Faster PET Reconstruction with Non-Smooth Priors by Randomization and Preconditioning

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Joint work with:

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PET imaging: P. Markiewicz, UCL, UK
J. Schott, UCL, UK

Outline

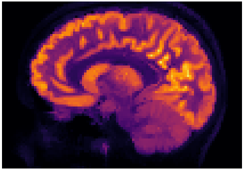
1) PET Reconstruction via Optimization (**Why?**)

$$\sum_{i=1}^{n} f_i(\mathbf{B}_i x) + g(x)$$

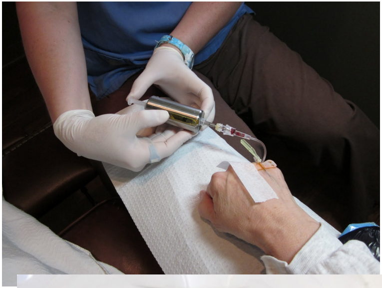
2) Randomized Algorithm for Convex Optimization (**How?**)

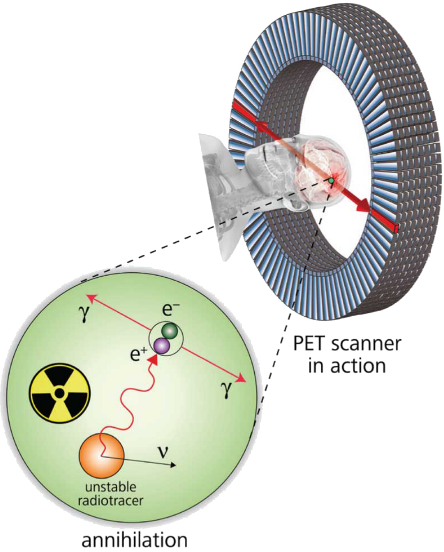
non-smooth
n large
$\mathbf{B}_i x$ expensive

3) Numerical Evaluation: PET imaging



Positron Emission Tomography (PET)

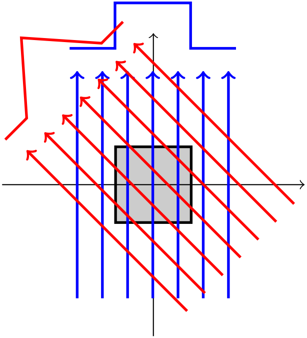


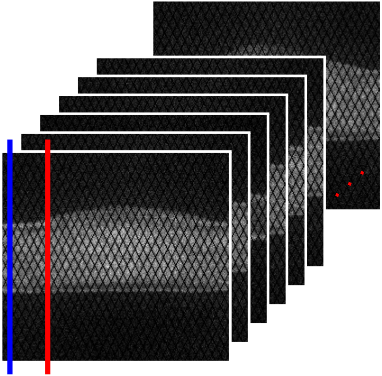


PET Modelling

$$b_i \sim \text{Poisson}(a_i^T u + r_i)$$

- data $b_i \in \mathbb{N}$
- background $r_i > 0$ (scatter, randoms)
- forward model $a_i^T u \approx \gamma_i \int_{L_i} u$ (x-ray transform)
- multiplicative correction $\gamma_i > 0$
- number of data / rays: 2D $N = 86k$, 3D $N = 355M$





PET Reconstruction[1]

$$u_\lambda \in \arg\min_u \left\{ \sum_{j=1}^m \mathcal{D}_j(\mathbf{A}_j u) + \lambda \mathcal{R}(u) + \imath_+(u) \right\}$$

- Group data in "subsets" $\mathbb{S}_1, \ldots, \mathbb{S}_m$

$$\mathcal{D}_j(\mathbf{A}_j u) := \sum_{i \in \mathbb{S}_j} \mathrm{KL}(a_i^T u + r_i; b_i)$$

