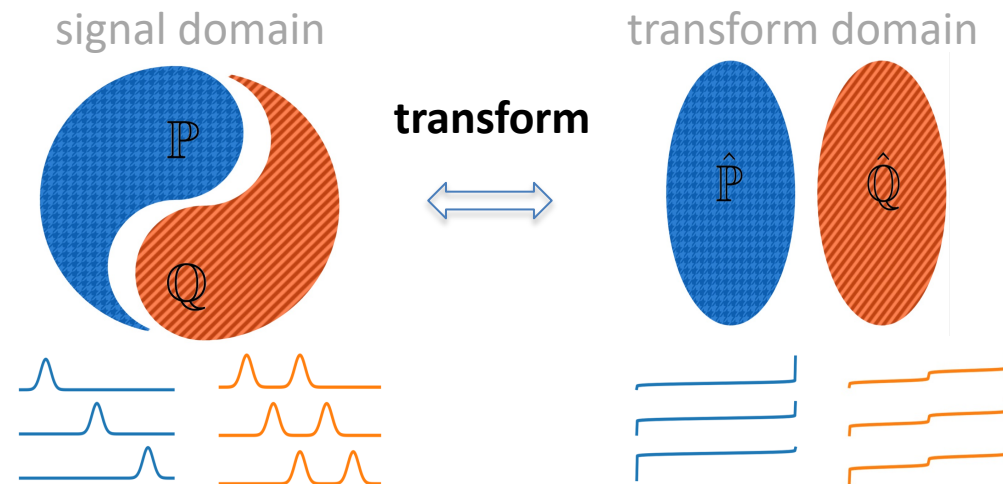


Transport transforms for signal analysis and machine learning: applications

Gustavo K. Rohde

Imaging and Data Science Laboratory

imagedatascience.com/transport
github.com/rohdelab/PyTransKit



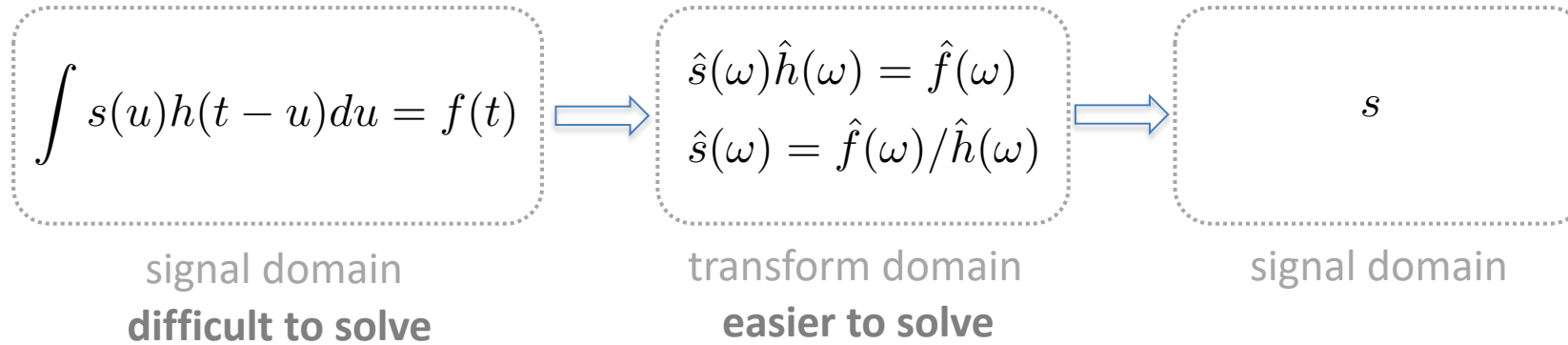
Fourier transform:

forward

$$\hat{s}(\omega) = \int s(t) e^{-j\omega t} dt$$

inverse

$$s(t) = \frac{1}{2\pi} \int \hat{s}(\omega) e^{j\omega t} d\omega$$



New signal transform:

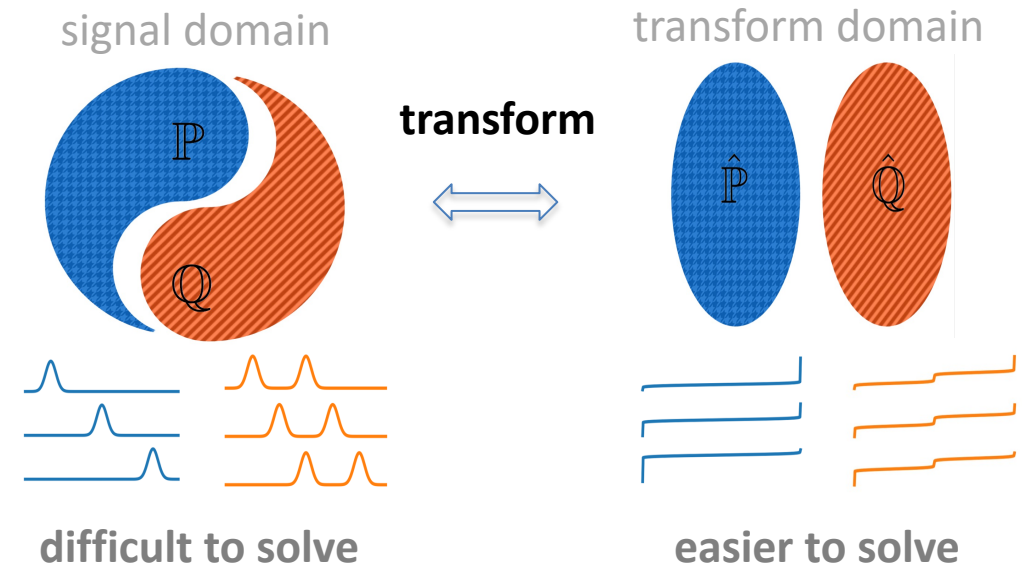
CDT,
SCDT
R-CDT
LOT

forward

$$\hat{s}(x) := S^{-1}(x)$$

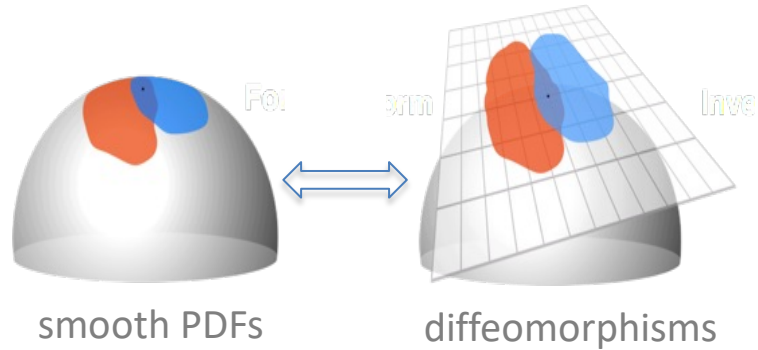
inverse

$$s(t) = \frac{d}{dt}(\hat{s})^{-1}$$



Summary: Transport & other Lagrangian Transforms

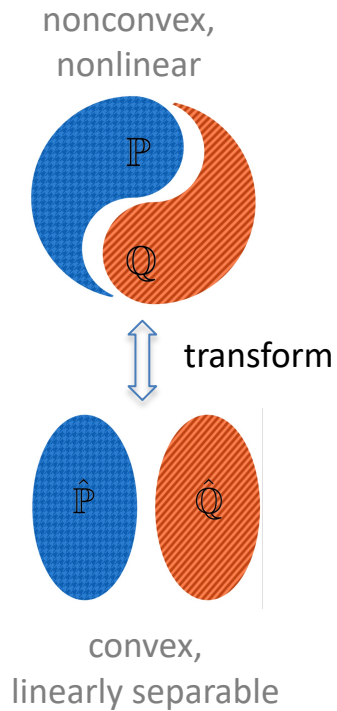
Nonlinear signal transform



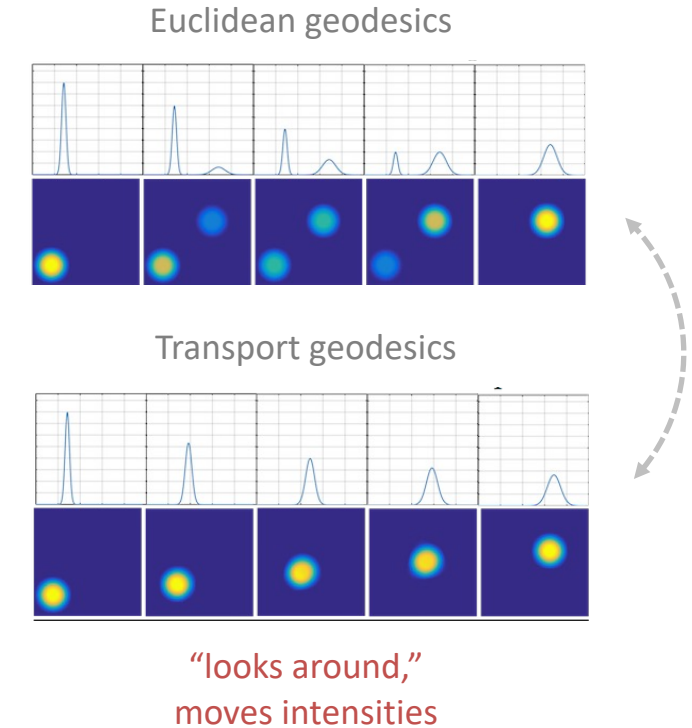
(LOT, CDT, R-CDT):

invertible transform framework for
Lagrangian modeling of signals & images
Connections to optimal transport

Properties



Intuition



Imagedatascience.com/transport

Topics covered

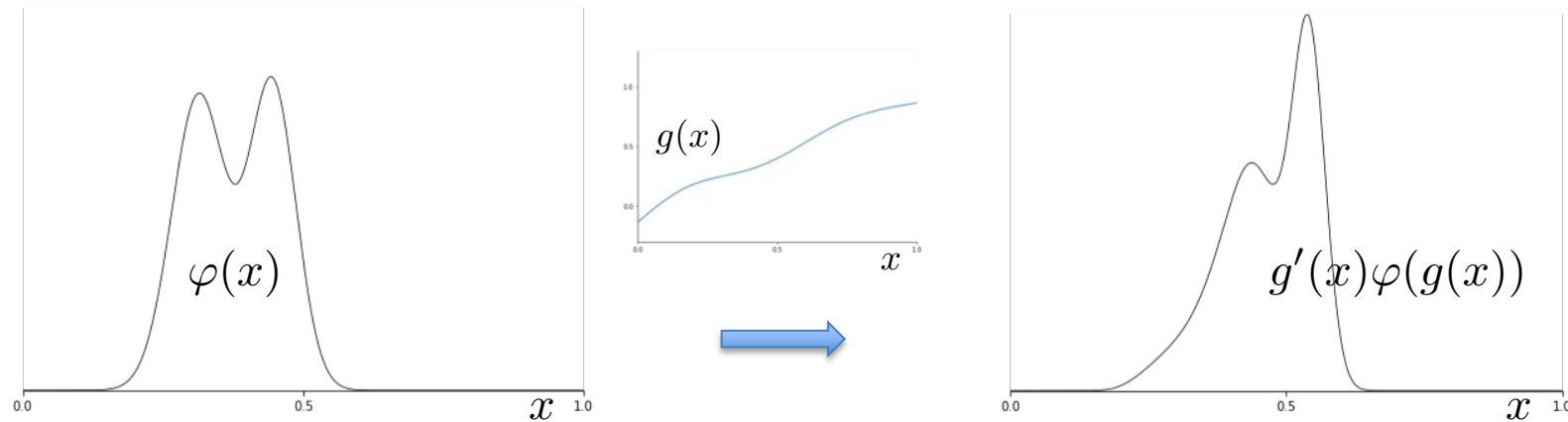
- Optimal transport overview
- Representing signals/images with transport transform/embeddings
- Applications
 - Nonlinear signal estimation
 - Model-based inverse problems
 - Transport-based morphometry (TBM)
 - Machine learning (e.g. classification)
- Summary

Outline

- **Motivation**
 - Transport-like processes
 - Nonlinear systems
- **Estimation**
 - Model training, parameter estimation
 - Inverse problems
- **Transport-based morphometry**
 - Cells, tissues, organs, faces, communications
 - Classification

Motivation

Model for signal/image deformations (transportations)



Translation:

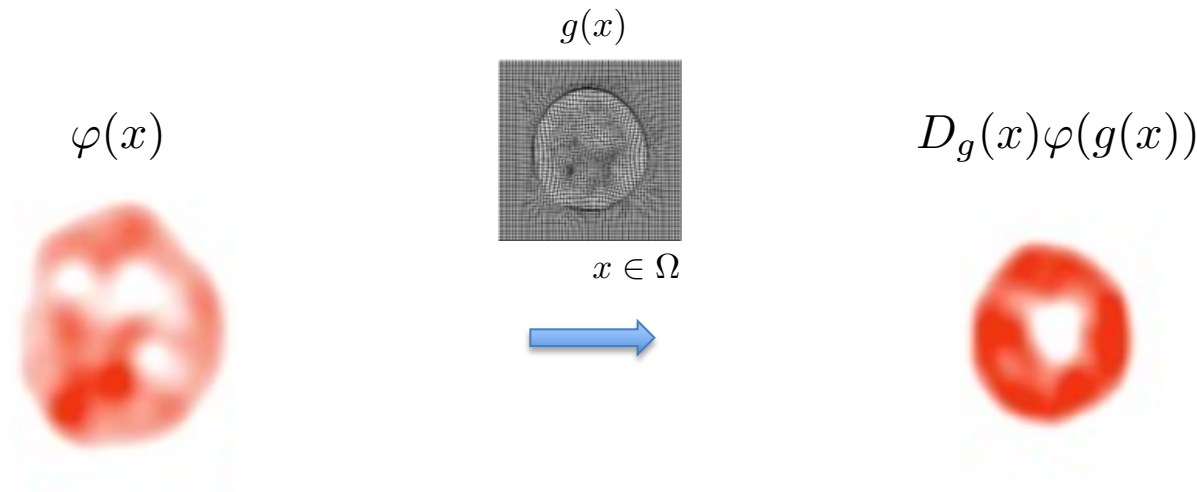
$$g(x) = x - \tau$$

Scaling:

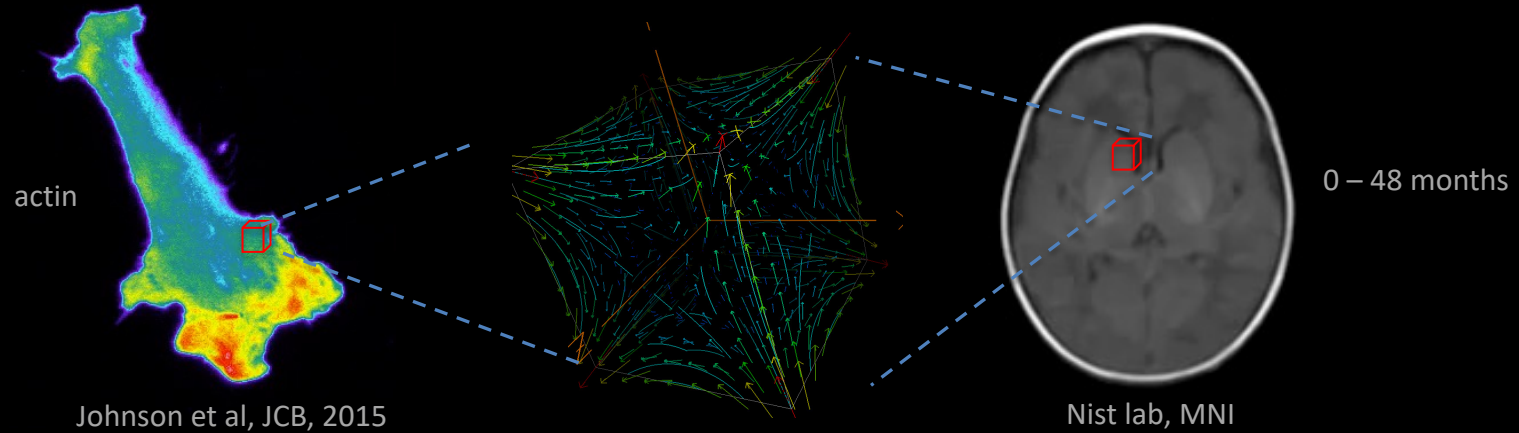
$$g(x) = ax$$

Nonrigid deformations:

$$g(x) = \sum_k c_k \phi_k(x)$$



What processes change signal/pixel intensity over time?



continuity equation

$$\underbrace{\frac{dI(x, y, z, t)}{dt}}_{\text{change in intensity at particular location}} = - \underbrace{\nabla \cdot (I(x, y, z, t) \mathbf{v}(x, y, z, t))}_{\text{net flux tissue velocity}} + \underbrace{\cancel{S(x, y, z, t)}}_{\text{source/sink term}}$$

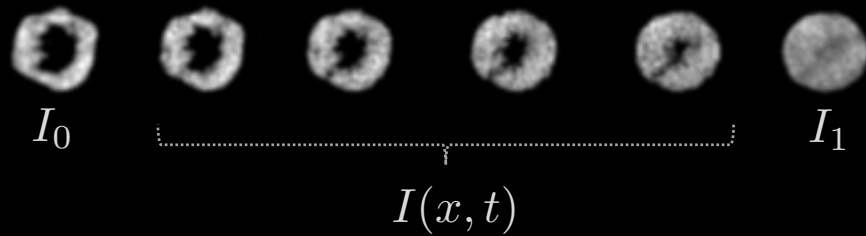
intensities not absolute

change in intensity at
particular location

net flux
tissue velocity

source/sink term

Transport with least action (optimal transport)



$$\left. \begin{array}{l} I(x, 0) = I_0(x) \\ I(x, 1) = I_1(x) \end{array} \right\} \begin{array}{l} \text{sample images} \\ \text{in a dataset} \end{array}$$

$$\frac{dI(x, t)}{dt} = -\nabla \cdot (I(x, y)v(x, t)) \quad \text{implies}$$

$$I(x, t) = D_f(x)I_0(f(x, t))$$

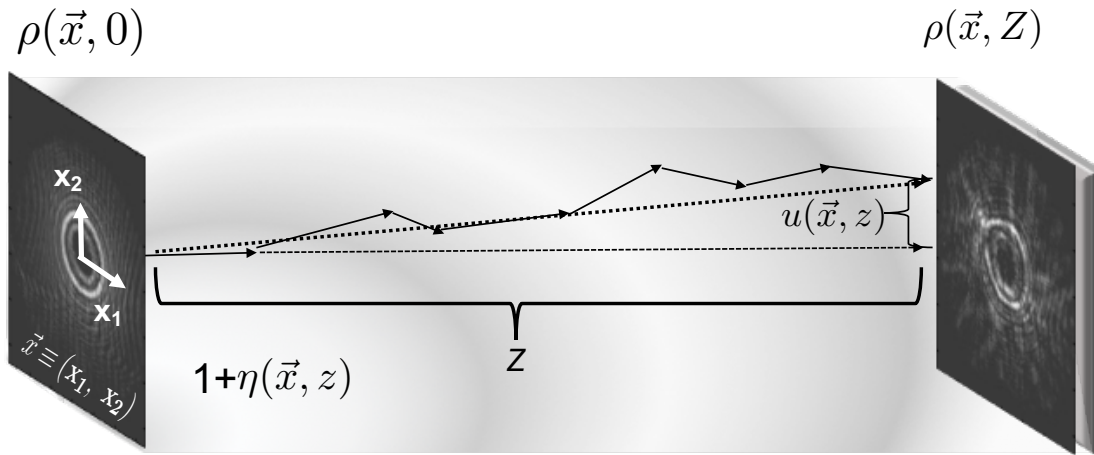
$$f(x, t) = \int_0^t v(x, t)dt$$

Theorem: [Benamou, Brenier, Numer. Math, 2000]

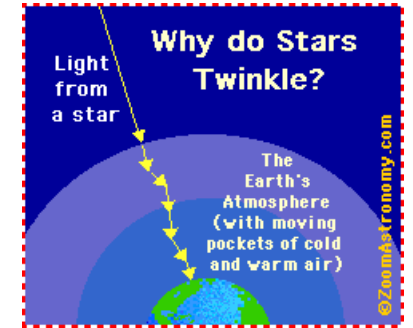
$$W^2(I_0, I_1) = \inf_v \int_0^1 \int_{\Omega} I(x, t)|v(x, t)|^2 dx dt$$

$$f(x, t) = (1 - t)x + t\nabla\phi \quad \text{gradient of convex function}$$

Modeling light propagation in turbulence



Light propagation path under turbulence



$$\frac{\partial \rho(\vec{x}, z)}{\partial z} + \nabla_X \cdot (\rho(\vec{x}, z) v(\vec{x}, z)) = 0$$

Continuity eq.

$$\frac{\partial v(\vec{x}, z)}{\partial z} + (v(\vec{x}, z) \cdot \nabla_X) v(\vec{x}, z) = 2 \nabla_X g(\eta(\vec{x}, z)).$$

Momentum eq.

$\rho(\vec{x}, z)$: magnitude of the EM field

$v(\vec{x}, z)$: velocity in the transverse plane

$u(\vec{x}, z)$: displacement in transverse plane

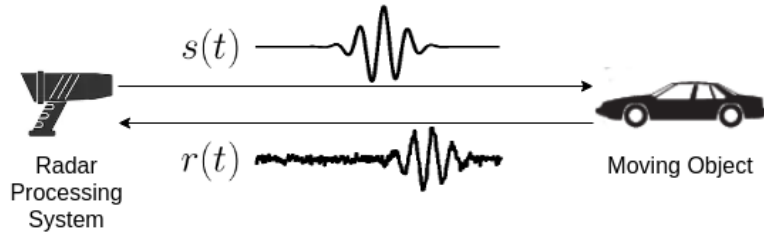
$\eta(\vec{x}, z)$: refractive index

Nichols, Emerson, Rohde, Journal of Modern Optics, 2019.

