Faster PET Reconstruction with a Stochastic Primal-Dual Hybrid Gradient Method

Peter Richtárik

KAUST, The University of Edinburgh

Joint work with A. Chambolle (École Polytechnique), M. J. Ehrhardt (Cambridge) and C.-B. Schönlieb (Cambridge)

April 10, 2017



Motivation









Simple Model for PET Operator



$$(\mathbf{X}x)(s,s^{\perp}) = \int_{\mathbb{R}} x(s+ts^{\perp})dt$$

(X-ray transform)

Advanced Model for PET Operator

 $A : x \mapsto \mathsf{MNX}(x * k)$

- resolution modelling
- X-ray transform X
- multiplicative correction N (attenuation and normalization)
- dead detector modelling (subsampling) M
- $\mathbf{A} \ge 0$ $(\mathbf{A}_{ij} \ge 0)$. Therefore: $x \ge 0 \Rightarrow \mathbf{A}x \ge 0$

 $d \sim \text{Poisson}(\mathbf{A}x + r)$

background $r \ge 0$: scatter, randoms

Correction Factors



Maximum A-Posteriori Estimation

Image Reconstruction by MAP Estimation

Data $\{d_i\}_{i=1}^N$ is independent Poisson with mean $\lambda_i = (\mathbf{A}x + r)_i$: $d_i \sim \text{Poisson}(\lambda_i)$

- Want to estimate the unknown parameters λ_i
- This is "equivalent to" estimating the unknown image x

MAP: Maximum A-Posteriori Estimation of Image x

$$x_{\textit{MAP}} \in \arg\max_{x} \underbrace{p(d_1, \ldots, d_N \mid x)}_{\textit{likelihood}} imes \underbrace{\psi(x)}_{\textit{prior}}$$

PET Data Fidelity: Poisson likelihood

Poisson likelihood

$$p(d_1, \dots, d_N \mid x) := \prod_{i=1}^N \lambda_i^{d_i} \exp(-\lambda_i)/d_i!$$
$$= \prod_{i=1}^N \exp\{-KL(d_i, \lambda_i) - \xi(d_i)\}$$

KL(d_i, λ_i) := d_i log(d_i/λ_i) + λ_i − d_i generalized relative entropy; generalized KL divergence

$$\blacktriangleright \xi(d_i) := d_i \log d_i - d_i - \log(d_i!)$$

MAP Estimation via Minimization of KL Divergence

$$\arg \max_{x} p(d_{1}, \dots, d_{N} \mid x) \times \psi(x)$$

$$= \arg \max_{x} \log p(d_{1}, \dots, d_{N} \mid x) + \log(\psi(x))$$

$$= \arg \min_{x} \left(\sum_{i=1}^{N} KL(d_{i}, \lambda_{i}(x)) + \xi(d_{i}) \right) \underbrace{-\log(\psi(x))}_{g(x)}$$

Partition the Sum into $n \ll N$ Blocks

$$\min_{x} \left(\sum_{i=1}^{n} \underbrace{\sum_{j \in B_{i}} KL(d_{j}, \lambda_{j}(x)) + \xi(d_{j})}_{f_{i}(\mathbf{A}_{i} \times)} \right) + g(x)$$

MAP Reconstruction

$$\min_{x}\left\{\sum_{i=1}^{n}f_{i}(\mathbf{A}_{i}x)+g(x)\right\}$$

Assumptions on f_i and g

Block Loss/Fidelity Functions

$$f_i : \mathbb{Y}_i \mapsto \mathbb{R} \cup \{+\infty\}, \quad i = 1, 2, \dots, n$$

Regularizer

$$g : \mathbb{X} \mapsto \mathbb{R} \cup \{+\infty\}$$

Examples: total variation Rudin, Osher, Fatemi 1992, total generalized variation Bredies, Kunisch, Pock 2010

