## $\ell^{1}$-regularization

Fallstudien der mathematischen Modellbildung, Teil 2
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## SPARSITY

- Enforcing structure helps with ill-conditioning and under-determined systems. A popular prior is sparsity, i.e. assuming the solution has only a few non-zero entries


■ Rationale: signals/data are often sparse in some basis / living on low-complexity domain.

## Regressor Selection

■ If $c_{i}, i=1, \ldots, n$ denotes the columns of $A$, the system rewrites

$$
y=\sum_{i=1}^{n} x_{i} c_{i}
$$

$\left(c_{i}\right)$ is an over-complete basis (or dictionary), and the goal is to select a subset of this basis that is sufficient to express $y \rightarrow$ regressor selection, or variable selection.

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- A natural candidate to promote sparsity of solutions is the $\ell^{0}$-norm

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! It is actually not a norm!

- The corresponding regularized problem is

$$
\min \|A x-y\|^{2}+\lambda\|x\|_{0}
$$

and in the noiseless case

$$
\min \|x\|_{0} \quad \text { s.t. } \quad A x=y
$$

## COMPUTATIONAL COMPLEXITY

- Remember that the penalized form is always equivalent to a constrained form with adequate parameter, i.e.

$$
\begin{equation*}
\min _{x \in \mathbb{R}^{n}}\|A x-y\|^{2} \quad \text { s.t. } \quad\|x\|_{0} \leqslant \tau \tag{1}
\end{equation*}
$$

■ NP-hard combinatorial, non-convex problem. Direct strategy: check every possible sparsity pattern, i.e. fix subsets J of non-zero entries in $x$ and solve the least-squares

$$
\min _{\tilde{x} \in \mathbb{R}^{n}}\left\|A_{j} \tilde{x}-y_{j}\right\|^{2}
$$

There are $\binom{n}{k}$ possible supports for each sparsity level $\rightarrow$ infeasible for large $n$

- Possible approximations of the problem:
- Greedy algorithms (e.g. orthogonal matching pursuit)
- Convex relaxation


## Convex envelope

- Definition (Convex envelope). The convex envelope of a function $I(x)$ is the largest convex $J(x)$ such that $J(x) \leqslant I(x)$.

- Theorem. The convex envelope of $\|x\|_{0}$ for $x$ restricted to $\|x\|_{\infty} \leqslant \alpha$ is $\|x\|_{1} / \alpha$



## CONVEX RELAXATION

- Relax $\ell^{0}$-penalty into $\ell^{1}$-penalty

$$
\begin{equation*}
\min \|A x-y\|_{2}^{2}+\lambda\|x\|_{1} \tag{LASso}
\end{equation*}
$$

Called LASSO ${ }^{1}$ (Least Absolute Shrinkage and Selection Operator) or basis pursuit denoising. When $\lambda=0$, we obtain the basis pursuit ${ }^{2}$ problem

$$
\begin{equation*}
\min \|x\|_{1} \quad \text { s.t. } \quad A x=y \tag{BP}
\end{equation*}
$$

- Main properties are:

Shrinkage: like Tikhonov regularization, LASSo penalizes large coefficients
Selection: unlike Tikhonov, LASso produces sparse estimates


[^0]
## LAGRANGE DUAL FUNCTION FOR LASSO

- We can reformulate the problem under a constrained form

$$
\min \frac{1}{2}\|z-y\|^{2}+\lambda\|x\|_{1} \quad \text { s.t. } \quad z=A x
$$

and deduce the Lagrangian:

$$
\mathcal{L}(x, z, \nu)=\frac{1}{2}\|z-y\|^{2}+\lambda\|x\|_{1}+\nu^{\top}(z-A x)
$$

- Minimization over $z$ yields $\tilde{z}=y-\nu$. Minimization over $x$ on the other hand is less obvious, since we have lost differentiability

$$
\inf _{x} \lambda\|x\|_{1}-\left\langle A^{\top} \nu, x\right\rangle=-\left(\sup _{x}\left\langle A^{\top} \nu, x\right\rangle-\lambda\|x\|_{1}\right)
$$

