Inverse Problems

Sommersemester 2023

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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_{90}	x_{91}	x_{92}	x_{93}	x_{94}	x_{95}	x_{96}	x_{97}	x_{98}	x_{99}
x_{80}	x_{81}	x_{82}	x_{83}	x_{84}	x_{85}	x_{86}	x_{87}	x_{88}	x_{89}
x_{70}	x_{71}	x_{72}	x_{73}	x_{74}	x_{75}	x_{76}	x_{77}	x_{78}	x_{79}
x_{60}	x_{61}	x_{62}	x_{63}	x_{64}	x_{65}	x_{66}	x_{67}	x_{68}	x_{69}
x_{50}	x_{51}	x_{52}	x_{53}	x_{54}	x_{55}	x_{56}	x_{57}	x_{58}	x_{59}
x_{40}	x_{41}	x_{42}	x_{43}	x_{44}	x_{45}	x_{46}	x_{47}	x_{48}	x_{49}
x_{30}	x_{31}	x_{32}	x_{33}	x_{34}	x_{35}	x_{36}	x_{37}	x_{38}	x_{39}
x_{20}	x_{21}	x_{22}	x_{23}	x_{24}	x_{25}	x_{26}	x_{27}	x_{28}	x_{29}
x_{10}	x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	x_{16}	x_{17}	x_{18}	x_{19}
x_{0}	x_{1}	x_{2}	x_{3}	x_{4}	x_{5}	x_{6}	x_{7}	x_{8}	x_{9}

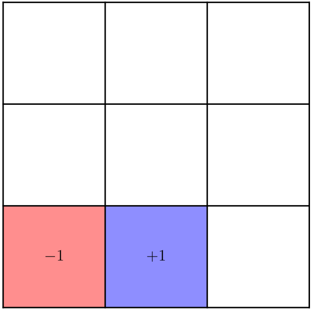
Recall that the vector x is related to the density matrix $(f_{i,j})$ of the computational domain via

$$x_{in+j} = f_{i,j}, \quad i, j \in \{0, \ldots, n-1\}.$$

`x = f.reshape((n*n,1))` and `f = x.reshape((n,n))` (Python)

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

Construction of L_H (periodic boundary conditions)



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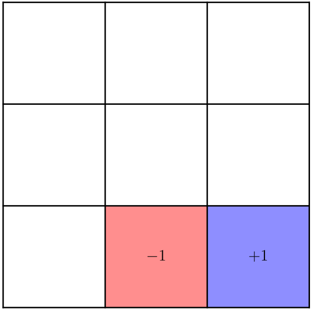
Construction of L_H (periodic boundary conditions)



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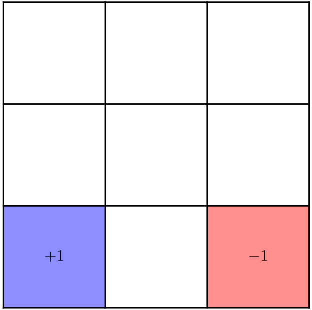

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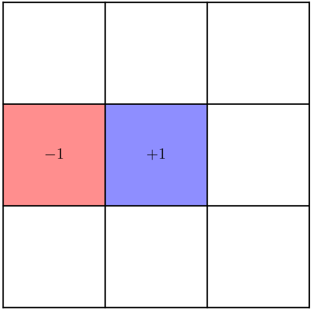

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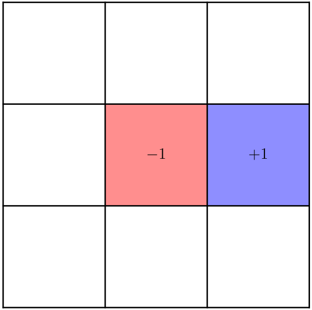

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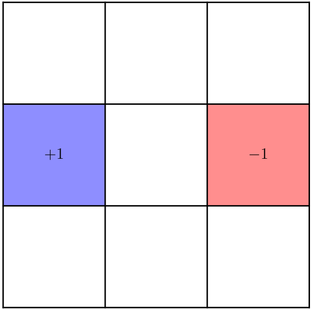

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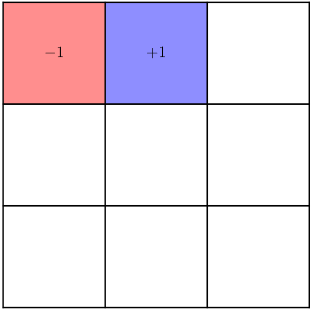

