ICASSP 2024 Tutorial T-10: Building White-Box Deep Neural Networks

Lecture I: *White-Box Architecture Design via Unrolled Optimization*

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TOYOTA TECHNOLOGICAL INSTITUTE AT CHICAGO

The Signal Processing Pipeline

Sensing, Compression

↓

Denoising, Deblurring, Superresolution

↓

Source Separation, Error Correction

↓

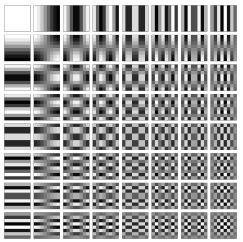
Completion, Generation, Prediction

The **pursuit of low-dimensional structure** is a universal task!

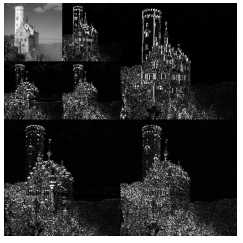
Historical Context: Quest for Low-Dimensionality

Fourier

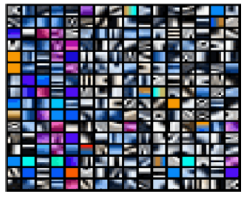
Wavelets



X-lets: Curvelets, Contourlets, Bandlets, ...



Learned Dictionaries

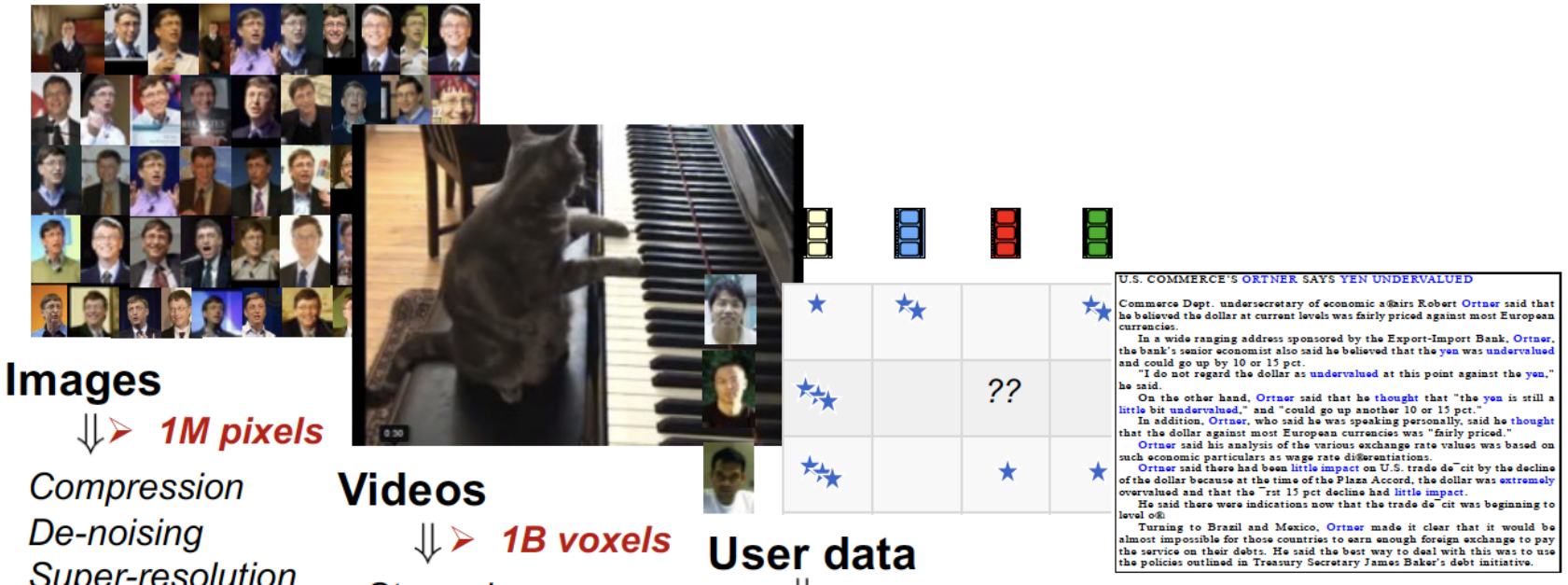


Learned Reconstruction Procedures

A continuing quest for **sparse signal representations** leveraging mathematics + massive data and computation!

A New Paradigm for Modern Data Science

Principles $\longleftarrow$ **Computation** $\longrightarrow$ **Applications**



Images

$\Downarrow\!\!\rightarrow$ *1M pixels*

Compression
De-noising
Super-resolution
Recognition…

Videos

$\Downarrow\!\!\rightarrow$ *1B voxels*

Streaming
Tracking
Stabilization…

User data

$\Downarrow\!\!\rightarrow$ *1B users*

Clustering
Classification
Collaborative filtering…

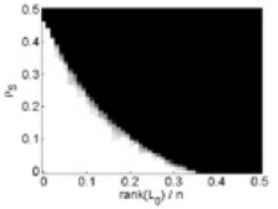
Web data

$\Downarrow\!\!\rightarrow$ *100B webpages*

Indexing
Ranking
Search…

How to extract low-dim structures from such high-dim data?

The (Pre-?) Modern Era: Massive Data and Computation



(a) Robust PCA, Random Signs

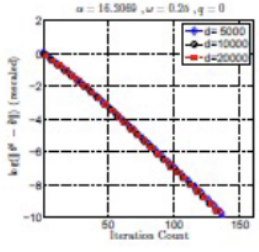
Mathematical Theory
(high-dimensional statistics, convex geometry, measure concentration, combinatorics…)

BIG DATA
(images, videos, voices, texts, biomedical, geospatial, consumer data…)

Cloud Computing
(parallel, distributed, scalable platforms)

Applications & Services
(data processing, analysis, compression, knowledge discovery, search, recognition…)

Computational Methods
(convex optimization, first-order algorithms, random sampling, deep networks…)



History: Principal Component Analysis (PCA)

[Pearson 1901, Hotelling 1933]

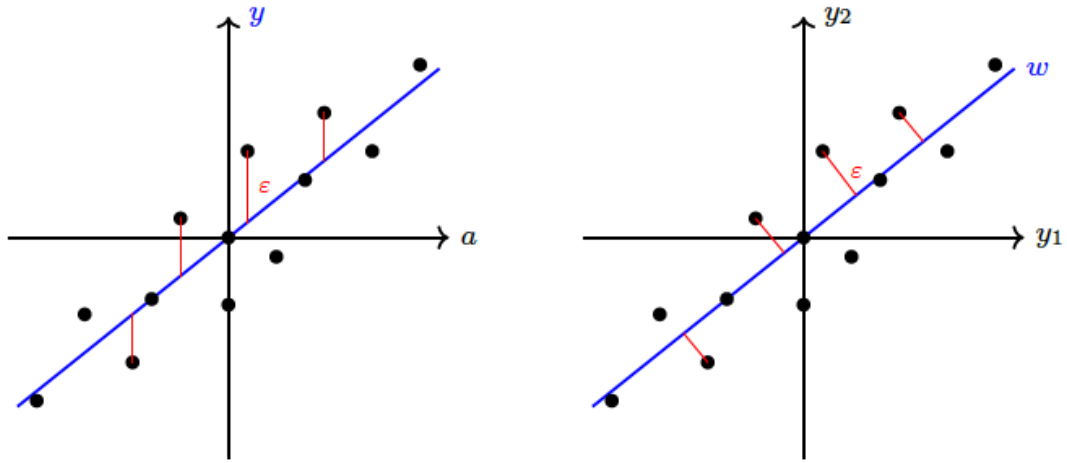


Figure 1: Left: regression; Right: principal component analysis.

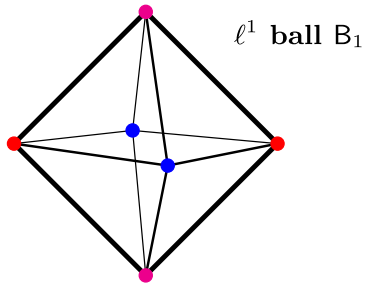
A high-dim random vector $\boldsymbol{y}$ is approximated by the $d < m$ components as:

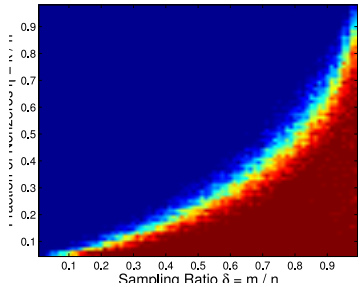
$$\boldsymbol{y} = \boldsymbol{u}_1 w_1 + \boldsymbol{u}_2 w_2 + \cdots + \boldsymbol{u}_d w_d + \boldsymbol{\epsilon} \doteq \boldsymbol{U}\boldsymbol{w} + \boldsymbol{\epsilon} \quad \in \mathbb{R}^m, \tag{1}$$

where $\boldsymbol{U} = [\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_d] \in \mathbb{R}^{m \times d}$, $\boldsymbol{w} = [w_1, w_2, \ldots, w_d]^* \in \mathbb{R}^d$, and the variance of the residual $\boldsymbol{\epsilon} \in \mathbb{R}^m$ is minimized:

$$\min \mathbb{E}\big[\|\boldsymbol{y} - \boldsymbol{U}\boldsymbol{w}\|_2^2\big]. \tag{2}$$

History: One Subspace to Many Independent Subspaces



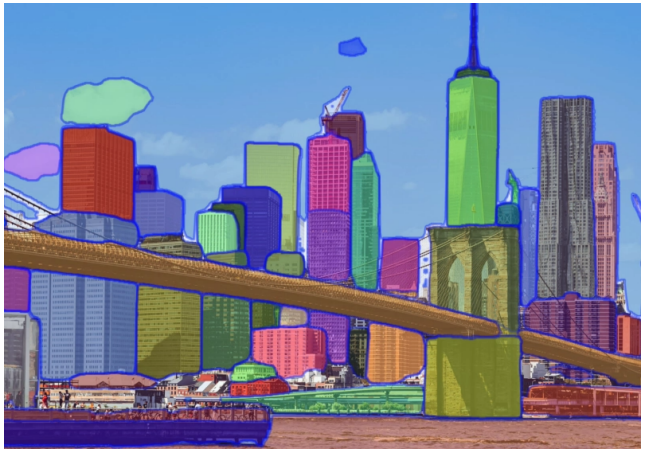


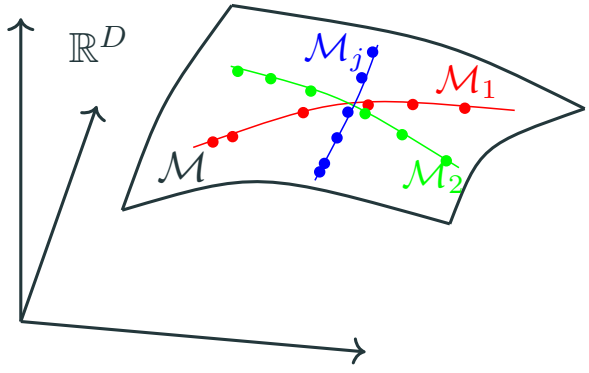
Model problem for signal representation—*sparse approximation*:

$$\boldsymbol{x} = \boldsymbol{A}\boldsymbol{z}, \quad \boldsymbol{z} \text{ sparse}, \quad \boldsymbol{A} \in \mathbb{R}^{m \times n} \text{ random}$$

1. *Piecewise linear model* for signals
2. Success determined by *intrinsic structure* of signal relative to model
3. Theory informs algorithm design (and vice versa)

Modern (Deep) Representation Learning

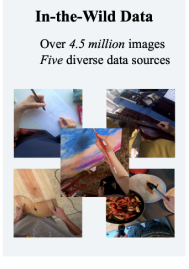


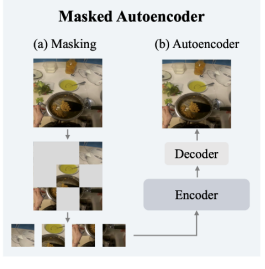


Understanding and interacting with the physical world

$\Longrightarrow$ **nonlinear signals**!

