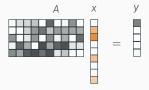
ℓ^1 -regularization

Fallstudien der mathematischen Modellbildung, Teil 2 20.10.2023 - 21.11.2023, paul.catala@tum.de 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.

If c_i , i = 1, ..., n denotes the columns of A, the system rewrites

$$y = \sum_{i=1}^{n} x_i c_i$$

 (c_i) 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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 \blacksquare A natural candidate to promote sparsity of solutions is the $\ell^0\text{-norm}$

$$\|x\|_0 = \# \{i \in \{1, \dots, n\} ; x_i \neq 0\}$$

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■ The corresponding regularized problem is

$$\min \|Ax - y\|^2 + \lambda \|x\|_0$$

and in the noiseless case

$$\min \|x\|_0 \quad \text{s.t.} \quad Ax = y$$

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

$$\min_{x \in \mathbb{R}^n} \|Ax - y\|^2 \quad \text{s.t.} \quad \|x\|_0 \leq \tau$$

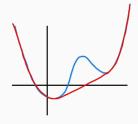
 NP-hard combinatorial, non-convex problem. Direct strategy: check every possible sparsity pattern, *i.e.* fix subsets J of non-zero entries in x and solve the least-squares

$$\min_{\tilde{x}\in\mathbb{R}^n}\|A_j\tilde{x}-y_j\|^2$$

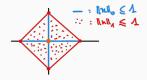
There are $\binom{n}{k}$ possible supports for each sparsity level \rightarrow infeasible for large n

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

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



Theorem. The convex envelope of $||x||_0$ for x restricted to $||x||_{\infty} \leq \alpha$ is $||x||_1/\alpha$



■ Relax ℓ^0 -penalty into ℓ^1 -penalty

$$\min \|Ax - y\|_2^2 + \lambda \|x\|_1 \tag{Lasso}$$

Called LASSO¹ (Least Absolute Shrinkage and Selection Operator) or basis pursuit denoising. When $\lambda = 0$, we obtain the basis pursuit² problem

$$\min \|x\|_1 \quad \text{s.t.} \quad Ax = y \tag{BP}$$

Main properties are:

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



¹Tibshirani, 1996

² Donoho, early 1990's

■ We can reformulate the problem under a constrained form

$$\min \frac{1}{2} \|z - y\|^2 + \lambda \|x\|_1 \quad \text{s.t.} \quad z = Ax$$

and deduce the Lagrangian:

coni

$$\mathcal{L}(x, z, \nu) = \frac{1}{2} \|z - y\|^2 + \lambda \|x\|_1 + \nu^\top (z - Ax)$$

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

$$\inf_{x} \lambda \|x\|_{1} - \langle A^{\top}\nu, x \rangle = -\left(\sup_{x} \langle A^{\top}\nu, x \rangle - \lambda \|x\|_{1}\right)$$
Definition (Conjugate function). The convex
conjugate of $f : \mathbb{R}^{n} \to \mathbb{R}$ is

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

With $J(x) := \lambda \|x\|_1$, the minimization over x and z yields,

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

DUAL NORM

Definition (Dual norm). Given a norm $\|\cdot\|$ 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

$$f^*(y) = egin{cases} 0 & ext{if} & \|y\|_* \leqslant 1 \ \infty & ext{otherwise} \end{cases}$$

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

$$y^{\top}x - \|x\| = t(y^{\top}w - \|w\|) \to \infty,$$

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

¹Boyd, Vandenberghe, Convex Optimization, Example 3.26

- If $J(x) = \lambda ||x||_1$, then $J^*(y)$ is the indicator of $\{||y||_{\infty} \leq \lambda\}$.
- Altogether, we obtain

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

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

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

SUBDIFFERENTIAL

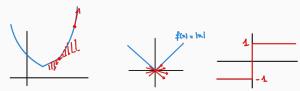
- $\|\cdot\|_1$ is convex but not differentiable at 0. How to derive optimality conditions?
 - Recall the standard inequality for convex functions

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

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

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

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



■ **Proposition.** For any function f,

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

Proof. x_* minimizer of $f \iff \forall x, f(x) \ge f(x_*) = f(x_*) + \langle 0, x - x^* \rangle \iff 0 \in \partial f(x).$

