A Randomized Algorithm for Non-Smooth Optimization and Medical Imaging Applications

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Joint work with:
Mathematics: Chambolle (Paris), Richtárik (KAUST), Schönlieb (Cambridge)
PET imaging: Markiewicz, Schott (both UCL)

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Outline

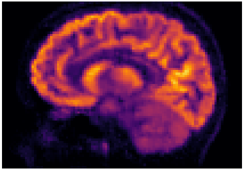
1) From Inverse Problems to Optimization (**Why?**)

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

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

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

3) Numerical Evaluation: PET imaging



From Inverse Problems to Optimization

What is an inverse problem? Inverse to what?

Forward problem: given u, compute $\mathbf{A}u = v$. Evaluate $\mathbf{A}$

- $\mathbf{A} : U \to V$ (non-)linear operator between spaces U and V

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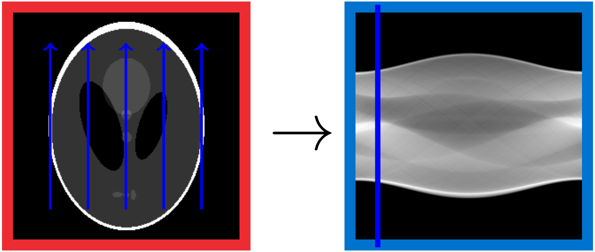
$$\mathbf{A}u(L) = \int_L u(r)dr$$



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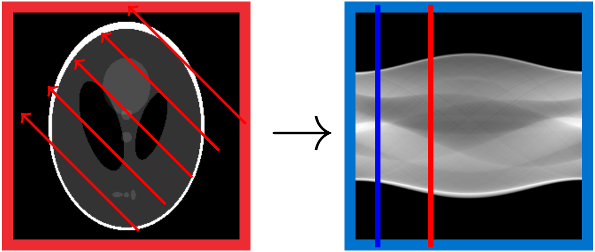

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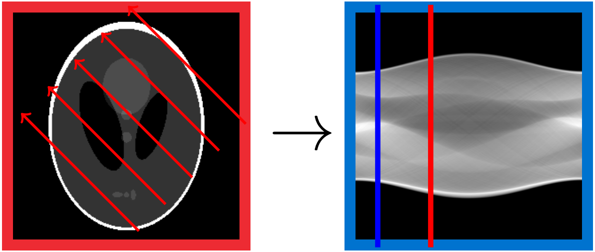
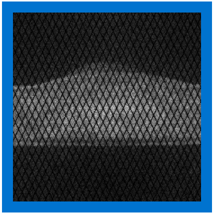


Inverse problem: given v, solve $\mathbf{A}u = v$. "Invert" $\mathbf{A}$

What is the problem with inverse problems?

- PET example: $\mathbf{A}u(L) = \int_L u(r)dr$



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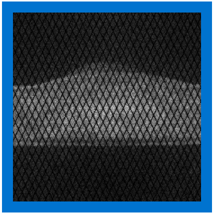

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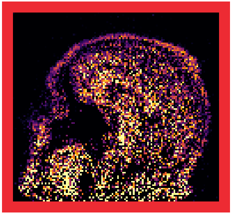

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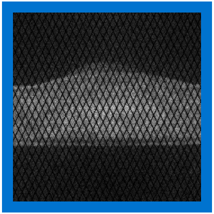
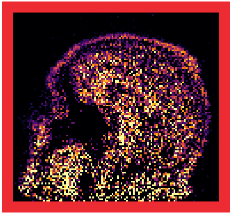
 $\longrightarrow$ 

Definition (Hadamard, 1902): We call an inverse problem $\mathbf{A}u = v$ **well-posed** if

(1) a solution u^* **exists**

(2) the solution u^* is **unique**

(3) u^* depends **continuously** on data v.

Otherwise, it is called **ill-posed**.

Jacques Hadamard

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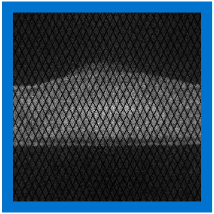

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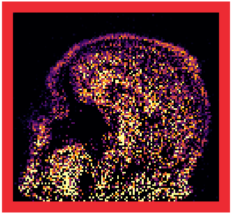

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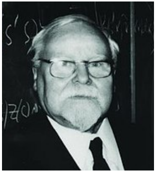
Most interesting problems are ill-posed, in particular (3) is violated.

