CSCI 1470/2470
Spring 2024

Ritambhara Singh

March 20, 2024
Wednesday

Interpretability cont. + Unsupervised learning

Deep Learning

Instructor office hours are cancelled this week!
No class this Friday!

ChatGPT prompt “minimalist landscape painting of a deep underwater scene with a blue tang fish in the bottom right corner”

Interpretation in DL

(1) Model architecture based methods

(2) Gradient-based methods

(3) Model agnostic methods

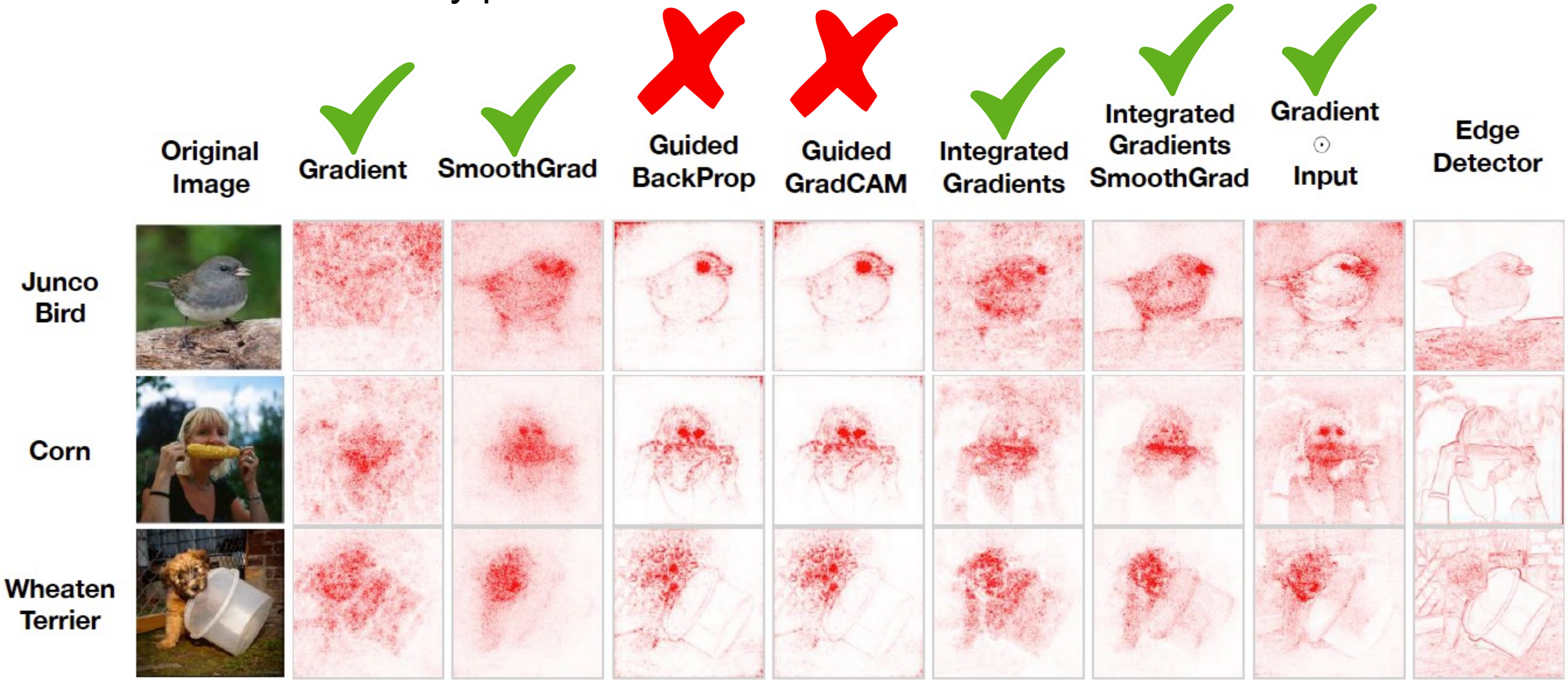
Testing different gradient-based methods

Model parameter randomization test compares the output of a saliency method on a trained model with the output of the saliency method on a randomly initialized untrained network of the same architecture.

Data randomization test compares a given saliency method applied to a model trained on a labeled data set with the method applied to the same model architecture but trained on a copy of the data set in which we randomly permuted all labels.

"We find that reliance, solely, on visual assessment can be misleading.

Through extensive experiments we show that some existing saliency methods are independent both of the model and of the data generating process."



[Sanity Checks for Saliency Maps]

Interpretation in DL

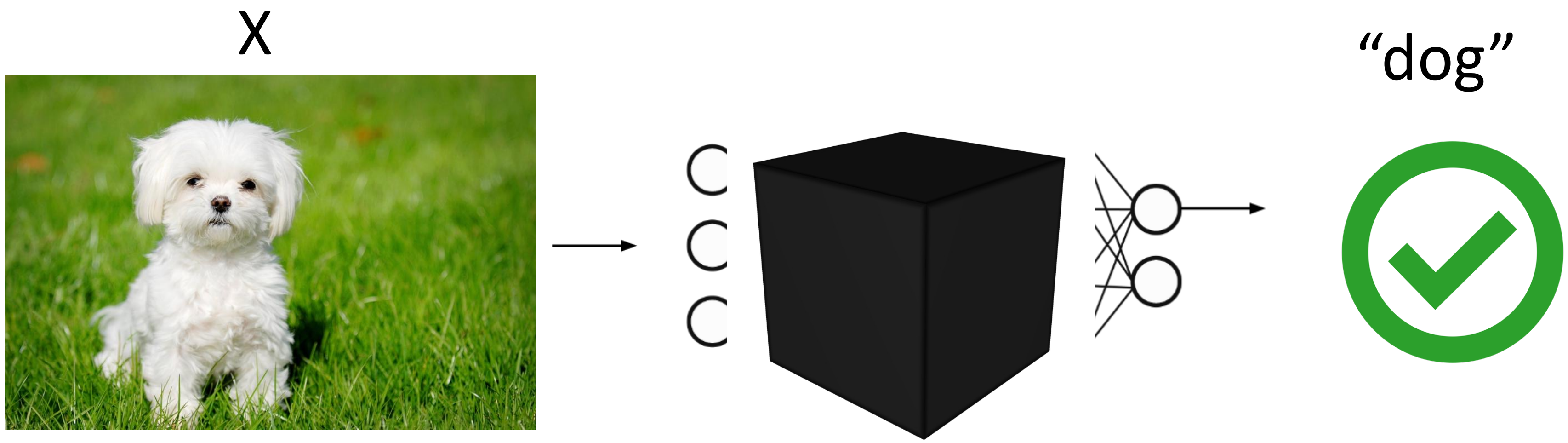
(1) Model architecture based methods

(2) Gradient-based methods

(3) Model agnostic methods

What is the simplest thing that comes to mind?

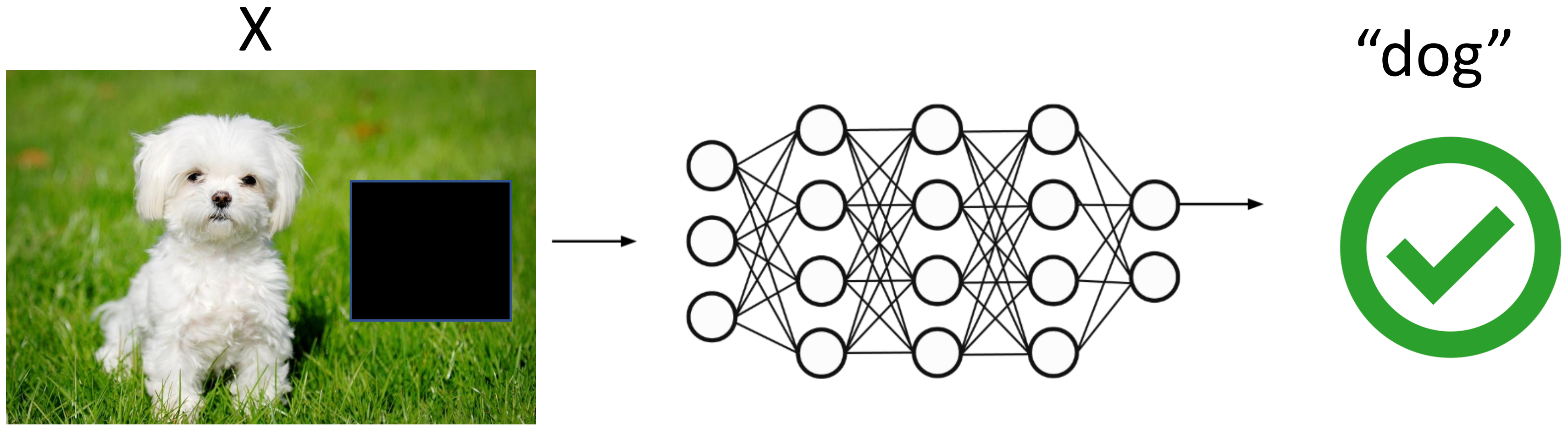
Task formulation



Which pixels are most important for classification?

Perturbation-based methods

- Let’s **perturb inputs**…
- omit or change words/parts of images, change word embedding values, etc.
- …**observe changed outputs**…



Perturbation-based methods

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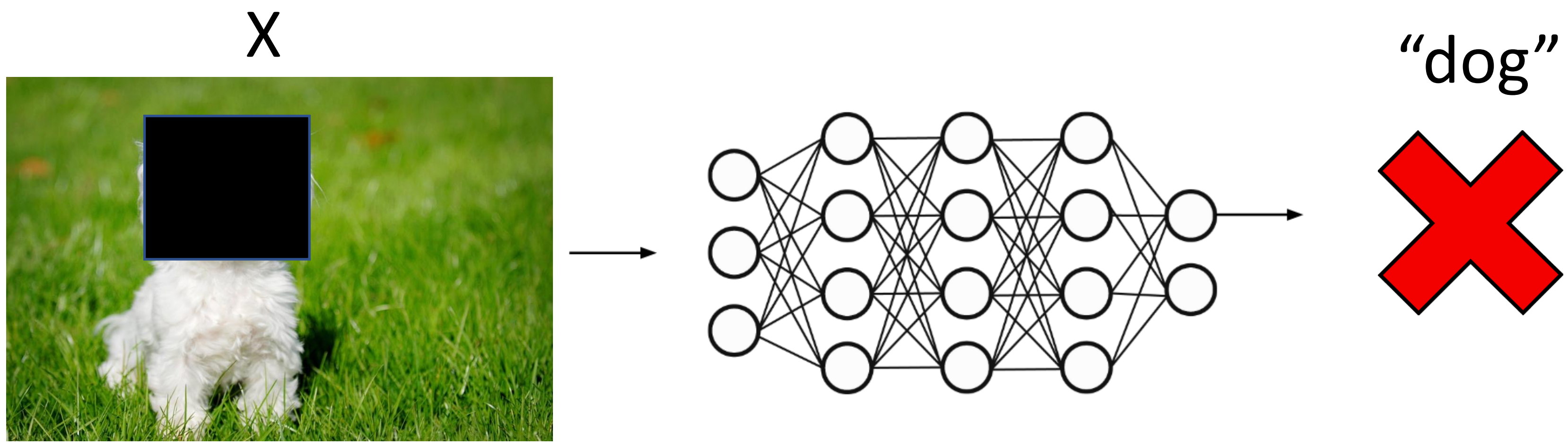


LIME

- Local Interpretable Model-Agnostic Explanations (LIME)
  - “Model-Agnostic”: treats every model as a black-box
- Let’s **perturb inputs**...
  - omit or change words/parts of images, change word embedding values, etc.
- ...**observe changed outputs**...
- ...and **approximate the underlying model** using a simple, interpretable model (like a linear classifier)
  - Interpretable because in $\sum w_i x_i$, the weights say “how much a particular input matters”

LIME example

- What makes this picture of a tree frog “tree frog”-y to a neural network?

Original Image

LIME example

- Perform a superpixel segmentation on the image
- Interpretable chunks in the image may be part of multiple superpixels
- But no superpixel will contain multiple interpretable parts

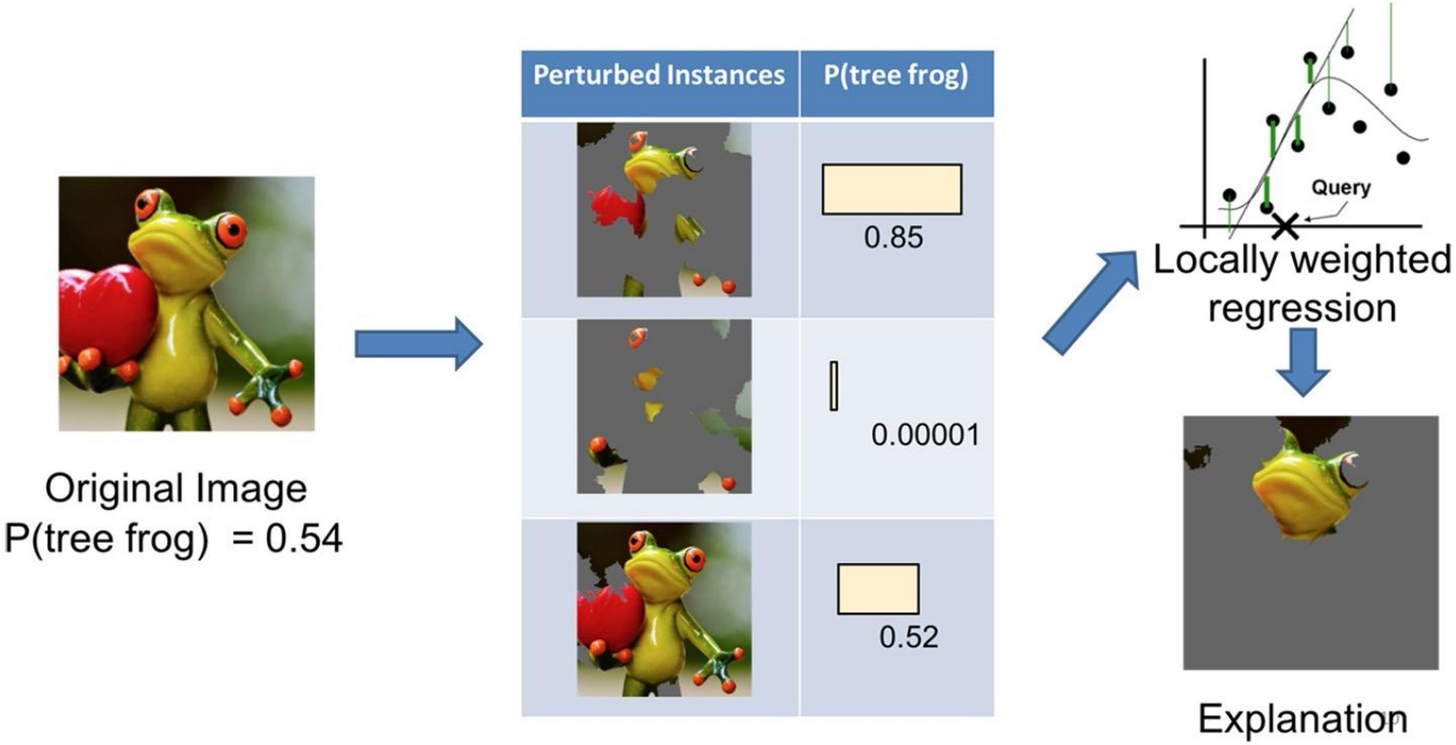
Original Image

Interpretable Components

Can we think of disadvantages of perturbation-based methods?

