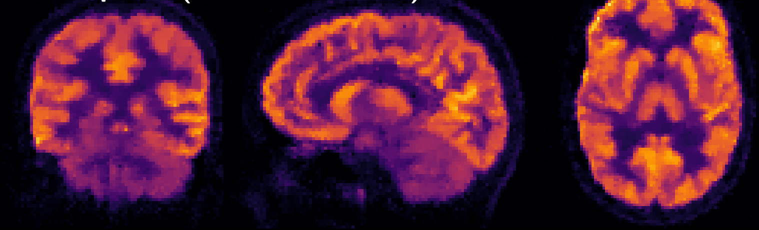
$$\min_x \left\{ \sum_{j=1}^{s} \|K_j x - b_j\|^2 + \lambda \|Dx\|_1 + \imath_+(x) \right\}$$

- Choose subsets S_i
- $A_i = (K_j)_{j \in S_i} : X \to \mathbb{R}^{|S_i|}$
- $f_i(y) = \sum_{j \in S_i} \|K_j x - b_j\|^2$
- n depends on the size of the subsets S_i
- $g(x) = \lambda \|Dx\|_1 + \imath_+(x)$

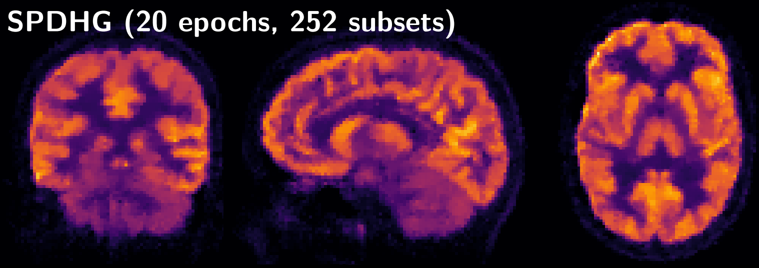
$$\min_x \left\{ \sum_{i=1}^{n} f_i(A_i x) + g(x) \right\}$$

PET: Sanity Check, Convergence to Saddle Point (TV)

saddle point (5000 iter PDHG)

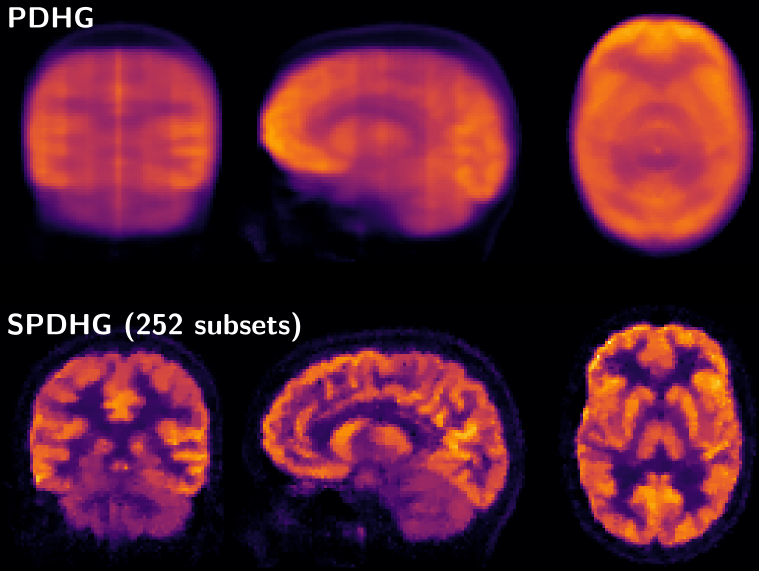


SPDHG (20 epochs, 252 subsets)



Ehrhardt, Markiewicz, Schönlieb '19

PET: Faster than PDHG, TV, 20 epochs

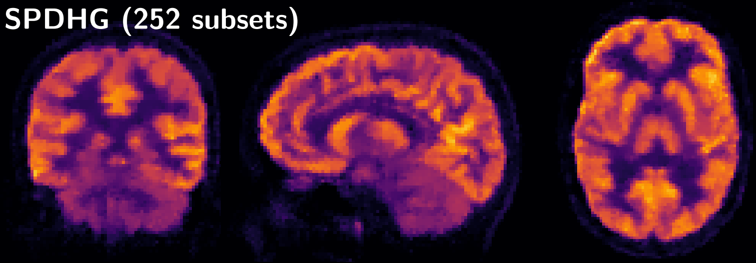


Ehrhardt, Markiewicz, Schönlieb '19

PET: Faster than PDHG, TV, 5 epochs

PDHG

SPDHG (252 subsets)