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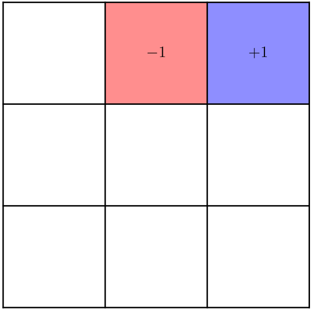

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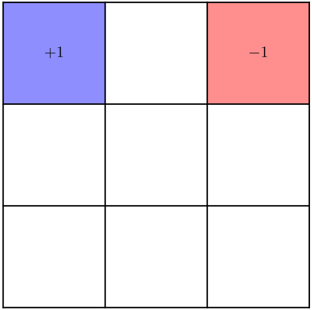

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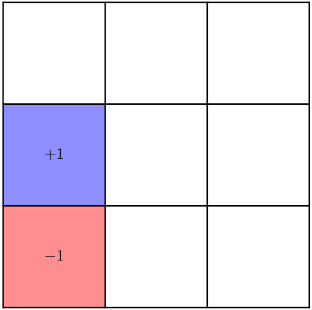
Python:

```
N = 3
block = sparse.spdiags(np.array([np.ones(N),-np.ones(N),np.ones(N)]),
                       np.array([1-N,0,1]),N,N) # form the 3x3 block
LH = sparse.block_diag([block]*N) # assemble the 9x9 block matrix
```

MATLAB:

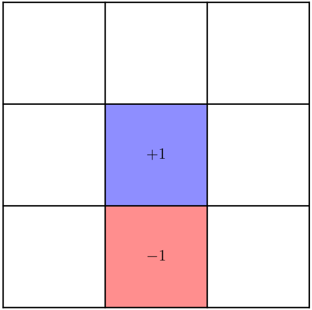
```
N = 3;
block = spdiags([1,-1,1].*ones(N,3),[1-N,0,1],N,N); % form the 3x3 block
LH = [];
for ii = 1:N
  LH = blkdiag(LH,block); % assemble the 9x9 block matrix
end
```

Construction of L_V (periodic boundary conditions)



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

Construction of L_V (periodic boundary conditions)



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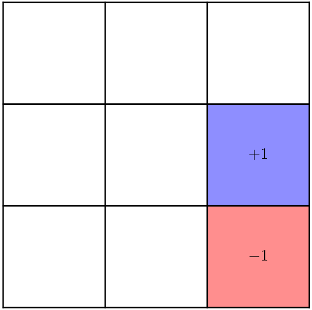

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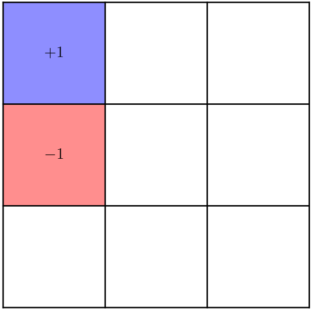

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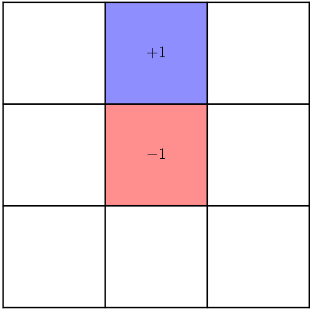

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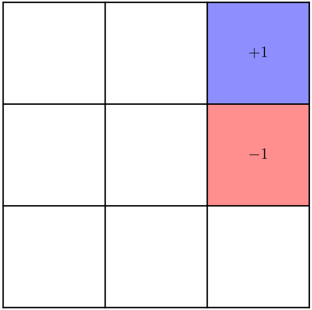

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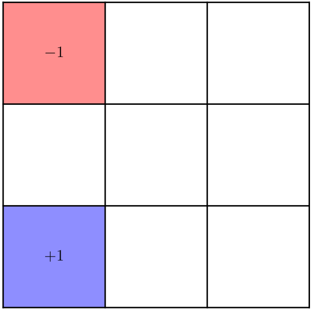

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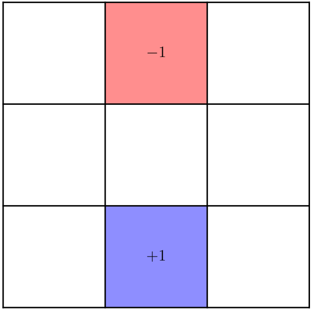
Construction of L_V (periodic boundary conditions)



