Deep Sparse Coding and Dictionary Learning

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1. Sparse Coding

- **Problem statement**: Given a signal $\boldsymbol{y} \in \mathbb{R}^m$ and an overcomplete dictionary $\mathbf{A} \in \mathbb{R}^{m\times n}$, find an s-sparse vector $\boldsymbol{x} \in \mathbb{R}^n$, $s \ll n$, such that $\boldsymbol{y} \approx \boldsymbol{Ax} \implies$ Basis selection: Express $\boldsymbol{y} = \sum_{i\in S} x_i \boldsymbol{a}_i$, $|S| = s$
- **Solution**: Seek the minimum ℓ_0-(quasi)-norm solution: NP-hard

$$\min_{\boldsymbol{x}} \|\boldsymbol{x}\|_0 \text{ subject to } \boldsymbol{y} = \boldsymbol{Ax}$$

2. Iterative Shrinkage-Thresholding Algorithm (ISTA)

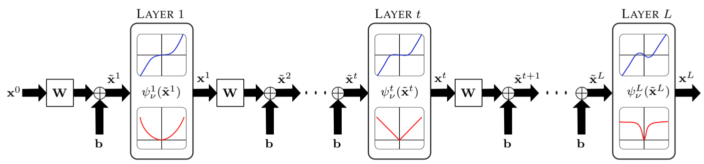
- **Relaxation techniques: Solve sparsity-regularized least-squares**

$$\hat{\boldsymbol{x}} = \arg\min_{\boldsymbol{x}} \underbrace{\frac{1}{2}\|\boldsymbol{y} - \boldsymbol{Ax}\|_2^2}_{f(\boldsymbol{x})} + \underbrace{\lambda\,\mathcal{R}(\boldsymbol{x})}_{\text{promotes sparsity}}$$

- **ISTA update**: $\boldsymbol{x}^{t+1} = T_{\lambda\eta}\left(\boldsymbol{x}^t - \eta\nabla f\left(\boldsymbol{x}^t\right)\right) \overset{\text{neural net.}}{\equiv} \boldsymbol{x}^{t+1} = \psi^t\left(\boldsymbol{W}\boldsymbol{x}^t + \boldsymbol{b}\right)$, where $\boldsymbol{W} = \boldsymbol{I} - \eta\boldsymbol{A}^\top\boldsymbol{A}$ and $\boldsymbol{b} = \eta\boldsymbol{A}^\top\boldsymbol{y}$
- **Our approach**: Learning the activation ψ^t in a data-driven manner
  - Advantage-1: Number of parameters to learn does not grow with n
  - Advantage-2: Possible to learn a rich variety of activations and regularizers

3. Architecture and Training of *LETnet*

***LETnet* architecture**: Model $\psi^t(u) = \sum_{k=1}^{K} c_k^t \phi_k(u)$, $\phi_k(u) = u\,\exp\left(-\frac{(k-1)u^2}{2\tau^2}\right)$



***LETnet* training**:

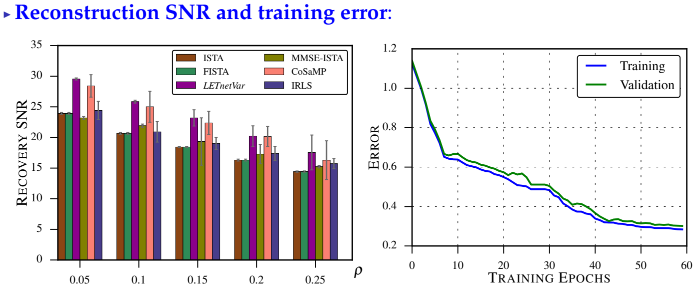
- Training cost $J(\mathbf{c}) = \frac{1}{2}\sum_{q=1}^{N} \|\mathbf{x}_q^L\left(\mathbf{y}_q, \mathbf{c}\right) - \mathbf{x}_q\|_2^2$, where $\mathbf{c} = \left(\mathbf{c}^1; \mathbf{c}^2; \cdots; \mathbf{c}^L\right)$
- Second-order Hessian-free optimization
  - $J_i^{(q)}\left(\mathbf{c}_i + \boldsymbol{\delta}_c\right) = J\left(\mathbf{c}_i\right) + \boldsymbol{\delta}_c^\top\mathbf{g}_i + \frac{1}{2}\boldsymbol{\delta}_c^\top\mathbf{H}_i\boldsymbol{\delta}_c$
  - Compute optimal direction using conjugate-gradient (CG) at every epoch i