- Kullback–Leibler divergence

$$\mathrm{KL}(y; b) = \begin{cases} y - b + b \log\left(\frac{b}{y}\right) & \text{if } y > 0 \\ \infty & \text{else} \end{cases}$$

- Constraint

$$\imath_+(u) = \begin{cases} 0, & \text{if } u_i \geq 0 \text{ for all } i \\ \infty, & \text{else} \end{cases}$$

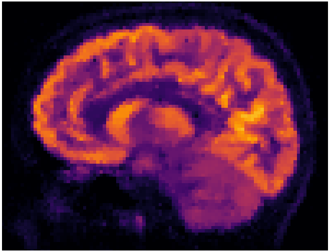
[1] Brune '10, Brune et al. '10, Setzer et al. '10, Müller et al. '11, Anthoine et al. '12, Knoll et al. '16, Ehrhardt et al. '16, Hohage and Werner '16, Schramm et al. '17, Rasch et al. '17, Ehrhardt et al. '17, Mehranian et al. '17 and many, many more

PET Reconstruction with TV

Total variation (TV)

Rudin, Osher, Fatemi 1992

$$\mathcal{R}(u) = \|\nabla u\|_1$$



$$\min_u \left\{ \sum_{j=1}^{m} \mathcal{D}_j(\mathbf{A}_j u) + \lambda \|\nabla u\|_1 + \imath_+(u) \right\}$$

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

$$n = m + 1 \quad g(x) = \imath_+(x)$$
$$\mathbf{B}_i = \mathbf{A}_i \quad f_i = \mathcal{D}_i \quad i \in [m]$$
$$\mathbf{B}_n = \nabla \quad f_n = \lambda \| \cdot \|_1$$

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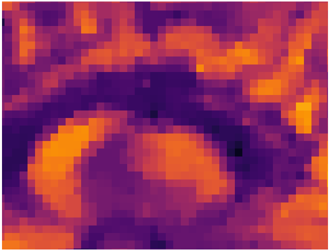

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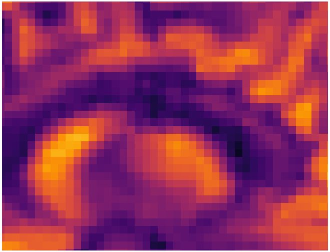
PET Reconstruction with TGV



Total generalized variation (TGV)

Bredies, Kunisch, Pock 2010

$$\mathcal{R}(u) = \min_v \|\nabla u - v\|_1 + \beta \|\mathbf{E} v\|_1$$

$$\min_{u,v} \left\{ \sum_{j=1}^{m} \mathcal{D}_j(\mathbf{A}_j u) + \lambda \|\nabla u - v\|_1 + \lambda\beta \|\mathbf{E} v\|_1 + \imath_+(u) \right\}$$

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

$$\begin{array}{ll} n = m + 2 & \\ x = (u; v) & g(x) = \imath_+(u) \\ \mathbf{B}_i = (\mathbf{A}_i, 0) & f_i = \mathcal{D}_i \quad i \in [m] \\ \mathbf{B}_{n-1} = (\nabla, -\mathbf{I}) & f_{n-1} = \lambda \|\cdot\|_1 \\ \mathbf{B}_n = (0, \mathbf{E}) & f_n = \lambda\beta \|\cdot\|_1 \end{array}$$

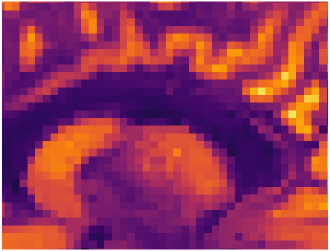
PET Reconstruction with dTV

Directional total variation (dTV)

Ehrhardt and Betcke 2016

$$\mathcal{R}(u) = \|\mathbf{D}\nabla u\|_1 = \sum_j \|\mathbf{D}_j(\nabla u)_j\|_1$$

$$\mathbf{D}_j = \mathbf{I} - \xi_j \xi_j^T$$



$$\min_u \left\{ \sum_{j=1}^m \mathcal{D}_j(\mathbf{A}_j u) + \lambda \|\mathbf{D}\nabla u\|_1 + \imath_+(u) \right\}$$

