Paired Autoencoders for Inference and Regularization

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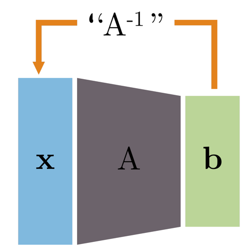
Introduction

- **Inverse problems** involve determining the causes or parameters of a system based on observed outcomes

$$A(\mathbf{x}) + \boldsymbol{\epsilon} = \mathbf{b}$$

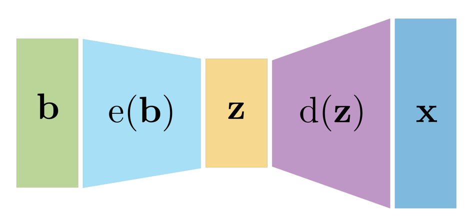
  - input observations $\mathbf{b} \in \mathbb{R}^m$
  - target parameters $\mathbf{x} \in \mathbb{R}^n$
  - forward process $A : \mathbb{R}^n \to \mathbb{R}^m$
  - noise $\boldsymbol{\epsilon} \in \mathbb{R}^m$



- **Machine learning** has been used to address many challenges in ill-posed and large-scale inverse problems, including full inversion (surrogate modeling), regularization, uncertainty quantification, and more
- **Encoder-decoder networks**

$$\mathbf{x} \approx (d \circ e)(\mathbf{b})$$

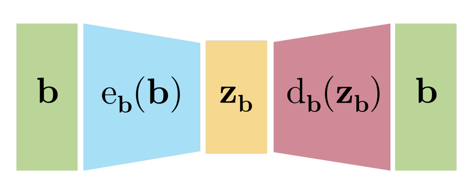
  - $e : \mathbb{R}^m \to \mathbb{R}^r$ maps $\mathbf{b}$ to a **latent variable z**
  - $d : \mathbb{R}^r \to \mathbb{R}^n$ maps from $\mathbf{z}$ to $\mathbf{x}$
  - ▹ Popular choice in many learning tasks
  - ▹ Can be used to directly learn map from $\mathbf{b}$ to $\mathbf{x}$



- **Autoencoders**

$$(d_b \circ e_b)(\mathbf{b}) \approx \mathbf{b}$$

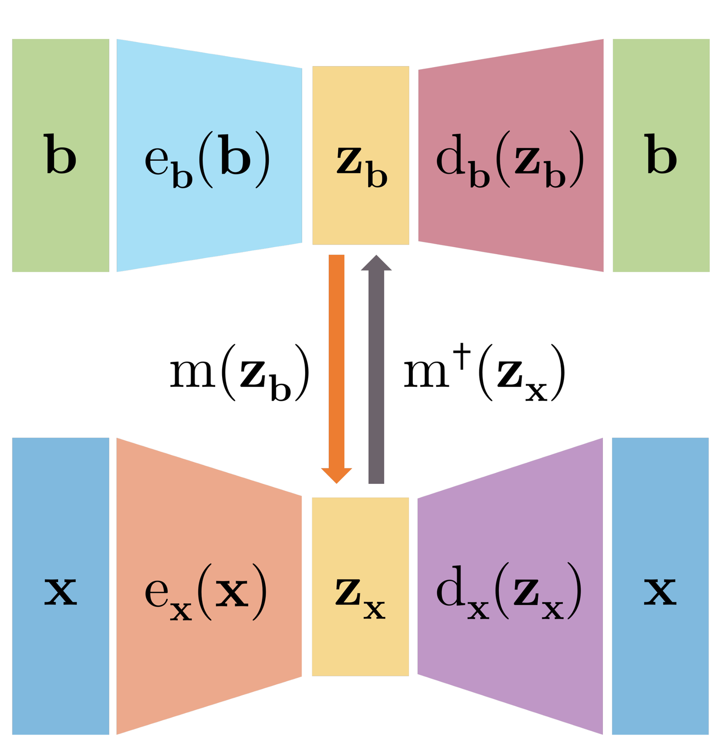
  - $e_\mathbf{b} : \mathbb{R}^m \to \mathbb{R}^{r_\mathbf{b}}$ compresses $\mathbf{b}$ to $\mathbf{z}_\mathbf{b}$
  - $d_\mathbf{b} : \mathbb{R}^{r_\mathbf{b}} \to \mathbb{R}^m$ expands $\mathbf{z}_\mathbf{b}$ to $\mathbf{b}$
  - ▹ Special case of an encoder-decoder network
  - ▹ Maps input $\mathbf{b}$ to itself
  - ▹ Used in dimensionality reduction, denoising