$$\boldsymbol{\delta}_c^* = \arg\min_{\boldsymbol{\delta}_c} J_i^{(q)}\left(\mathbf{c}_i + \boldsymbol{\delta}_c\right) + \gamma\left\|\boldsymbol{\delta}_c\right\|_2^2$$

  - Update parameters as $\mathbf{c}_{i+1} \leftarrow \mathbf{c}_i + \boldsymbol{\delta}_c^*$
- Two ingredients of CG
  - Gradient $\mathbf{g}_i = \nabla J(\mathbf{c})|_{\mathbf{c}=\mathbf{c}_i}$ and the Hessian-vector product $\mathbf{H}_i\mathbf{u}$, for any $\mathbf{u}$
  - Computing the hessian-vector product
    - $\mathcal{R}_\mathbf{u}(\mathbf{h}(\mathbf{c})) = \lim_{\alpha\to 0}\frac{\mathbf{h}(\mathbf{c}+\alpha\mathbf{u}) - \mathbf{h}(\mathbf{c})}{\alpha} \implies \mathbf{H}_i\mathbf{u} = \mathcal{R}_\mathbf{u}\left(\nabla_\mathbf{c} J(\mathbf{c})\right)|_{\mathbf{c}=\mathbf{c}_i}$
  - $\mathbf{g}_i$ and $\mathbf{H}_i\mathbf{u}$ are computed using back-propagation

4. Validation on Synthetic Signals

- **Data generation**:
  - $n = 256$, $m = \lceil 0.7n\rceil$
  - $A_{i,j} \sim \mathcal{N}(0, 1/m)$
  - $\boldsymbol{x} = \boldsymbol{x}_{\text{supp}} \odot \boldsymbol{x}_{\text{mag}}$, where $\boldsymbol{x}_{\text{supp}} \sim \text{Bernoulli}(\rho)$ and $\boldsymbol{x}_{\text{mag}} \sim \mathcal{N}(0,1)$
  - $0 < \rho < 1$: smaller the value of ρ, sparser the vector $\boldsymbol{x}$
  - λ chosen optimally using cross-validation
  - 100 examples used for training and testing
  - Performance averaged over 10 independent trials
- **Reconstruction SNR and training error**:

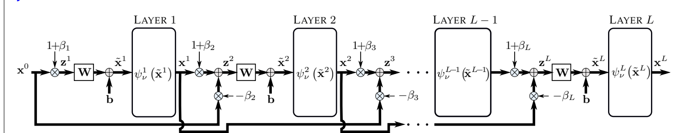


(a) $SNR_{input} = 20$ dB (b) Training and validation error

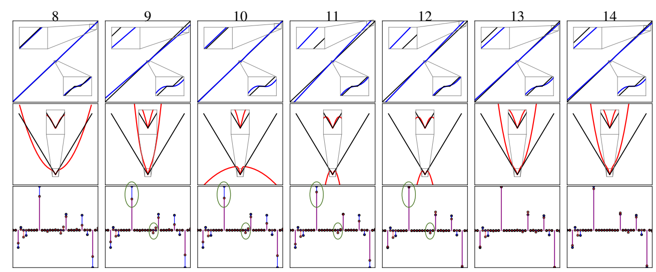
- Both training and validation errors decrease; no overfitting

