

The rise and fall of regularizations: *l*₁ vs. *l*₂ representer theorems

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OUTLINE

- Linear inverse problems and regularization
 - Tikhonov regularization
 - The sparsity (r)evolution
 - Compressed sensing and l₁ minimization
- Part I: Discrete-domain regularization (l₂ vs. l₁)
- Part II: Continuous-domain regularization (L₂ vs. gTV)
 - Classical *L*₂ regularization: theory of RKHS
 - Splines and operators
 - Minimization of gTV: the optimality of splines
 - Enabling components for the proof
 - Special case TV in 1D













CS: Three fundamental ingredients

(Donoho, IEEE T. Inf. Theo. 2006)

1. Existence of sparsifying transform (W or L)

- Wavelet basis
- Dictionary
- Differential operator (Gradient)

2. Incoherence of sensing matrix A

- Restricted isometry; few linearly dependent columns (spark)
- Quasi-random and delocalized structure: Gaussian matrix with i.i.d. entries, random sampling in Fourier domain
- 3. Non-linear signal recovery (l_1 minimization)

CS: Examples of applications in imaging

- Magnetic resonance imaging (MRI) (Lustig, *Mag. Res. Im.* 2007) - Radio Interferometry (Wiaux, Notic. R. Astro. 2007) - Teraherz Imaging (Chan, Appl. Phys. 2008) - Digital holography (Brady, Opt. Express 2009; Marim 2010) - Spectral-domain OCT (Liu, Opt. Express 2010) (Arce, IEEE Sig. Proc. 2014) - Coded-aperture spectral imaging - Localization microscopy (Zhu, Nat. Meth. 2012) - Ultrafast photography (Gao, *Nature* 2014) 8

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(Candès-Romberg, Inv. Prob. 2007)



Classical regularized least-squares estimator

Linear measurement model:

 \Rightarrow

- $y_m = \langle \mathbf{h}_m, \mathbf{x} \rangle + n[m], \quad m = 1, \dots, M$
- \blacksquare System matrix of size $M\times N$: $\ \mathbf{H}=[\mathbf{h}_{1}\cdots\mathbf{h}_{M}]^{T}$

$$\mathbf{x}_{\text{LS}} = \arg\min_{\mathbf{x}\in\mathbb{R}^N} \|\mathbf{y} - \mathbf{H}\mathbf{x}\|_2^2 + \lambda \|\mathbf{x}\|_2^2$$

$$\mathbf{x}_{\text{LS}} = (\mathbf{H}^T \mathbf{H} + \lambda \mathbf{I}_N)^{-1} \mathbf{H}^T \mathbf{y}$$
$$= \mathbf{H}^T \mathbf{a} = \sum_{m=1}^M a_m \mathbf{h}_m \quad \text{where} \quad \mathbf{a} = (\mathbf{H} \mathbf{H}^T + \lambda \mathbf{I}_M)^{-1} \mathbf{y}$$

Interpretation: $\mathbf{x}_{\text{LS}} \in \text{span}\{\mathbf{h}_m\}_{m=1}^M$

Lemma $(\mathbf{H}^T\mathbf{H} + \lambda \mathbf{I}_N)^{-1}\mathbf{H}^T = \mathbf{H}^T(\mathbf{H}\mathbf{H}^T + \lambda \mathbf{I}_M)^{-1}$

Generalization: constrained *l*₂ **minimization**

- Discrete signal to reconstruct: $x = (x[n])_{n \in \mathbb{Z}}$
- Sensing operator $H : \ell_2(\mathbb{Z}) \to \mathbb{R}^M$ $x \mapsto \mathbf{z} = H\{x\} = (\langle x, h_1 \rangle, \dots, \langle x, h_M \rangle) \text{ with } h_m \in \ell_2(\mathbb{Z})$
- Closed convex set in measurement space: $\mathcal{C} \subset \mathbb{R}^M$

