

Inverse Problems

Sommersemester 2022

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Total variation regularization for X-ray tomography

Some helpful resources on the Chambolle–Pock algorithm:

-  A. Chambolle and T. Pock. A first-order primal-dual algorithm for convex problems with applications to imaging. *J. Math. Imaging Vision* **40**:120–145, 2011.
-  L. Condat. A generic proximal algorithm for convex optimization – application to total variation minimization. *IEEE Signal Proc. Letters* **21**(8):985–989, 2014.
-  E. Y. Sidky, J. H. Jørgensen, and X. Pan. Convex optimization problem prototyping for image reconstruction in computed tomography with the Chambolle-Pock algorithm. *Phys. Med. Biol.* **57**:3065–3091, 2012.
-  Operator Discretization Library. https://odl.readthedocs.io/math/solvers/nonsmooth/chambolle_pock.html, 2017.
-  PORTAL. portal.readthedocs.io/en/latest/chambollepock.html, written by P. Paleo, 2015.

Additional resources on total variation regularization for X-ray tomography:

-  J. L. Mueller and S. Siltanen. Linear and Nonlinear Inverse Problems with Practical Applications. 2012.
-  S. Siltanen. Total variation regularization for X-ray tomography. FIPS Computational Blog, <https://blog.fips.fi/tomography/x-ray-total-variation-regularization-for-x-ray-tomography/>, 2017.

Recall that the discrete measurement model for X-ray tomography can be expressed as

$$y = Ax.$$

This time, we consider solving the inverse problem of recovering x based on noisy measurements y .

We are interested in *anisotropic total variation regularization*

$$\arg \min_{x \geq 0} \left\{ \frac{1}{2} \|y - Ax\|^2 + \lambda \|Dx\|_1 \right\}, \quad \lambda > 0,$$

where $\|x\|_1 = \sum_i |x_i|$, $D = \begin{bmatrix} L_H \\ L_V \end{bmatrix}$ is the discretized (image) gradient operator,

$$\|Dx\|_1 = \sum_j |(Dx)_j| = \sum_j |(L_H x)_j| + \sum_j |(L_V x)_j|,$$

and L_H and L_V denote the horizontal and vertical (image) finite difference matrices, respectively.

Special feature: TV regularization preserves sharp edges.

x_{91}	x_{92}	x_{93}	x_{94}	x_{95}	x_{96}	x_{97}	x_{98}	x_{99}	x_{100}
x_{81}	x_{82}	x_{83}	x_{84}	x_{85}	x_{86}	x_{87}	x_{88}	x_{89}	x_{90}
x_{71}	x_{72}	x_{73}	x_{74}	x_{75}	x_{76}	x_{77}	x_{78}	x_{79}	x_{80}
x_{61}	x_{62}	x_{63}	x_{64}	x_{65}	x_{66}	x_{67}	x_{68}	x_{69}	x_{70}
x_{51}	x_{52}	x_{53}	x_{54}	x_{55}	x_{56}	x_{57}	x_{58}	x_{59}	x_{60}
x_{41}	x_{42}	x_{43}	x_{44}	x_{45}	x_{46}	x_{47}	x_{48}	x_{49}	x_{50}
x_{31}	x_{32}	x_{33}	x_{34}	x_{35}	x_{36}	x_{37}	x_{38}	x_{39}	x_{40}
x_{21}	x_{22}	x_{23}	x_{24}	x_{25}	x_{26}	x_{27}	x_{28}	x_{29}	x_{30}
x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	x_{16}	x_{17}	x_{18}	x_{19}	x_{20}
x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}

Recall that the vector x is related to the density matrix ($f_{i,j}$) of the computational domain via

$$x_{(j-1)n+i} = f_{i,j}, \quad i, j \in \{1, \dots, n\}.$$

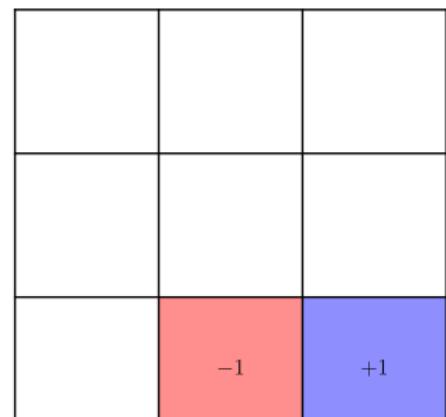
`x = f(:) and f = reshape(x,n,n)`

Construction of L_H (periodic boundary conditions)