5. *fLETnet*: A Deep Architecture Motivated by FISTA

- **FISTA iterations unfolded**
  1. $\mathbf{z}^t = (1+\beta_t)\mathbf{x}^{t-1} - \beta_t\mathbf{x}^{t-2}$
  2. $\mathbf{x}^t = T_\nu\left(\tilde{\mathbf{x}}^t\right)$, where $\tilde{\mathbf{x}}^t = \mathbf{W}\mathbf{z}^t + \mathbf{b}$ for $t = 1, 2, \cdots, L$
- ***fLETnet* architecture**:



- **Key Features of *fLETnet***:
  - Direct links from two previous layers (second-order memory)
  - Circumvents the issue of vanishing/exploding gradient
  - The resulting architecture *fLETnet* is essentially a deep residual network
  - Equivalent performance as the *LETnet* with half as many layers
- **What regularizers does the *fLETnet* learn?**

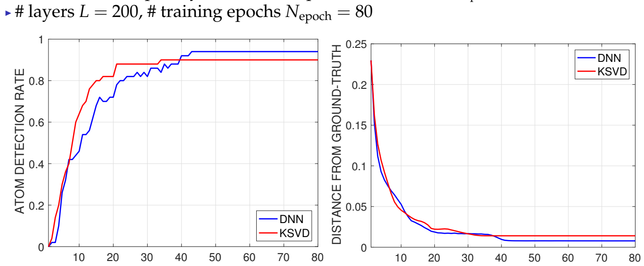


6. Comparison of Testing Run-times

Algorithm	per iteration/layer run-time (in milliseconds)	# layers/ iterations	total time (in milliseconds)
ISTA	0.0331	1000	33.10
FISTA	0.0394	1000	39.40
LETnet	0.0895	100	8.95
fLETnet	0.1088	50	5.44
MMSE-ISTA	0.6184	1000	618.40
CoSaMP	11.7672	50	588.36
IRLS	5.2784	50	263.92

7. Deep Dictionary Learning

- **Problem statement**: Given a set of signals $\left\{\boldsymbol{y}_j\right\}_{j=1}^N \in \mathbb{R}^m$, learn an overcomplete dictionary $\mathbf{A} \in \mathbb{R}^{m\times n}$ and s-sparse vectors $\{\boldsymbol{x}_j\}_{j=1}^N \in \mathbb{R}^n$, $s \ll n$, such that $\boldsymbol{y}_j \approx \boldsymbol{A}\boldsymbol{x}_j$ for all j
- **Proposed approach**: $\hat{\boldsymbol{A}} = \min_{\boldsymbol{A}} \sum_{j=1}^N \left\|\boldsymbol{A}\,\text{net}_{\boldsymbol{y}_j}(\boldsymbol{A}) - \boldsymbol{y}_j\right\|_2^2$
  - $\text{net}_{\boldsymbol{y}_j}(\boldsymbol{A})$ is the output of ISTA corresponding to the signal $\boldsymbol{y}_j$ and dictionary $\boldsymbol{A}$
  - Gradient descent: $\boldsymbol{A} \leftarrow \boldsymbol{A} - \mu\nabla J(\boldsymbol{A})$, $\nabla J(\boldsymbol{A})$ requires only matrix-vector products
- **Advantages over conventional dictionary learning algorithms**:
  - Online and distributed implementations
  - Certain desirable properties on the dictionary, such as incoherence, can be promoted by adding a penalty and appropriately modifying the gradient
- **Performance metrics**:
  - Atom detection rate: $\frac{\#\{\text{recovered atoms}\}}{n}$
  - Distance of $\hat{\boldsymbol{A}}$ from $\boldsymbol{A}^*$: $\kappa = \frac{1}{n}\sum_{i=1}^{n}\min_{1\leqslant j\leqslant n}\left(1 - \left|\boldsymbol{a}_j^T\boldsymbol{a}_i^*\right|\right)$
- **Experimental validation**:
  - $n = 50$, $m = 20$, sparsity $s = 3$, # examples $N = 2000$, $\text{SNR}_{\text{input}} = 30$ dB
  - # layers $L = 200$, # training epochs $N_{\text{epoch}} = 80$



Acknowledgement: This is a joint work with Debabrata Mahapatra.

