Regularizing inverse problems using sparsity-based signal models



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Why

Low-dose X-ray CT imaging Accelerated MR imaging Other inverse problems

How

MAP estimation for inverse problems Classical regularization methods (some sparsity based) Contemporary regularization methods (all sparsity based)



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Improving X-ray CT image reconstruction



- A picture is worth 1000 words
- (and perhaps several 1000 seconds of computation?)



Thin-slice FBP Seconds ASIR (denoise) A bit longer Statistical Much longer

Today's talk: less about computation, more about image quality Right image used edge-preserving regularization

Accelerating MR imaging





(a) $4 \times$ under-sampled MR kspace

(b) zero-filled reconstruction (c) "compressed sensing" reconstruction with TV regularization (d) adaptive dictionary learning regularization [1, Fig. 10]

(c)

(d)

Other ill-posed inverse problems



$$y = Ax + \varepsilon$$

- compressed sensing
- deblurring (restoration)
- in-painting
- denoising (not ill posed)



(*A* random, wide) (*A* Toeplitz, wide?) (*A* subset of rows of *I*) (*A* = *I*)





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If we have a prior p(x), then the MAP estimate is:

$$\hat{\boldsymbol{x}} = \operatorname*{arg\,max}_{\boldsymbol{x}} \operatorname{p}(\boldsymbol{x} \mid \boldsymbol{y}) = \operatorname*{arg\,max}_{\boldsymbol{x}} \log \operatorname{p}(\boldsymbol{y} \mid \boldsymbol{x}) + \log \operatorname{p}(\boldsymbol{x}).$$

For gaussian measurement errors and linear model:

$$-\log p(\boldsymbol{y} \mid \boldsymbol{x}) \equiv \frac{1}{2} \| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{x} \|_{\boldsymbol{W}}^2$$

where $\|\boldsymbol{y}\|_{\boldsymbol{W}}^2 = \boldsymbol{y}' \boldsymbol{W} \boldsymbol{y}$ and $\boldsymbol{W}^{-1} = \text{Cov}\{\boldsymbol{y} \mid \boldsymbol{x}\}$ is known (**A** from physics, **W** from statistics)



▶ If all images x are "plausible" (have non-zero probability) then

$$p(\mathbf{x}) \propto e^{-R(\mathbf{x})} \Longrightarrow -\log p(\mathbf{x}) \equiv R(\mathbf{x})$$

(from fantasy / imagination / wishful thinking)

• MAP \equiv regularized weighted least-squares (WLS) estimation:

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\operatorname{arg\,max}} \log p(\boldsymbol{y} \mid \boldsymbol{x}) + \log p(\boldsymbol{x})$$
$$= \underset{\boldsymbol{x}}{\operatorname{arg\,min}} \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_{\boldsymbol{W}}^2 + R(\boldsymbol{x})$$

- ► A regularizer R(x), aka log prior, is essential for high-quality solutions to ill-conditioned / ill-posed inverse problems.
- Why ill-posed? High ambitions...

Example of ill-conditioned inverse problem

Two-pixel, two-ray "X-ray tomography" model:

 $\mathsf{cond}(\textit{\textbf{A}'}\textit{\textbf{A}})\approx 400$



log-likelihood log p(y|x):







Assuming x lies in a sufficiently low-dimensional subspace could make an inverse problem well conditioned.

 x_1 Assume $\boldsymbol{x} = \boldsymbol{D} \boldsymbol{z}$ where $\boldsymbol{D} = \left[egin{array}{c} 1 \\ 1 \end{array}
ight]$ and $\boldsymbol{z} \in \mathbb{R}^1$ (*z* has only one nonzero element so very sparse!?) Estimate coefficient(s): $\hat{z} = \arg \min_{z} ||y - ADz||_{2}^{2}$, then $\hat{x} = D\hat{z}$, where $\boldsymbol{B} \triangleq \boldsymbol{A}\boldsymbol{D} = \begin{bmatrix} 2\\ 0.1 \end{bmatrix}$ and $\operatorname{cond}(\boldsymbol{B}'\boldsymbol{B}) = 1$ which is perfect! イロト 不得 トイヨト イヨト 二日

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Candès and Romberg (2005) [2] used 22 (noiseless) projection views, each with 256 samples. $22 \cdot 256 = 5632$ measured values, vs $256^2 = 65536$ unknown pixels



Subspace representation (using pixel basis) is undesirably coarse.