- **Aim** to leverage latent representations through **Paired Autoencoders for Inference and Regularization** (**PAIR**)

PAIR

- The PAIR framework is data-driven, and requires learning:
  - ▹ input $\mathbf{b}$ autoencoder, $(d_\mathbf{b} \circ e_\mathbf{b}) : \mathbb{R}^m \to \mathbb{R}^m$, unsupervised
  - ▹ target $\mathbf{x}$ autoencoder, $(d_\mathbf{x} \circ e_\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}^n$, unsupervised
  - ▹ latent inverse map, $m^\dagger : \mathbb{R}^{r_\mathbf{b}} \to \mathbb{R}^{r_\mathbf{x}}$, supervised
  - ▹ latent forward map, $m : \mathbb{R}^{r_\mathbf{x}} \to \mathbb{R}^{r_\mathbf{b}}$, supervised



- Potential uses:
  - ▹ $\mathbf{x} \approx (d_\mathbf{x} \circ m^\dagger \circ e_\mathbf{b})(\mathbf{b})$ can approximate the inverse process
  - ▹ $\mathbf{b} \approx (d_\mathbf{b} \circ m \circ e_\mathbf{x})(\mathbf{x})$ can approximate the forward model

Linear PAIR for Computed Tomography

Linear Autoencoders:

$$(d_\mathbf{x} \circ e_\mathbf{x})(\mathbf{x}) = \mathbf{DEx}$$

$$e_\mathbf{x}(\mathbf{x}) = \mathbf{Ex} = \mathbf{z}_\mathbf{x}, \qquad \mathbf{E} \in \mathbb{R}^{r \times n}$$
$$d_\mathbf{x}(\mathbf{z}_\mathbf{x}) = \mathbf{D}\mathbf{z}_\mathbf{x} \approx \mathbf{x}, \qquad \mathbf{D} \in \mathbb{R}^{n \times r}$$

Empirical Bayes risk approach:

- Work directly with realizations of random variable X

$$\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_N] \in \mathbb{R}^{n \times N}$$

- An optimal choice of encoder and decoder

$$\widehat{\mathbf{E}} = \mathbf{U}_{\mathbf{X},r}^\top \qquad \widehat{\mathbf{D}} = \mathbf{U}_{\mathbf{X},r}$$

  from left singular vectors of $\mathbf{X}$ corresponding to the r largest singular values [2, 3]

Linear Latent Mappings:
To find the optimal mapping between latent spaces, let

$$\mathbf{Z_X} = \begin{bmatrix} | & & | \\ e_\mathbf{x}(\mathbf{x}_1) & \ldots & e_\mathbf{x}(\mathbf{x}_N) \\ | & & | \end{bmatrix}$$

$$\mathbf{Z_B} = \begin{bmatrix} | & & | \\ e_\mathbf{b}(\mathbf{b}_1) & \ldots & e_\mathbf{b}(\mathbf{b}_N) \\ | & & | \end{bmatrix}$$

- Optimal linear latent inverse mapping

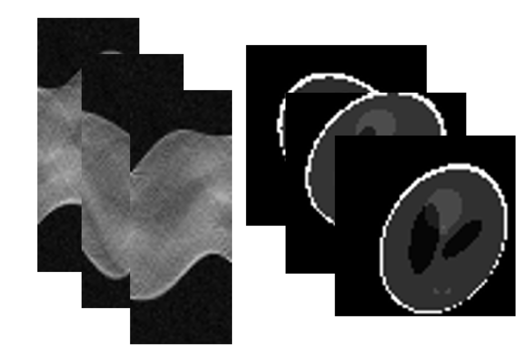
$$\mathbf{M}^\dagger = \underset{\widehat{\mathbf{M}}}{\arg\min} \left\| \widehat{\mathbf{M}}\mathbf{Z_B} - \mathbf{Z_X} \right\|_\mathrm{F}^2 = \mathbf{Z_X}(\mathbf{Z_B}^\top\mathbf{Z_B})^{-1}\mathbf{Z_B}^\top$$