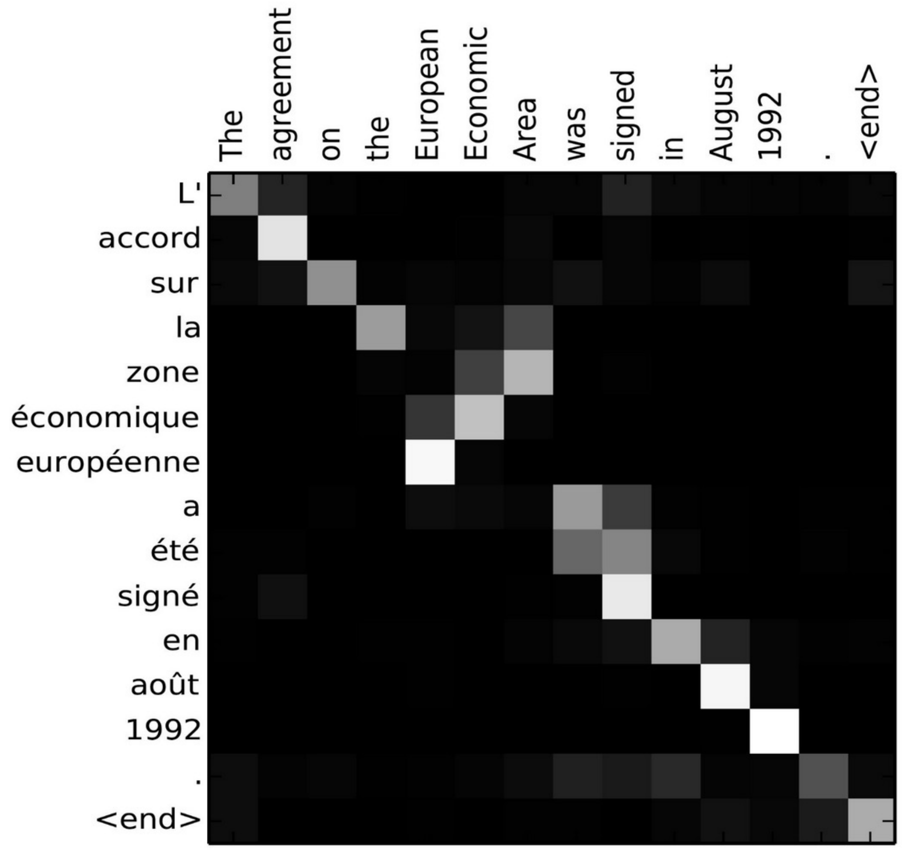
LIME example

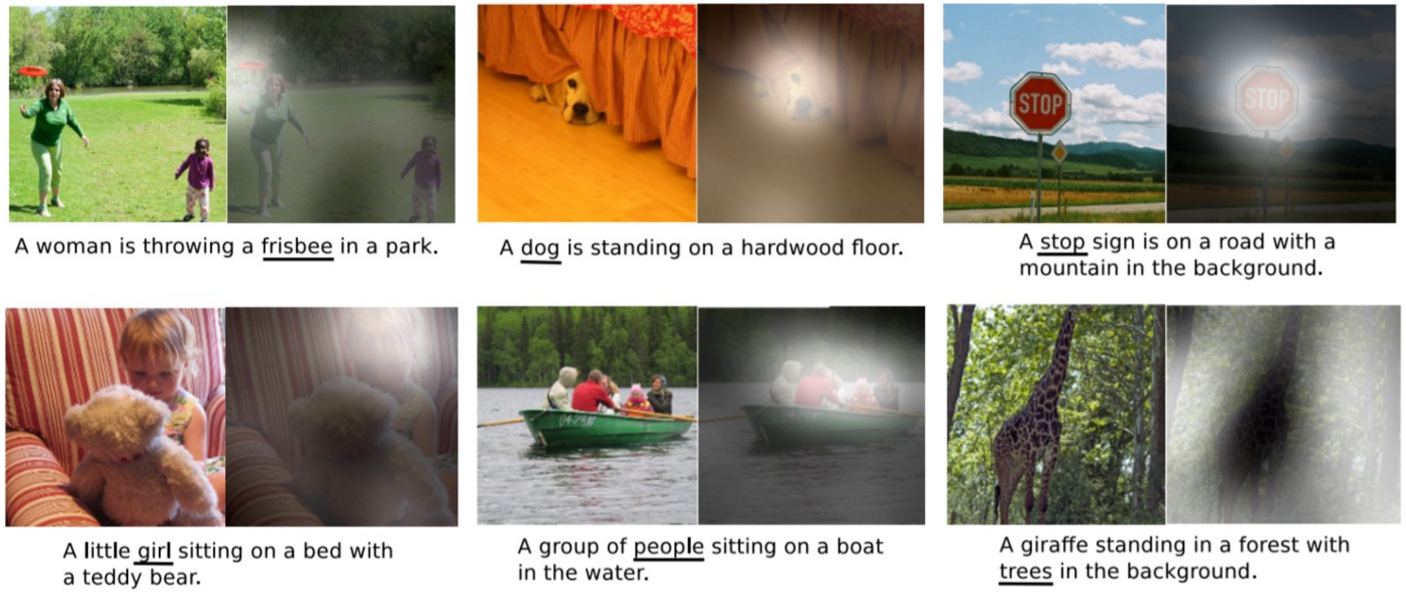
- Different combinations of chunks put through the net yield different probabilities
- Learn a linear model to predict the probability from these different combos
- Chunks with high weight in the linear model “matter more” for the classification result



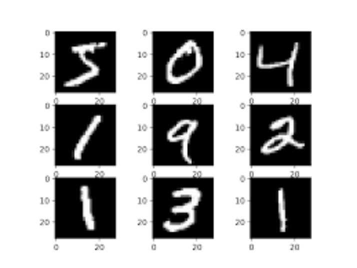
Any questions?

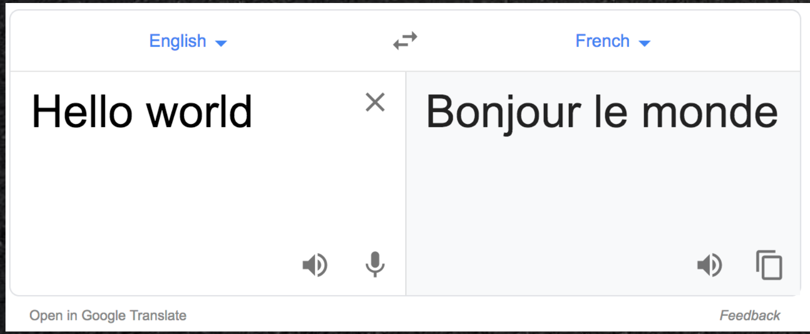
Attention as interpretation method





Roadmap





Supervised machine learning

Perceptron

Fully Connected Neural Networks

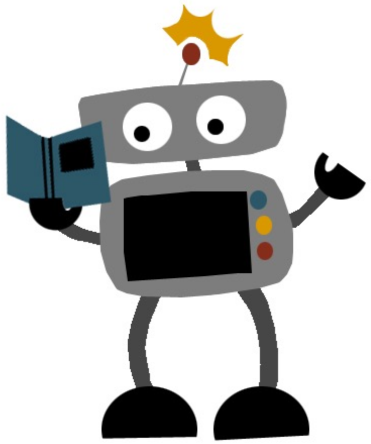
Convolutional Neural Networks

Language models

Recurrent Neural Networks

Transformers (Seq2seq)

Recap: What is Machine Learning?



Input: X

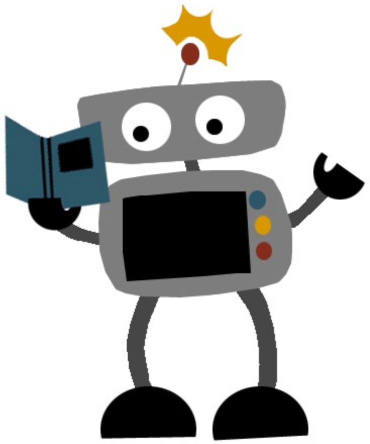
Output: Y

”Cooking?”

Function: f

$\boxed{f(X) \rightarrow Y}$

Recap: What is Machine Learning?



Supervised Learning

Input: X

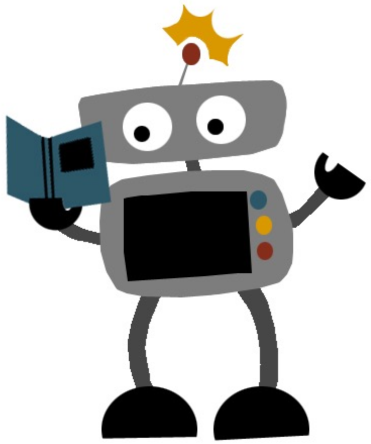
Learned function: f

Output: Y

”Cooking?”

$f(X) \rightarrow Y$

What if you don’t have any labels?



Input: X

Unsupervised Learning

What can you learn from just input data without labels?

Today's goal – learn about unsupervised learning using deep learning models

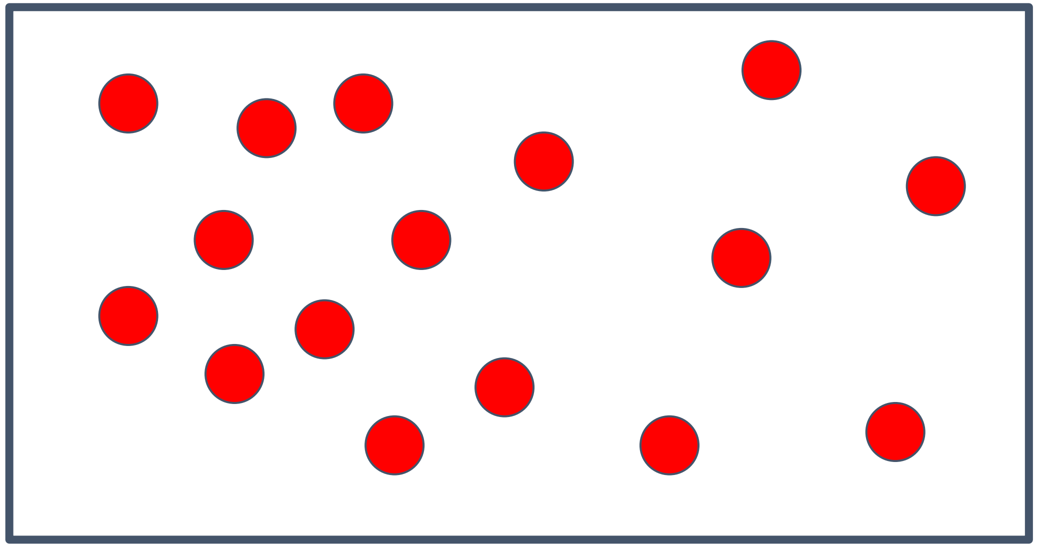
(1) Unsupervised Learning

(2) Auto-encoders (AE)

Unsupervised Learning

- What can we learn from input data when there are no labels?
  - We can only analyze the structure of the data itself

Data:

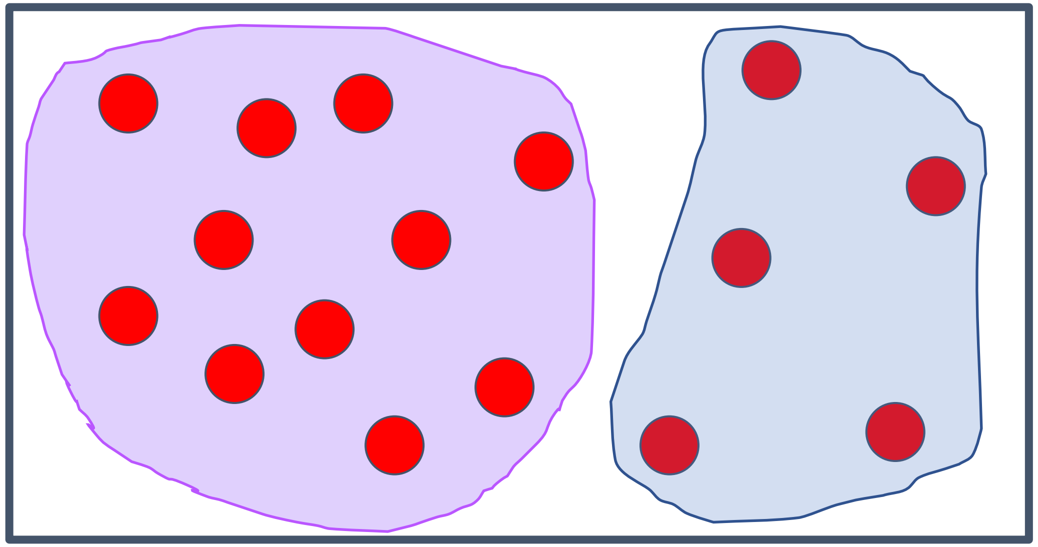


Clustering

The organization of unlabeled data into similarity groups called "clusters."