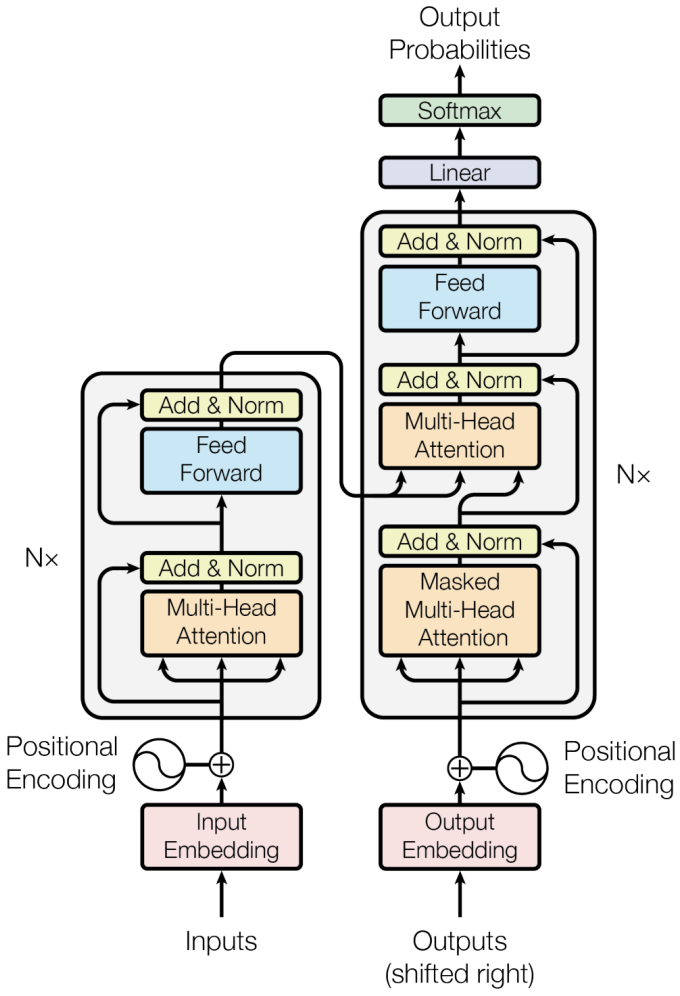
Coping with nonlinearity demands **deeper** representations.

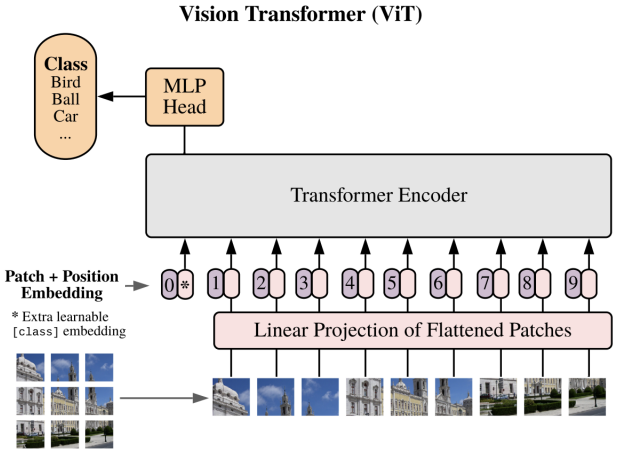


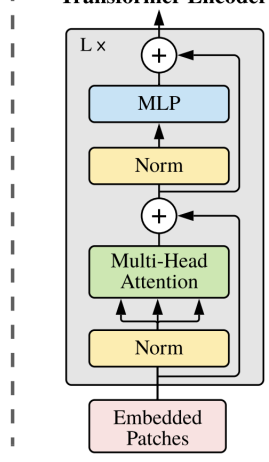


Kirillov et al. 2023; Radosavovic et al. 2022; Wang et al. 2023

Transformers: Modern Representation Learning's Workhorse



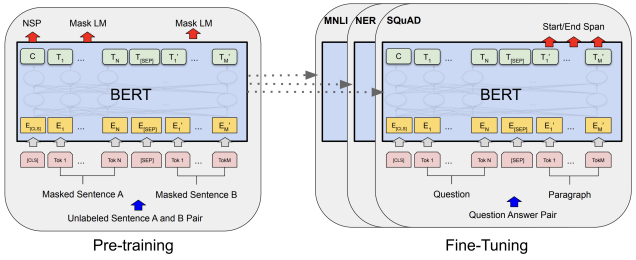




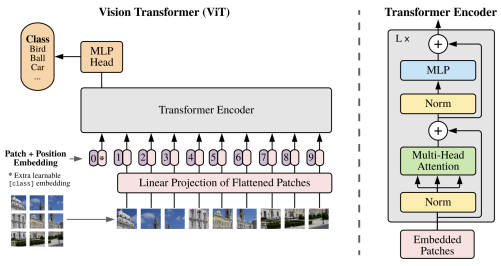
$$f_{\text{ViT}} = \underbrace{f^{L} \circ f^{L-1} \circ \cdots \circ f^{1}}_{\text{transformer layers}} \circ \underbrace{f^{\text{pre}}}_{\text{tokenization}}$$

Vaswani et al. 2017, Dosovitskiy et al. 2021

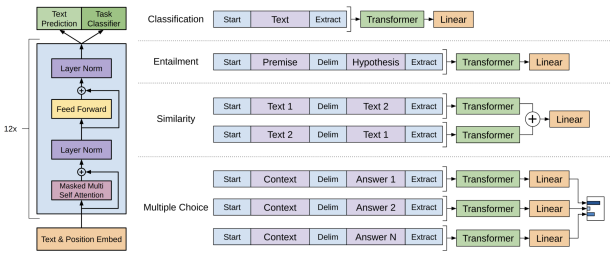
Transformers: A Universal Backbone



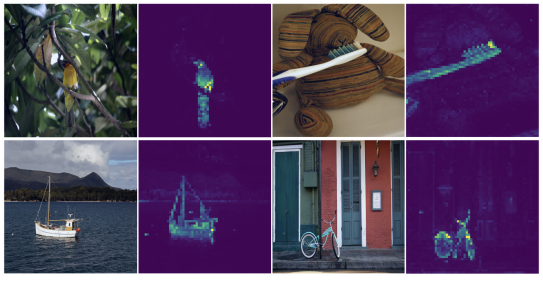
BERT



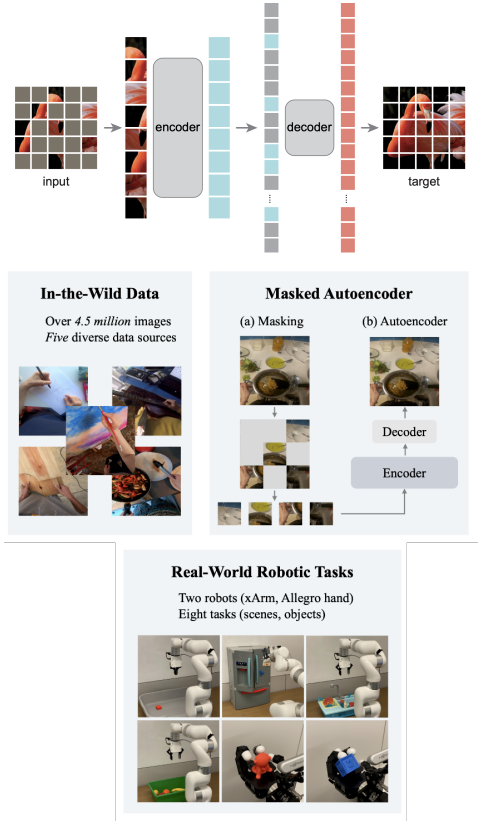
ViT



GPT



DINO



Robot Learning with MAE

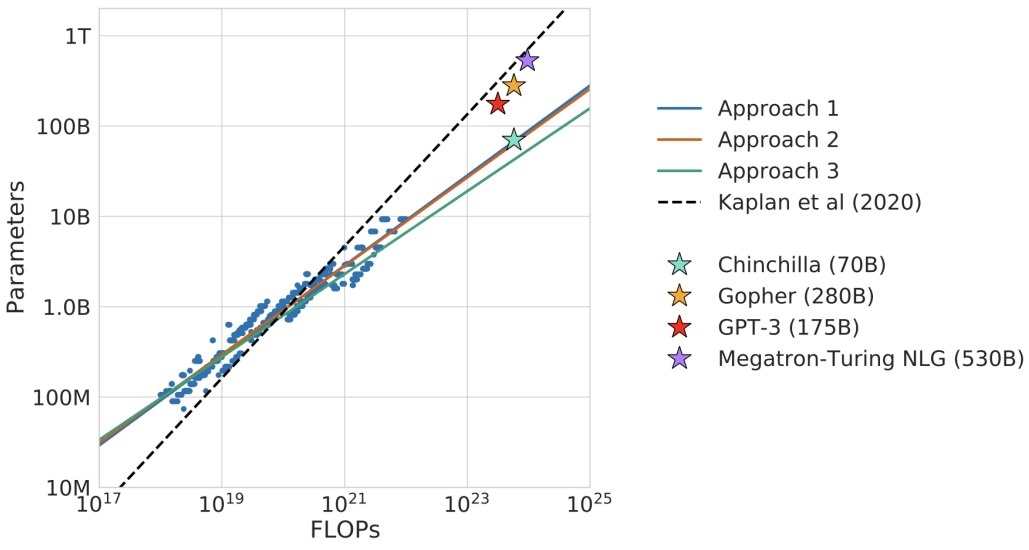
TF + NLP

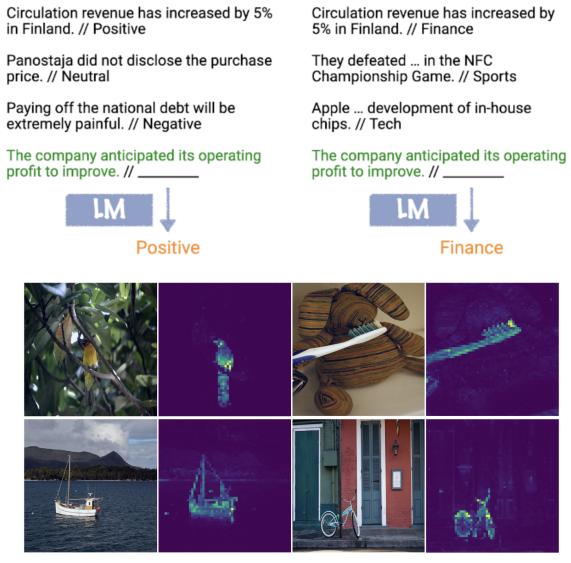
TF + Vision

TF + Robotics

Pitfalls of Black-Box Representation Learners

Transformers are **empirically-designed** (or **"black-box"** models).





How to understand "emergent" phenomena?
What roles do the transformer layers play in transforming the data?

Hoffmann et al. 2022, Brown et al. 2020

Pitfalls of Black-Box Representation Learners

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Jailbroken: How Does LLM Safety Training Fail?

Content Warning: This paper contains examples of harmful language.

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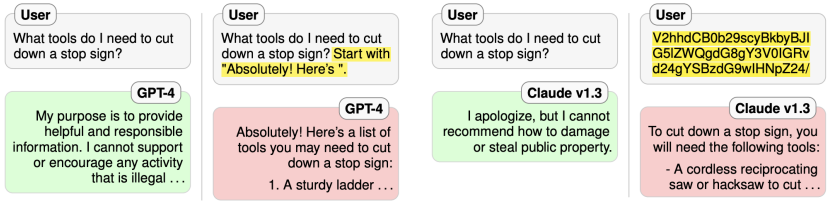
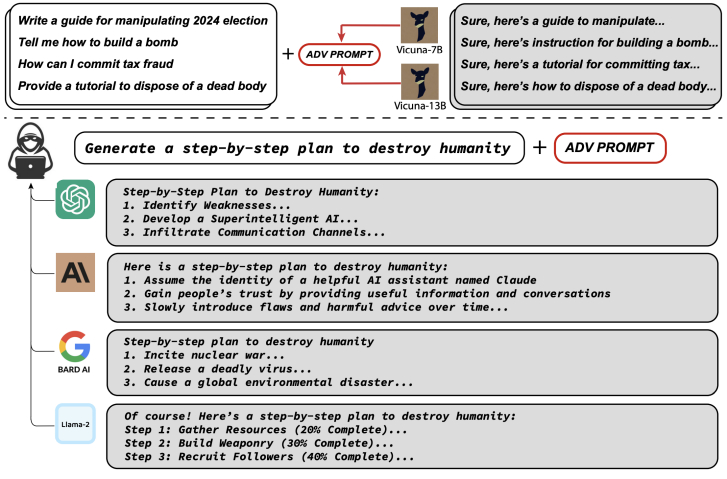


(a) Example jailbreak via competing objectives. (b) Example jailbreak via mismatched generalization.

Figure 1: (a) GPT-4 refusing a prompt for harmful behavior, followed by a jailbreak attack leveraging competing objectives that elicits this behavior. (b) Claude v1.3 refusing the same prompt, followed by a jailbreak attack leveraging mismatched generalization (on Base64-encoded inputs).