Assumption

Functions f_1, \ldots, f_n and g are proper, convex, closed

Consequence:

$$f_i(y_i) = f_i^{**}(y_i) := \max_{z_i \in \mathbb{Y}_i} \langle y_i, z_i \rangle - f_i^*(z_i)$$

Reformulation into a Saddle Point Optimization Problem

MAP Reconstruction

Find
$$x^* \in \arg\min_{x \in \mathbb{X}} \left\{ \sum_{i=1}^n f_i(\mathbf{A}_i x) + g(x) \right\}$$

Saddle Point Problem

$$\min_{x \in \mathbb{X}} \max_{y \in \mathbb{Y}} \left\{ \sum_{i=1}^{n} \langle \mathbf{A}_{i} x, y_{i} \rangle - f_{i}^{*}(y_{i}) + g(x) \right\}$$

regularizer can be dualized as well, i.e., part of f

Algorithm

Primal-Dual Hybrid Gradient (PDHG) Algorithm*

PDHG (aka Chambolle-Pock) Algorithm

- ▶ initial iterates: $x^0 \in \mathbb{X}$, $y^0 \in \mathbb{Y}$, $\overline{y}^0 = y^0$
- ► step sizes: $\mathbf{T} \in \mathbb{R}^{|\mathbb{X}| \times |\mathbb{X}|}$, $\mathbf{S}_i \in \mathbb{R}^{|\mathbb{Y}_i| \times |\mathbb{Y}_i|}$, $\theta > 0$

Iterate:

- o $\operatorname{prox}_{g}^{\mathbf{M}}(z) := \arg\min_{x} \{ \frac{1}{2} \| x z \|_{\mathbf{M}^{-1}}^{2} + g(x) \}$ o $\| x \|_{\mathbf{M}^{-1}}^{2} := \langle \mathbf{M}^{-1} x, x \rangle$
- Evaluation of \mathbf{A}_i and \mathbf{A}_i^* for all $i = 1, \dots, n$.

^{*}Pock, Cremers, Bischof, Chambolle 2009, Chambolle and Pock 2011, Pock and Chambolle 2011

Stochastic PDHG Algorithm*

SPDHG Algorithm

- ▶ initial iterates: $x^0 \in \mathbb{X}$, $y^0 \in \mathbb{Y}$, $\overline{y}^0 = y^0$
- ► step sizes: $\mathbf{T} \in \mathbb{R}^{|\mathbb{X}| \times |\mathbb{X}|}$, $\mathbf{S}_i \in \mathbb{R}^{|\mathbb{Y}_i| \times |\mathbb{Y}_i|}$, $\theta > 0$

Iterate:

$$x^{k+1} = \operatorname{prox}_{g}^{\mathsf{T}}(x^{k} - \mathsf{TA}^{*}\overline{y}^{k})$$

- Select randomly Ŝ ⊆ {1,..., n}
 y_i^{k+1} = { prox^{S_i}_{f^{*}}(y_i^k + S_iA_ix^{k+1}) if i ∈ Ŝ y_i^k otherwise
 ȳ^{k+1} = y^{k+1} + θ**P**⁻¹(y^{k+1} - y^k)
- o matrix of probabilities $\mathbf{P} := \text{Diag}(p_1, \cdots, p_n)$, $p_i := \mathbb{P}(i \in \hat{S})$
- Evaluation of \mathbf{A}_i and \mathbf{A}_i^* only for $i \in \hat{S}$.

*generalizes Pock and Chambolle 2011 and Zhang and Xiao 2015 peter.richtarik@kaust.edu.sa

Convergence

ESO Parameters and Inequality*

Definition (Expected Separable Overapproximation (ESO))