- Optimal linear latent forward mapping

$$\mathbf{M} = \mathbf{Z_B}(\mathbf{Z_X}^\top\mathbf{Z_X})^{-1}\mathbf{Z_X}^\top$$

Note: also holds for nonlinear autoencoders

Computed Tomography Example:

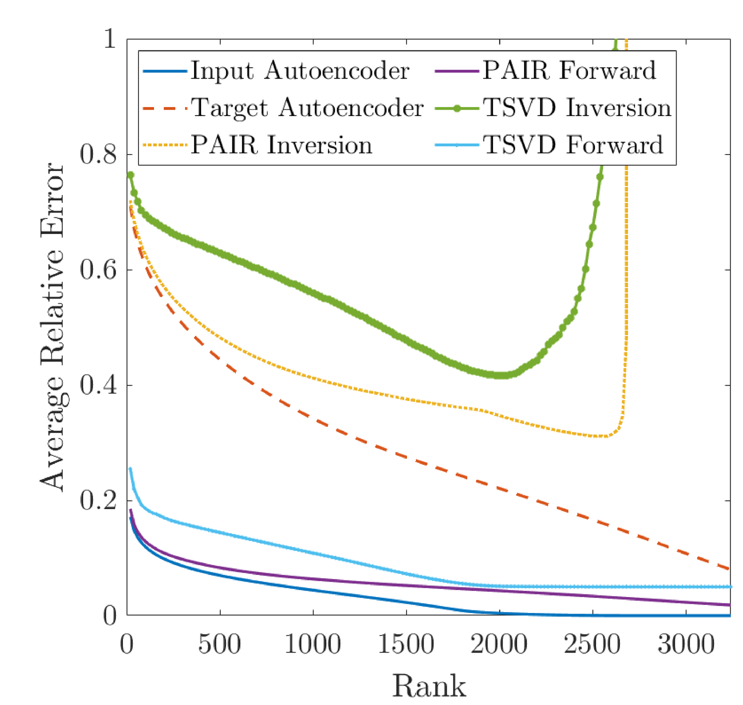


Inputs:

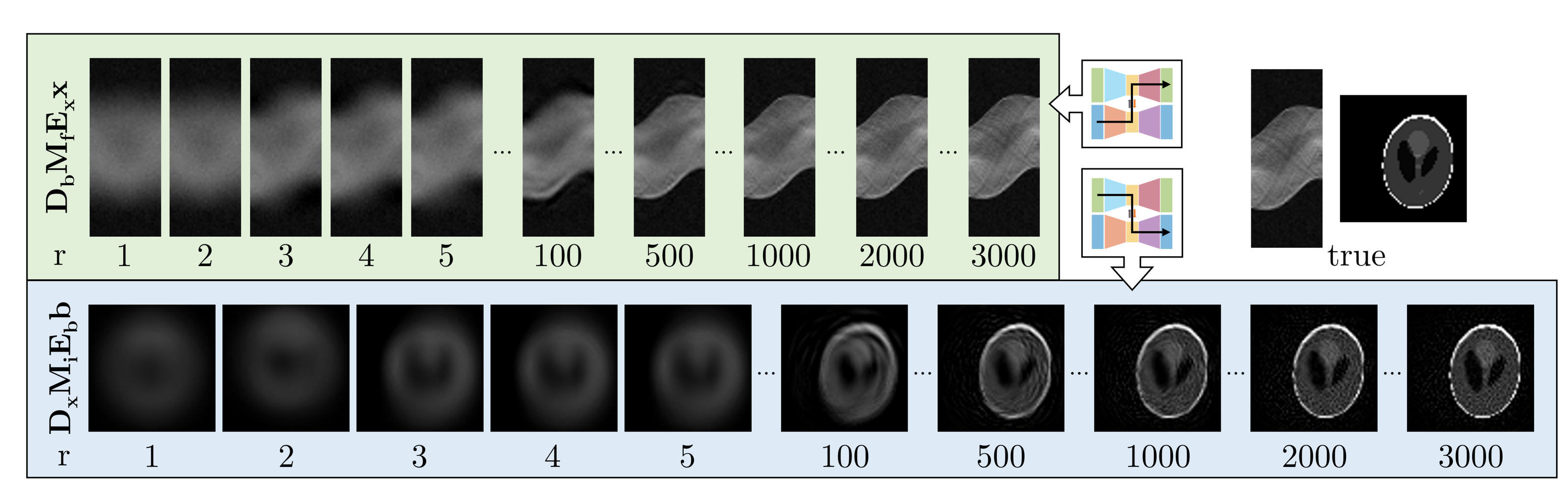
- Sinogram observations with 5% noise
- 90×36 pixels, vectorized to $\mathbf{b} \in \mathbb{R}^{3240}$