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

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$\mathbf{B}_i = \mathbf{A}_i \quad f_i = \mathcal{D}_i \quad i \in [m]$

$\mathbf{B}_n = \mathbf{D}\nabla \quad f_n = \lambda \| \cdot \|_1$

Observations

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

- **Proper** $f : X \mapsto \mathbb{R} \cup \{\infty\}$ and $f \not\equiv \infty$, **convex** and **lower semi-continuous (lsc)** $x_k \to x$ then $f(x) \leq \liminf_{k\to\infty} f(x_k)$
- $f(z) = \sum_i f_i(z_i)$ is "**separable**". Not separable in x.
- f_i, g are **non-smooth** but **proximal operator** has closed-form

$$\mathrm{prox}_f^{\mathbf{T}}(x) = \arg\min_z \left\{ \frac{1}{2}\|z - x\|_{\mathbf{T}}^2 + f(z) \right\}, \quad \|x\|_{\mathbf{T}}^2 := \langle \mathbf{T}^{-1}x, x\rangle$$

Note: $\mathrm{prox}_f^{\tau\mathbf{I}} = \mathrm{prox}_{\tau f}^{1}$

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Problem 1: Cannot compute $\text{prox}_{f_i \circ B_i}$

Problem 2: n is large and/or $\mathbf{B}_i x$ expensive

Algorithm

The way out: Saddle Point Problem

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

- $f(y) := \sum_i f_i(y_i)$, $\mathbf{B} = [\mathbf{B}_1; \ldots; \mathbf{B}_n]$

$$x^\sharp \in \arg\min_x \{ f(\mathbf{B}x) + g(x) \}$$

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Definition: The **convex conjugate** of f is given by

$$f^*(y) := \sup_z \langle z, y\rangle - f(z).$$

Theorem: Let f be proper, convex and lsc, then

$$f(z) = (f^*)^*(z) = \sup_y \langle z, y\rangle - f^*(y).$$

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$$(x^\sharp, y^\sharp) \in \arg\min_x \sup_y \left\{ \langle \mathbf{B}x, y \rangle - f^*(y) + g(x) \right\}$$

Primal-Dual Hybrid Gradient (PDHG) Algorithm[1]

Given $x^0, y^0, \overline{y}^0 = y^0$
Iterate

(1) $x^{k+1} = \mathrm{prox}_g^{\mathbf{T}}(x^k - \mathbf{T}\mathbf{B}^*\overline{y}^k)$

(2) $y^{k+1} = \mathrm{prox}_{f^*}^{\mathbf{S}}(y^k + \mathbf{S}\mathbf{B}x^{k+1})$

(3) $\overline{y}^{k+1} = y^{k+1} + \theta(y^{k+1} - y^k)$

- evaluation of $\mathbf{B}$ and $\mathbf{B}^*$
- proximal operator
- convergence: $\theta = 1, \|\mathbf{S}^{1/2}\mathbf{B}\mathbf{T}^{1/2}\|^2 < 1$, cf. $\sigma\tau\|\mathbf{B}\|^2 < 1$

[1] Pock, Cremers, Bischof, Chambolle '09, Esser, Zhang, Chan '10, Chambolle and Pock '11

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- $f(y) := \sum_i f_i(y_i)$, $[\text{prox}_{f^*}(y)]_i = \text{prox}_{f_i^*}(y_i)$
- $\mathbf{B} = [\mathbf{B}_1; \ldots; \mathbf{B}_n]^T$, $\mathbf{B}^* y = \sum_{i=1}^n \mathbf{B}_i^* y_i$
- $z^k = \sum_{i=1}^n \mathbf{B}_i^* y_i^k$