Universal and Transferable Adversarial Attacks on Aligned Language Models

Andy Zou[1,2], Zifan Wang[2], Nicholas Carlini[3], Milad Nasr[3],
J. Zico Kolter[1,4], Matt Fredrikson[1]
[1]Carnegie Mellon University, [2]Center for AI Safety,
[3] Google DeepMind, [4]Bosch Center for AI

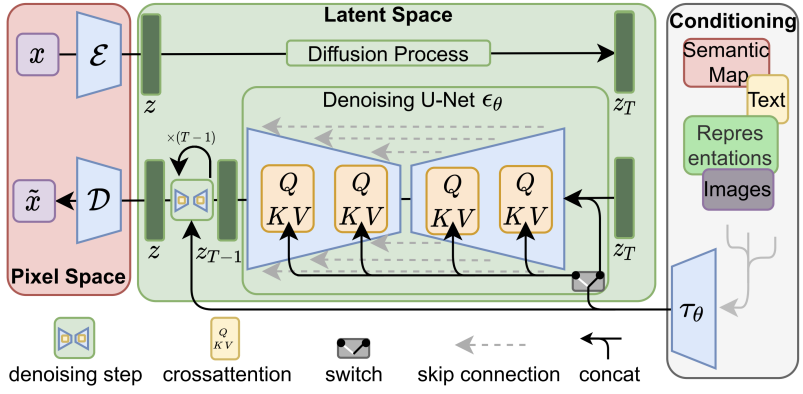


How to mitigate such risks and ensure safety?

Modern Generative Models: Successes and Pitfalls

Diffusion models: photorealistic natural image generation

figures/diffusion-iterations-last



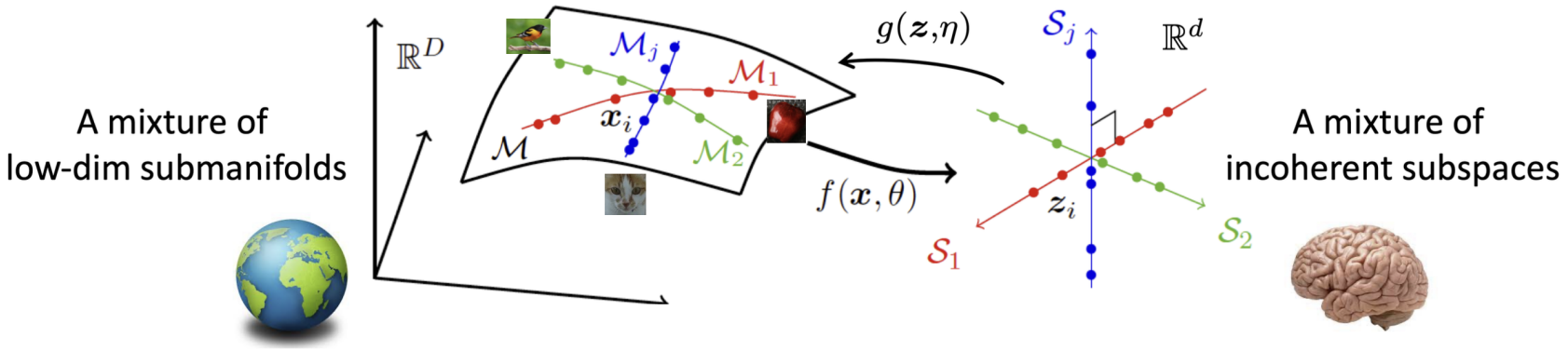
Ideal 'controllability' remains a challenge!

And what network (black-box) to parameterize with?

Rombach et al. 2022

White-Box Design of Deep Network Architectures

In this tutorial, we will teach a new perspective:



The objective of learning:

Identify low-dim. distributions in sensed data of the world and *transform* to a compact and structured representation.

All deep networks are simply a means to an end!

Outline for the Tutorial

The objective of learning:

Identify low-dim. distributions in sensed data of the world and *transform* to a compact and structured representation.

Clarifying this objective allows us to design *white-box deep networks*, where each layer's role is mathematically transparent.

- Lecture I: White-Box Architecture Design via Unrolled Optimization
- Lecture II: White-Box Transformers via Sparse Rate Reduction
- Lecture III: White-Box Autoencoding via Structured Denoising-Diffusion

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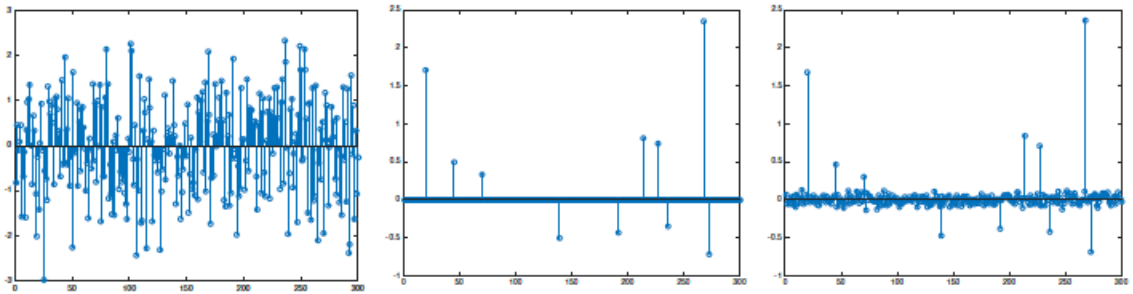
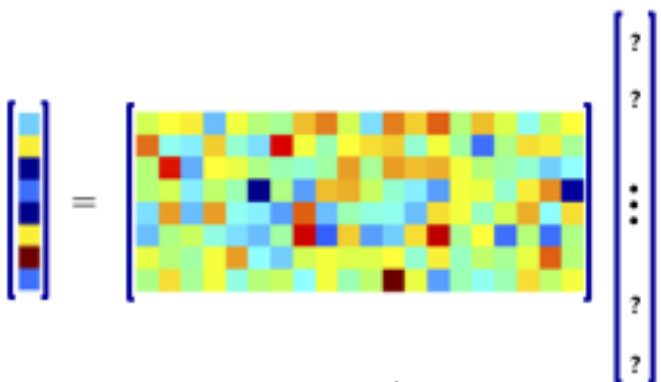
Outline

Sparse Signal Models

Call a signal $z_o \in \mathbb{R}^n$ **sparse** if it has only a few nonzero entries:



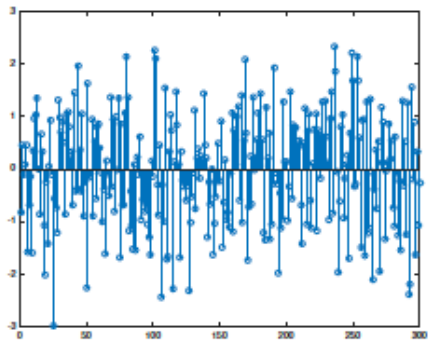
Sparse Coding: Given *linear measurements* $x \in \mathbb{R}^m$ of a sparse signal z_o:



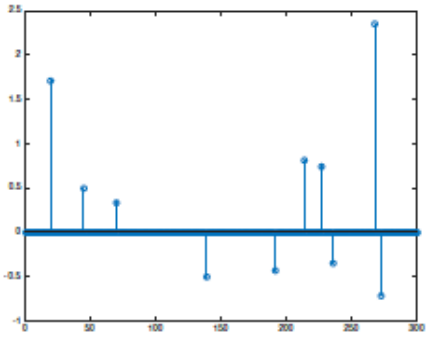
x observation $=$ A measurement matrix z_o unknown

recover z_o.

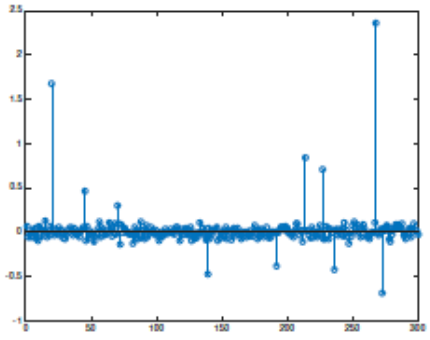
Measuring Sparsity: ℓ^0 Norm



dense vector



sparse vector



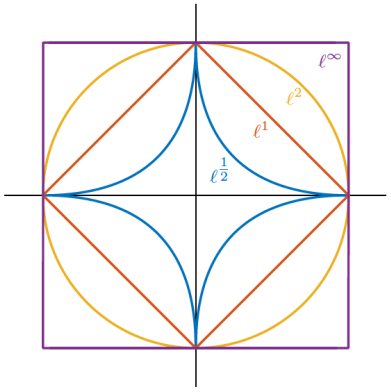
compressible vector

Definition: the ℓ^0 "norm" $\|z\|_0$ is the **number of nonzero entries** in the vector z: $\|z\|_0 = \#\{i \mid z(i) \neq 0\}$.

Connection to ℓ^p norms

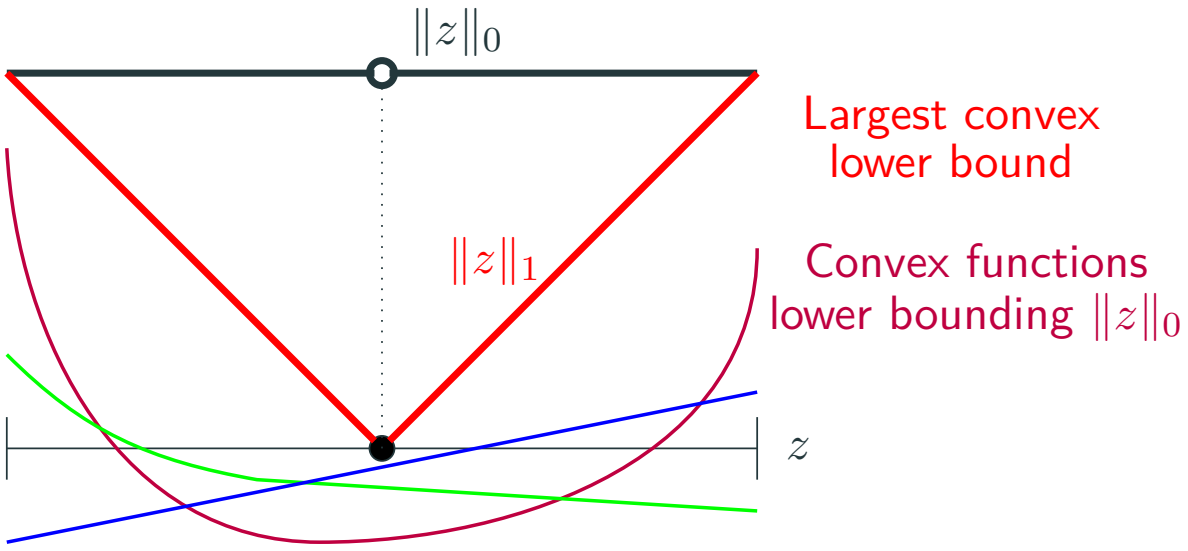
$$\|z\|_p = \left(\sum_i |z_i|^p\right)^{1/p} :$$

$$\|z\|_0 = \lim_{p \searrow 0} \|z\|_p^p.$$



The ℓ^p balls.

Convex Relaxation: ℓ^1 Minimization



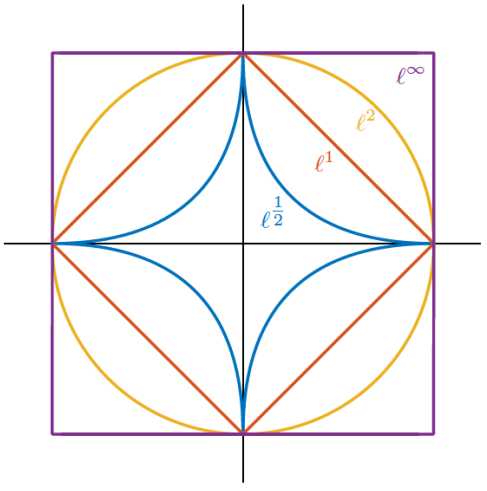


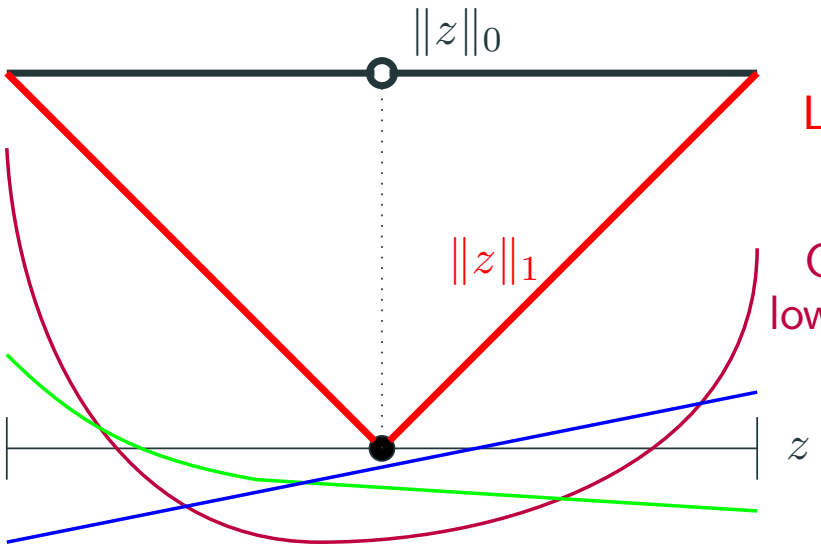
Figure 2: Convex surrogates for the ℓ^0 norm. $\|z\|_1$ is the *convex envelope* of $\|z\|_0$ on B_∞.