Some basic rules

- $\partial f(x) = \{\nabla f(x)\}$ if f is differentiable at x
- $\partial(\alpha f) = \alpha \partial f$ if $\alpha > 0$
- $\partial(f_1 + f_2)(x) = \partial f_1(x) + \partial f_2(x)$ (except in pathological cases: according to Moreau-Rockafellar theorem, if there exists a point $x_0 \in \text{dom}(f_1 + f_2)$ such that f_1 is continuous at x_0 , then the equality holds for any $x \in \text{dom}(f_1 + f_2)$).
- if g(x) = f(Ax + b) where f is convex, then $\partial g(x) = A^{\top} \partial f(Ax + b)$

Subdifferential of $\|\cdot\|_1$

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

$$(\forall z \in \mathbb{R}, |z| \ge yz) \iff y \in [-1, 1]$$

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

$$\partial |x| = \begin{cases} \{1\} & \text{if } x > 0\\ [-1,1] & \text{if } x = 0\\ \{-1\} & \text{if } x < 0 \end{cases}$$

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Generalization:

$$v \in \partial \|x\|_1 \iff v_i = \begin{cases} v_i = \operatorname{sign}(x_i) & \text{if } x_i \neq 0\\ v_i \in [-1, 1] & \text{if } x_i = 0 \end{cases}$$

Proof. We have, by applying the calculus rules

$$||x||_1 = \sum |x_i| = \sum |e_i^{\top}x|$$

hence

$$\partial \|\mathbf{x}\|_1 = \sum \partial |\mathbf{e}_i^\top \mathbf{x}| = \sum \mathbf{e}_i \partial |\mathbf{x}_i|$$

which leads to the desired result.

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

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

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

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

Proof. We have

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

OPTIMALITY CONDITIONS FOR LASSO

■ The Lasso objective

$$f(x) := \frac{1}{2} \|Ax - y\|^2 + \lambda \|x\|_1$$
 (LASSO)

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

$$0 \in \partial f(x) = A^{\top}(Ax - y) + \lambda \partial \|x\|_{1}^{2}$$

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

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

where

$$\begin{cases} \eta_i = \operatorname{sign}(x_{*i}) & \text{if } x_{*i} \neq 0\\ \eta_i \in [-1, 1] & \text{if } x_{*i} = 0 \end{cases}$$

■ If A satisfies A^TA = I, there is a closed-form solution given by the soft thresholding operator

$$S_{\lambda}(x) = \begin{cases} x_i + \lambda & \text{if } x_i < -\lambda \\ 0 & \text{if } |x_i| \leq \lambda \\ x_i - \lambda & \text{if } x_i > \lambda \end{cases}$$



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In that case

$$\min \frac{1}{2} \|Ax - y\|^2 + \lambda \|x\|_1 = \frac{1}{2} \sum_i (x_i - (A^\top y)_i)^2 + \lambda \sum_i |x_i|,$$

so we may solve the minimization component by component (separable problem).

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$$0 \in \partial h(x) = \begin{cases} x - z - \lambda & \text{if } x < 0\\ -z + \lambda[-1, 1] & \text{if } x = 0 \\ x - z + \lambda & \text{if } x > 0 \end{cases} \iff \begin{cases} x = z + \lambda & \text{if } z < -\lambda \\ x = 0 & \text{if } -\lambda \leqslant z \leqslant \lambda \\ x = z - \lambda & \text{if } z > \lambda \end{cases}$$

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• Therefore, a solution obeys $x_* = S_{\lambda}(A^{\top}y)$

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- Gradient descent evolves in the direction of the negative gradient

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

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

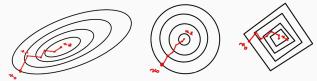


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Subgradient descent uses any vector in the subdifferential instead of the gradient

 $x_{k+1} = x_k - \gamma g_k$, where $g_k \in \partial f(x_k)$

- ✓ simple and cheap
- X sub-optimal solutions
- **X** slow, with convergence $f(x_t) f(x_*) = O(1/\sqrt{t})$

$$\operatorname{prox}_{\gamma f}(x) = \operatorname{argmin}_{y} \frac{1}{2} \|x - y\|^{2} + \gamma f(y)$$

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• Connection with gradient descent: If $f \in C^1$, first order optimality yields

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i.e. y is the point from which if you look *backwards* along $-\nabla f(y)$, you reach x

- Gradient step: $y x = -\gamma \nabla f(\mathbf{x})$ (forward step)
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If $f \in C^0$, then

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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.