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Stochastic PDHG Algorithm[1]

Given $x^0, y^0, z^0 = \overline{z}^0 = \mathbf{B}^* y^0$, e.g. all equal 0

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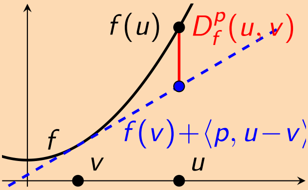
unbiased: $\mathbb{E}_j \frac{\theta}{p_j}(z^{k+1} - z^k) =$ deterministic update with all data

[1] Chambolle, E, Richtárik, Schönlieb '18

Convergence of SPDHG

Definition: Let $p \in \partial f(v)$. The **Bregman distance** of f is defined as

$$D_f^p(u, v) = f(u) - \left[f(v) + \langle p, u - v \rangle \right].$$



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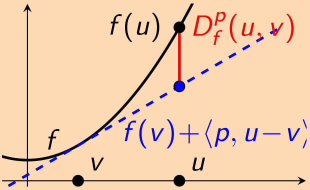

Theorem: Chambolle, E, Richtárik, Schönlieb '18
Let $(x^\sharp, y^\sharp)$ be a saddle point, $\theta = 1$ and choose $\mathbf{S}_i, \mathbf{T} := \min_i \mathbf{T}_i$ such that

$$\left\| \mathbf{S}_i^{1/2} \mathbf{B}_i \mathbf{T}_i^{1/2} \right\|^2 < p_i \quad i = 1, \ldots, n.$$

Then

- Almost surely: $D_g^{r^\sharp}(x^k, x^\sharp) + D_{f^*}^{q^\sharp}(y^k, y^\sharp) \to 0$
- Rate for ergodic sequence $(X^k, Y^k) = \frac{1}{k}\sum_{j=1}^k (x^j, y^j)$

$$\mathbb{E}\left\{ D_g^{r^\sharp}(X^k, x^\sharp) + D_{f^*}^{q^\sharp}(Y^k, y^\sharp) \right\} \le \frac{C}{k}$$

Step-sizes and Preconditioning

Theorem: E, Markiewicz, Schönlieb '18

Let $\rho < 1$ and $\gamma > 0$. Then $\|\mathbf{S}_i^{1/2}\mathbf{B}_i\mathbf{T}_i^{1/2}\|^2 < p_i$ is satisfied by

$$\mathbf{S}_i = \frac{\gamma\rho}{\|\mathbf{B}_i\|}\mathbf{I}\,, \quad \mathbf{T}_i = \frac{\rho p_i}{\gamma\|\mathbf{B}_i\|}\mathbf{I}\,.$$

If $\mathbf{B}_i \geq 0$, then the step-size condition is also satisfied for

$$\mathbf{S}_i = \operatorname{diag}\left(\frac{\gamma\rho}{\mathbf{B}_i 1}\right)\,, \quad \mathbf{T}_i = \operatorname{diag}\left(\frac{\rho p_i}{\gamma\mathbf{B}_i^T 1}\right)\,.$$

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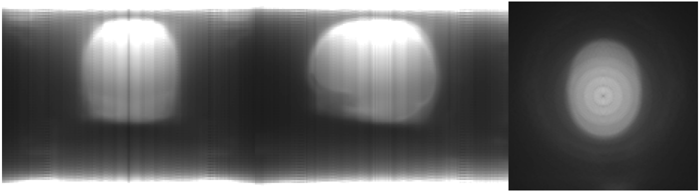
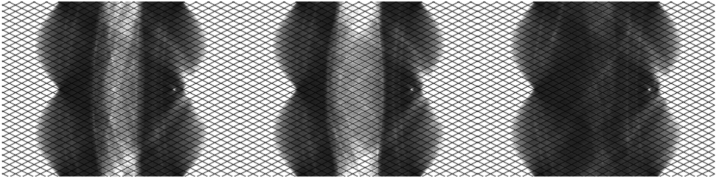
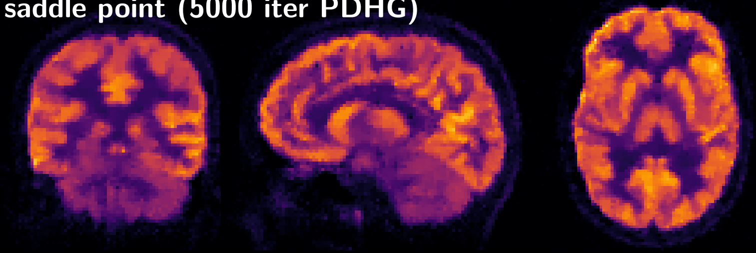