A cluster is a collection of data items which are "similar" between them, and "dissimilar" to data items in other clusters.

Data:



?

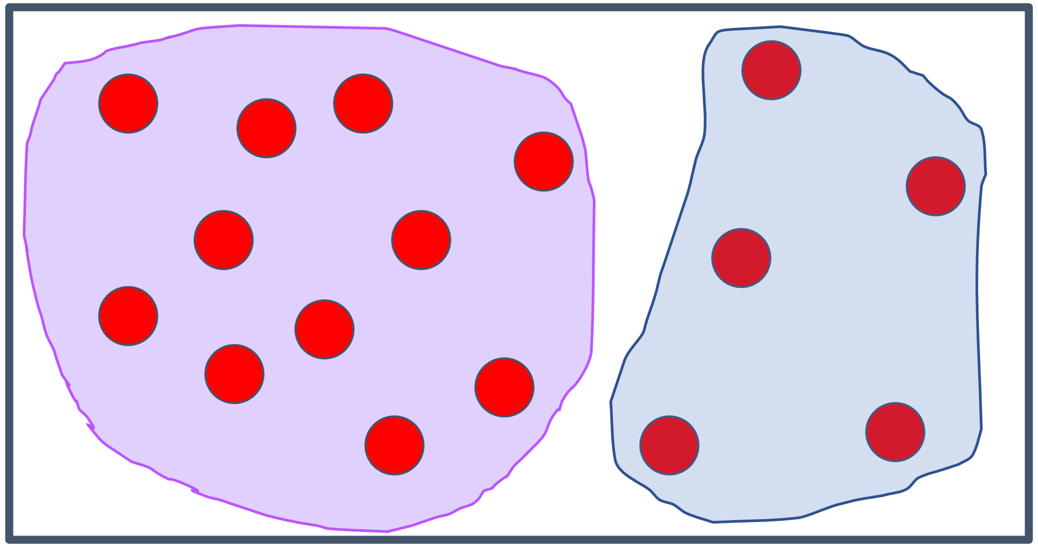






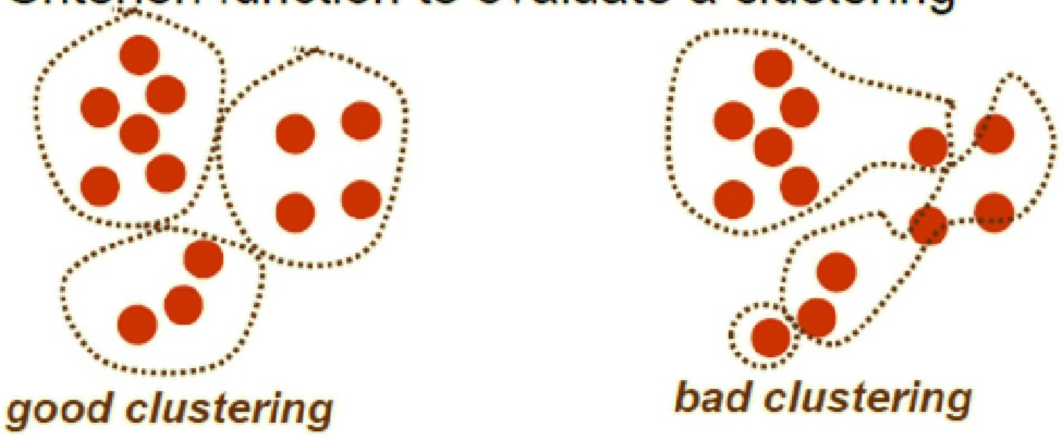
How does the machine do the clustering?

Data:



1. Proximity measure, *either*
   - similarity measure $\mathbf{s}(\mathbf{x}_i,\mathbf{x}_k)$: large if $\mathbf{x}_i,\mathbf{x}_k$ are similar
   - dissimilarity(or distance) measure $\mathbf{d}(\mathbf{x}_i,\mathbf{x}_k)$: small if $\mathbf{x}_i,\mathbf{x}_k$ are similar

2. Criterion function to evaluate a clustering

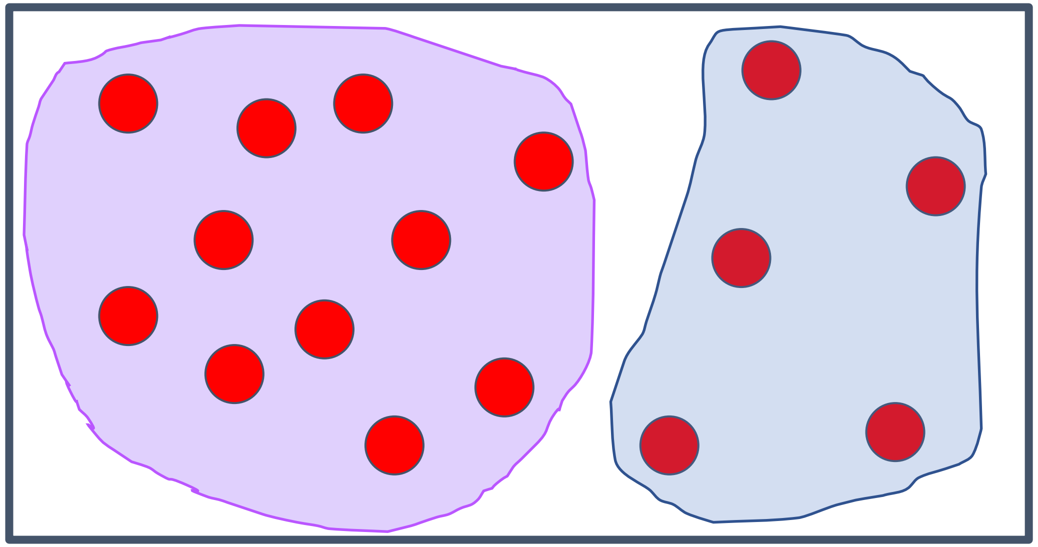


3. Algorithm to compute clustering
   - For example, by optimizing the criterion function

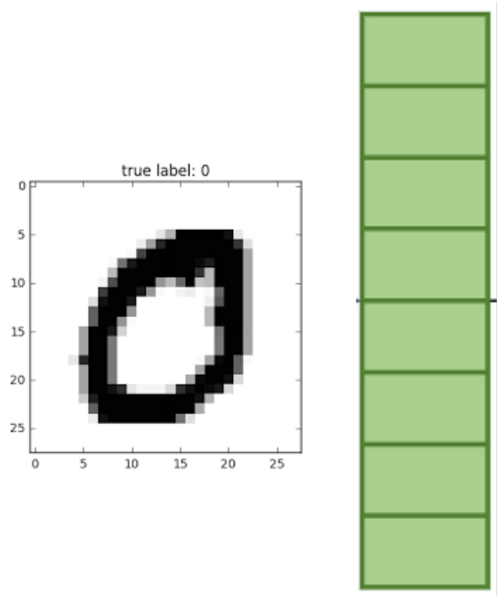
http://www.mit.edu/~9.54/fall14/slides/Class13.pdf

Data in high dimension

Data:



What about an image?

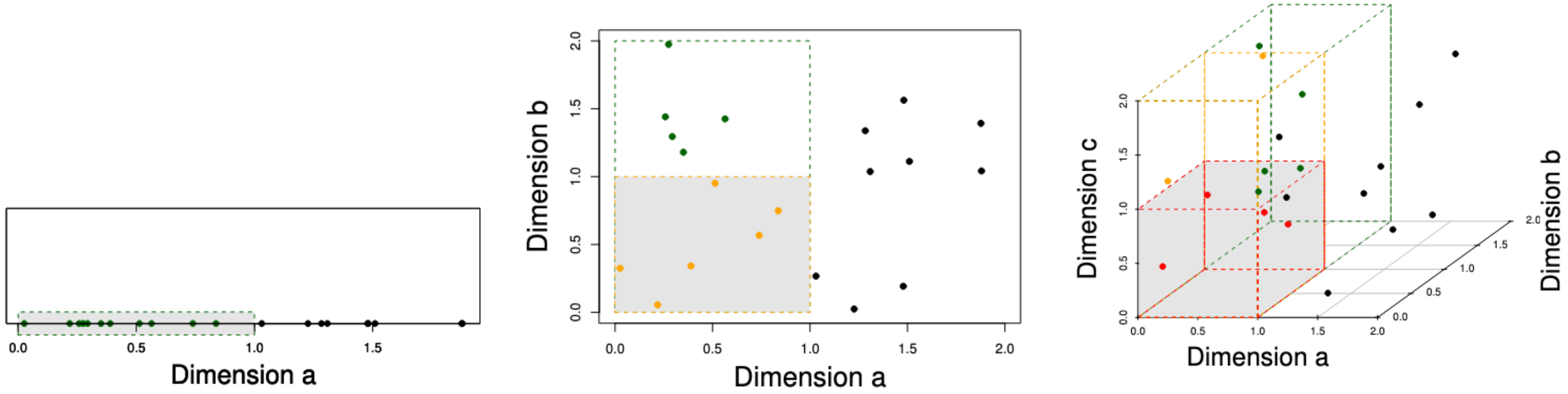


$\mathbb{R}^{784}$

Curse of dimensionality in clustering

What can we do?

Adding a dimension stretches the points across that dimension, pushing them further apart.



(a) 11 Objects in One Unit Bin (b) 6 Objects in One Unit Bin (c) 4 Objects in One Unit Bin

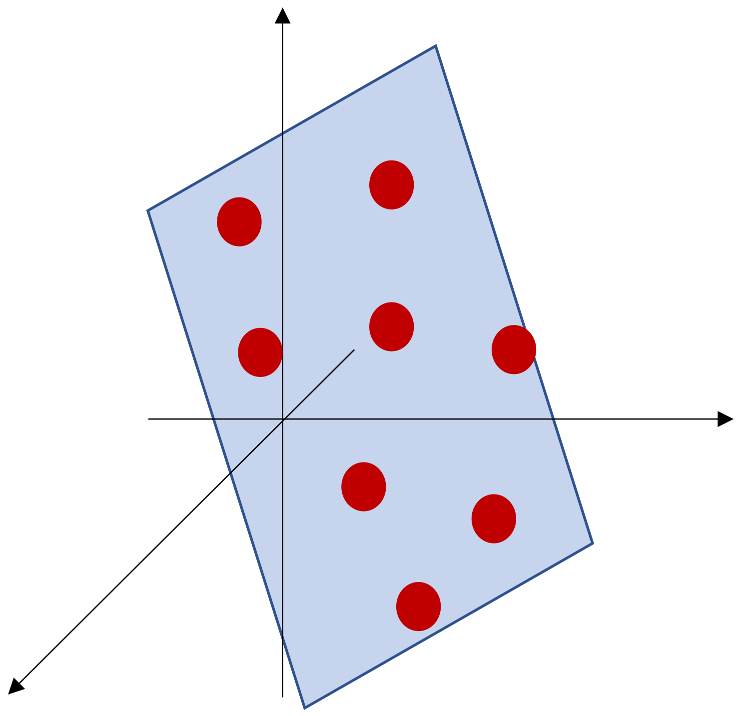
The points continue to spread out, when more dimensions are being added, until they are equidistant from each other and distance is not very meaningful.

https://www.kdd.org/exploration_files/parsons.pdf

https://delta1epsilon.github.io/2019/Gotchas-with-clustering/

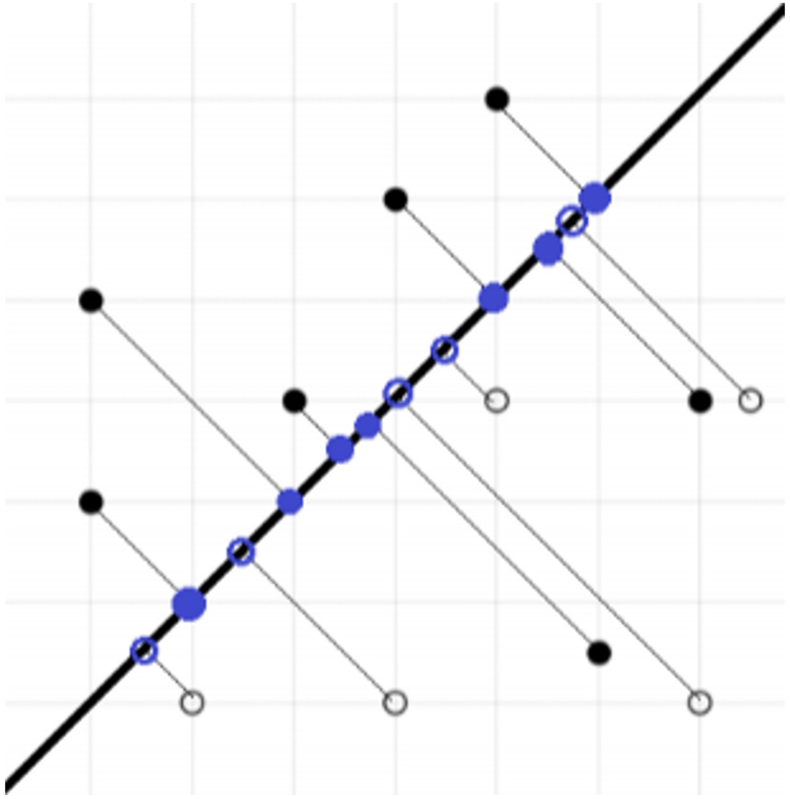
Dimensionality Reduction

- Represent the data with fewer dimensions
- The key idea: While the data may exist in a high dimensional space, it may actually lie along a lower dimensional subspace
  - Ex: data in $\mathbb{R}^3$ may lie along a plane
  - i.e. the ***intrinsic dimensionality*** of the data is actually 2 (not 3)



Dimensionality Reduction using projection

- Data may not lie exactly on a lower-dimensional subspace
- Can still represent it fairly well (with some degree of error)



