Inverse problem regularization using adaptive signal models



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Work with Sai Ravishankar, II Yong Chun, Raj Nadakuditi, Yong Long, Xuehang Zheng, ...

IMACCS

2018-06-04



• Forward problem (data acquisition):



SPECT, PET, X-ray CT, MRI, optical

Inverse problem (image formation):



 Image reconstruction topics: physics models, measurement statistical models, regularization / object priors, optimization.



- "Analytical" methods FBP for SPECT / PET / X-ray CT, IFFT for MRI, ...
- 2. Iterative / statistical methods
 - LS / ML methods
 - regularized / Bayesian methods
- 3. Adaptive / data-driven methods

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



Commercial availability of iterative methods for human scanners per FDA 510(k) dates:

► PET/SPECT

Unregularized OS-EM \approx 1997

► X-ray CT

Regularized MBIR [2011-11-09 for GE Veo] (Installed at UM in Jan. 2012)

► PET

Regularized EM variant (Q.Clear) 2014-03-21

► MRI

Compressed sensing! (Sparsity-based regularization) [2017-01-27 for Siemens Cardiac Cine] [2017-04-20 for GE HyperSense]

Ultrasound?



Accelerating MR imaging using adaptive regularization



(b)

(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]









Background

Ill-posed problems and regularization Classical "hand crafted" regularizers

Adaptive regularization

Patch-based adaptive regularizers Convolutional adaptive regularizers Blind dictionary learning

Summary



- $y = Ax + \varepsilon$
- y : measurements ε : noise
- x : unknown image A : system matrix (typically wide)
- ► compressed sensing (*e.g.*, MRI) (*A* "random" rows of DFT)





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

(A Toeplitz)(A subset of rows of I)(A = I)

Why under-sample?



Why under-sample in MRI?

- Reduce scan time (?)
 - Patient comfort
 - Scan cost / throughput
 - Motion artifacts (Philips at ISMRM 2017)
- Improve spatial resolution (collect higher k-space lines)
- Improve scan diversity for quantitative MRI
- Improve temporal resolution trade-off in dynamic MRI

Why under-sample or reduce intensity in CT?

Reduce X-ray dose

(But under-sampling leads to ill-posed inverse problems...)





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 a linear forward model:

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

where $\|\mathbf{y}\|_{\mathbf{W}}^2 = \mathbf{y}' \mathbf{W} \mathbf{y}$ and $\mathbf{W}^{-1} = \text{Cov}\{\mathbf{y} \mid \mathbf{x}\}$ 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 / data)

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

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

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



- 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



Neighboring pixels tend to have similar values except near edges: x_i

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







- 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_i $\mathsf{R}(\mathbf{x}) = \beta \mathrm{TV}(\mathbf{x}) = \beta \|\Delta \mathbf{x}\|_{1}$ $= \beta \sum_{i} |x_{j} - x_{j-1}|$ Potential function ψ : x_{j-1} b(z)0 -1 0

- 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...



- ► Transforms: wavelets, curvelets,
- Markov random field models
- Graphical models

All "hand crafted" ...

...



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III-posed problems and regularization Classical "hand crafted" regularizers

Adaptive regularization

Patch-based adaptive regularizers Convolutional adaptive regularizers Blind dictionary learning

Summary



Data

- Population adaptive methods (e.g., X-ray CT)
- Patient adaptive methods
- Spatial structure
 - Patch-based models
 - Convolutional models
- Regularizer formulation
 - Synthesis (dictionary) approach
 - Analysis (sparsifying transforms) approach

Many options...



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Assumption: if x is a plausible image, then each $\Omega P_m x$ is sparse.

- ► **P**_m**x** extracts the *m*th of *M* patches from **x**
- Ω is a square sparsifying transform matrix







Given training images x_1, \ldots, x_L from a representative population, find transform Ω_* that best sparsifies their patches:

$$\boldsymbol{\Omega_*} = \mathop{\arg\min}_{\boldsymbol{\Omega}} \min_{\text{unitary}} \min_{\{\boldsymbol{z}_{l,m}\}} \sum_{l=1}^{L} \sum_{m=1}^{M} \|\boldsymbol{\Omega}\boldsymbol{P}_{m}\boldsymbol{x}_{l} - \boldsymbol{z}_{l,m}\|_{2}^{2} + \alpha \|\boldsymbol{z}_{l,m}\|_{0}$$