-1	+1	

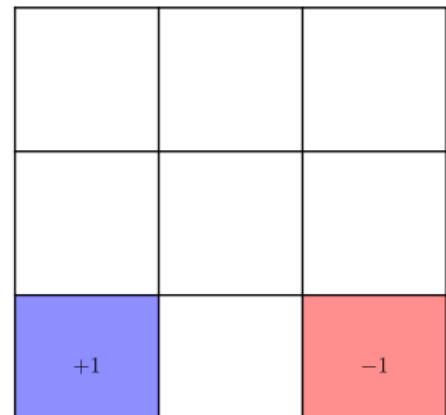
$$\begin{bmatrix} -1 & 1 \end{bmatrix}$$

Construction of L_H (periodic boundary conditions)



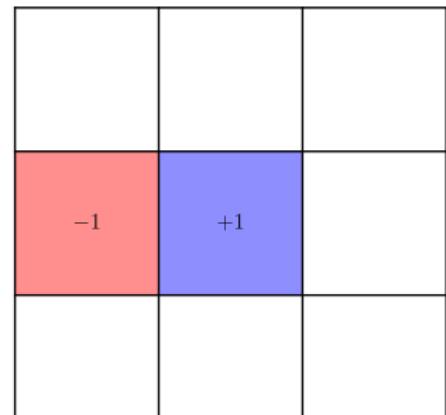
$$\begin{bmatrix} & -1 & 1 \\ & -1 & 1 \\ \end{bmatrix}$$

Construction of L_H (periodic boundary conditions)



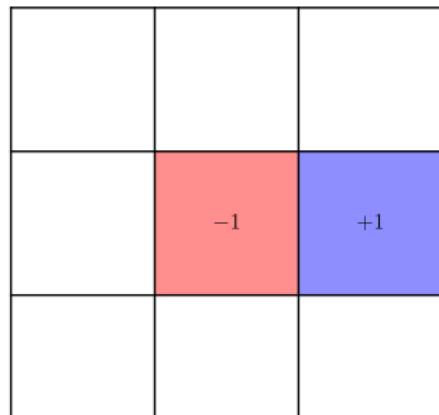
$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$

Construction of L_H (periodic boundary conditions)



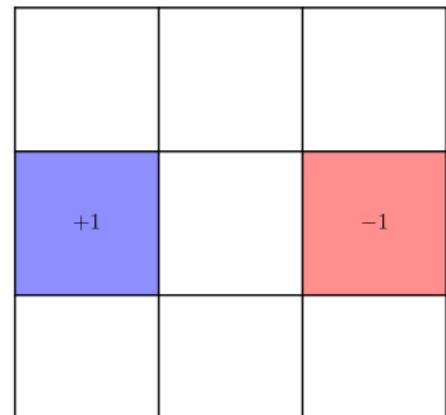
$$\begin{bmatrix} & -1 & 1 \\ & -1 & 1 \\ 1 & & -1 \\ & & -1 & 1 \end{bmatrix}$$

Construction of L_H (periodic boundary conditions)



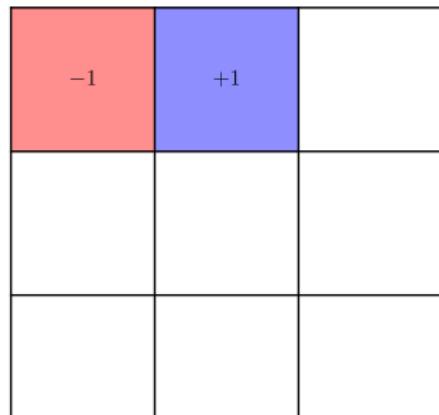
$$\begin{bmatrix} & \begin{matrix} -1 & 1 \\ -1 & 1 \end{matrix} & \\ \begin{matrix} -1 & 1 \\ 1 & -1 \end{matrix} & & \begin{matrix} -1 & 1 \\ -1 & 1 \end{matrix} \\ & \begin{matrix} -1 & 1 \\ -1 & 1 \end{matrix} & \end{bmatrix}$$

Construction of L_H (periodic boundary conditions)



