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Unsupervised methods

Diving deep into autoencoders

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Introduction

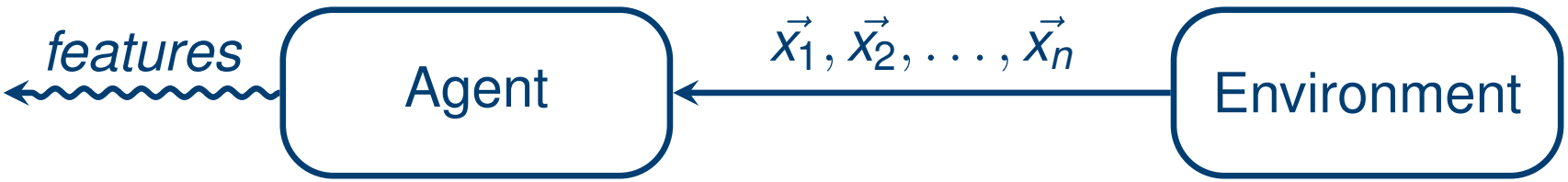
- In this lecture, I will guide you through the essentials of using deep neural networks for *unsupervised learning*.
- We will focus primarily on **autoencoders**, which offer a good tradeoff between model capacity and ease of training—and are still widely used both industrially and in research.
- For completeness, we will also briefly survey two historically used architectures for unsupervised learning (*RBMs* and *DBNs*), and a bleeding-edge *GAN* architecture (more details on Advanced Deep Learning & Reinforcement Learning. . .)

The three “flavours” of machine learning

- Unsupervised learning
- Supervised learning
  (more details next week!)
- Reinforcement learning
  (more details on Advanced DL & RL)

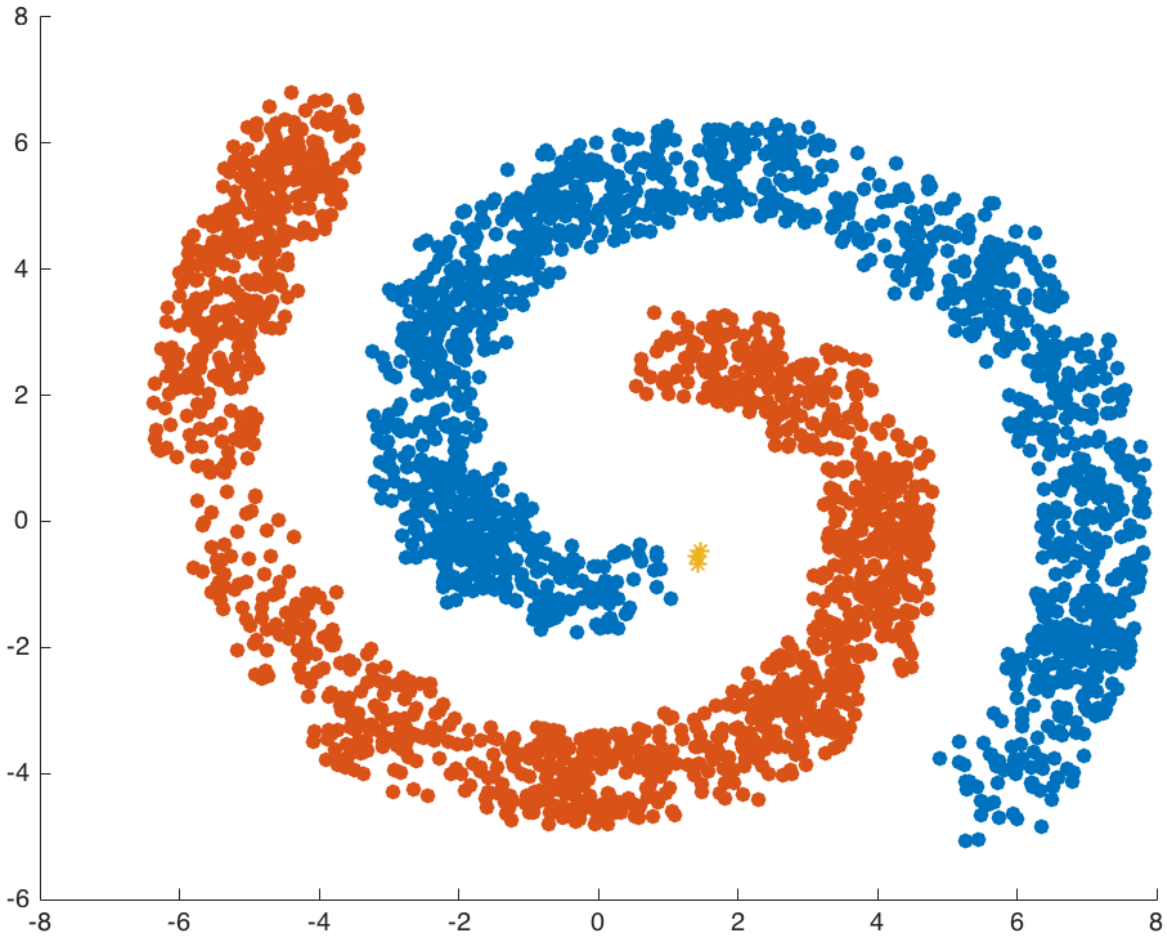
Unsupervised learning

- The environment gives you *unlabelled data*—and asks you to assign useful features/structure to it.



- Example: study data from patients suffering from a disease, in order to discover different (previously unknown) types of it.

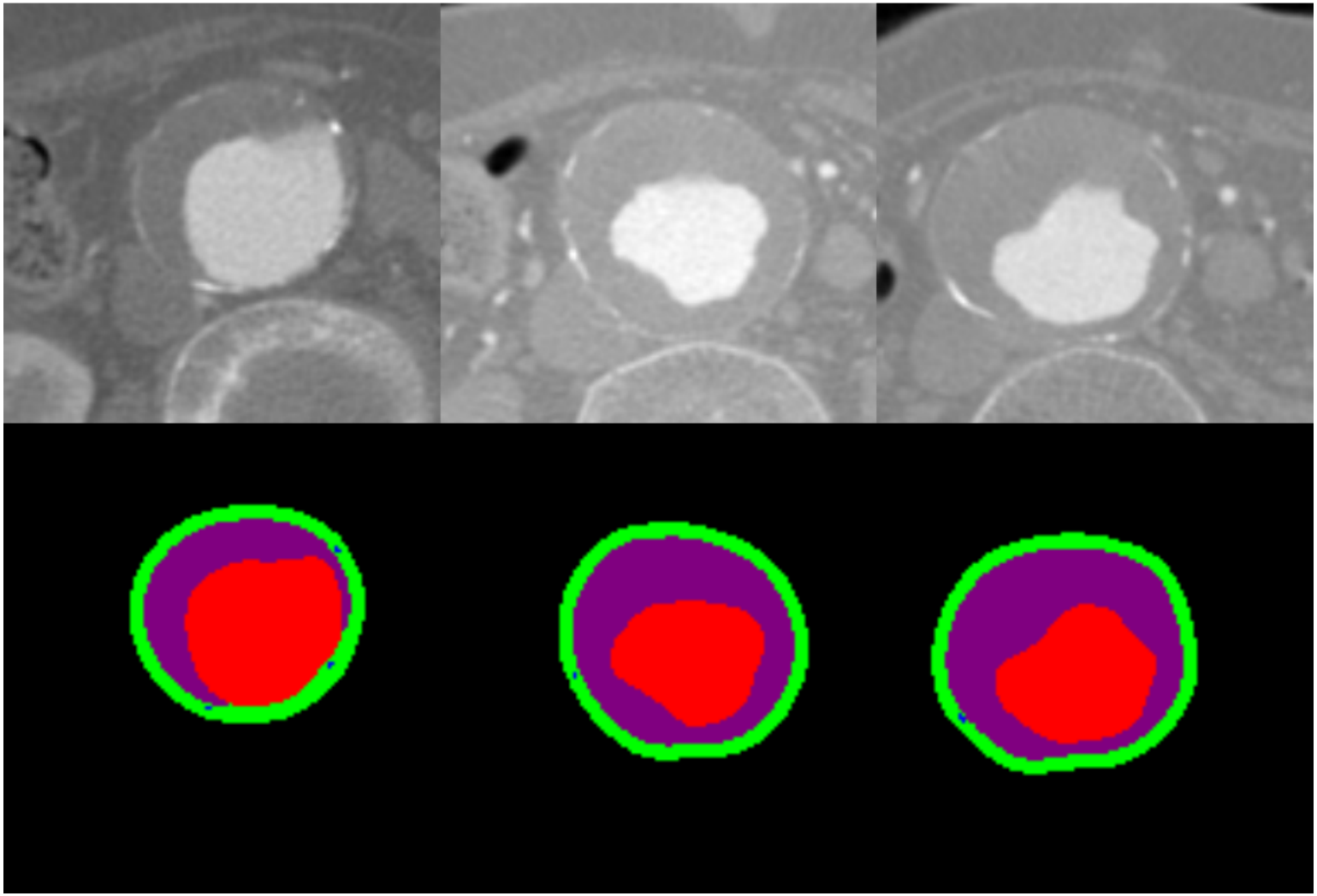
Example: Clustering



What's the point if we don't have labels?