A way to solve inverse problems

Tikhonov regularization (1943)

Approximate a solution u^* of $\mathbf{A}u = v$ via

$$u_\lambda = \arg\min_u \left\{ \|\mathbf{A}u - v\|^2 + \lambda \|u\|^2 \right\}$$
$$= (\mathbf{A}^*\mathbf{A} + \lambda I)^{-1}\mathbf{A}^* v$$



Andrey Tikhonov

A way to solve inverse problems

Variational regularization

Approximate a solution u^* of $\mathbf{A}u = v$ via

$$u_\lambda = \arg\min_u \left\{ D(\mathbf{A}u, v) + \lambda R(u) \right\}$$

- **data fit** D: quantify fit of prediction $\mathbf{A}u$ to data v. Usually a "divergence", i.e. $D(x, y) \geq 0$ and $D(x, y) = 0$ iff $x = y$

$$D(x, y) = \|x - y\|_2^2, \|x - y\|_1, \int x - y + y \log(y/x), \dots$$

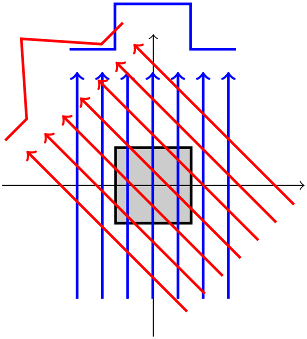
- **regularizer** R: penalize unwanted features, ensures stability

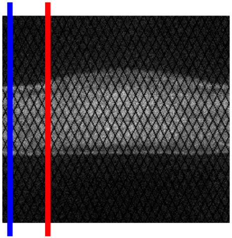
$$R(x) = \|x\|_2^2, \|x\|_1, \mathrm{TV}(x) = \|\nabla x\|_1, \mathrm{TGV}, \dots$$

PET Modelling

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

- data $b_i \in \mathbb{N}$
- forward model $a_i^T u \approx \gamma_i \int_{L_i} u$ (x-ray transform)
- multiplicative correction $\gamma_i > 0$ (attenuation, normalisation)
- background $r_i > 0$ (scatter, randoms)





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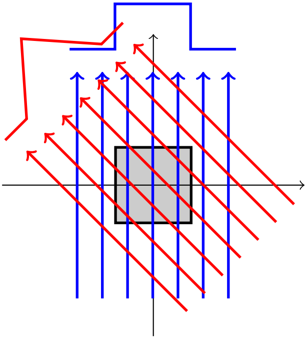
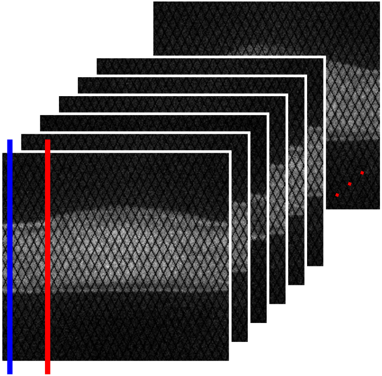
- number of data / rays: 2D $N = 86k$, 3D $N = 355M$





PET Reconstruction[1]

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

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

$$\mathcal{D}_j(y) := \sum_{i \in \mathbb{S}_j} \mathrm{KL}(y_i; b_i)$$

- Kullback–Leibler divergence

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

- Regularizer $\mathcal{R}$, see next page
- Constraint

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

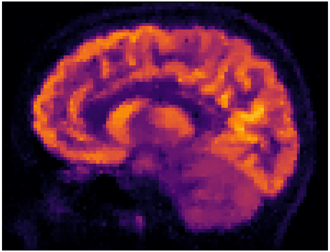
[1] Brune '10, Brune et al. '10, Setzer et al. '10, Müller et al. '11, Anthoine et al. '12, Knoll et al. '16, Ehrhardt et al. '16, Hohage and Werner '16, Schramm et al. '17, Rasch et al. '17, Ehrhardt et al. '17, Mehranian et al. '17 and many, many more

