Introduction	Material decomposition	Constrained algorithm	Numerical experiments	Results	Conclusion

An ADMM algorithm for constrained material decomposition in spectral CT

May, 23th, 2018

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Spectra	I CT				



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Attenuation coefficients depend on energy



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Allow decomposing materials



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Introdu	ction				

Introduction

Previous work

- A Gauss-Newton algorithm was developed [1]
 - + Fast convergence
 - + Better decomposition error than first order algorithms
 - + Spatially regularized
 - Can have negative values



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Constrained algorithms

Positivity constraints were added for materials decomposition

- Long and Fessler 2014 [2]
- Noh and Fessler 2009 [3]
- Sidky and Pan 2014 [4]
- Ding and Long 2017 [5]

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First oder algorithms in projection and image domain

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- } Second order algorithm in image domain

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Propose	ed method				

Positivity / Inequality

• We propose to enforce the positivity of the materials maps

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Propose	ed method				

Positivity / Inequality

• We propose to enforce the positivity of the materials maps

Equality

- Quantity of injected marker is known
- Should be retrieved in the decompositions

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Proposed method

Positivity / Inequality

• We propose to enforce the positivity of the materials maps

Equality

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Algorithm

• Use of an alternating direction method of multipliers (ADMM) : update of a with a second order algorithm

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Forward	l problem				

Denoting $\mathbf{s} \in \mathbb{R}^{IP}$ the data vector and $\mathbf{a} \in \mathbb{R}^{MP}$ the materials maps, we have :

$$\mathbf{s} = [s_{1,1}, \dots, s_{l,1}, \dots, s_{l,P}]^{\mathrm{T}}$$
$$\mathbf{a} = [a_{1,1}, \dots, a_{m,1}, \dots, a_{M,P}]^{\mathrm{T}}$$

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$$\mathbf{a} = [a_{1,1}, ..., a_{m,1}, ..., a_{M,P}]^{\mathrm{T}}$$

Using the standard spectral CT forward model is :

$$\mathbf{s}_{i,p} = \int_{\mathbf{R}} n_i^0(E) \exp\left(-\sum_{m=1}^M a_{m,p} \tau_m(E)\right) \mathrm{d}E$$

with $n_i^0(E)$ the effective spectrum, $\tau_m(E)$ a function representing the material attenuation and $a_{m,p}$ the projected mass of material m on pixel p.

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Inverse	problem				

• We propose to solve :

$$\min_{\mathbf{a}} \mathcal{C}(\mathbf{a}, \mathbf{s}) \quad \text{s.t} \quad \begin{cases} \mathbf{a} \ge \mathbf{0} \\ \sum_{p} a_{m,p} = c_{m} \end{cases}$$
(1)

with c_m is the quantity of *m*th material.

• We chose

$$C(\mathbf{a}, \mathbf{s}) = D(\mathbf{a}, \mathbf{s}) + \alpha_{\mathrm{R}} \mathcal{R}(\mathbf{a})$$

where

$$\begin{split} \mathcal{D}(\mathbf{a},\mathbf{s}) &= ||\mathbf{s} - \mathcal{F}(\mathbf{a})||_{\mathbf{W}}^{2} \\ \mathcal{R}(\mathbf{a}) &= ||\Delta \mathbf{a}_{\text{soft}}||_{2}^{2} + ||\nabla \mathbf{a}_{\text{bone}}||_{1} + ||\nabla \mathbf{a}_{\text{Gd}}||_{1} \end{split}$$

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ADMM					

The Lagrangian function is minimized by an ADMM algorithm :

$$egin{aligned} \mathcal{L}(\mathbf{a},\mathbf{b},oldsymbollpha_{\mathrm{I}},lpha_{\mathrm{E}},\mathbf{s}) &= \mathcal{D}(\mathbf{a},\mathbf{s}) + lpha_{\mathrm{R}}\mathcal{R}(\mathbf{a}) \ &+ \mathcal{H}_{\mathrm{E}}(\mathbf{a},lpha_{\mathrm{E}}) + \mathcal{G}_{\mathrm{E}}(\mathbf{a}) \ &+ \mathcal{H}_{\mathrm{I}}(\mathbf{a},\mathbf{b},oldsymbollpha_{\mathrm{I}}) + \mathcal{G}_{\mathrm{I}}(\mathbf{a},\mathbf{b}) + \mathbf{1}(\mathbf{b}) \end{aligned}$$