Example: $C_{\mathbf{y}} = \{ \mathbf{z} \in \mathbb{R}^M : \|\mathbf{y} - \mathbf{z}\|_2^2 \le \sigma^2 \}$

Representer theorem for constrained ℓ_2 minimization

(P2)
$$\min_{x \in \ell_2(\mathbb{Z})} \|x\|_{\ell_2}^2 \text{ s.t. } H\{x\} \in \mathcal{C}$$

The problem (P2) has a unique solution of the form

$$x_{\rm LS} = \sum_{m=1}^{M} a_m h_m = \mathrm{H}^*\{\mathbf{a}\}$$

with expansion coefficients $\mathbf{a} = (a_1, \cdots, a_M) \in \mathbb{R}^M$.

(U.-Fageot-Gupta IEEE Trans. Info. Theory, Sept. 2016) 11

Constrained l_1 **minimization** \Rightarrow **sparsifying effect**

- Discrete signal to reconstruct: $x = (x[n])_{n \in \mathbb{Z}}$
- Sensing operator $H : \ell_1(\mathbb{Z}) \to \mathbb{R}^M$ $x \mapsto \mathbf{z} = H\{x\} = (\langle x, h_1 \rangle, \dots, \langle x, h_M \rangle) \text{ with } h_m \in \ell_\infty(\mathbb{Z})$
- Closed convex set in measurement space: $\mathcal{C} \subset \mathbb{R}^M$

Representer theorem for constrained ℓ_1 minimization

P1)
$$\mathcal{V} = \arg\min_{x \in \ell_1(\mathbb{Z})} \|x\|_{\ell_1} \text{ s.t. } H\{x\} \in \mathcal{C}$$

is convex, weak*-compact with extreme points of the form

$$x_{\text{sparse}}[\cdot] = \sum_{k=1}^{K} a_k \delta[\cdot - n_k] \quad \text{with} \quad K = \|x_{\text{sparse}}\|_0 \le M.$$

If CS condition is satisfied, then solution is unique

(U.-Fageot-Gupta IEEE Trans. Info. Theory, Sept. 2016)

Controlling sparsity

Measurement model: y_n

$$a_n = \langle h_m, x \rangle + n[m], \quad m = 1, \dots, M$$

$$x_{\text{sparse}} = \arg\min_{x \in \ell_1(\mathbb{Z})} \left(\sum_{m=1}^M |y_m - \langle h_m, x \rangle|^2 + \lambda ||x||_{\ell_1} \right)$$



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Geometry of *l*₂ vs. *l*₁ minimization







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Continuous-domain regularization (L ₂ scenario)			
Regularization functional:	$\ \mathbf{L}f\ _{L_{2}}^{2} = \int_{\mathbb{R}^{d}} \mathbf{L}f(\mathbf{a}) ^{2}$	$oldsymbol{x}) ^2\mathrm{d}oldsymbol{x}$	
	L: suitable differentia	al operator	
Theory of reproducing kernel Hilbert spaces (Aronszajn 1950)			
$\langle f,g angle_{\mathcal{H}} = \langle \mathcal{L}f, \mathcal{L}g angle$			
Interpolation and approximation theory			
Smoothing splines (Sch		nberg 1964, Kimeldorf-Wahba 1971)	
Thin-plate splines, radial basis functions		(Duchon 1977)	
Machine learning			
Radial basis functions, kernel methods		(Poggio-Girosi 1990)	
 Representer theorem(s) 			



Sparsity and continuous-domain modeling

Compressed sensing (CS)			
Generalized sampling and infinite-dimension	sional CS (Adcock-Hansen, 2011)		
Xampling: CS of analog signals	(Eldar, 2011)		
Splines and approximation theory			
• L_1 splines	(Fisher-Jerome, 1975)		
Locally-adaptive regression splines	(Mammen-van de Geer, 1997)		
Generalized TV	(Steidl et al. 2005; Bredies et al. 2010)		
Statistical modeling			
Sparse stochastic processes	(Unser et al. 2011-2014)		