- Encourage aggregate sparsity, not patch-wise sparsity (cf K-SVD [2])
- Non-convex due to unitary constraint and $\left\|\cdot\right\|_{0}$
- Efficient alternating minimization algorithm [3]
 - z update is simply hard thresholding
 - Ω update is an orthogonal Procrustes problem (SVD)
 - Subsequence convergence guarantees [3]

Example of learned sparsifying transform





 $\begin{array}{l} (\text{2D slices in x-y, x-z, y-z}) \\ 8\times8\times8 \text{ patches} \Longrightarrow \mathbf{\Omega}_{*} \text{ is } 8^{3}\times8^{3} = 512\times512 \\ \text{ top } 8\times8 \text{ slice of } 256 \text{ of the } 512 \text{ rows of } \mathbf{\Omega}_{*} \uparrow \end{array}$



Regularized inverse problem [4]:

$$\hat{\boldsymbol{x}} = \operatorname*{arg\,min}_{\boldsymbol{x}} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{y}\|_{\boldsymbol{W}}^2 + \beta \, \mathsf{R}(\boldsymbol{x})$$

$$\mathsf{R}(\boldsymbol{x}) = \arg\min_{\{\boldsymbol{z}_m\}} \sum_{m=1}^{M} \|\boldsymbol{\Omega}_* \boldsymbol{P}_m \boldsymbol{x} - \boldsymbol{z}_m\|_2^2 + \alpha \|\boldsymbol{z}_m\|_0.$$

 Ω_* adapted to population training data

Alternating minimization optimizer:

- *z_m* update is simple hard thresholding
- ➤ x update is a quadratic problem: many options Linearized augmented Lagrangian method (LALM) [5]

Example: low-dose 3D X-ray CT simulation













X. Zheng, S. Ravishankar, Y. Long, JF: IEEE T-MI, June 2018 [4]

3D X-ray CT simulation Error maps





RMSE in HU

X-ray Intensity	FDK	EP	ST Ω _*	ULTRA	ULTRA- $\{\tau_j\}$
$1 imes 10^4$	67.8	34.6	32.1	30.7	29.2
$5 imes 10^3$	89.0	41.1	37.3	35.7	34.2

- Physics / statistics provides dramatic improvement
- Data adaptive regularization further reduces RMSE



Given training images x_1, \ldots, x_L from a representative population, find a set of transforms $\{\hat{\Omega}_k\}_{k=1}^{K}$ that best sparsify image patches:

$$\begin{cases} \hat{\boldsymbol{\Omega}}_{\boldsymbol{k}} \end{cases} = \underset{\{\boldsymbol{\Omega}_{\boldsymbol{k}} \text{ unitary}\}}{\arg\min} \underset{\{\boldsymbol{k}_{l,m} \in \{1,...,K\}\}}{\min} \underset{\{\boldsymbol{z}_{l,m}\}}{\min} \\ \sum_{l=1}^{L} \sum_{m=1}^{M} \left\| \boldsymbol{\Omega}_{\boldsymbol{k}_{l,m}} \boldsymbol{P}_{m} \boldsymbol{x}_{l} - \boldsymbol{z}_{l,m} \right\|_{2}^{2} + \alpha \left\| \boldsymbol{z}_{l,m} \right\|_{0}$$

- Joint unsupervised clustering / sparsification
- Further nonconvexity due to clustering
- Efficient alternating minimization algorithm [6]

Example: 3D X-ray CT learned set of transforms





X. Zheng, S. Ravishankar, Y. Long, JF: IEEE T-MI, June 2018 [4]







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Drawback of basic patch-based methods: $512 \times 512 \times 512$ 3D X-ray CT image volume $8 \times 8 \times 8$ patches $\implies 512^3 \cdot 8^3 \cdot 4 = 256$ Gbyte of patch data for stride=1

Convolutional sparsity model



Assumption: There is a set of filters $\{\boldsymbol{h}_k\}_{k=1}^{K}$ such that $\{\boldsymbol{h}_k * \boldsymbol{x}\}$ are sparse for a plausible image \boldsymbol{x} .