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April 7, 2017
EECS Divisional Symposium, 2017

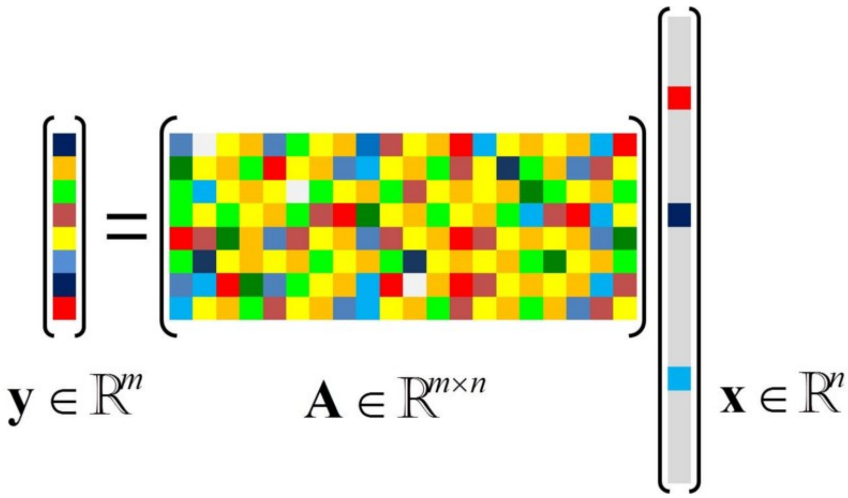
SPECTRUM LAB

Outline

- What is sparse coding?
- Iterative shrinkage-thresholding algorithms (ISTA)
  - Iterative unfolding and connections to deep neural networks (DNNs)
  - Building a learnable model for sparse coding
- Our contributions
  - Modeling the non-linearity using a linear expansion of thresholds (LETs)
  - Parametric flexibility for designing regularizers
  - Efficient second-order (Hessian-free) optimization for learning
  - Reducing the number of layers and link with deep residual networks
  - Building a deep architecture for dictionary learning
- Simulation results and insights
- Summary and future works

What is sparse coding?

- Problem statement: Given a signal $\boldsymbol{y} \in \mathbb{R}^m$ and an overcomplete dictionary $\mathbf{A} \in \mathbb{R}^{m\times n}$, find an s-sparse vector $\boldsymbol{x} \in \mathbb{R}^n$, $s \ll n$, such that $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$



- Basis selection: Express $\boldsymbol{y} = \sum_{i\in S} x_i \boldsymbol{a}_i$, $|S| = s$
  - Estimating $\boldsymbol{A}$ from given data is the problem of dictionary learning
- Solution: Seek the minimum ℓ_0-(quasi)-norm solution: Combinatorially hard

$$\min_{\boldsymbol{x}} ||\boldsymbol{x}||_0 \text{ subject to } \boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$$

Iterative shrinkage-thresholding algorithm (ISTA) meets neural network

- Relaxation techniques: Solve sparsity-regularized least-squares

$$\hat{\boldsymbol{x}} = \arg\min_{\boldsymbol{x}} \underbrace{\frac{1}{2}\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2}_{f(\boldsymbol{x})} + \underbrace{\lambda \mathcal{R}(\boldsymbol{x})}_{\text{promotes sparsity}}$$