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The Lagrangian function is minimized by an ADMM algorithm :

$$\begin{split} \mathcal{L}(\mathbf{a},\mathbf{b},\pmb{\alpha}_{\mathrm{I}},\alpha_{\mathrm{E}},\mathbf{s}) &= \mathcal{D}(\mathbf{a},\mathbf{s}) + \alpha_{\mathrm{R}}\mathcal{R}(\mathbf{a}) \\ &+ \mathcal{H}_{\mathrm{E}}(\mathbf{a},\alpha_{\mathrm{E}}) + \mathcal{G}_{\mathrm{E}}(\mathbf{a}) \\ &+ \mathcal{H}_{\mathrm{I}}(\mathbf{a},\mathbf{b},\pmb{\alpha}_{\mathrm{I}}) + \mathcal{G}_{\mathrm{I}}(\mathbf{a},\mathbf{b}) + \mathbf{1}(\mathbf{b}) \end{split}$$

where

Equality : $\sum_{p} a_{m,p} = c_m$ $\mathcal{H}_{\mathrm{E}}(\mathbf{a}, \alpha_{\mathrm{E}}) = \alpha_{\mathrm{E}} \left(\sum_{p=1}^{P} \frac{a_{\mathrm{gd},p}}{c_{\mathrm{gd}}} - 1 \right)$ $\mathcal{G}_{\mathrm{E}}(\mathbf{a}) = \frac{\beta_{\mathrm{E}}}{2} \left(\sum_{p=1}^{P} \frac{a_{\mathrm{gd},p}}{c_{\mathrm{gd}}} - 1 \right)^2$ with $\alpha_{\mathrm{E}} \in \mathbf{R}$ and $\beta_{\mathrm{E}} \in \mathbf{R}$.

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$$egin{aligned} \mathcal{L}(\mathbf{a},\mathbf{b},oldsymbollpha_{\mathrm{I}},lpha_{\mathrm{E}},\mathbf{s}) &= \mathcal{D}(\mathbf{a},\mathbf{s}) + lpha_{\mathrm{R}}\mathcal{R}(\mathbf{a}) \ &+ \mathcal{H}_{\mathrm{E}}(\mathbf{a},lpha_{\mathrm{E}}) + \mathcal{G}_{\mathrm{E}}(\mathbf{a}) \ &+ \mathcal{H}_{\mathrm{I}}(\mathbf{a},\mathbf{b},oldsymbollpha_{\mathrm{I}}) + \mathcal{G}_{\mathrm{I}}(\mathbf{a},\mathbf{b}) + \mathbf{1}(\mathbf{b}) \end{aligned}$$

where

Inequality : $\mathbf{a} \ge \mathbf{0}$

Inequalities need an auxiliary variable, b, such that the constraint becomes a=b and $b\geq 0.$

$$egin{aligned} \mathcal{H}_{\mathrm{I}}(\mathbf{a},\mathbf{b},oldsymbollpha_{\mathrm{I}}) &= oldsymbollpha_{\mathrm{I}}^{\mathrm{T}}(\mathbf{b}-\mathbf{a}) \ \mathcal{G}_{\mathrm{I}}(\mathbf{a},\mathbf{b}) &= rac{eta_{\mathrm{I}}}{2}||\mathbf{b}-\mathbf{a}||_2^2 \end{aligned}$$

and

$$\mathbf{1}(\mathbf{b}) = \begin{cases} 0, & \text{if } \mathbf{b} \geq 0 \\ \infty, & \text{otherwise} \end{cases}$$

with $\alpha_{I} \in \mathbf{R}^{MP}$ and $\beta_{I} \in \mathbf{R}$.

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Minimiz	ation scheme				

• Minimization of $\mathcal{L}(\mathbf{a}, \mathbf{b}, \alpha_{I}, \alpha_{E}, \mathbf{s})$ is done by finding the saddle point [6], through alternating updates :

