

Stochastic Primal-Dual Hybrid Gradient Algorithm with Arbitrary Sampling and Imaging Applications

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■ Set-up:

- $\mathbb{X}, \mathbb{Y}_i, i = 1, \dots, n$: real Hilbert spaces.
- $\mathbb{Y} = \prod_{i=1}^n \mathbb{Y}_i := \{y = (y_1, \dots, y_n) : y_i \in \mathbb{Y}_i, i = 1, \dots, n\}$
- $A_i : \mathbb{X} \rightarrow \mathbb{Y}_i, i = 1, \dots, n$: bounded linear operators
- $A : \mathbb{X} \rightarrow \mathbb{Y}$: $Ax = (A_1x, \dots, A_nx)$
- $f : \mathbb{Y} \rightarrow \mathbb{R}_{\infty}$ and $g : \mathbb{X} \rightarrow \mathbb{R}_{\infty}$ are convex.
- f is separable: $f(y) = \sum_{i=1}^n f_i(y_i)$, $f_i : \mathbb{Y}_i \rightarrow \mathbb{R}_{\infty}$

■ Objective function:

$$\min_{x \in \mathbb{X}} \left\{ \Phi(x) := \sum_{i=1}^n f_i(A_i x) + g(x) \right\}$$

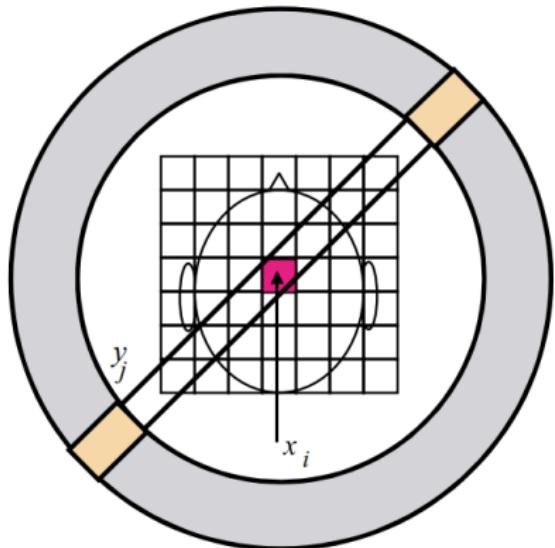
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Reconstruct image from intensity measurements!



Schematic of PET scanner

- n voxels or grid of boxes imposed over the emitting objects
- ξ_i : Number of emissions from the voxel- i .
 $\xi_i \sim \text{Poisson}(x_i)$, are independent.
- y_j : Intensity measurement at the j -th detector pairs/conincidence line, $j = 1, \dots, N$.

- $C_{i,j} \propto$ probability of the emission from voxel- i being detected by the j -th detector pair or hitting the j -th coincidence line
- $\Xi_{i,j} = C_{i,j}\xi_i$ number of emissions from voxel- i hitting the j -th coincidence line
- $y_j = \sum_{i=1}^n \Xi_{i,j}$: measurement at the j -th detector pair

To estimate the true emission intensities x_i using the measurements y_j

- Maximize the likelihood function:

$$l(x | y) \equiv p(y | x) = \prod_{j=1}^N \frac{1}{y_j!} e^{-\sum_{i=1}^n C_{i,j}\xi_i} \left(\sum_{i=1}^n C_{i,j}\xi_i \right)^{y_j}$$

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An optimization problem

- Maximize the log-likelihood function or equivalently the function:

$$\Phi(x) := -Ce_Nx + \sum_{j=1}^N y_j \log(C^T x)_j$$

- Define

$$g : \mathbb{R}^n \longrightarrow \mathbb{R} \quad \text{as} \quad g(x) := -Ce_Nx$$

$$A_j : \mathbb{R}^n \longrightarrow \mathbb{R} \quad \text{as} \quad A_j := C_j^T x = (C^T x)_j$$

$$f_j : \mathbb{R} \longrightarrow \mathbb{R} \quad \text{as} \quad f_j(x) := y_j \log((C^T x)_j)$$

$$f : \mathbb{R}^N = \underbrace{\mathbb{R} \times \cdots \times \mathbb{R}}_{N \text{ times}} \longrightarrow \mathbb{R} \quad \text{as} \quad f(z) := \sum_{j=1}^N y_j \log(z_j)$$