Nichols, Emerson, Cattell, Park, Kanaev, Bucholtz, Watnik, Doster, GK Rohde, Applied Optics, 2018

Model/parameter estimation

Parametric signal estimation



Static object: $r(t) = s(t - \tau) + \eta(t)$

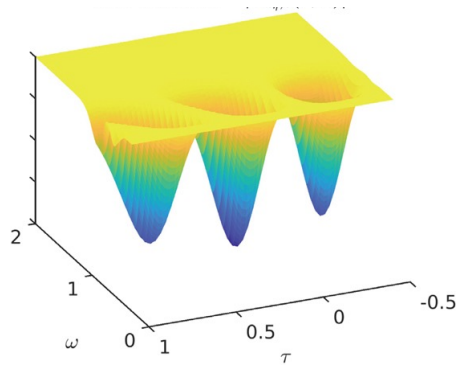
$$g_p(t) = \omega t - \tau$$

Moving object: $r(t) = s(\omega t - \tau) + \eta(t)$

Traditional approach:

$$A_{r,s}(\tau, \omega) = \sqrt{\omega} \int r(t) s(\omega t - \tau) dt$$

$$\arg \min_{\tau, \omega} -|A_{r,s}(\tau, \omega)|$$

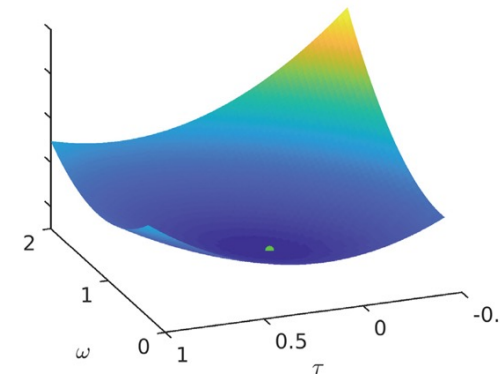


computationally expensive
global optimization required

Wasserstein minimization

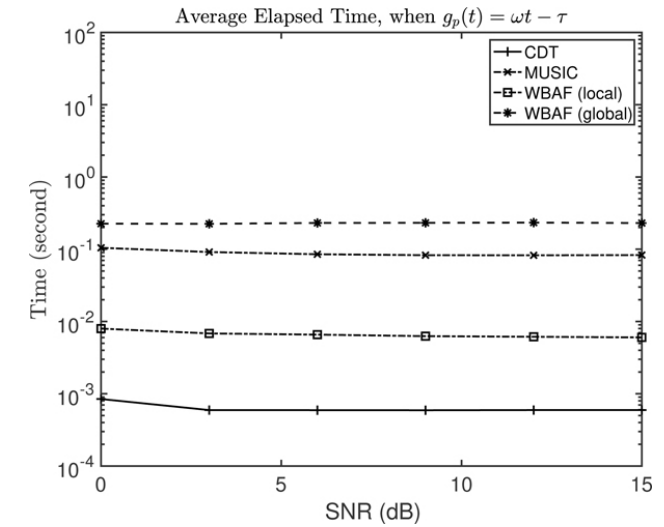
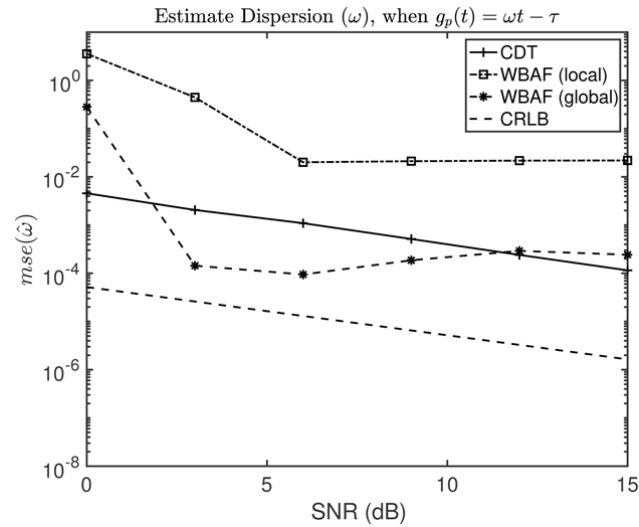
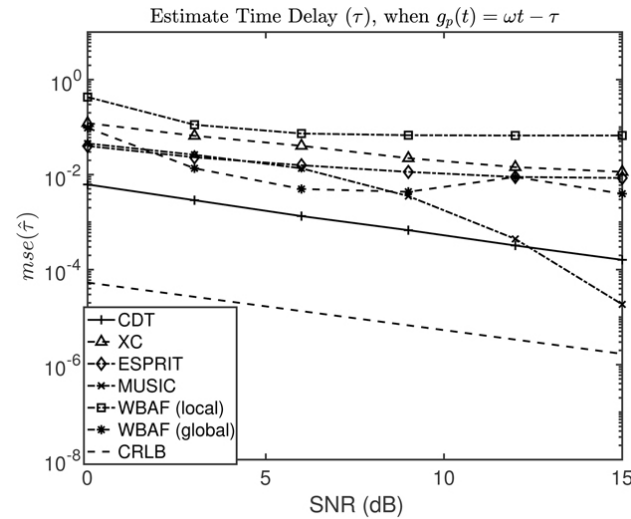
$$W^2(r, s) = \|\omega \hat{r} - \tau - \hat{s}\|^2$$

$$\arg \min_{\tau, \omega} \|\omega \hat{r} - \tau - \hat{s}\|^2$$



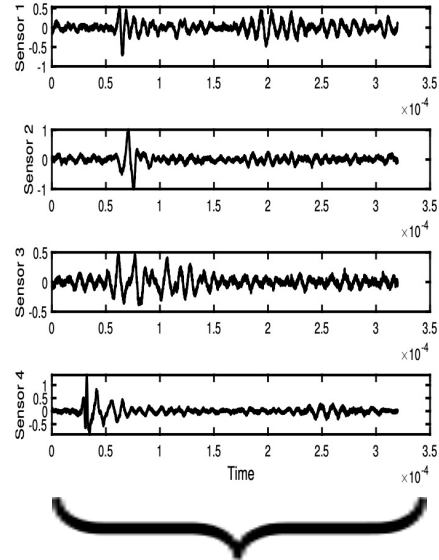
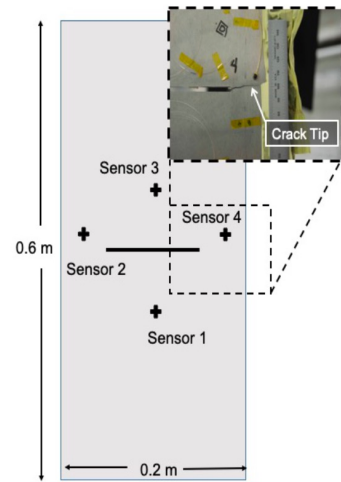
linear least squares
cheap to compute

Parametric signal estimation



orders of magnitude cheaper to compute

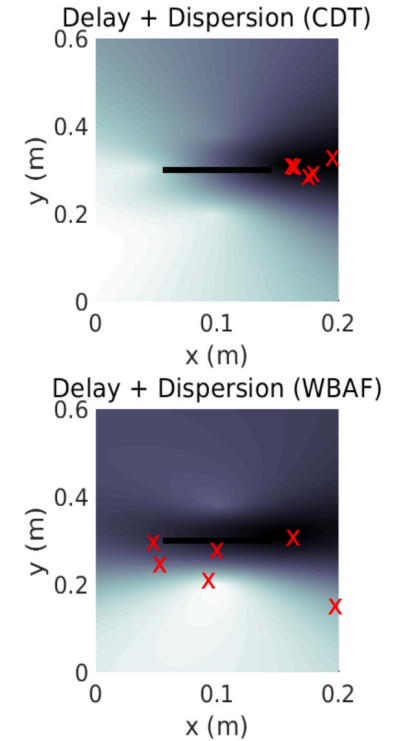
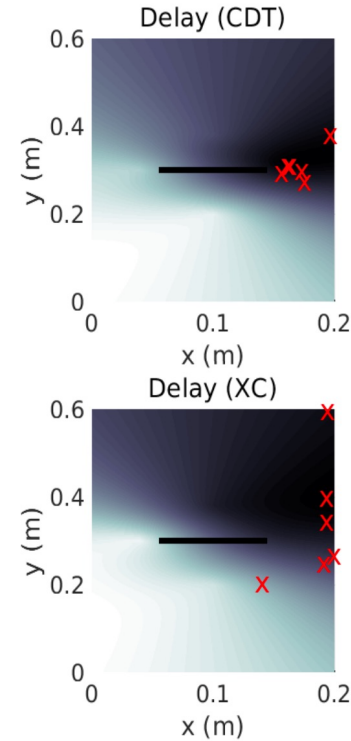
Parametric signal estimation in structural health monitoring



Crack localization



Estimate
TDOA in
CDT
domain



Model-based inverse problems

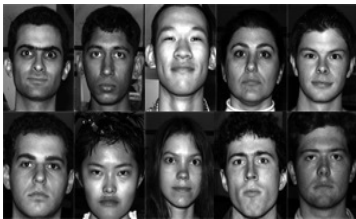
Enhancing an image

Find model parameters that best match data

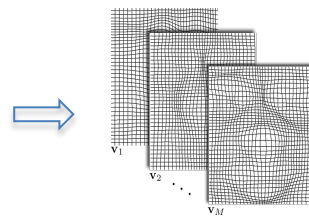


Modeling phase

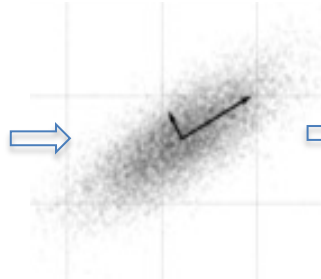
sample database



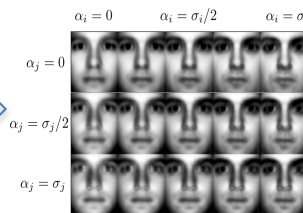
transform



PCA



model



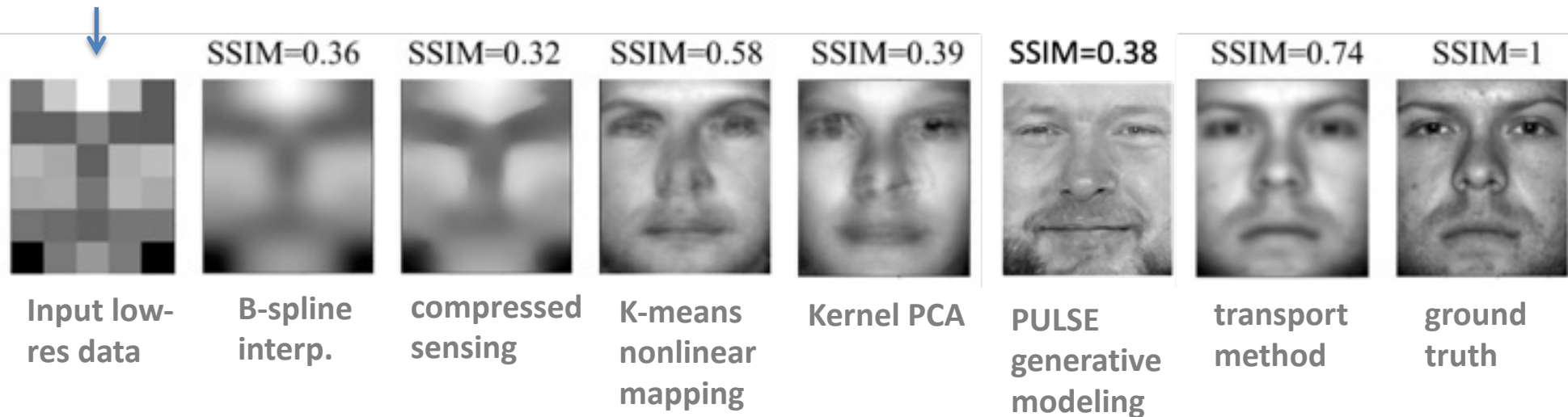
Model: $M_\alpha = D_{f_\alpha}(x)I_0(f_\alpha(x)) \quad f_\alpha(x) = \sum_k \alpha_k \phi_k(x)$

Fit: $\min_\alpha \|I - \underset{\text{degradation}}{V} M_\alpha\|^2$

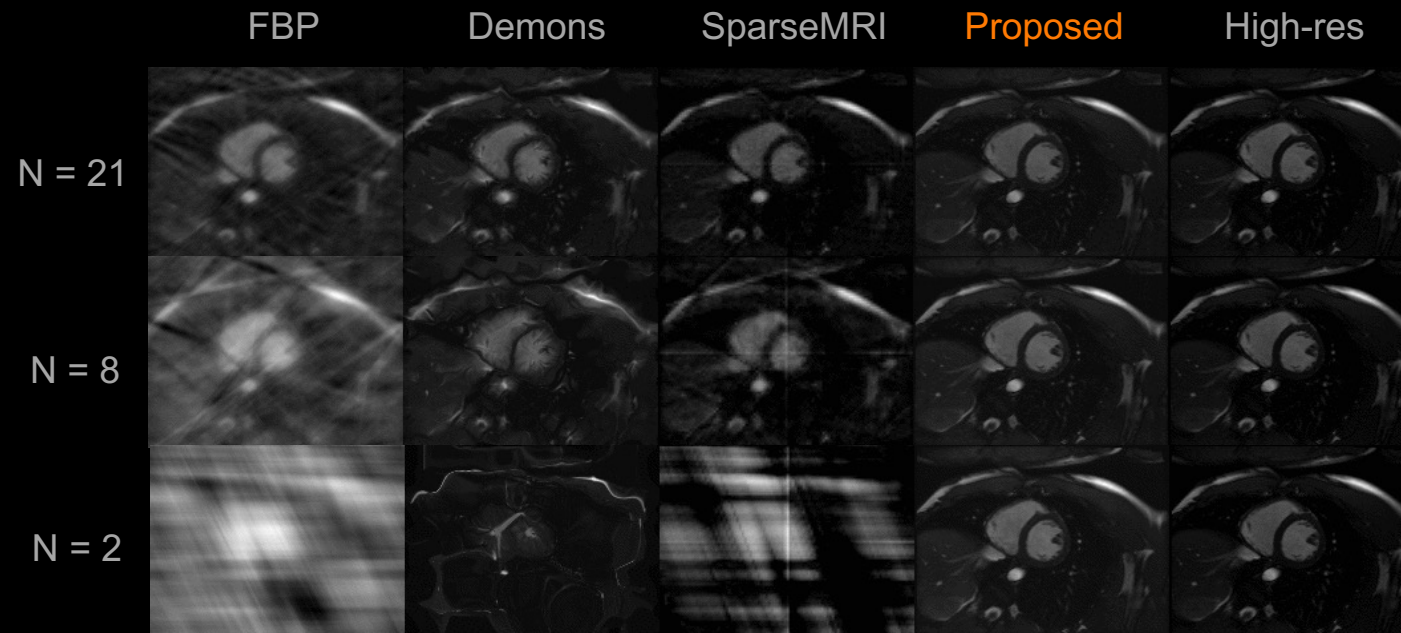
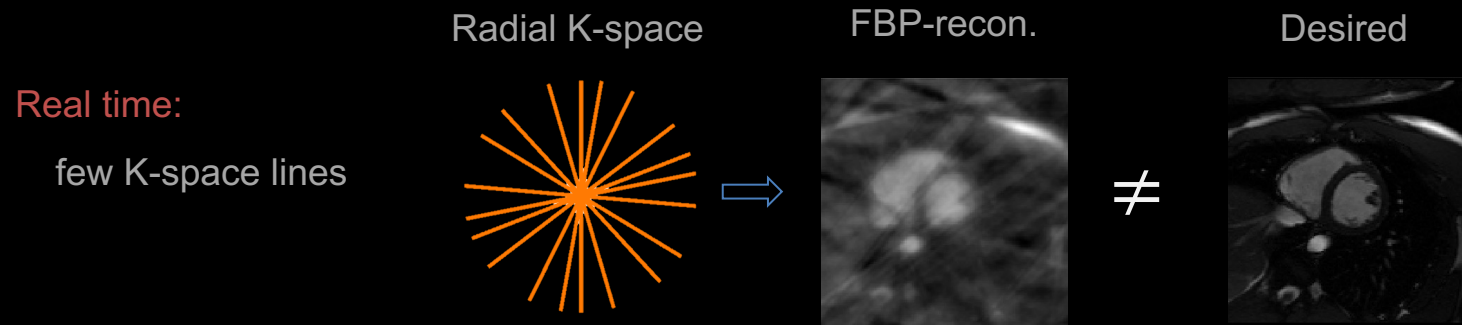
low-res data

Transport PCA trained on high res database

5x6 pixels!



Application: real time cardiac MRI



[Cattell, Meyer, Epstein, Rohde, IEEE Asilomar 17]

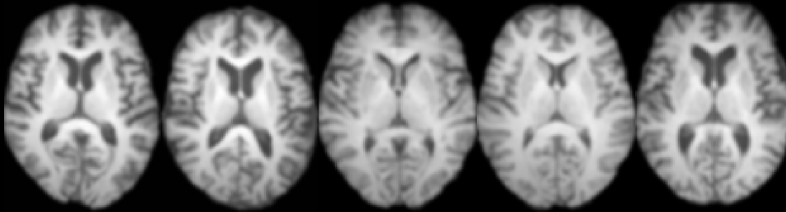
Transport-based Morphometry (TBM)

Biomedical image data science

Are fitness and gray matter morphology related?

Class 1:

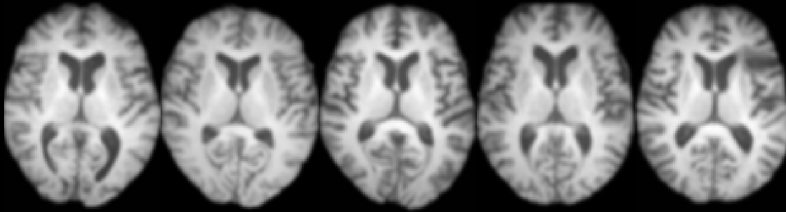
persons with low
fitness index



magnetic
resonance
imaging (MRI)

Class 2:

persons with high
fitness index



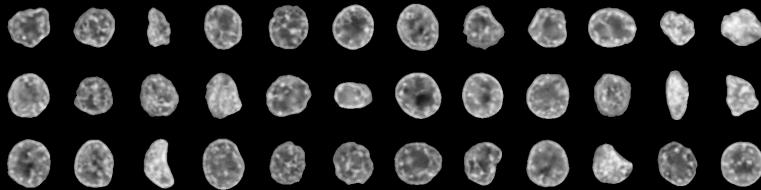
Hypothesis testing

Are there differences?

Is nuclear morphology related to cancer?

Class 1:

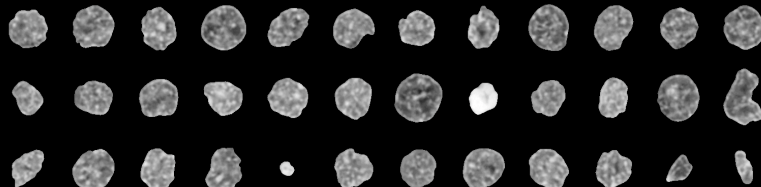
nuclei from
benign tissues



digital pathology
(microscopy)

Class 2:

nuclei from
malignant tissues

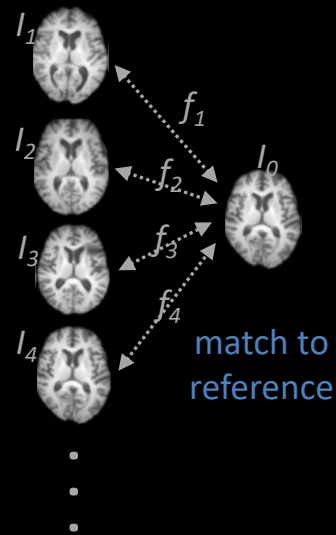


Understanding

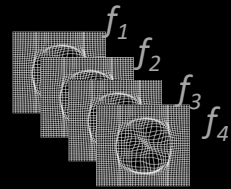
If so, can we model them?

Transport-based morphometry (TBM)

1) Transform



transport maps



2) regression

modeling variations

- PCA, least squares, ...

modeling differences

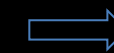
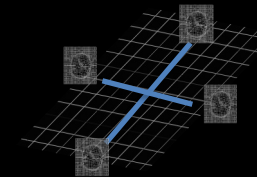
- LDA, SVM, ...

modeling relationships

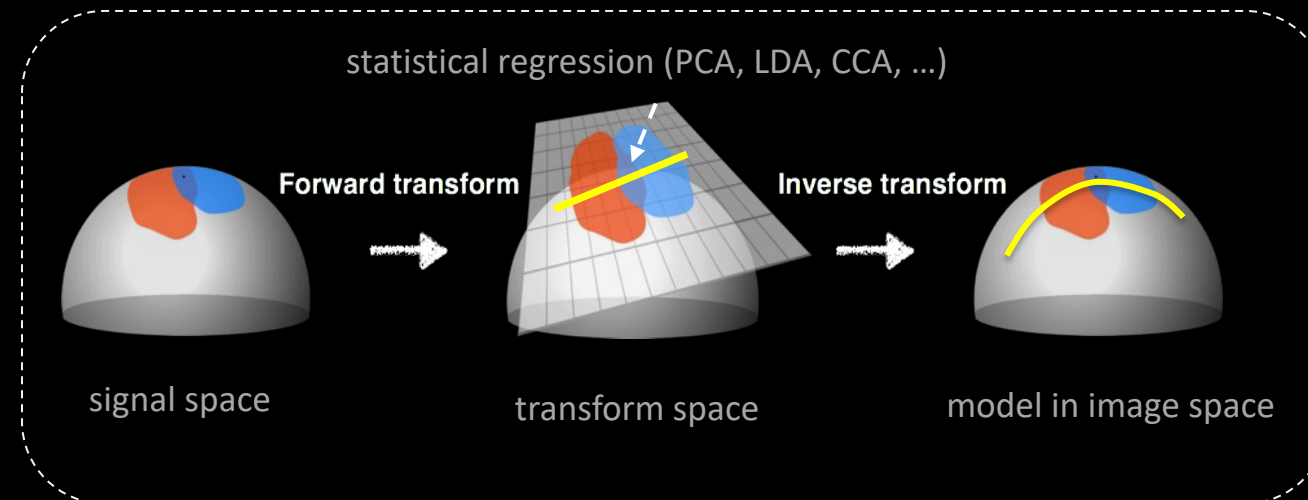
- CCA, ...