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- Tikhonov regularization (IID gaussian prior)
- Roughness penalty (Basic MRF prior)
- Sparsity in ambient space
- Edge-preserving regularization
- Total-variation (TV) regularization
- Black-box denoiser like NLM

Tikhonov regularization





 $\mathsf{R}(\boldsymbol{x}) = \beta \|\boldsymbol{x}\|_2^2$

- Colors show equivalent (normalized) prior $p(x) / p(0) = e^{-R(x)}$
- Equivalent to IID gaussian prior on x
- Makes any ill-conditioned / ill-posed problem well conditioned
- Ignores correlations between pixels

Sparsity regularization in ambient space





$$\mathsf{R}(\mathbf{x}) = \beta \|\mathbf{x}\|_0 = \beta \sum_j \mathbb{I}_{\{x_j \neq 0\}}$$

- Approximate Bayesian interpretation
- Non-convex
- IID \implies also ignores correlations

Sparsity regularization: convex relaxation





$$\mathsf{R}(\mathbf{x}) = \beta \|\mathbf{x}\|_1 = \beta \sum_j |x_j|$$

- Equivalent to IID Laplacian prior on x
- Also ignores correlations





Caution: Shepp-Logan phantom [3] was designed for testing non-Bayesian methods, not for designing signal models. Q: What causes the spread??



Edge-preserving regularization

Neighboring pixels tend to have similar values except near edges:

$$\mathsf{R}(\boldsymbol{x}) = \beta \sum_{j} \psi(x_j - x_{j-1})$$

Potential function ψ :





- Equivalent to improper prior (agnostic to DC value)
- Accounts for spatial correlations, but only very locally
- Used clinically now for low-dose X-ray CT image reconstruction

Total-variation (TV) regularization



Neighboring pixels tend to have similar values except near edges ("gradient sparsity"): x_2

$$\begin{aligned} \mathsf{R}(\boldsymbol{x}) &= \beta \operatorname{TV}(\boldsymbol{x}) = \beta \|\boldsymbol{C}\boldsymbol{x}\|_{1} \\ &= \beta \sum_{j} |x_{j} - x_{j-1}| \end{aligned}$$





- Equivalent to improper prior (agnostic to DC value)
- Accounts for correlations, but only very locally
- Well-suited to piece-wise constant Shepp-Logan phantom!
- Used in many academic publications...



Noisy image \rightarrow Denoiser \rightarrow Denoised image

- Example: Non-local means (NLM)
- Corresponding regularizer [4]–[6]:

$$\mathsf{R}(\boldsymbol{x}) = \beta \frac{1}{2} \|\boldsymbol{x} - \mathsf{NLM}(\boldsymbol{x})\|_2^2$$

- Encourages self-consistency with denoised version of image
- No evident Bayesian interpretation
- Variable splitting can facilitate minimization [7].



- Transforms: wavelets, curvelets, ...
- Markov random field models
- Graphical models
- ▶ ...



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- Convolutional sparsity
- Union of subspaces
- Sparse coding with dictionary
- manifolds? [8]



Idea:

$$x[\vec{n}] \approx \sum_{k=1}^{K} h_k[\vec{n}] * z_k[\vec{n}]$$

- where each $h_k[ec{n}]$ is a FIR filter with $\|oldsymbol{h}_k\|=1$
- and each coefficient image $z_k[\vec{n}]$ is sparse [9]–[11]. Equivalent matrix-vector representation:

$$\mathbf{x} pprox \sum_{k=1}^{K} \mathbf{H}_k \mathbf{z}_k$$

where H_k is a Toeplitz (or circulant) matrix corresponding to h_k .

Convolutional sparsity: example





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Recall $\boldsymbol{x} \approx \sum_{k=1}^{K} \boldsymbol{H}_{k} \boldsymbol{z}_{k}$ Natural corresponding regularizer:

$$\mathsf{R}(\boldsymbol{x}) = \min_{\{\boldsymbol{z}_k\}} \min_{\substack{\{\boldsymbol{h}_k\}\\ \|\boldsymbol{h}_k\| = 1}} \left(\left\| \boldsymbol{x} - \sum_{k=1}^{K} \boldsymbol{H}_k \boldsymbol{z}_k \right\|_2^2 + \lambda^2 \sum_{k=1}^{K} \|\boldsymbol{z}_k\|_0 \right)$$

Adapts FIR filters $\{h_k\}$ and coefficients $\{z_k\}$ to candidate x.