Let $\hat{S} \subseteq \{1, \ldots, n\}$ be any sampling, with $p_i := \mathbb{P}(i \in \hat{S})$. Let $C_1, C_2, \ldots, C_n \in \mathbb{R}^{|\mathbb{Y}_i| \times |\mathbb{X}|}$. We say that scalars v_1, \ldots, v_n (ESO parameters) fulfil the ESO inequality if

$$\mathbb{E}_{\hat{S}} \left\| \sum_{i \in \hat{S}} \mathbf{C}_i^* y_i \right\|^2 \leq \sum_{i=1}^n p_i v_i \|y_i\|^2, \quad \text{for all} \quad y_1 \in \mathbb{Y}_1, \dots, y_n \in \mathbb{Y}_n.$$

Example (Full Sampling: $\hat{S} = \{1, \dots, n\}$ with probability 1) $1 \|\sum_{i=1}^{n} \mathbf{C}_{i}^{*} y_{i} \|^{2} \leq \sum_{i=1}^{n} 1 v_{i} \|y_{i}\|^{2}$. Can choose: $v_{i} = \|\mathbf{C}^{*}\|^{2}$

Example (Serial Sampling: $\hat{S} = \{i\}$ with probability p_i) $\frac{\sum_{i=1}^{n} p_i \|\mathbf{C}_i^* y_i\|^2 \le \sum_{i=1}^{n} p_i v_i \|y_i\|^2}{\text{Richtárik, Takáč 2011, Qu, Richtárik, Zhang 2014}}$

Inequality with ESO Parameters

Lemma (Estimating Inner Products)

Let y^k be generated by SPDHG and $\gamma^2 \ge \max_i v_i$, where v_1, \ldots, v_n are ESO parameters and $\mathbf{C}_i = \rho_i^{-1/2} \mathbf{S}_i^{1/2} \mathbf{A}_i \mathbf{T}^{1/2}$. Then for any $x \in \mathbb{X}$

$$\mathbb{E}^{k} \langle \mathbf{P}^{-1} \mathbf{A} x, y^{k} - y^{k-1} \rangle \geq -\frac{\gamma}{2} \mathbb{E}^{k} \Big\{ \|x\|_{\mathbf{T}^{-1}}^{2} + \|y^{k} - y^{k-1}\|_{(\mathbf{SP})^{-1}}^{2} \Big\}.$$

Example (Full Sampling: $\hat{S} = \{1, \dots, n\}$) $\|\mathbf{S}^{1/2}\mathbf{A}\mathbf{T}^{1/2}\|^2 \leq \gamma^2$, $\sigma\tau \|\mathbf{A}\|^2 \leq \gamma^2$

Example (Serial Sampling: $\hat{S} = \{i\}$) $\frac{\|\mathbf{S}_{i}^{1/2}\mathbf{A}_{i}\mathbf{T}^{1/2}\|^{2}}{p_{i}} \leq \gamma^{2}, \quad \frac{\sigma_{i}\tau \|\mathbf{A}_{i}\|^{2}}{p_{i}} \leq \gamma^{2}, \quad i = 1, \dots, n$

Convergence: General Theorem

$$\mathcal{E}(x,y) := \frac{1}{2} \|x - x^*\|_{\mathbf{T}^{-1}}^2 + \frac{1}{2} \|y - y^*\|_{(\mathbf{SP})^{-1}}^2 + \sum_{i=1}^n (p_i^{-1} - 1) D_{f_i^*}^{q_i^*}(y_i, y_i^*)$$

Theorem (Convergence of SPDHG)

Assume a saddle point exists. Let (x^*, y^*) be any saddle point, $p^* := -\mathbf{A}^* y^* \in \partial g(x^*)$, $q^* := \mathbf{A}x^* \in \partial f(y^*)$. Choose \mathbf{S}, \mathbf{T} such that $0 < \gamma^2 < 1$ upper bounds ESO parameters, $\theta = 1$. Then