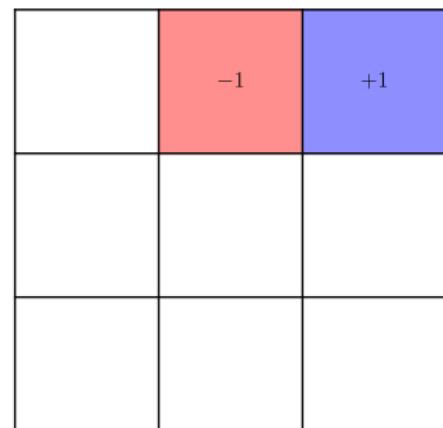
$$\begin{bmatrix} -1 & 1 & \\ & -1 & 1 \\ 1 & & -1 & \\ & & & -1 & 1 \\ & & & & -1 \\ & & & 1 & & -1 \end{bmatrix}$$

Construction of L_H (periodic boundary conditions)



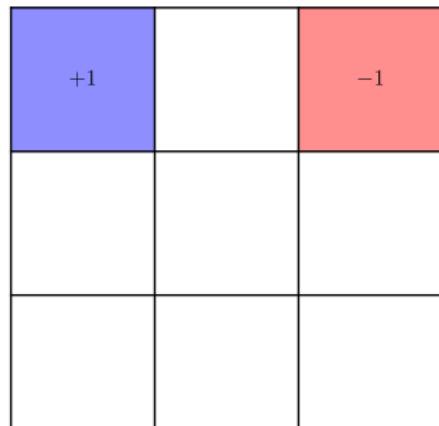
$$\begin{bmatrix} -1 & 1 & \\ 1 & -1 & 1 \\ & -1 & 1 \\ & 1 & -1 \\ & & -1 & 1 \end{bmatrix}$$

Construction of L_H (periodic boundary conditions)



$$\begin{bmatrix} -1 & 1 & \\ 1 & -1 & 1 \\ & -1 & 1 \\ & 1 & -1 \\ & & -1 & 1 \\ & & -1 & 1 \end{bmatrix}$$

Construction of L_H (periodic boundary conditions)



$$\begin{bmatrix} -1 & 1 & \\ 1 & -1 & 1 \\ & -1 & 1 \\ & 1 & -1 \\ & -1 & 1 \\ 1 & & -1 \end{bmatrix}$$

Construction of L_H (periodic boundary conditions)

$$\begin{bmatrix} -1 & 1 & & & & & & & \\ & -1 & 1 & & & & & & \\ 1 & & -1 & & & & & & \\ & & & -1 & 1 & & & & \\ & & & & -1 & 1 & & & \\ & & & 1 & & -1 & & & \\ & & & & & & -1 & 1 & \\ & & & & & & & -1 & 1 \\ & & & & & & 1 & & -1 \end{bmatrix}$$

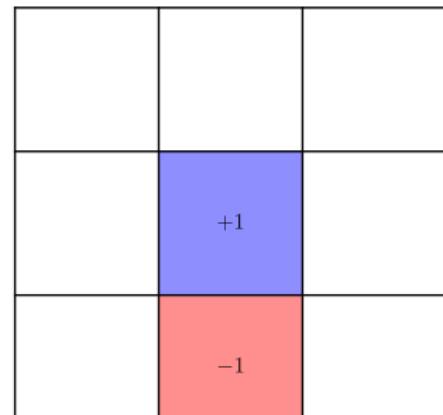
```
n = 3;
block = spdiags([1,-1,1].*ones(n,3),[1-n,0,1],n,n);
%block = -eye(n)+diag(ones(n-1,1),1); block(end,1) = 1;
LH = [];
for ii = 1:n
    LH = blkdiag(LH,block); % form the 9x9 block matrix
end
```

Construction of L_V (periodic boundary conditions)

+1		
-1		

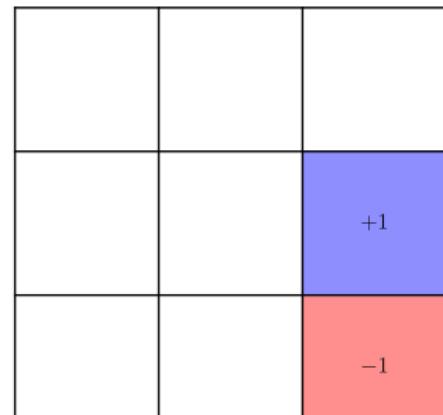
$$\begin{bmatrix} & -1 & 1 \\ & & \end{bmatrix}$$

Construction of L_V (periodic boundary conditions)