Definition (Conjugate function). The convex conjugate of $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$ is

$$
f^{*}(y)=\sup _{x}\langle y, x\rangle-f(x)
$$



With $J(x):=\lambda\|x\|_{1}$, the minimization over $x$ and $z$ yields,

$$
\mathcal{L}(\tilde{x}, \tilde{z}, \nu)=\nu^{\top} y-\frac{1}{2}\|\nu\|^{2}-J^{*}\left(A^{\top} \nu\right)
$$

## DUAL NORM

■ Definition (Dual norm). Given a norm \|.\| on $\mathbb{R}^{n}$, the associated dual norm is

$$
\|y\|_{*}=\sup \left\{y^{\top} x ;\|x\| \leqslant 1\right\}
$$

Example. $\|\cdot\|_{1}$ and $\|\cdot\|_{\infty}$ are dual to each other.

- Proposition. The conjugate function of $\|x\|$ is

$$
f^{*}(y)=\left\{\begin{array}{lc}
0 & \text { if }\|y\|_{*} \leqslant 1 \\
\infty & \text { otherwise }
\end{array}\right.
$$

Proof. ${ }^{1}$ If $\|y\|_{*}>1$, then by definition there exists $w \in \mathbb{R}^{n}$ such that $\|w\| \leqslant 1$ and $y^{\top} w>1$. Taking $x=$ tw and letting $t \rightarrow \infty$ we obtain

$$
y^{\top} x-\|x\|=t\left(y^{\top} w-\|w\|\right) \rightarrow \infty
$$

hence $f^{*}(y)=\infty$. If $\|y\|_{*} \leqslant 1$, since $y^{\top} x \leqslant\|x\|\|y\|_{*}$ for all $x$, then $y^{\top} x-\|x\| \leqslant 0$, and $x=0$ is the maximizer.

[^1]
## DUAL LASSO

- If $J(x)=\lambda\|x\|_{1}$, then $J^{*}(y)$ is the indicator of $\left\{\|y\|_{\infty} \leqslant \lambda\right\}$.
- Altogether, we obtain

$$
\mathcal{L}(\tilde{x}, \tilde{z}, \nu)=\nu^{\top} y-\frac{1}{2}\|\nu\|^{2}-i_{\left\{\nu:\|\nu\|_{\infty} \leqslant \lambda\right\}}\left(A^{\top} \nu\right)
$$

where we denote $i_{C}$ the indicator function of the set $C$. Hence the LASso dual problem reads

$$
\max \nu^{\top} y-\frac{1}{2}\|\nu\|^{2} \quad \text { s.t. } \quad\left\|A^{\top} \nu\right\|_{\infty} \leqslant \lambda
$$

## SUBDIFFERENTIAL

$\|\cdot\|_{1}$ is convex but not differentiable at 0 . How to derive optimality conditions?

- Recall the standard inequality for convex functions

$$
f(y) \geqslant f(x)+\langle\nabla f(x), y-x\rangle
$$

■ Definition (Sub-differential). The sub-differential of $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$ at $x$ is

$$
\partial f(x)=\left\{v \in \mathbb{R}^{n} ; \forall y \in \mathbb{R}^{n}, f(y) \geqslant f(x)+\langle v, y-x\rangle\right\}
$$

Note that $\partial f(x)$ is convex. If $f$ is differentiable, then $\partial f(x)=\{\nabla f(x)\}$.



- Proposition. For any function $f$,

$$
x_{*}=\operatorname{argmin}_{x} f(x) \Longleftrightarrow 0 \in \partial f(x)
$$

Proof. $x_{*}$ minimizer of $f \Longleftrightarrow \forall x, f(x) \geqslant f\left(x_{*}\right)=f\left(x_{*}\right)+\left\langle 0, x-x^{*}\right\rangle \Longleftrightarrow 0 \in \partial f(x)$.