- So maximizing the likelihood is of the form

$$\min_{x \in \mathbb{X}} \left\{ \Phi(x) := \sum_{i=1}^n f_i(A_i x) + g(x) \right\}$$

- Saddle point problem:

$$\min_{x \in \mathbb{S}} \sup_{y \in \mathbb{Y}} \left\{ \Psi(x, y) := \sum_{i=1}^n \langle A_i x, y_i \rangle - f_i^*(y_i) + g(x) \right\}$$

- Optimality conditions: A saddle point $(x^\sharp, y^\sharp) \in \mathbb{X} \times \mathbb{Y}$ satisfies

$$\begin{aligned} A_i x^\sharp &\in \partial f_i^*(y^\sharp), \quad i = 1, \dots, n \\ -A^* y^\sharp &\in \partial g(x^\sharp) \end{aligned}$$

- Primal-Dual update:

$$x^{(k+1)} = \text{Prox}_g^T \left(x^{(k)} - T A^* \bar{y}^{(k)} \right)$$

$$y_i^{(k+1)} = \text{Prox}_{f_i^*}^{S_i} \left(y_i^{(k)} + S_i A_i x^{(k+1)} \right), \quad i = 1, \dots, n,$$

$$\bar{y}^{(k+1)} = y^{(k+1)} + \theta \left(y^{(k+1)} - y^{(k)} \right)$$

- T and $S = \text{diag}(S_1, \dots, S_n)$ are symmetric and positive definite.
- Guaranteed convergence under $\|S^{1/2}AT^{1/2}\| < 1$ and $\theta = 1$

Update a *random* subset of the dual variables at every iteration

- To sample a random subset \mathbb{S} of indices $\{1, \dots, n\} =: [n]$
- \mathbb{S} is a random variable defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and taking values in $2^{[n]}$
- \mathbb{S} induces a probability distribution $P_{\mathbb{S}}$ on $2^{[n]}$ given by
$$P_{\mathbb{S}}(S) := \mathbb{P}\{\mathbb{S} = S\}, \quad S \subseteq [n].$$
- The probability of an integer/index i being included in the random set \mathbb{S} is

$$p_i := \mathbb{P}\{i \in \mathbb{S}\} = \sum_S \mathbb{1}_{\{i \in S\}} \mathbb{P}\{\mathbb{S} = S\}, \quad i = 1, \dots, n.$$

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Algorithm 1 Input: $x^{(0)}, y^{(0)}, S = \text{diag}(S_1, \dots, S_n), T, \theta, \mathbb{S}^{(k)}, K.$
Initialize: $\bar{y}^{(0)} = y^{(0)}$

- 1: **for** $k = 0, \dots, K - 1$ **do**
- 2: $x^{(k+1)} = \text{Prox}_g^T(x^{(k)} - TA^*\bar{y}^{(k)})$
- 3: Select $\mathbb{S}^{(k+1)} \subset \{1, \dots, n\}$
- 4: $y_i^{(k+1)} = \begin{cases} \text{Prox}_{f_i^*}^{S_i} \left(y_i^{(k)} + S_i A_i x^{(k+1)} \right) & \text{if } i \in \mathbb{S}^{(k+1)} \\ y_i^{(k)} & \text{else} \end{cases}$
- 5: $\bar{y}^{(k+1)} = y^{(k+1)} + \theta Q(y^{(k+1)} - y^{(k)})$
- 6: **end for**

- $Q := \text{diag} \left(\frac{1}{p_1} I_1, \dots, \frac{1}{p_n} I_n \right)$

Bregman distance $D_f^q(x, y)$:

For any function $f : \mathbb{X} \rightarrow \mathbb{R}_\infty$, $x, y \in \mathbb{X}$, and a subgradient $q \in \partial f(y)$ of f at y ,

$$D_f^q(x, y) := f(x) - f(y) - \langle q, x - y \rangle$$

Distance functions

$$\mathcal{F}_i(y_i|\tilde{x}, \tilde{y}_i) := f_i^*(y_i) - f_i^*(\tilde{y}_i) - \langle A_i \tilde{x}, y_i - \tilde{y}_i \rangle, \quad i = 1, \dots, n.$$

$$\mathcal{F}(y|\tilde{x}, \tilde{y}) := \sum_{i=1}^n \mathcal{F}_i(y_i|\tilde{x}, \tilde{y}_i).$$

$$\mathcal{F}^P(y|\tilde{x}, \tilde{y}) := \sum_{i=1}^n \left(\frac{1}{p_i} - 1 \right) \mathcal{F}_i(y_i|\tilde{x}, \tilde{y}_i).$$

$$\mathcal{G}(x|\tilde{x}, \tilde{y}) := g(x) - g(\tilde{x}) - \langle -A^* \tilde{y}, x - \tilde{x} \rangle.$$