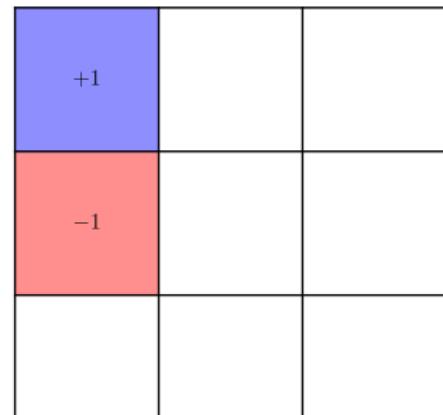
$$\begin{bmatrix} -1 & & 1 \\ & -1 & \\ & & 1 \end{bmatrix}$$

Construction of L_V (periodic boundary conditions)



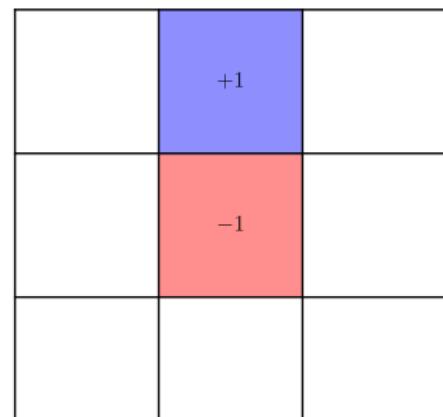
$$\begin{bmatrix} & -1 & & 1 & \\ & & -1 & & 1 \\ & & & -1 & \\ & & & & 1 \end{bmatrix}$$

Construction of L_V (periodic boundary conditions)



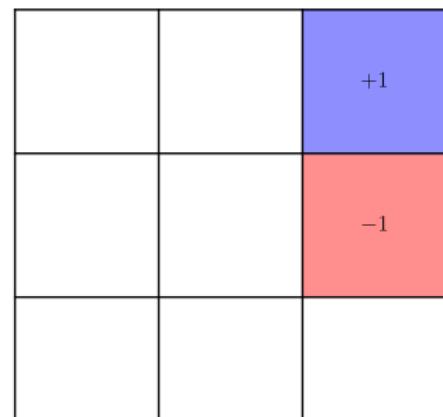
$$\begin{bmatrix} -1 & & 1 & & \\ & -1 & & 1 & \\ & & -1 & & 1 \\ & & & -1 & \\ & & & & 1 \end{bmatrix}$$

Construction of L_V (periodic boundary conditions)



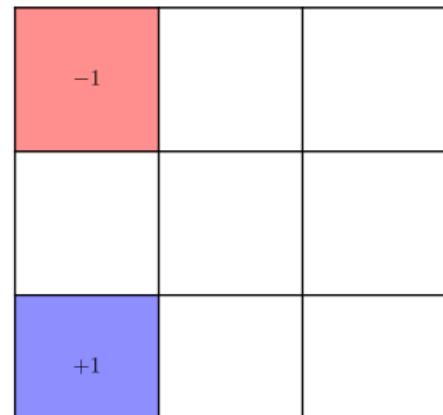
$$\begin{bmatrix} -1 & & 1 & & \\ & -1 & & 1 & \\ & & -1 & & 1 \\ & & & -1 & \\ & & & & -1 \end{bmatrix}$$

Construction of L_V (periodic boundary conditions)



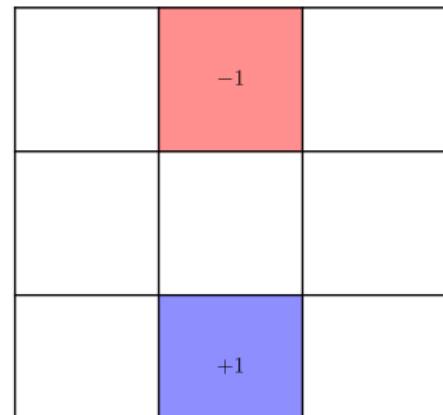
$$\begin{bmatrix} -1 & & 1 & & \\ & -1 & & 1 & \\ & & -1 & & 1 \\ & & & -1 & & 1 \\ & & & & -1 & \\ & & & & & -1 \end{bmatrix}$$

Construction of L_V (periodic boundary conditions)



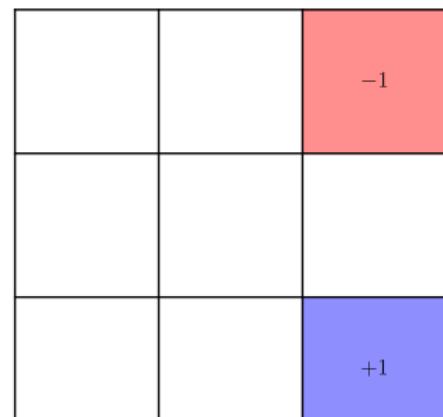
$$\begin{bmatrix} -1 & & & & & & & & \\ & -1 & & & & & & & \\ & & 1 & & & & & & \\ & & & 1 & & & & & \\ & & & & -1 & & & & \\ & & & & & -1 & & & \\ & & & & & & 1 & & \\ & & & & & & & -1 & \\ & & & & & & & & 1 \\ 1 & & & & & & & & \end{bmatrix}$$