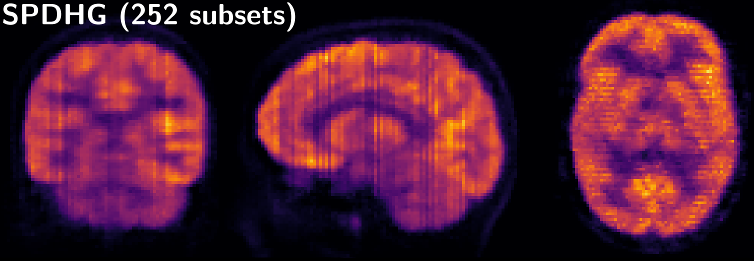


Ehrhardt, Markiewicz, Schönlieb '19

PET: Faster than PDHG, TV, 1 epochs

PDHG

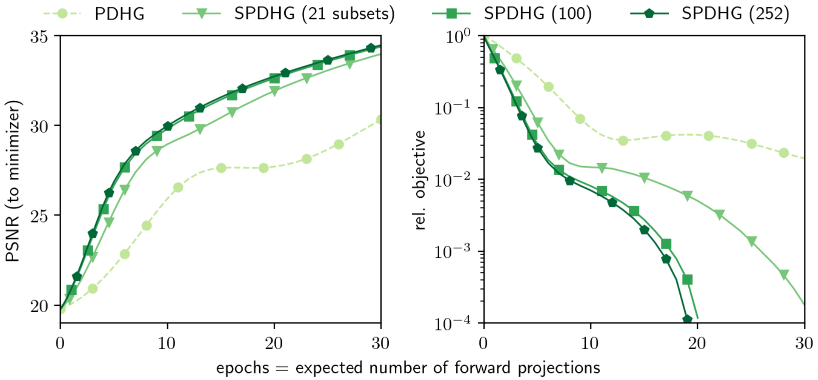
SPDHG (252 subsets)



Ehrhardt, Markiewicz, Schönlieb '19

PET: More subsets are faster

$n = 1, 21, 100, 252$



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Step-size condition of SPDHG

$$\sigma\tau < 1/(n \max_i \|A_i\|^2)$$

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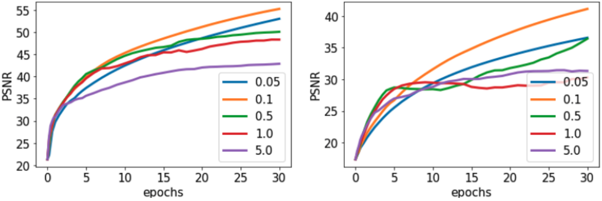
- Is the ratio σ/τ important? Yes Delplancke et al. '20



(a) synthetic data (b) real data

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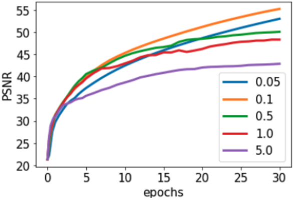
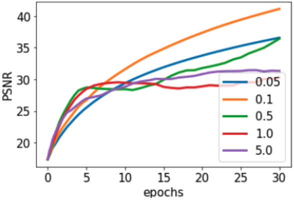


(a) synthetic data



(b) real data

- How to choose the ratio σ/τ? Open question

Adaptive step-sizes

- Idea: let σ and τ vary with iterations
- PDHG: a bit of theory + emprical results Goldstein et al. '15
- SPDHG: empirical results for MPI Zdun and Brandt '21

