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Introduction

Adaptive regularization

Patch-based adaptive regularizers Convolutional adaptive regularizers Blind dictionary learning Supervised adaptive regularization

Summary

Bibliography





Introduction

Adaptive regularization

Summary

Bibliography

Image reconstruction background



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...

Generations of medical image reconstruction methods

- 70's "Analytical" methods (integral equations) FBP for SPECT / PET / X-ray CT, IFFT for MRI, ...
- 2. 80's Algebraic methods (as in "linear algebra") Solve y = Ax
- 3. 90's Statistical methods
 - \bullet LS / ML methods
 - Bayesian methods (Markov random fields, ...)
 - regularized methods
- 4. 00's Compressed sensing methods (mathematical sparsity models)
- 5. 10's Adaptive / data-driven methods machine learning, deep learning, ...



Two important milestones for clinical CT



• Deep-learning image reconstruction

FDA approved 2019 [2, 3]



Sparse-view CT: Under-determined inverse problem

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Data model:

 $y = Ax + \varepsilon$

- **y** : measurements (sinogram)
- e : noise
- **x** : unknown image
- ► A : system matrix (often wide)





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 $\|m{y}\|_{m{W}}^2 = m{y}'m{W}m{y}$

and $W^{-1} = Cov\{y | x\}$ is known (**A** from physics, **W** from statistics)



Priors for MAP estimation

▶ 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 / under-determined inverse problems.
- Why under-determined? Often high ambitions...



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Non-adaptive regularizers



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- Tikhonov regularization (IID gaussian prior)
- Markov random field (MRF) models
- Roughness penalty (cf MRF prior)
- Edge-preserving regularization (used in clinical CT scanners)
- Total-variation (TV) regularization (not used in clinical CT scanners)
- Black-box denoiser like NLM, e.g., plug-and-play ADMM [4]
- Sparsity in ambient space
- Sparsifying transforms: wavelets, curvelets,
- Graphical models

▶ ...

All "hand crafted" from statistical / mathematical models ...





Introduction

Adaptive regularization

Patch-based adaptive regularizers Convolutional adaptive regularizers Blind dictionary learning Supervised adaptive regularization

Summary

Bibliography

Data

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

Many options...



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Introduction

Adaptive regularization

Patch-based adaptive regularizers Convolutional adaptive regularizers Blind dictionary learning Supervised adaptive regularization

Summary

Bibliography

Patch-based regularization and TV

Anisotropic discrete TV regularizer: $R(\mathbf{x}) = \|\mathbf{T}\mathbf{x}\|_{1}$ where \mathbf{T} is finite-differences \equiv patches of size 2 × 1.

Larger patches provide more context for distinguishing signal from noise.

cf. CNN approaches

Patch-based regularizers:

- synthesis models
- analysis methods







X-ray CT with learned sparsifying transforms

Data

- Population adaptive methods
- Patient adaptive methods
- Spatial structure
 - Patch-based models
 - Convolutional models
- Regularizer formulation
 - Synthesis (dictionary) approach
 - Analysis (sparsifying transform) approach



Patch-wise transform sparsity model

Assumption: if x is a plausible image, then each $TP_m x$ is sparse.

- $P_m x$ extracts the *m*th of *M* patches from x
- **T** is a (often square) sparsifying transform matrix.







Sparsifying transform learning (population adaptive)

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

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

- Encourage aggregate sparsity, not patch-wise sparsity (cf K-SVD [5])
- Non-convex due to unitary constraint and $\|\cdot\|_0$
- Efficient alternating minimization algorithm [6]
 - z update : simple hard thresholding
 - **T** update : orthogonal Procrustes problem (SVD)
 - Subsequence convergence guarantees [6]



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Example of learned sparsifying transform



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3D X-ray training data



Parts of learned sparsifier T_*



(2D slices in x-y, x-z, y-z, from 3D image volume) $8 \times 8 \times 8$ patches $\implies T_*$ is $8^3 \times 8^3 = 512 \times 512$ top 8 \times 8 slice of 256 of the 512 rows of $\textit{\textbf{T}}_{*}\uparrow_{_{18/53}}$