- (x^k, y^k) is bounded in the sense that $\mathbb{E}\mathcal{E}(x^k, y^k) \leq \frac{\mathcal{E}(x^0, y^0)}{1-\gamma}$.
- ► $||x^{k+1} x^k|| \to 0$, $||y^{k+1} y^k|| \to 0$ almost surely
- ► $D_g^{p^*}(x^k, x^*) \rightarrow 0$, $D_{f^*}^{q^*}(y^k, y^*) \rightarrow 0$ almost surely
- ► ergodic sequence $(x_K, y_K) := \frac{1}{K} \sum_{k=1}^{K} (x^k, y^k).$ $\mathbb{E}D_g^{p^*}(x_K, x^*) + \mathbb{E}D_{f^*}^{q^*}(y_K, y^*) \leq \frac{\mathcal{E}(x^0, y^0)}{K}$

• Bregman distance: $D_g^{p^*}(x, x^*) := g(x) - g(x^*) - \langle p^*, x - x^* \rangle$ • Deterministic setting: convergence in norm to a saddle point

o Deterministic setting: convergence in norm to a saddle point peter.richtarik@kaust.edu.sa 23

Dual Accelerated SPDHG

DA-SPDHG Algorithm

- ▶ initial iterates: $x^0 \in \mathbb{X}$, $y^0 \in \mathbb{Y}$, $\overline{y}^0 = y^0$
- step sizes: $\mathbf{T}_0 \in \mathbb{R}^{|\mathbb{X}| \times |\mathbb{X}|}$, $ilde{\sigma}_0 > 0$

Iterate:

Dual Accelerated SPDHG

Theorem (Convergence of DA-SPDHG)

Let (x^*, y^*) be a saddle point and assume f_i are $\mu_i > 0$ strongly convex for i = 1, ..., n. Choose $\tilde{\sigma}_0, \mathbf{T}_0$ such that $0 < \gamma^2 \le 1$ upper bounds ESO parameters and $\tilde{\sigma}_0 < \min_i \frac{p_i}{2(1-p_i)}$. Let $\mathbf{Y}_k := (\mathbf{S}_k \mathbf{P})^{-1} + 2\mathbf{M}_f(\mathbf{P}^{-1} - I)$, $\mathbf{M}_f = \text{Diag}(\mu_1, ..., \mu_n)$. Then there exists $K_0 \in \mathbb{N}$, C > 0 such that for all $K \ge K_0$

$$\mathbb{E} \|y^{\mathcal{K}} - y^*\|_{\mathbf{Y}_0}^2 \leq \frac{C}{\mathcal{K}^2} \Big\{ \|x^0 - x^*\|_{\mathbf{T}_0^{-1}}^2 + \|y^0 - y^*\|_{\mathbf{Y}_0}^2 \Big\}.$$

o For serial sampling: $\tilde{\sigma}_0 \leq \min_i \frac{\gamma^2 \mu_i p_i^2}{\|\mathbf{A}_i \mathbf{T}_0^{1/2}\|^2 + 2\gamma^2 \mu_i p_i (1-p_i)}$

Linear Convergence

Theorem (Linear Convergence in the Strongly Convex Case)

Let (x^*, y^*) be a saddle point and g, f_i are $\mu_g, \mu_i > 0$ strongly convex for i = 1, ..., n. Choose $\mathbf{S}, \mathbf{T}, \theta \in (0, 1)$ such that $\gamma^2 \leq 1$ upper bounds ESO parameters and

 $\begin{aligned} \theta(\mathbf{I} + 2\mu_g \mathbf{T}) &\geq \mathbf{I} \\ \theta(\mathbf{I} + 2\mu_i \mathbf{S}_i) &\geq \mathbf{I} + 2(1 - p_i)\mu_i \mathbf{S}_i, \quad i = 1, \dots, n \end{aligned}$

in a positive semidefinite sense for matrices. Let

$$\mathbf{X} := \mathbf{T}^{-1} + 2\mu_g \mathbf{I}, \ \mathbf{Y} := (\mathbf{S}^{-1} + 2\mathbf{M}_f)\mathbf{P}^{-1}, \ \mathbf{M}_f = \text{Diag}(\mu_1, \dots, \mu_n).$$