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$$\mathcal{G}(x|\tilde{x}, \tilde{y}) := g(x) - g(\tilde{x}) - \langle -A^* \tilde{y}, x - \tilde{x} \rangle.$$

Partial primal-dual gap:

$$G_{\mathbb{B}_1 \times \mathbb{B}_2}(x, y) := \sup_{\tilde{y} \in \mathbb{B}_2} \Psi(x, \tilde{y}) - \inf_{\tilde{x} \in \mathbb{B}_1} \Psi(\tilde{x}, y), \quad \mathbb{B}_1 \times \mathbb{B}_2 \subset \mathbb{X} \times \mathbb{Y}$$

Relation to the distance functions

$$G_{\mathbb{B}_1 \times \mathbb{B}_2}(x, y) = \sup_{(\tilde{x}, \tilde{y}) \in \mathbb{B}_1 \times \mathbb{B}_2} [\mathcal{F}(y|\tilde{x}, \tilde{y}) + \mathcal{G}(x|\tilde{x}, \tilde{y})]$$

Theorem (4.3)

Then the Bregman distance between iterates of Algorithm 1 $(x^{(k)}, y^{(k)}) \in \mathbb{X} \times \mathbb{Y}$ and any saddle point $(x^\#, y^\#) \in \mathbb{X} \times \mathbb{Y}$ converges to zero almost surely,

$$D_{f^*+g}^q((x^{(k)}, y^{(k)}), (x^\#, y^\#)) \rightarrow 0 \quad \text{a.s.}$$

Moreover, the ergodic sequence $(x_{(K)}, y_{(K)}) := \frac{1}{K} \sum_{k=1}^K (x^{(k)}, y^{(k)})$ converges with rate $1/K$ in an expected partial primal-dual gap sense; i.e., for any set $\mathbb{B} := \mathbb{B}_1 \times \mathbb{B}_2 \subset \mathbb{W}$ it holds that

$$\mathbb{E} G_{\mathbb{B}}(x_{(K)}, y_{(K)}) \leq \frac{C_{\mathbb{B}}}{K},$$

where the constant is given by

$$C_{\mathbb{B}} := \sup_{x \in \mathbb{B}_1} \frac{1}{2} \|x^{(0)} - x\|_{T^{-1}}^2 + \sup_{y \in \mathbb{B}_2} \frac{1}{2} \|y^{(0)} - y\|_{QS^{-1}}^2 + \sup_{w \in \mathbb{B}} \mathcal{F}^p(y^{(0)}|w).$$

The same rate holds for the expected Bregman distance, $\mathbb{E} D_{f^*+g}^q \leq C_{\{(x^\#, y^\#)\}}/K$.

Lemma (4.4)

Consider the deterministic updates

$$x^{(k+1)} = \text{Prox}_g^{\mathbf{T}^{(k)}} \left(x^{(k)} - \mathbf{T}_{(k)} \mathbf{A}^* \bar{y}^{(k)} \right),$$

$$\hat{y}_i^{(k+1)} = \text{Prox}_{f_i^*}^{S_{(k)}^i} \left(y_i^{(k)} + S_{(k)}^i \mathbf{A}_i x^{(k+1)} \right), \quad i = 1, \dots, n,$$

with iteration varying step sizes $\mathbf{T}_{(k)}$ and $S_{(k)} = \text{diag}(S_{(k)}^1, \dots, S_{(k)}^n)$. Then for any $(x, y) \in \mathbb{W}$ it holds that