- Literature focuses on the minimization problem (sparse coding)
- Yet to be explored as regularizer for inverse problems
- Inherently shift-invariant representation; no "patches" needed

Union of subspaces model

- Dimensionality reduction?
- ▶ cf. classification / clustering motivation [12]
- (Extension to union of "flats" (linear varieties) is possible [13].)

Given (?) collection of K subspace bases D_1, \ldots, D_K (dictionaries with full column rank):

$$R(\mathbf{x}) = \underbrace{\min_{k}}_{\text{"classification"}} \underbrace{\min_{\mathbf{z}_{k}} \quad \beta \frac{1}{2} \|\mathbf{x} - \mathbf{D}_{k} \mathbf{z}_{k}\|_{2}^{2}}_{\text{regression}}$$
$$= \min_{k} \beta \frac{1}{2} \|\mathbf{x} - \mathbf{D}_{k} \mathbf{D}_{k}^{+} \mathbf{x}\|_{2}^{2}$$

- $R(\mathbf{x}) = 0$ if \mathbf{x} lies in the span of any of the dictionaries $\{\mathbf{D}_k\}$.
- otherwise, distance to nearest subspace (discourage, not constrain)
- Non-convex (highly?) (cf. preceding picture)
- Apply to image patches to be practical
- Equivalent Bayesian interpretation? (not a mixture model here)

Assume $x \approx Dz$ where D is a dictionary (often over-complete) and z is a sparse coefficient vector. Corresponding regularizers:

$$\mathsf{R}(\boldsymbol{x}) = \min_{\boldsymbol{z} : \|\boldsymbol{z}\|_{\rho} \leq s} \beta \frac{1}{2} \|\boldsymbol{x} - \boldsymbol{D}\boldsymbol{z}\|_{2}^{2}$$

$$\mathsf{R}(\boldsymbol{x}) = \min_{\boldsymbol{z}} \left(\beta_1 \frac{1}{2} \| \boldsymbol{x} - \boldsymbol{D} \boldsymbol{z} \|_2^2 + \beta_2 \| \boldsymbol{z} \|_p \right)$$

- Convex in \boldsymbol{z} (for given \boldsymbol{x}) if $p \geq 1$.
- R(x) typically non-convex in x.
- Could be equivalent to a union-of-subspaces regularizer if *D* = [*D*₁ ... *D*_K] and if we constrain coefficient vector *z* in a non-standard way.

Union-of-subspaces vs sparse-coding-with-dictionary

Consider union-of-subspaces model with $D_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$, $D_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$. So D_1 spans x-y plane and D_2 spans z-axis. A dictionary model with $D = [D_1 \ D_2] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ and sparsity s = 2, happily represents all three cardinal planes

Thus dictionary model seems "less constrained" than union-of-subspaces model. (Still, focus on sparse dictionary representation hereafter.)

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Dictionary learning from training data

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- Given training data $\pmb{x}_1,\ldots,\pmb{x}_N\in\mathbb{R}^d$ (image patches)
- Assumed model: $\boldsymbol{x}_n \approx \boldsymbol{D} \boldsymbol{z}_n$
- unknown $d \times J$ dictionary $\boldsymbol{D} = [\boldsymbol{d}_1 \ \dots \ \boldsymbol{d}_J]$
- coefficient vectors $\pmb{z}_1,\ldots,\pmb{z}_{\pmb{N}}\in\mathbb{R}^J$ assumed "sparse"

K-SVD dictionary learning formulation [14]:

$$D^* = \underset{D \in \mathbb{R}^{d \times J}}{\arg\min} \sum_{n=1}^{N} \underset{z_n \in \mathbb{R}^J}{\min} \|x_n - Dz_n\|_2 \quad \text{s.t.} \quad \begin{aligned} \|d_j\| &= 1 \ \forall j \\ \|z_n\|_0 \leq s \ \forall n \end{aligned}$$
$$= \underset{D \in \mathbb{R}^{d \times J}}{\arg\min} \underset{Z \in \mathbb{R}^{J \times N}}{\min} \|X - DZ\|_F \quad \text{s.t.} \quad \begin{aligned} \|d_j\| &= 1 \ \forall j \\ \|z_n\|_0 \leq s \ \forall n \end{aligned}$$

 $\mathbf{X} \triangleq [\mathbf{x}_1 \ \dots \ \mathbf{x}_N], \ \mathbf{Z} \triangleq [\mathbf{z}_1 \ \dots \ \mathbf{z}_N]$ Computationally expensive and no convergence guarantees. Inherently non-convex due to product of unknowns \mathbf{DZ} .