3) Inverse transform

PCA, LDA, CCA, ...



visualization

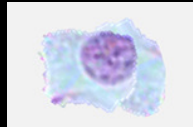
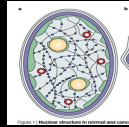


Example: nuclear structure in cancer

Aberrations in genetic
code and/or increase in
transcriptional activity



Unfolding/repackaging
of chromatin → change
in nuclear configuration

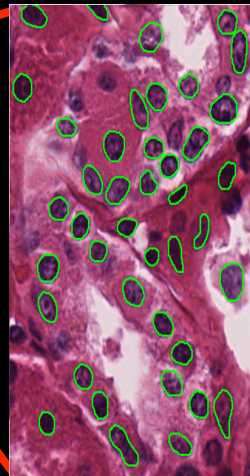
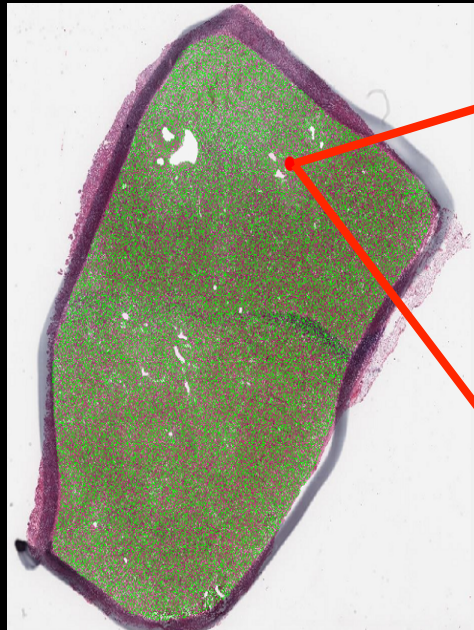


normal



cancer

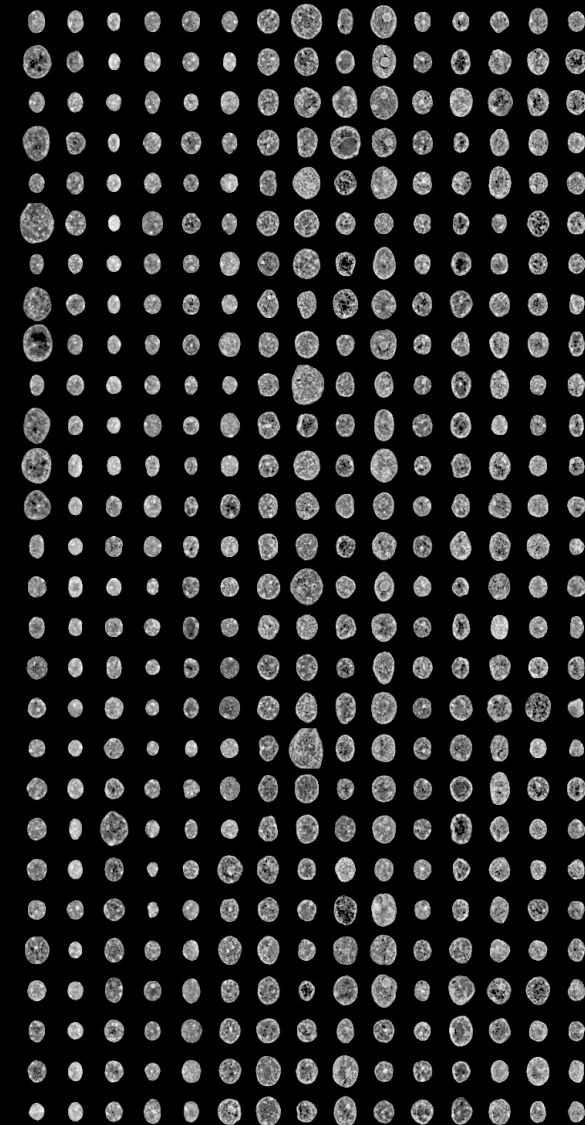
Pathology, whole slide imaging



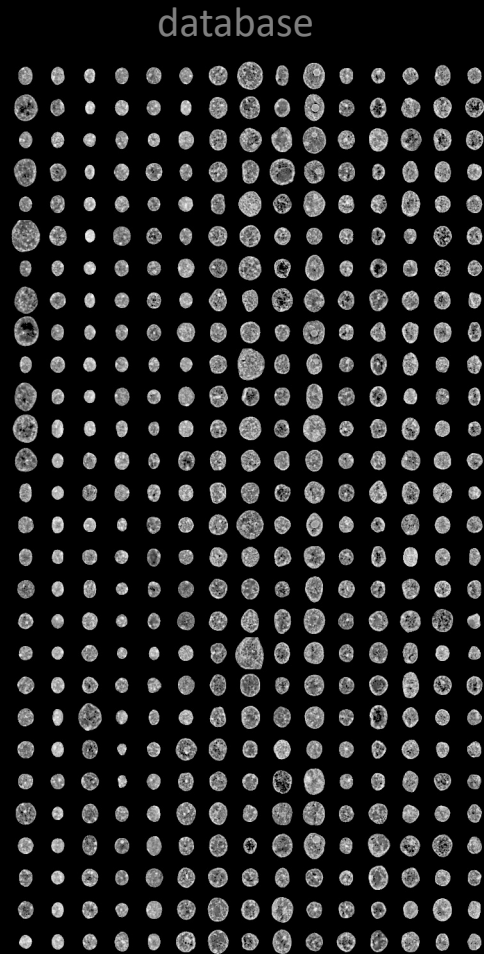
segmentation



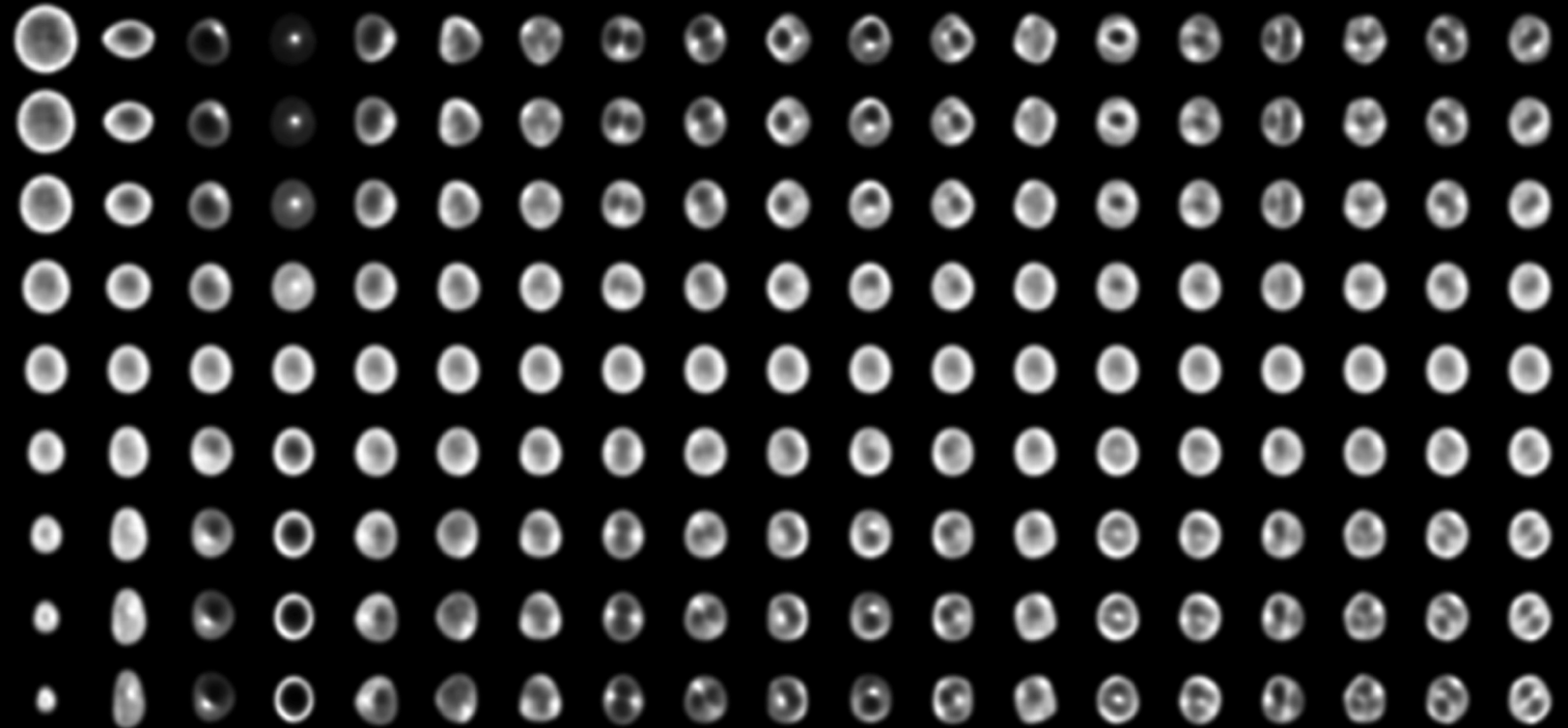
segmented nuclei



Exploratory analysis: PCA on transport maps



Modeling chromatin variation in liver cancer (shape + texture)



learned "features"

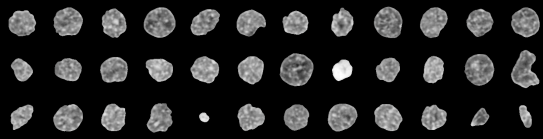
$$D_{f_\alpha^{-1}}(x)s_0(f_\alpha^{-1}(x))$$

$$f_\alpha(x) = \underbrace{f(x)}_{\text{mean}} + \alpha w(x) \leftarrow \text{PCA eigenvector}$$

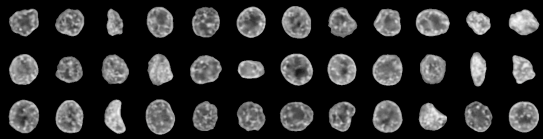
TBM: modeling discriminant information

[Basu et al, PNAS 2014]

Class 1: benign cells

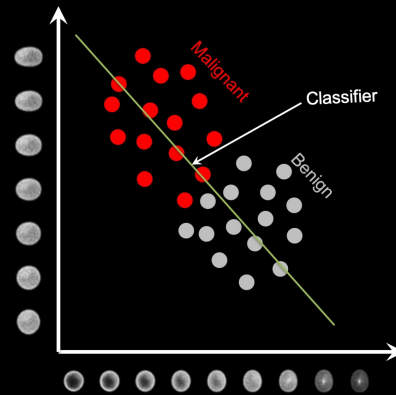


Class 2: malignant cells



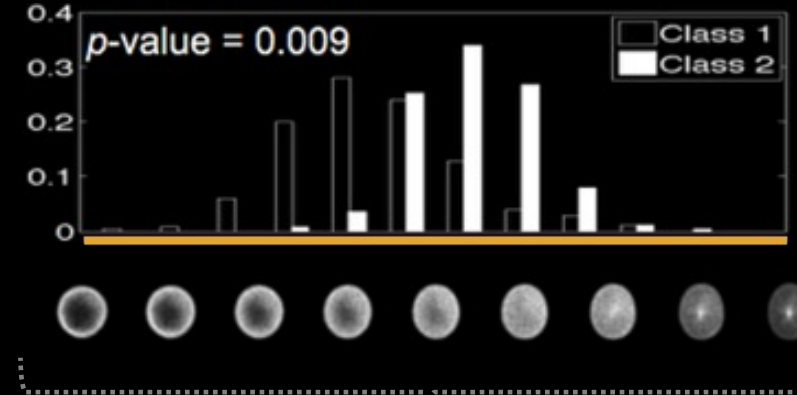
forward
→

LDA in transport space



inverse
→

Fetal-type hepatoblastoma



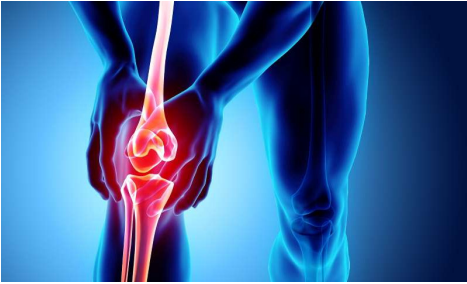
Inverse of classification function

$$D_{f_{\alpha}^{-1}}(x) s_0(f_{\alpha}^{-1}(x))$$

$$f_{\alpha}(x) = \underbrace{f(x)}_{\text{mean}} + \alpha w(x)$$

← classifier

TBM in early detection of osteoarthritis (OA)

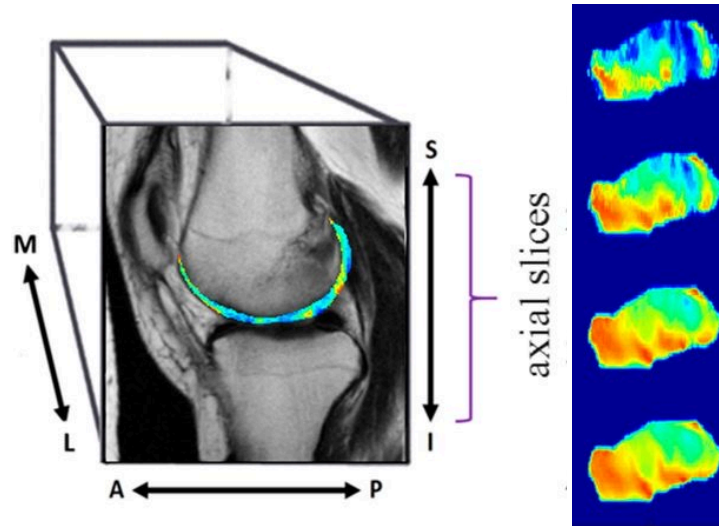


- OA affects 1 in 4 adults.
- Today OA is diagnosed at an irreversible stage.
- Diagnosis requires X-ray confirmation of bone damage.
- Early detection could prevent further development of disease.
- Early detection could stratify patient populations for treatment discovery.

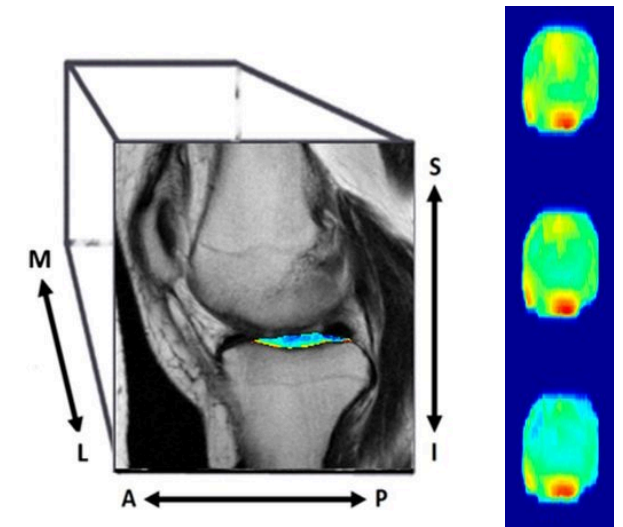
T2-MRI of knee cartilage

- water molecules
- proteoglycans
- orientation of collagen fibers

medial femoral cartilage

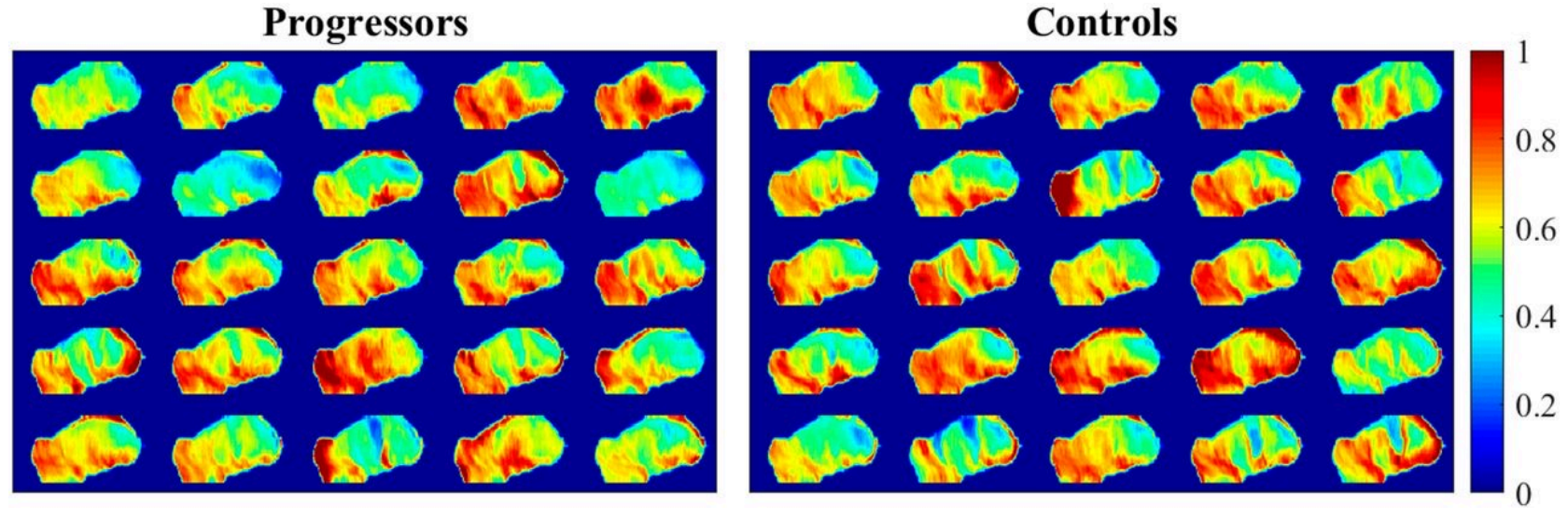


medial tibial cartilage



TBM in early detection of osteoarthritis (OA)

Images acquired 3 years prior to symptoms



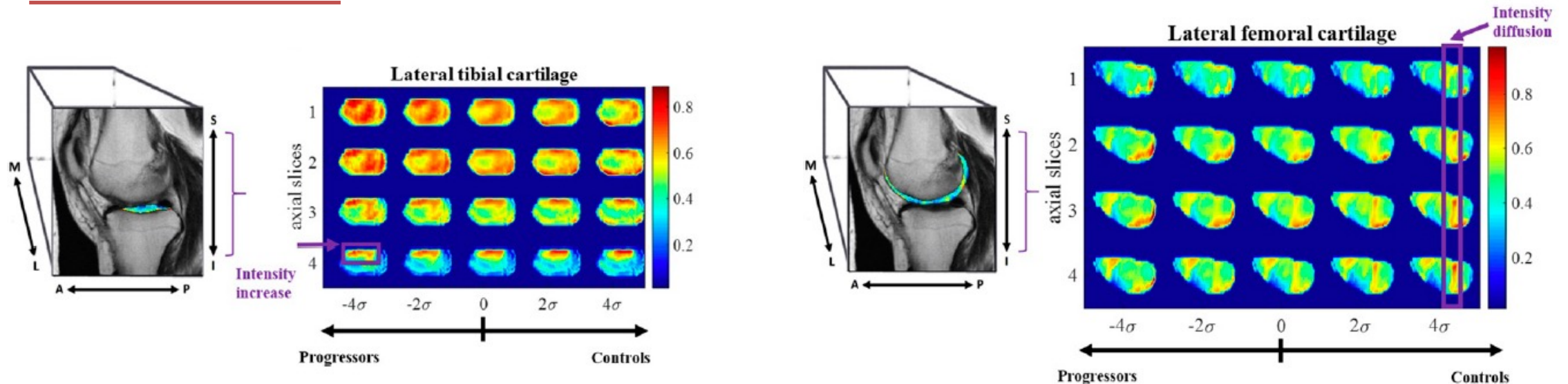
Can we predict which ones will progress to be symptomatic 3 years in the future?