$$\begin{aligned} & \|x^{(k)} - x\|_{\mathbf{T}_{(k)}^{-1}}^2 + \|y^{(k)} - y\|_{S_{(k)}^{-1}}^2 \geq \|x^{(k+1)} - x\|_{\mathbf{T}_{(k)}^{-1} + \mu_g \mathbf{I}}^2 + \|\hat{y}^{(k+1)} - y\|_{S_{(k)}^{-1} + M}^2 \\ & + 2 \left(\mathcal{G} \left(x^{(k+1)} | w \right) + \mathcal{F} \left(\hat{y}^{(k+1)} | w \right) \right) - 2 \left\langle \mathbf{A} \left(x^{(k+1)} - x \right), \hat{y}^{(k+1)} - \bar{y}^{(k)} \right\rangle \\ & + \|x^{(k+1)} - x^{(k)}\|_{\mathbf{T}_{(k)}^{-1}}^2 + \|\hat{y}^{(k+1)} - y^{(k)}\|_{S_{(k)}^{-1}}^2 \end{aligned}$$

- $y_i^{(k)}$ at step- k is updated only if i gets picked in the random subset \mathbb{S} , i.e.,

$$y_i^{(k+1)} = \begin{cases} \hat{y}_i^{(k+1)}, & \text{if } i \in \mathbb{S} \\ y_i^{(k)}, & \text{if } i \notin \mathbb{S} \end{cases}.$$

- A key initial step:

$$\begin{aligned} \mathbb{E}^{(k+1)} [\varphi(y_i^{(k+1)})] &= \mathbb{E}_{\mathbb{S}^{(k)}} [\varphi(y_i^{(k+1)})] \\ &= \varphi(\hat{y}_i^{(k+1)}) \mathbb{P}\{i \in \mathbb{S}\} + \varphi(y_i^{(k)}) \mathbb{P}\{i \notin \mathbb{S}\} \\ \Rightarrow \varphi(\hat{y}_i^{(k+1)}) &= \left(\frac{1}{p_i} - 1 \right) \mathbb{E}^{(k+1)} [\varphi(y_i^{(k+1)})] \\ &\quad - \left(\frac{1}{p_i} - 1 \right) \varphi(y_i^{(k)}) + \mathbb{E}^{(k+1)} [\varphi(y_i^{(k+1)})]. \end{aligned}$$

- Will need to bound terms involving inner products

Expected Separable Overapproximation (ESO)

For a bounded linear operator $C : \mathbb{X} \longrightarrow \mathbb{Y}$, a vector $v = (v_1, \dots, v_n) \in \mathbb{R}^n$ satisfies the ESO inequality if

$$\mathbb{E}_{\mathbb{S}} \left\| \sum_{i \in \mathbb{S}} z_i C_i^* \right\|^2 \leq \sum_{i=1}^n p_i v_i \|z_i\|^2, \quad \forall z = (z_1, \dots, z_n) \in \mathbb{Y}.$$

The parameters v_i , $i = 1, \dots, n$ are called as ESO parameters of C and \mathbb{S} .

Lemma (4.2)

Let $y_i^+ = \begin{cases} \hat{y}_i, & \text{if } i \in \mathbb{S} \\ y_i, & \text{otherwise} \end{cases}$ and let $\{v_i\}_{i=1}^n$ be some ESO parameters of $\mathbb{S}^{1/2} \mathbf{A} \mathbf{T}^{1/2}$. Then for any $x \in \mathbb{X}$ and $c > 0$,

$$2\mathbb{E}_{\mathbb{S}} \langle \mathbf{Q} \mathbf{A} x, y^+ - y \rangle \geq -\mathbb{E}_{\mathbb{S}} \left\{ \frac{1}{c} \|x\|_{\mathbf{T}^{-1}}^2 + c \max_{1 \leq i \leq n} \frac{v_i}{p_i} \|y^+ - y\|_{\mathbf{Q} \mathbf{S}^{-1}}^2 \right\}$$

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$$2\mathbb{E}_{\mathbb{S}} \langle QAx, y^+ - y \rangle \geq -\mathbb{E}_{\mathbb{S}} \left\{ \frac{1}{c} \|x\|_{T^{-1}}^2 + c \max_{1 \leq i \leq n} \frac{v_i}{p_i} \|y^+ - y\|_{QS^{-1}}^2 \right\}$$

Algorithm 2 SPDHG with acceleration on the dual variable (DA-SPDHG)

Input: $x^{(0)}, y^{(0)}, \tau_{(0)} \in \mathbb{R}, \tilde{\sigma}_{(0)} \in \mathbb{R}, \mathbb{S}^{(k)}, K$.

Initialize: $\bar{y}^{(0)} = y^{(0)}$.