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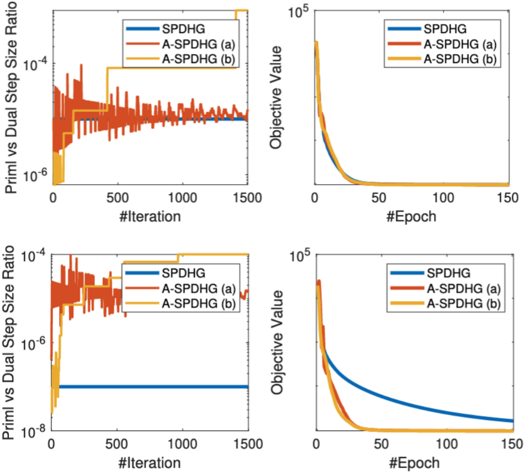
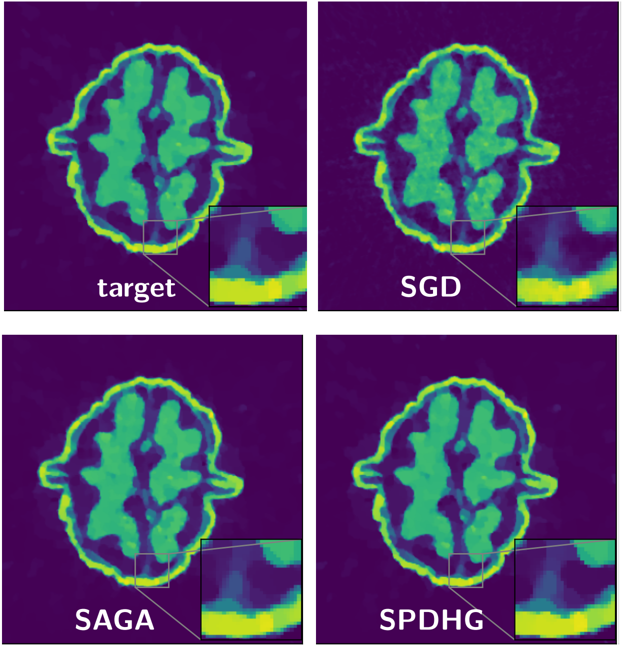
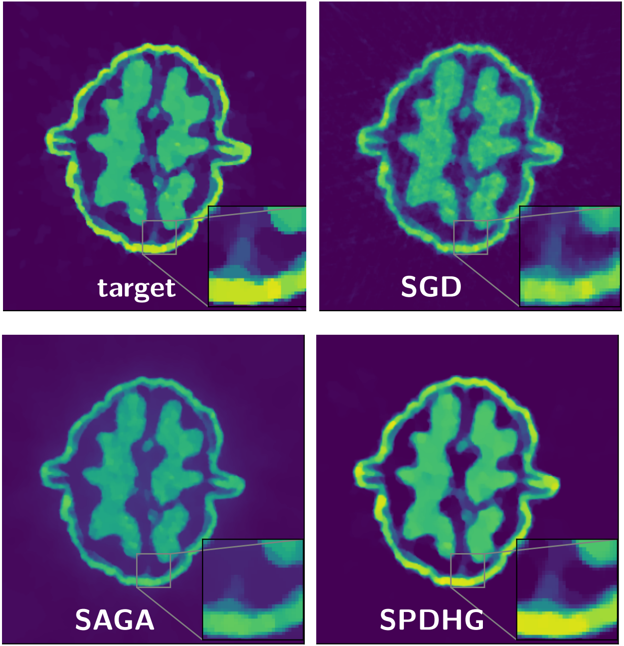
- SPDHG: theory + numerics for CT Chambolle, Ehrhardt et al. '24



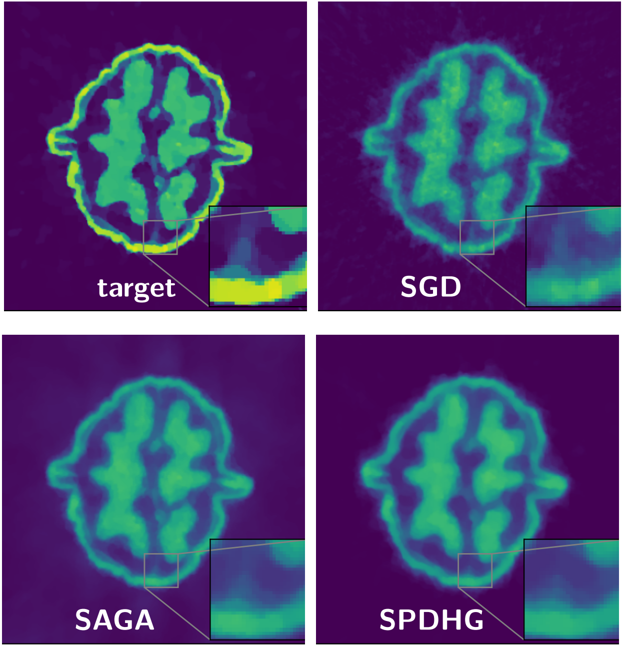
CT: 10 epochs Ehrhardt, Kereta, Liang, Tang '24