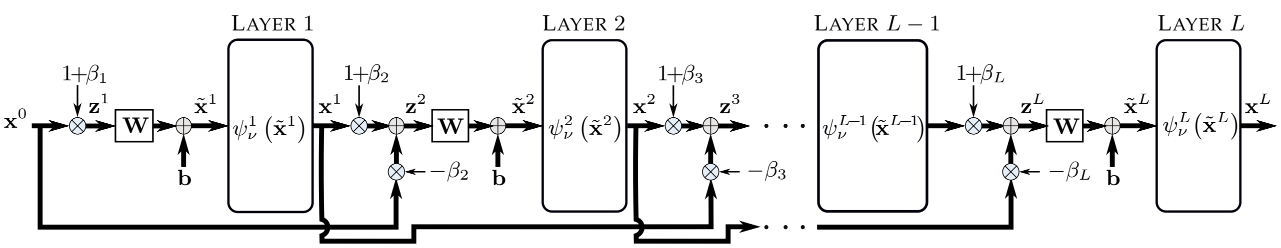
- ISTA update rule (Daubechies et al., 2004)
  - $\boldsymbol{x}^{t+1} = T_{\lambda\eta}\left(\boldsymbol{x}^t - \eta \nabla f\left(\boldsymbol{x}^t\right)\right)$, where T_ν denotes soft-thresholding with threshold ν
- Unfolding of ISTA iterations

$$\boldsymbol{x}^{t+1} = \underbrace{\psi^t}_{\text{non lin.}}\left(\underbrace{\boldsymbol{W}\boldsymbol{x}^t + \boldsymbol{b}}_{\text{affine}}\right), \text{ where } \boldsymbol{W} = \boldsymbol{I} - \eta \boldsymbol{A}^\top \boldsymbol{A} \text{ and } \boldsymbol{b} = \eta \boldsymbol{A}^\top \boldsymbol{y}$$

- Building learnable models
  - Learn the linear transformation parameters $\boldsymbol{W}$ and $\boldsymbol{b}$ from the data – data-intensive
  - Learn the nonlinear shrinkage function
- *LETnet*: Modeling the activation nonlinearity using LETs
  - LET modeling: $\psi^t(u) = \sum_{k=1}^{K} c_k^t \phi_k(u)$, where $\phi_k(u) = u \exp\left(-\frac{(k-1)u^2}{2\tau^2}\right)$

Unfolding of FISTA (Nesterov, 1980s) and the *fLETnet*

- FISTA iterations unfolded
  1. $\mathbf{z}^t = (1+\beta_t)\mathbf{x}^{t-1} - \beta_t \mathbf{x}^{t-2}$
  2. $\tilde{\mathbf{x}}^t = \mathbf{W}\mathbf{z}^t + \mathbf{b}$
  3. $\mathbf{x}^t = T_\nu\left(\tilde{\mathbf{x}}^t\right)$, for $t = 1, 2, \cdots, L$



- *fLETnet*: Network architecture motivated by FISTA
  - Replace T_ν with a parametric activation ψ^t
  - Direct links from two previous layers (second-order memory)
  - -1 link: identity mapping; thus no new parameters to learn
  - Circumvents the issue of vanishing/exploding gradient
  - The *fLETnet* architecture is essentially a deep residual network (He et al., 2015)
  - Results in equivalent performance as the *LETnet* with half as many layers

Training the *LETnet* and the *fLETnet*

- Training dataset $\mathcal{D}$ consists of N examples $\{(\mathbf{y}_q, \mathbf{x}_q)\}_{q=1}^{N}$, where $\mathbf{y}_q = \mathbf{A}\mathbf{x}_q + \xi_q$, for a given $\boldsymbol{A}$
- Training cost $J(\boldsymbol{c}) = \frac{1}{2}\sum_{q=1}^{N} \|\mathbf{x}_q^L\left(\boldsymbol{y}_q, \boldsymbol{c}\right) - \mathbf{x}_q\|_2^2$, where $\boldsymbol{c} = \left(\boldsymbol{c}^1; \boldsymbol{c}^2; \cdots; \boldsymbol{c}^L\right)$
- Second-order optimization
  - Quadratic approximation in the i^{th} training epoch

$$J_i^{(q)}\left(\boldsymbol{c}_i + \delta_{\boldsymbol{c}}\right) = J\left(\boldsymbol{c}_i\right) + \delta_{\boldsymbol{c}}^{\top}\boldsymbol{g}_i + \frac{1}{2}\delta_{\boldsymbol{c}}^{\top}\mathbf{H}_i\delta_{\boldsymbol{c}}$$