Joint work with Sai Ravishankar and Raj Nadakuditi [15]-[18]

• Write sparse representation as Sum of OUter Products (SOUP):

$$oldsymbol{X} pprox oldsymbol{D}oldsymbol{Z} = oldsymbol{D}oldsymbol{C}' = \sum_{j=1}^J oldsymbol{d}_joldsymbol{c}_j'$$

where $\mathbf{Z}' = \mathbf{C} = [\mathbf{c}_1 \ \dots \ \mathbf{c}_J] \in \mathbb{R}^{N \times J}$ (coefficients for each atom) • Replace individual atom sparsity constraint $\|\mathbf{z}_n\|_0 \leq s$ with aggregate sparsity regularizer: $\|\|\mathbf{Z}\|\|_0 = \|\|\mathbf{C}\|\|_0$.

- Natural for Dictionary Learning (DIL) from training data
- Unnatural for image compression using sparse coding

SOUP-DIL ℓ_0 formulation:

$$\boldsymbol{D}^{*} = \underset{\boldsymbol{D} \in \mathbb{R}^{d \times J}}{\operatorname{arg\,min}} \min_{\boldsymbol{C} \in \mathbb{R}^{N \times J}} \| \boldsymbol{X} - \boldsymbol{D} \boldsymbol{C}' \|_{F}^{2} + \lambda^{2} \| \boldsymbol{C} \|_{0} \quad \text{s.t.} \quad \frac{\|\boldsymbol{d}_{j}\|_{2}}{\|\boldsymbol{c}_{j}\|_{\infty}} \leq L \ \forall j$$

SOUP-DIL algorithm

SOUP-DIL formulation:

$$\boldsymbol{D}^{*} = \operatorname*{arg\,min}_{\boldsymbol{D} \in \mathbb{R}^{d \times J}} \min_{\boldsymbol{C} \in \mathbb{R}^{N \times J}} \| \boldsymbol{X} - \boldsymbol{D}\boldsymbol{C}' \|_{F}^{2} + \lambda^{2} \| \boldsymbol{C} \|_{0} \quad \text{s.t.} \quad \frac{\|\boldsymbol{d}_{j}\|_{2} = 1 \ \forall j}{\|\boldsymbol{c}_{j}\|_{\infty} \leq L \ \forall j}$$

- Block coordinate descent (BCD) algorithm
 - Sparse coding step for *C*
 - Dictionary update step for *D*
- Very simple update rules (low compute cost)
- Monotone descent of $\Psi(\boldsymbol{D}, \boldsymbol{C})$
- Convergence theorem: for any given initialization (D⁰, C⁰), all accumulation points of sequence (D, C)
 - are critical points of cost Ψ and
 - are equivalent (reach same cost function value Ψ^*).
 - Furthermore: $\left\{ \left\| \boldsymbol{D}^{(k)} \boldsymbol{D}^{(k-1)} \right\| \right\} \rightarrow 0$. Same for $\left\{ \boldsymbol{C}^{(k)} \right\}$.

$$\boldsymbol{D}^{*} = \underset{\boldsymbol{D} \in \mathbb{R}^{d \times J}}{\operatorname{arg\,min}} \min_{\boldsymbol{C} \in \mathbb{R}^{N \times J}} \| \boldsymbol{X} - \boldsymbol{D}\boldsymbol{C}' \| _{F}^{2} + \lambda^{2} \| \boldsymbol{C} \|_{0} \quad \text{s.t.} \quad \frac{\|\boldsymbol{d}_{j}\|_{2}}{\|\boldsymbol{c}_{j}\|_{\infty}} \leq L \ \forall j$$

Alternate: update one column d_j of D then one column c_j of C.