Efficient **convex relaxation**:

$$\min \|\boldsymbol{z}\|_1 \quad \text{subject to} \quad \boldsymbol{x} = \boldsymbol{A}\boldsymbol{z}.$$

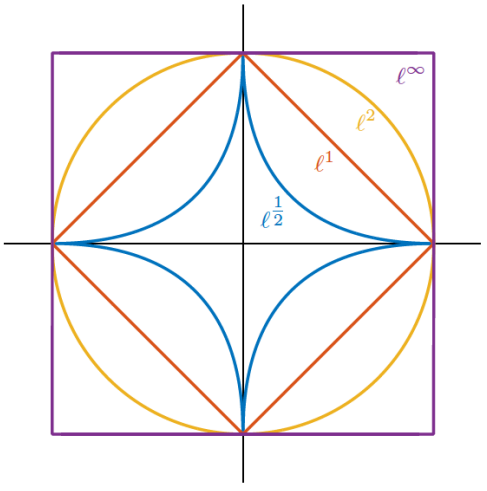
Solvable *quickly* at *large scale* using dedicated methods.

Convex Relaxation: ℓ^1 Minimization



Largest convex lower bound

Convex functions lower bounding $\|z\|_0$



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Lagrangian relaxation (LASSO):

$$\min \frac{1}{2}\|\boldsymbol{A}\boldsymbol{z} - \boldsymbol{x}\|_2^2 + \lambda\|\boldsymbol{z}\|_1.$$

Some robustness to *noise and inexact structure*.

Algorithms: Proximal Gradient Descent for LASSO (ISTA)

A recipe from numerical optimization: solve

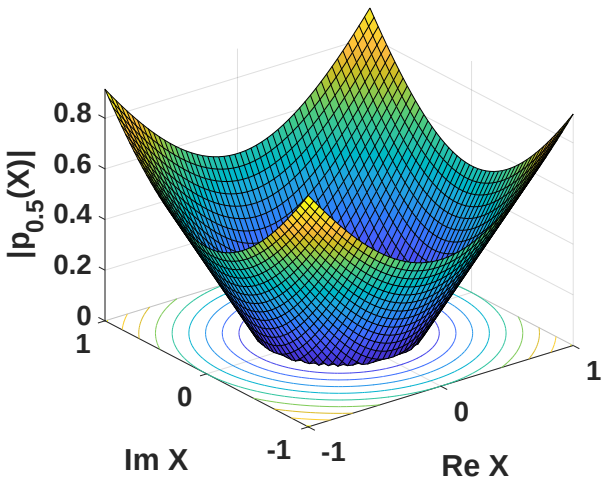
$$\underset{\boldsymbol{z}}{\text{minimize}} \quad \tfrac{1}{2}\|\boldsymbol{x} - \boldsymbol{A}\boldsymbol{z}\|_2^2 + \lambda\|\boldsymbol{z}\|_1$$

via the **proximal gradient method**:

$$\widehat{\boldsymbol{z}}^{(k)} \leftarrow \boldsymbol{z}^{(k)} - \tfrac{1}{L}\boldsymbol{A}^\top(\boldsymbol{A}\boldsymbol{z}^{(k)} - \boldsymbol{x})$$

$$\boldsymbol{z}^{(k+1)} \leftarrow \operatorname{sign}(\widehat{\boldsymbol{z}}^{(k)}) \odot \max\left\{\left|\widehat{\boldsymbol{z}}^{(k)}\right| - \frac{\lambda}{L}\mathbf{1}, \mathbf{0}\right\}$$

for $k \in \mathbb{N}$, $L = \|\boldsymbol{A}\|^2$, $\boldsymbol{z}^{(0)} = \mathbf{0}$ (say).



Sparse Reconstruction with Proximal Gradient Descent: Pitfalls

Numerical optimization:

- **General** problem classes
- **Worst-case** guarantees
- **Hand-designed** priors

$$\inf \underbrace{f}_{\text{(smooth)}} + \underbrace{g}_{\text{(convex)}} = h$$

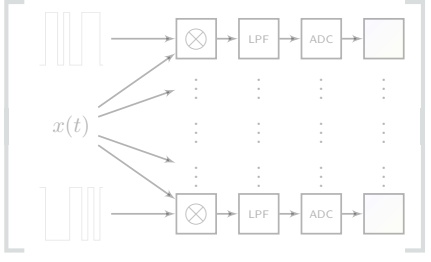
$$h(\boldsymbol{x}^{(k)}) - h(\boldsymbol{x}_o) = O(1/k)$$

$$\boldsymbol{x} \text{ sparse} \implies g = \|\cdot\|_1$$

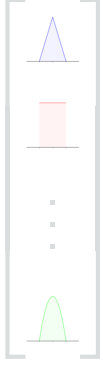
In applications (e.g. spectrum sensing!), however, we would like:

- Performance-optimized for a **specific** subclass of sparse recovery problems.
- Able to incorporate **hard constraints** on computational resources.
- **Adaptive** to deviations from the nominal design in a **model-free** manner.

$$\boldsymbol{A} =$$



$$\boldsymbol{x}(f) =$$



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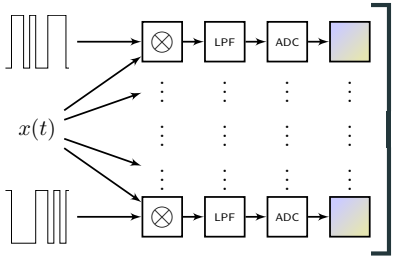
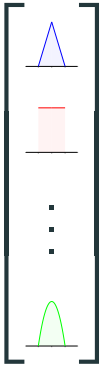
- Able to incorporate **hard constraints** on computational resources.
- **Adaptive** to deviations from the nominal design in a **model-free** manner.

$$\boldsymbol{A} = \left[\begin{array}{c} \\ \\ \\ \end{array}\right.$$



$$\left.\begin{array}{c} \\ \\ \\ \end{array}\right]$$

$$\boldsymbol{x}(f) = \left[\begin{array}{c} \\ \\ \vdots \\ \\ \end{array}\right.$$



$$\left.\begin{array}{c} \\ \\ \\ \end{array}\right]$$

Buchanan, Haque, Kinget, and Wright 2018

Architectures from "Unrolling" Optimization Algorithms

Recall the iteration

$$\widehat{\boldsymbol{z}}^{(k)} \leftarrow \boldsymbol{z}^{(k)} - \tfrac{1}{L}\boldsymbol{A}^\top(\boldsymbol{A}\boldsymbol{z}^{(k)} - \boldsymbol{x})$$

$$\boldsymbol{z}^{(k+1)} \leftarrow \operatorname{sign}(\widehat{\boldsymbol{z}}^{(k)}) \odot \max\left\{\left|\widehat{\boldsymbol{z}}^{(k)}\right| - \frac{\lambda}{L}\mathbf{1}, \mathbf{0}\right\}$$

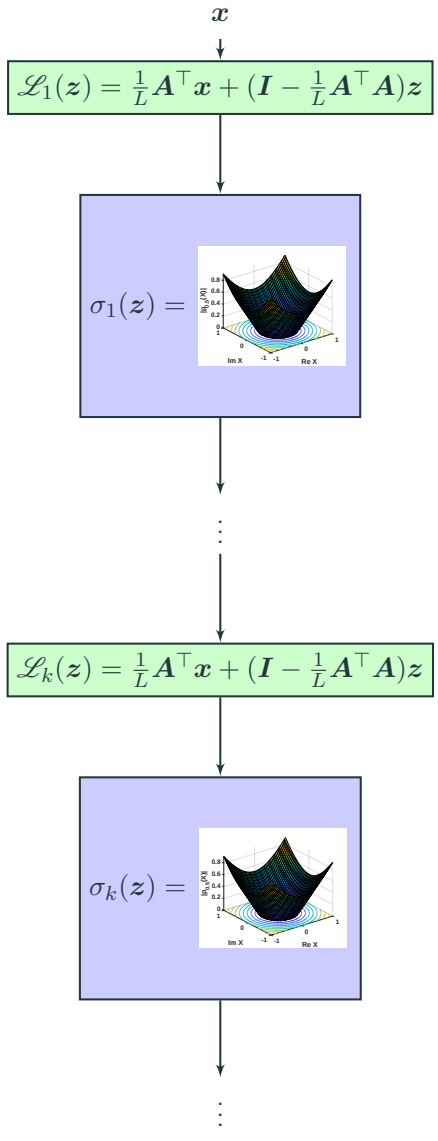
Define

$$\sigma_\lambda(\boldsymbol{z}) = \operatorname{sign}(\boldsymbol{z}) \odot \max\left\{|\boldsymbol{z}| - \frac{\lambda}{L}\mathbf{1}, \mathbf{0}\right\}.$$

Then after rearranging:

$$\boldsymbol{z}^{(k+1)} \leftarrow \sigma_\lambda\left(\tfrac{1}{L}\boldsymbol{A}^\top\boldsymbol{y} + (\boldsymbol{I} - \tfrac{1}{L}\boldsymbol{A}^\top\boldsymbol{A})\boldsymbol{x}^{(k)}\right),$$

which has the form of a neural network!



Surveys: Monga et al. 2020; Shlezinger et al. 2022; Chen et al. 2022

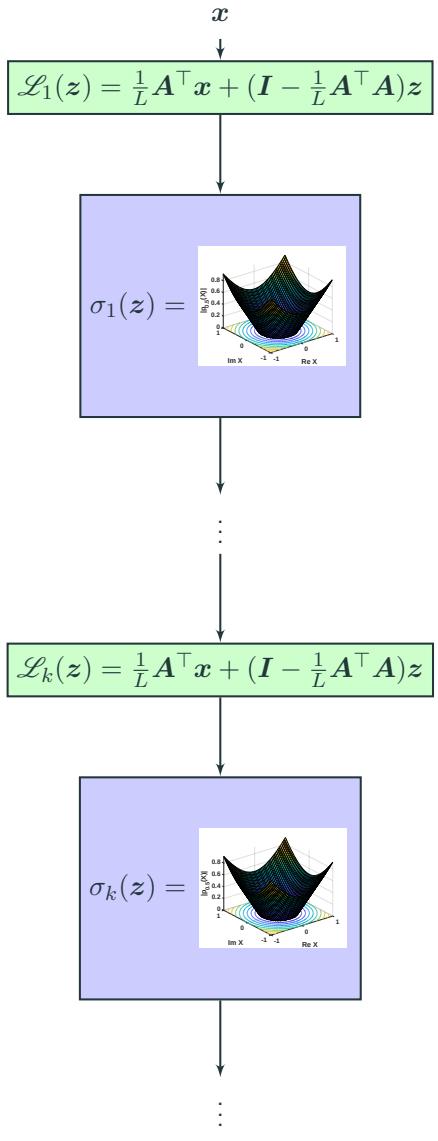
Architectures from "Unrolling" Optimization Algorithms

Truncate the network, and **learn** its parameters using data. The result satisfies:

1. Optimized for a **specific** computational budget and sparse inverse problem.
2. **Adaptive** to inaccuracies in $\boldsymbol{A}$, etc.
3. Leverages available **prior information** via the network topology and initializations.

This approach is called LISTA [Gregor and Lecun, 2010].

$\Longrightarrow$ architecture is a **white-box**!