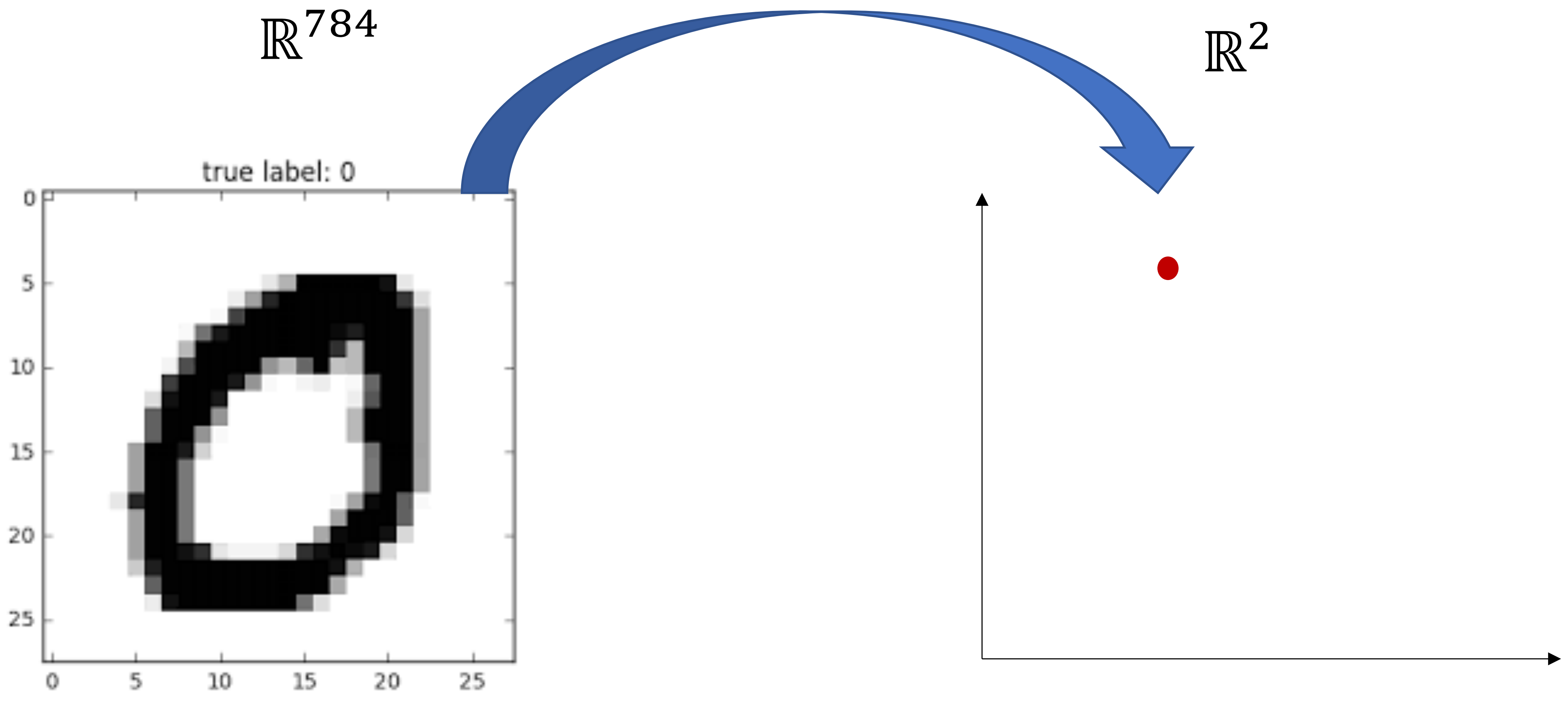
2D data projected to 1 dimension

Any questions?

Dimensionality Reduction: Why?

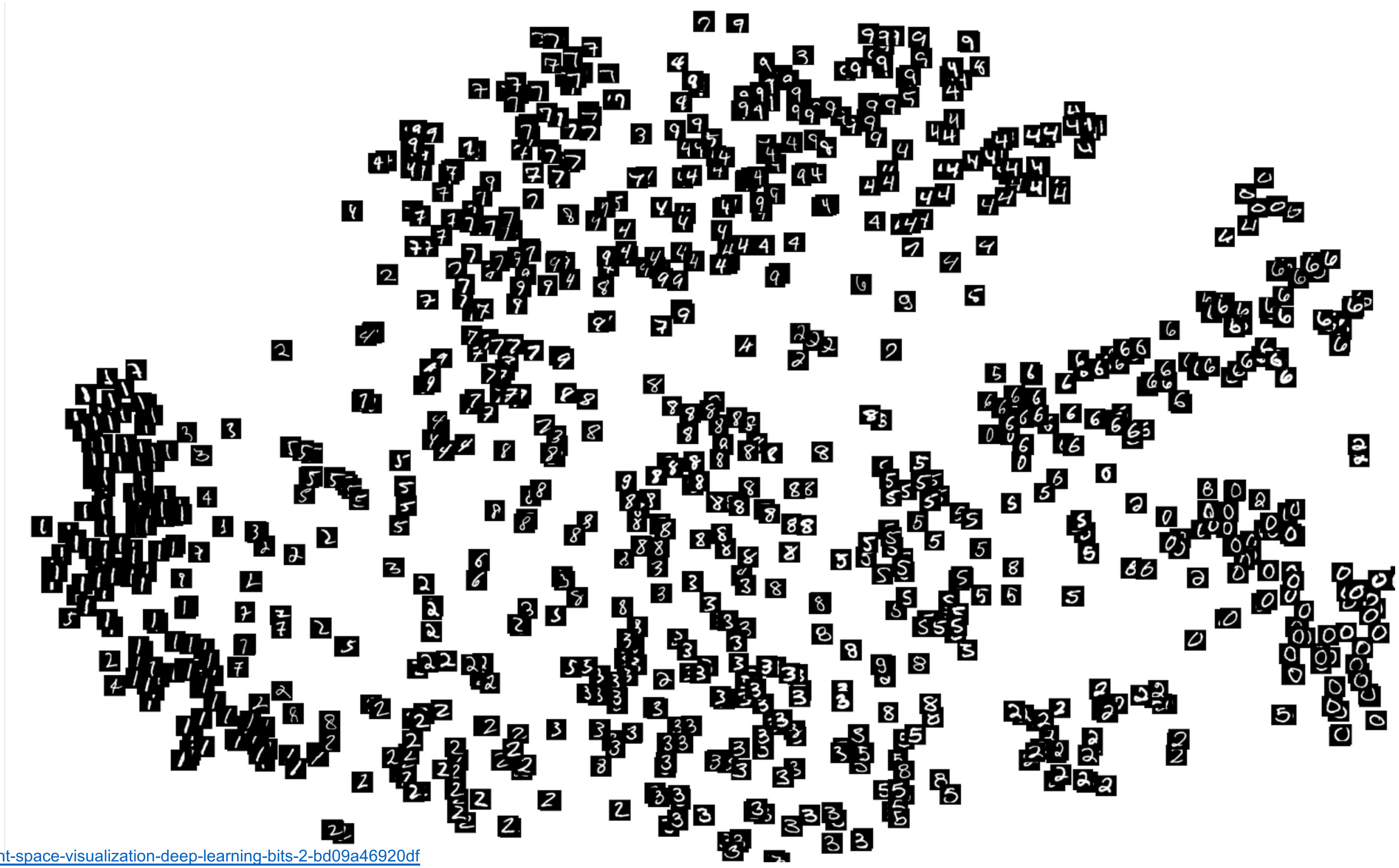
- Lots of benefits to making the data lower-dimensional
  - Many clustering algorithms behave better in lower dimensions
  - Takes less storage/memory → if you're trying to analyze a huge dataset
  - More efficient to search using approximate nearest neighbor algorithms
  - Easier to ***visualize*** (if you reduce the data to 2 or 3 dimensions)

Dimensionality Reduction: Visualization



https://hackernoon.com/latent-space-visualization-deep-learning-bits-2-bd09a46920df

Dimensionality Reduction: Visualization



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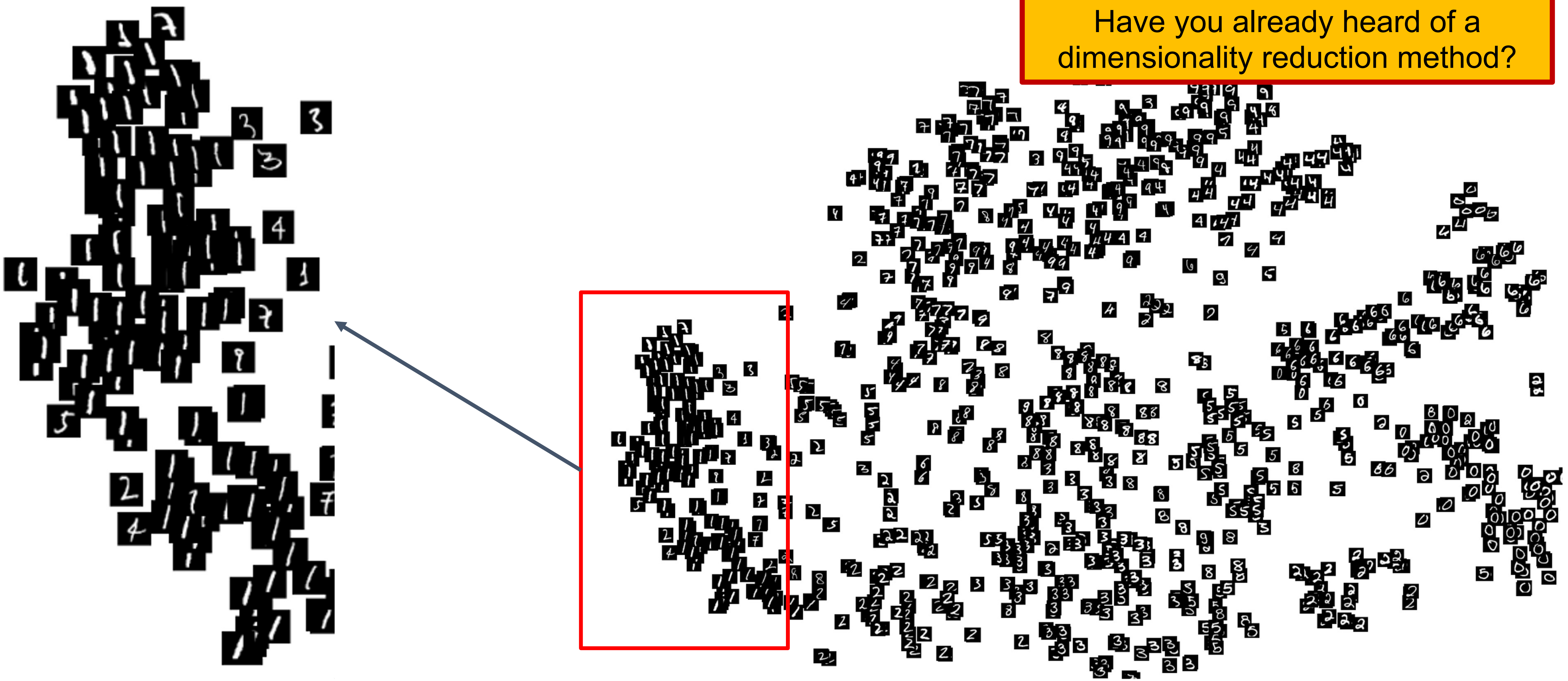
Dimensionality Reduction: Visualization

Have you already heard of a dimensionality reduction method?



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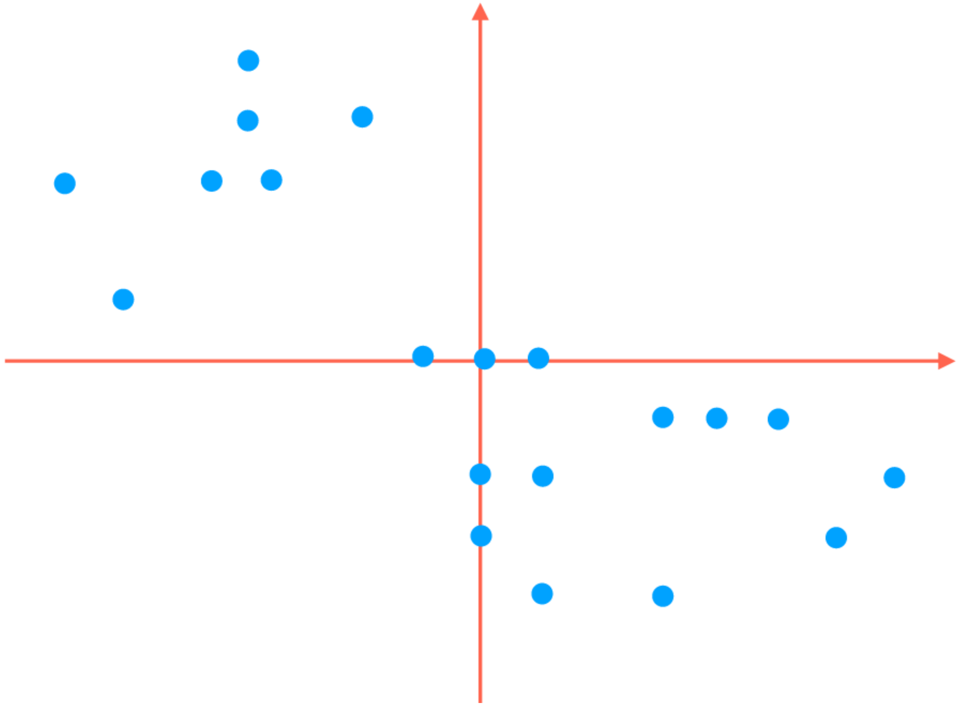
Principal Component Analysis (PCA)

How to project 2D data down to 1D?



https://www.andrew.cmu.edu/user/georgech/95-865/Lectures/Lecture%20-%2003_essence.pdf