## SUBDIFFERENTIAL CALCULUS

Some basic rules

- $\partial f(x)=\{\nabla f(x)\}$ if $f$ is differentiable at $x$
- $\partial(\alpha f)=\alpha \partial f$ if $\alpha>0$
- $\partial\left(f_{1}+f_{2}\right)(x)=\partial f_{1}(x)+\partial f_{2}(x)$ (except in pathological cases: according to Moreau-Rockafellar theorem, if there exists a point $x_{0} \in \operatorname{dom}\left(f_{1}+f_{2}\right)$ such that $f_{1}$ is continuous at $x_{0}$, then the equality holds for any $x \in \operatorname{dom}\left(f_{1}+f_{2}\right)$ ).
- if $g(x)=f(A x+b)$ where $f$ is convex, then $\partial g(x)=A^{\top} \partial f(A x+b)$


## SUBDIFFERENTIAL OF $\|\cdot\|_{1}$

- $|x|$ is differentiable at any $x \neq 0$ with derivative $\pm 1$. At 0 ,

$$
(\forall z \in \mathbb{R},|z| \geqslant y z) \Longleftrightarrow y \in[-1,1]
$$

so $\partial 0=[-1,1]$, and

$$
\partial|x|=\left\{\begin{array}{lll}
\{1\} & \text { if } & x>0 \\
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- Generalization:

$$
v \in \partial\|x\|_{1} \Longleftrightarrow v_{i}=\left\{\begin{array}{l}
v_{i}=\operatorname{sign}\left(x_{i}\right) \quad \text { if } \quad x_{i} \neq 0 \\
v_{i} \in[-1,1] \quad \text { if } \quad x_{i}=0
\end{array}\right.
$$

Proof. We have, by applying the calculus rules

$$
\|x\|_{1}=\sum\left|x_{i}\right|=\sum\left|e_{i}^{\top} x\right|
$$

hence

$$
\partial\|x\|_{1}=\sum \partial\left|e_{i}^{\top} x\right|=\sum e_{i} \partial\left|x_{i}\right|
$$

which leads to the desired result.

## Subdifferential and Conjugate Function

Let $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$. By definition of the conjugate function

$$
\forall x, y \in \mathbb{R}^{n}, \quad x^{\top} y \leqslant f(x)+f^{*}(y)
$$

Equality occurs when $y \in \partial f(x)$, i.e.

$$
\forall x, y \in \mathbb{R}^{n}, \quad x^{\top} y=f(x)+f^{*}(y) \Longleftrightarrow y \in \partial f(x)
$$

Proof. We have

$$
\begin{aligned}
x^{\top} y \geqslant f(x)+f^{*}(y) & \Longleftrightarrow x^{\top} y \geqslant f(x)+z^{\top} y-f(z) \quad \forall z \in \mathbb{R}^{n} \\
& \Longleftrightarrow f(z) \geqslant f(x)+\langle y, z-x\rangle \quad \forall z \in \mathbb{R}^{n} \\
& \Longleftrightarrow y \in \partial f(x)
\end{aligned}
$$

## OPTIMALITY CONDITIONS FOR LASSO

- The LASso objective

$$
\begin{equation*}
f(x):=\frac{1}{2}\|A x-y\|^{2}+\lambda\|x\|_{1} \tag{LASSO}
\end{equation*}
$$

is not always strictly convex: it can have several minimizers. This is in constrast for instance with the Tikhonov regularization

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- We can derive optimality conditions for Lasso

$$
0 \in \partial f(x)=A^{\top}(A x-y)+\lambda \partial\|x\|_{1}
$$

Proposition (LASSO optimality). $x_{*}$ is a minimizer of (LASSO) if and only if there exists $\eta \in \mathbb{R}^{n}$ such that

$$
A^{\top}\left(A x^{*}-y\right)+\lambda \eta=0
$$

where

$$
\left\{\begin{array}{l}
\eta_{i}=\operatorname{sign}\left(x_{* i}\right) \quad \text { if } \quad x_{* i} \neq 0 \\
\eta_{i} \in[-1,1] \quad \text { if } \quad x_{* i}=0
\end{array}\right.
$$