- 1: **for** $k = 0, \dots, K - 1$ **do**
- 2: $x^{(k+1)} = \text{Prox}_g^{\tau_{(k)}}(x^k - \tau_{(k)} A^* \bar{y}^{(k)})$
- 3: Select $\mathbb{S}^{(k+1)} \subset \{1, \dots, n\}$
- 4: $\sigma_i^{(k)} = \frac{\tilde{\sigma}_{(k)}}{\mu_i [p_i - 2(1 - p_i) \tilde{\sigma}_{(k)}]}, \quad i \in \mathbb{S}^{(k+1)}$
- 5: $y_i^{(k+1)} = \begin{cases} \text{Prox}_{f_i^*}^{\sigma_i^{(k)}}(y_i^{(k)} + \sigma_i^{(k)} A_i x^{(k+1)}) & \text{if } i \in \mathbb{S}^{(k+1)} \\ y_i^{(k)} & \text{else} \end{cases}$
- 6: $\theta_{(k)} = (1 + 2\tilde{\sigma}_{(k)})^{-1/2}, \quad \tau_{(k+1)} = \tau_{(k)}/\theta_{(k)}, \quad \tilde{\sigma}_{(k+1)} = \theta_{(k)}\tilde{\sigma}_{(k)}$
- 7: $\bar{y}^{(k+1)} = y^{(k+1)} + \theta_{(k)} Q(y^{(k+1)} - y^{(k)})$
- 8: **end for**

Theorem (5.1)

Let f_i^* be strongly convex with constants $\mu_i > 0, i = 1, \dots, n$. Let the initial step sizes $\tilde{\sigma}_{(0)}, \tau_{(0)}$ be chosen such that

$$\tilde{\sigma}_{(0)} < \min_i \frac{p_i}{2(1-p_i)},$$

and for the ESO parameters $\{v_i\}$ of $S_{(0)}^{1/2} A \tau_{(0)}^{1/2}$ it holds that

$$v_i \leq p_i, \quad i = 1, \dots, n$$

with $[S_{(k)}]_i = \sigma_i^{(k)} I$ and

$$\sigma_i^{(k)} = \frac{\tilde{\sigma}_{(k)}}{\mu_i [p_i - 2(1-p_i) \tilde{\sigma}_{(k)}]}.$$

Then there exists $\tilde{K} \in \mathbb{N}$ such that for all $K \geq \tilde{K}$ it holds that

$$\mathbb{E} \|y^{(K)} - y^\sharp\|_{Y_{(0)}}^2 \leq \frac{2}{K^2} \left[\|x^{(0)} - x^\sharp\|_{\tau_{(0)}}^2 + \|y^{(0)} - y^\sharp\|_{Y_{(0)}}^2 \right],$$

where the metric on \mathbb{Y} is defined by $Y_{(k)} := Q S_{(k)}^{-1} + 2M(Q - I)$.

Theorem (6.1)

Let the step sizes $\tau, \sigma_1, \dots, \sigma_n, 0 < \theta < 1$ be chosen such that the ESO parameters $\{v_i\}$ of $S^{1/2}A\tau^{1/2}$ can be estimated as

$$v_i < p_i/\theta, \quad i = 1, \dots, n$$

and the extrapolation θ satisfies the lower bounds

$$\theta \geq \frac{1}{1 + 2\mu_g\tau}, \quad \theta \geq \frac{1 + 2(1 - p_i)\mu_i\sigma_i}{1 + 2\mu_i\sigma_i}, \quad i = 1, \dots, n$$

Then the iterates of Algorithm 1 converge linearly to the saddle point; in particular

$$\begin{aligned} \mathbb{E} \left\{ (1 - \gamma^2\theta) \|x^{(K)} - x^\#\|_X^2 + \|y^{(K)} - y^\#\|_Y^2 \right\} \leq \\ \theta^K \left\{ \|x^{(0)} - x^\#\|_X^2 + \|y^{(0)} - y^\#\|_Y^2 \right\} \end{aligned}$$

holds where the metrics are given by $X := (\tau^{-1} + 2\mu_g)I$, $Y := (S^{-1} + 2M)Q$, and $\gamma^2 = \max_i v_i/p_i$.