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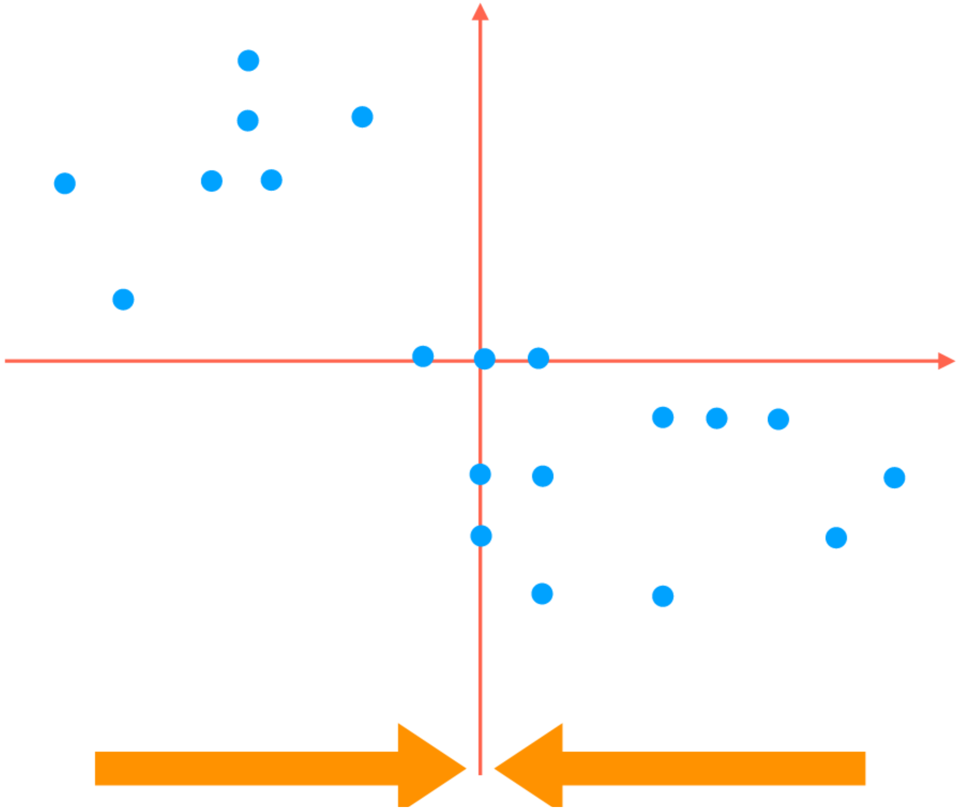

Simplest thing to try: flatten to one of the red axes

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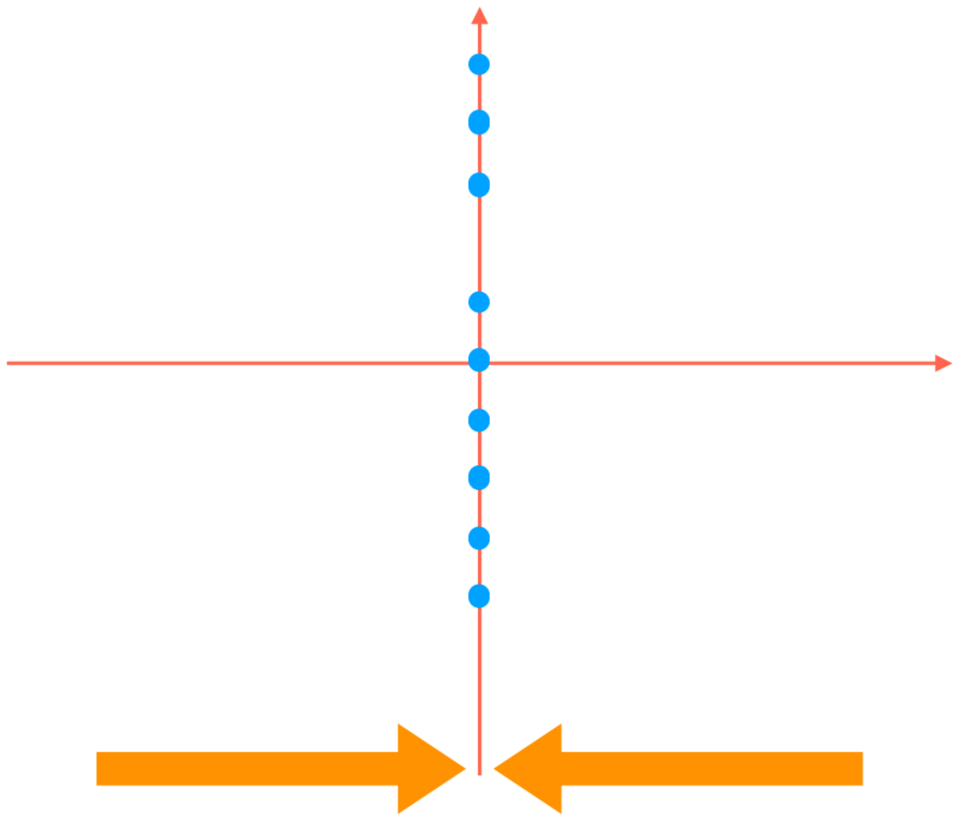

Simplest thing to try: flatten to one of the red axes

(We could of course flatten to the other red axis)

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Principal Component Analysis (PCA)

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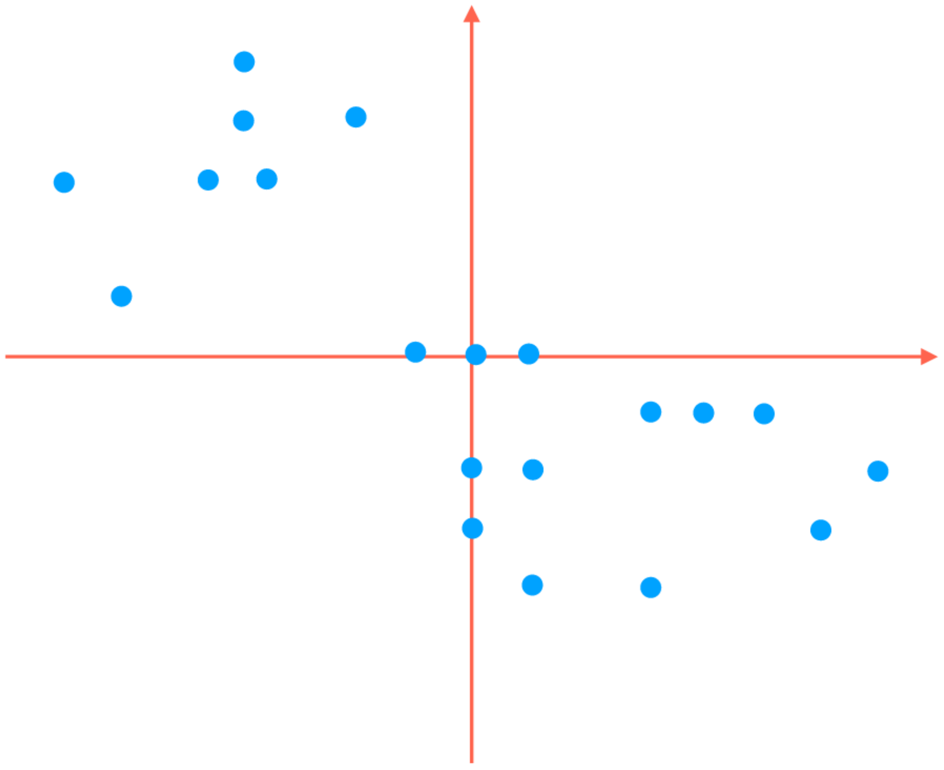
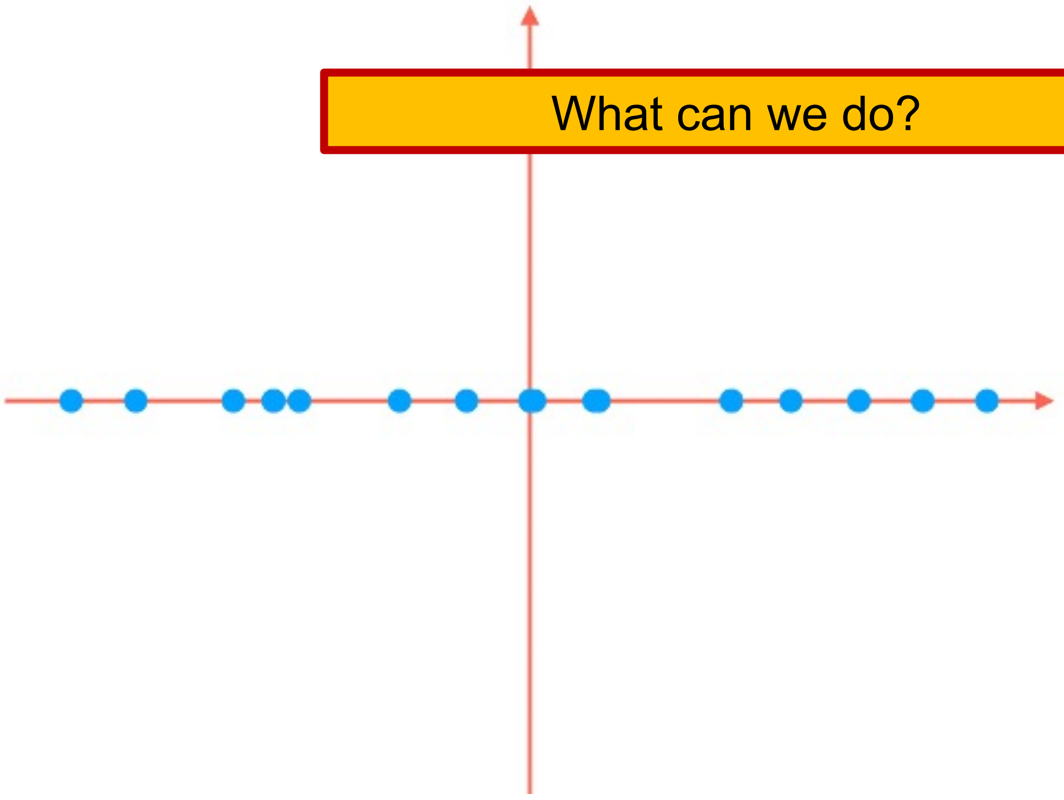


What is the issue here?

What can we do?



But notice that most of the variability in the data is *not* aligned with the red axes!

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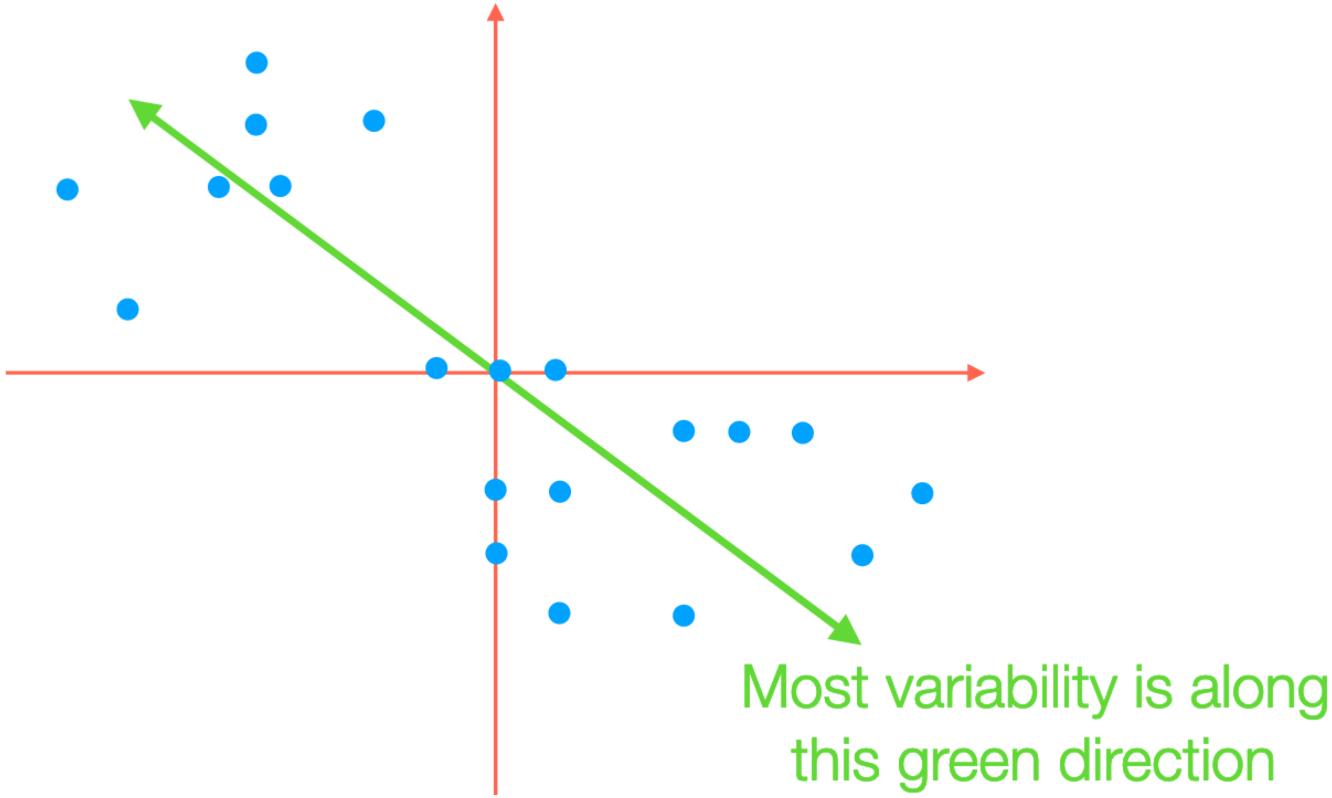