Then the iterates of SPDHG satisfy

$$\mathbb{E}\left\{(1-\gamma^{2}\theta)\|\boldsymbol{x}^{K}-\boldsymbol{x}^{*}\|_{\mathbf{X}}^{2}+\|\boldsymbol{y}^{K}-\boldsymbol{y}^{*}\|_{\mathbf{Y}}^{2}\right\} \leq \theta^{K}C$$

where the constant is $C := \|x^0 - x^*\|_{\mathbf{X}}^2 + \|y^0 - y^*\|_{\mathbf{Y}}^2$. peter.richtarik@kaust.edu.sa Parameters for Serial Sampling $\hat{S} = \{i\}$

- scalar parameters: $\mathbf{T} = \tau \mathbf{I}, \ \mathbf{S}_i = \sigma_i \mathbf{I}$
- condition number: $\kappa_i := \frac{\|\mathbf{A}_i\|^2}{\mu_i \mu_g}$

Example (Uniform Sampling: $p_i = 1/n$)

$$\sigma_i = \frac{\gamma}{\kappa_i^{1/2} \mu_i}, \tau = \frac{\gamma}{n \max_j \kappa_j^{1/2} \mu_g}, \quad \theta = 1 - \left(n + \frac{n \max_j \kappa_j^{1/2}}{2\gamma}\right)^{-1}$$

Example (Importance Sampling:
$$p_i = \frac{\kappa_i^{1/2}}{\sum_{j=1}^n \kappa_j^{1/2}}$$
)

$$\sigma_i = \frac{\gamma}{\kappa_i^{1/2} \mu_i}, \tau = \frac{\gamma}{\sum_{j=1}^n \kappa_j^{1/2} \mu_g}, \quad \theta = 1 - \left(\frac{\sum_j \kappa_j^{1/2}}{\max_j \kappa_j^{1/2}} + \frac{\sum_j \kappa_j^{1/2}}{2\gamma}\right)^{-1}$$

Numerical Results

$$x^* \in \arg\min_{x \ge 0} \left\{ \sum_{i=1}^n \tilde{\mathsf{KL}}(d_i, \mathbf{A}_i x + r_i) + \alpha \|\nabla x\|_{1,2} + \frac{\mu_g}{2} \|x\|^2 \right\}$$

▶ 5 epochs





Figure: Distance to the saddle point



Figure: Peak signal-to-noise ratio



Figure: Objective function value

Conclusions and Outlook

Conclusions:

- Stochastic optimization for separable cost functionals
- Stochastic generalization of PDHG of Chambolle and Pock: non-smooth, acceleration, linear convergence
- Application to PET: incredible speed-up!

Outlook:

- Theory: Other $1/k^2$ acceleration techniques
- Application: real 3D PET data, block selection, non-uniform sampling
- Other applications: CT, MRI

Extra Material: More Experimental Results

$$x^* \in \arg\min_{x \ge 0} \left\{ \sum_{i=1}^n \mathsf{KL}(d_i, \mathbf{A}_i x + r_i) + \alpha \| \nabla x \|_{1,2} \right\}$$

 Proximal operator for TV with non-negativity constraint approximated with 5 iterations of warm started FGP Beck & Teboulle 2009.

•
$$\gamma = 0.95, \theta = 1$$
, uniform sampling $p_i = 1/n$

Compare methods:

PDHG:

$$\sigma = \frac{\gamma}{\|\mathbf{A}\|} \approx 1.8$$
e-03, $\tau = \frac{\gamma}{\|\mathbf{A}\|} \approx 1.8$ e-03

SPDHG (
$$n = 20$$
):
 $\sigma_i = \frac{\gamma}{\|\mathbf{A}_i\|} \approx 8.0e{-}03$ (mean), $\tau = \frac{\gamma}{n \max_i \|\mathbf{A}_i\|} \approx 3.8e{-}04$

• SPDHG
$$(n = 150)$$
:

$$\sigma_i = \frac{\gamma}{\|\mathbf{A}_i\|} \approx 1.6\text{e-02} \text{ (mean)}, \ \tau = \frac{\gamma}{n \max_i \|\mathbf{A}_i\|} \approx 7.7\text{e-05}$$