Update	Algorithm used
$a^{\ell+1}\in \operatorname{argmin}\mathcal{L}(a,b^\ell,lpha^\ell_\mathrm{E},oldsymbollpha^\ell_\mathrm{I})$	Iterative Gauss-Newton
$\mathbf{b}^{\ell+1} \in \mathop{\mathrm{argmin}}_{\mathbf{b}} \mathcal{L}(\mathbf{a}^{\ell+1}, \mathbf{b}, lpha^{\ell}_{\mathrm{E}}, oldsymbol{lpha}^{\ell}_{\mathrm{I}})$	Proximal algorithm
$lpha_{ ext{E}}^{\ell+1} \in \operatorname{argmax}_{\mathcal{L}} \mathcal{L}(a^{\ell+1}, b^{\ell+1}, lpha_{ ext{E}}, \boldsymbol{lpha}_{ ext{I}}^{\ell})$	Ascent gradient
$oldsymbol{lpha}_{\mathrm{I}}^{\ell+1} \in \operatorname*{argmax}_{oldsymbol{lpha}_{\mathrm{I}}} \mathcal{L}(\mathbf{a}^{\ell+1}, \mathbf{b}^{\ell+1}, lpha_{\mathrm{E}}^{\ell+1}, oldsymbol{lpha}_{\mathrm{I}})$	Ascent gradient

• Moreover, at each iteration ℓ , Lagrangian parameters are increasing

$$\begin{split} \beta_{\rm E}^{\ell+1} &= \omega \beta_{\rm E}^\ell \\ \beta_{\rm I}^{\ell+1} &= \omega \beta_{\rm I}^\ell \end{split}$$

• Until they reach the maximum allow value β_{\max} .

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D					

Parameters

Phantom

- Thorax : 84×306 pixels
- 3 materials : soft tissues, bones and gadolinium (portal vein)
- 4 energy bins

Algorithm

• $\mathbf{a}^0 = 0 \mathrm{g.cm}^{-2}$

•
$$\alpha_{\mathrm{R}} = 1$$
, $\alpha_{\mathrm{E}}^{0} = 0$, $\boldsymbol{\alpha}_{\mathrm{I}}^{0} = 0$

•
$$eta_{ ext{E}}^{ ext{0}}=10^{ ext{0}}$$
, $eta_{ ext{I}}^{ ext{0}}=10^{-2}$, $\omega=1.5$

•
$$\beta_{\rm max} = 10^{10}$$

- Stopping criteria
 - The inner loop stops if
 - $\bullet\,$ the relative decrease of the cost function is too low (10^{-3})
 - it made more than 30 iterations
 - The outer loop stops if

• the equality is respected :
$$|\left(\sum_{
ho}^{P} rac{\delta_{\mathrm{gd},\mathrm{P}}^{\ell}}{c_{\mathrm{gd}}} - 1
ight)| < 10^{-3}$$

- \bullet the inequality is respected : $|| \boldsymbol{a}^\ell \boldsymbol{b}^\ell || < 10^{-3}$
- Decomposition for $\theta = [0^{\circ}, 359^{\circ}]$

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Projection domain



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Drainet	ion domain				

Projection domain



Evaluation of the decomposition with the $\ell_2\text{-norm}$:

$$\xi_{\mathrm{D}}^{ heta} = \sum_{m}^{M} ||\mathbf{a}_{m}^{ heta} - \mathbf{a}_{m}^{\mathrm{truth}, heta}||_{2}$$

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Image domain



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Image domain							



Evaluation of the reconstructed materials with the $\ell_2\text{-norm}$:

$$\chi^{z}_{\mathrm{D}} = \sum_{m}^{M} || \boldsymbol{\rho}^{\mathrm{z}}_{m} - \boldsymbol{\rho}^{\mathrm{truth},\mathrm{z}}_{m} ||_{2}$$

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Conclusion					

- Equality and inequality constraints give a better decomposition and visualization
- Decrease cross-talk
- However, it needs more iteration

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Conclus	sion				

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- However, it needs more iteration

And next :

• Application of this algorithm to real data

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Thank you for your attention ! Questions? :)