PET Reconstruction with TV

Total variation (TV)

Rudin, Osher, Fatemi 1992

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

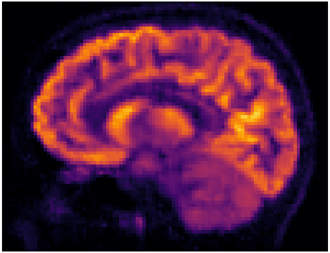


$$\min_u \left\{ \sum_{j=1}^{m} \mathcal{D}_j(\mathbf{A}_j u) + \lambda \|\nabla u\|_1 + \imath_+(u) \right\}$$

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

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

PET Reconstruction with TGV



Total generalized variation (TGV)

Bredies, Kunisch, Pock 2010

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

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

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

$n = m + 2$

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

Observations

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

- **Proper:** Extended valued $f : X \mapsto \mathbb{R} \cup \{\infty\}$ and $f \not\equiv \infty$
- **Convex:** e.g. C convex $\Rightarrow \imath_C$ convex
- **Lower semi-continuous (lsc):** $x_k \to x$ then

$$f(x) \leq \liminf_{k\to\infty} f(x_k)$$

  - continuous $\Rightarrow$ lsc
  - C closed $\Rightarrow \imath_C$ lsc
- $f(z) = \sum_i f_i(z_i)$ is "**separable**". Not separable in x.

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Problem 1: The functions f_i, g are non-smooth but "simple"
Problem 2: n is large and/or $\mathbf{B}_i x$ expensive

Optimization

Subgradient

If f is convex and smooth, then for all $x, y \in X$ we have

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle$$

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Extend definition to non-differentiable functions:

Definition: $f : X \mapsto \mathbb{R} \cup \{\infty\}$ is **subdifferentiable** at $x \in X$ if there exists a **subgradient** $p \in X$ such that for all $y \in X$

$$f(y) \geq f(x) + \langle p, y - x \rangle$$

holds. The set of all subgradients at $x \in X$ is called the **subdifferential** and denoted by $\partial f(x)$.

Example: $f(x) = |x|$

$$\partial f(x) = \begin{cases} \{1\} & \text{if } x > 0 \\ [-1, 1] & \text{if } x = 0 \\ \{-1\} & \text{if } x < 0 \end{cases}$$

Proximal Operators: A **gradient descent** point of view

(Sub-)Gradient descent: $p \in \partial f(x) \quad (= \{\nabla f(x)\}$ if f is diff.)

$$x^+ = x - p$$

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Definition: The **proximal operator** of f is defined as

$$\operatorname{prox}_f(x) := (I + \partial f)^{-1}(x)\,.$$

prox_f has *many* names:
prox / proximal / proximity / resolvent operator

Proximal Operators: A **minimization** point of view

Definition: The **proximal operator** of f is defined as

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"Proof":

$$\begin{aligned}
& x^+ = \arg\min_z \left\{ \frac{1}{2}\|z - x\|^2 + f(z) \right\} \\
\Leftrightarrow \quad & 0 \in \partial \left\{ \frac{1}{2}\|x^+ - x\|^2 + f(x^+) \right\} \\
\Leftrightarrow \quad & 0 \in x^+ - x + \partial f(x^+) \\
\Leftrightarrow \quad & x \in (I + \partial f)x^+ \\
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\end{aligned}$$

Proximal operator: properties and examples

$$\operatorname{prox}_f(x) = \arg\min_z \left\{ \frac{1}{2}\|z - x\|^2 + f(z) \right\}$$

Many rules: e.g.

Proposition: Let f be separable, i.e. $f(x) = \sum_i f_i(x_i)$. Then

$$\operatorname{prox}_f(x)_i = \operatorname{prox}_{f_i}(x_i)\,.$$

Examples:

- $f(x) = \frac{1}{2}\|x\|_2^2$: $\operatorname{prox}_f(x) = \frac{1}{2}x$
- $f(x) = \|x\|_1$:

$$\operatorname{prox}_f(x)_i = \begin{cases} x_i - 1 & \text{if } x_i > 1 \\ 0 & |x_i| \leq 1 \\ x_i + 1 & \text{if } x_i < -1 \end{cases}$$

- $f = \imath_C$: $\operatorname{prox}_f(x) = \operatorname{proj}_C(x)$
- $f = \imath_{\geq 0}$: $\operatorname{prox}_f(x)_i = \max(x_i, 0)$

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Problem: What is the proximal operator of $f(x) = \|\mathbf{C}x\|_1$?