- As in the above example, unsupervised learning can often be a *precursor to supervised learning*, if we don't even know what the labels should be (e.g. disease subtypes)!
- Often vastly increases the amount of data available! Obtaining labelled data is not always:
  - Appropriate (e.g. if, as above, *we don't even know the labels*);
  - Cheap (e.g. *segmenting medical images*);
  - Feasible (e.g. clinical studies for *extremely rare diseases*).
- Can aid better *dimensionality reduction*, simplifying the work of other algorithms, allow for *synthesising new training data*. . . and much more.
- Humans are essentially learning (mostly) unsupervised!

Example: Medical image segmentation



How can unlabelled data help?

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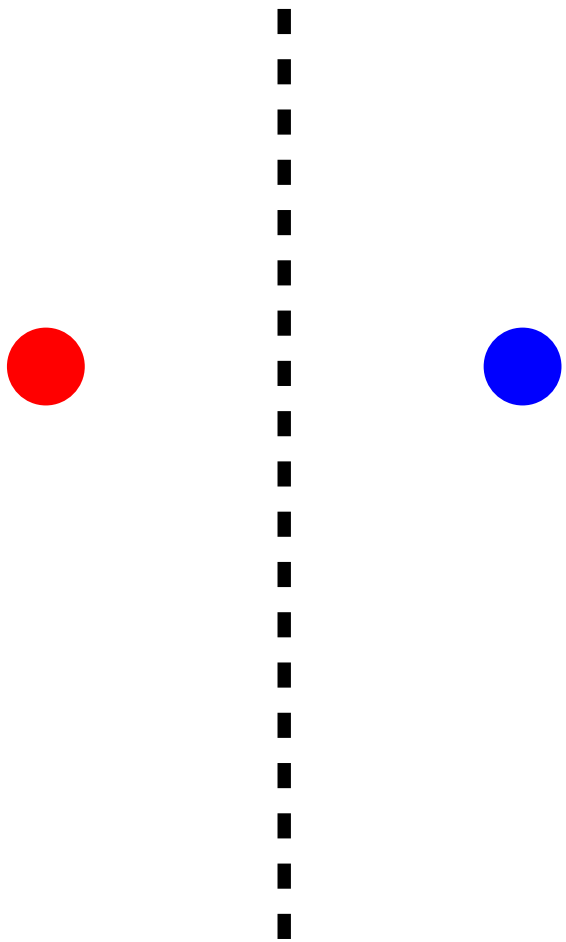
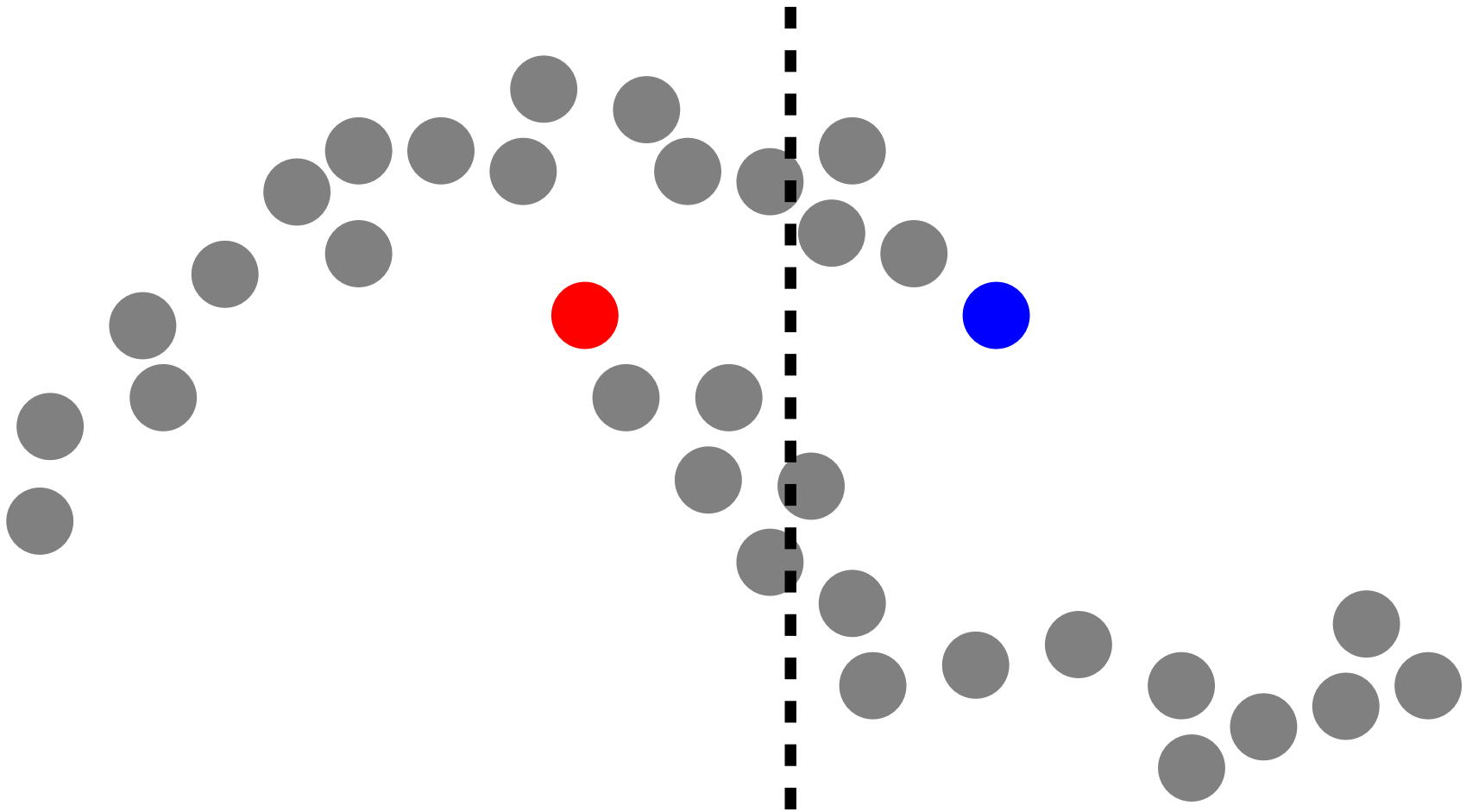
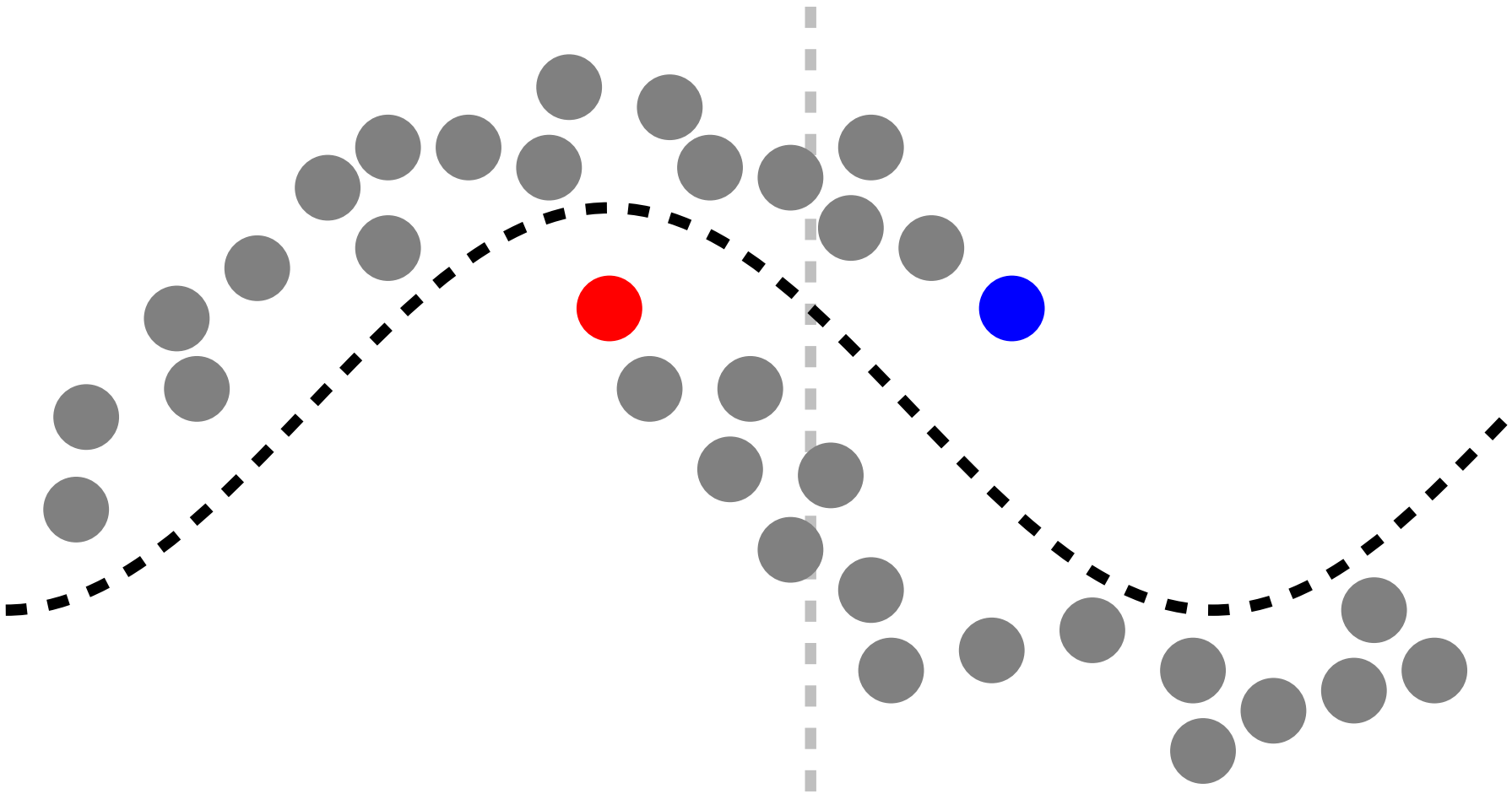


How can unlabelled data help?