Construction of L_V (periodic boundary conditions)



$$\begin{bmatrix} -1 & & 1 & & \\ & -1 & & 1 & \\ & & -1 & & 1 \\ & & & -1 & & 1 \\ 1 & & 1 & & -1 & & -1 \\ & & & & & -1 & & 1 \end{bmatrix}$$

Construction of L_V (periodic boundary conditions)



$$\begin{bmatrix} -1 & & 1 & & \\ & -1 & & 1 & \\ & & -1 & & 1 \\ & & & -1 & & 1 \\ 1 & & 1 & & -1 & & \\ & 1 & & 1 & & -1 & & \\ & & & 1 & & & -1 & & \\ & & & & 1 & & & -1 & & \end{bmatrix}$$

Construction of L_V (periodic boundary conditions)

$$\begin{bmatrix} -1 & & 1 & & & \\ & -1 & & 1 & & \\ & & -1 & & 1 & \\ & & & -1 & & 1 \\ & & & & -1 & & 1 \\ 1 & & & & & -1 & \\ & 1 & & & & & -1 \\ & & 1 & & & & \end{bmatrix}$$

$n = 3;$

```
LV = spdiags([1,-1,1].*ones(n^2,3),[-n^2+n,0,n],n^2,n^2);  
%LV = -eye(n^2)+diag(ones(n^2-n,1),n)+diag(ones(n,1),n-n^2);
```

Let $F^*: \mathbb{R}^M \rightarrow \mathbb{R} \cup \{+\infty\}$ and $G: \mathbb{R}^N \rightarrow \mathbb{R} \cup \{+\infty\}$ be convex lower semicontinuous functions and $K \in \mathbb{R}^{M \times N}$. Consider the abstract problem

$$\min_{x \in \mathbb{R}^N} \max_{\eta \in \mathbb{R}^M} \{\langle Kx, \eta \rangle + G(x) - F^*(\eta)\}.$$

The general form of the Chambolle–Pock algorithm can be written as

$$\eta_{k+1} = \text{prox}_{\sigma F^*}(\eta_k + \sigma K \tilde{x}_k), \quad (\text{update dual variable})$$

$$x_{k+1} = \text{prox}_{\tau G}(x_k - \tau K^T \eta_{k+1}), \quad (\text{update primal variable})$$

$$\tilde{x}_{k+1} = x_{k+1} + \theta(x_{k+1} - x_k), \quad (\text{extrapolation})$$

where $\tau > 0$ is the primal step size, $\sigma > 0$ is the dual step size, $\theta > 0$ is an extrapolation parameter, and the *proximal operator* of a function f is defined as

$$\text{prox}_f(\eta) := \arg \min_x \left\{ f(x) + \frac{1}{2} \|x - \eta\|^2 \right\}.$$

If $\sigma\tau \leq 1/L^2$, $L = \|K\|_2$ (operator norm), and $\theta = 1$, then the algorithm can be shown to converge at linear rate $\mathcal{O}(k^{-1})$ [Chambolle and Pock 2011].

Let us recast the TV regularization problem

$$\min_{x \geq 0} \left\{ \frac{1}{2} \|y - Ax\|^2 + \lambda \|Dx\|_1 \right\}, \quad \lambda > 0, \quad (1)$$

in the above framework.

- Note that

$$\frac{1}{2} \|Ax - y\|^2 = \max_q \left\{ \langle Ax - y, q \rangle - \frac{1}{2} \|q\|^2 \right\},$$

since $0 = \nabla_q (\langle Ax - y, q \rangle - \frac{1}{2} \|q\|^2) = Ax - y - q$ iff $q = Ax - y$.

- Since $\|x\|_1 = \sum_i |x_i| = \langle |x|, 1 \rangle = \langle x, \text{sign}(x) \rangle$,

$$\lambda \|Dx\|_1 = \max_{\|z\|_\infty \leq 1} \langle Dx, \lambda z \rangle = \max_{\|z\|_\infty \leq \lambda} \langle Dx, z \rangle = \max_z \left\{ \langle Dx, z \rangle - \iota_\lambda(z) \right\},$$

where $\iota_\lambda(z) = 0$ if $\|z\|_\infty \leq \lambda$ and $\iota_\lambda(z) = +\infty$ otherwise.