The way out: Saddle Point Problems

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

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

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

(1) $x^{k+1} = \text{prox}_{\tau g}(x^k - \tau \mathbf{B}^* \overline{y}^k)$

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

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

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

[1] Pock, Cremers, Bischof, Chambolle '09, Chambolle and Pock '11

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(3) $\bar{y}_i^{k+1} = y_i^{k+1} + \theta(y_i^{k+1} - y_i^k) \quad i = 1, \ldots, n$

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

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(3) $\bar{y}_i^{k+1} = y_i^{k+1} + \theta(y_i^{k+1} - y_i^k) \quad i = 1, \ldots, n$

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

[1] Pock, Cremers, Bischof, Chambolle '09, Chambolle and Pock '11

Stochastic PDHG Algorithm[1]

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

(1) $x^{k+1} = \mathrm{prox}_{\tau g}(x^k - \sum_{i=1}^n \mathbf{B}_i^* \overline{y}_i^k)$

Select $\mathbb{S}^{k+1} \subset \{1, \dots, n\}$ randomly.

(2) $y_i^{k+1} = \begin{cases} \mathrm{prox}_{\sigma_i f_i^*}(y_i^k + \sigma_i \mathbf{B}_i x^{k+1}) & i \in \mathbb{S}^{k+1} \\ y_i^k & \text{else} \end{cases}$

(3) $\overline{y}_i^{k+1} = y_i^{k+1} + \frac{\theta}{p_i}(y_i^{k+1} - y_i^k) \quad i = 1, \dots, n$

- probabilities $p_i := \mathbb{P}(i \in \mathbb{S}^{k+1}) > 0$ (**proper** sampling)
- $\sum_{i=1}^n \mathbf{B}_i^* \overline{y}_i^k$ can be computed using only $\mathbf{B}_i^*$ for $i \in \mathbb{S}^k$
- evaluation of $\mathbf{B}_i$ and $\mathbf{B}_i^*$ only for $i \in \mathbb{S}^{k+1}$.

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

Convergence Guarantees

Step Size Condition with ESO[1]

Tall matrix $\mathbf{C} = [\mathbf{C}_1; \ldots; \mathbf{C}_n]$, $\mathbf{C}^* h = \sum_{i=1}^n \mathbf{C}_i^* h_i$

Definition (Expected Separable Overapproximation, ESO):
Random subset $\mathbb{S} \subset \{1, \ldots, n\}$. The ESO parameters v_i fulfill the ESO inequality if for all h

$$\mathbb{E}_{\mathbb{S}} \left\| \sum_{i \in \mathbb{S}} \mathbf{C}_i^* h_i \right\|^2 \leq \sum_{i=1}^n p_i v_i \|h_i\|^2 \,.$$

[1] Qu, Richtárik, Zhang '14

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Example (Full Sampling): $\mathbb{S} = \{1, \ldots, n\}, p_i = 1,\ v_i = \|\mathbf{C}\|^2$

$$LHS = \|\mathbf{C}^* h\|^2$$

[1] Qu, Richtárik, Zhang '14

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$$LHS = \|\mathbf{C}^* h\|^2 \leq \|\mathbf{C}^*\|^2 \|h\|^2 = \sum_{i=1}^n \|\mathbf{C}^*\|^2 \|h_i\|^2$$

[1] Qu, Richtárik, Zhang '14

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$$LHS = \|\mathbf{C}^* h\|^2 \leq \|\mathbf{C}^*\|^2 \|h\|^2 = \sum_{i=1}^n \|\mathbf{C}^*\|^2 \|h_i\|^2$$