Regularizer based on learned sparsifying transform

Regularized inverse problem [7]:

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

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

 $\boldsymbol{\mathcal{T}}_*$ adapted to population training data

Alternating minimization optimizer:

- ► *z_m* update : simple hard thresholding
- x update : quadratic problem (many options) Linearized augmented Lagrangian method (LALM) [8]



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



X. Zheng, S. Ravishankar, Y. Long, JF:

IEEE T-MI, June 2018 [7]



3D X-ray CT simulation Error maps





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

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

$$\left\{\hat{\boldsymbol{T}}_{k}\right\} = \underset{\{\boldsymbol{T}_{k} \text{ unitary}\}}{\arg\min} \min_{\{\boldsymbol{z}_{l,m}\}} \sum_{l=1}^{L} \sum_{m=1}^{M} \left(\min_{k \in \{1,\dots,K\}} \|\boldsymbol{T}_{k}\boldsymbol{P}_{m}\boldsymbol{x}_{l} - \boldsymbol{z}_{l,m}\|_{2}^{2} + \alpha \|\boldsymbol{z}_{l,m}\|_{0} \right)$$

- Joint unsupervised clustering / sparsification
- Further nonconvexity due to clustering
- Efficient alternating minimization algorithm [9]

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







Example: 3D X-ray CT ULTRA for chest scan





Zheng et al., IEEE T-MI, June 2018 [7]

Matlab code: http://web.eecs.umich.edu/~fessler/irt/reproduce/

 ${\tt https://github.com/xuehangzheng/PWLS-ULTRA-for-Low-Dose-3D-CT-Image-Reconstruction}$





Introduction

Adaptive regularization

Patch-based adaptive regularizers Convolutional adaptive regularizers Blind dictionary learning Supervised adaptive regularization

Summary

Bibliography



Data

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- Patient adaptive methods
- Spatial structure
 - Patch-based models
 - Convolutional models
- Regularizer formulation
 - Synthesis (dictionary) approach
 - Analysis (sparsifying transform) approach

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: analysis model

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Assumption: For a plausible image \boldsymbol{x} , the filter outputs $\{\boldsymbol{h}_k * \boldsymbol{x}\}$ are sparse, for some filters $\{\boldsymbol{h}_k\}_{k=1}^{K}$ [10]

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



Outputs $\mathbf{z}_1, \ldots, \mathbf{z}_4$



Sparsifying filter learning (population adaptive)

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Given training images $\mathbf{x}_1, \ldots, \mathbf{x}_L$ from a representative population, find filters $\{\hat{\mathbf{h}}_k\}_{k=1}^K$ 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:

•
$$\mathcal{H} = \{\boldsymbol{H} : \boldsymbol{H}\boldsymbol{H}' = \boldsymbol{I}\}, \ \boldsymbol{H} = [\boldsymbol{h}_1 \ \dots \ \boldsymbol{h}_K]$$

- *cf.* tight-frame condition $\sum_{k=1}^{K} \| \boldsymbol{h}_k * \boldsymbol{x} \|_2^2 \propto \| \boldsymbol{x} \|_2^2$
- Encourage aggregate sparsity, period
- ▶ Non-convex due to constraint \mathcal{H} and $\|\cdot\|_0$
- Efficient alternating minimization algorithm [11]
 - z update is simply hard thresholding
 - Filter update uses diagonal majorizer, proximal map (SVD)
 - Subsequence convergence guarantees [11]

Examples of learned sparsifying filters

 $\alpha = \overline{10^{-4}}$



-0.099

 $\alpha = \overline{2 \times 10^{-3}}$





-0.16

Regularizer based on learned sparsifying filters

Regularized inverse problem [11]:

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

 $\left\{ \hat{oldsymbol{h}}_k
ight\}$ 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 [11]



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

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123 views (out of usual 984) \implies 8× dose reduction 25 filters 5 × 5

RMSE (in HU):

FBP	82.8
EP	40.8
Adaptive filters	35.2

- Physics / statistics provides dramatic improvement
- Data-adaptive regularization further reduces RMSE, improves fine details

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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:

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



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Learning 2 layers of filters [11]:

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

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 [11]

Use multi-level learned filters as (interpretable?) regularizer for CT.