Then (1) is equivalent to

$$\min_x \max_{q,z} \left\{ \langle Ax - y, q \rangle + \langle Dx, z \rangle - \frac{1}{2} \|q\|^2 - \iota_\lambda(z) + \iota_+(x) \right\},$$

where $\iota_+(x) = 0$ if $x \geq 0$ and $\iota_+(x) = +\infty$ otherwise.

It is easy to see that

$$\min_x \max_{q,z} \left\{ \langle Ax - y, q \rangle + \langle Dx, z \rangle - \frac{1}{2} \|q\|^2 - \iota_\lambda(z) + \iota_+(x) \right\}$$

is tantamount to

$$\min_x \max_{q,z} \left\{ \left\langle Kx, \begin{bmatrix} q \\ z \end{bmatrix} \right\rangle + G(x) - F^*(q, z) \right\},$$

where

$$G(x) = \iota_+(x),$$

$$F^*(q, z) = \langle y, q \rangle + \frac{1}{2} \|q\|^2 + \iota_\lambda(z),$$

$$K = \begin{bmatrix} A \\ D \end{bmatrix}.$$

Note that if $A \in \mathbb{R}^{Q \times N}$ and $D \in \mathbb{R}^{L \times N}$, then $K \in \mathbb{R}^{(Q+L) \times N}$ and we identify the dual variable as the pair $\eta = (q, z) \in \mathbb{R}^M$, where $q \in \mathbb{R}^Q$, $z \in \mathbb{R}^L$, and $M = Q + L$.

The proximal mapping corresponding to G is simply the projection onto $\{x \geq 0 \mid x \in \mathbb{R}^N\}$:

$$\text{prox}_{\tau G}(x) = (\max(x_i, 0))_i = \max(x, 0).$$

On the other hand,

$$\text{prox}_{\sigma F^*}(q, z) = \left(\frac{q - \sigma y}{1 + \sigma}, \frac{\lambda z}{\max(\lambda, |z|)} \right). \quad (\text{N.B. } \eta = (q, z))$$

Noting that $K^T = [A^T, D^T]$, the Chambolle–Pock algorithm takes the form

$$\begin{cases} \eta_{k+1} = \text{prox}_{\sigma F^*}(\eta_k + \sigma K \tilde{x}_k) \\ x_{k+1} = \text{prox}_{\tau G}(x_k - \tau K^T \eta_{k+1}) \\ \tilde{x}_{k+1} = x_{k+1} + \theta(x_{k+1} - x_k) \end{cases} \Leftrightarrow \begin{cases} q_{k+1} = \frac{q_k + \sigma A \tilde{x}_k - \sigma y}{1 + \sigma} \\ z_{k+1} = \frac{\lambda(z_k + \sigma D \tilde{x}_k)}{\max(\lambda, |z_k + \sigma D \tilde{x}_k|)} \\ x_{k+1} = \max(x_k - \tau A^T q_{k+1} - \tau D^T z_{k+1}, 0) \\ \tilde{x}_{k+1} = x_{k+1} + \theta(x_{k+1} - x_k). \end{cases} \begin{matrix} & \text{(elementwise division)} \\ & \text{(elementwise max)} \end{matrix}$$

Pseudocode for the Chambolle–Pock algorithm

Given: projection matrix A , data y , regularization parameter λ .

1. Form the difference matrices L_H and L_V . Set $D = [L_H; L_V]$;
 2. $L = \text{svds}([A; D], 1)$; % alt. use the power method
 3. $\tau = 1/L$, $\sigma = 1/L$, $\theta = 1$;
 4. $x = \text{zeros}(\text{size}(A, 2), 1)$, $q = \text{zeros}(\text{size}(A, 1), 1)$;
 5. $z = \text{zeros}(\text{size}(D, 1), 1)$, $\hat{x} = x$;
Repeat
 6. $q = (q + \sigma * (A * \hat{x} - y)) / (1 + \sigma)$;
 7. $z = \lambda * (z + \sigma * D * \hat{x}) ./ \max(\lambda, \text{abs}(z + \sigma * D * \hat{x}))$;
 8. $x_{\text{old}} = x$;
 9. $x = \max(x - \tau * A' * q - \tau * D' * z, 0)$;
 10. $\hat{x} = x + \theta * (x - x_{\text{old}})$;
- until convergence.