Geometry of *l*₂ vs. *l*₁ minimization

Prototypical inverse problem

 $\min_{\mathbf{x}} \left\{ \|\mathbf{y} - \mathbf{H}\mathbf{x}\|_{\ell_2}^2 + \lambda \, \|\mathbf{x}\|_{\ell_2}^2 \right\} \ \Leftrightarrow \ \min_{\mathbf{x}} \|\mathbf{x}\|_{\ell_2} \ \text{subject to} \ \|\mathbf{y} - \mathbf{H}\mathbf{x}\|_{\ell_2}^2 \le \sigma^2$

 $\min_{\mathbf{x}} \left\{ \|\mathbf{y} - \mathbf{H}\mathbf{x}\|_{\ell_2}^2 + \lambda \|\mathbf{x}\|_{\ell_1} \right\} \iff \min_{\mathbf{x}} \|\mathbf{x}\|_{\ell_1} \text{ subject to } \|\mathbf{y} - \mathbf{H}\mathbf{x}\|_{\ell_2}^2 \le \sigma^2$



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Splines are analog and intrinsically sparse

 $L\{\cdot\}$: admissible differential operator

 $\delta(\cdot - oldsymbol{x}_0)$: Dirac impulse shifted by $oldsymbol{x}_0 \in \mathbb{R}^d$

Definition

The function $s: \mathbb{R}^d \to \mathbb{R}$ is a (non-uniform) L-spline with knots $(\boldsymbol{x}_k)_{k=1}^K$ if

 $L\{s\} = \sum_{k=1}^{K} a_k \delta(\cdot - \boldsymbol{x}_k) = \boldsymbol{w}_{\delta}$: spline's innovation

Spline theory: (Schultz-Varga, 1967)

FRI signal processing: Innovation variables (2K) (Vetterli et al., 2002)

 a_k

 $\mathbf{L} = \frac{\mathbf{d}}{\mathbf{d}x}$

- Location of singularities (knots) : $\{x_k\}_{k=1}^K$
- Strength of singularities (linear weights): $\{a_k\}_{k=1}^K$



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Spline synthesis: generalization

L: spline admissible operator (LSI)

 $ho_{\mathrm{L}}(oldsymbol{x}) = \mathrm{L}^{-1}\{\delta\}$: Green's function of L

Finite-dimensional null space: $\mathcal{N}_{L} = \operatorname{span}\{p_n\}_{n=1}^{N_0}$



Principled operator-based approach

- Biorthogonal basis of $\mathcal{N}_{\mathrm{L}} = \mathrm{span}\{p_n\}_{n=1}^{N_0}$
 - $\phi = (\phi_1, \cdots, \phi_{N_0})$ such that $\langle \phi_m, p_n \rangle = \delta_{m,n}$
 - Projection operator: $p=\sum_{n=1}^{N_0}\langle\phi_n,p
 angle p_n$ for all $p\in\mathcal{N}_{\mathrm{L}}$

Operator-based spline synthesis

Boundary conditions: $\langle s, \phi_n \rangle = \mathbf{b_n}, \ n = 1, \cdots, N_0$

Spline's innovation:
$$L\{s\} = w_{\delta} = \sum_{k} a_{k} \delta(\cdot - \boldsymbol{x}_{k})$$

 $s(\boldsymbol{x}) = L_{\boldsymbol{\phi}}^{-1}\{w_{\delta}\}(\boldsymbol{x}) + \sum_{n=1}^{N_{0}} \boldsymbol{b}_{n} p_{n}(\boldsymbol{x})$

Existence of L_{ϕ}^{-1} as a stable right-inverse of L ? (see **Theorem 1**)

$$LL_{\phi}^{-1}w = w$$

$$\boldsymbol{\phi}(\mathbf{L}_{\boldsymbol{\phi}}^{-1}w) = \mathbf{0}$$

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From Dirac impulses to Borel measures

 $\mathcal{S}(\mathbb{R}^d)$: Schwartz's space of smooth and rapidly decaying test functions on \mathbb{R}^d