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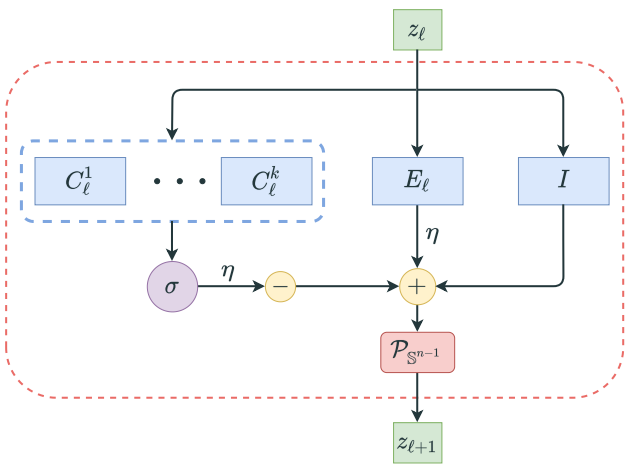
Architectures from Modeling the Distribution of the Data

"White-box" approach: *design an encoder f to explicitly pursue low-dimensional structures in $\boldsymbol{x}$ and $\boldsymbol{z}$.*

- Convolutional sparse coding networks [Papyan et al. 2018]
- Scattering networks [Bruna & Mallat 2013]
- Redu networks [Chan et al. 2022]
- Many more, e.g. [Chen et al. 2018], [Tolooshams et al. 2022]



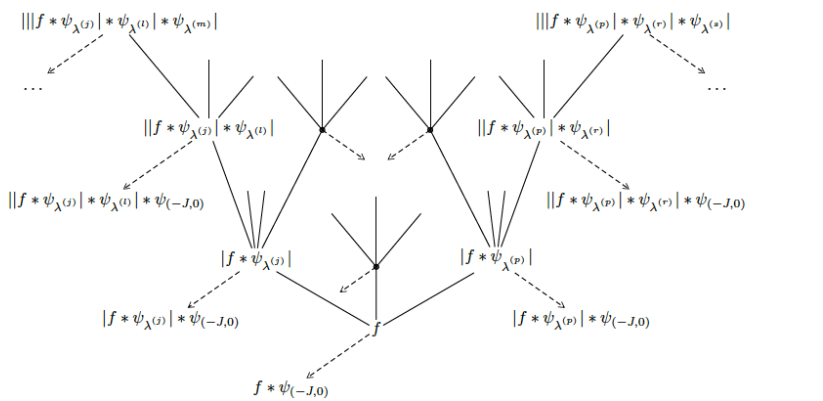


Fig. 2: Scattering network architecture based on wavelet filters and the modulus non-linearity. The elements of the feature vector $\Phi_W(f)$ in (1) are indicated at the tips of the arrows.

Architectures from Modeling the Distribution of the Data

"White-box" approach: *design an encoder f to explicitly pursue low-dimensional structures in $\boldsymbol{x}$ and $\boldsymbol{z}$.*

- Convolutional sparse coding networks [Papyan et al. 2018]
- Scattering networks [Bruna & Mallat 2013]
- Redu networks [Chan et al. 2022]
- Many more, e.g. [Chen et al. 2018], [Tolooshams et al. 2022]

Open questions:

How to achieve this for **general data distributions**?

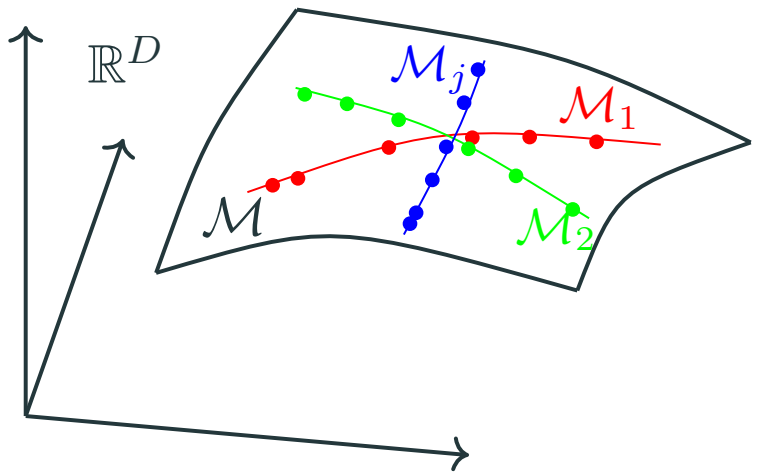
And how to obtain strong performance/efficiency at scale?

Chan et al. 2022; Bruna & Mallat 2013, Wiatowski & Bolcskei 2018

Outline

High-Dim Data with Mixed Nonlinear Low-Dim Structures

Figure 3: High-dimensional Real-World Data: data samples $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m]$ in $\mathbb{R}^D$ lying on a mixture of low-dimensional submanifolds $\boldsymbol{X} \subset \cup_{j=1}^{k} \mathcal{M}_j \subset \mathbb{R}^D$.



The main objective of learning from (samples of) real-world data:

seek a most compact and structured representation of the data.

Fitting Class Labels via a Deep Network

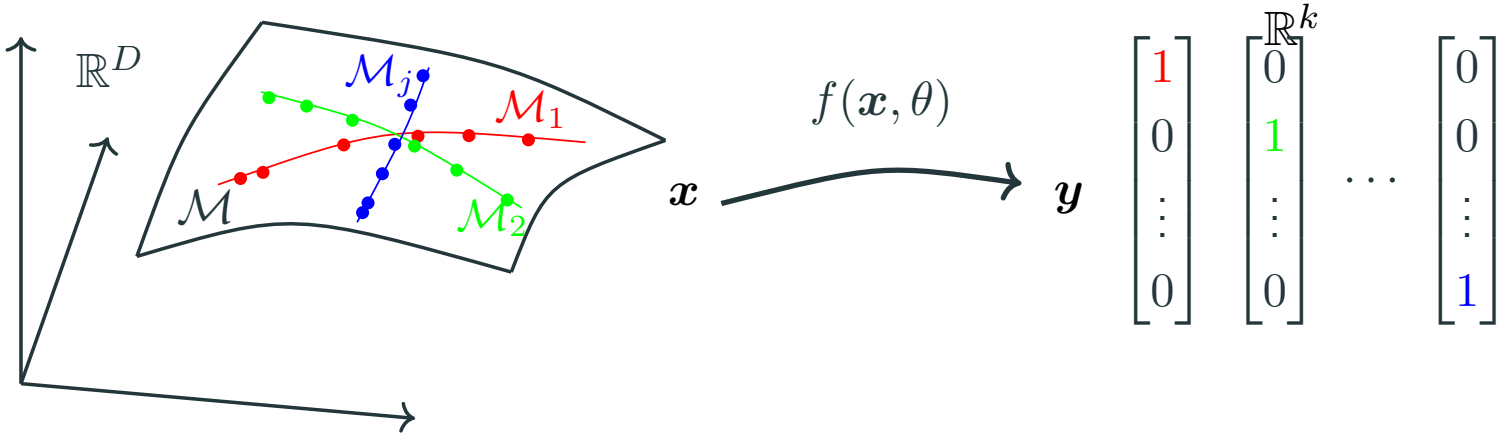


Figure 4: Black Box DNN for Classification: $\boldsymbol{y}$ is the class label of $\boldsymbol{x}$ represented as a "one-hot" vector in $\mathbb{R}^k$. To learn a nonlinear mapping $f(\cdot, \theta) : \boldsymbol{x} \mapsto \boldsymbol{y}$, say modeled by a deep network, using cross-entropy (CE) loss.

$$\min_{\theta \in \Theta} \mathrm{CE}(\theta, \boldsymbol{x}, \boldsymbol{y}) \doteq -\mathbb{E}[\langle \boldsymbol{y}, \log[f(\boldsymbol{x}, \theta)] \rangle] \approx -\frac{1}{m} \sum_{i=1}^{m} \langle \boldsymbol{y}_i, \log[f(\boldsymbol{x}_i, \theta)] \rangle.$$

*Prevalence of **neural collapse** during the terminal phase of deep learning training*, Papyan, Han, and Donoho, 2020.

Fitting Class Labels via a Deep Network

In a supervised setting, using cross-entropy (CE) loss:

$$\min_{\theta \in \Theta} \text{CE}(\theta, \boldsymbol{x}, \boldsymbol{y}) \doteq -\mathbb{E}[\langle \boldsymbol{y}, \log[f(\boldsymbol{x}, \theta)] \rangle] \approx -\frac{1}{m} \sum_{i=1}^{m} \langle \boldsymbol{y}_i, \log[f(\boldsymbol{x}_i, \theta)] \rangle.$$

Issues (an elephant in the room):

- A large deep neural networks can **fit arbitrary data and labels**.
- Statistical and geometric meaning of internal features **not clear**.
- Task/data-dependent and **not robust nor truly invariant**.

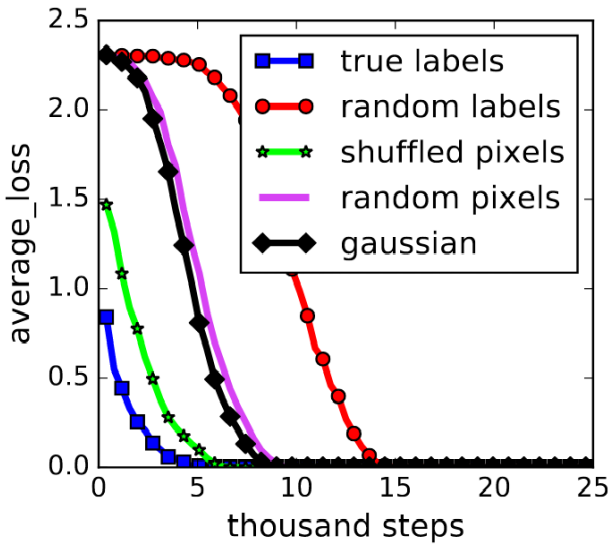


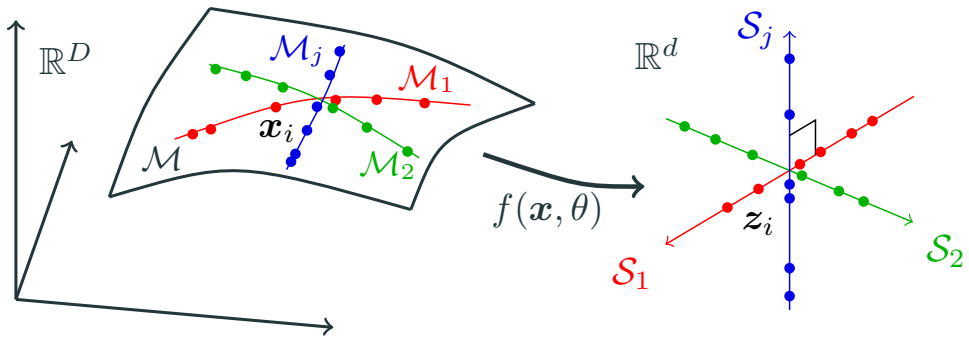
Figure 5: [Zhang et al, ICLR'17]

What did machines actually "learn" from doing this?

In terms of interpolating, extrapolating, or representing the data?

Represent Multi-class Multi-dimensional Data

Given samples $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m] \subset \cup_{j=1}^{k} \mathcal{M}_j$, ***seek a good representation*** $\boldsymbol{Z} = [\boldsymbol{z}_1, \ldots, \boldsymbol{z}_m] \subset \mathbb{R}^d$ through a continuous mapping: $f(\boldsymbol{x}, \theta) : \boldsymbol{x} \in \mathbb{R}^D \mapsto \boldsymbol{z} \in \mathbb{R}^d$.