How can unlabelled data help?



Unsupervised learning is the future! (*LeCun, 2017*)

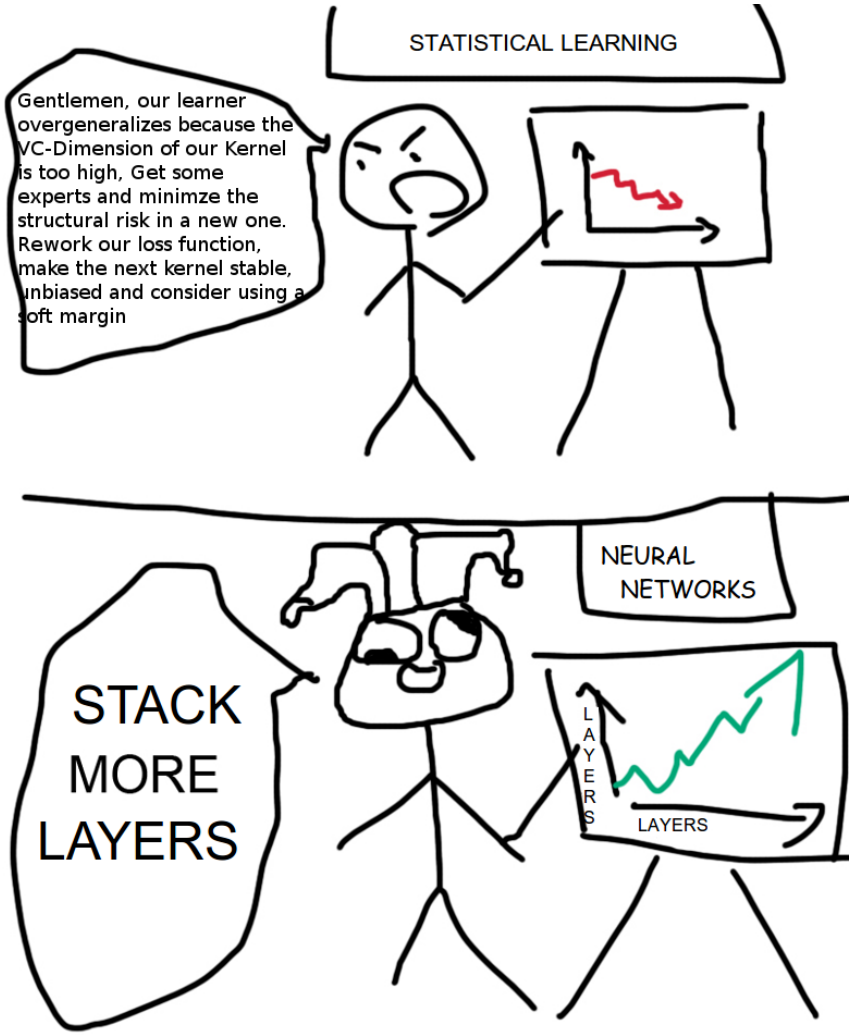
How Much Information Does the Machine Need to Predict?

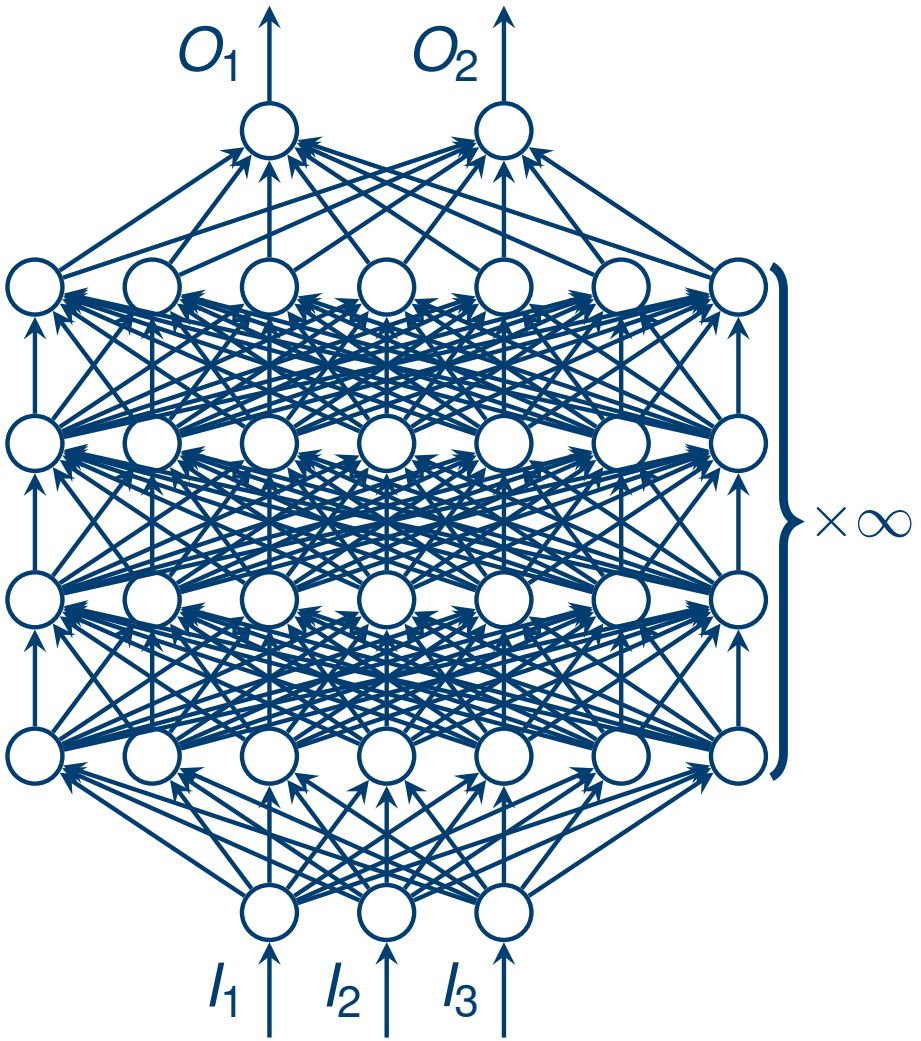
Y LeCun

- "Pure" Reinforcement Learning (cherry)
  - The machine predicts a scalar reward given once in a while.
  - **A few bits for some samples**
- Supervised Learning (icing)
  - The machine predicts a category or a few numbers for each input
  - Predicting human-supplied data
  - **10→10,000 bits per sample**
- Unsupervised/Predictive Learning (cake)
  - The machine predicts any part of its input for any observed part.
  - Predicts future frames in videos
  - **Millions of bits per sample**

- (Yes, I know, this picture is slightly offensive to RL folks. But I'll make it up)

(Re)introducing neural networks and deep learning



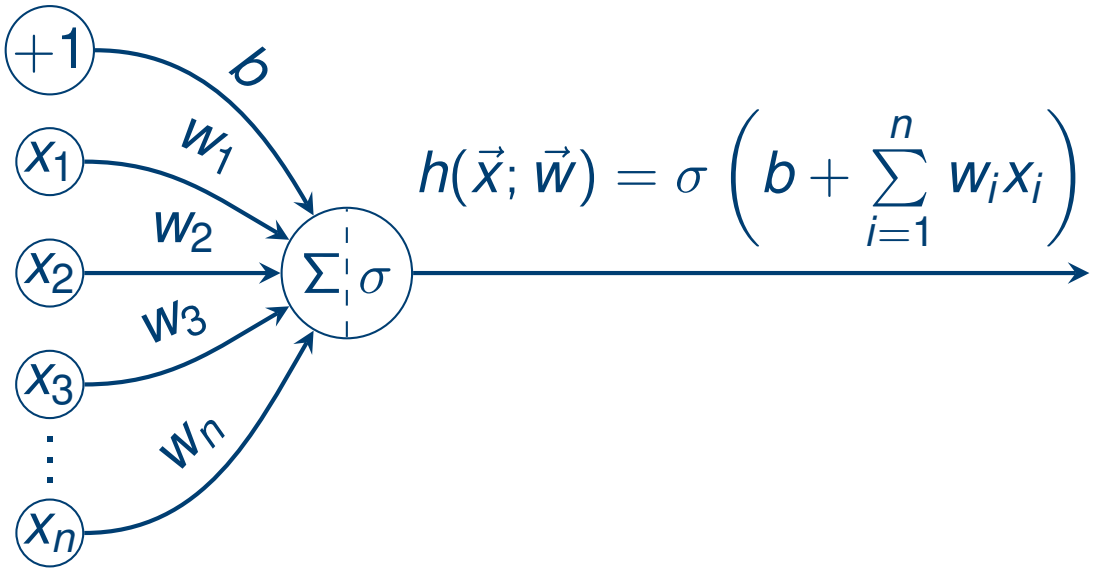


Neural networks

- To make life simpler (esp. notationally!), let's start with a slightly more thorough introduction to simple neural networks.
- This might restate some of the material you've already seen, with the aim of making notation more consistent!
- **Neural networks** are structures of interconnected processing units (*neurons*).
- Each neuron computes a linear combination of its *inputs*, afterwards potentially applying an *activation function*, to produce its *output*.
- Occasionally, I will illustrate how to specify neural networks of interest using *Keras* (`keras.io`). (**highly recommended!**)