## The Othonormal Case

- If $A$ satisfies $A^{\top} A=I$, there is a closed-form solution given by the soft thresholding operator

$$
S_{\lambda}(x)= \begin{cases}x_{i}+\lambda & \text { if } \quad x_{i}<-\lambda \\ 0 & \text { if } \quad\left|x_{i}\right| \leqslant \lambda \\ x_{i}-\lambda & \text { if } \quad x_{i}>\lambda\end{cases}
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- In that case

$$
\min \frac{1}{2}\|A x-y\|^{2}+\lambda\|x\|_{1}=\frac{1}{2} \sum_{i}\left(x_{i}-\left(A^{\top} y\right)_{i}\right)^{2}+\lambda \sum_{i}\left|x_{i}\right|
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so we may solve the minimization component by component (separable problem). Let $z:=A^{\top} y$ and $h: \mathbb{R} \rightarrow \mathbb{R}, h(x):=\frac{1}{2}(x-z)^{2}+\lambda|x|$. Then the optimality conditions give

$$
0 \in \partial h(x)=\left\{\begin{array} { l l } 
{ x - z - \lambda } & { \text { if } x < 0 } \\
{ - z + \lambda [ - 1 , 1 ] \text { if } x = 0 } \\
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- Therefore, a solution obeys $x_{*}=S_{\lambda}\left(A^{\top} y\right)$


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- Gradient descent evolves in the direction of the negative gradient

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x_{k+1}=x_{k}-\gamma \nabla f\left(x_{k}\right)
$$

$\checkmark$ simple and cheap
$\checkmark$ can be fast for smooth (well-conditioned), strongly convex functions, with convergence at least $f\left(x_{t}\right)-f\left(x_{*}\right)=O\left(c^{-t}\right)$
$\boldsymbol{x}$ usually slow, with convergence $f\left(x_{t}\right)-f\left(x_{*}\right)=O(1 / t)$
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$x$ cannot handle non-differentiable functions


- Subgradient descent uses any vector in the subdifferential instead of the gradient

$$
x_{k+1}=x_{k}-\gamma g_{k}, \quad \text { where } \quad g_{k} \in \partial f\left(x_{k}\right)
$$

$\checkmark$ simple and cheap
$x$ sub-optimal solutions
$\boldsymbol{x}$ slow, with convergence $f\left(x_{t}\right)-f\left(x_{*}\right)=O(1 / \sqrt{t})$

## PROXIMAL METHODS

■ Definition (Proximal Operator). For a convex $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$ (or $\overline{\mathbb{R}}$ ), we define its proximal operator as

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\operatorname{prox}_{\gamma f}(x)=\operatorname{argmin}_{y} \frac{1}{2}\|x-y\|^{2}+\gamma f(y)
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i.e. y is the point from which if you look backwards along $-\nabla f(y)$, you reach $x$

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- Proximal operator generalizes projection: if $f(x)=\mathbb{1}_{C}(x)$ is an indicator function of a convex set, then $\operatorname{prox}_{\gamma f}(x)=\operatorname{Proj}_{C}(x)$. More generally, $\operatorname{prox}_{\gamma f}(x)$ is an orthogonal projection on a level set of $f$.


## OPTIMALITY CERTIFICATE

- Proposition (Fixed point). Let $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$ (or $\overline{\mathbb{R}}$ ) be continuous convex. For any $\gamma>0$,

$$
x_{*} \in \operatorname{argmin} f(x) \Longleftrightarrow x_{*}=\operatorname{prox}_{\gamma f}\left(x_{*}\right)
$$

Proof. We can assume without loss of generality that $\gamma=1$. Suppose $f(x) \geqslant f\left(x_{*}\right)$ for all $x$. Then