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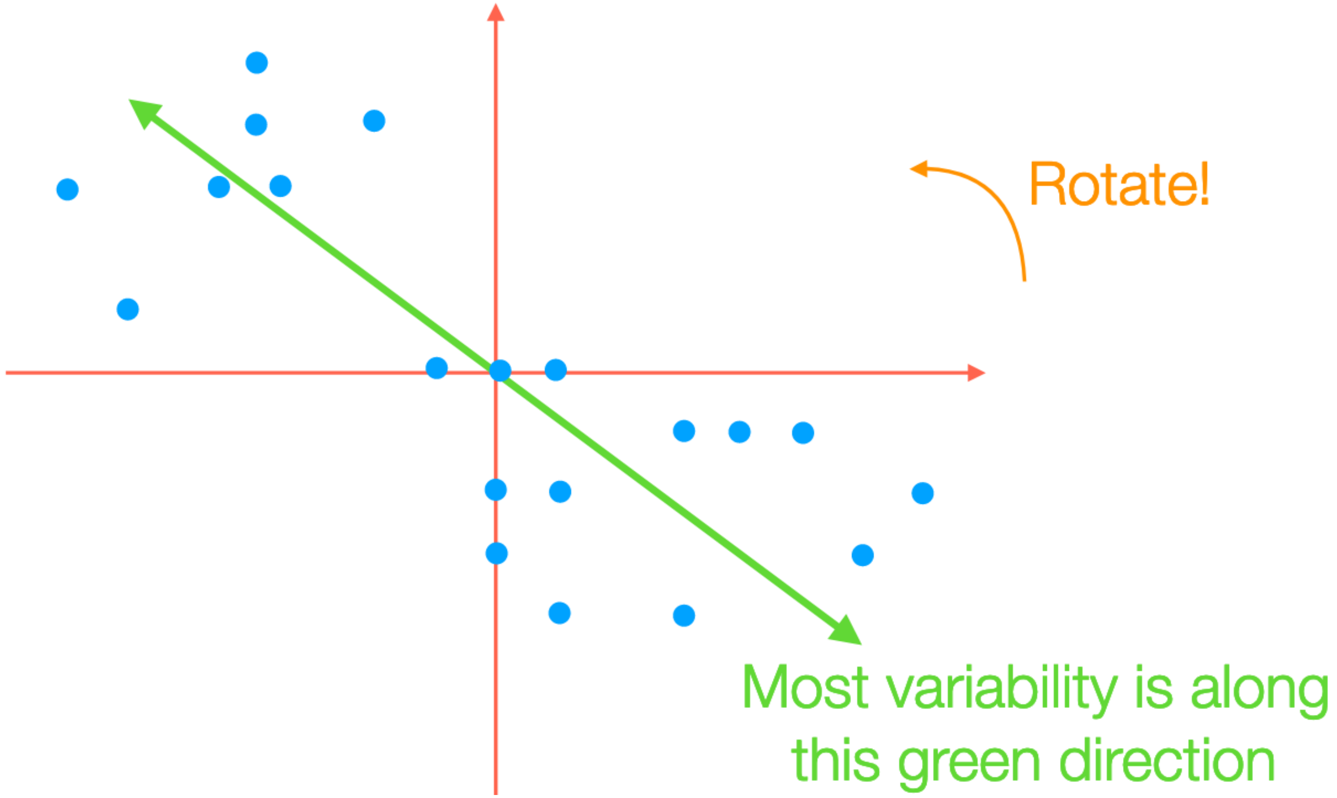

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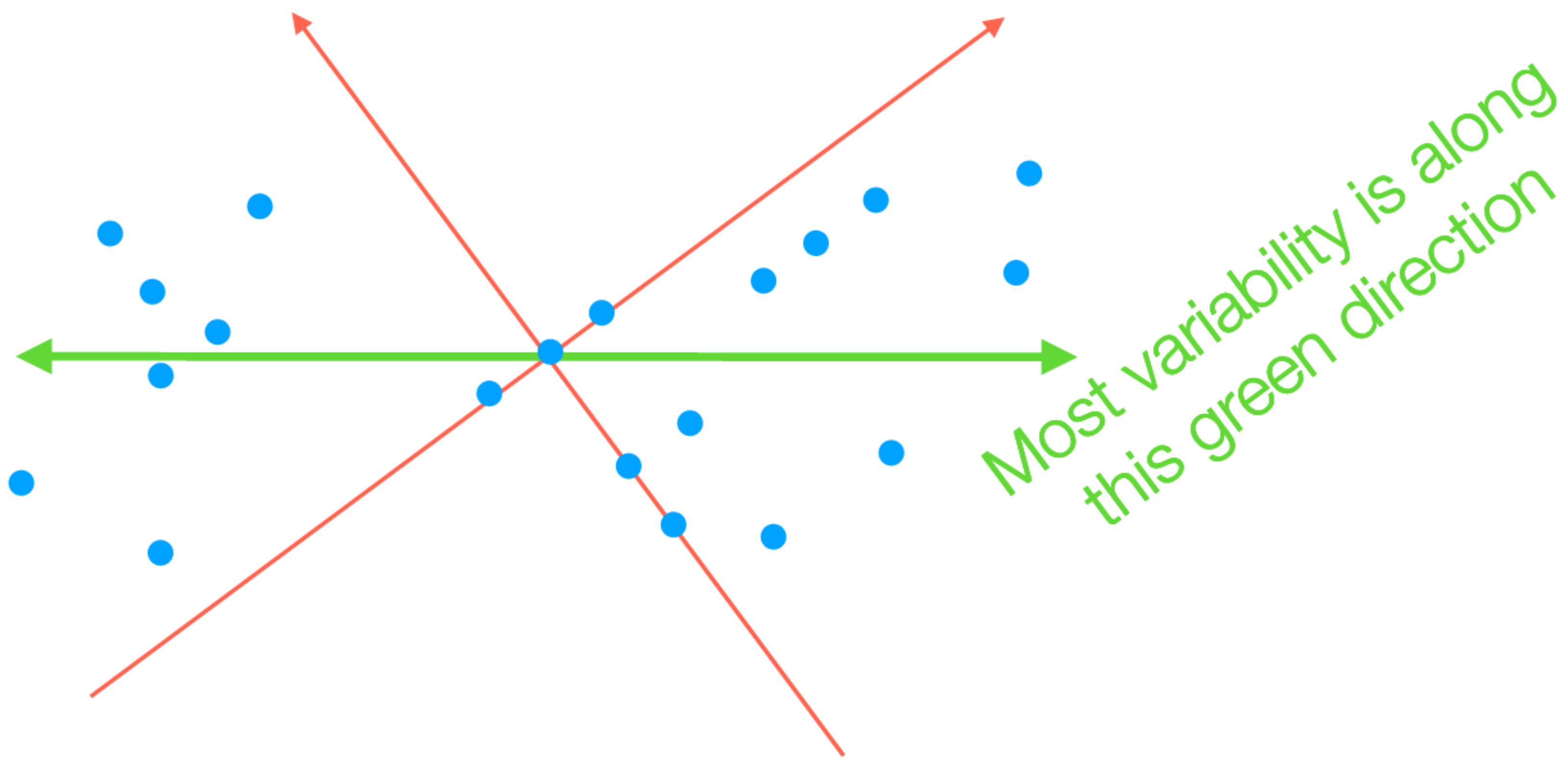

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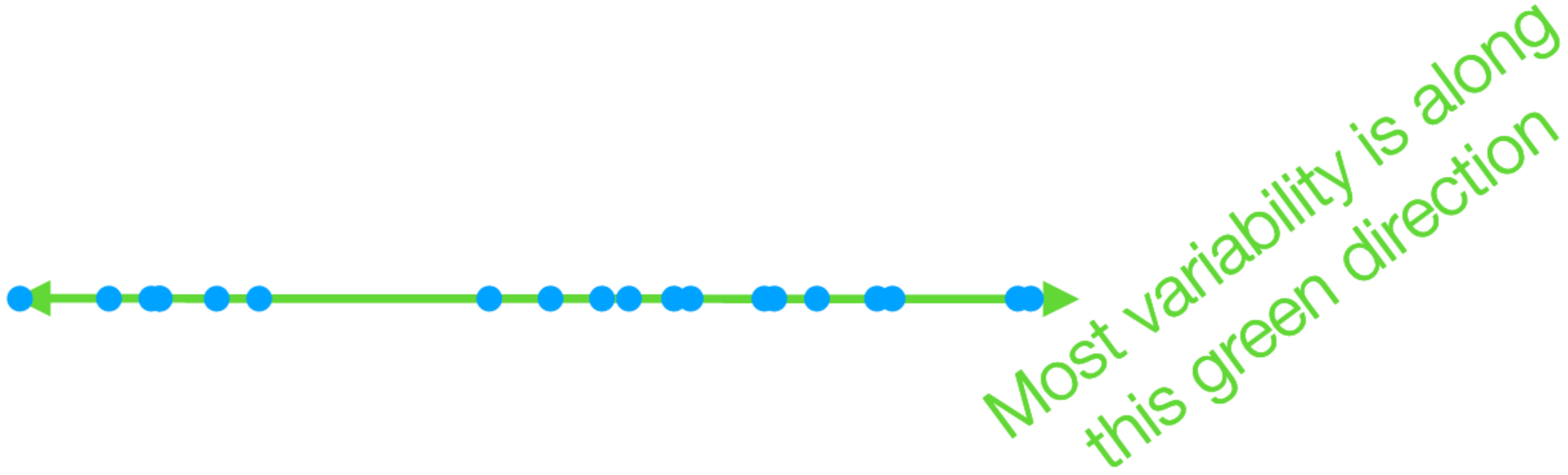

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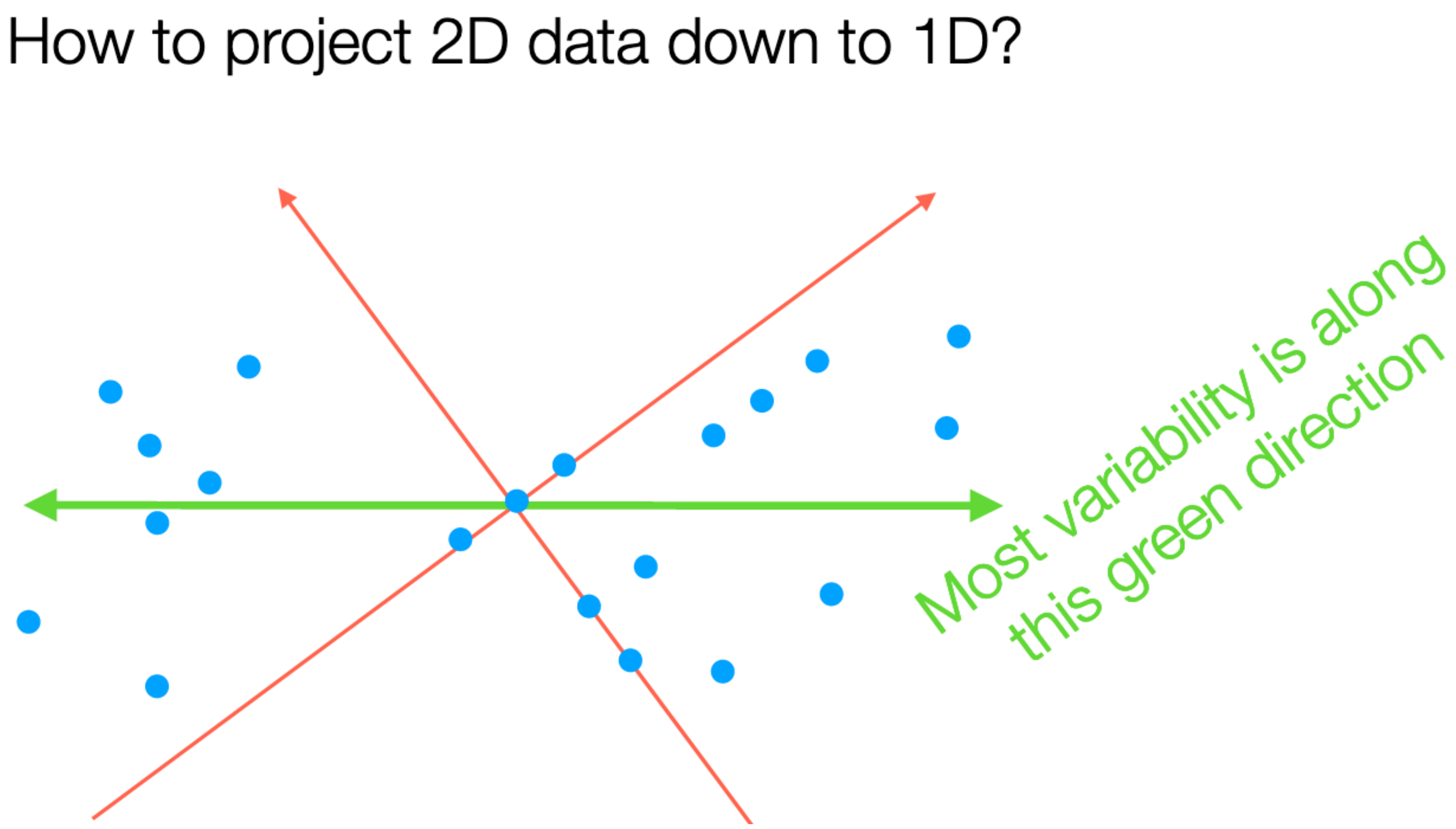
Principal Component Analysis (PCA)



The idea of PCA actually works for 2D ➔ 2D as well
(and just involves rotating, and not “flattening” the data)

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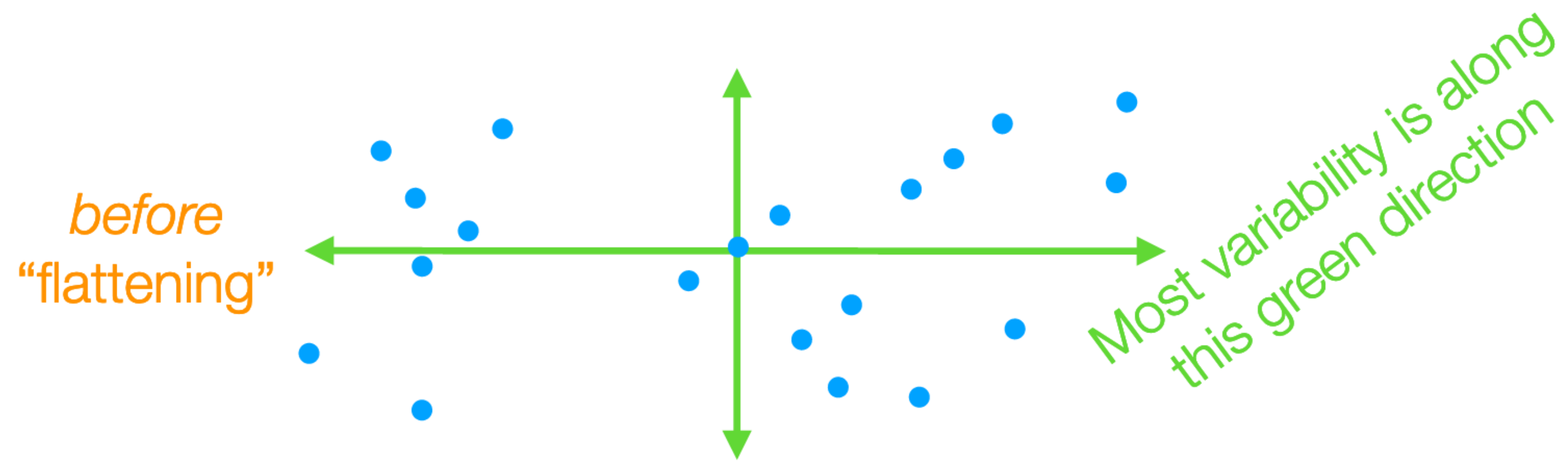
Principal Component Analysis (PCA)

~~How to project 2D data down to 1D?~~

How to rotate 2D data so 1st axis has most variance



The idea of PCA actually works for 2D ➔ 2D as well
(and just involves rotating, and not "flattening" the data)

2nd green axis chosen to be 90° ("orthogonal") from first green axis

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Principal Component Analysis (PCA)

- Finds top *k* orthogonal directions that explain the most variance in the data

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Principal Component Analysis (PCA)

- Finds top *k* orthogonal directions that explain the most variance in the data
  - 1st component: explains most variance along 1 dimension
  - 2nd component: explains most of remaining variance along next dimension that is orthogonal to 1st dimension
  - …

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Any questions?