Introduction

Adaptive regularization

Patch-based adaptive regularizers Convolutional adaptive regularizers Blind dictionary learning Supervised adaptive regularization

Summary

Bibliography

MR with adapted patch dictionary

Data

- Population adaptive methods
- Patient adaptive methods
- Spatial structure
 - Patch-based models
 - Convolutional models
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 - Synthesis (dictionary) approach
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Patch-wise dictionary sparsity model

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Assumption: if \boldsymbol{x} is a plausible image, then each patch has

 $P_{p}x pprox Dz_{p},$

for a sparse coefficient vector z_p . (Synthesis approach.)

- $P_p x$ extracts the *p*th of *P* patches from x
- **D** is a (typically overcomplete) dictionary for patches



MR reconstruction using adaptive dictionary regularizer

Dictionary-blind MR image reconstruction:

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

where P_m extracts *m*th of *M* image patches.

In words: of the many images...

Alternating (nested) minimization:

- Fixing \boldsymbol{x} and \boldsymbol{D} , update each row of $\boldsymbol{Z} = [\boldsymbol{z}_1 \ldots \boldsymbol{z}_M]$ sequentially via hard-thresholding.
- Fixing *x* and *Z*, update *D* using SOUP-DIL [12].
- 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 [12].



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2D CS MRI results I





2D CS MRI results II

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

Matlab code: http://web.eecs.umich.edu/~fessler/irt/reproduce/ https://gitlab.eecs.umich.edu/fessler/soupdil_dinokat















PSNR:

lm.	Samp.	Acc.	0-fill	Sparse MRI	PANO	DLMRI	SOUP- DILLI	SOUP- DILLO
а	Cart.	7×	27.9	28.6	31.1	31.1	30.8	31.1
b	Cart.	2.5×	27.7	31.6	41.3	40.2	38.5	42.3
с	Cart.	2.5×	24.9	29.9	34.8	36.7	36.6	37.3
с	Cart.	4×	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
е	Cart.	2.5×	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.				[13]	[14]	[15]	[12]	[12]

2D CS MRI results IV

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

Summary of patch-based, data-driven adaptive regularizers

Use training data to learn:

- dictionary **D** (for patches)
- sparsifying transform(s) T (for patches)

• or convolutional versions thereof [10, 17]

ML-based regularized optimization problem using M image patches:

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\arg\min} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{y}\|_{2}^{2} + \beta R_{\mathrm{ML}}(\boldsymbol{x})$$

$$R_{\mathrm{ML-DL}}(\boldsymbol{x}) = \underset{\{\boldsymbol{z}_{m}\}}{\min} \sum_{m=1}^{M} \|\boldsymbol{P}_{m}\boldsymbol{x} - \boldsymbol{D}\boldsymbol{z}_{m}\|_{2}^{2} + \alpha \|\boldsymbol{z}_{m}\|_{0}$$

$$R_{\mathrm{ML-ST}}(\boldsymbol{x}) = \underset{\{\boldsymbol{z}_{m}\}}{\min} \sum_{m=1}^{M} \|\boldsymbol{T}\boldsymbol{P}_{m}\boldsymbol{x} - \boldsymbol{z}_{m}\|_{2}^{2} + \alpha \|\boldsymbol{z}_{m}\|_{0}$$

Alternative: blind adaptive learned dictionary [15] or learned sparsifying transform [18]. Double minimization (so very "deep?") More interpretable than CNNs?