A single neuron

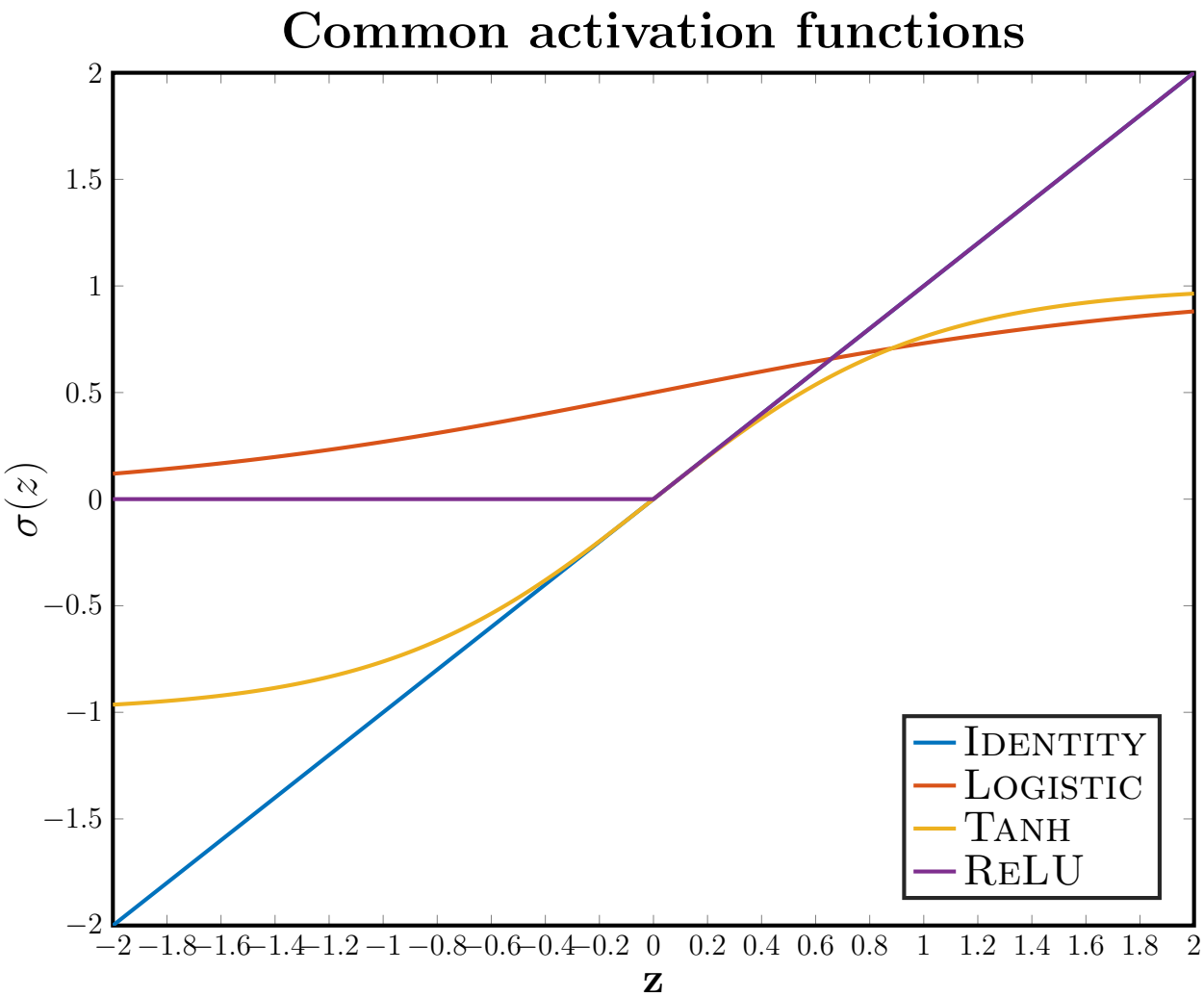
Within this context sometimes also called a *perceptron* (. . .)



Popular choices for the activation function σ:

- *Identity*: $\sigma(x) = x$;
- *Rectified linear unit (ReLU)*: $\sigma(x) = \max(0, x)$;
- *Sigmoid functions*: $\sigma(x) = \frac{1}{1+\exp(-x)}$ (*logistic*); $\sigma(x) = \tanh x$.

Activation functions



Neural networks and deep learning

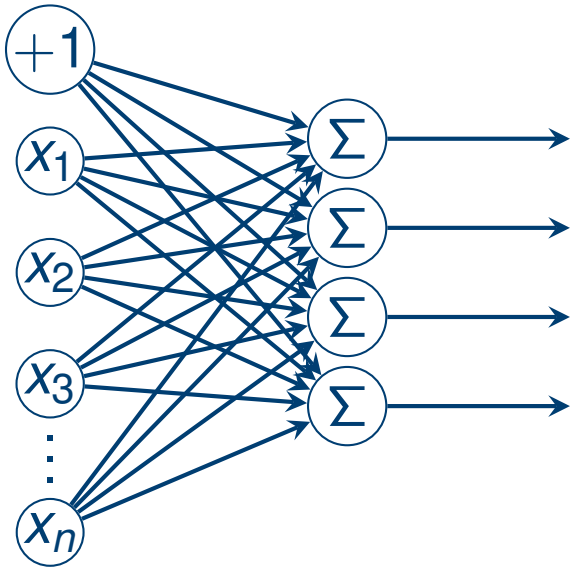
- It is easy to extend a single neuron to a *neural network*—simply connect outputs of neurons to inputs of other neurons.
- We may do this in two ways:
  - **Feedforward**: the computation graph does not have cycles;
  - **Recurrent**: the computation graph has cycles.
- Typically we organise neural networks in a sequence of *layers*, such that a single layer only processes output from the previous layer. Everything with $>$ 1 hidden layer is *"deep"*!

A few details on training

- Neural networks are trained from known (input, output) samples. The training algorithm adapts the neurons' weights to maximise *predictive power* on the training examples.
- This is done, for a single training example $(\vec{x}, y)$, by:
  - Computing the output of the network $y' = h(\vec{x}; \vec{w})$;
  - Determining the *loss* of this output $\mathcal{L}(y, y')$;
  - Computing partial derivatives of the loss with respect to each weight, $\frac{\partial \mathcal{L}}{\partial \vec{w}}$, and using these to update weights.
  - Key words: *backpropagation*, *stochastic gradient descent*.
- More details next week!

A simple classifier

Let's ignore the activation functions and "deep learning" for now. . . here is a simple, shallow, 4-class classifier.

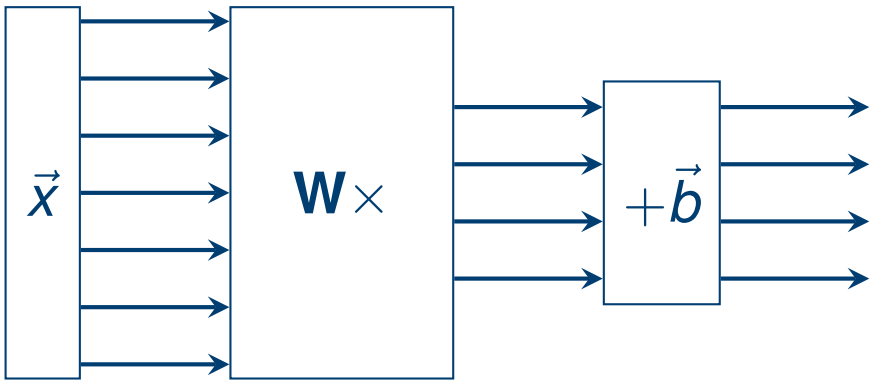


Choose the class which has the maximal *output*:

$$C = \text{argmax}_j \left\{ b_j + \sum_{i=1}^{n} w_{ij} x_i \right\}$$

Block notation

Note that this layer is essentially doing a matrix multiplication. . .



$$C = \text{argmax}_j \left(\mathbf{W}\vec{x} + \vec{b} \right)_j$$

N.B. W of size $4 \times n$, $\vec{b}$ of size 4.