  - Compute optimal direction using conjugate-gradient (CG) at every epoch i

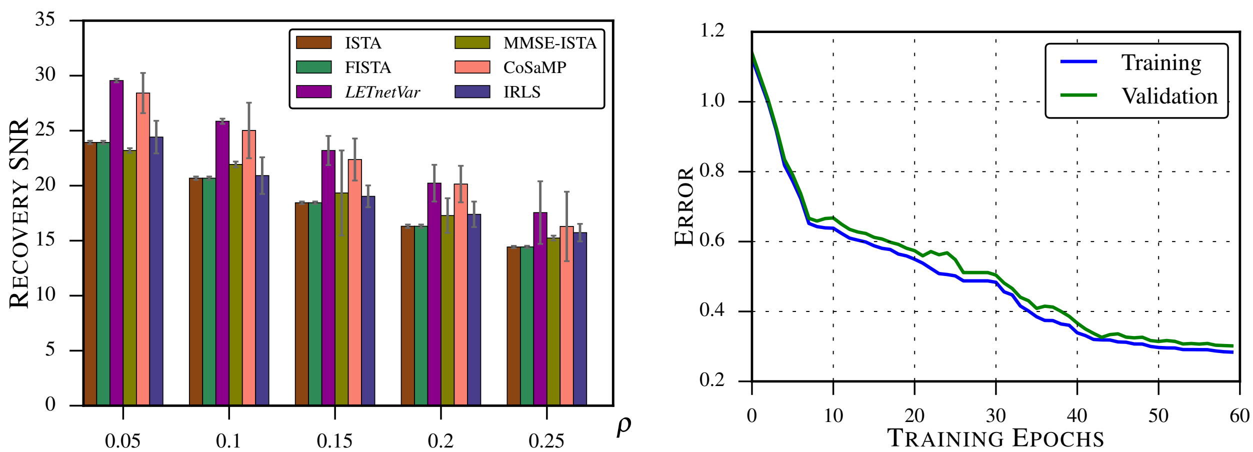
$$\delta_{\boldsymbol{c}}^{*} = \arg\min_{\delta_{\boldsymbol{c}}} J_i^{(q)}\left(\boldsymbol{c}_i + \delta_{\boldsymbol{c}}\right) + \gamma\|\delta_{\boldsymbol{c}}\|_2^2$$

  - Update parameters as $\boldsymbol{c}_{i+1} \leftarrow \boldsymbol{c}_i + \delta_{\boldsymbol{c}}^{*}$
- Two ingredients of CG
  - Gradient $\boldsymbol{g}_i = \nabla J(\boldsymbol{c})\big|_{\boldsymbol{c}=\boldsymbol{c}_i}$
  - Hessian-vector product $\mathbf{H}_i\boldsymbol{u}$ for any vector $\boldsymbol{u}$, where $\mathbf{H}_i = \nabla^2 J(\boldsymbol{c})\big|_{\boldsymbol{c}=\boldsymbol{c}_i}$
    - $\mathcal{R}_{\mathbf{u}}(\mathbf{h}(\mathbf{c})) = \lim_{\alpha\to 0}\frac{\mathbf{h}(\mathbf{c}+\alpha\mathbf{u})-\mathbf{h}(\mathbf{c})}{\alpha} \implies \mathbf{H}_i\mathbf{u} = \mathcal{R}_{\mathbf{u}}\left(\nabla_{\mathbf{c}}J(\mathbf{c})\right)\big|_{\mathbf{c}=\mathbf{c}_i}$

Experimental details and parameter settings

- Data generation
  - $n = 256$, $m = \lceil 0.7n \rceil$
  - $A_{i,j} \sim \mathcal{N}(0, 1/m)$
  - $\boldsymbol{x} = \boldsymbol{x}_{\text{supp}} \odot \boldsymbol{x}_{\text{mag}}$, where $\boldsymbol{x}_{\text{supp}} \sim \text{Bernoulli}(\rho)$ and $\boldsymbol{x}_{\text{mag}} \sim \mathcal{N}(0, 1)$
  - $0 < \rho < 1$: smaller the value of ρ, sparser the vector $\boldsymbol{x}$
  - λ chosen optimally using cross-validation
  - $N_{\text{train}} = 100$ examples used for training
  - $N_{\text{test}} = 100$ examples used for testing
  - Performance averaged over 10 independent trials

Performance assessment of *LETnetVar*



(a) $SNR_{input} = 20$ dB (b) Training and validation error

Figure: Comparison of ensemble-averaged reconstruction SNR and its standard deviation.