(ground truth diagnosis based on WOMAC score, 86 subjects)

Presymptomatic prediction accuracy

Classifier for cartilage texture maps	Test accuracy, %	Sensitivity, %	Specificity, %	Cohen's kappa	<i>P</i>
Original image pLDA	64.5	61.5	67.4	0.29	< 0.001
Original image SVM (Gaussian kernel)	63.2	65.5	60.9	0.26	<0.001
Original image RF	54.9	39.0	70.7	0.10	<0.001
TBM pLDA	78.0	76.9	79.0	0.56	<0.001
TBM SVM (Gaussian kernel)	74.1	78.0	70.2	0.48	<0.001
TBM RF	70.2	65.0	75.3	0.40	<0.001
WNDCHRM features pLDA	60.8	60.6	61.0	0.22	0.02
WNDCHRM features SVM (Gaussian kernel)	53.3	62.7	43.9	0.07	0.19
WNDCHRM features RF	55.6	48.6	62.6	0.11	<0.001

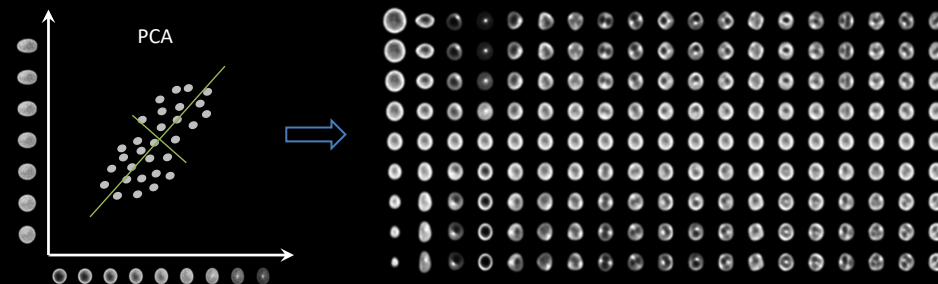
Classifier inverse:



Summary: transport-based morphometry

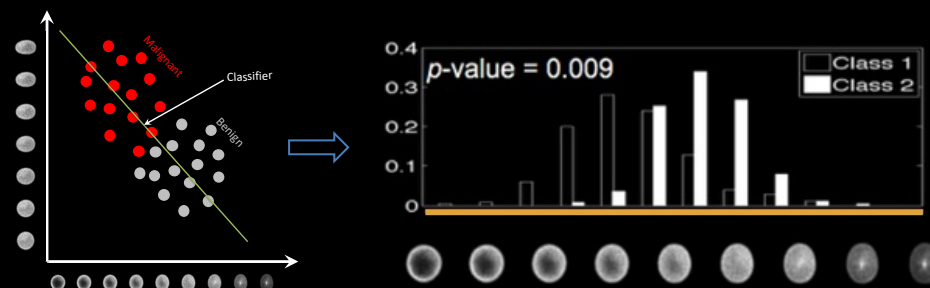
1) Exploratory analysis

- Transport PCA, subspace learning, ...
- Models texture & shape simultaneously
- Visualizes variations within dataset



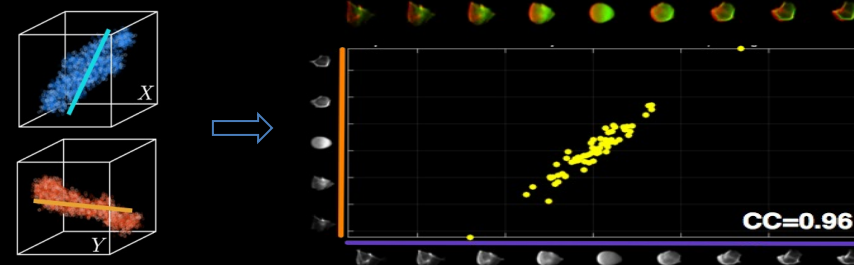
2) Discriminant models

- SVM, LDA, pLDA, ...
- Visualizes most discriminative information



3) Functional relationships

- CCA
- Study & visualize relationship between different measurements



Signa/image classification

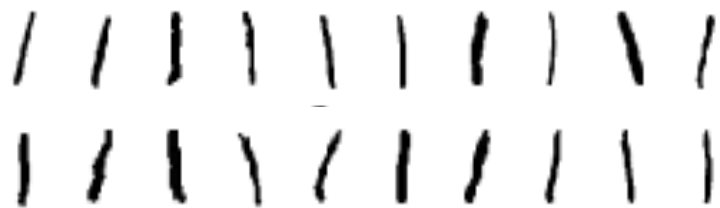
Algebraic generative model for signal/image classes

An image class is modeled as

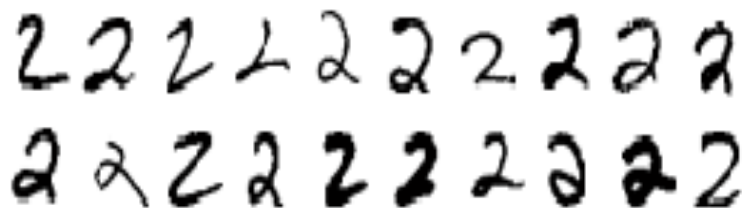
a set of transport maps $g_j \in \mathcal{G}$
 applied to a template $\varphi^{(k)}$

unknown

$\mathbb{S}^1$: class for digit 1



$\mathbb{S}^2$: class for digit 2



$$\mathbb{S}^{(1)} = \left\{ s_j^{(1)} \mid s_j^{(1)} = |\det J g_j| \varphi^{(1)} \circ g_j, \forall g_j \in \mathcal{G} \right\}$$

template for class 1 $\varphi^{(1)} = |$

“confound”

$$\mathbb{S}^{(2)} = \left\{ s_j^{(2)} \mid s_j^{(2)} = |\det J g_j| \varphi^{(2)} \circ g_j, \forall g_j \in \mathcal{G} \right\}$$

template for class 2 $\varphi^{(2)} = 2$

Model for 1D signal classes

$\mathbb{S}^{(1)}$: class for normal ECG heartbeats



$$\mathbb{S}^{(1)} = \{s_j^{(1)} \mid s_j^{(1)} = g'_j \varphi^{(1)} \circ g_j, \forall g_j \in \mathcal{G}\}$$

template for class 1: $\varphi^{(1)}$

$\mathbb{S}^{(2)}$: class for premature ventricular contraction beats



$$\mathbb{S}^{(2)} = \{s_j^{(2)} \mid s_j^{(2)} = g'_j \varphi^{(2)} \circ g_j, \forall g_j \in \mathcal{G}\}$$

template for class 2: $\varphi^{(2)}$

Problem statement (supervised learning)

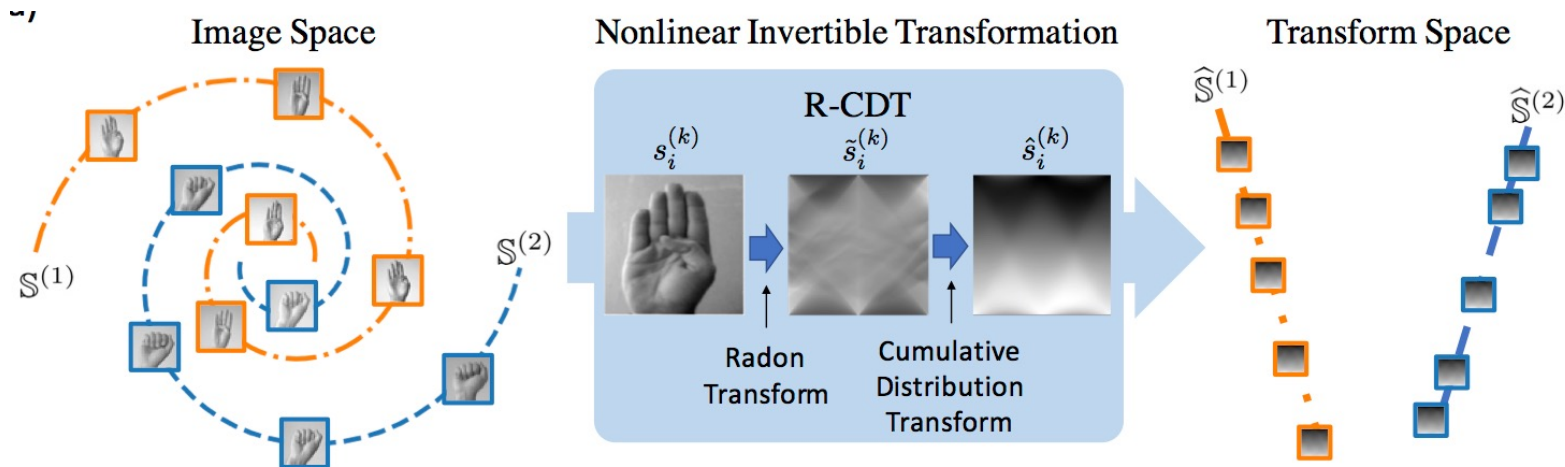
Training: given sample signals/images from different classes

$$\{s_1^{(1)}, s_2^{(1)}, \dots\} \quad s_j^{(k)} \in \mathbb{S}^{(k)} = \left\{ s_j^{(k)} \mid s_j^{(k)} = |\det J g_j| \varphi^{(k)} \circ g_j, \forall g_j \in \mathcal{G} \right\}$$

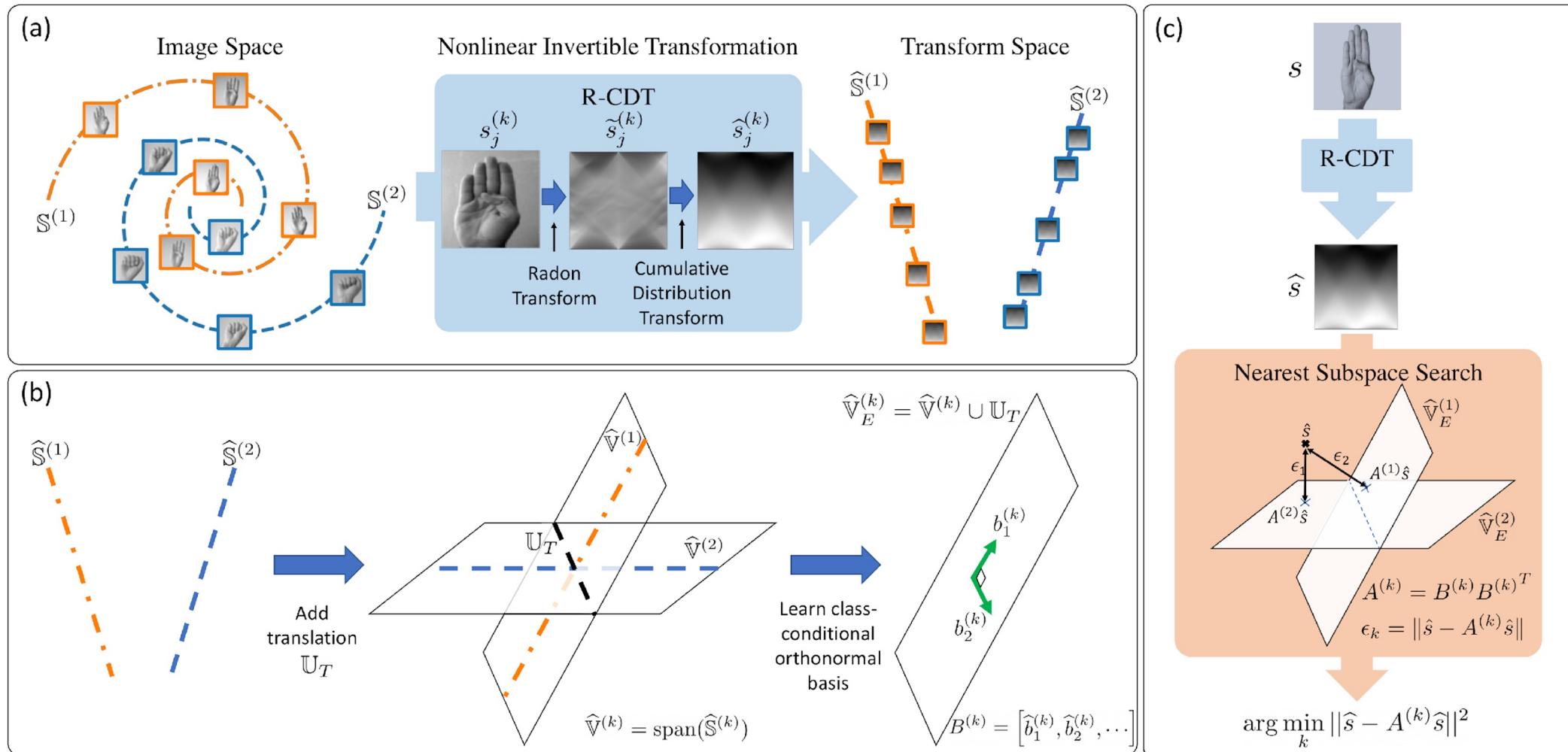
$$\{s_1^{(2)}, s_2^{(2)}, \dots\} \quad \varphi^{(k)} \text{ unknown} \\ g_j \in \mathcal{G} \text{ unknown}$$

Testing: find the class that a test sample s originated from.

Solution overview

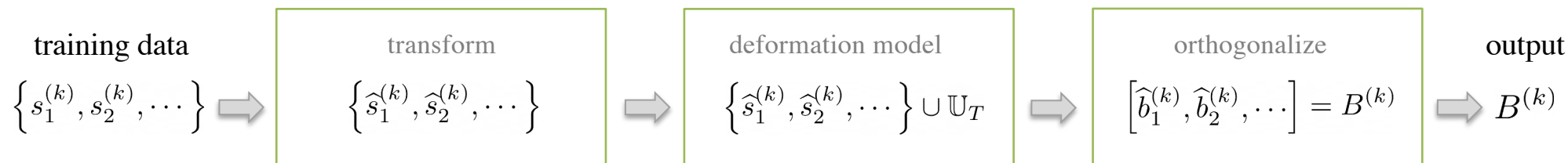


RCDT – nearest subspace

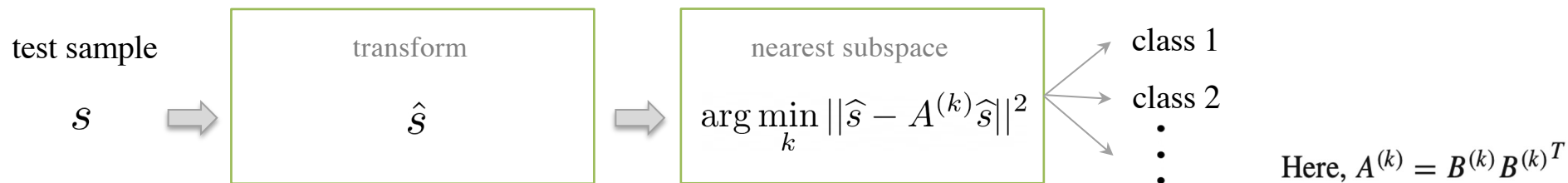


RCDT – nearest subspace

Training: estimating basis vectors for subspaces corresponding to each class



Testing : predicting the test sample as belonging to the class corresponding to the nearest subspace



Translation $\mathbb{U}_T = \{u_T^{(1)}(t, \theta), u_T^{(2)}(t, \theta)\}$, with $u_T^{(1)}(t, \theta) = \cos \theta$ and $u_T^{(2)}(t, \theta) = \sin \theta$
Isotropic scaling $\mathbb{U}_D = \emptyset$

Two important aspects of the method:

1. The method can learn from datasets
2. The method can learn from mathematically prescribed sets without explicitly using the training data

Datasets

Chinese printed character
dataset



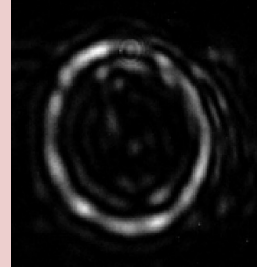
MNIST dataset



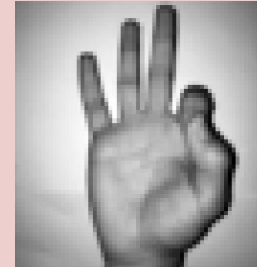
Affine-MNIST dataset



Optical OAM dataset



Sign language dataset

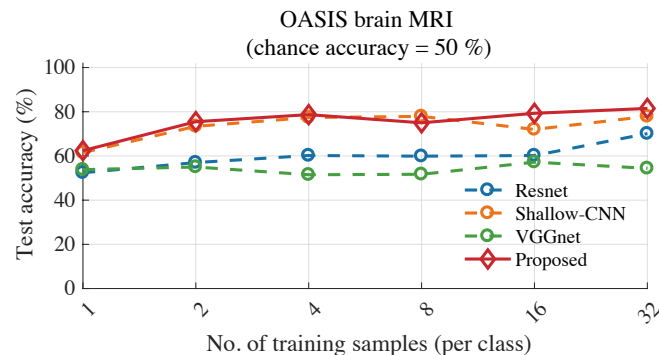
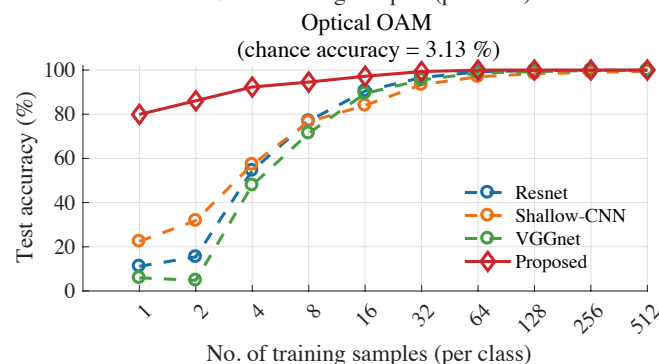
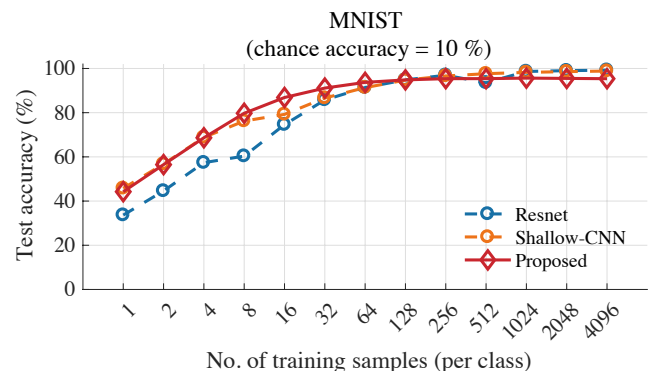
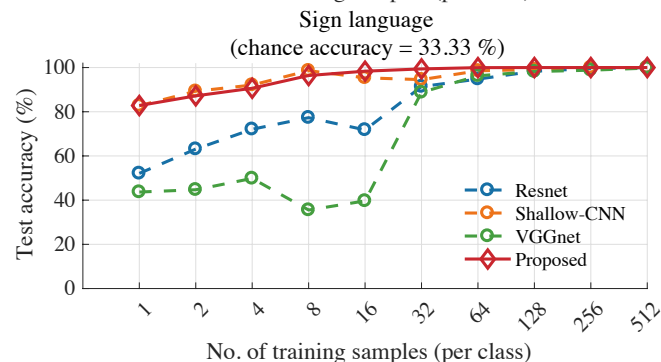
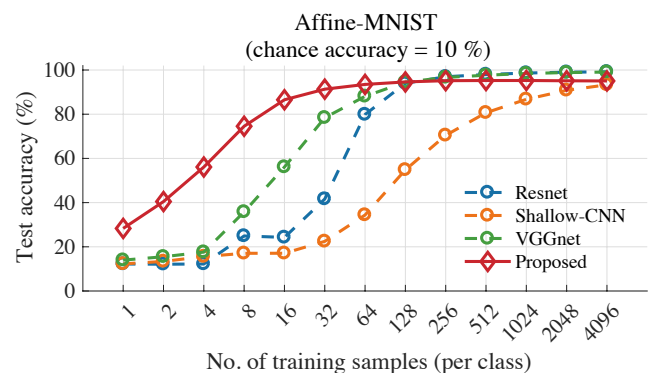
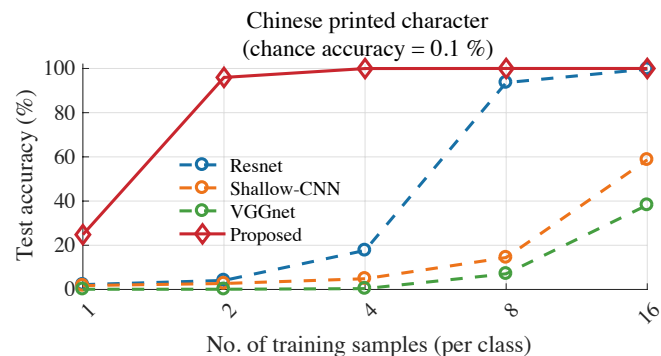


OASIS Brain MRI
dataset

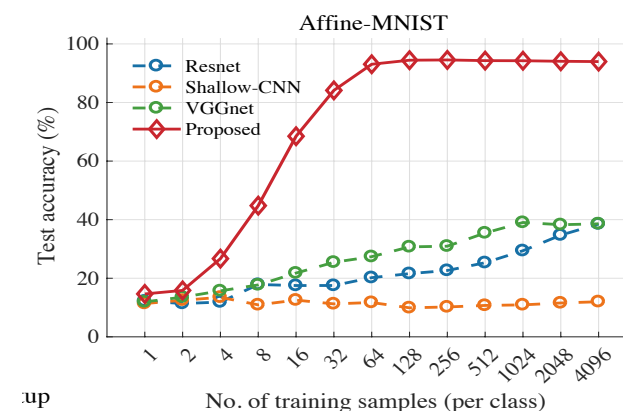
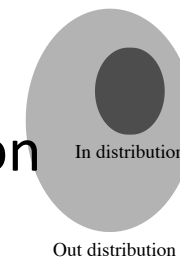


Results and comparisons with deep learning

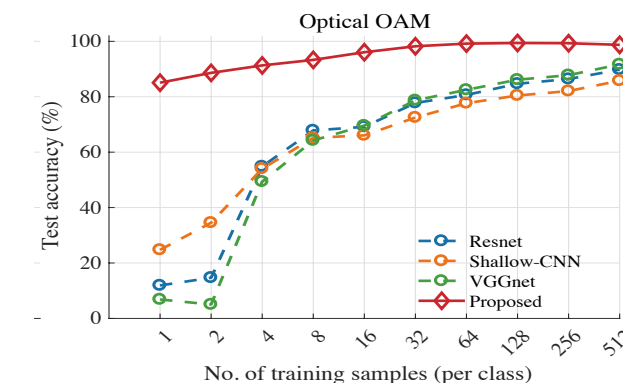
[Shifat-E-Rabbi et al, JMIV 2021]