Example (Serial Sampling): $\mathbb{S} = \{i\},\ v_i = \|\mathbf{C}_i\|^2$

$$LHS = \sum_{i=1}^n p_i \|\mathbf{C}_i^* h_i\|^2$$

[1] Qu, Richtárik, Zhang '14

Step Size Condition with ESO[1]

Tall matrix $\mathbf{C} = [\mathbf{C}_1; \dots; \mathbf{C}_n]$, $\mathbf{C}^* h = \sum_{i=1}^n \mathbf{C}_i^* h_i$

Definition (Expected Separable Overapproximation, ESO): Random subset $\mathbb{S} \subset \{1, \dots, n\}$. The ESO parameters v_i fulfill the ESO inequality if for all h

$$\mathbb{E}_{\mathbb{S}} \left\| \sum_{i \in \mathbb{S}} \mathbf{C}_i^* h_i \right\|^2 \leq \sum_{i=1}^n p_i v_i \|h_i\|^2 .$$

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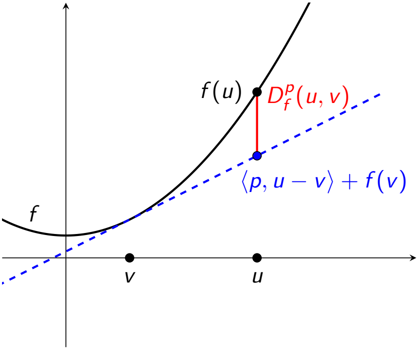
[1] Qu, Richtárik, Zhang '14

Bregman Distance

Definition: The **Bregman distance** of f is defined as

$$D_f^p(u,v) = f(u) - f(v) - \langle p, u-v \rangle, \qquad p \in \partial f(v).$$



Convergence of SPDHG

Theorem: Chambolle, E, Richtárik, Schönlieb '18
Let $(x^\sharp, y^\sharp)$ be a saddle point, $\theta = 1$ and choose σ_i, τ such that there exist ESO parameters v_i of $\mathbf{C} = [\mathbf{C}_1; \dots, \mathbf{C}_n]$ with $\mathbf{C}_i = \sqrt{\sigma_i \tau}\mathbf{B}_i$ which satisfy

$$v_i < p_i.$$

Then

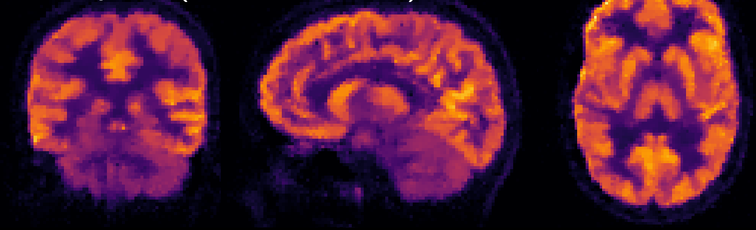
- Almost surely: $D_g^{r^\sharp}(x^k, x^\sharp) + D_{f^*}^{q^\sharp}(y^k, y^\sharp) \to 0$
- Rate for ergodic sequence $(x_K, y_K) = \frac{1}{K}\sum_{k=1}^K (x^k, y^k)$

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

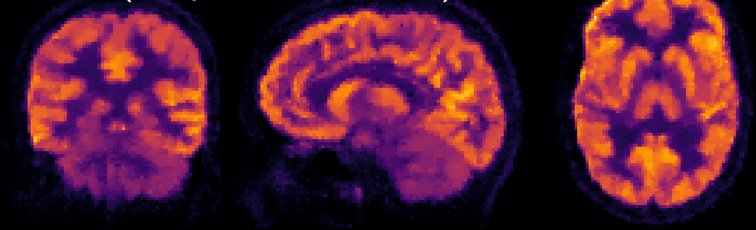
Applications

Sanity Check: Convergence to Saddle Point (TV)

saddle point (5000 iter PDHG)