- For more plausible images, $\{h_k * x\}$ is more sparse.
- * denotes convolution
- Inherently shift invariant and no patches

Example:



Sparsifying filter learning (population adaptive)



Given training images x_1, \ldots, x_L from a representative population, find filters $\left\{ \hat{h}_k \right\}_{k=1}^{K}$ that best sparsify them:

$$\left\{ \hat{\boldsymbol{h}}_{k} \right\} = \underset{\{\boldsymbol{h}_{k}\}\in\mathcal{H}}{\arg\min} \min_{\{\boldsymbol{z}_{l,k}\}} \sum_{l=1}^{L} \sum_{k=1}^{K} \|\boldsymbol{h}_{k} * \boldsymbol{x}_{l} - \boldsymbol{z}_{l,k}\|_{2}^{2} + \alpha \|\boldsymbol{z}_{l,k}\|_{0}$$

► To encourage filter diversity: • H = {H : HH' = I}, H = [h₁ ... h_K] • cf. tight-frame condition ∑^K_{k=1} ||h_k * x||²₂ ∝ ||x||²₂

- Encourage aggregate sparsity, period
- Non-convex due to constraint \mathcal{H} and $\|\cdot\|_0$
- Efficient alternating minimization algorithm [7]
 - z update is simply hard thresholding
 - Filter update uses diagonal majorizer, proximal map (SVD)
 - Subsequence convergence guarantees [7]

Examples of learned sparsifying filters







Regularized inverse problem [7]:

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x} \succeq \boldsymbol{0}}{\arg\min} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{y}\|_{\boldsymbol{W}}^2 + \beta \operatorname{\mathsf{R}}(\boldsymbol{x})$$
$$\operatorname{\mathsf{R}}(\boldsymbol{x}) = \underset{\{\boldsymbol{z}_k\}}{\arg\min} \sum_{k=1}^K \left\| \hat{\boldsymbol{h}}_k * \boldsymbol{x} - \boldsymbol{z}_k \right\|_2^2 + \alpha \|\boldsymbol{z}_k\|_0.$$

$$\left\{ oldsymbol{\hat{h}}_k
ight\}$$
 adapted to population training data

Block proximal gradient with majorizer (BPG-M) optimizer:

- *z_k* update is simple hard thresholding
- x update is a quadratic problem: diagonal majorizer
- I. Y. Chun, JF, 2018, arXiv 1802.05584 [7]

Example: sparse-view 2D X-ray CT simulation





35 / 50



123 views (out of usual 984) \Longrightarrow 8× dose reduction

RMSE (in HU):					
FBP	82.8				
EP	40.8				
Adaptive filters	35.2				

- Physics / statistics provides dramatic improvement
- Data-adaptive regularization further reduces RMSE

Extension to multiple layers (cf CNN) I



Convolutional sparsity model: $h_k * x$ is sparse for $k = 1, ..., K_1$ Learning 1 "layer" of filters:

$$\{\hat{\boldsymbol{h}}_{k}^{[1]}\} = \underset{\{\boldsymbol{h}_{k}^{[1]}\}\in\mathcal{H}}{\arg\min\min} \min_{\{\boldsymbol{z}_{l,k}^{[1]}\}} \sum_{l=1}^{L} \sum_{k=1}^{K_{1}} \left\|\boldsymbol{h}_{k}^{[1]} * \boldsymbol{x}_{l} - \boldsymbol{z}_{l,k}^{[1]}\right\|_{2}^{2} + \alpha \left\|\boldsymbol{z}_{l,k}^{[1]}\right\|_{0}^{2}$$



Learning 2 layers of filters [7]:

$$\begin{pmatrix} \{ \hat{\boldsymbol{h}}_{k}^{[1]} \}, \{ \hat{\boldsymbol{h}}_{k}^{[2]} \} \end{pmatrix} = \underset{\{ \boldsymbol{h}_{k}^{[1]} \}, \{ \boldsymbol{h}_{k}^{[2]} \} \in \mathcal{H} \{ \boldsymbol{z}_{l,k}^{[1]} \} \{ \boldsymbol{z}_{l,k}^{[2]} \} \\ \sum_{l=1}^{L} \sum_{k=1}^{K_{1}} \left\| \boldsymbol{h}_{k}^{[1]} * \boldsymbol{x}_{l} - \boldsymbol{z}_{l,k}^{[1]} \right\|_{2}^{2} + \alpha \left\| \boldsymbol{z}_{l,k}^{[1]} \right\|_{0} \\ + \sum_{l=1}^{L} \sum_{k=1}^{K_{2}} \left\| \boldsymbol{h}_{k}^{[2]} * \left(\boldsymbol{P}_{k} \boldsymbol{z}_{l}^{[1]} \right) - \boldsymbol{z}_{l,k}^{[2]} \right\|_{2}^{2} + \alpha \left\| \boldsymbol{z}_{l,k}^{[2]} \right\|_{0}$$

Here P_k is a pooling operator for the output of first layer Block proximal gradient with majorizer (BPG-M) optimizer I. Y. Chun, JF, 2018, arXiv 1802.05584 [7]



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Assumption: if x is a plausible image, then each patch has

$P_m x \approx D z_m$

for a sparse coefficient vector \boldsymbol{z}_m . (Synthesis approach.)