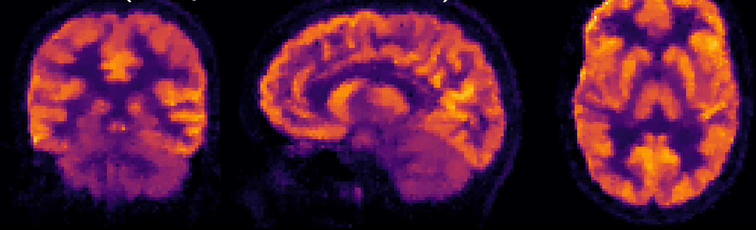
Applications

Sanity Check: Convergence to Saddle Point (TV)

saddle point (5000 iter PDHG)

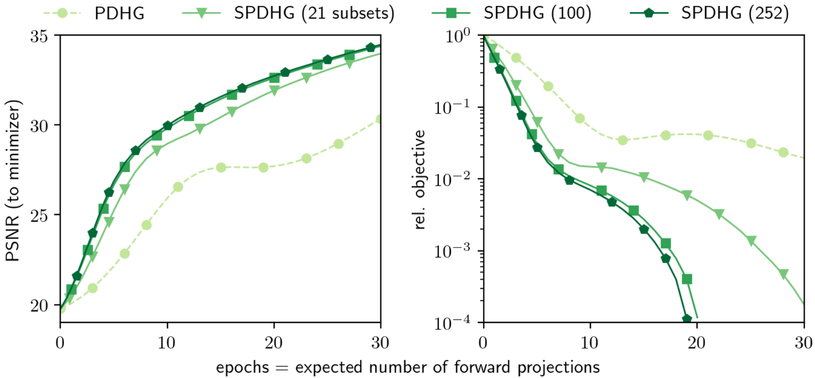


SPDHG (20 epochs, 252 subsets)