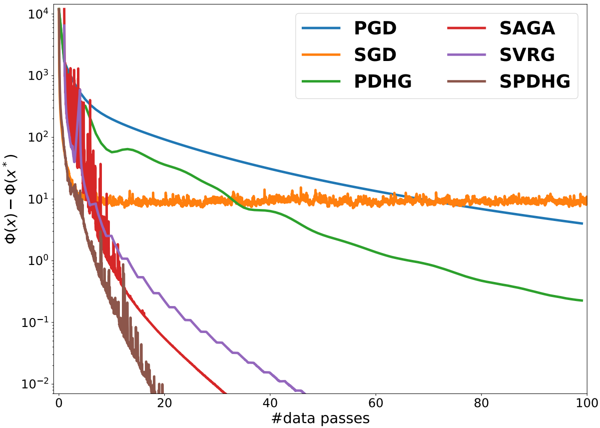
CT: 3 epochs Ehrhardt, Kereta, Liang, Tang '24



CT: 1 epoch Ehrhardt, Kereta, Liang, Tang '24

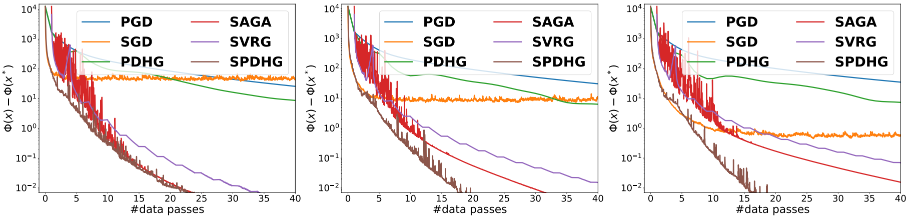


CT: Quantitative Comparison



Ehrhardt, Kereta, Liang, Tang '24

CT: Quantitative Comparison, Noise

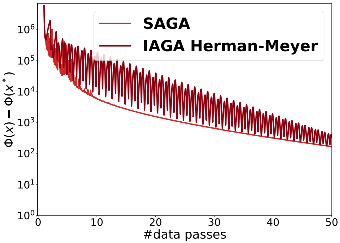


high noise **medium noise (shown)** **low noise**

- Speed seems to depend on noise in the data
- Gradient based methods more effected

Ehrhardt, Kereta, Liang, Tang '24

CT: Random v Deterministic



30 subsets

- similar convergence for 30 subsets (similar to literature)

Herman and Meyer '93, Ehrhardt, Kereta, Liang, Tang '24

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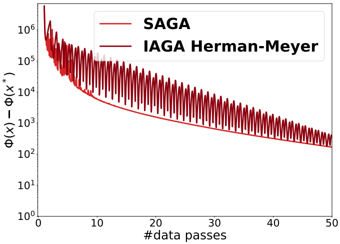

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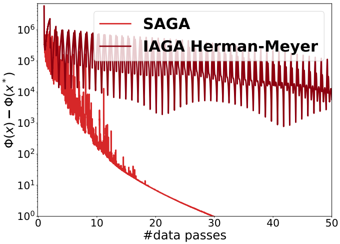


240 subsets

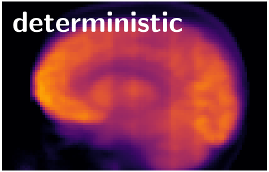
- similar convergence for 30 subsets (similar to literature)
- big difference for 240 subsets

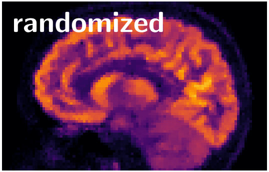
Herman and Meyer '93, Ehrhardt, Kereta, Liang, Tang '24

Conclusions and Outlook

Conclusions:

- **Zoo** of stochastic algorithms exists (gets larger and larger)
- **Randomness** seems important in general and not just mathematical convenience
- **Speeds up** reconstruction of inverse problems; e.g. PET, listmode PET (randomize over events), CT, parallel MRI, motion-corrected CT, magnetic particle imaging





Future directions:

- Tighter analysis
- Inverse problems specific analysis
- Learned algorithms