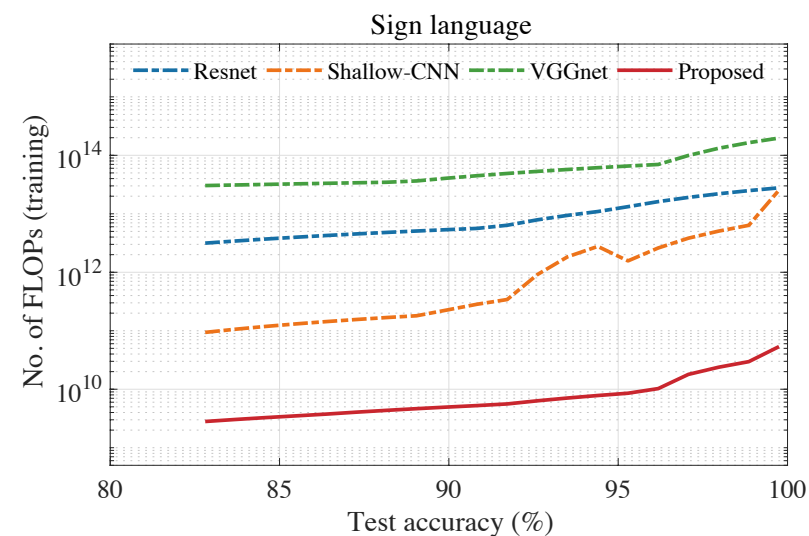
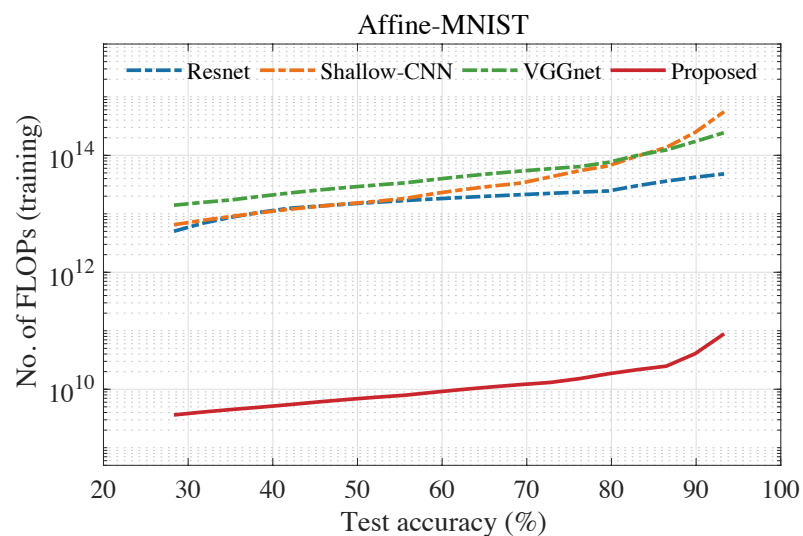
Out of distribution testing



up



Results and comparisons with deep learning



Limitations

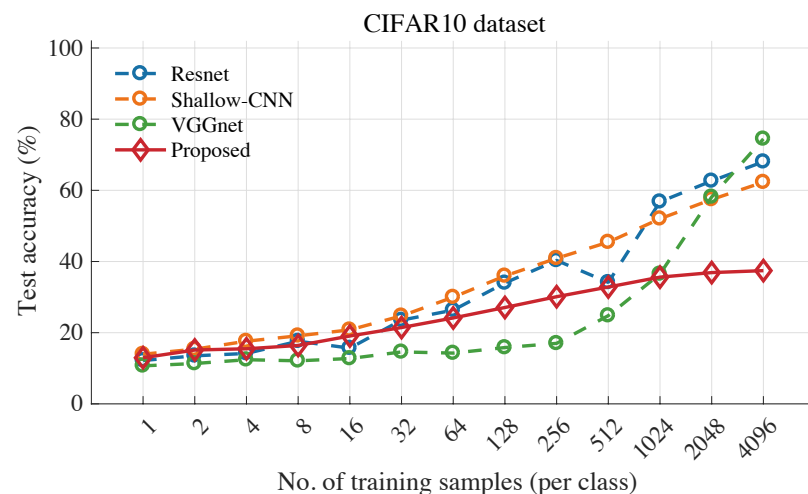
$$\mathbb{P} = \{p_g : g \in \mathcal{C}\} \quad \mathbb{Q} = \{q_g : g \in \mathcal{C}\}$$

where

$$p_g(x) = g'(x)p_0(g(x))$$

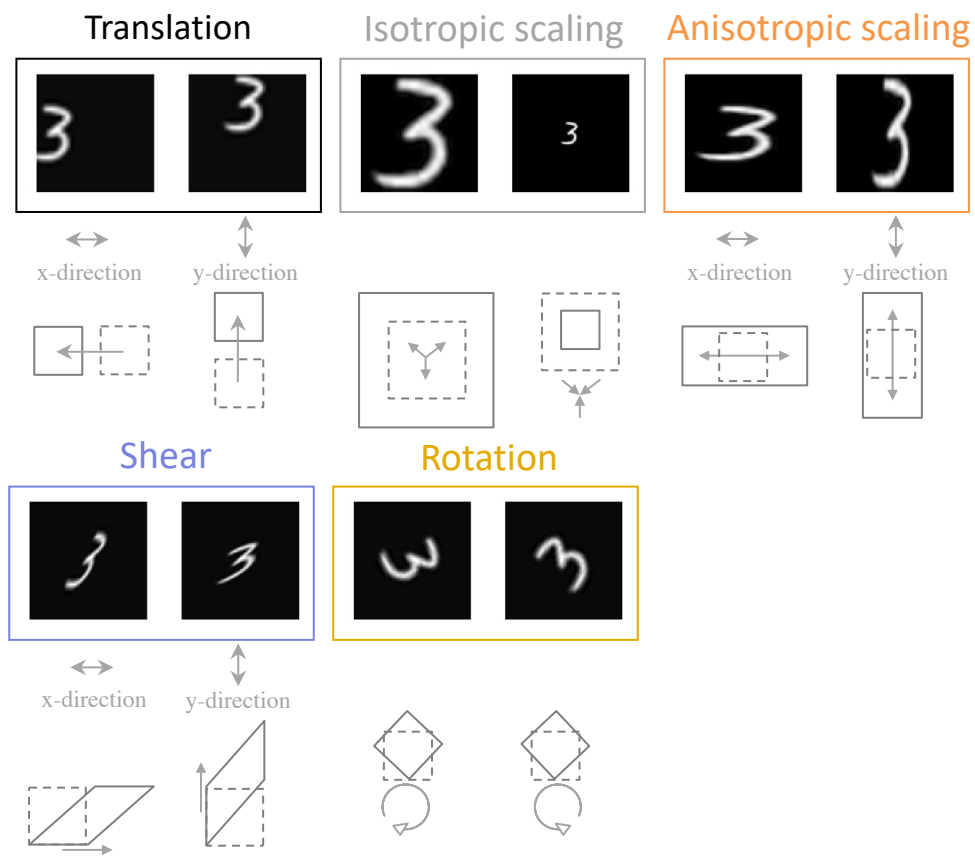
$$q_g(x) = g'(x)q_0(g(x))$$

It doesn't seem to work as well for
general object detection



Invariance encoding

Aim: Can we mathematically model invariances ?

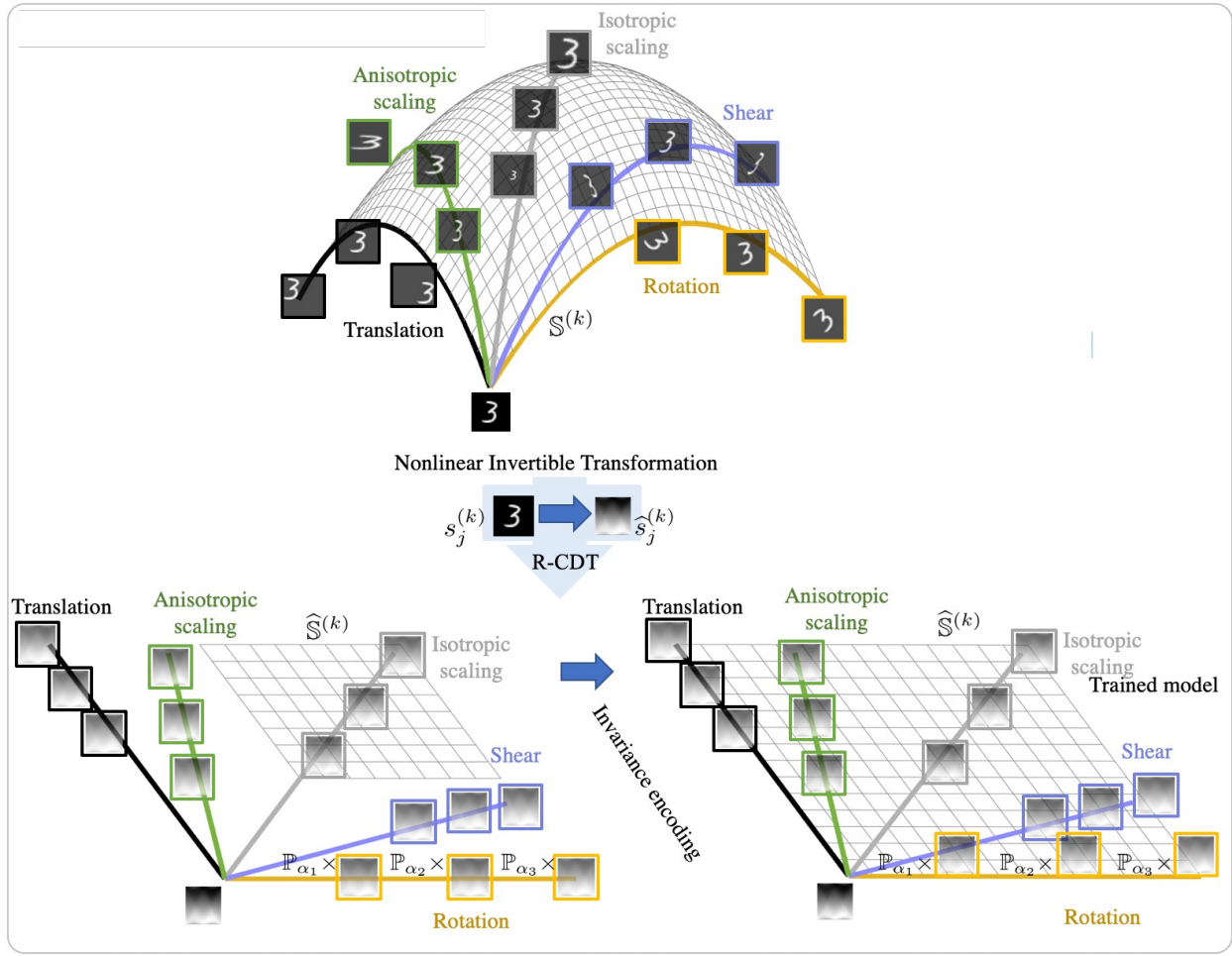


$\{s_1^{(1)}, s_2^{(1)}, \dots\} \quad \{s_1^{(2)}, s_2^{(2)}, \dots\}$

$s_j^{(k)} \in \mathbb{S}^{(k)} = \left\{s_j^{(k)} \mid s_j^{(k)} = |\det J g_j| \varphi^{(k)} \circ g_j, \forall g_j \in \mathcal{G}\right\}$

$\varphi^{(k)}$ unknown $g_j \in \mathcal{G}$ unknown + affine

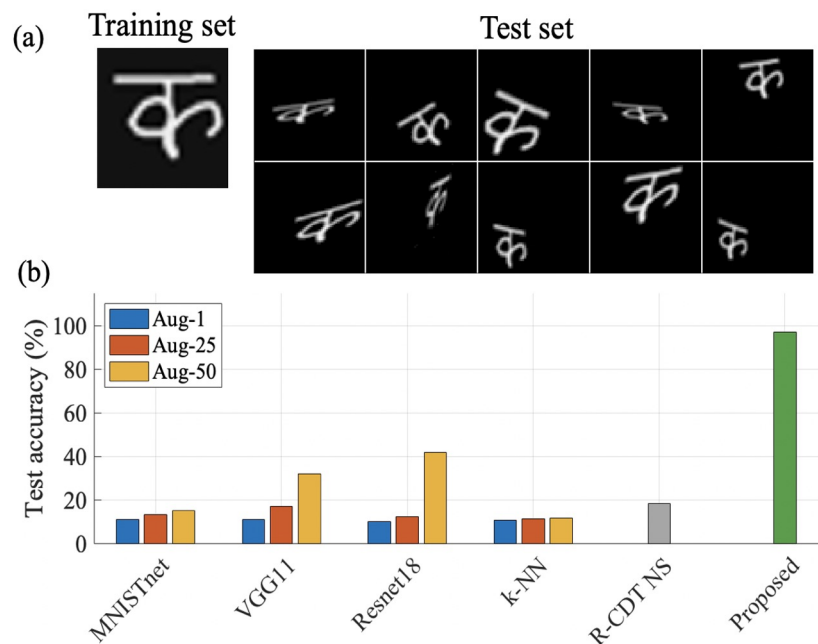
Solution overview:



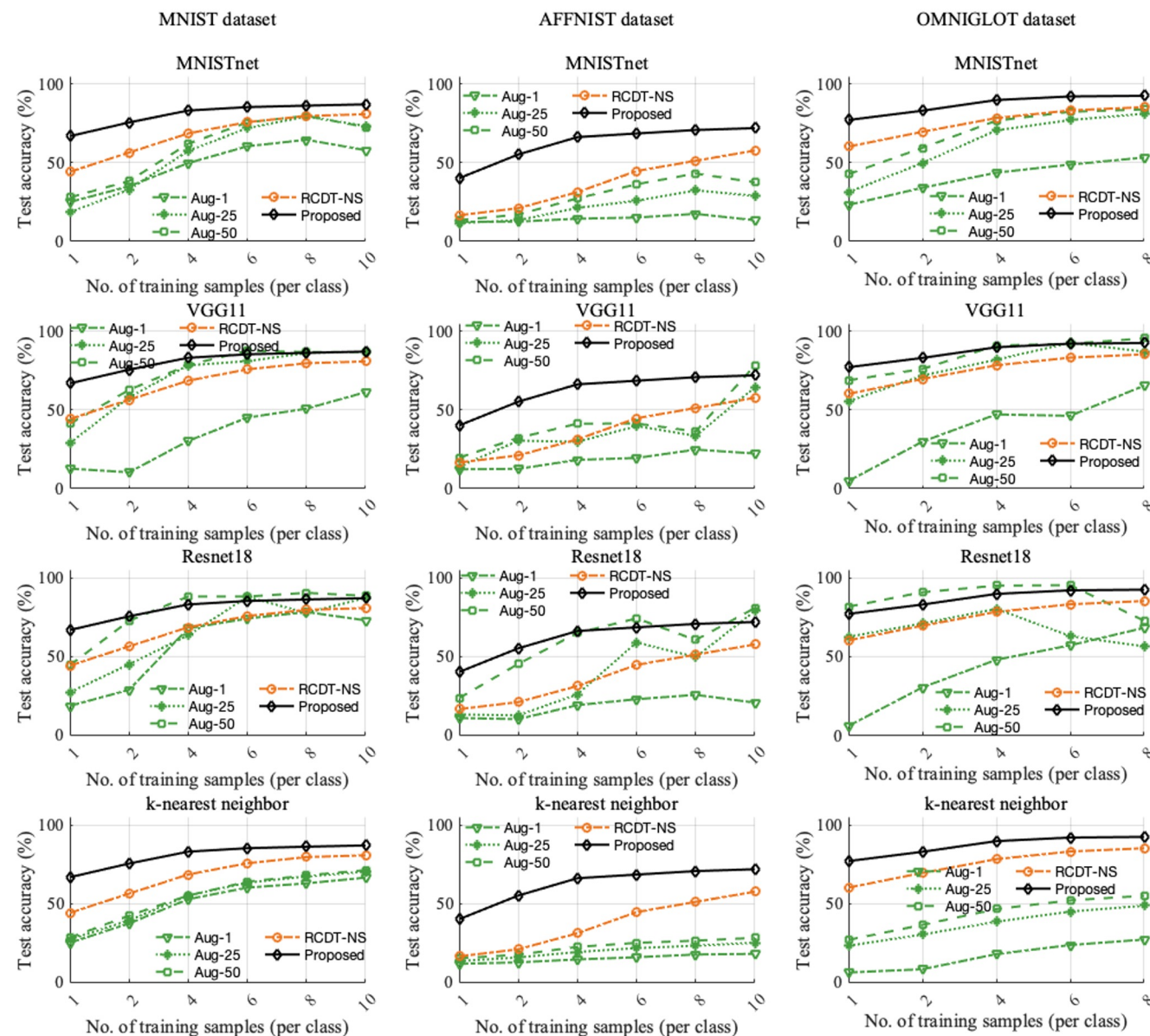
Results and comparisons with deep learning

[Shifat-E-Rabbi et al, arxiv 2022]

Synthetic data



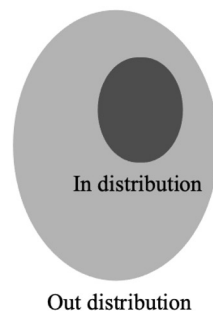
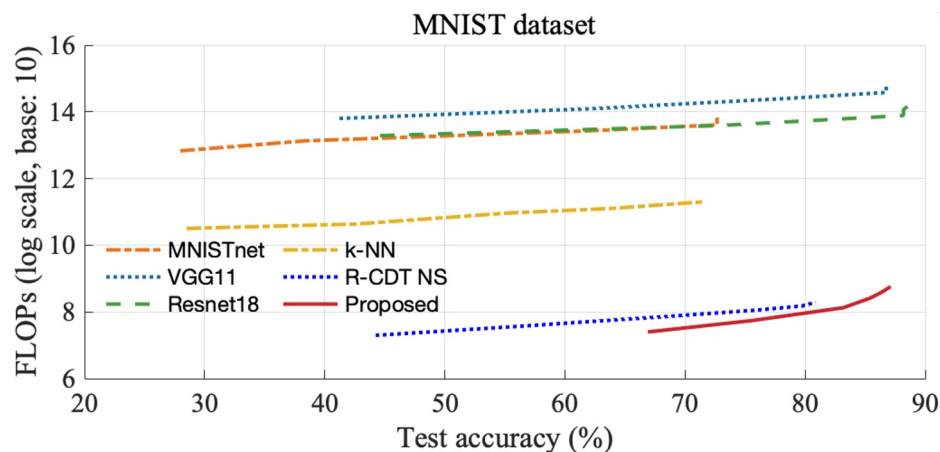
Real data



Results and comparisons with deep learning

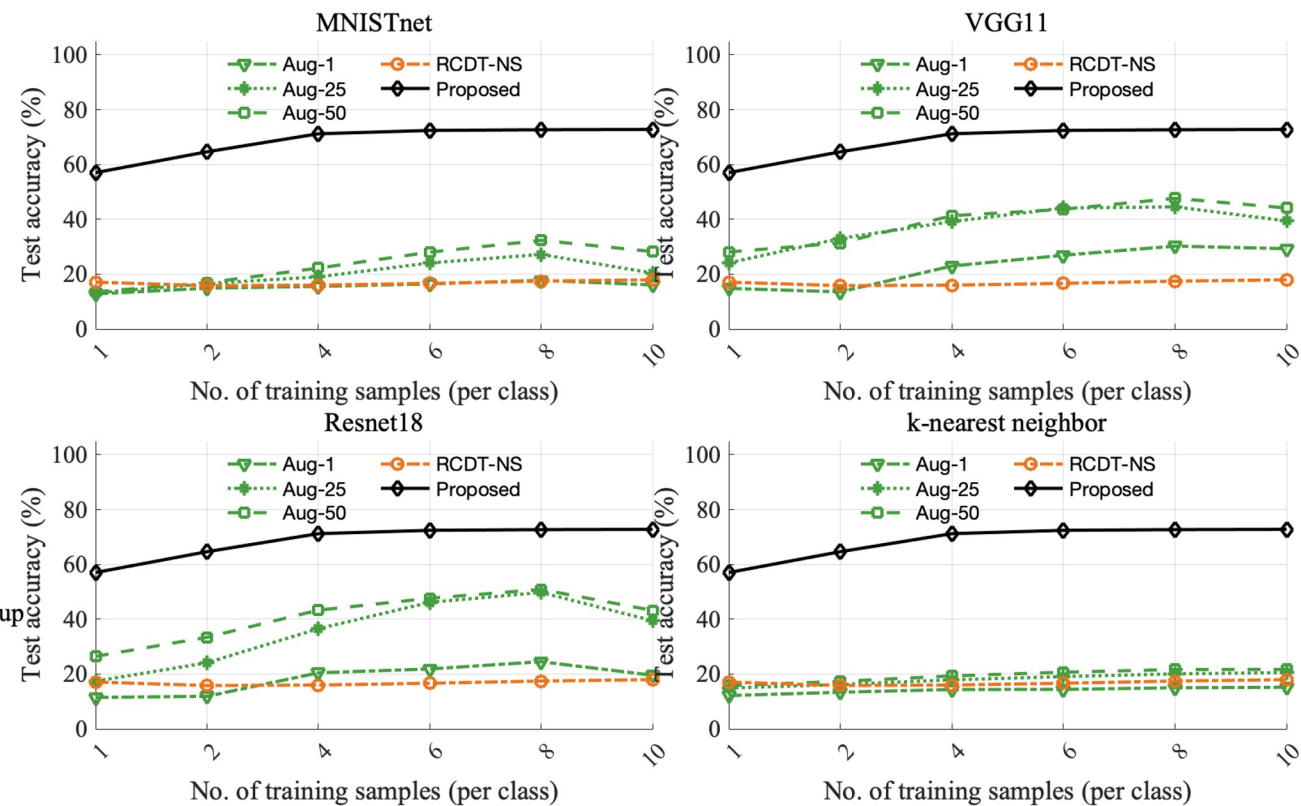
[Shifat-E-Rabbi et al, arxiv 2022]