Softmax

- **Problem**: what should the targets be?
- Outputs are *unbounded*! For an example of the second class, the targets should be $\vec{y} = \begin{bmatrix} -\infty & +\infty & -\infty & -\infty \end{bmatrix} \ldots$
- **Solution**: transform the outputs monotonically to the $[0, 1]$ range, using the *softmax* function:

$$softmax(\vec{z})_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

Probabilistic classification

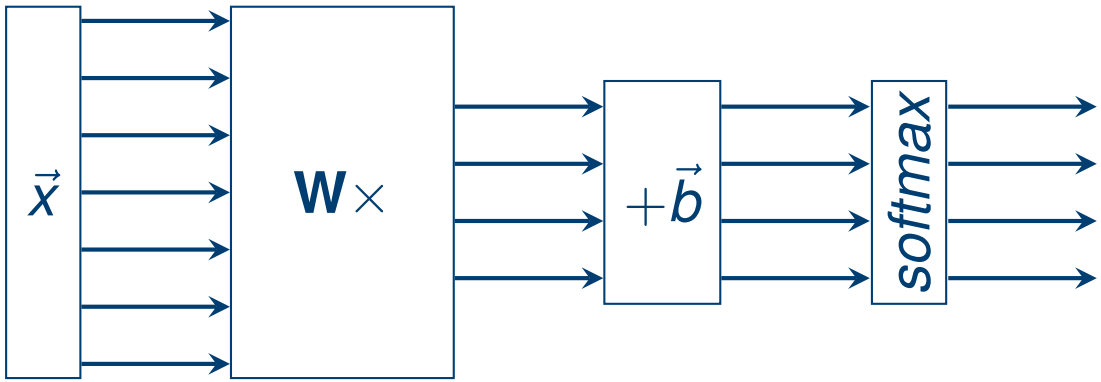
- This conveniently also makes the outputs add up to 1, so we can interpret $y'_i = \mathit{softmax}(h(\vec{x}))_i = \mathbb{P}(\vec{x} \textit{ in class } i)$.
- Now the target for an example of the second class should be $\vec{y} = \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}$ ($\sim$ one-hot encoding).
- Typically express the loss function as the *cross-entropy*:

$$\mathcal{L}(\vec{y}, \vec{y}') = -\sum_{i=1}^{K} y_i \log y'_i$$

where K is the number of classes.

Back in business

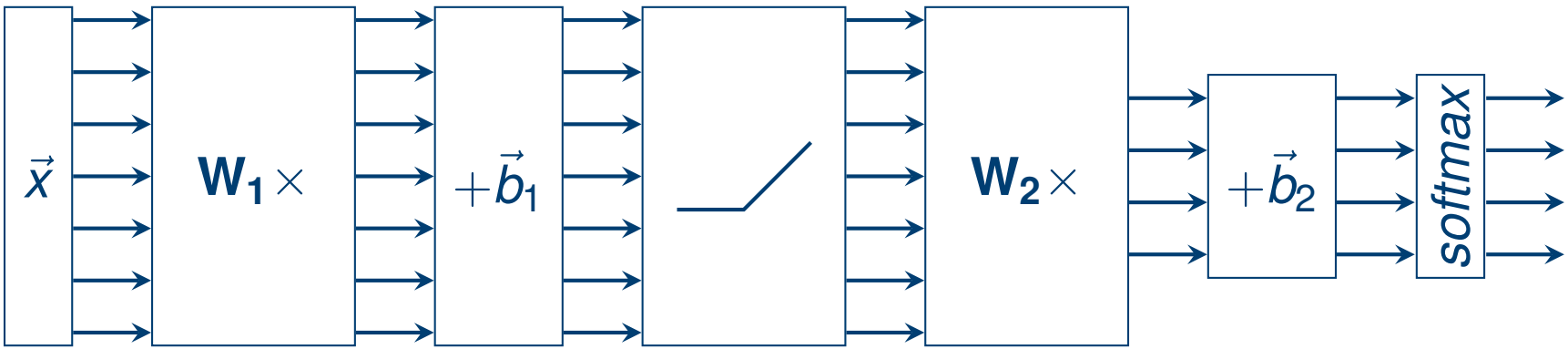
Integrating into our simple classifier:



$$C = \text{argmax}_j \left\{ softmax \left(\mathbf{W}\vec{x} + \vec{b} \right)_j \right\}$$

Going deeper with LEGO™

Making things *deep* is now easy…

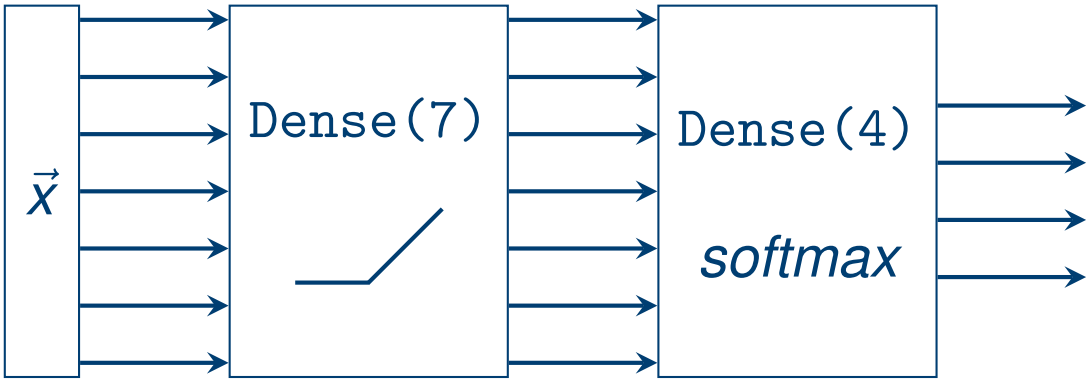


$$C = \text{argmax}_j \left\{ softmax \left(\mathbf{W_2} ReLU \left(\mathbf{W_1} \vec{x} + \vec{b}_1 \right) + \vec{b}_2 \right)_j \right\}$$

N.B. the ReLU is *important*! A composition of linear functions is itself a linear function… (at least in theory—thank you, OpenAI :))

Fully connected layers

The “matrix-multiply–bias–activation” (sometimes also called *fully connected* or `Dense`) layer is a common building block of neural networks.



Keras code:

```
x = Input(shape=(7,))
h = Dense(7, activation='relu')(x)
y = Dense(4, activation='softmax')(h)
```

Working with images

- Simple fully-connected neural networks (as described already) typically fail on high-dimensional datasets (e.g. images).
  - Treating each pixel as an independent input...
  - ...results in $h \times w \times d$ new parameters per neuron in the first hidden layer...
  - ...quickly deteriorating as images become larger—requiring exponentially more data to properly fit those parameters!
- **Key idea:** downsample the image until it is small enough to be tackled by such a network!
  - Would ideally want to extract some useful features first...
- $\implies$ exploit spatial structure!

The *convolution* operator

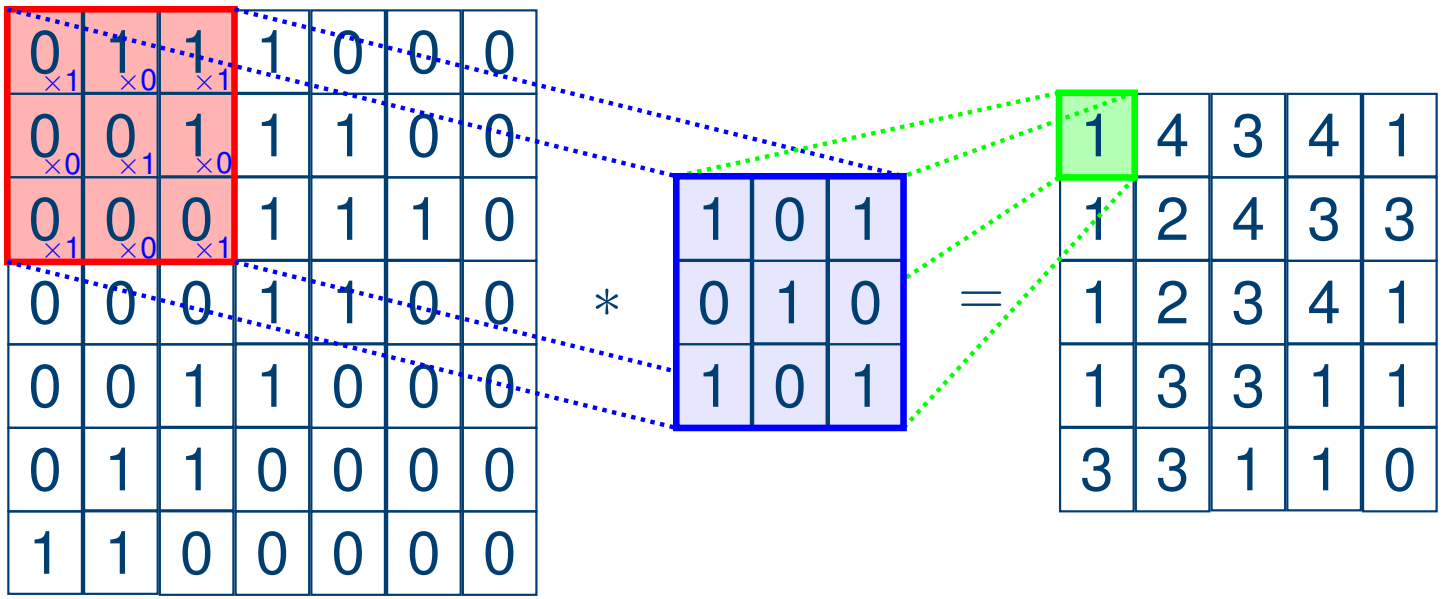
Enter the *convolution* operator

- Define a small (e.g. 3×3) matrix (the kernel, $\mathbf{K}$).
- Overlay it in all possible ways over the input image, $\mathbf{I}$.
- Record sums of elementwise products in a new image.