► Sparse coding step: update c_j using residual $E_j \triangleq \sum_{k \neq j} d_k c'_k$

$$\min_{\boldsymbol{c}_{j}} \left\| \boldsymbol{E}_{j} - \boldsymbol{d}_{j} \boldsymbol{c}_{j}^{\prime} \right\|_{F}^{2} + \lambda^{2} \left\| \boldsymbol{c}_{j} \right\|_{0} \quad \text{s.t.} \quad \left\| \boldsymbol{c}_{j} \right\|_{\infty} \leq L$$

Truncated (via *L*) hard thresholding of $E'_j d_j$ with threshold λ • Dictionary atom step: update d_j

$$\min_{\boldsymbol{d}_j} \| \boldsymbol{E}_j - \boldsymbol{d}_j \boldsymbol{c}_j' \|_F^2 \quad \text{s.t.} \quad \| \boldsymbol{d}_j \|_2 = 1$$

Constrained least-squares solution: $d_j = (\boldsymbol{E}_j \boldsymbol{c}_j) / \|\boldsymbol{E}_j \boldsymbol{c}_j\|_2$

Truncated hard thresholding for SOUP-DIL

(Algorithm also provides a simple sparse coding method.)

Example: dictionary learning for Barbara

Barbara

K-SVD D

SOUP-DIL **D**

Denoising PSNR (dB) from [15]					
	σ	Noisy	0-DCT	K-SVD	SOUP-DIL
	20	22.13	29.95	30.83	30.79
	25	20.17	28.68	29.63	29.64
	30	18.59	27.62	28.54	28.63
	100	8.11	21.87	21.87	21.97

SOUP-DIL faster than K-SVD

- Large image \boldsymbol{x} , extract M patches $\boldsymbol{X} = [\boldsymbol{P}_1 \boldsymbol{x} \dots \boldsymbol{P}_M \boldsymbol{x}]$
- ► Assume patch x_m = P_mx ≈ Dz_m has (aggregate) sparse representation in dictionary D ∈ ℝ^{d×J} where d is patch size

$$\mathsf{R}(\boldsymbol{x}) = \mathsf{R}(\boldsymbol{X}) = \min_{\boldsymbol{C} \in \mathbb{R}^{M \times J}} \| \boldsymbol{X} - \boldsymbol{D}\boldsymbol{C}' \|_{F}^{2} + \lambda^{2} \| \boldsymbol{C} \|_{0} \quad \text{s.t.} \| \boldsymbol{c}_{j} \|_{\infty} \leq L \,\forall j$$

- ► R(x) = 0 if patches can be represented exactly with "sufficiently few" non-zero coefficients (depends on λ)
- Ignore constraint $\|\boldsymbol{c}_j\|_{\infty} \leq L$
- Bayesian interpretation?

CT reconstruction using (known) dictionary regularizer

$$\hat{\boldsymbol{x}} = \arg\min_{\boldsymbol{x}} \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_{\boldsymbol{W}}^2 + \beta \operatorname{R}(\boldsymbol{x})$$

=
$$\arg\min_{\boldsymbol{x}} \min_{\boldsymbol{C} \in \mathbb{R}^{M \times J}} \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_{\boldsymbol{W}}^2 + \frac{\beta}{2} \left(\|\|\boldsymbol{X} - \boldsymbol{D}\boldsymbol{C}'\|\|_F^2 + \lambda^2 \|\|\boldsymbol{C}\|\|_0 \right)$$

Alternating (nested) minimization:

- Fixing *x*, updating each column of *C* sequentially involves (truncated?) hard-thresholding
- Fixing \boldsymbol{C} , updating \boldsymbol{x} is (large-scale) quadratic problem

$$g(\boldsymbol{x}) = \frac{1}{2} \|\boldsymbol{X} - \boldsymbol{D}\boldsymbol{C}'\|_{F}^{2} = \sum_{m=1}^{M} \frac{1}{2} \|\boldsymbol{P}_{m}\boldsymbol{x} - \boldsymbol{D}\boldsymbol{P}_{m}\boldsymbol{C}'\|_{2}^{2}$$

$$abla^2 g({m x}) = \sum_{m=1}^M {m P}_m' {m P}_m ~~$$
 is diagonal

Work in progress...

- Numerous "normal-dose" CT images!
- learn D, or most of it, from "big data"
- learn statistics of sparse coefficients Z?
- replace generic $\|\boldsymbol{Z}\|_0$ with $p(\boldsymbol{Z})$?

Extensions / future work

- Use majorization to update multiple columns of *D* or *C* simultaneously
- DC atom
- Rotate/flip atoms [19] [20]
- rank constraints on dictionary atoms [16]
- Tensor structured atoms for 3D / dynamic imaging
- Combined transform learning / dictionary learning
- Union of manifolds instead of union of subspaces?
- ▶ ...

Open problems

- Model selection
- Parameter selection
- Performance guarantees

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