Computational complexity



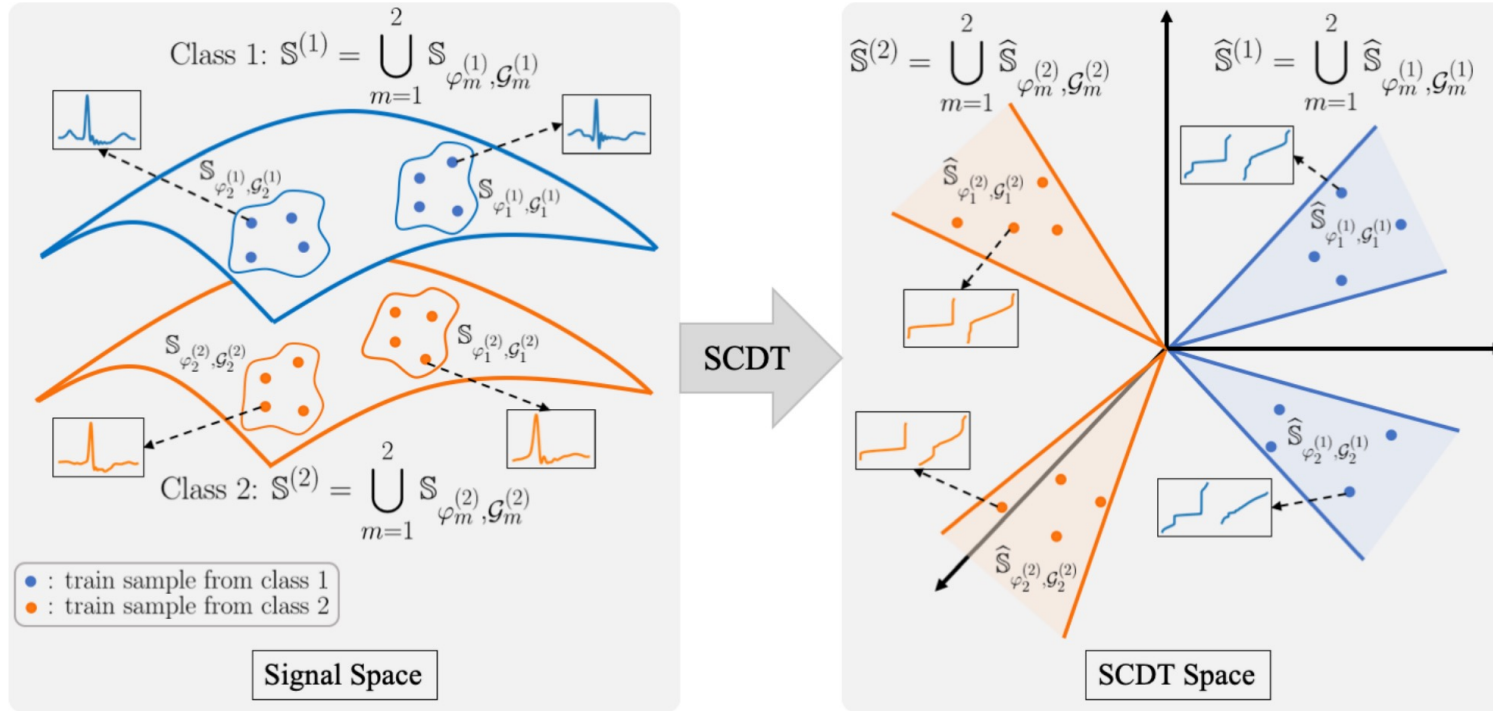
Out of distribution setup

Out-of-distribution experiment



End-to-End Time Series Classification [Rubaiyat et al, ArXiv 2022]

Generative Model:



$$\mathbb{S}^{(c)} = \bigcup_{m=1}^{M_c} \mathbb{S}_{\varphi_m^{(c)}, \mathcal{G}_m^{(c)}},$$

$$\mathbb{S}_{\varphi_m^{(c)}, \mathcal{G}_m^{(c)}} = \left\{ s_{j,m}^{(c)} \mid s_{j,m}^{(c)} = g_j' \varphi_m^{(c)} \circ g_j, g_j' > 0, g_j \in \mathcal{G}_m^{(c)} \right\},$$

$$\left(\mathcal{G}_m^{(c)} \right)^{-1} = \left\{ \sum_{i=1}^k \alpha_i f_{i,m}^{(c)}, \alpha_i \geq 0 \right\}$$

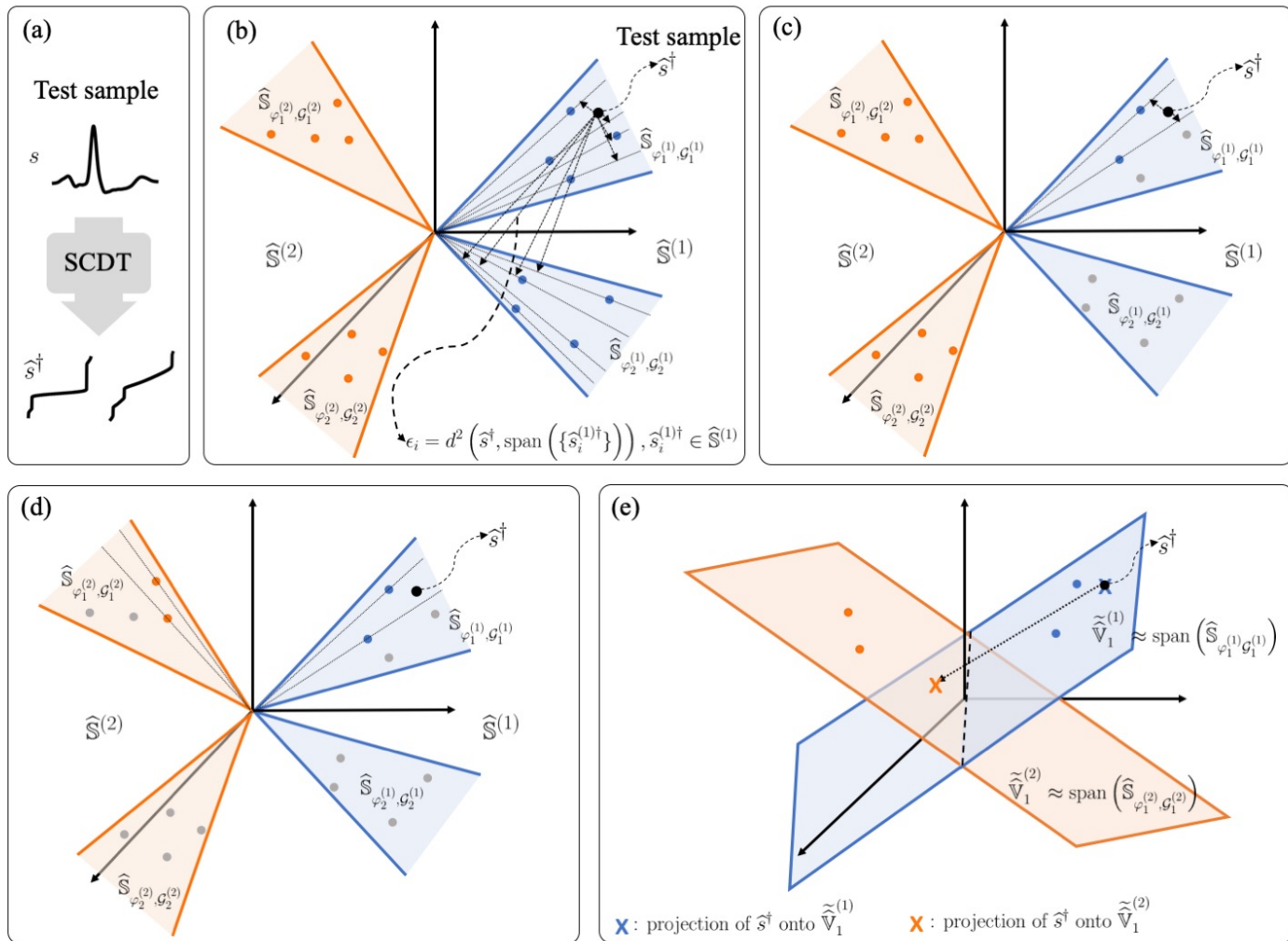
$$\hat{\mathbb{S}}^{(c)} = \bigcup_{m=1}^{M_c} \hat{\mathbb{S}}_{\varphi_m^{(c)}, \mathcal{G}_m^{(c)}},$$

$$\hat{\mathbb{S}}_{\varphi_m^{(c)}, \mathcal{G}_m^{(c)}} = \left\{ \hat{s}_{j,m}^{(c)} \mid \hat{s}_{j,m}^{(c)} = g_j^{-1} \circ \hat{\varphi}_m^{(c)}, g_j \in \mathcal{G}_m^{(c)} \right\},$$

$$\left(\mathcal{G}_m^{(c)} \right)^{-1} = \left\{ \sum_{i=1}^k \alpha_i f_{i,m}^{(c)}, \alpha_i \geq 0 \right\}$$

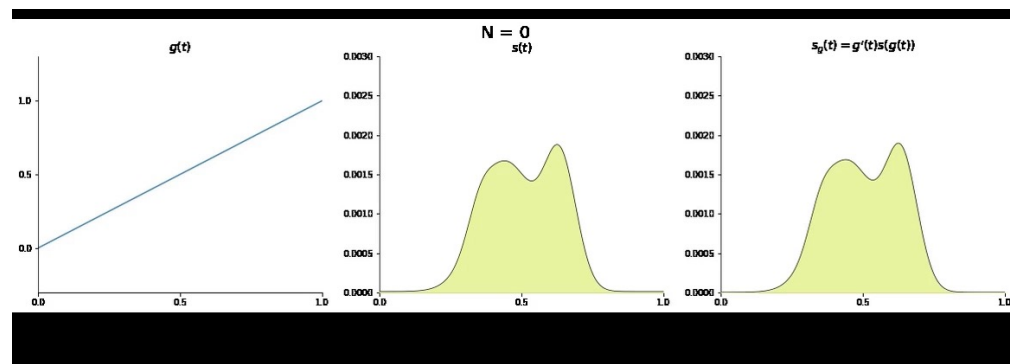
End-to-End Time Series Classification [Rubaiyat et al, ArXiv 2022]

NLS algorithm:

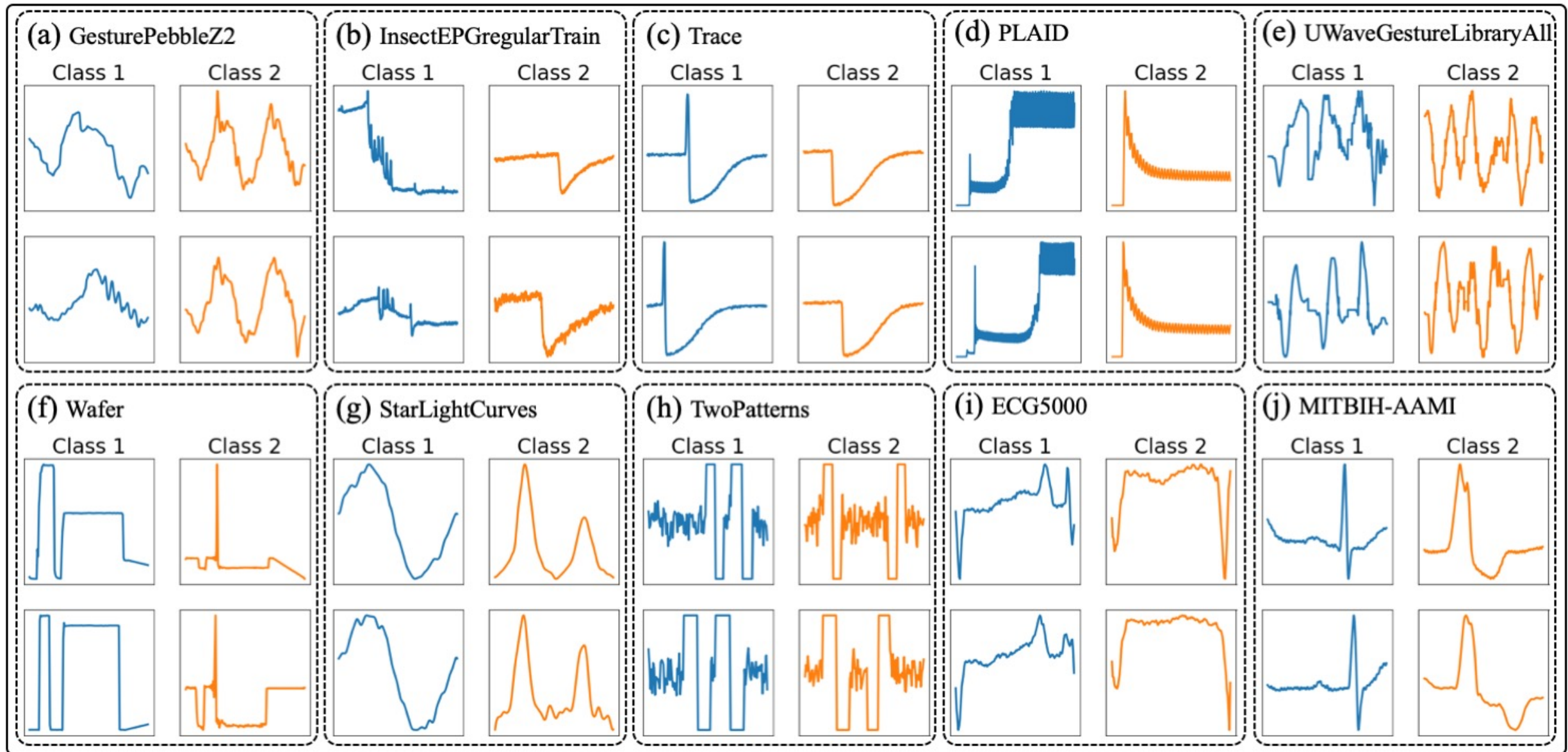


Subspace Enrichment:

$$\hat{\tilde{V}}_m^{(c)} = \text{span} \left(\{\hat{z}_1^{(c)\dagger}, \dots, \hat{z}_k^{(c)\dagger}\} \cup \mathbb{U}_T \cup \mathbb{U}_H \right)$$



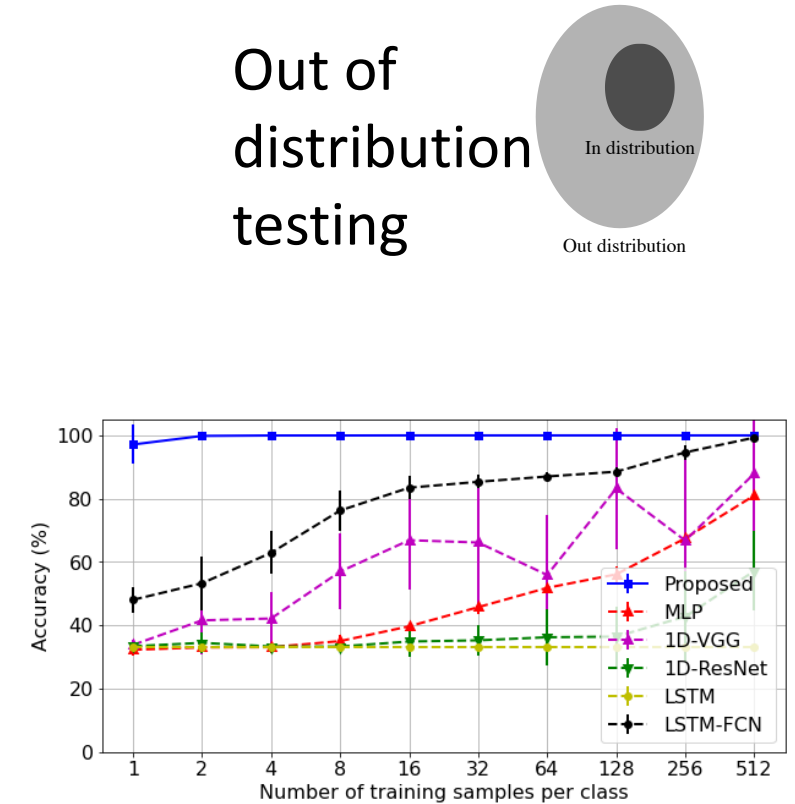
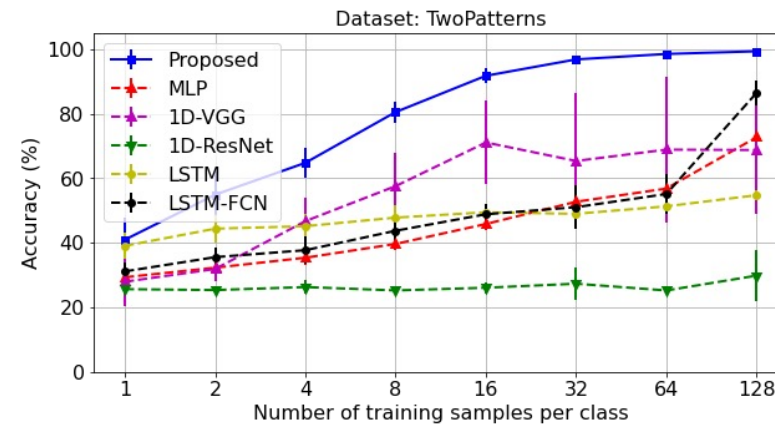
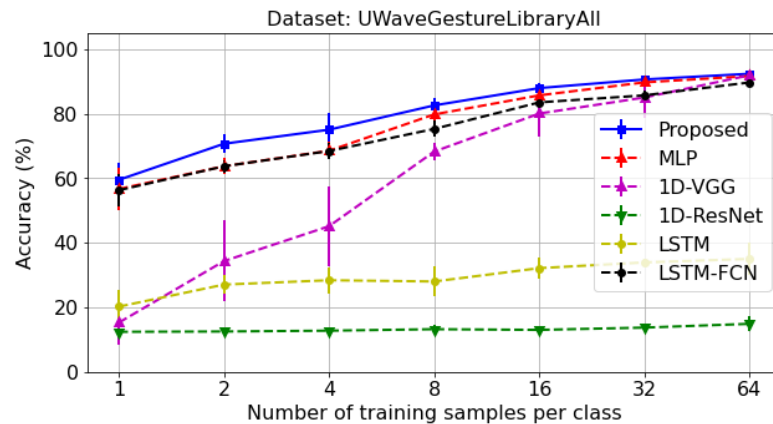
Solution is given by: $\arg \min_c d^2 \left(\hat{s}, \hat{\tilde{V}}_m^{(c)} \right)$



Results and comparisons with deep learning

[Rubaiyat et al, ArXiv 2022]

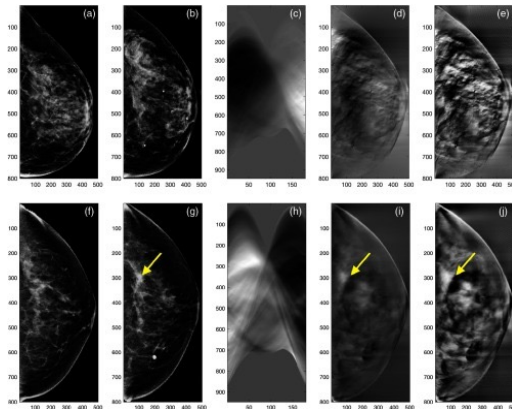
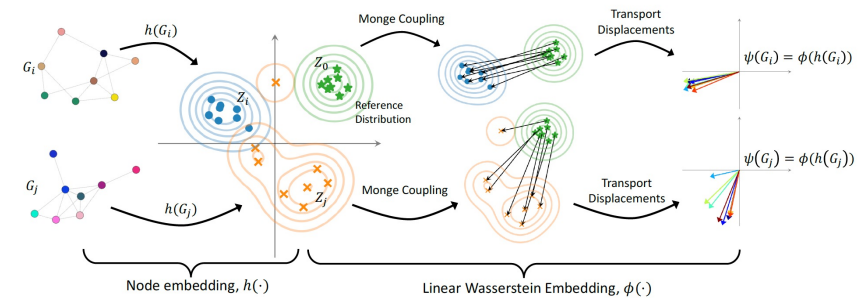
Dataset	MLP	1D-VGG	1D-ResNet	LSTM	LSTM-FCN	SCDT-NS	Proposed
GesturePebbleZ2	83.92	48.99	63.23	60.19	85.82	81.64	86.07
InsectEPGRegularTrain	80.92	82.07	50.58	57.05	59.95	73.43	90.82
Trace	64.0	35.8	25.9	28.2	58.1	85.0	88.0
PLAID	39.65	19.35	29.81	26.35	39.57	58.29	70.02
UWaveGestureLibraryAll	94.74	96.42	42.86	30.72	94.16	90.4	94.92
Wafer	68.69	94.03	53.66	51.36	86.70	92.75	95.53
StarLightCurves	75.85	70.0	56.53	60.54	74.38	77.4	84.2
TwoPatterns	88.12	95.15	87.42	80.62	98.47	95.15	99.92
ECG5000	98.9	98.92	98.92	98.36	98.76	93.4	97.4
MITBIH-AAMI	65.54	82.94	59.13	55.34	79.46	62.9	84.05
Win	0	2	1	0	0	0	8
AVG arithmetic ranking	3.5	3.5	5.6	6.3	3.6	3.8	1.6
AVG geometric ranking	3.42	2.8	5.07	6.27	3.46	3.49	1.28
MPCE	0.072	0.065	0.125	0.127	0.066	0.059	0.030



Other applications

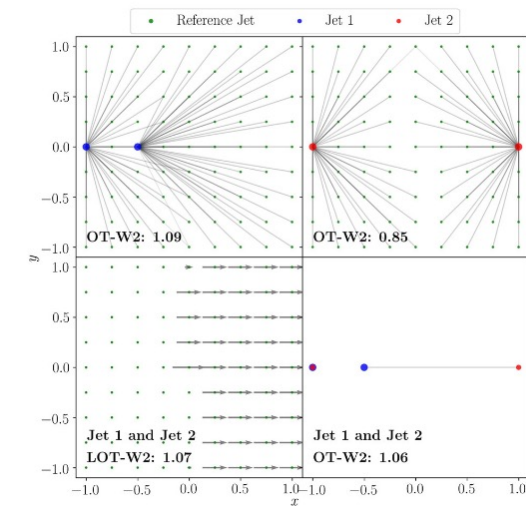
Kolouri et al, *Wasserstein Embedding for Graph Learning*, ICLR 2021

Uses LOT to obtain embedding for graph features for classification

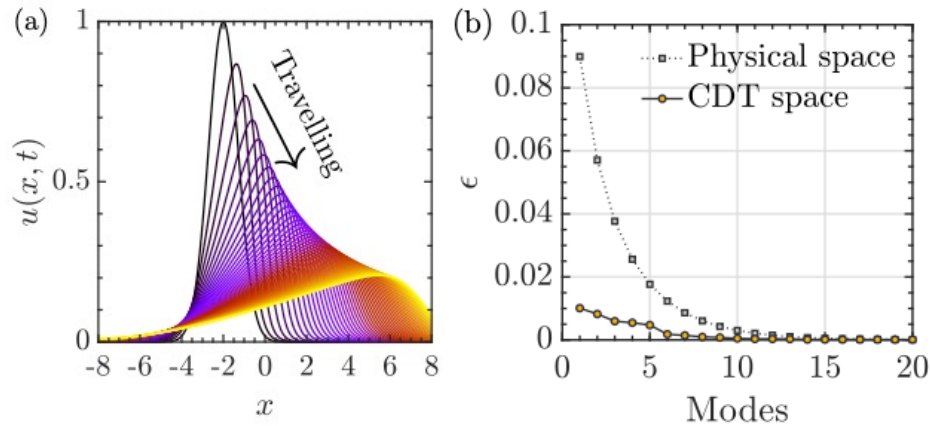
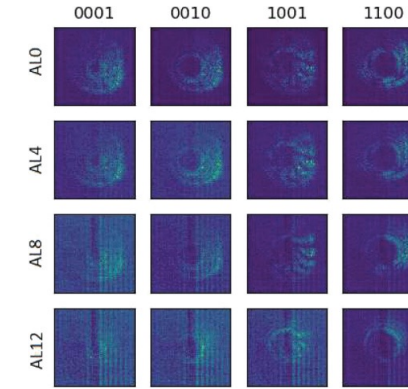


Lee et al, *Detecting mammographically occult cancer in women with dense breasts using deep convolutional neural network and Radon Cumulative Distribution Transform*, Journal of Medical Imaging 2019.