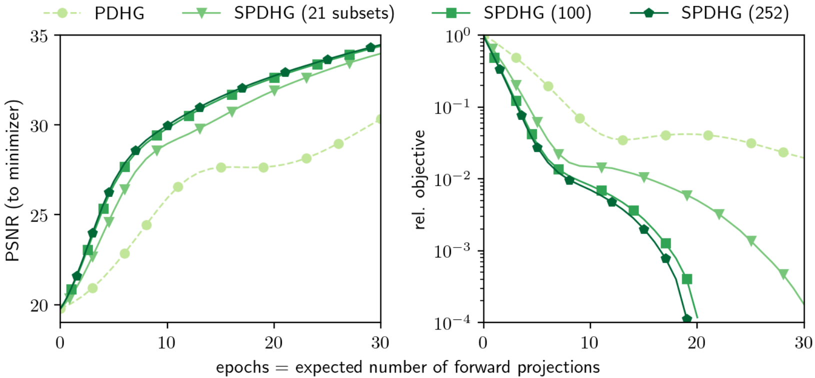


SPDHG (20 epochs, 252 subsets)



More subsets are faster

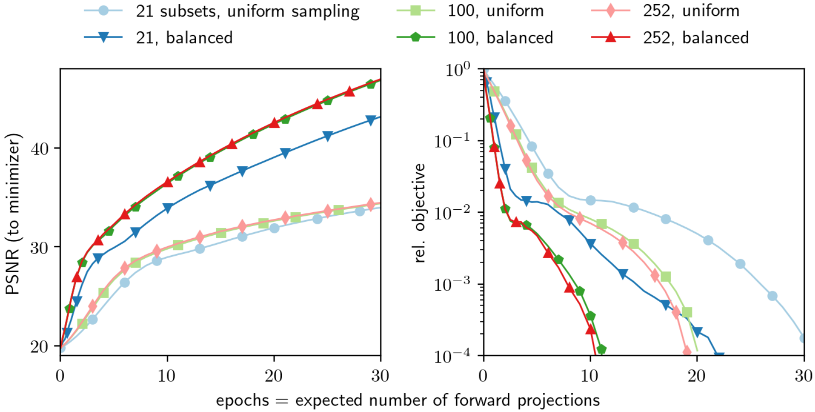
$$m = 1, 21, 100, 252$$



"Balanced sampling" is faster

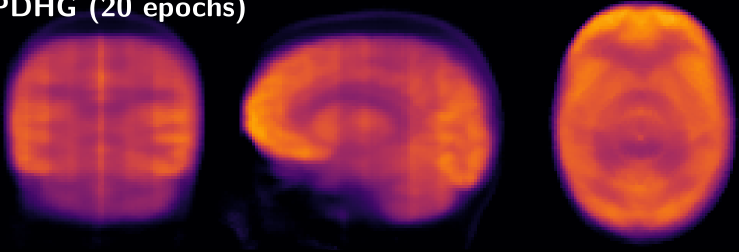
uniform sampling: $p_i = 1/n$

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

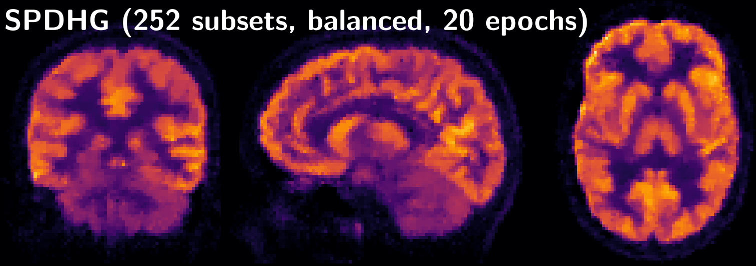


Faster than PDHG, TV

PDHG (20 epochs)



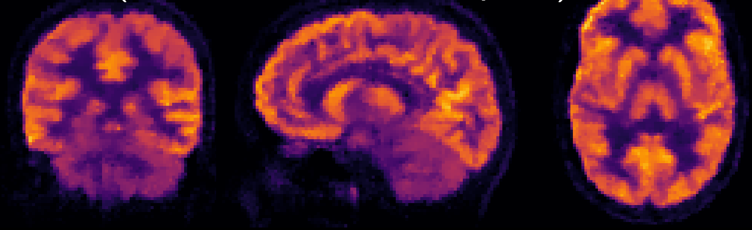
SPDHG (252 subsets, balanced, 20 epochs)



Faster than PDHG, TV

PDHG (5 epochs)