Targets:

- Randomized Shepp Logan Phantoms, representing brain anatomy
- 64×64 pixels, vectorized to $\mathbf{x} \in \mathbb{R}^{4096}$



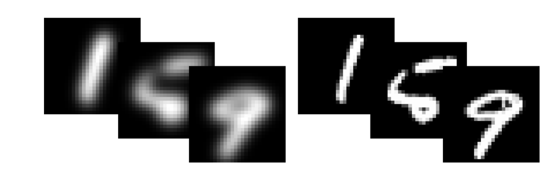
Average relative error norms for test dataset comparing autoencoders, PAIR approximations, and TSVD approximations for inversion and forward propagation.



Linear PAIR approximations for different sized latent spaces. Note that $r_\mathbf{x}$ and $r_\mathbf{b}$ are not required to be equal, but in this case we take $r_\mathbf{x} = r_\mathbf{b} = r$.

Nonlinear PAIR for Deblurring Example

MNIST Deblurring Example:



Inputs:

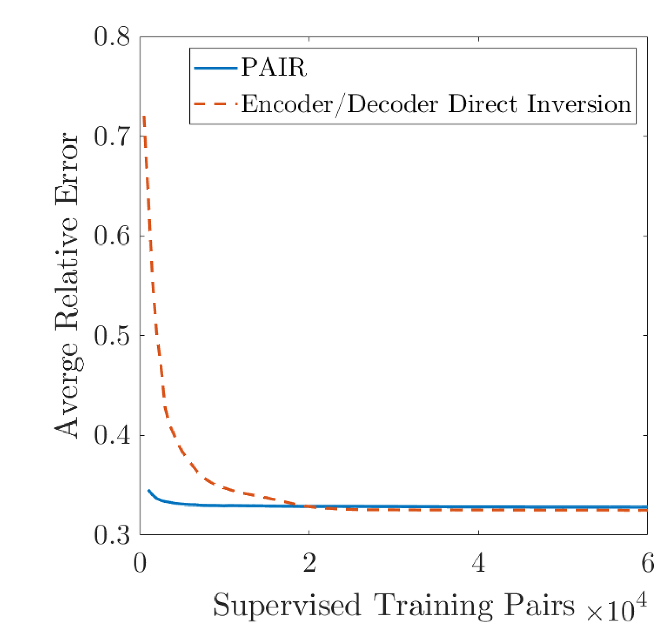
- Blurred (Gaussian) MNIST digits
- 28×28 pixels

Targets:

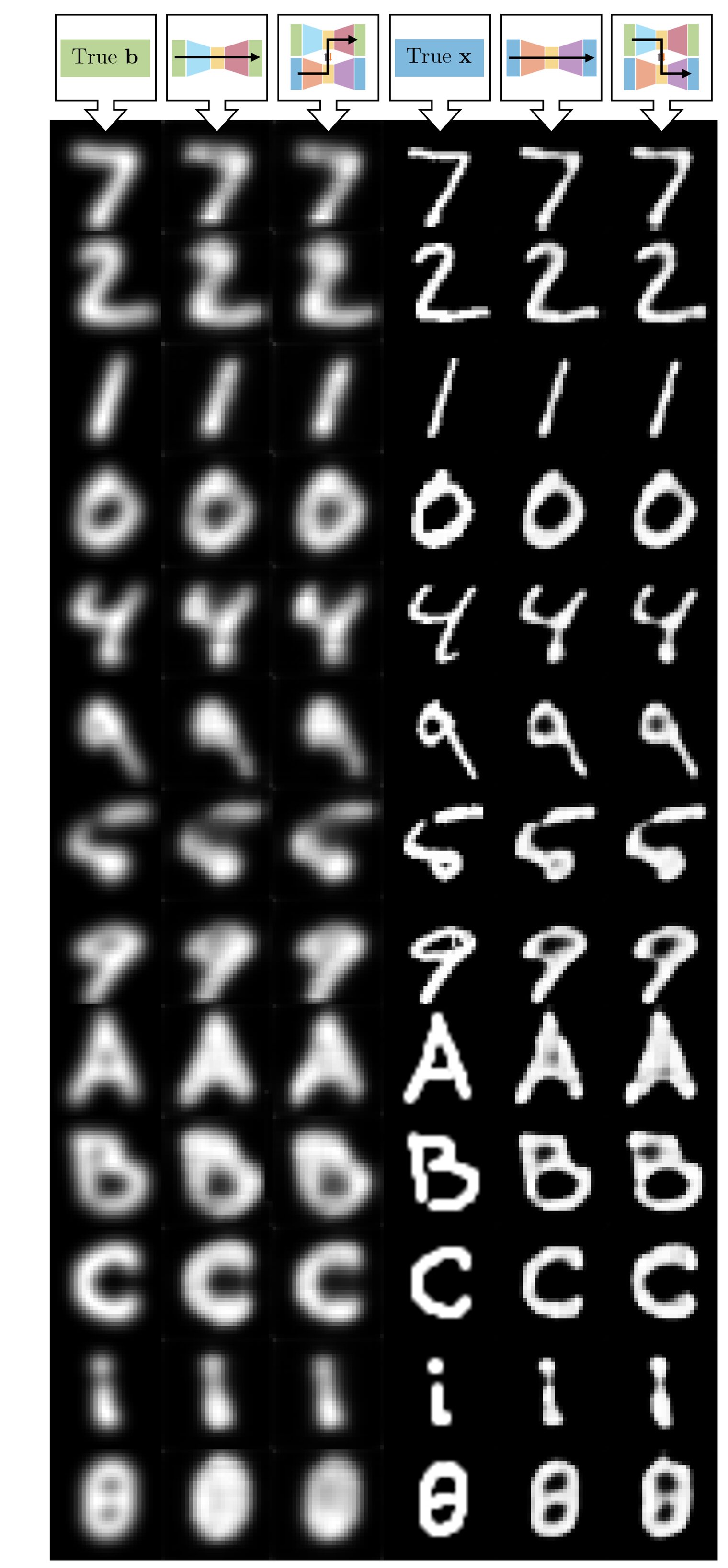
- Original MNIST digits
- 28×28 pixels

Autoencoder Architecture:

- 5 layer CNN, 236 parameters
- $\mathbf{z}_\mathbf{b}, \mathbf{z}_\mathbf{x} \in \mathbb{R}^{7 \times 7 \times 3}$
- Linear latent mappings



PAIR inversion vs encoder-decoder direct inversion for different numbers of supervised samples



Test examples and out-of-sample images

Conclusions

- PAIR is a new data-driven framework for inverse problems
- Theory for linear PAIR exploits a low-rank SVD approximation with inherent regularization
- Optimal linear latent maps defined for both linear and nonlinear autoencoders
- Superior for problems with many unpaired samples but few paired samples
- Numerical results show generalizability

Future Applications of PAIR:

- Approximate adjoints
- Define new data-driven priors (e.g., approximate mean and prior covariance)
- Create surrogate models using a reduced model for forward propagation of dynamical systems

References

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Acknowledgements

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