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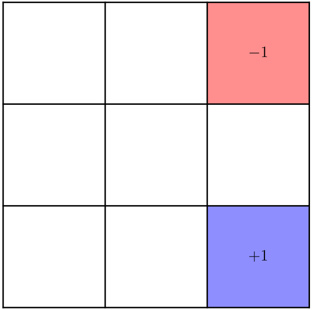

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Construction of L_V (periodic boundary conditions)

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Python:

```
N = 3
LV = sparse.spdiags(np.array([np.ones(N**2),-np.ones(N**2),np.ones(N**2)]),
                    np.array([-N**2+N,0,N]),N**2,N**2)
```

MATLAB:

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

Let $F^*\colon \mathbb{R}^M \to \mathbb{R} \cup \{+\infty\}$ and $G\colon \mathbb{R}^N \to \mathbb{R} \cup \{+\infty\}$ 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

$$\begin{aligned}
\eta_{k+1} &= \mathrm{prox}_{\sigma F^*}(\eta_k + \sigma K\widetilde{x}_k), && \text{(update dual variable)}\\
x_{k+1} &= \mathrm{prox}_{\tau G}(x_k - \tau K^{\mathrm{T}}\eta_{k+1}), && \text{(update primal variable)}\\
\widetilde{x}_{k+1} &= x_{k+1} + \theta(x_{k+1} - x_k), && \text{(extrapolation)}
\end{aligned}$$

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

$$\mathrm{prox}_f(\eta) := \arg\min_x \big\{ f(x) + \tfrac{1}{2}\|x - \eta\|^2 \big\}.$$

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

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

in the above framework.

- Note that

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

  since $0 = \nabla_q(\langle Ax - y, q\rangle - \frac{1}{2}\|q\|^2) = Ax - y - q$ iff $q = Ax - y$.
- Since $\|x\|_1 = \sum_i |x_i| = \langle |x|, 1\rangle = \langle x, \mathrm{sign}(x)\rangle$,

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

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

Then (1) is equivalent to

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

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

It is easy to see that

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

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

$$\begin{aligned} G(x) &= \iota_+(x), \\ F^*(q,z) &= \langle y, q \rangle + \tfrac{1}{2}\|q\|^2 + \iota_\lambda(z), \\ K &= \begin{bmatrix} A \\ D \end{bmatrix}. \end{aligned}$$

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 $\{x \geq 0 \mid x \in \mathbb{R}^N\}$:

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

On the other hand,

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

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

$$\begin{cases} \eta_{k+1} = \mathrm{prox}_{\sigma F^*}(\eta_k + \sigma K \widetilde{x}_k) \\ x_{k+1} = \mathrm{prox}_{\tau G}(x_k - \tau K^{\mathrm{T}} \eta_{k+1}) \\ \widetilde{x}_{k+1} = x_{k+1} + \theta(x_{k+1} - x_k) \end{cases}$$

$$\Leftrightarrow \quad \begin{cases} q_{k+1} = \frac{q_k + \sigma A \widetilde{x}_k - \sigma y}{1 + \sigma} \\ z_{k+1} = \frac{\lambda(z_k + \sigma D \widetilde{x}_k)}{\max(\lambda, |z_k + \sigma D \widetilde{x}_k|)} & \text{(elementwise division)} \\ x_{k+1} = \max(x_k - \tau A^{\mathrm{T}} q_{k+1} - \tau D^{\mathrm{T}} z_{k+1}, 0) & \text{(elementwise } \max) \\ \widetilde{x}_{k+1} = x_{k+1} + \theta(x_{k+1} - x_k). \end{cases}$$

Pseudocode for the Chambolle–Pock algorithm

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

1. Form the difference matrices $\mathtt{L_H}$ and $\mathtt{L_V}$. Set `D = [L_H;L_V];`
2. `L = svds([A;D],1);`
3. `tau = 1/L, sigma = 1/L, theta = 1;`
4. `x = zeros(size(A,2),1), q = zeros(size(A,1),1);`
5. `z = zeros(size(D,1),1), xhat = x;`

   Repeat

   6. `q = (q+sigma*(A*xhat-y))/(1+sigma);`
   7. `z = lambda * (z+sigma*D*xhat)./max(lambda,abs(z+sigma*D*xhat));`
   8. `xold = x;`
   9. `x = max(x-tau*A'*q-tau*D'*z,0);`
   10. `xhat = x+theta*(x-xold);`

   until convergence.