 $\mathcal{S}'(\mathbb{R}^d)$: Schwartz's space of tempered distributions

Space of real-valued, countably additive Borel measures on \mathbb{R}^d

$$\mathcal{M}(\mathbb{R}^d) = \left(C_0(\mathbb{R}^d)\right)' = \left\{ w \in \mathcal{S}'(\mathbb{R}^d) : \|w\|_{\mathcal{M}} = \sup_{\varphi \in \mathcal{S}(\mathbb{R}^d) : \|\varphi\|_{\infty} = 1} \langle w, \varphi \rangle < \infty \right\},$$

where $w : \varphi \mapsto \langle w, \varphi \rangle = \int_{\mathbb{R}^d} \varphi(\mathbf{r}) w(\mathbf{r}) \mathrm{d}\mathbf{r}$

Equivalent definition of "total variation" norm

 $\|w\|_{\mathcal{M}} = \sup_{\varphi \in C_0(\mathbb{R}^d) : \|\varphi\|_{\infty} = 1} \langle w, \varphi \rangle$

Basic inclusions

- $\delta(\cdot x_0) \in \mathcal{M}(\mathbb{R}^d)$ with $\|\delta(\cdot x_0)\|_{\mathcal{M}} = 1$ for any $x_0 \in \mathbb{R}^d$
- $\| \| f \|_{\mathcal{M}} = \| f \|_{L_1(\mathbb{R}^d)} \text{ for all } f \in L_1(\mathbb{R}^d) \quad \Rightarrow \quad L_1(\mathbb{R}^d) \subseteq \mathcal{M}(\mathbb{R}^d)$

Optimality result for Dirac measures

- **F**: linear continuous map $\mathcal{M}(\mathbb{R}^d) \to \mathbb{R}^M$
- \mathcal{C} : convex compact subset of \mathbb{R}^M
- Generic constrained TV minimization problem

$$\mathcal{V} = \arg\min_{w \in \mathcal{M}(\mathbb{R}^d) : \mathbf{F}(w) \in \mathcal{C}} \|w\|_{\mathcal{M}}$$

Generalized Fisher-Jerome theorem

The solution set \mathcal{V} is a **convex, weak***-**compact** subset of $\mathcal{M}(\mathbb{R}^d)$ with **extremal points** of the form

$$w_{\delta} = \sum_{k=1}^{K} a_k \delta(\cdot - \boldsymbol{x}_k)$$

with $K \leq M$ and $\boldsymbol{x}_k \in \mathbb{R}^d$.

(U.-Fageot-Ward, ArXiv 2016)

Jerome-Fisher, 1975: Compact domain & scalar intervals

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General convex problems with gTV regularization

$$\mathcal{M}_{\mathcal{L}}(\mathbb{R}^d) = \left\{ s : gTV(s) = \|\mathcal{L}\{s\}\|_{\mathcal{M}} = \sup_{\|\varphi\|_{\infty} \le 1} \langle \mathcal{L}\{s\}, \varphi \rangle < \infty \right\}$$

- Linear measurement operator $\mathcal{M}_{L}(\mathbb{R}^{d}) \to \mathbb{R}^{M} : f \mapsto \mathbf{z} = \mathrm{H}\{f\}$
- \mathcal{C} : **convex** compact subset of \mathbb{R}^M
- Finite-dimensional null space $\mathcal{N}_{L} = \{q \in \mathcal{M}_{L}(\mathbb{R}^{d}) : L\{q\} = 0\}$ with basis $\{p_{n}\}_{n=1}^{N_{0}}$
 - Admissibility of regularization: $H\{q_1\} = H\{q_2\} \Leftrightarrow q_1 = q_2$ for all $q_1, q_2 \in \mathcal{N}_L$