More subsets are faster

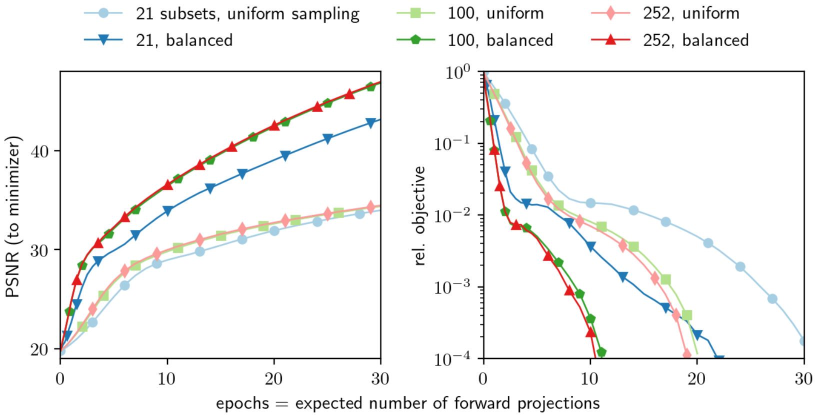
$$m = 1, 21, 100, 252$$



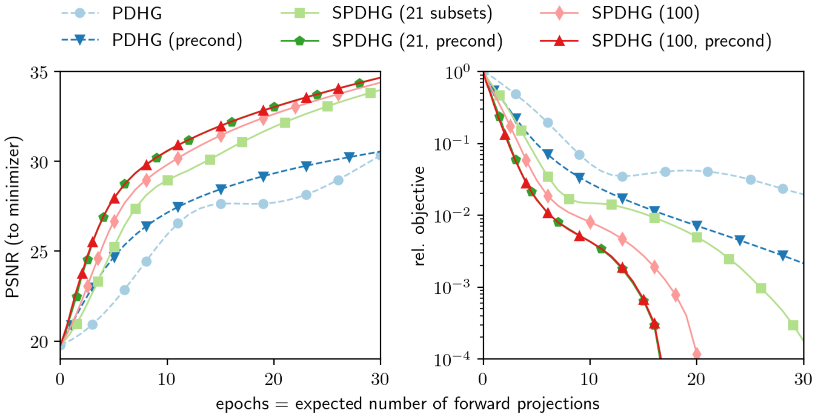
"Balanced sampling" is faster

$$\text{uniform sampling: } p_i = 1/n$$

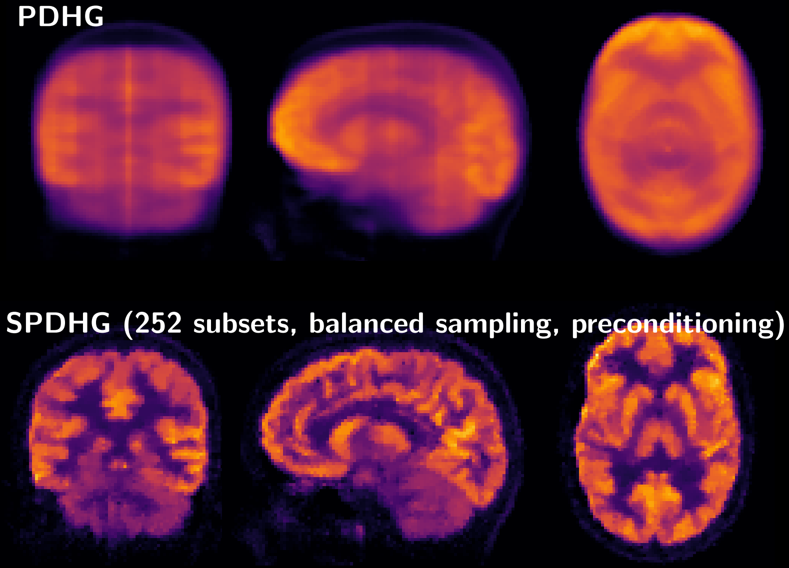
$$\text{balanced sampling: } p_i = \begin{cases} \frac{1}{2m} & i < n \\ \frac{1}{2} & i = n \end{cases}$$