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

$$X_* \in \operatorname{argmin} f(X) \iff X_* = \operatorname{prox}_{\gamma f}(X_*)$$

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

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

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

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Suggests updates of the form

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

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Iterative Soft-thresholding Algorithm (ISTA)

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

• Choice of regularization parameter λ 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.* $\langle f, \psi_{a,b} \rangle \simeq 0$ often.



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Wavelet Sparse Regularization

$$\min_{\mathbf{x}\in\mathbb{R}^n} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|^2 + \|\mathbf{x}\|_1$$
 (synthesis)

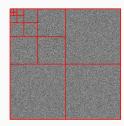
and the reconstructed image is then given by $f = \Psi x$, or

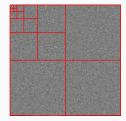
$$\min_{\boldsymbol{\in}\mathbb{R}^{q}} \|\boldsymbol{y} - \boldsymbol{K}\boldsymbol{f}\|^{2} + \|\boldsymbol{\Psi}^{\top}\boldsymbol{f}\|_{1}$$
 (analysis)

WAVELET DENOISING

Corresponds to $A = I_n$: solution is given in closed-form by soft-thresholding.







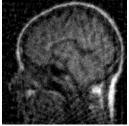
Soft denoising, SNR=17.6

$$\min_{f} \|y - \mathcal{R}f\|^2 + \|\Psi^{\top}f\|, \quad \text{where} \quad \mathcal{R}f(s, u) = \int_{\mathbb{R}} f(su + tu^{\top}) dt$$



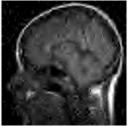
Original

SNR=9.16dB



Pseudo-inverse

Sparsity in Orthogonal Wavelets, SNR=11.1dB





■ 1D discrete total variation

$$\min_{x} \|Ax - y\|^{2} + \lambda \|Dx\|_{1} \text{ where } D = \begin{bmatrix} 1 & -1 & & \\ & 1 & -1 & \\ & & \ddots & \\ & & 1 & -1 \end{bmatrix} \in \mathbb{R}^{(n-1) \times n}$$

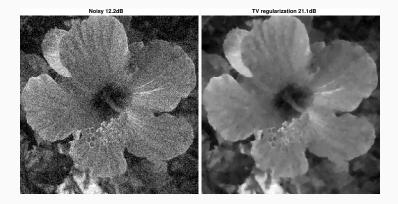
Penalizes "edges" in x, tends to produce results piecewise constant (sparse gradient)
nD, continuous (infinite dimensional): for smooth f,

$$\min \left\| \int K(s,t)f(t) \mathrm{d}t - y(s) \right\|_{\mathsf{L}^2}^2 + \lambda \|\nabla f\|_1$$

 $J(f) = \|\nabla f\|_1$ 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.



• The proximal operator for $TV : x \mapsto ||Dx||_1$ has no closed-form

$$x = \operatorname{prox}_{\gamma \operatorname{TV}}(z) \iff z \in S^{\top} x + \gamma \operatorname{sign}(Dx)$$

where
$$S = \begin{bmatrix} 0 & & \\ 1 & 0 & \\ 1 & 1 & 0 \\ 1 & \dots & 1 & 1 \end{bmatrix}$$
 (it is the matrix such that $DS = I$)]

Alternating Directions Method of Multipliers considers the augmented Lagrangian

$$\mathcal{L}(x, z, \nu) = \frac{1}{2} \|Ax - y\|^2 + \lambda \|z\|_1 + \nu^\top (Dx - z) + \frac{\rho}{2} \|Dx - z\|^2$$

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

Alternating Directions Method of Multipliers considers the augmented Lagrangian

$$\mathcal{L}(\mathbf{X}, \mathbf{Z}, \nu) = \frac{1}{2} \|A\mathbf{X} - \mathbf{y}\|^2 + \lambda \|\mathbf{Z}\|_1 + \nu^\top (D\mathbf{X} - \mathbf{Z}) + \frac{\rho}{2} \|D\mathbf{X} - \mathbf{Z}\|^2$$

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

 Majorization-Minimization algorithm compute s at each step a (quadratic) majorant of TV(x), and minimize it