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\begin{aligned}
f(x)+\frac{1}{2}\left\|x-x_{*}\right\|^{2} \geqslant f\left(x_{*}\right)+\frac{1}{2}\left\|x_{*}-x_{*}\right\|^{2} & \Longrightarrow x_{*}=\operatorname{argmin}_{x} f(x)+\frac{1}{2}\left\|x-x_{*}\right\|^{2} \\
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On the other hand, assume that $x_{*}=\operatorname{prox}_{f}\left(x_{*}\right)$. Then

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0 \in \partial f\left(x_{*}\right)+x_{*}-x_{*} \Longrightarrow 0 \in \partial f\left(x_{*}\right)
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0 \in \partial f\left(x_{*}\right)+x_{*}-x_{*} \Longrightarrow 0 \in \partial f\left(x_{*}\right)
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which shows that $x_{*}$ minimizes $f$.

- Proximal iterations: $x_{k+1}=\operatorname{prox}_{\gamma f}\left(x_{k}\right)$ (fixed-point iterations)

Remark. prox is usually not a contraction (contraction $=\|h(x)-h(y)\| \leqslant \rho\|x-y\|$ with $\rho<1$ ), but it is nonexpansive, and slightly more, which ensures the convergence of fixed point iterations.

## Proximal Splitting

- Consider the generic problem

$$
\min F(x)+G(x)
$$

where $F \in C^{1}$ is differentiable, and $G \in C^{0}$ is "proximable" (i.e. we can easily project on its level lines).

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where $F \in C^{1}$ is differentiable, and $G \in C^{0}$ is "proximable" (i.e. we can easily project on its level lines). Then

$$
\begin{aligned}
0 \in \nabla F(x)+\partial G(x) & \Longleftrightarrow 0 \in(\lambda \nabla F(x)-x)+(x-\partial G(x)) \\
& \Longleftrightarrow(I-\gamma \nabla F)(x) \in(I+\gamma \partial G)(x)
\end{aligned}
$$

- Suggests updates of the form

$$
x_{k+1}=\operatorname{prox}_{\gamma F}\left(x_{k}-\gamma \nabla F\left(x_{k}\right)\right)
$$

This algorithm is called proximal gradient method, or forward-backward splitting.

## PROXIMAL SPLITTING

- Consider the generic problem

$$
\min F(x)+G(x)
$$

where $F \in C^{1}$ is differentiable, and $G \in C^{0}$ is "proximable" (i.e. we can easily project on its level lines). Then

$$
\begin{aligned}
0 \in \nabla F(x)+\partial G(x) & \Longleftrightarrow 0 \in(\lambda \nabla F(x)-x)+(x-\partial G(x)) \\
& \Longleftrightarrow(I-\gamma \nabla F)(x) \in(I+\gamma \partial G)(x)
\end{aligned}
$$

- Suggests updates of the form

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$$

This algorithm is called proximal gradient method, or forward-backward splitting.

- Convergence with rate $O(1 / k)$ when $\gamma \in[0,1 / L]$ fixed, where $\nabla F$ is $L$-Lipschitz ( $L$ corresponds to the conditioning of $A$ in our case).


## Proximal Splitting for Lasso

- Recall the LASSO

$$
\min \frac{1}{2}\|A x-y\|^{2}+\lambda\|x\|_{1}=\text { "smooth" }+ \text { "simple" }
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■ Proximal operator for $\|\cdot\|_{1}$

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- Iterative Soft-thresholding Algorithm (ISTA)

$$
x_{k+1}=S_{\lambda}\left(x_{k}-\frac{1}{\kappa(A)} A^{\top}\left(A x_{k}-y\right)\right)
$$

- Choice of regularization parameter $\lambda$ is, as always, sensitive


## Wavelet Sparsity

- Wavelet basis = orthonormal (Hilbert) basis of $L^{2}(\Omega)$, and a fortiori of $\mathbb{R}^{n}$

$$
\psi_{a, b}^{(\theta)}(x)=\frac{1}{\sqrt{a}} \psi^{(\theta)}\left(\frac{x-b}{a}\right)
$$