Representer theorem for gTV regularization The extremal points of the constrained minimization problem $\mathcal{V} = \arg \min_{f \in \mathcal{M}_{\mathrm{L}}(\mathbb{R}^d)} \|\mathrm{L}\{f\}\|_{\mathcal{M}}$ s.t. $\mathrm{H}\{f\} \in \mathcal{C}$ are necessarily of the form $f(x) = \sum_{k=1}^{K} a_k \rho_{\mathrm{L}}(x - x_k) + \sum_{n=1}^{N_0} b_n p_n(x)$ with $K \leq M - N_0$; that is, **non-uniform** L-**splines** with knots at the x_k and $\|\mathrm{L}\{f\}\|_{\mathcal{M}} = \sum_{k=1}^{L} |a_k|$. The full solution set is the **convex hull** of those extremal points.

(U.-Fageot-Ward, ArXiv 2016) 30

Enabling components for proof of the theorem



Existence of stable right-inverse operator

 $L_{\infty,n_0}(\mathbb{R}^d) = \{f: \mathbb{R}^d \to \mathbb{R}: \sup_{\boldsymbol{x} \in \mathbb{R}^d} \left(|f(\boldsymbol{x})| (1+\|\boldsymbol{x}\|)^{-n_0} \right) < +\infty \}$

Theorem 1 (U.-Fageot-Ward, ArXiv 2016)

Let L be a spline-admissible operator with a N_0 -dimensional null space $\mathcal{N}_L \subseteq L_{\infty,n_0}(\mathbb{R}^d)$ such that $p = \sum_{n=1}^{N_0} \langle p, \phi_n \rangle p_n$ for all $p \in \mathcal{N}_L$. Then, there exists a **unique and stable operator** $L_{\phi}^{-1} : \mathcal{M}(\mathbb{R}^d) \to L_{\infty,n_0}(\mathbb{R}^d)$ such that, for all $w \in \mathcal{M}(\mathbb{R}^d)$,

- Right-inverse property: $LL_{\phi}^{-1}w = w$,
- Boundary conditions: $\phi(L_{\phi}^{-1}w) = 0$ with $\phi = (\phi_1, \cdots, \phi_{N_0})$.

Its generalized impulse response $g_{\phi}(x,y) = L_{\phi}^{-1} \{ \delta(\cdot - y) \}(x)$ is given by

$$g_{\boldsymbol{\phi}}(\boldsymbol{x}, \boldsymbol{y}) =
ho_{\mathrm{L}}(\boldsymbol{x} - \boldsymbol{y}) - \sum_{n=1}^{N_0} p_n(\boldsymbol{x}) q_n(\boldsymbol{y})$$

with $\rho_{\rm L}$ such that ${\rm L}\{\rho_{\rm L}\} = \delta$ and $q_n(\boldsymbol{y}) = \langle \phi_n, \rho_{\rm L}(\cdot - \boldsymbol{y}) \rangle$.

Characterization of generalized Beppo-Levi spaces

Regularization operator $L: \mathcal{M}_L(\mathbb{R}^d) \to \mathcal{M}(\mathbb{R}^d)$

$$f \in \mathcal{M}_{\mathcal{L}}(\mathbb{R}^d) \quad \Leftrightarrow \quad \mathrm{gTV}(f) = \|\mathcal{L}\{f\}\|_{\mathcal{M}} < \infty$$

Theorem 2 (U.-Fageot-Ward, ArXiv 2016)

Let L be a spline-admissible operator that admits a stable right-inverse L_{ϕ}^{-1} of the form specified by Theorem 1. Then, any $f \in \mathcal{M}_{L}(\mathbb{R}^{d})$ has a unique representation as

 $f = \mathcal{L}_{\phi}^{-1}w + p,$

where $w = L\{f\} \in \mathcal{M}(\mathbb{R}^d)$ and $p = \sum_{n=1}^{N_0} \langle \phi_n, f \rangle p_n \in \mathcal{N}_L$ with $\phi_n \in (\mathcal{M}_L(\mathbb{R}^d))'$. Moreover, $\mathcal{M}_L(\mathbb{R}^d)$ is a Banach space equipped with the norm