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```
while Stopping criteria aren't met for the
outer loop do
while Stopping criteria aren't met for
the inner loop do
| solve(H^k \delta a^k = -g^k) | a^{k+1} = a^k + \lambda^k \delta a^k | k = k + 1
end
a^{\ell+1} = a^{k-1}
```

 $\bullet~$ Update of a : Gauss-Newton algorithm

 $\begin{array}{l} \mbox{while Stopping criteria aren't met for the} \\ \mbox{outer loop do} \\ \mbox{while Stopping criteria aren't met for} \\ \mbox{the inner loop do} \\ \mbox{solve} \left(\mathsf{H}^k \delta a^k = - \mathbf{g}^k \right) \\ \mbox{a}^{k+1} = \mathbf{a}^k + \lambda^k \delta \mathbf{a}^k \\ \mbox{k} = \mathbf{k} + 1 \\ \mbox{end} \\ \mbox{a}^{\ell+1} = \mathbf{a}^{k-1} \\ \mbox{b}^{\ell+1} = \Pi (\mathbf{a}^{\ell+1} - \frac{\mathbf{a}_1^\ell}{\beta_1}) \end{array}$

- $\bullet~$ Update of a : Gauss-Newton algorithm
- $\bullet~$ Update of b~: Proximal algorithm

- $\bullet~$ Update of a : Gauss-Newton algorithm
- $\bullet~$ Update of b~: Proximal algorithm
- $\bullet~$ Update of α_E : Ascent gradient

 $\begin{array}{l} \mbox{while Stopping criteria aren't met for the} \\ \mbox{outer loop do} \\ \mbox{while Stopping criteria aren't met for} \\ \mbox{the inner loop do} \\ \mbox{loop above } \left(\begin{array}{l} \mbox{solve} \left(\mathsf{H}^k \delta \mathbf{a}^k = -\mathbf{g}^k \right) \\ \mbox{solve} \left(\mathsf{H}^k \delta \mathbf{a}^k = -\mathbf{g}^k \right) \\ \mbox{a}^{k+1} = \mathbf{a}^k + \lambda^k \delta \mathbf{a}^k \\ \mbox{loop k} = k+1 \\ \mbox{end} \\ \mbox{a}^{\ell+1} = \mathbf{a}^{k-1} \\ \mbox{b}^{\ell+1} = \Pi(\mathbf{a}^{\ell+1} - \frac{\mathbf{a}^\ell_1}{\beta_1}) \\ \mbox{a}^{\ell+1}_E = \alpha^\ell_E + \beta_E \frac{\mathcal{H}_E(\mathbf{a}^{\ell+1}_E)}{\alpha^\ell_E} \\ \mbox{a}^{\ell+1} = \mathbf{a}^\ell_1 + \beta_1(\mathbf{b}^{\ell+1} - \mathbf{a}^{\ell+1}) \end{array} \right)$

- $\bullet~$ Update of a : Gauss-Newton algorithm
- Update of \mathbf{b} : Proximal algorithm
- $\bullet~$ Update of α_E : Ascent gradient
- Update of $\pmb{\alpha}_{\mathrm{I}}$: Ascent gradient

- Update of **a** : Gauss-Newton algorithm
- $\bullet~$ Update of b~: Proximal algorithm
- $\bullet~$ Update of α_E : Ascent gradient
- Update of $\pmb{\alpha}_{\mathrm{I}}$: Ascent gradient
- Update of the β s

while Stopping criteria aren't met for the outer loop do while Stopping criteria aren't met for the inner loop do solve $(\mathbf{H}^k \delta \mathbf{a}^k = -\mathbf{g}^k)$ $a^{k+1} = a^k + \lambda^k \delta a^k$ k = k + 1end $a^{\ell+1} = a^{k-1}$ $\mathbf{b}^{\ell+1} = \Pi(\mathbf{a}^{\ell+1} - \frac{\mathbf{a}_{\mathrm{I}}^{\ell}}{\beta_{\mathrm{r}}})$ $\alpha_{\rm E}^{\ell+1} = \alpha_{\rm E}^{\ell} + \beta_{\rm E} \frac{\mathcal{H}_{\rm E}(\mathbf{a}_m^{\ell+1})}{\alpha_{\rm E}^{\ell}}$ $\boldsymbol{\alpha}_{\mathrm{I}}^{\ell+1} = \boldsymbol{\alpha}_{\mathrm{I}}^{\ell} + \beta_{\mathrm{I}}(\mathbf{b}^{\ell+1} - \mathbf{a}^{\ell+1})$ $\beta_{\rm E}^{\ell+1} = \omega \beta_{\rm E}^{\ell}$ $\beta_{\rm T}^{\ell+1} = \omega \beta_{\rm T}^{\ell}$ if $\beta_{\rm E}^{\ell+1} > \beta_{\rm max}$ then $\vec{\beta}_{\mathrm{F}}^{\ell+1} = \beta_{\mathrm{max}}$ end if $\beta_{\mathrm{I}}^{\ell+1} > \beta_{\mathrm{max}}$ then $\beta_{\rm I}^{\ell+1} = \beta_{\rm max}$ end $\ell = \ell + 1$ end

- Update of **a** : Gauss-Newton algorithm
- Update of **b** : Proximal algorithm
- Update of $\alpha_{\rm E}$: Ascent gradient
- Update of \pmb{lpha}_{I} : Ascent gradient
- Update of the β s
- Make sure that the values aren't too high