- ► **P**_m**x** extracts the *m*th of *M* patches from **x**
- ► **D** is a (typically overcomplete) dictionary for patches



MR reconstruction using adaptive dictionary regularizer



Dictionary-blind MR image reconstruction:

$$\hat{\boldsymbol{x}} = \arg\min_{\boldsymbol{x}} \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_{2}^{2} + \beta \operatorname{R}(\boldsymbol{x})$$
$$\operatorname{R}(\boldsymbol{x}) = \min_{\boldsymbol{D} \in \mathcal{D}} \min_{\boldsymbol{z}' \in \mathcal{C}} \sum_{m=1}^{M} \left(\|\boldsymbol{P}_{m}\boldsymbol{x} - \boldsymbol{D}\boldsymbol{z}_{m}\|_{2}^{2} + \lambda^{2} \|\boldsymbol{z}_{m}\|_{0} \right)$$

where P_m extracts *m*th of *M* image patches. In words: of the many images...

Alternating (nested) minimization:

- ► Fixing x and D, update each row of Z = [z₁ ... z_M] sequentially via hard-thresholding.
- Fixing x and Z, update D using SOUP-DIL [8].
- Fixing Z and D, updating x is a quadratic problem.
 Efficient FFT solution for single-coil Cartesian MRI.
 Use CG for non-Cartesian and/or parallel MRI.
- Non-convex, but monotone decreasing and some convergence theory [8].

2D CS MRI results I





Sampling $(2.5\times)$

_
_
_
_
-
_
-

Initial **D**



Learned real {**D**}

$$\begin{split} & \textbf{6} \times \textbf{6} \text{ patches} \\ & \textbf{\textit{D}} \in \mathbb{C}^{6^2 \times 144} \\ & [8] \end{split}$$

2D CS MRI results II





(SNR compared to fully sampled image.) Using $\|\boldsymbol{z}_m\|_0$ leads to higher SNR then $\|\boldsymbol{z}_m\|_1$. Adaptive case is non-convex anyway...





lm.	Samp.	Acc.	0-fill	Sparse MRI	PANO	DLMRI	SOUP- DILLI	SOUP- DILLO
а	Cart.	7x	27.9	28.6	31.1	31.1	30.8	31.1
b	Cart.	2.5x	27.7	31.6	41.3	40.2	38.5	42.3
с	Cart.	2.5x	24.9	29.9	34.8	36.7	36.6	37.3
с	Cart.	4x	25.9	28.8	32.3	32.1	32.2	32.3
d	Cart.	2.5×	29.5	32.1	36.9	38.1	36.7	38.4
e	Cart.	2.5x	28.1	31.7	40.0	38.0	37.9	41.5
f	2D rand.	5×	26.3	27.4	30.4	30.5	30.3	30.6
g	Cart.	2.5x	32.8	39.1	41.6	41.7	42.2	43.2
Ref.				[9]	[10]	[1]	[8]	[8]

2D CS MRI results IV





Summary: 2D static MR reconstruction from under-sampled data with adaptive dictionary learning and convergent algorithm, faster than K-SVD approach of DLMRI.





Data-driven / adaptive regularization

- Beneficial for low-dose CT and under-sampled MRI reconstruction
- Dictionary atom structure (e.g., low rank) further helpful for dynamic MRI
- Block proximal methods provide reasonably computational efficiency
- Convergence theory (unlike KSVD)

Future work:

- Synthesis (*e.g.*, dictionary) vs analysis (*e.g.*, transform learning) formulations Begs for some principled model comparison...
- Online methods for reduced memory, better adaptation [12-15]
- Adaptive methods versus "deep" methods?
- Prospective use



June 2016 special issue of IEEE Trans. on Medical Imaging [16]:



IEEE TRANSACTIONS ON MEDICAL IMAGING, VOL. 37, NO. 6, JUNE 2018

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Image Reconstruction Is a New Frontier of Machine Learning

Ge Wang[®], *Fellow, IEEE*, Jong Chu Ye[®], *Senior Member, IEEE*, Klaus Mueller[®], *Senior Member, IEEE*, and Jeffrey A. Fessler[®], *Fellow, IEEE*

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