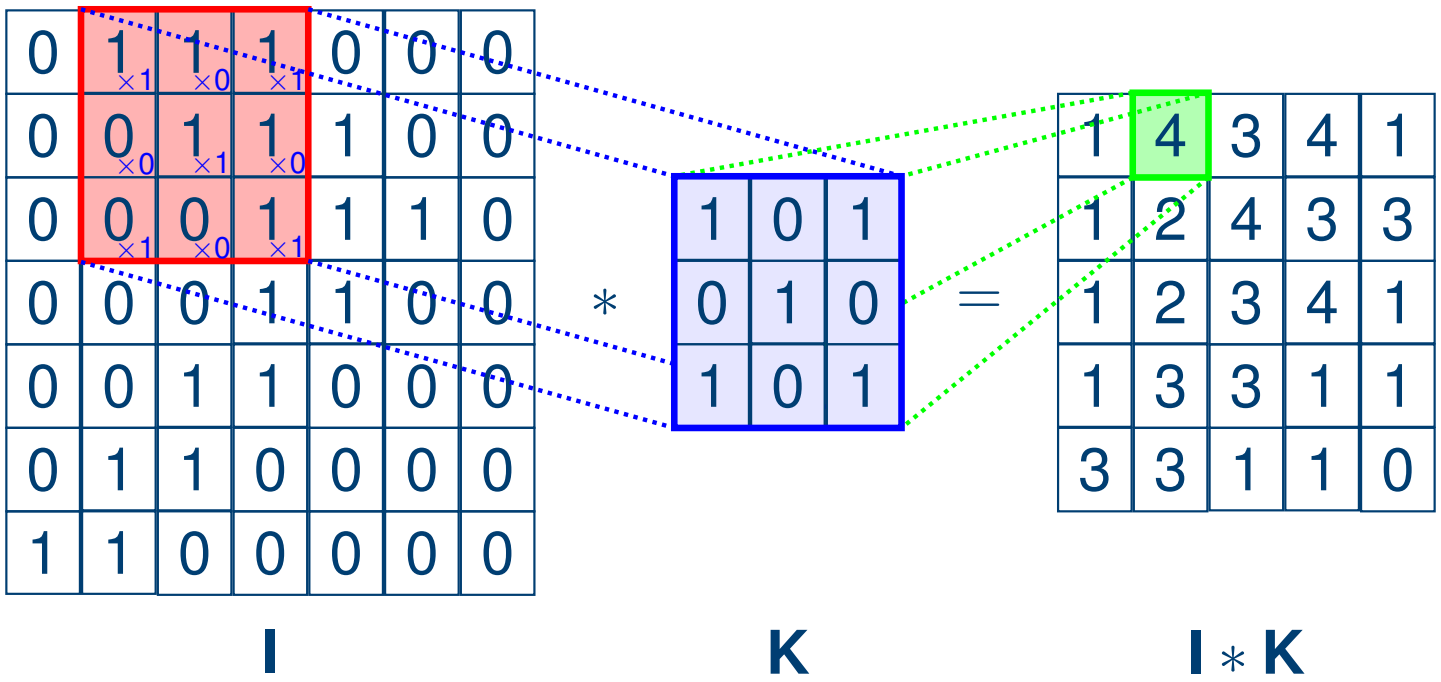
$$(\mathbf{I} * \mathbf{K})_{xy} = \sum_{i=1}^{h} \sum_{j=1}^{w} \mathbf{K}_{ij} \cdot \mathbf{I}_{x+i-1,y+j-1}$$

- This operator exploits structure—neighbouring pixels influence one another stronger than ones on opposite corners!
- Start with *random kernels*—and let the network find the optimal ones on its own!