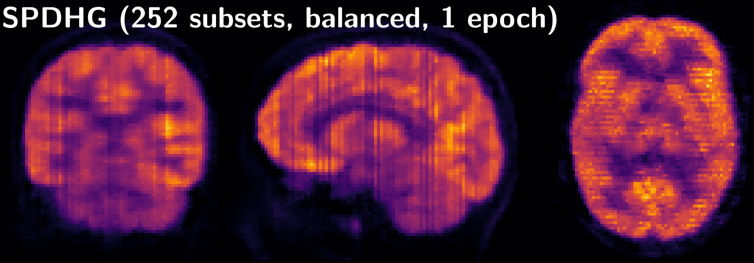
SPDHG (252 subsets, balanced, 5 epochs)



Faster than PDHG, TV

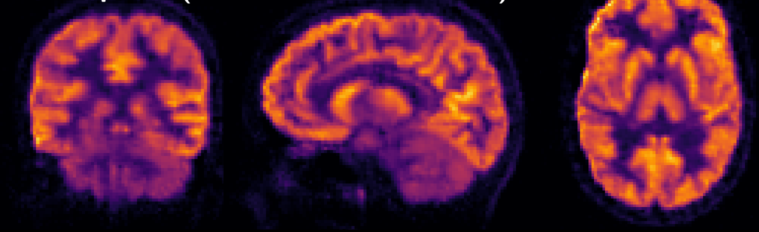
PDHG (1 epoch)

SPDHG (252 subsets, balanced, 1 epoch)

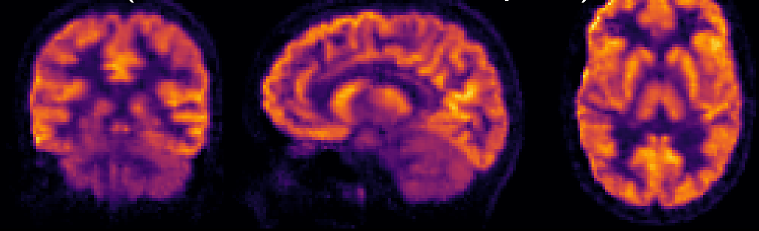


Total Generalized Variation

saddle point (PDHG, 5000 iterations)

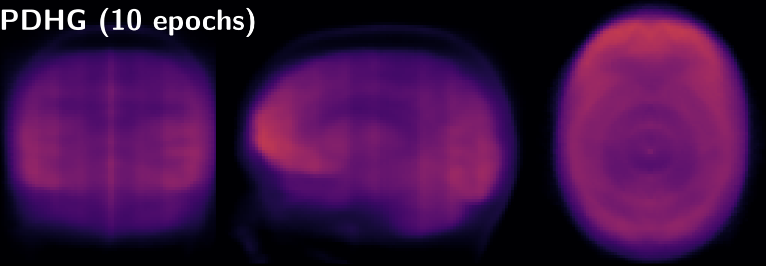


SPDHG (252 subsets, balanced, 10 epochs)

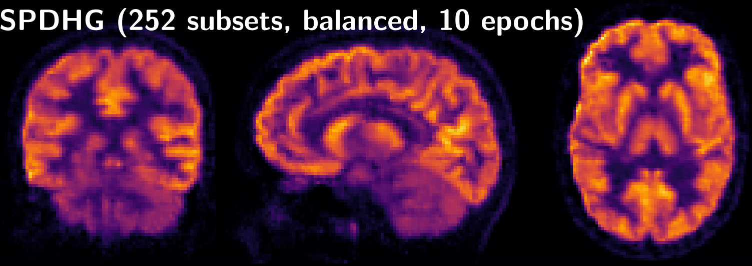


Total Generalized Variation

PDHG (10 epochs)



SPDHG (252 subsets, balanced, 10 epochs)



Conclusions and Outlook

Summary:

- **Randomized** optimization for cost functionals with “separable structure”
- **Generalisation** of PDHG ($n = 1$)
- Convergence for **arbitrary sampling**
- **Much faster** PET reconstruction: advanced models feasible for clinical data

Not shown today:

- Convergence theorems: 1) $\mathcal{O}(1/k^2)$ acceleration, 2) linear convergence

Future work:

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