Cai et al, *Linearized optimal transport for collider events*. Physical Review D, 2020.

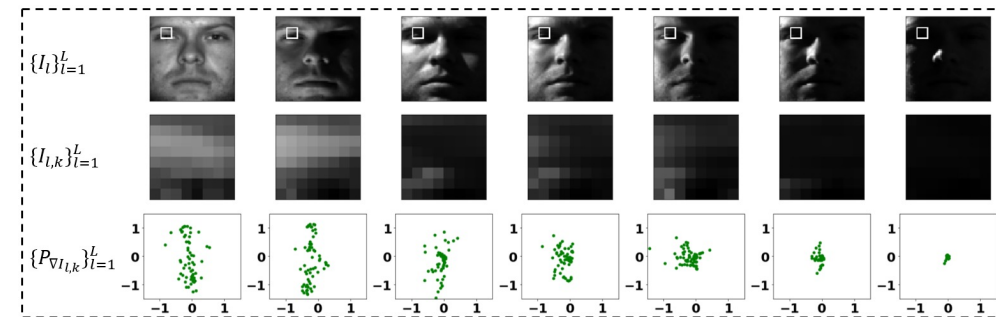


Neary et al, *Tranposrt-based pattern recognition versus deep neural networks in underwater OAM communications*, JOSA (A), 2021.

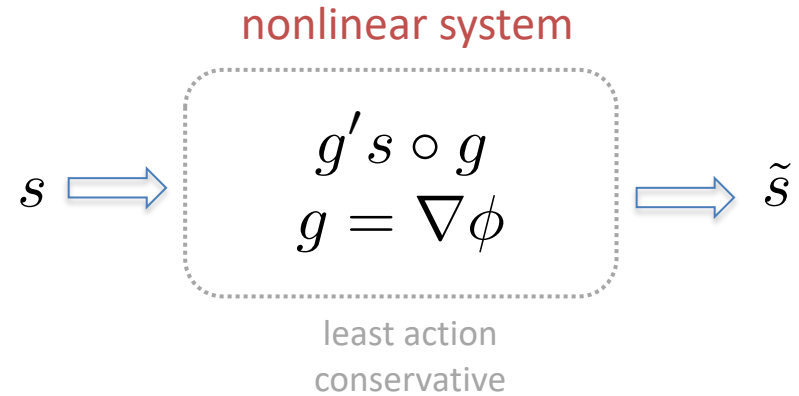


Ren et al, *Model reduction of traveling-wave problems via Radon cumulative distribution transform*, Physical Review Fluids, 2021.

Zhuang et al, *Local sliced-Wasserstein features sets for illumination-invariant face recognition*, ArXiv, 2022.



Summary



Solution



Extra slides

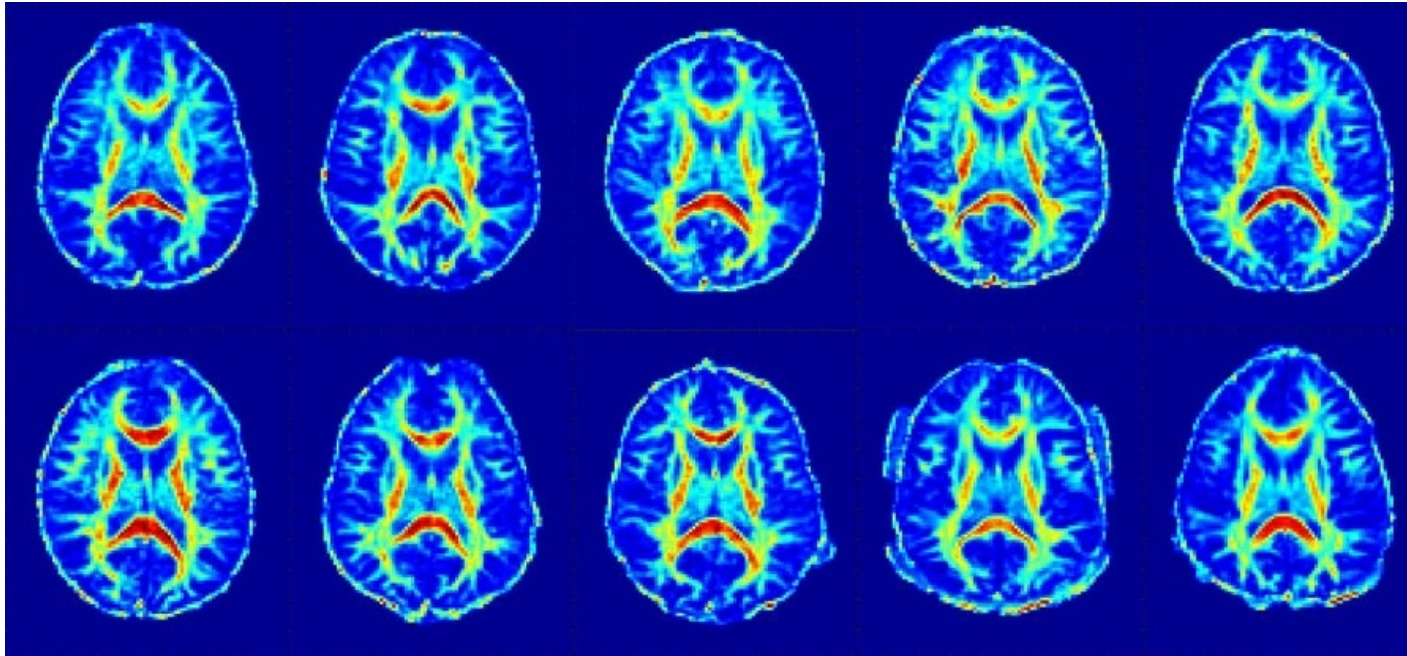
Post-concussive cognitive changes

- Immediate and transient alteration in brain function
- Cognitive changes are common after mild traumatic brain injury and predictive of poor post-concussive outcome (Himanen et al. 2005; Bigler, 2004)
- However, the underlying **structural substrates** are poorly understood
- Diffuse axonal injury implicated in decrease in working memory (Niogi et al. 2008)



Kundu, Ghodadra, Fakhra, Alhilali, Rohde, Assessing Post-concussive reaction time using TBM of diffusion tensor images, American Journal of Neuroradiology, 2019.

Goals

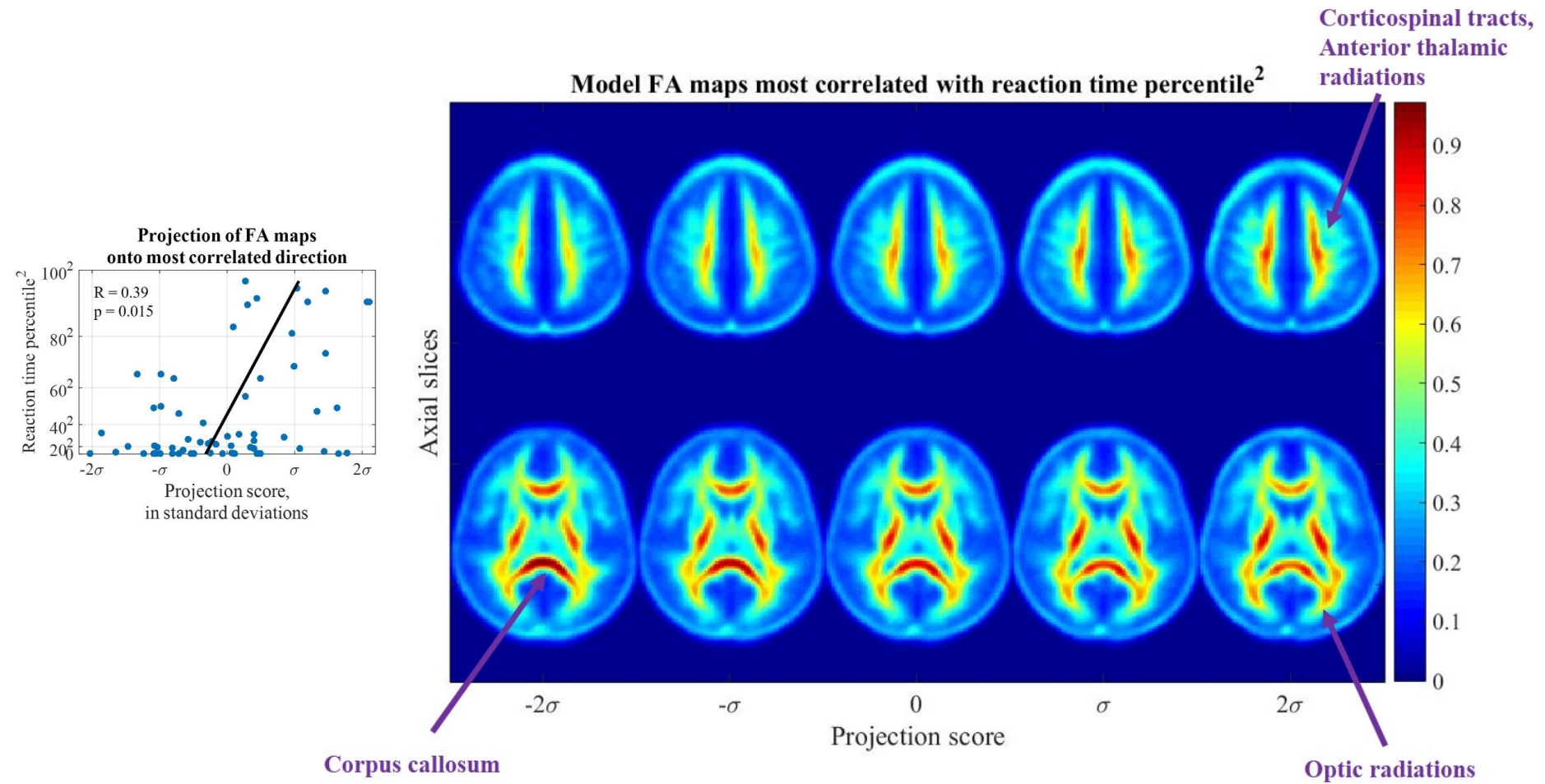


Best reaction
times

Worst reaction
times

- Are there identifiable **patterns** that are hidden from human view?
- If so, **how can we find them?**

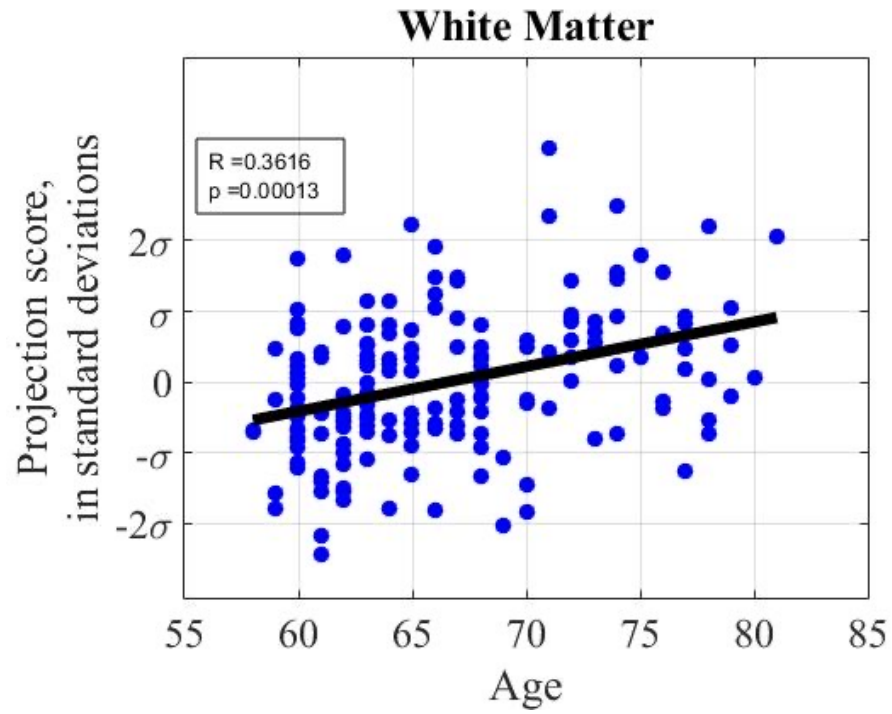
Visualization of dynamic morphology changes



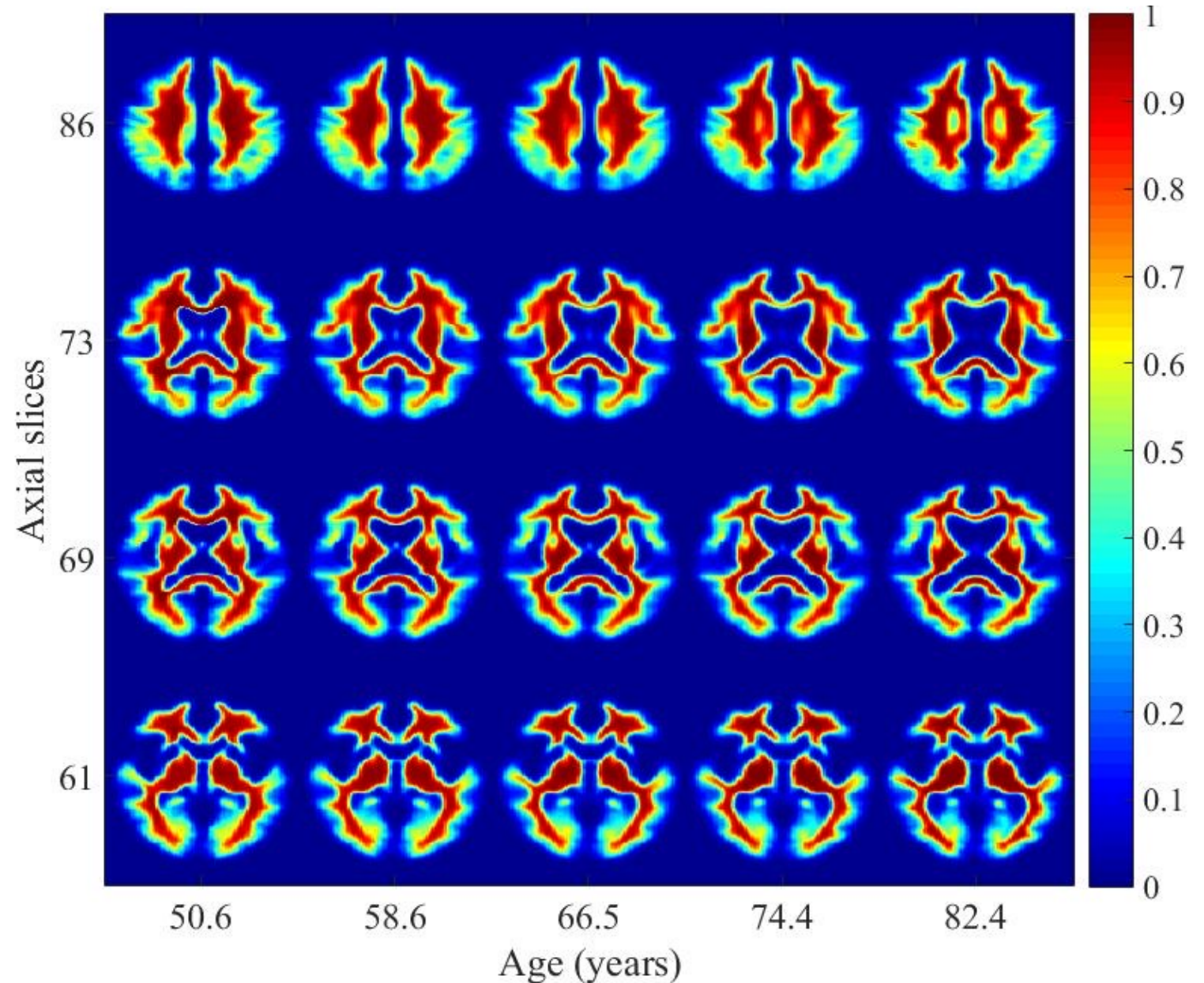
Kundu, Ghodadra, Fakhra, Alhilali, Rohde, Assessing Post-concussive reaction time using TBM of diffusion tensor images, American Journal of Neuroradiology, 2019.

T1 images and aging

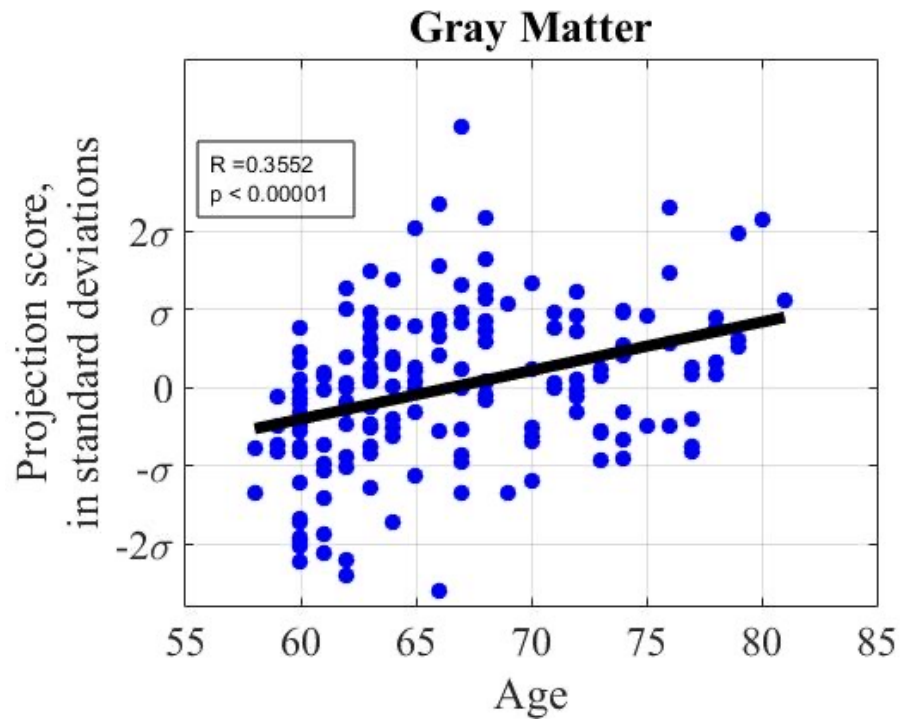
White matter with age



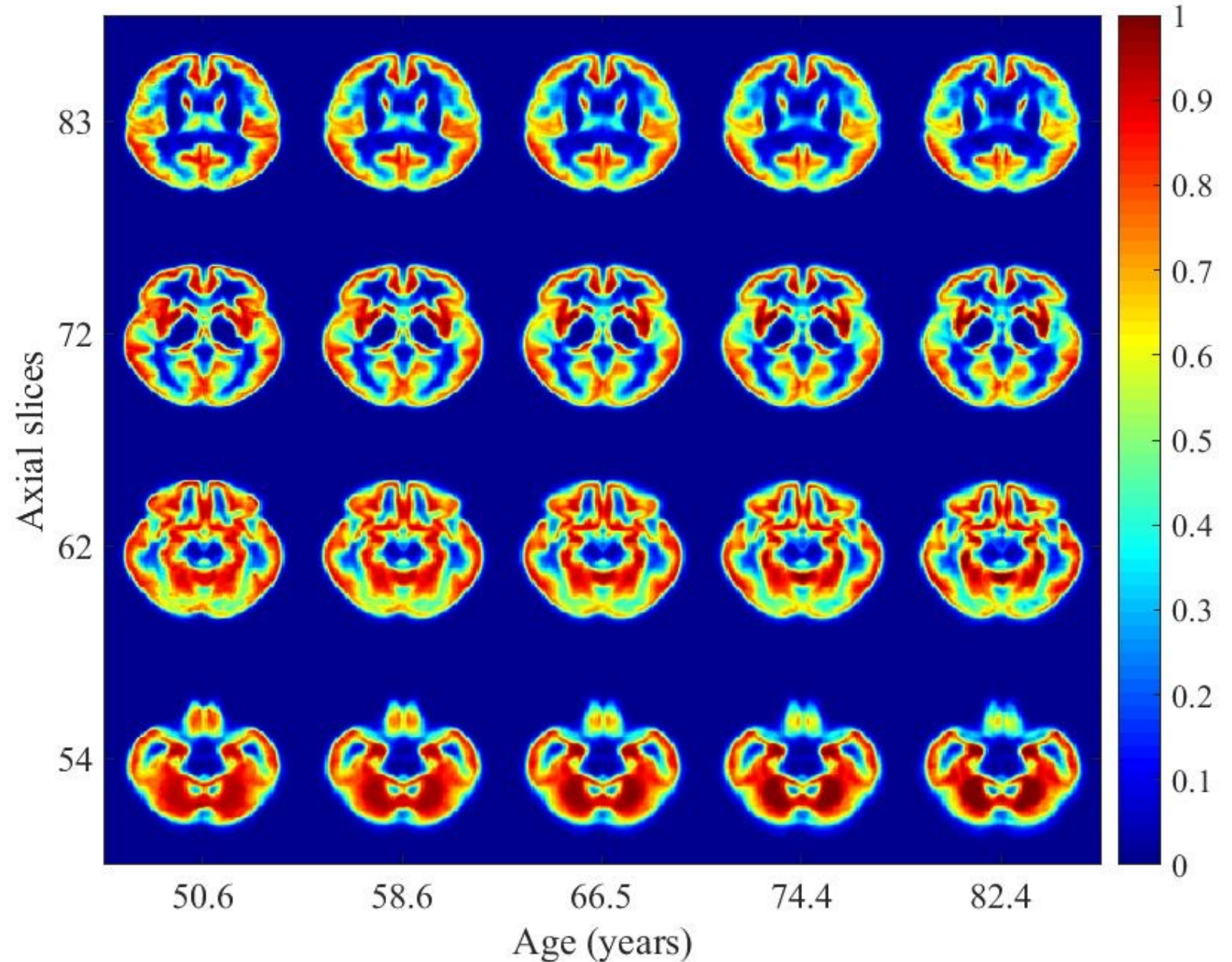
0.31 mm shift in GM distribution with every 10 year increase age.