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Introduction

Adaptive regularization

Patch-based adaptive regularizers Convolutional adaptive regularizers Blind dictionary learning Supervised adaptive regularization

Summary

Bibliography

Convolutional sparsity revisted

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Cost function for convolutional sparsity regularization:

$$\arg\min_{\boldsymbol{x}} \frac{1}{2} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{y}\|_{\boldsymbol{W}}^{2} + \beta \left(\min_{\boldsymbol{\zeta}} \sum_{k=1}^{K} \frac{1}{2} \|\boldsymbol{h}_{k} \ast \boldsymbol{x} - \boldsymbol{\zeta}_{k}\|_{2}^{2} + \alpha \|\boldsymbol{\zeta}_{k}\|_{1}\right)$$

Alternating minimization updates:

Sparse code:
$$\boldsymbol{\zeta}_k^{(n+1)} = \operatorname{soft} \{ \boldsymbol{h}_k * \boldsymbol{x}^{(n)}, \alpha \}$$

Image:
$$\mathbf{x}^{(n+1)} = \arg\min_{\mathbf{x}} F(\mathbf{x}; \mathbf{y}, \mathbf{z}^{(n)})$$

 $F(\mathbf{x}; \mathbf{y}, \mathbf{z}^{(n)}) \triangleq \frac{1}{2} \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_{\mathbf{W}}^{2} + \beta \left(\sum_{k=1}^{K} \frac{1}{2} \|\mathbf{h}_{k} * \mathbf{x} - \boldsymbol{\zeta}_{k}^{(n+1)}\|_{2}^{2} + \alpha \|\boldsymbol{\zeta}_{k}^{(n+1)}\|_{1} \right)$
 $= \frac{1}{2} \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_{\mathbf{W}}^{2} + \beta \frac{1}{2} \|\mathbf{x} - \mathbf{z}^{(n)}\|_{2}^{2} \quad (\text{quadratic but } \text{large} \Longrightarrow \text{majorize})$
 $\mathbf{z}^{(n)} = \mathcal{R}(\mathbf{z}^{(n)}) = \sum_{k=1}^{K} \text{flip}(\mathbf{h}_{k}) * \text{soft}\{\mathbf{h}_{k} * \mathbf{x}^{(n)}\} \quad (\text{denoise} \Longrightarrow \text{learn})$





Unrolled loop network with momentum and quadratic majorizer:

► Diagonal majorizer: $M = \text{diag}\{A'WA1\} + \beta I \succeq A'WA + \beta I$

Learn image mapper ("refiner") R from training data (supervised). cf CNN: filter → threshold → filter



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- $\blacktriangleright \text{ Image mapper } \mathcal{R} \text{ is shallow}$
 - \implies less risk of over-fitting / hallucination
- Momentum accelerates convergence (fewer layers)
- First unrolled loop approach to have convergence theory (under suitable assumptions on *R*)
- Image update uses original CT sinogram y and imaging physics A

[19]

II Yong Chun, Zhengyu Huang, Hongki Lim, J A Fessler Momentum-Net: Fast and convergent iterative neural network for inverse problems

http://arxiv.org/abs/1907.11818

Momentum-Net preliminary results

Illustration of benefits of momentum:



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Momentum-Net preliminary image results



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Sparse-view CT with 123/984 views, $I_0 = 10^5$, 800-1200 mod. HU display.



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Introduction

Adaptive regularization

Summary

Bibliography





- CT image reconstruction has evolved greatly in the 50+ years since Allan Cormack's seminal papers [20, 21]
 - physics
 - statistics
 - regularization and optimization
 - data adaptive methods inspired by machine learning
- Machine learning has great potential for medical imaging
- Much excitement but many challenges
- Image reconstruction seems especially suitable for ML ideas
- Data-driven, adaptive regularizers beneficial for low-dose CT
- More comparisons between model-based methods with adaptive regularizers and CNN-based methods needed

Resources

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Talk and code available online at http://web.eecs.umich.edu/~fessler



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