Preconditioning is faster

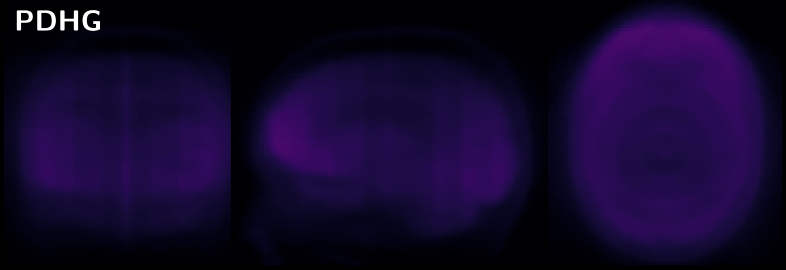


Faster than PDHG (TV), 20 epochs

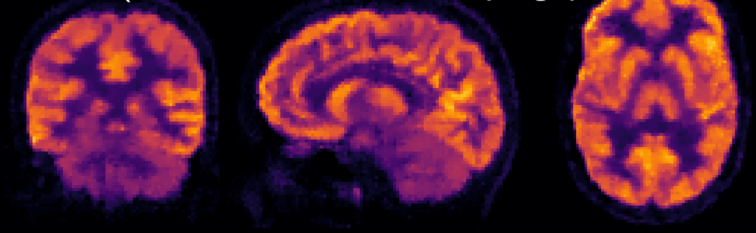


Faster than PDHG (TV), 5 epochs

PDHG



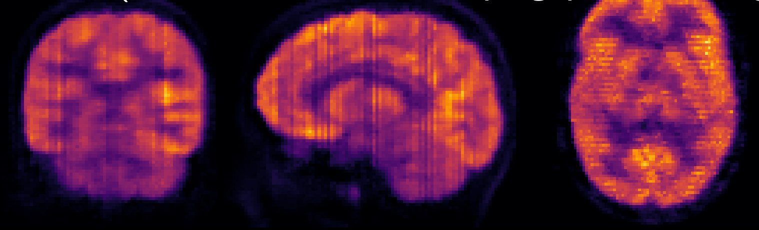
SPDHG (252 subsets, balanced sampling, preconditioning)



Faster than PDHG (TV), 1 epoch

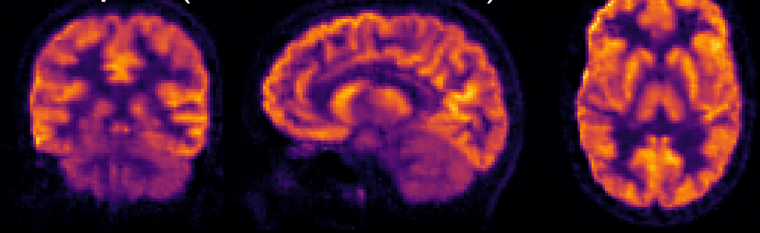
PDHG

SPDHG (252 subsets, balanced sampling, preconditioning)

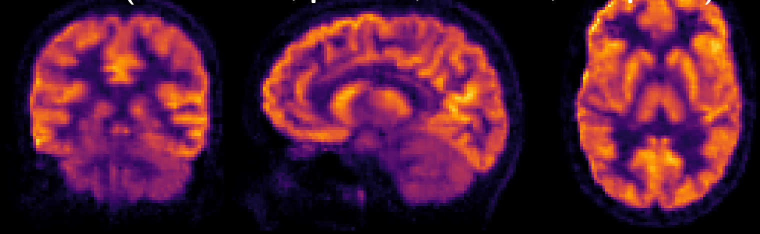


Total Generalized Variation

saddle point (PDHG, 5000 iteration)



SPDHG (252 subsets, precond, balanced, 10 epochs)



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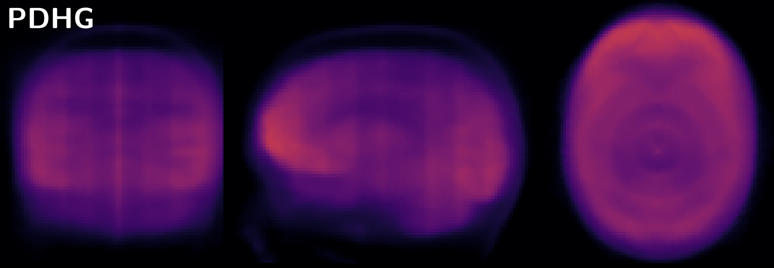
PDHG