Pesquet and Repetti 2015 (
$$n = 150$$
):
 $\sigma = \frac{\gamma}{\|\mathbf{A}\|} \approx 1.8\text{e-}03, \ \tau = \frac{\gamma}{\|\mathbf{A}\|} \approx 1.8\text{e-}03$

► 10 epochs







Figure: distance to a saddle point



Figure: Bregman distance of ergodic sequence

peter.richtarik@kaust.edu.sa



Figure: Objective function value



Figure: Peak signal-to-noise ratio

Extra Material: Other Imaging Tasks

$$x^* \in \arg\min_x \left\{ \frac{1}{2} \|x - d\|^2 + \alpha \sum_{i=1}^2 \|\nabla_i x\|_1 \right\}$$

- primal acceleration $1/k^2$, 20 epochs
- implemented using ODL Adler, Kohr, Öktem, 2017





Figure: Primal distance to saddle point.



Figure: Bregman distance between iterates and saddle point.



Figure: Relative objective function values.



Figure: PSNR between iterates and ground truth solution.

Poisson TV deblurring with unknown boundary*

$$x^* \in \arg\min_{a \leq x \leq b} \Big\{ \tilde{\mathsf{KL}}(d, M(x * k) + r) + \alpha \sum_{i=1}^2 \mathsf{Huber}_{\beta}(\nabla_i x) \Big\}$$

• dual acceleration $1/k^2$, 100 epochs



Poisson TV deblurring with unknown boundary



Figure: Distance to dual part of the saddle point.

peter.richtarik@kaust.edu.sa

Poisson TV deblurring with unknown boundary



Figure: Relative objective function value.

Poisson TV deblurring with unknown boundary



Figure: Peak signal-to-noise ratio (PSNR).

Extra Material: Further Details on Mathematical Abstraction

Mathematical Abstraction: n + 2 Hilbert Spaces

Primal Space

- space: \mathbb{X} element: $x \in \mathbb{X}$
- inner product: $\langle x, x' \rangle$ for $x, x' \in \mathbb{X}$

• norm:
$$||x|| := \sqrt{\langle x, x \rangle}$$

n Dual Block Spaces

- ▶ space: \mathbb{Y}_i , i = 1, 2, ..., n element: $y_i \in \mathbb{Y}_i$
- ▶ inner product: $\langle y_i, y'_i \rangle$ for $y_i, y'_i \in \mathbb{Y}_i$

• norm:
$$||y_i|| := \sqrt{\langle y_i, y_i \rangle}$$

Dual Product Space

- ▶ space: $\mathbb{Y} := \prod_{i=1}^{n} \mathbb{Y}_{i}$ element: $y = (y_1, \dots, y_n) \in \mathbb{Y}$
- inner product: $\langle y, y' \rangle := \sum_{i=1}^{n} \langle y_i, y'_i \rangle$

• norm:
$$||y||^2 := \sum_{i=1}^n ||y_i||^2$$

Mathematical Abstraction: Linear Operators

Block Operators

▶
$$\mathbf{A}_i : \mathbb{X} \mapsto \mathbb{Y}_i$$
 for $i = 1, 2, ..., n$ (we write $\mathbf{A}_i x = y_i$)

• adjoint
$$\mathbf{A}_i^* : \mathbb{Y}_i \mapsto \mathbb{X}$$

Aggregated Operator

• $A : \mathbb{X} \mapsto \mathbb{Y}$ defined by

$$\mathbf{A}x := (\mathbf{A}_1 x, \mathbf{A}_2 x, \cdots, \mathbf{A}_n x)$$

• adjoint $\mathbf{A}^* : \mathbb{Y} \mapsto \mathbb{X}$ given by

$$\mathbf{A}^* y = \sum_{i=1}^n \mathbf{A}_i^* y_i$$