Principal Component Analysis (PCA)

- Finds top *k* orthogonal directions that explain the most variance in the data
  - 1st component: explains most variance along 1 dimension
  - 2nd component: explains most of remaining variance along next dimension that is orthogonal to 1st dimension
  - …
- "Flatten" data to the top *k* dimensions to get lower dimensional representation (if *k* < original dimension)

https://www.andrew.cmu.edu/user/georgech/95-865/Lectures/Lecture%20-%2003_essence.pdf

3D example from:

https://setosa.io/ev/principal-component-analysis/

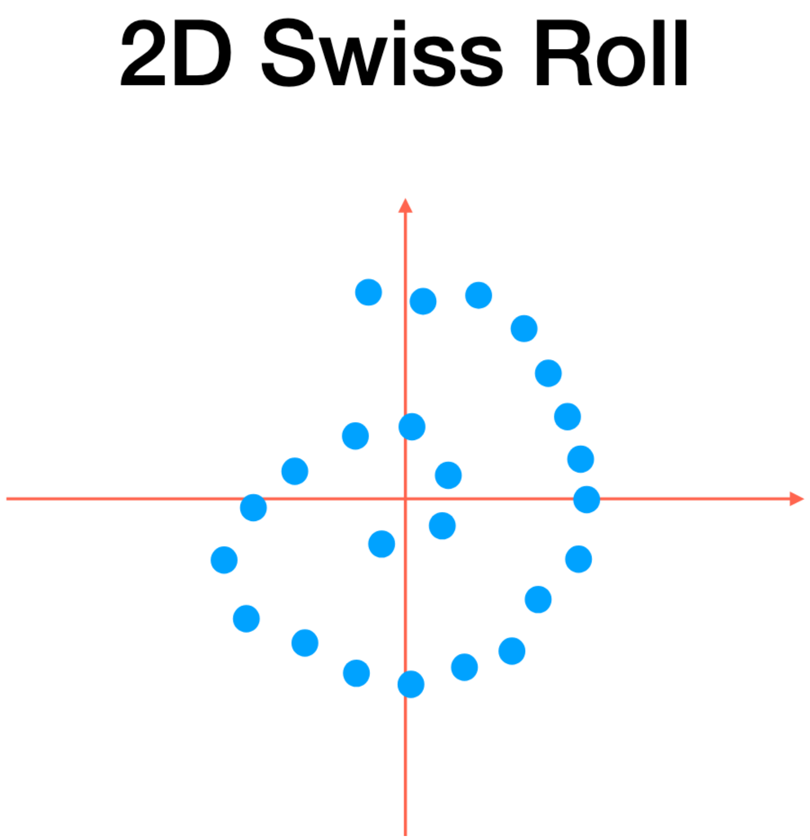
PCA reorients data so axes explain variance in “decreasing order”
➔ can “flatten” (*project*) data onto a few axes that captures most variance

https://www.andrew.cmu.edu/user/georgech/95-865/Lectures/Lecture%20-%2003_essence.pdf

Limitations of PCA

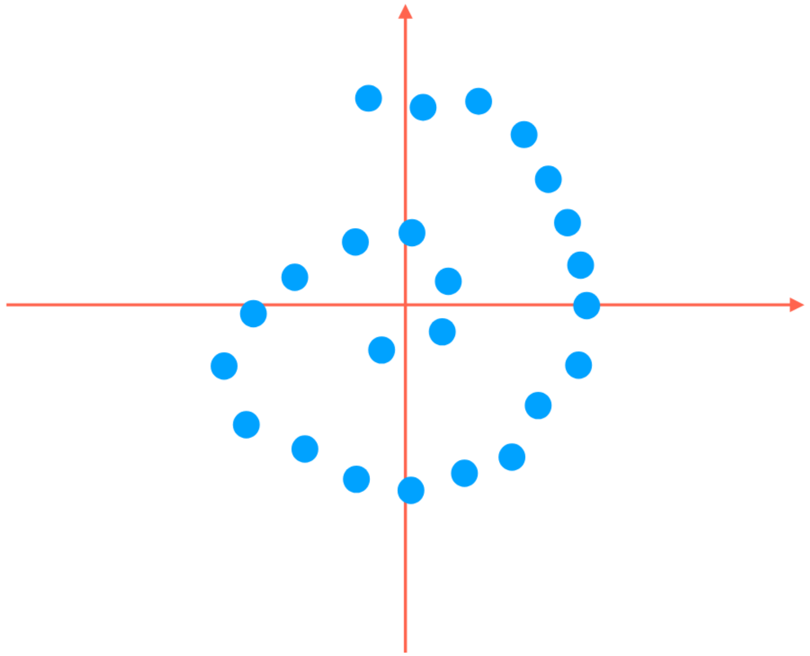
https://www.foodnetwork.com/recipes/food-network-kitchen/hot-cocoa-cake-roll-4553196

Limitations of PCA



Limitations of PCA

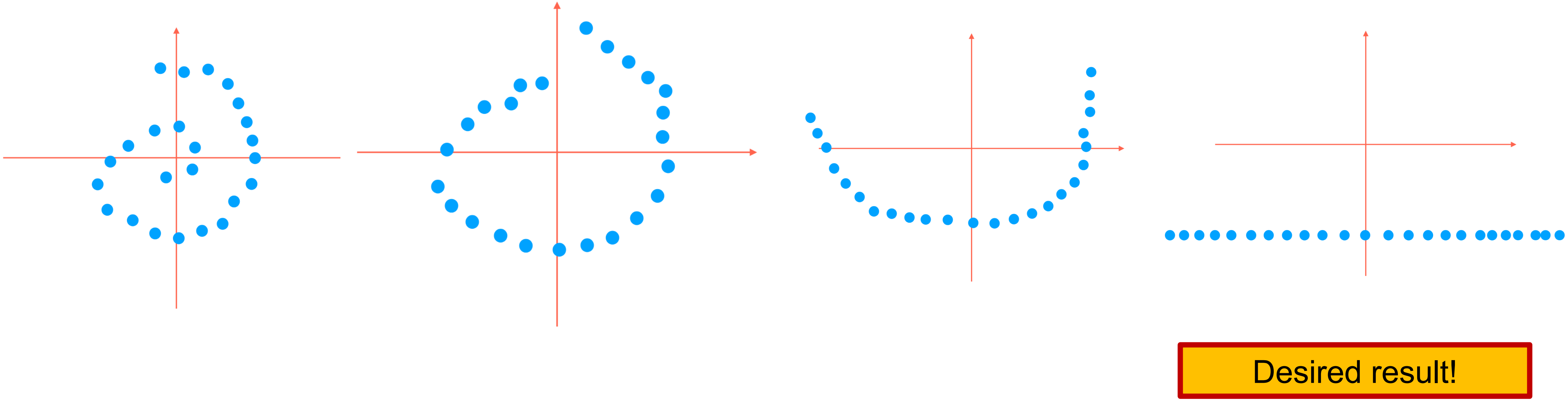
2D Swiss Roll



PCA would just flatten this thing and
lose the information that the data actually lives on a 1D line that has been curved!

https://www.andrew.cmu.edu/user/georgech/95-865/Lectures/Lecture%20-%2003_essence.pdf

Limitations of PCA



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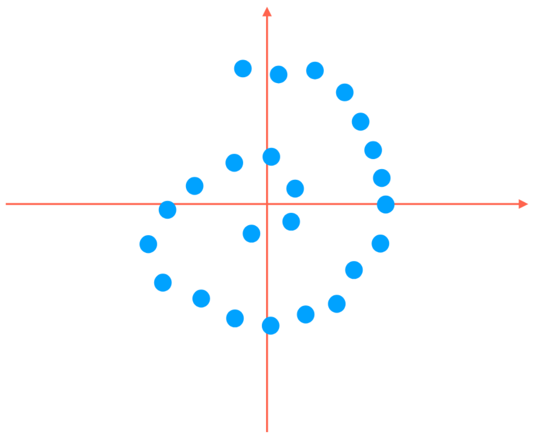
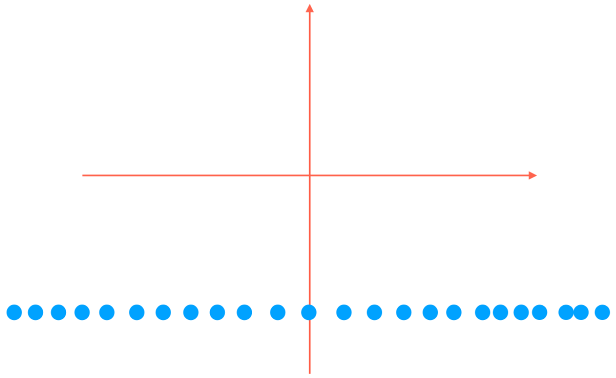
How to dimension-reduce gnarly datasets?

- The Swiss Roll has an intrinsic dimensionality of 1
  - i.e. "how far along the curve a point is"
- But PCA can't figure this out because the projection from $\mathbb{R}^2$ to $\mathbb{R}^1$ is ***non-linear***
  - i.e. "unroll" the curve and lay it flat along a number line
- How can we compute non-linear projections?



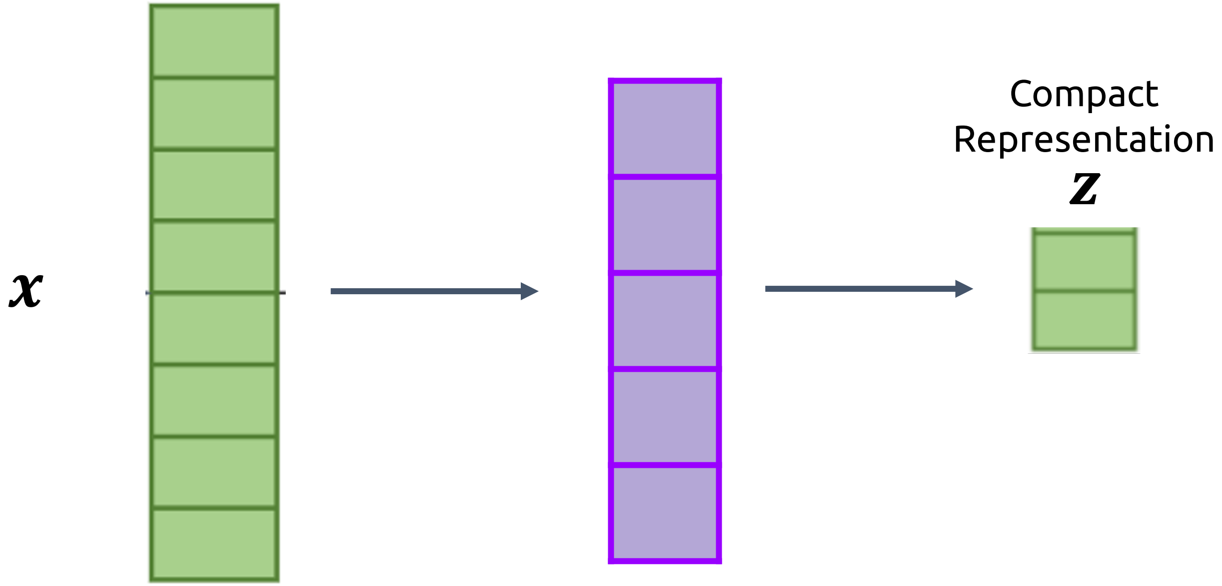


“I hear these neural nets are pretty good at learning non-linear functions”

Can we use a neural net to learn a non-linear projection to a lower-dimensional space?

A nonlinear projection neural net

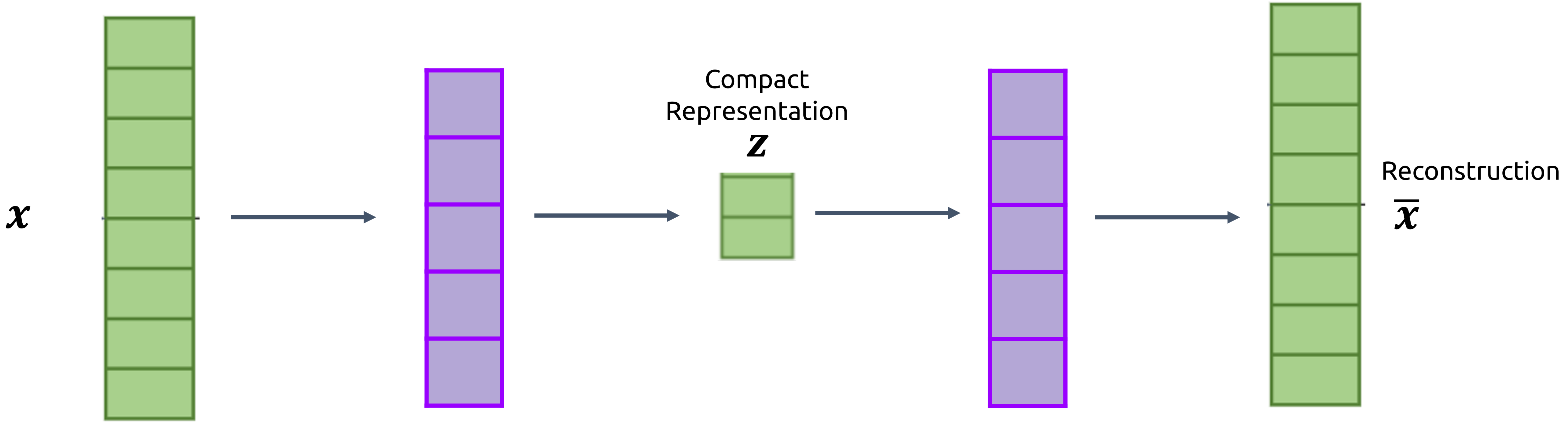
- We could just use a regular neural net architecture (e.g. fully connected) to take a vector input $\boldsymbol{x}$ and output a lower-dimensional vector $\boldsymbol{z}$



- But how do we train this thing?
- What's the loss for "be a good nonlinear projection of x?"