Comparable to Fourier basis, but extracts both spatial and frequency information. Images have sparse representation with respect to wavelets, i.e. $\left\langle f, \psi_{a, b}\right\rangle \simeq 0$ often. $x \in \mathbb{R}^{n}$ coefficients $\quad f=\Psi x \in \mathbb{R}^{q}$ image $\quad y=K f+\delta \in \mathbb{R}^{m}$ data


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- Wavelet Sparse Regularization

$$
\min _{x \in \mathbb{R}^{n}}\|y-A x\|^{2}+\|x\|_{1}
$$

(synthesis)
and the reconstructed image is then given by $f=\Psi_{x}$, or

$$
\min _{f \in \mathbb{R}^{q}}\|y-K f\|^{2}+\left\|\Psi^{\top} f\right\|_{1}
$$

## Wavelet Denoising

Corresponds to $A=I_{n}$ : solution is given in closed-form by soft-thresholding.


## TOMOGRAPHY

$$
\min _{f}\|y-\mathcal{R} f\|^{2}+\left\|\Psi^{\top} f\right\|, \quad \text { where } \quad \mathcal{R} f(s, u)=\int_{\mathbb{R}} f\left(s u+t u^{\top}\right) \mathrm{d} t
$$



Original


Pseudo-inverse

Sparsity in Orthogonal Wavelets, SNR=11.1dB


ISTA

## TV REGULARIZATION

- 1D discrete total variation

$$
\min _{x}\|A x-y\|^{2}+\lambda\|D x\|_{1} \quad \text { where } \quad D=\left[\begin{array}{cccc}
1 & -1 & & \\
& 1 & -1 & \\
& & \ddots & \\
& 1 & -1
\end{array}\right] \in \mathbb{R}^{(n-1) \times n}
$$

Penalizes "edges" in $x$, tends to produce results piecewise constant (sparse gradient)

- nD, continuous (infinite dimensional): for smooth $f$,

$$
\min \left\|\int K(s, t) f(t) \mathrm{d} t-y(s)\right\|_{L^{2}}^{2}+\lambda\|\nabla f\|_{1}
$$

$J(f)=\|\nabla f\|_{1}$ is the total variation of $f$, and it can be extended to non-smooth images with discontinuities (edges).
$J(f)$ corresponds to the total length of its level sets.
Difficult to minimize: $\nabla J(f)=\operatorname{div}(\nabla f /\|\nabla f\|)$ is not well defined everywhere.

## TV DENOISING

Noisy 12.2 dB


TV regularization 21.1 dB


## Optimality Conditions for TV Denoising

- The proximal operator for TV : $x \mapsto\|D x\|_{1}$ has no closed-form

$$
\begin{aligned}
& x=\operatorname{prox}_{\gamma \mathrm{TV}}(z) \Longleftrightarrow \\
\text { where } S & \left.\left.=\left[\begin{array}{llll}
0 & & \\
1 & 0 & & \\
1 & 1 & 0 & \\
1 & \ldots & 1 & 1
\end{array}\right] \text { (it is the matrix such that } D S=I\right)\right]
\end{aligned}
$$

## Solving the TV Denoising Problem

■ Alternating Directions Method of Multipliers considers the augmented Lagrangian

$$
\mathcal{L}(x, z, \nu)=\frac{1}{2}\|A x-y\|^{2}+\lambda\|z\|_{1}+\nu^{\top}(D x-z)+\frac{\rho}{2}\|D x-z\|^{2}
$$

and solves it iteratively minimizing over $x$ (proximal step), $z$ (proximal step) and maximizing over $\nu$ (gradient ascent).

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■ Majorization-Minimization algorithm compute s at each step a (quadratic) majorant of $\operatorname{TV}(x)$, and minimize it





[^0]:    ${ }^{1}$ Tibshirani, 1996
    ${ }^{2}$ Donoho, early 1990's

[^1]:    ${ }^{1}$ Boyd, Vandenberghe, Convex Optimization, Example 3.26