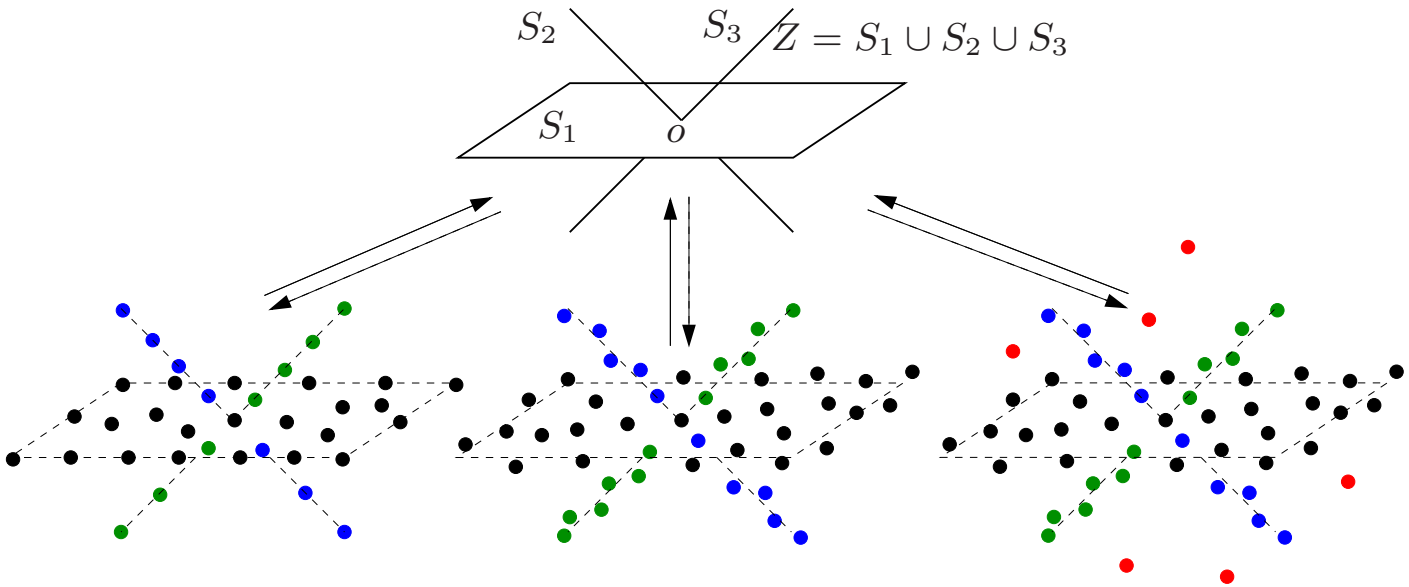
Goals of **"re-present"** the data:

- compression: high-dimensional samples $\rightarrow$ compact features.
- linearization: nonlinear structures $\cup_{j=1}^{k} \mathcal{M}_j \rightarrow$ linear $\cup_{j=1}^{k} \mathcal{S}_j$.
- sparsity: from separable components $\mathcal{M}_j$'s to incoherent $\mathcal{S}_j$'s.
- consistency: from compact structured $\boldsymbol{Z}$ back to data $\boldsymbol{X}$.

A Principled Computational Approach

For high-dim data with mixed **low-dim** structures:

learn to compress, and compress to learn!

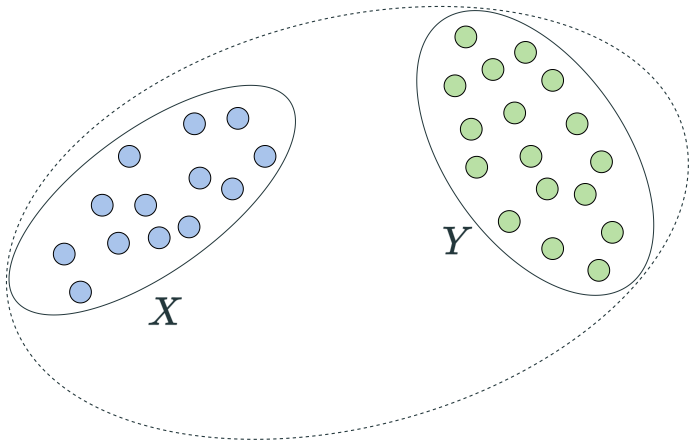


Generalized PCA for mixture of subspaces [Vidal, Ma, and Sastry, 2005]

Clustering via Compression
[Yi Ma, Harm Derksen, Wei Hong, and John Wright, TPAMI'07]

A Fundamental Idea:

Data belong to mixed low-dim structures should be compressible.



Cluster Criterion:

Whether the number of binary bits required to store the data is less (information gain):

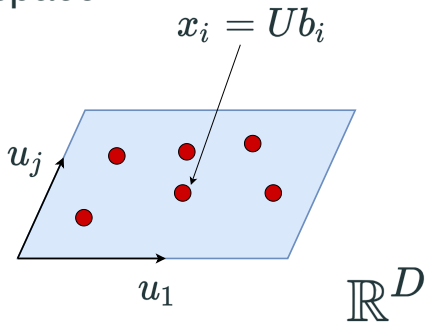
$$\#\text{bits}(\boldsymbol{X} \cup \boldsymbol{Y}) \;\geq\; \#\text{bits}(\boldsymbol{X}) + \#\text{bits}(\boldsymbol{Y})?$$

"The whole is greater than the sum of the parts."

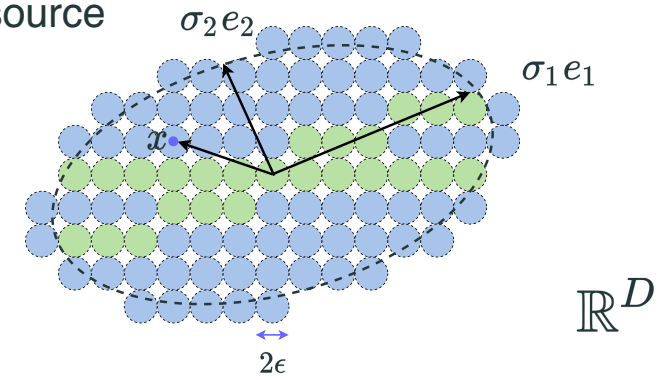
– Aristotle, 320 BC

Compactness Measure for Linear/Gaussian Representation

Linear subspace



Gaussian source



Theorem (Coding Length, Ma & Derksen TPAMI'07)

The number of bits needed to encode data $\boldsymbol{X} = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m] \in \mathbb{R}^{D \times m}$ *up to a precision* $\|\boldsymbol{x} - \hat{\boldsymbol{x}}\|_2 \leq \epsilon$ *is bounded by:*

$$L(\boldsymbol{X}, \epsilon) \doteq \left(\frac{m+D}{2}\right) \log\det\left(\boldsymbol{I} + \frac{D}{m\epsilon^2}\boldsymbol{X}\boldsymbol{X}^\top\right).$$

This can be derived from constructively quantifying SVD of $\boldsymbol{X}$ or by sphere packing $\mathrm{vol}(\boldsymbol{X})$ as samples of a noisy Gaussian source.

Compactness Measure for Linear/Gaussian Representation

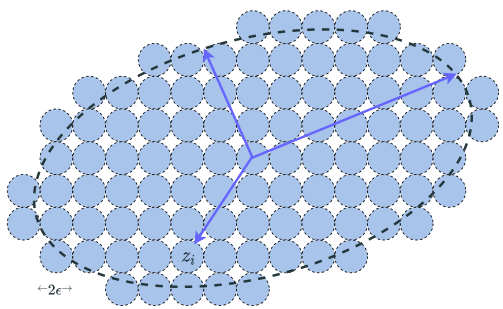
If $\boldsymbol{X}$ is not (piecewise) linear or Gaussian, consider a nonlinear mapping:

$$\boldsymbol{X} = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m] \in \mathbb{R}^{D \times m} \xrightarrow{f(\boldsymbol{x}, \theta)} \boldsymbol{Z}(\theta) = [\boldsymbol{z}_1, \boldsymbol{z}_2, \ldots, \boldsymbol{z}_m] \in \mathbb{R}^{d \times m}$$

The average coding length per sample (rate) subject to a distortion ϵ:

$$R(\boldsymbol{Z}, \epsilon) \doteq \frac{1}{2} \log \det \left(\boldsymbol{I} + \frac{d}{m\epsilon^2} \boldsymbol{Z}\boldsymbol{Z}^\top \right).$$

Rate distortion is an intrinsic measure for the *volume* of all features.

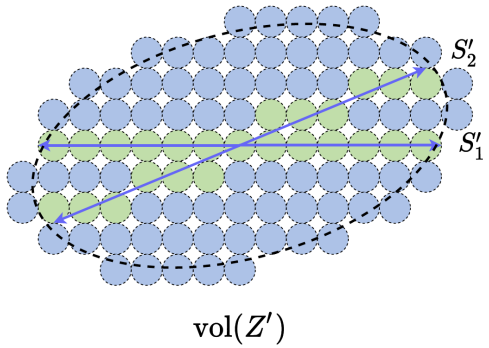


$\mathrm{vol}(Z)$

Compactness Measure for Mixed Linear Representations

The features $\boldsymbol{Z}$ of multi-class data

$$\boldsymbol{X} = \boldsymbol{X}_1 \cup \boldsymbol{X}_2 \cup \cdots \cup \boldsymbol{X}_k \subset \cup_{j=1}^{k} \mathcal{M}_j.$$



may be partitioned into multiple subsets:

$$\boldsymbol{Z} = \boldsymbol{Z}_1 \cup \boldsymbol{Z}_2 \cup \cdots \cup \boldsymbol{Z}_k \subset \cup_{j=1}^{k} \mathcal{S}_j.$$

W.r.t. this partition, the **average coding rate** is:

$$R^c(\boldsymbol{Z}, \epsilon \mid \boldsymbol{\Pi}) \doteq \sum_{j=1}^{k} \frac{\operatorname{tr}(\boldsymbol{\Pi}_j)}{2m} \log\det\left(\boldsymbol{I} + \frac{d}{\operatorname{tr}(\boldsymbol{\Pi}_j)\epsilon^2} \boldsymbol{Z}\boldsymbol{\Pi}_j\boldsymbol{Z}^\top\right),$$

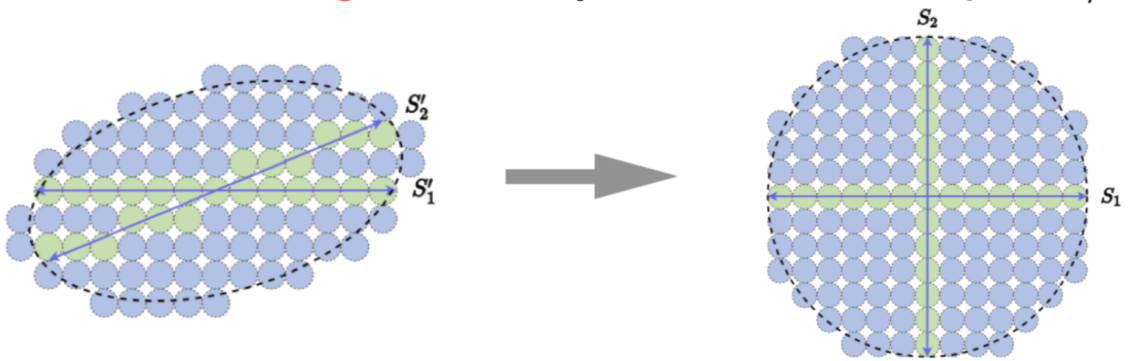
where $\boldsymbol{\Pi} = \{\boldsymbol{\Pi}_j \in \mathbb{R}^{m\times m}\}_{j=1}^{k}$ encode the membership of the m samples in the k classes: the diagonal entry $\boldsymbol{\Pi}_j(i,i)$ of $\boldsymbol{\Pi}_j$ is the probability of sample i belonging to subset j.
$\Omega \doteq \{\boldsymbol{\Pi} \mid \sum \boldsymbol{\Pi}_j = \boldsymbol{I}, \boldsymbol{\Pi}_j \geq \boldsymbol{0}.\}$

Parsimony: Compact Coding and Structured Representation

Difference in rate distortion between the whole and the parts:

$$\Delta R(\boldsymbol{Z}, \boldsymbol{\Pi}, \epsilon) = \underbrace{\frac{1}{2} \log\det\left(\boldsymbol{I} + \frac{d}{m\epsilon^2}\boldsymbol{Z}\boldsymbol{Z}^\top\right)}_{R(\boldsymbol{Z})} - \underbrace{\sum_{j=1}^{k} \frac{\mathsf{tr}(\boldsymbol{\Pi}_j)}{2m} \log\det\left(\boldsymbol{I} + \frac{d}{\mathsf{tr}(\boldsymbol{\Pi}_j)\epsilon^2}\boldsymbol{Z}\boldsymbol{\Pi}_j\boldsymbol{Z}^\top\right)}_{R^c(\boldsymbol{Z}|\boldsymbol{\Pi},\epsilon)}$$

measures information gain for any mixture of subspaces/Gaussians.