- Observations
  - *LETnetVar* with 100 layers performs 3 to 4 dB better than ISTA, with optimally chosen hyper-parameter (λ).
  - When measurements are more noisy, the improvement in recovery SNR of *LETnet* was found to be higher.
  - Training and validation errors reduce monotonically with training epochs

What regularizers did the *fLETnet* learn?

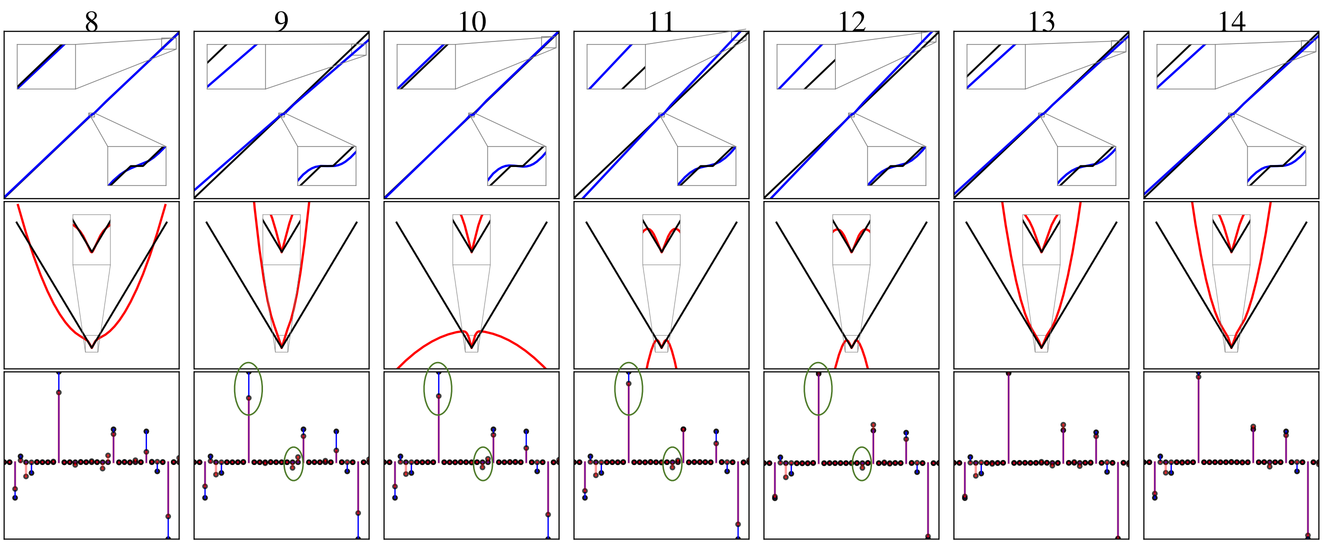


Figure: The learnt LET functions (blue) of *fLETnet* and the corresponding induced regularizers (red).