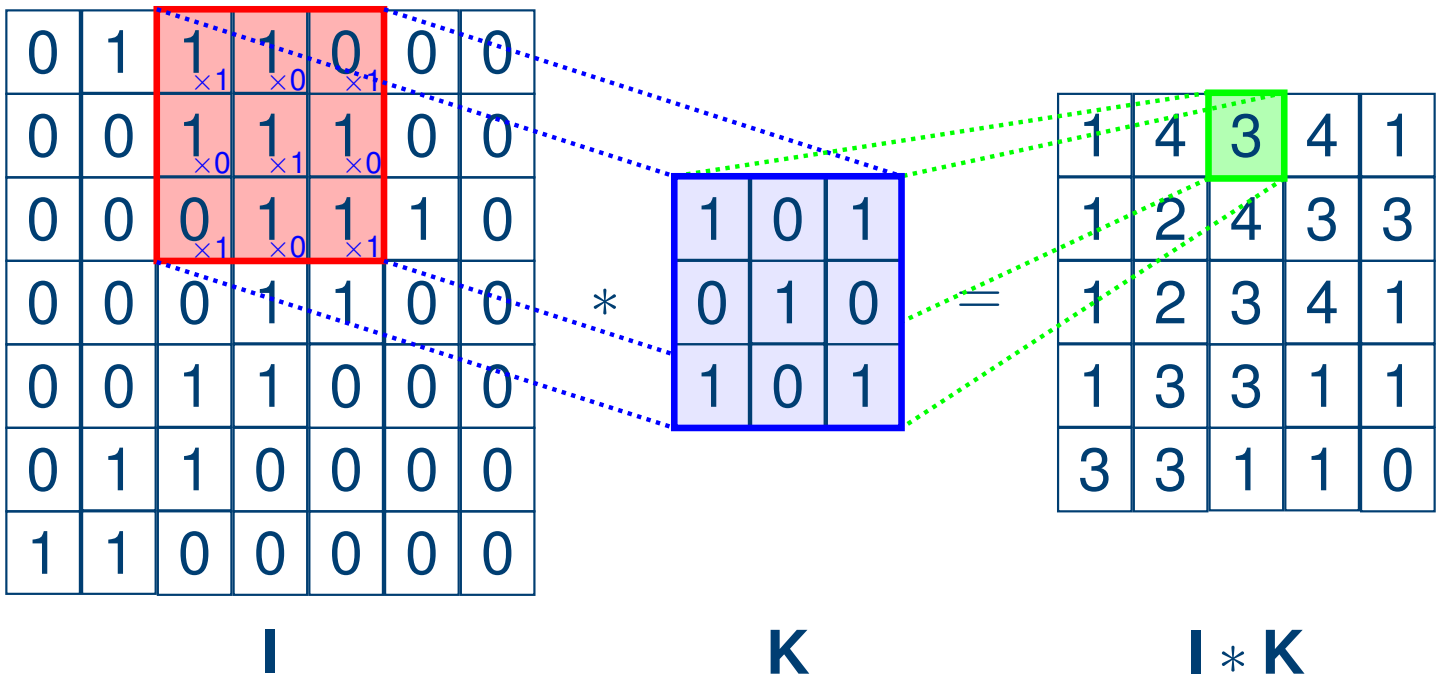
Convolution example



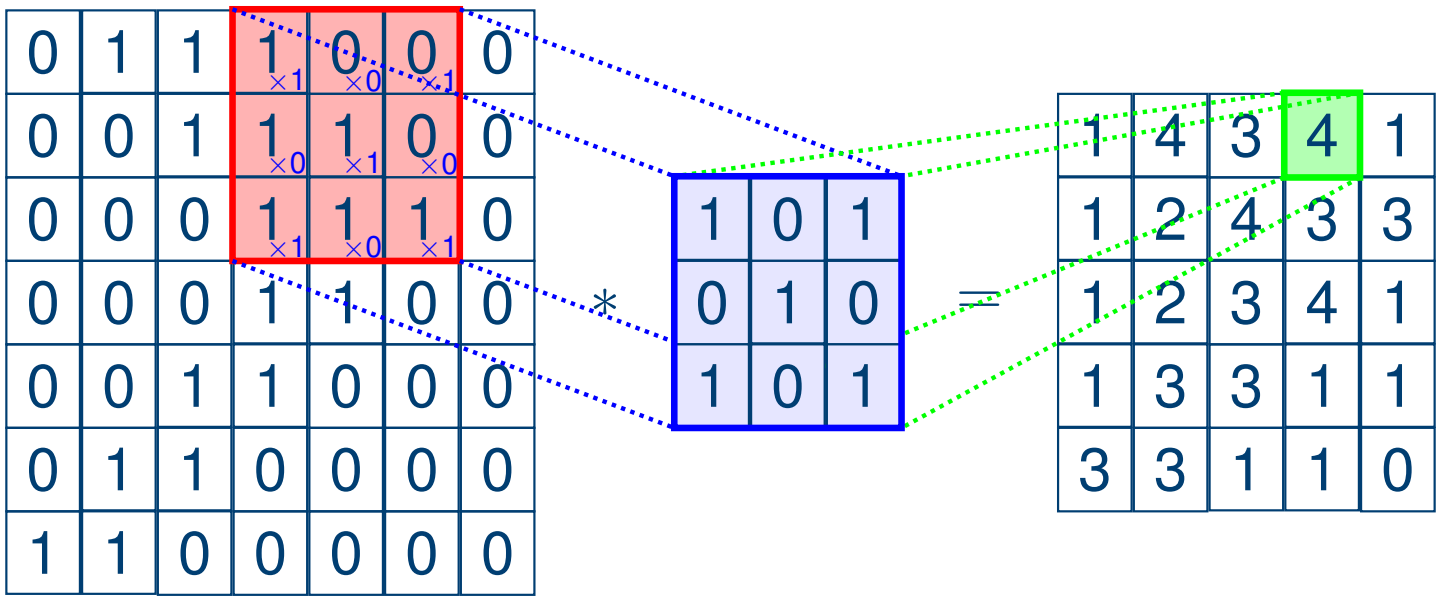
Convolution example



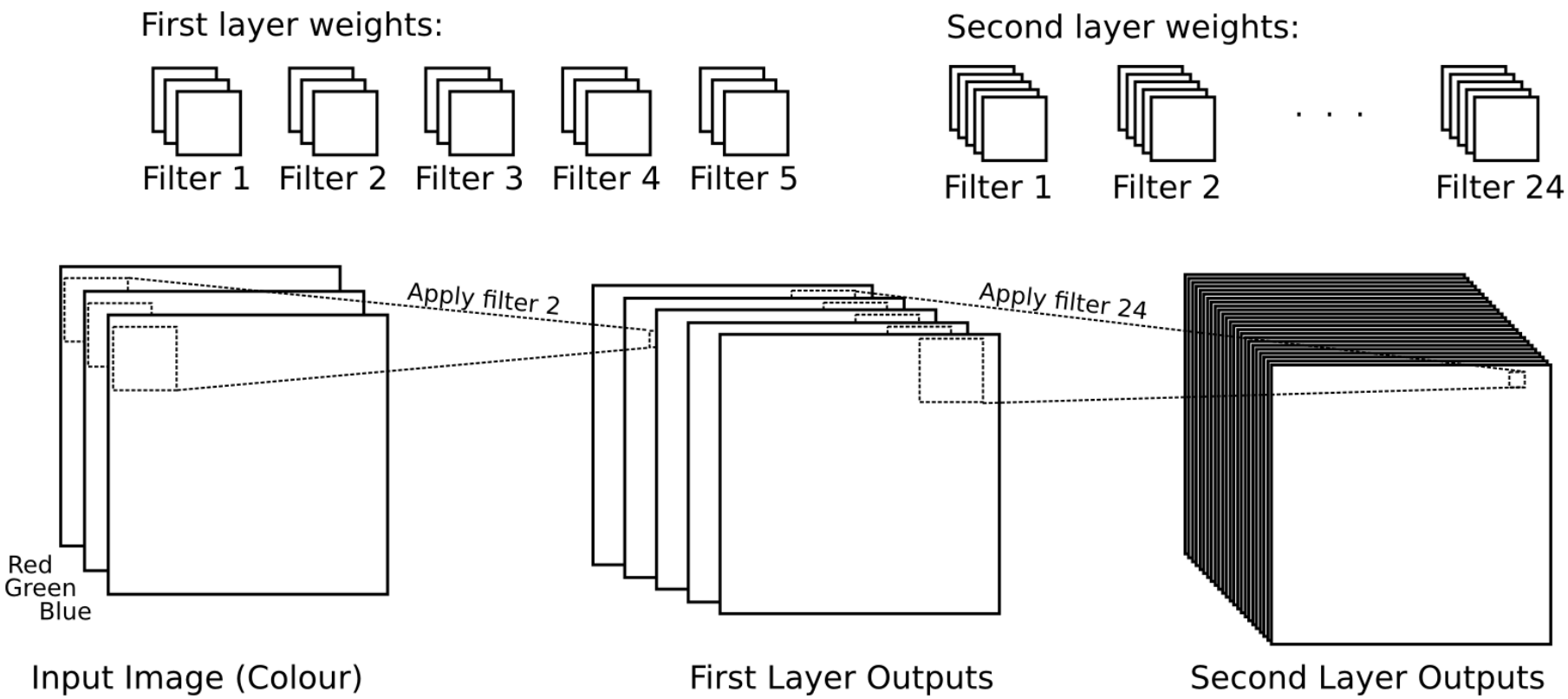
Convolution example



Convolution example

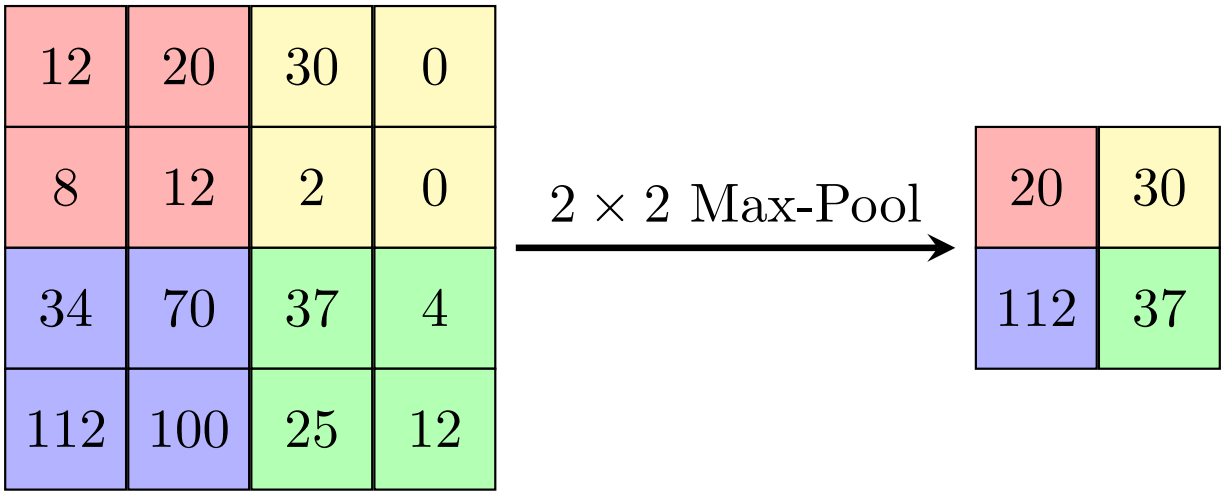


Stacking convolutions

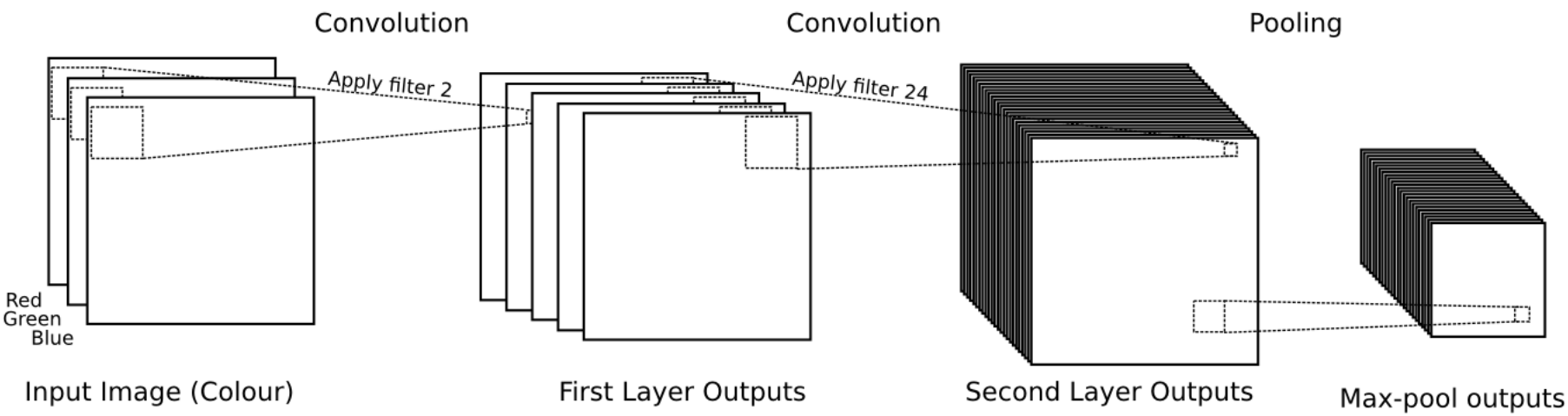


Downsampling ($\sim$ *max-pooling*)

Convolutions *light up* when they detect a particular feature in a region of the image. Therefore, when downsampling, it is a good idea to preserve maximally activated parts. This is the inspiration behind the *max-pooling* operation.