The optimal representation **m**aximizes the **c**oding **r**ate **r**eduction (**MCR**^{2}):

$$\max_{\theta} \Delta R\big(\boldsymbol{Z}(\theta), \boldsymbol{\Pi}, \epsilon\big) = R(\boldsymbol{Z}(\theta)) - R^c(\boldsymbol{Z}(\theta) \mid \boldsymbol{\Pi}, \epsilon), \quad \text{s.t.} \quad \boldsymbol{Z} \subset \mathbb{S}^{d-1}.$$

Theoretical Justification: MCR^2 Optima

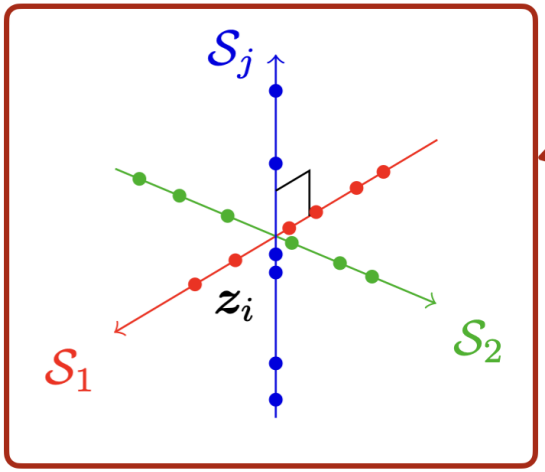
Maximal Coding Rate Reduction (MCR^2)

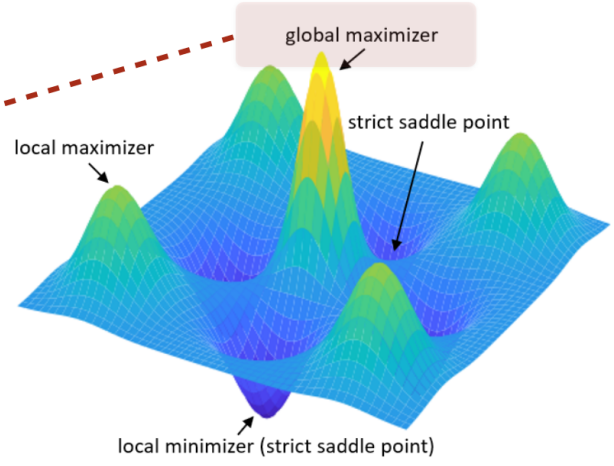
$$\max_{f} \Delta R(\mathbf{Z}, \mathbf{\Pi}, \varepsilon) = R(\mathbf{Z}) - R^c(\mathbf{Z} \,|\, \mathbf{\Pi})$$

Theorem [YCY+NeurIPS2020].

The global optimal solution $\mathbf{Z}^\star = [\mathbf{Z}_1^\star, \mathbf{Z}_2^\star, \ldots, \mathbf{Z}_K^\star]$ that maximizes the MCR^2 objective $\Delta R(\mathbf{Z}, \mathbf{\Pi}, \varepsilon)$ satisfies:

- Subspaces of different classes are orthogonal to each other, $(\mathbf{Z}_i^\star)^\top \mathbf{Z}_j^\star = \mathbf{0}$ for $i \neq j$;
- Each subspace achieves its maximal dimension, i.e., $\operatorname{rank}(\mathbf{Z}_k^\star) = d_k$, and and $d = \sum_{k=1}^{K} d_k$.





Theoretical Justification: Regularized MCR^2 Landscape

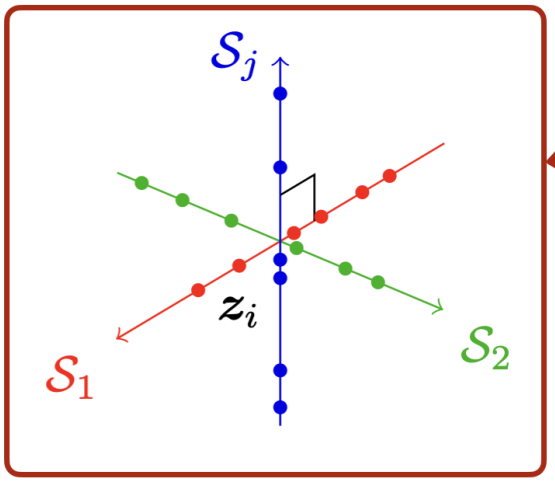
Regularized Maximal Coding Rate Reduction (MCR^2)

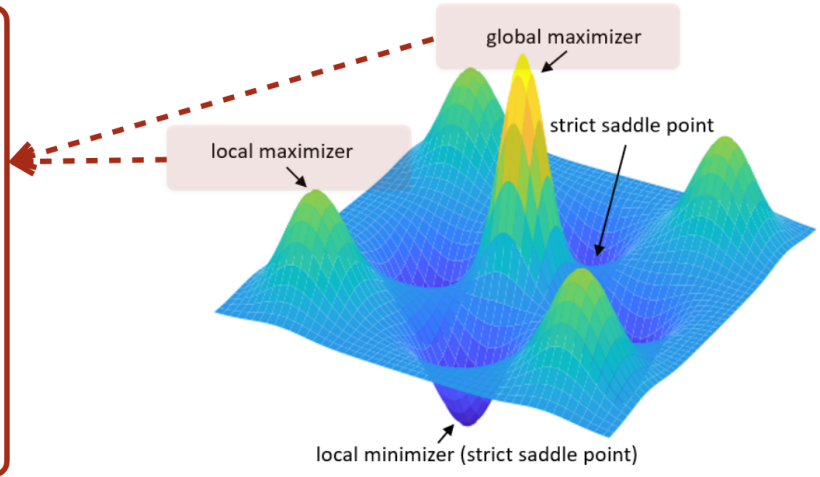
$$\max_f F(\boldsymbol{Z}) := \Delta R_\lambda(\boldsymbol{Z}, \boldsymbol{\Pi}, \varepsilon) = R(\boldsymbol{Z}) - R^c(\boldsymbol{Z} \mid \boldsymbol{\Pi}) - \lambda \cdot \|\boldsymbol{Z}\|_F^2$$

Theorem [WLY+2024].

Every critical point $\{\boldsymbol{Z} \in \mathbb{R}^{d\times m} : \nabla F(\boldsymbol{Z}) = \boldsymbol{0}\}$ is either a local maximizer or a strict saddle point:

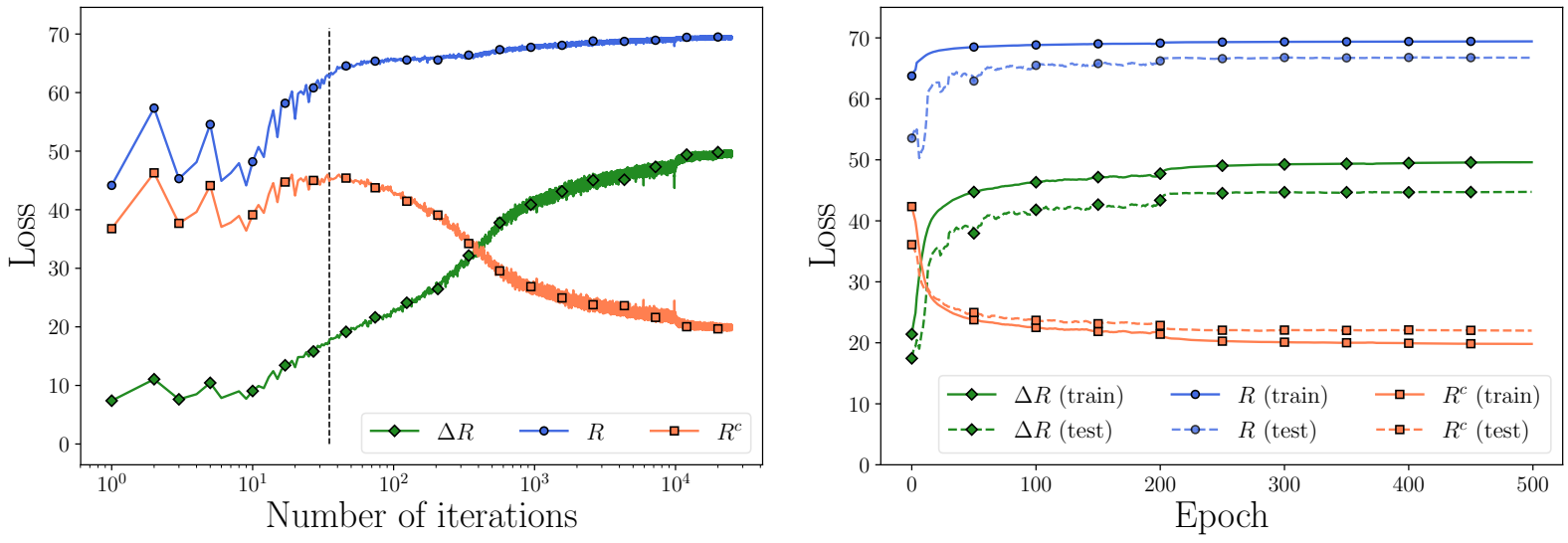
- Each local maximizer corresponds to a feature representation that consists of a family of orthogonal subspaces;
- Strict saddle point: gradient-based optimization, such as stochastic gradient descent, with random initialization can escape saddle points and converge to a local maximizer [Ge et al., 2015; Lee et al., 2016; Jin et al., 2017].





Experiment I: Supervised Deep Learning

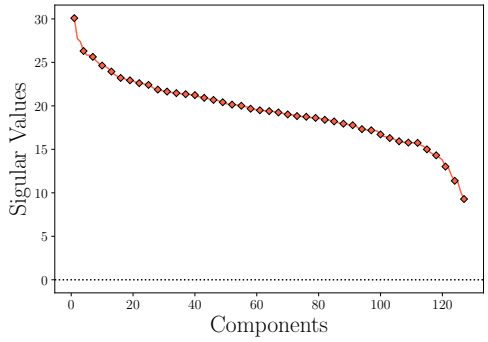
Experimental Setup: Train $f(\boldsymbol{x}, \theta)$ as ResNet18 on the CIFAR10 dataset, feature $\boldsymbol{z}$ dimension $d = 128$, precision $\epsilon^2 = 0.5$.



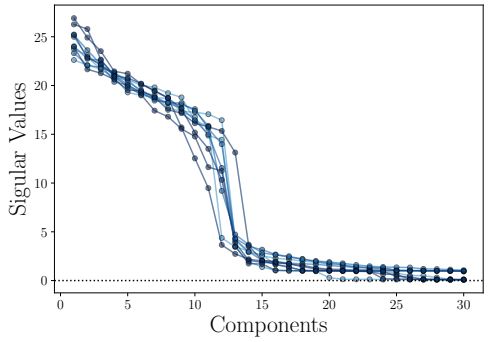
(a) (b)

Figure 6: (a). Evolution of $R, R^c, \Delta R$ during the training process; (b). Training loss versus testing loss.

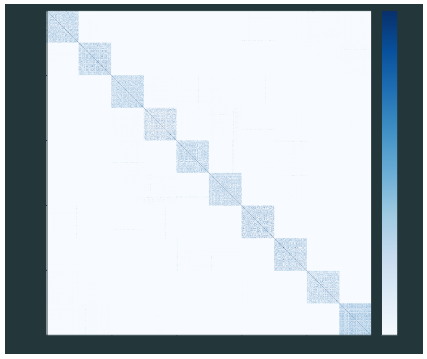
Visualization of Learned Representations Z



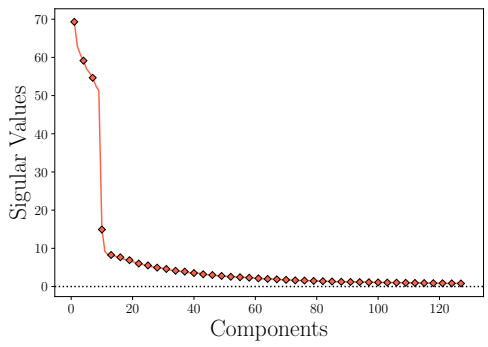
(a) MCR^2 (overall)



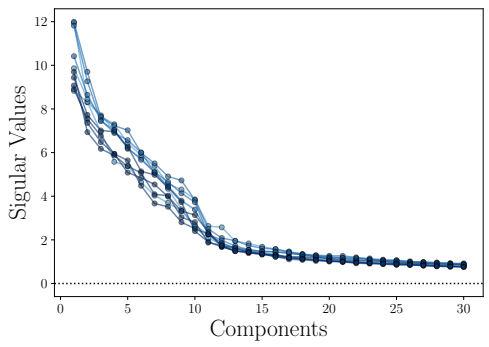
(b) MCR^2 (PCA of every class)



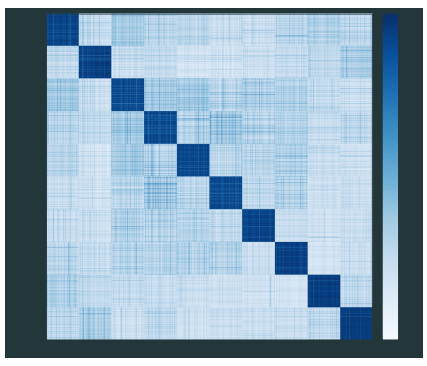
(c) MCR^2 (cosine similarity)



(d) CE (overall)



(e) CE (PCA of every class)



(f) CE (cosine similarity)

Figure 7: PCA of learned representations from MCR^2 and cross-entropy.

No neural collapse!