A nonlinear projection neural net

- Idea: a compact representation $\boldsymbol{z}$ is a good non-linear projection of $\boldsymbol{x}$ if it's possible to reconstruct $\boldsymbol{x}$ well from $\boldsymbol{z}$

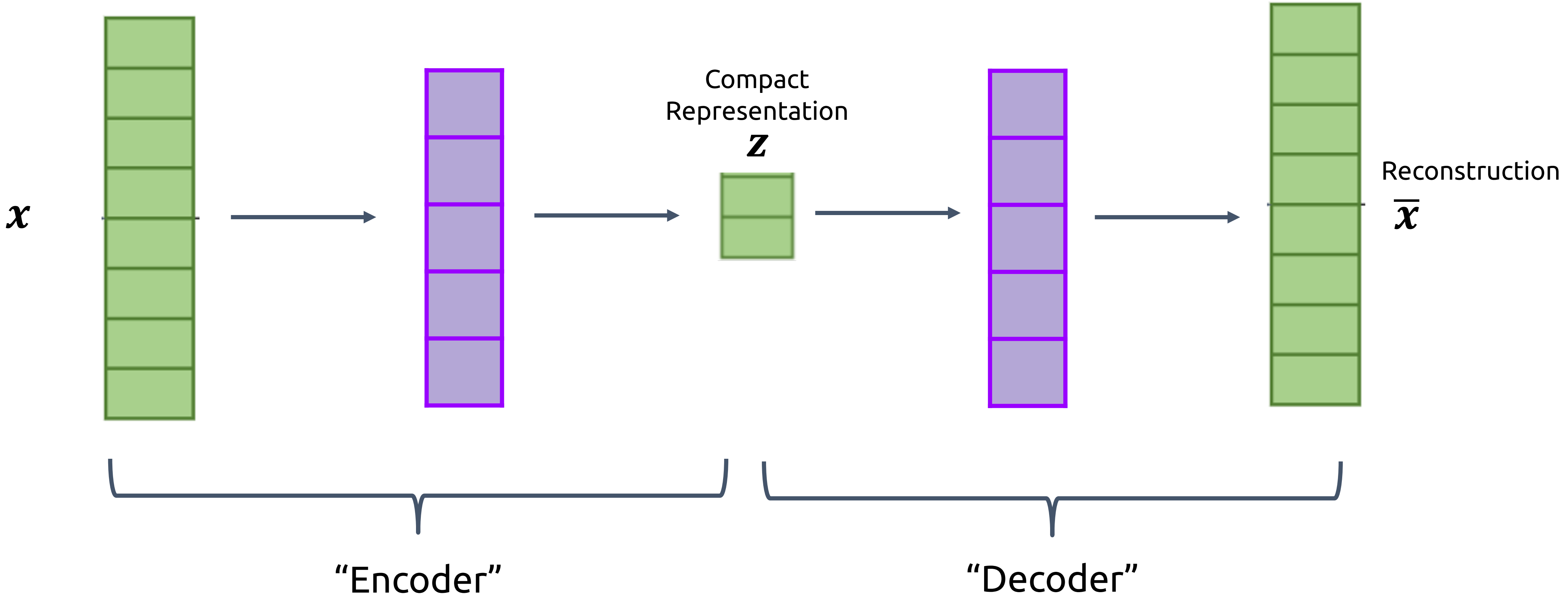


- What loss function makes sense here?
  - $L(\boldsymbol{x}, \overline{\boldsymbol{x}}) = (\boldsymbol{x} - \overline{\boldsymbol{x}})^2$ (squared error loss)
- This architecture is called an ***autoencoder***

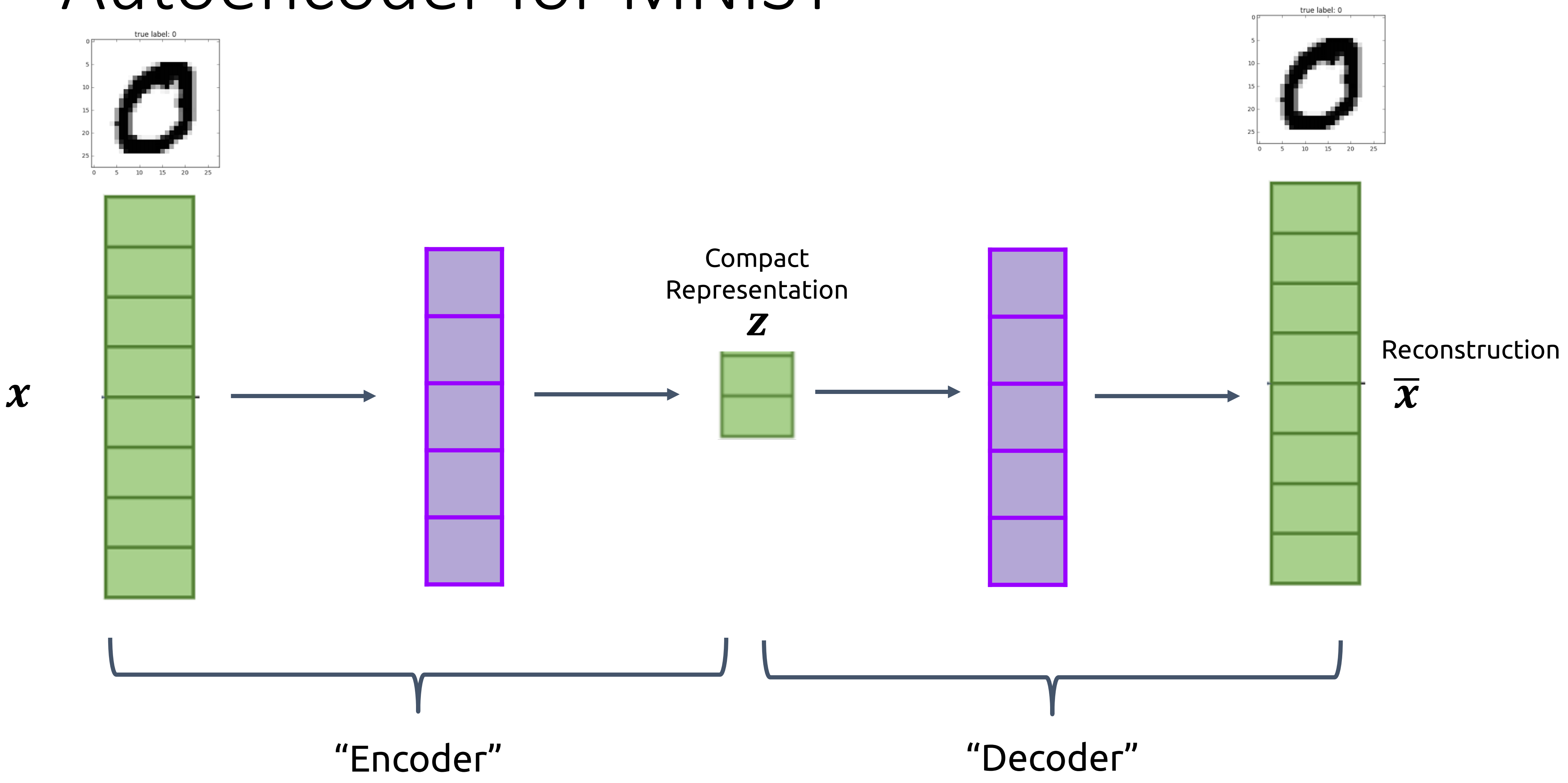
Autoencoder

How is this different from the Seq2seq encoder/decoder setup?

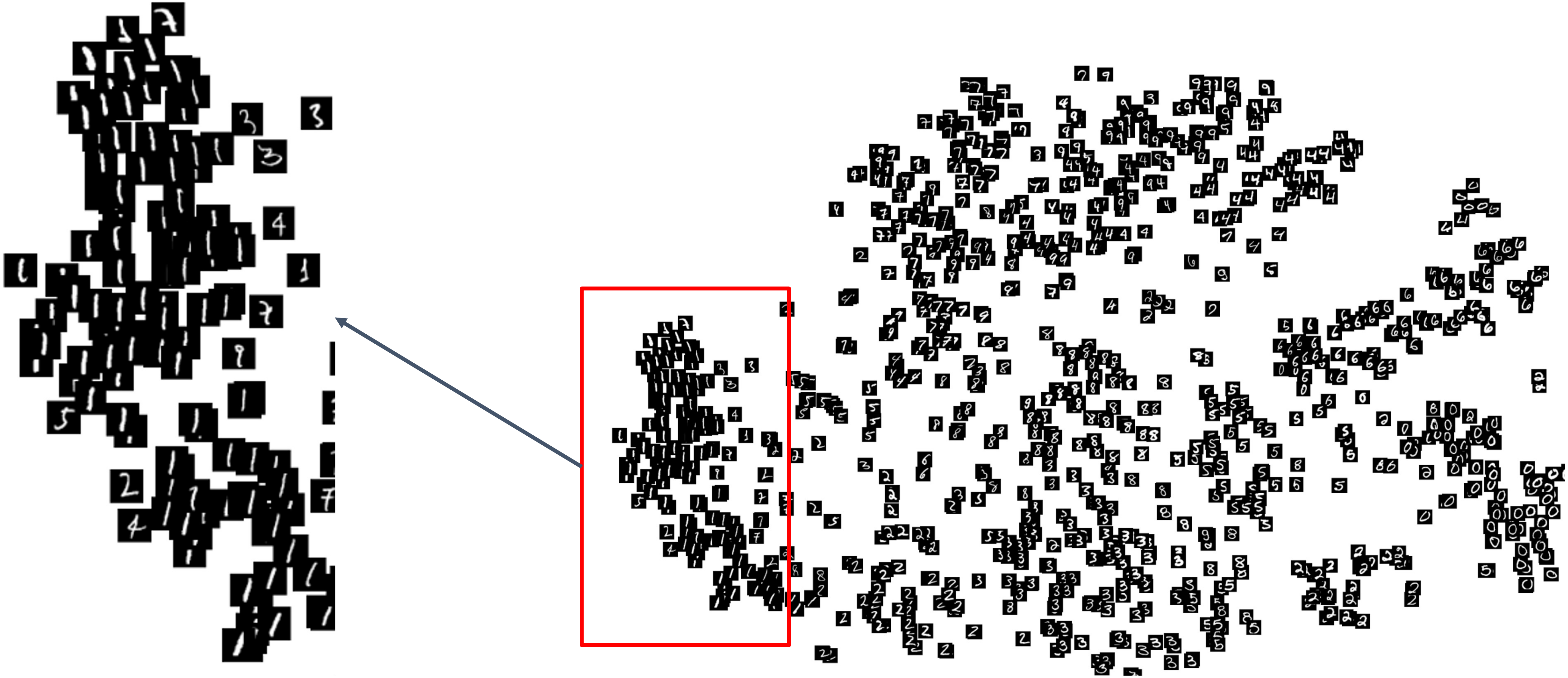
- Reconstruction loss: $L(\boldsymbol{x}, \overline{\boldsymbol{x}}) = (\boldsymbol{x} - \overline{\boldsymbol{x}})^2$



Autoencoder for MNIST



This visualization? Autoencoder

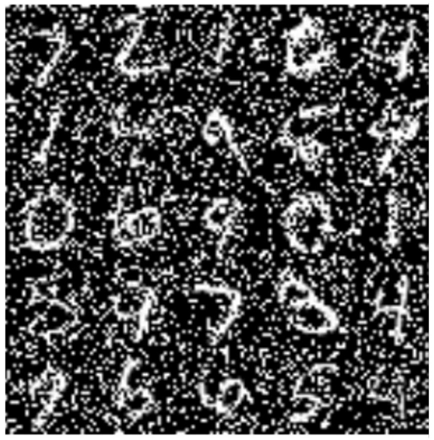


https://hackernoon.com/latent-space-visualization-deep-learning-bits-2-bd09a46920df

Other Autoencoder applications

Denoising Autoencoder

Input: Noisy Images

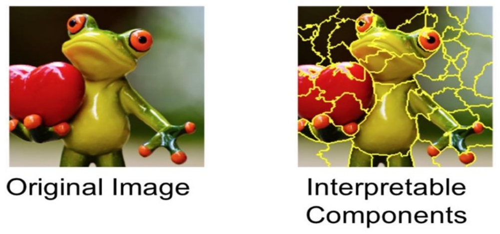


Output: Restored Image

Recap

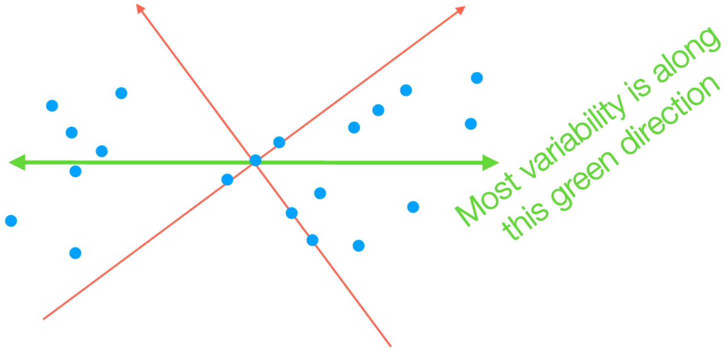
Model agnostic interpretation

- LIME (or perturbation-based)
- Attention (inbuilt interpretation)



Unsupervised Learning

- Learning the structure in the data
- Clustering
- Dimensionality reduction using PCA



Auto-encoders (AEs)

- Perform non-linear dimensionality reduction
- Architecture and loss function