- Space of tracer distributions or images: $\mathbb{X} = \mathbb{R}^{d_1 \times d_2}$, $d_1 = d_2 = 250$.
- Data spaces: $\mathbb{Y}_i = \mathbb{R}^{|\mathbb{B}_i|}$
 - $\mathbb{B}_i \subset [200 \times 250]$, $\mathbb{B}_i \cap \mathbb{B}_j = \emptyset$, $\bigcup_{i=1}^n \mathbb{B}_i = [200 \times 250]$
 - $f_i(y) = \begin{cases} \sum_{j \in \mathbb{B}_i} \left[y_j + r_j - b_j + b_j \log \left(\frac{b_j}{y_j + r_j} \right) \right], & \text{if } y_j + r_j > 0, \\ +\infty, & \text{else.} \end{cases}$
- Operator A is a scaled X-ray transform where in each of 200 directions 250 line integrals are computed.
- TV prior: $g(x) = \alpha \|\nabla x\|_{2,1} + \iota_{\geq 0}(x)$
 - $\alpha = 0.2$, $\nabla x = (\nabla_1 x, \nabla_2 x) \in \mathbb{R}^{d_1 d_2 \times 2}$.

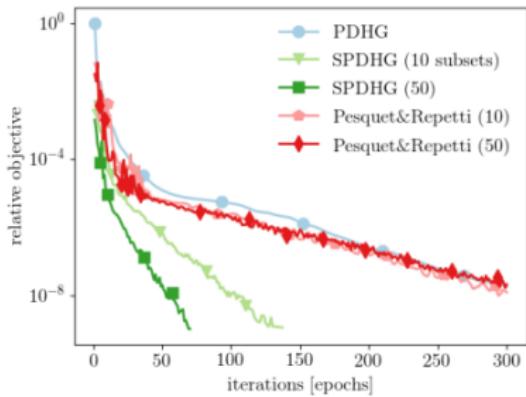
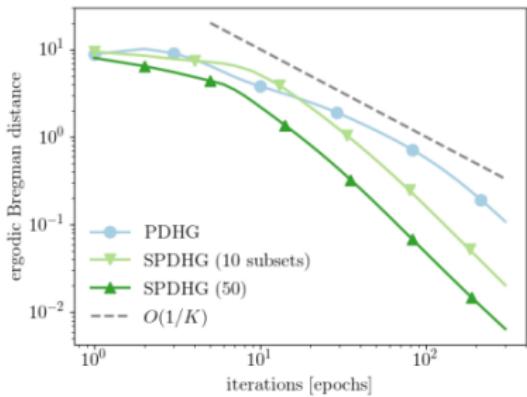


FIG. 1. PET reconstruction with TV solved as a nonstrongly convex problem. Left: As proven in Theorem 4.3, the ergodic Bregman distances converge indeed with rate $O(1/K)$. Right: Speed comparison measured in terms of relative objective $[\Phi(x^{(K)}) - \Phi(x^\#)] / [\Phi(x^{(0)}) - \Phi(x^\#)]$. The proposed algorithm SPDHG converges faster than the algorithm of Pesquet and Repetti [35] and the deterministic PDHG.

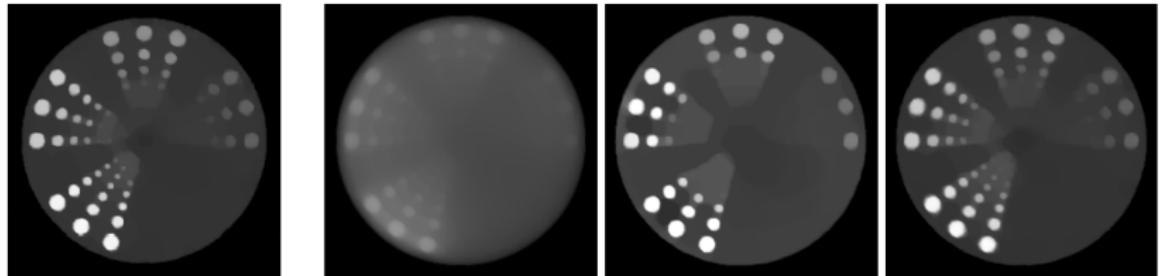


FIG. 2. PET reconstruction results after 5 epochs with uniform sampling of 50 subsets. From left to right: Approximate primal part of saddle point, PDHG, Pesquet and Repetti [35], and SPDHG. With the same number of operator evaluations, both stochastic algorithms make much more progress towards the saddle point.