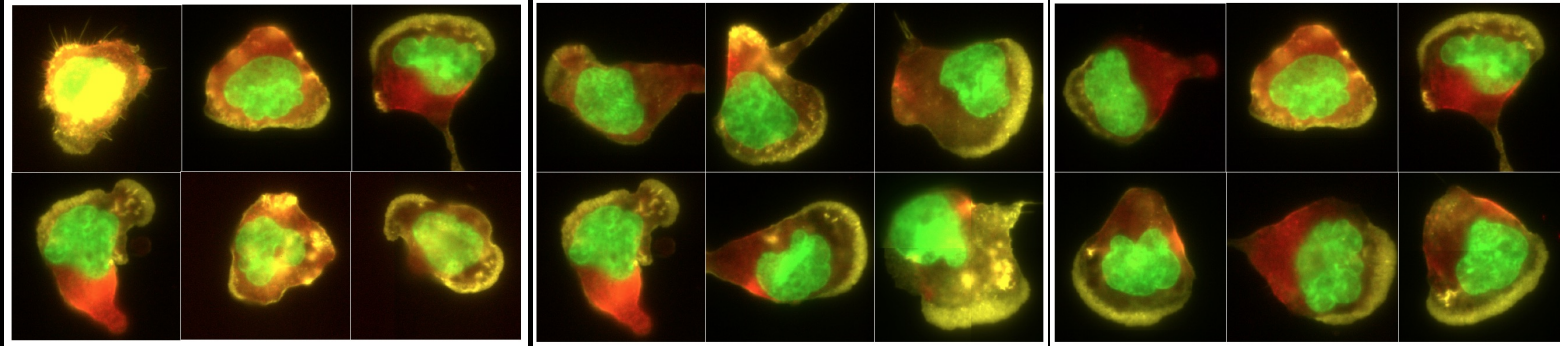
Gray matter with age



0.66 mm shift in GM distribution with every 10 year increase age.

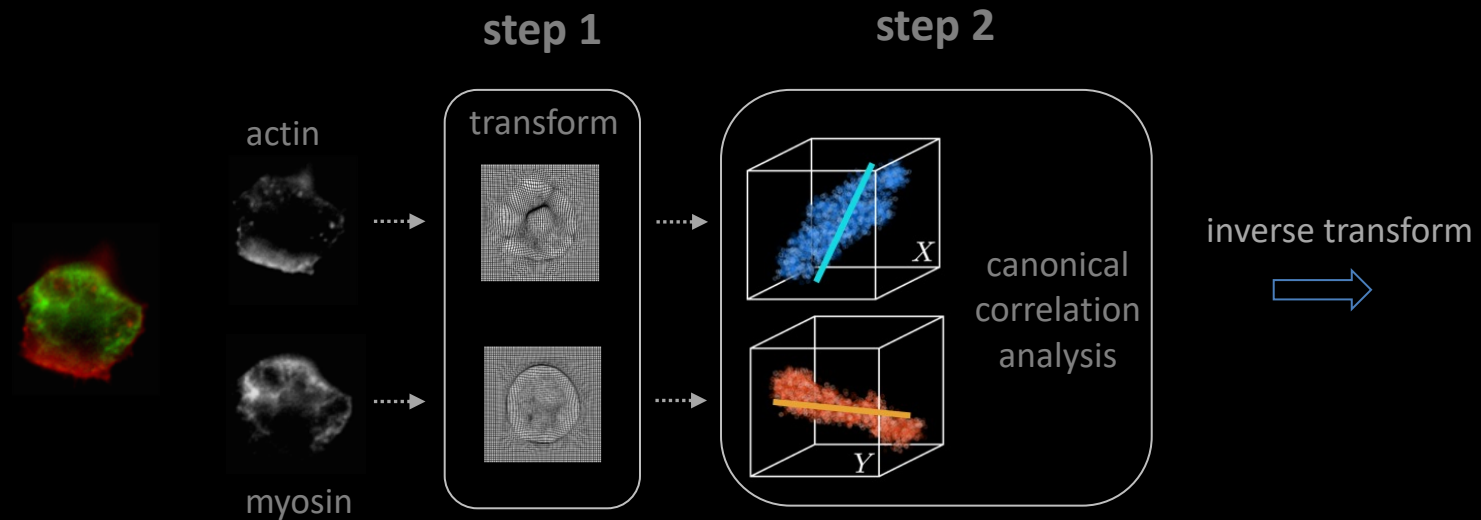


Example: Can we model the dependency between **myosin** and **actin** in neutrophils?

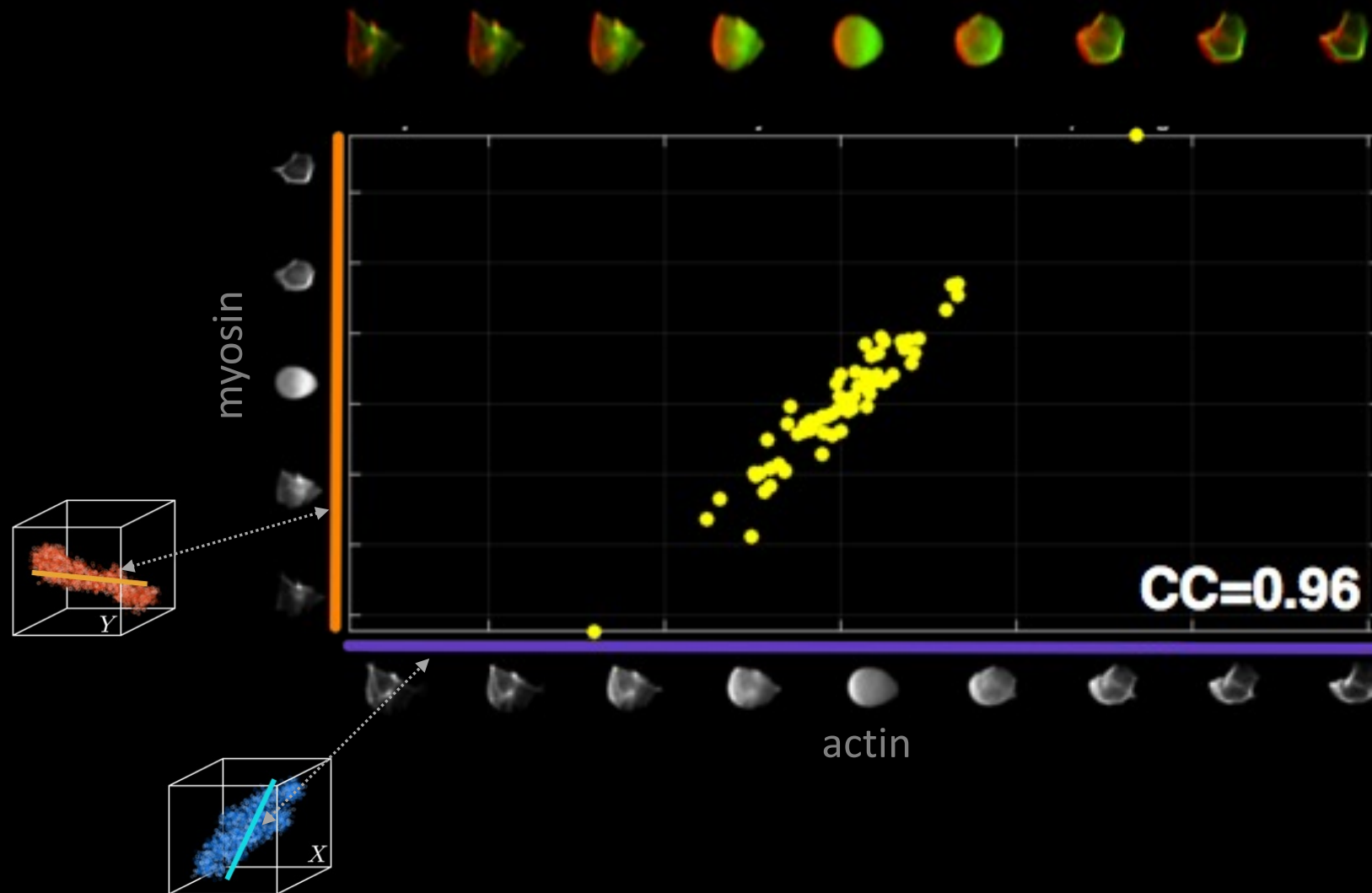


Courtesy: Theriot Lab (Stanford)

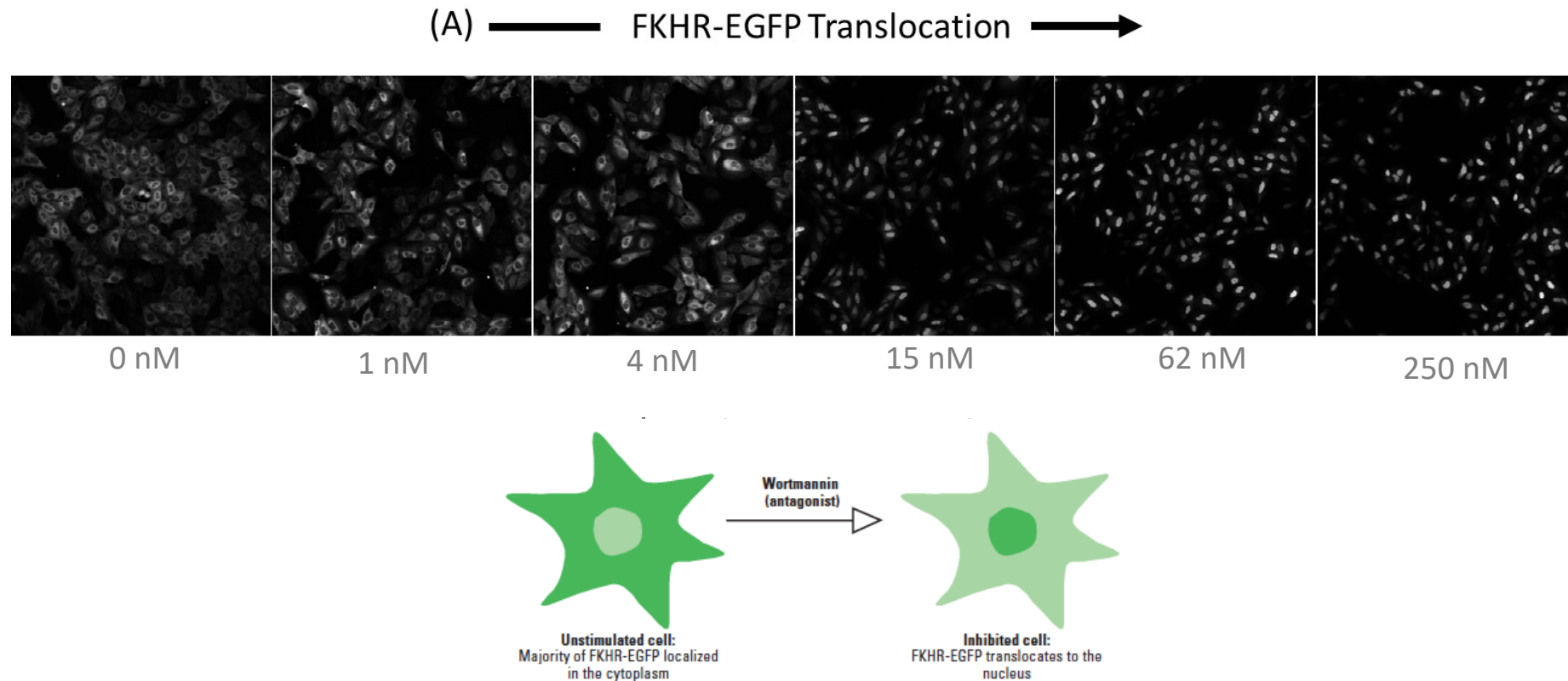
Solution:



Result: Antipodal relationship between actin and myosin

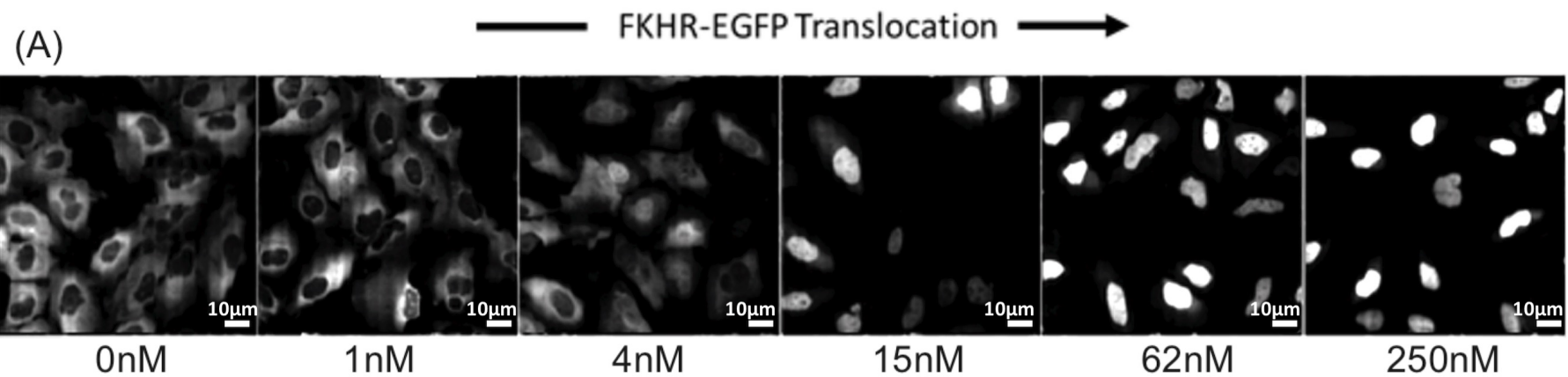


Forkhead protein translocation (drug screening)

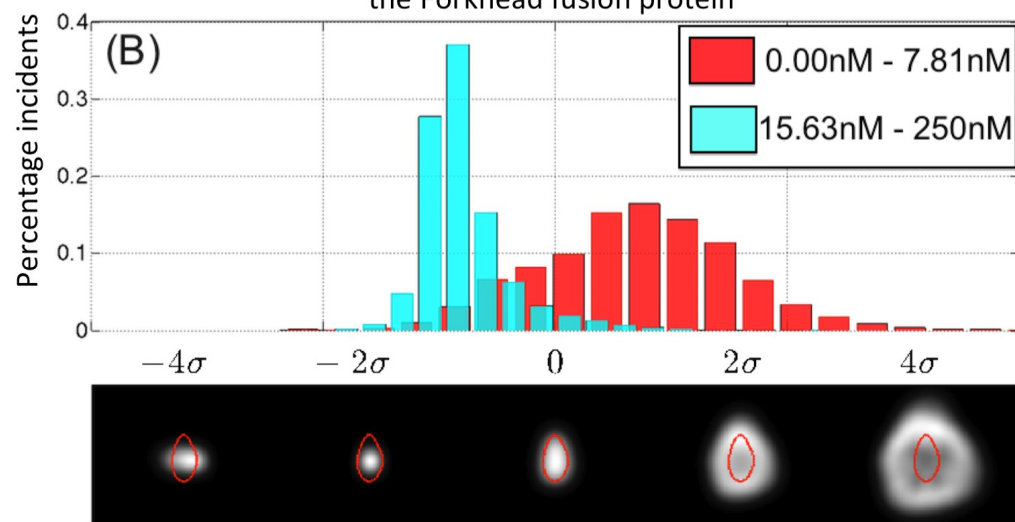


Problem statement

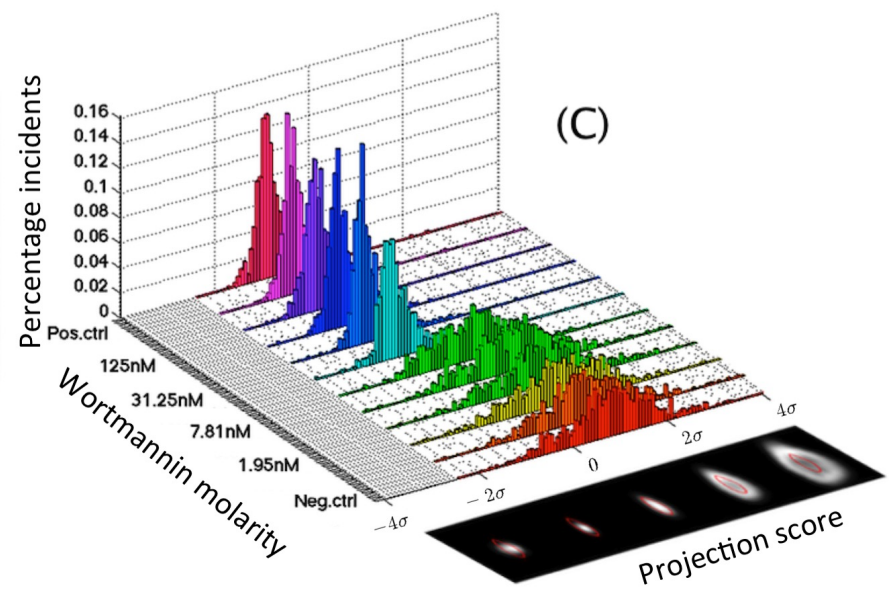
Can we automatically “decode” the effects of Worthamin concentration?

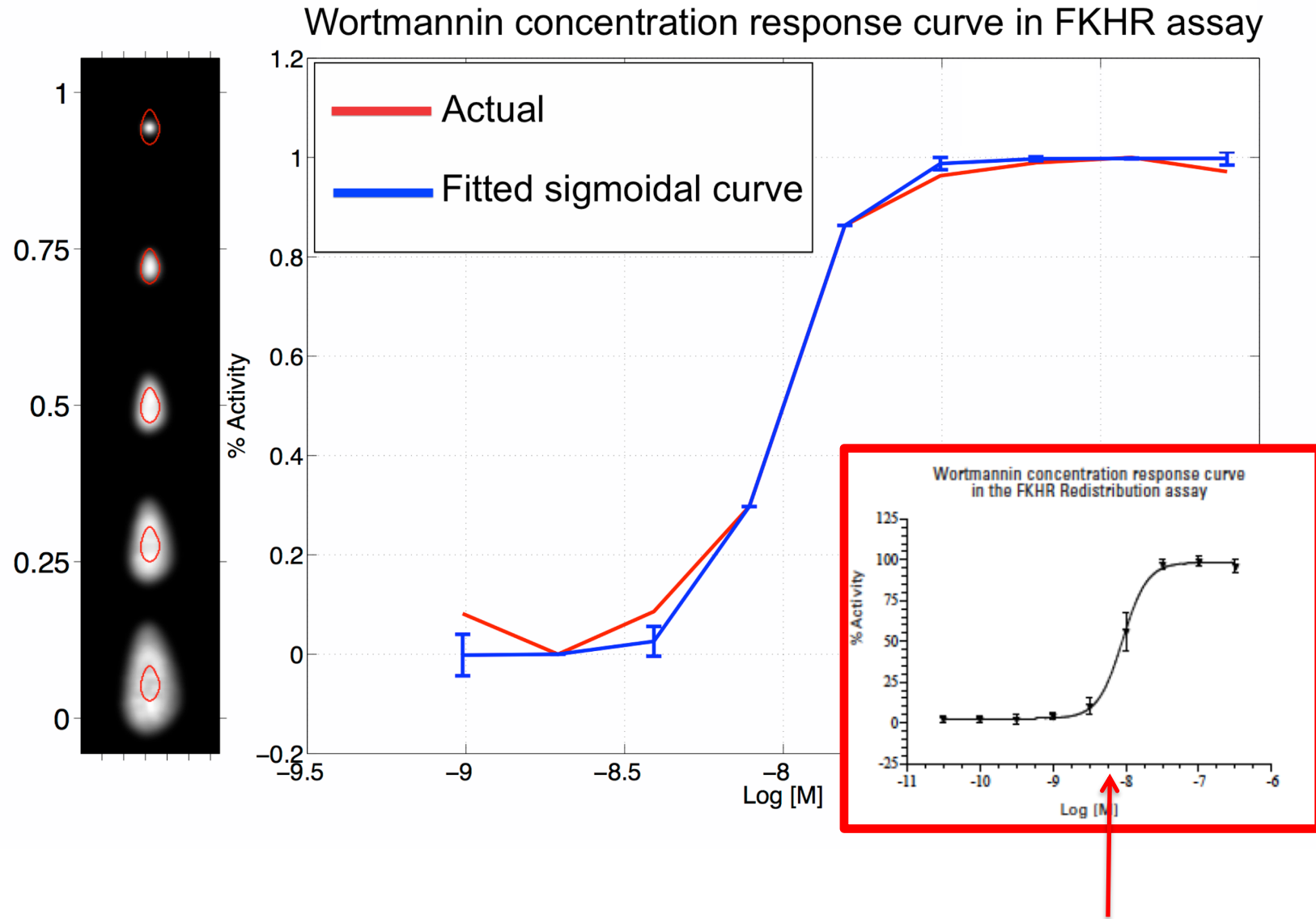


The effect of Wortmannin on cytoplasm to nucleus translocation of the Forkhead fusion protein



Projection score





Basu, Kolouri, Rohde, PNAS 2014

From Thermo-Fisher