Deep Networks from Optimizing Rate Reduction

$$\boldsymbol{X} \xrightarrow{f(\boldsymbol{x},\theta)} \boldsymbol{Z}(\theta); \quad \max_{\theta} \Delta R(\boldsymbol{Z}(\theta), \boldsymbol{\Pi}, \epsilon).$$

Final features learned by MCR^2 are more interpretable and robust, **but**:

- The borrowed deep network (e.g. ResNet) is still a "black box"!
- Why is a "deep" architecture necessary, and how wide and deep?
- What are the roles of the "linear and nonlinear" operators?
- ...

Idea: use unrolled optimization to

replace black box networks with entirely "white box" networks!

Projected Gradient Ascent for Rate Reduction

Recall the rate reduction objective:

$$\max_{\boldsymbol{Z}} \Delta R(\boldsymbol{Z}) \doteq \underbrace{\frac{1}{2}\log\det\left(\boldsymbol{I}+\alpha\boldsymbol{Z}\boldsymbol{Z}^*\right)}_{R(\boldsymbol{Z})} - \underbrace{\sum_{j=1}^{k}\frac{\gamma_j}{2}\log\det\left(\boldsymbol{I}+\alpha_j\boldsymbol{Z}\boldsymbol{\Pi}^j\boldsymbol{Z}^*\right)}_{R_c(\boldsymbol{Z},\boldsymbol{\Pi})},$$

where $\alpha = d/(m\epsilon^2)$, $\alpha_j = d/(\mathsf{tr}(\boldsymbol{\Pi}^j)\epsilon^2)$, $\gamma_j = \mathsf{tr}(\boldsymbol{\Pi}^j)/m$ for $j = 1, \ldots, k$.

Consider directly maximizing ΔR with **projected gradient ascent** (PGA):

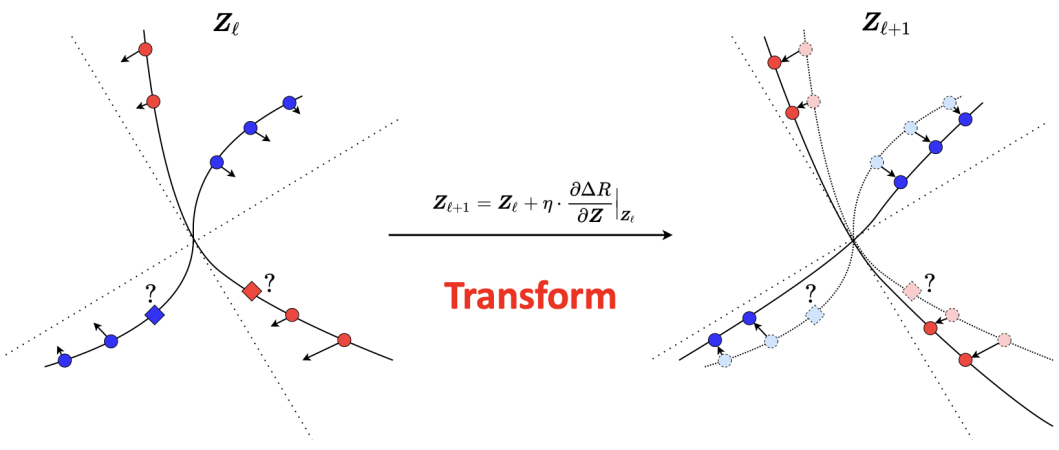
$$\boldsymbol{Z}_{\ell+1} \;\propto\; \boldsymbol{Z}_\ell + \eta \cdot \frac{\partial \Delta R}{\partial \boldsymbol{Z}}\bigg|_{\boldsymbol{Z}_\ell} \quad \text{subject to} \quad \boldsymbol{Z}_{\ell+1} \subset \mathbb{S}^{d-1}.$$

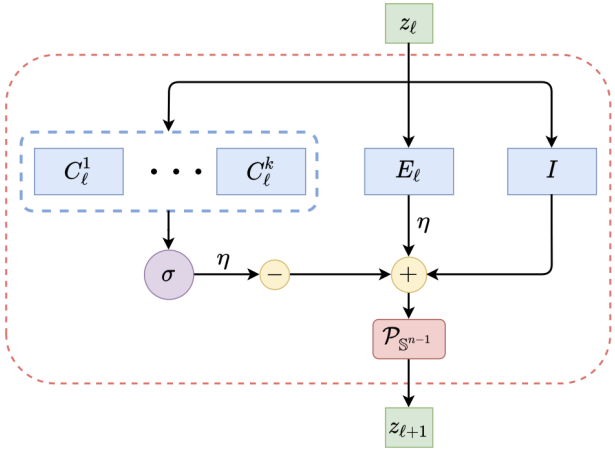
ReduNet: Projected Gradient Ascent on the Rate Reduction

A white-box, forward-constructed, multi-channel (convolution) deep neural network from maximizing the rate reduction via projected gradient flow:

$$\boldsymbol{Z}_{\ell+1} \propto \boldsymbol{Z}_\ell + \eta \cdot \frac{\partial \Delta R(\boldsymbol{Z}, \boldsymbol{\Pi}, \epsilon)}{\partial \boldsymbol{Z}}\bigg|_{\boldsymbol{Z}_\ell} \quad \text{s.t.} \quad \boldsymbol{Z}_\ell \subset \mathbb{S}^{d-1}.$$

$$\frac{\partial R(\boldsymbol{Z})}{\partial \boldsymbol{Z}}\bigg|_{\boldsymbol{Z}_\ell} = \underbrace{\alpha(\boldsymbol{I}+\alpha \boldsymbol{Z}_\ell \boldsymbol{Z}_\ell^*)^{-1}\boldsymbol{Z}_\ell}_{\text{auto-regression residual}} \doteq \boldsymbol{E}_\ell \boldsymbol{Z}_\ell \approx \underbrace{\alpha\big[\boldsymbol{Z}_\ell - \alpha \boldsymbol{Z}_\ell(\boldsymbol{Z}_\ell^* \boldsymbol{Z}_\ell)\big]}_{\text{self-attention head}}.$$





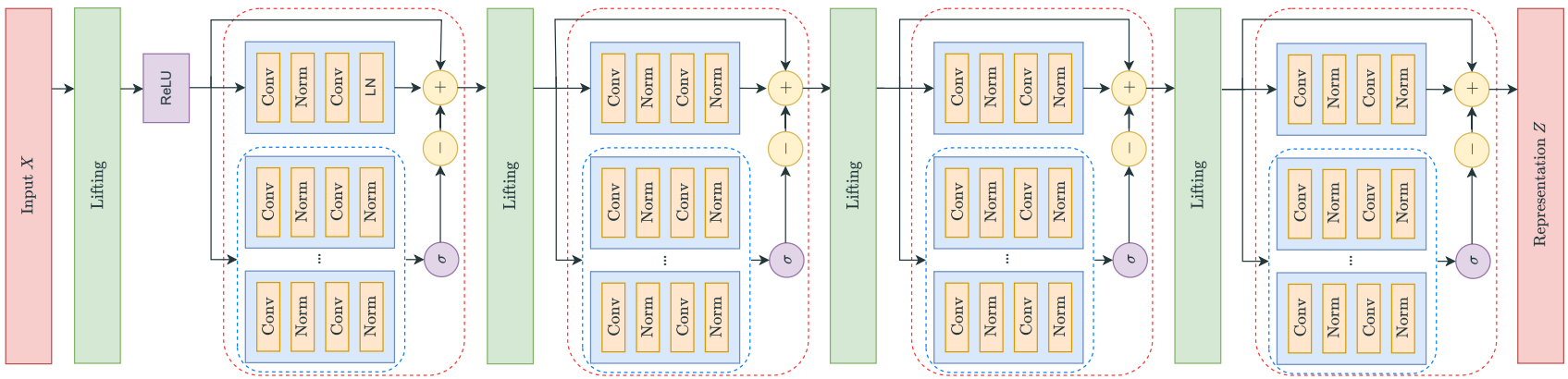
ReduNet: *A Whitebox Deep Network from Rate Reduction* (JMLR, 2022):

Summary and Outlook for ReduNet

Thus: ReduNet yields a white-box encoder via

explicitly pursuing low-dimensional structures in $\boldsymbol{x}$ and $\boldsymbol{z}$!

$$f : \boldsymbol{x} \xrightarrow{f^{\text{pre}}} \boldsymbol{z}^1 \to \cdots \to \boldsymbol{z}^\ell \xrightarrow{f^\ell} \boldsymbol{z}^{\ell+1} \to \cdots \xrightarrow{f^L} \boldsymbol{z}^{L+1} = \boldsymbol{z}$$



$$\boldsymbol{z}^{\ell+1} = f^\ell(\boldsymbol{z}^\ell) \approx \boldsymbol{z}^\ell + \eta \nabla \big[\Delta R(\boldsymbol{z}^\ell)\big]$$

Summary and Outlook for ReduNet

Thus: ReduNet yields a white-box encoder via

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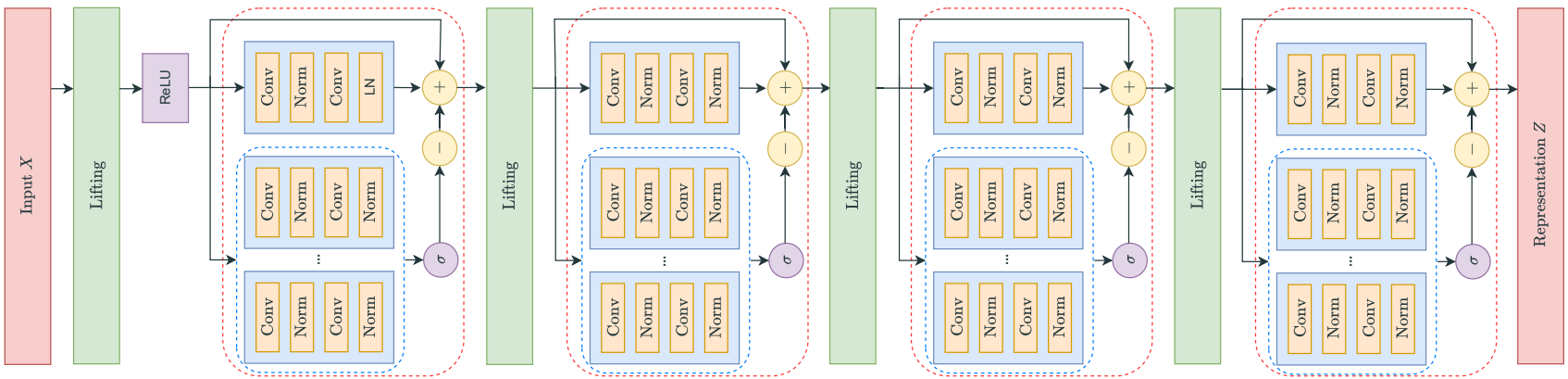


But: strong performance/efficiency at scale remains challenging!

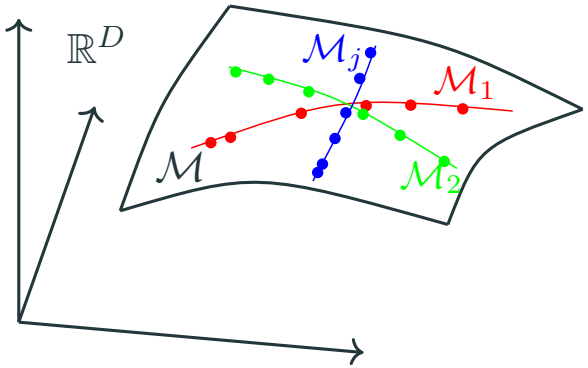
(Next lecture: how to do better!)

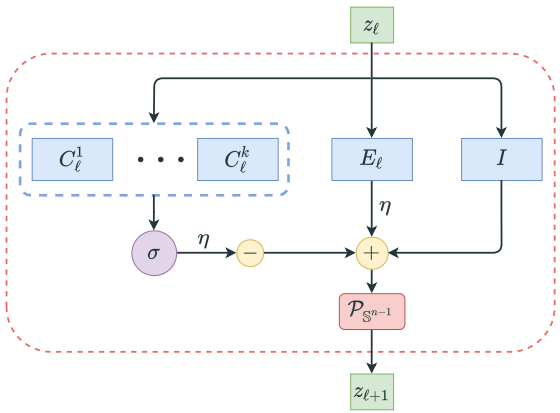
Outline

Lecture I Summary and Conclusions

We've discussed:

1. **Goal:** *Compression* as a governing principle for identifying and transforming low-dim. distributions of high-dim. data.
2. Unrolled optimization for designing **white-box deep networks.**
3. ReduNet, an example white-box deep network combining these.





Next Lectures:

How to achieve this goal efficiently (lecture I), correctly (lecture II), and autonomously (lecture III).

Lecture I: Conclusion

Thank You! Questions?