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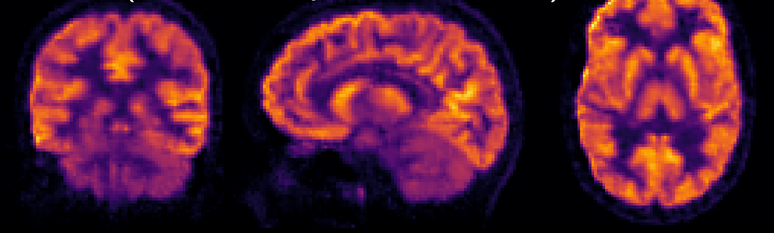
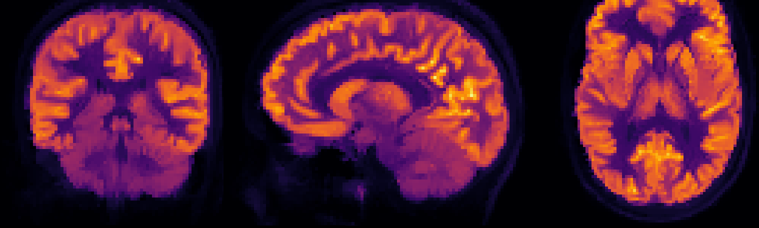
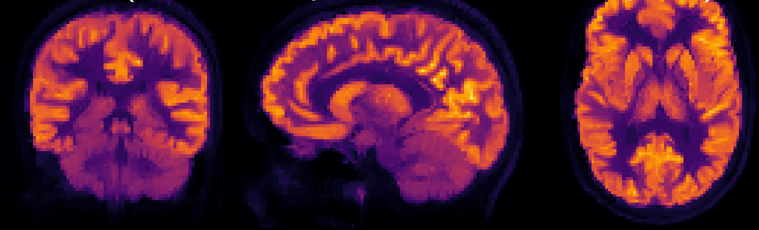


Directional Total Variation

saddle point (PDHG, 5000 iteration)

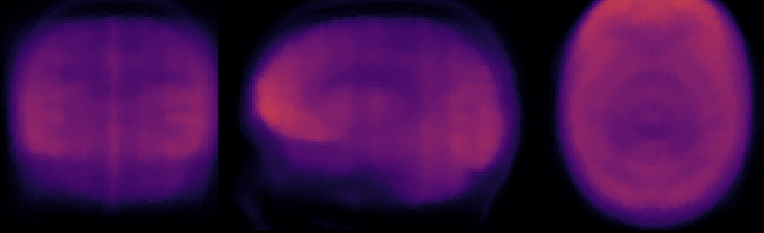


SPDHG (252 subsets, precond, balanced, 10 epochs)

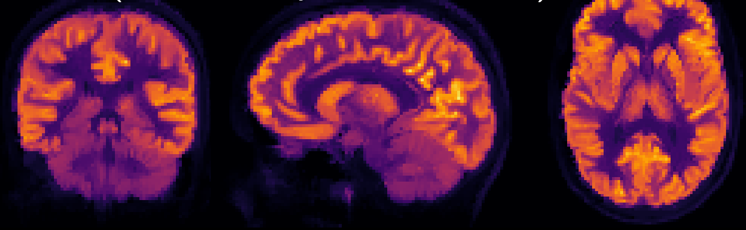


Directional Total Variation, 10 epochs

PDHG



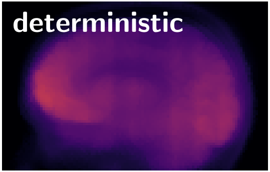
SPDHG (252 subsets, precond, balanced)



Conclusions and Outlook

Summary:

- **Randomized** optimization for cost functionals with "separable structure"
- **Generalisation** of PDHG ($n = 1$)
- **Randomization**, **preconditioning** and **balanced sampling** all speed up SPDHG
- **Much faster** PET reconstruction: advanced models feasible for clinical data



Future work:

- almost sure convergence of iterates
- biased extrapolation
- sampling: 1) optimal, 2) adaptive

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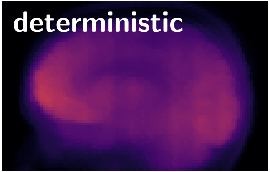

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Job Opportunity:

- PostDoc in Bath, UK on imaging and machine learning; talk to me!