- Key observations
  - Can learn a wide variety of regularizers
  - Signal component missed in a layer can be recovered subsequently
  - Balance between signal preservation and noise cancellation

A comparison of testing run-times

Algorithm	per iteration/layer run-time (in milliseconds)	number of layers/ iterations	total time (in milliseconds)
ISTA	0.0331	1000	33.10
FISTA	0.0394	1000	39.40
LETnet	0.0895	100	8.95
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Deep dictionary learning

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- Proposed approach:

$$\hat{\boldsymbol{A}} = \min_{\boldsymbol{A}} \sum_{j=1}^N \left\|\boldsymbol{A}\ \mathrm{net}_{\boldsymbol{y}_j}(\boldsymbol{A}) - \boldsymbol{y}_j\right\|_2^2$$

  - $\mathrm{net}_{\boldsymbol{y}_j}(\boldsymbol{A})$ is the output of ISTA corresponding to the signal $\boldsymbol{y}_j$ and dictionary $\boldsymbol{A}$
  - Gradient descent: $\boldsymbol{A} \leftarrow \boldsymbol{A} - \mu\nabla J(\boldsymbol{A})$
  - Computing $\nabla J(\boldsymbol{A})$ requires only matrix-vector products
- Advantages over conventional dictionary learning algorithms:
  - Online implementation
  - Distributed implementation for a large training dataset
  - Certain desirable properties on the dictionary, such as incoherence, can be promoted by adding a penalty and appropriately modifying the gradient

Deep dictionary learning: Performance validation

- Data generation
  - $n = 50$, $m = 20$
  - Number of examples $N = 2000$
  - Sparsity $s = 3$
  - Number of layers $L = 200$
  - Add noise to the training dataset such that $\mathrm{SNR}_{\mathrm{input}} = 30$ dB

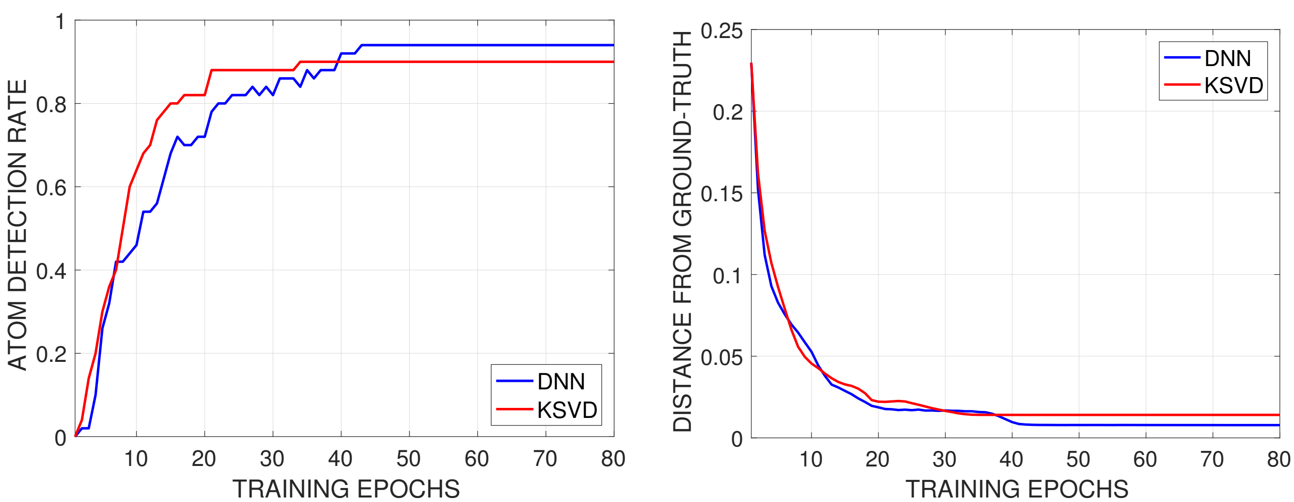

Figure: Comparison of DNN-based dictionary learning with K-SVD

Summary and future works

Summary

- Sparse coding as a function approximation problem
- Link between ISTA and a DNN
- Learning data-driven parameterized nonlinearities
- Efficient Hessian-free second-order optimization for training the network
- Link between FISTA and deep residual network
- The induced regularizers are nonstandard! Go beyond ℓ_1 and ℓ_0
- Extension to dictionary learning

Future works

- Restricted to a fixed dictionary. How about adaptive/slowly varying dictionaries?
- A generic DNN solution to any iterative algorithm for inverse problems?