 $||f||_{\mathcal{L},\phi} = ||\mathcal{L}f||_{\mathcal{M}} + ||\phi(f)||_2.$

Generalized Beppo-Levi space: $\mathcal{M}_{L}(\mathbb{R}^{d}) = \mathcal{M}_{L, \phi}(\mathbb{R}^{d}) \oplus \mathcal{N}_{L}$

$$\mathcal{M}_{\mathrm{L}, \boldsymbol{\phi}}(\mathbb{R}^d) = \left\{ f \in \mathcal{M}_{\mathrm{L}}(\mathbb{R}^d) : \boldsymbol{\phi}(f) = \mathbf{0}
ight\}$$

$$\mathcal{N}_{\mathrm{L}} = \left\{ p \in \mathcal{M}_{\mathrm{L}}(\mathbb{R}^d) : \mathrm{L}\{p\} = 0 \right\}$$

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Example: Convex problem with TV regularization

$$L = D = \frac{d}{dx}$$

$$\mathcal{N}_{D} = \operatorname{span}\{p_{1}\}, \quad p_{1}(x) = 1$$

$$\rho_{D}(x) = \mathbb{1}_{+}(x): \text{Heaviside function}$$

General linear-inverse problem with TV regularization

 $\min_{s \in \mathcal{M}_{\mathrm{D}}(\mathbb{R})} \|\mathrm{D}\{s\}\|_{\mathcal{M}} \quad \text{s.t.} \quad \mathrm{H}\{s\} = (\langle h_1, s \rangle, \cdots, \langle h_M, s \rangle) \in \mathcal{C}(\mathbf{y})$

Generic form of the solution (by Theorem 4)

$$s(x) = b_1 + \sum_{k=1}^{K} a_k \mathbb{1}_+ (x - x_k)$$

with K < M and free parameters b_1 and $(a_k, x_k)_{k=1}^K$

SUMMARY: Sparsity in infinite dimensions

Discrete-domain formulation

- Contrasting behavior of l_1 vs. l_2 regularization
- Minimization of l₁ favors sparse solutions (independently of sensing matrix)
- Continuous-domain formulation $s \in \mathcal{X}$ $s \mapsto \mathbf{z} = \mathbf{H}\{s\}$ $\mathbf{L}s = w \quad \Rightarrow \quad s = \mathbf{L}^{-1}w$ Linear measurement model Linear signal model: PDE
 - L-splines = signals with "sparsest" innovation $gTV(s) = ||Ls||_{\mathcal{M}}$

- Deterministic optimality result
 - gTV regularization: favors "sparse" innovations
 - Non-uniform L-splines: universal solutions of linear inverse problems

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Preprints and demos: <u>http://bigwww.epfl.ch/</u>



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For splines: see chapter 6

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Link with "Total variation" of Rudin-Osher



"Total variation of function" \neq "total variation of a measure"

Total variation in 1D: $TV(f) = \sup_{\|\varphi\|_{\infty} \leq 1} \langle Df, \varphi \rangle = \|Df\|_{\mathcal{M}}$

→ perfect equivalence (with L=D)

■ Usual total variation in 2D: $TV(f) = \sup_{\|\varphi\|_{\infty} \leq 1} \langle \nabla f, \varphi \rangle$

Problem: $\boldsymbol{\nabla} = (\partial_x, \partial_y)$ is not a scalar operator

 L_1 version of the 2D total variation:

$$TV(f) = \int_{\mathbb{R}^2} |\nabla f(x, y)| dx dy = \frac{1}{4} \int_0^{2\pi} \|D_{u_\theta} f\|_{\mathcal{M}} d\theta \quad \Rightarrow \text{angular averaging}$$
(rotation invariance)

 $D_{u_{\theta}}f = \langle u_{\theta}, \nabla f \rangle$: directional derivative of f along $u_{\theta} = (\cos \theta, \sin \theta)$

Present theory explains the regularisation effect of $\|D_{u_{\theta}}f\|_{\mathcal{M}}$