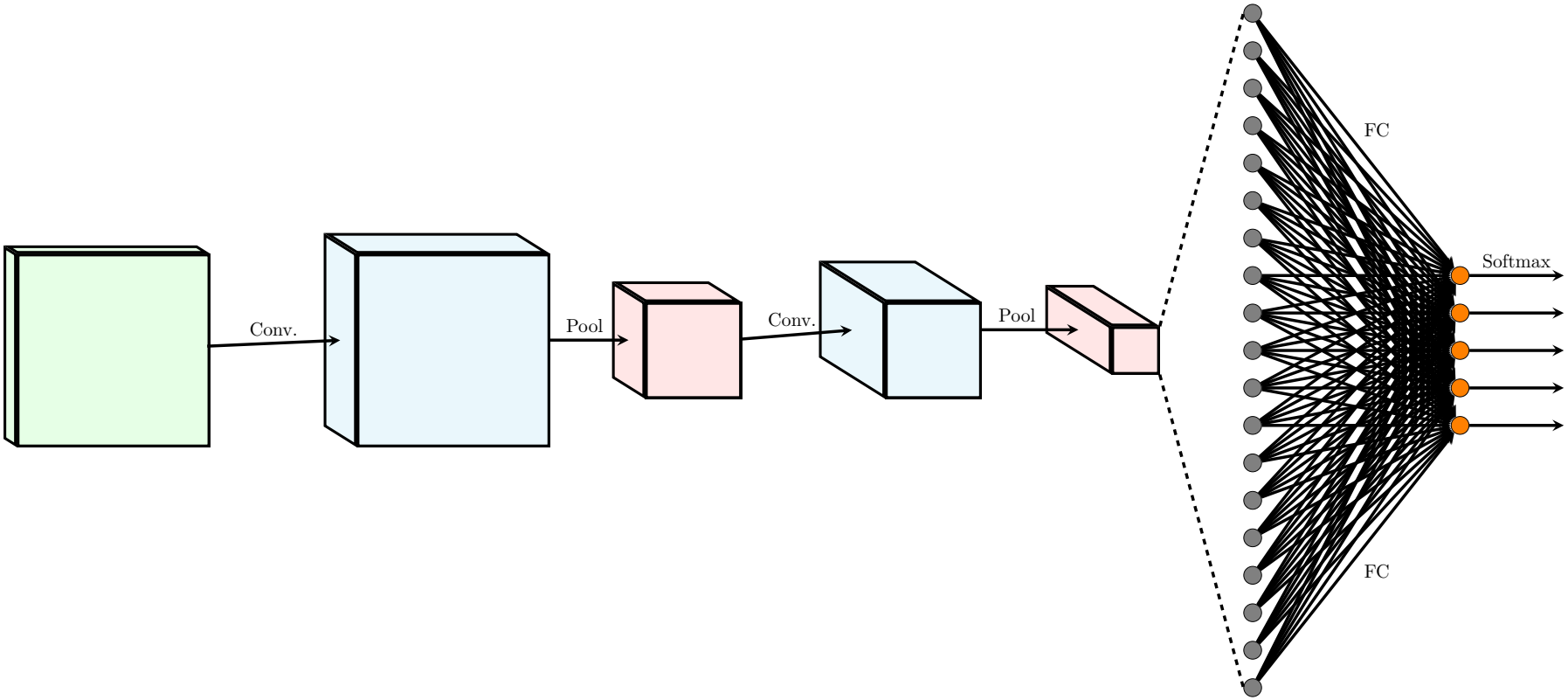


Stacking convolutions and poolings



Stacking convolutions and poolings

Rough rule of thumb: increase the *depth* (number of convolutions) as the *height* and *width* decrease.



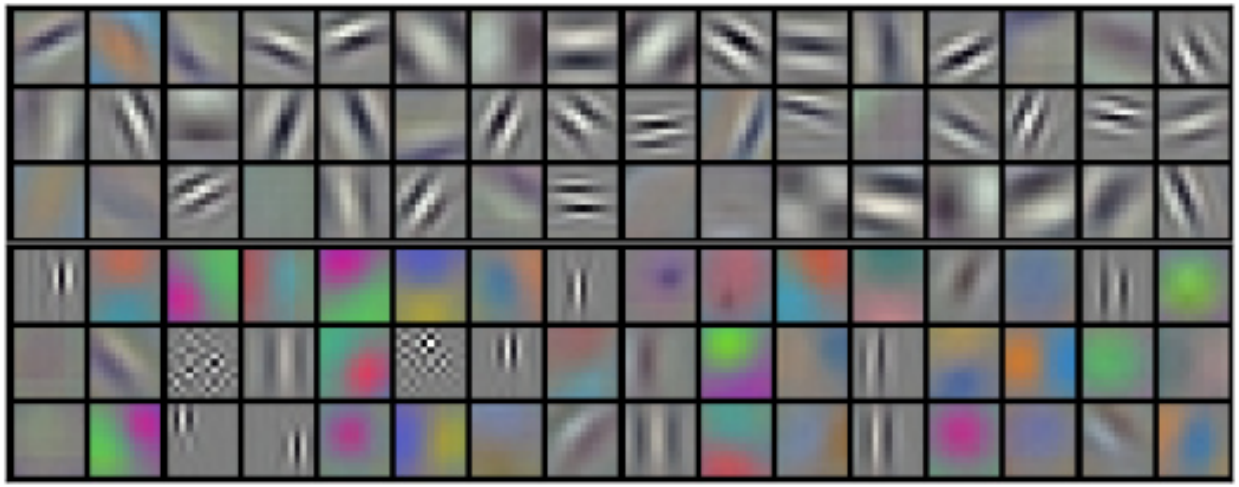
CNN representations

Three ways to examine the CNN's internal representations:

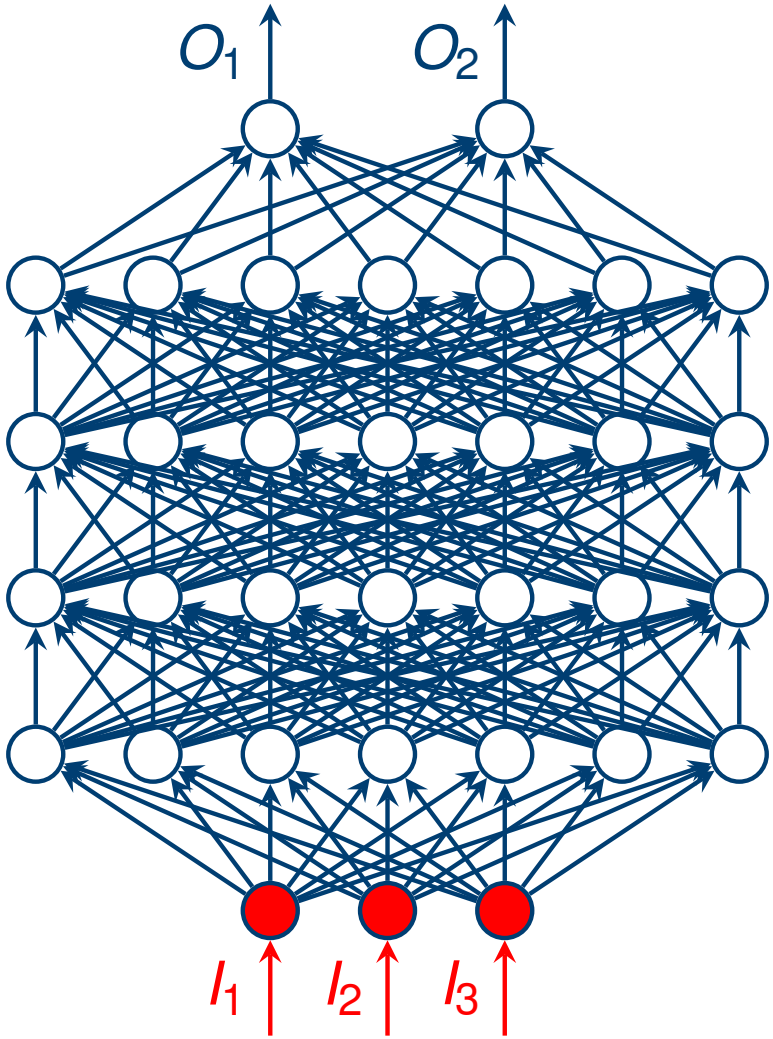
1. Observe the learnt *kernels*;
2. Pass an input through the network, observe the *activations*;
3. Coming later in this lecture. . .

Observing kernels

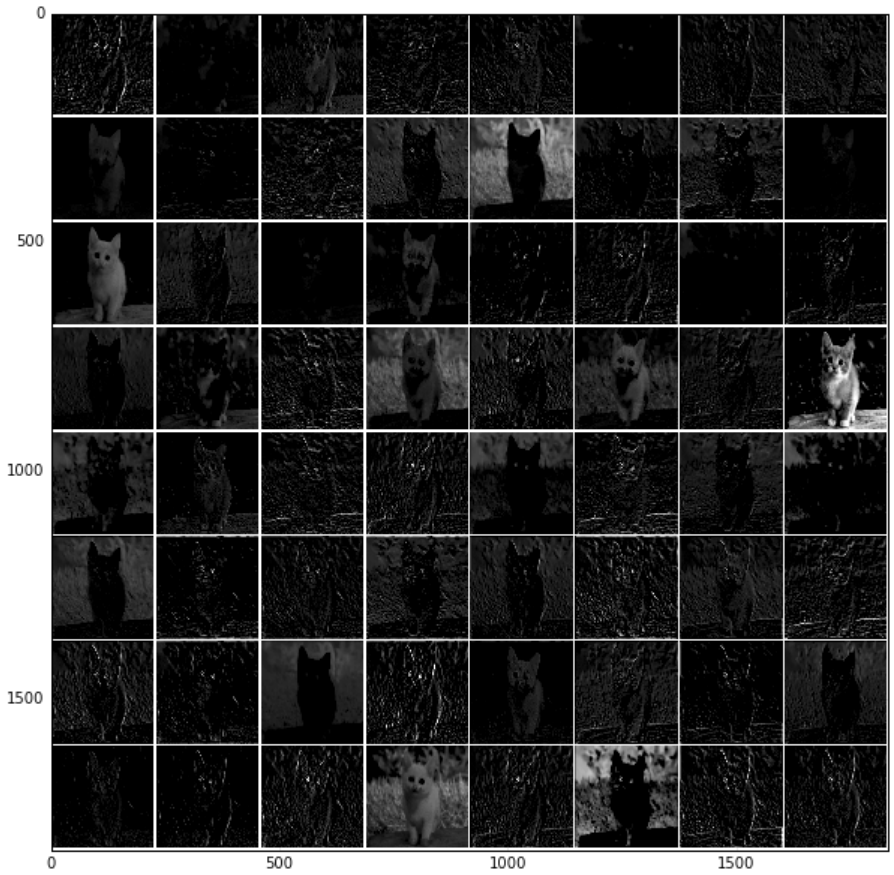
- Typically, as the kernels are small, gaining useful information from them becomes difficult already *past the first layer*.
- However, the first layer of kernels reveals something *magical*... In almost all cases, these kernels will learn to become *edge detectors*!

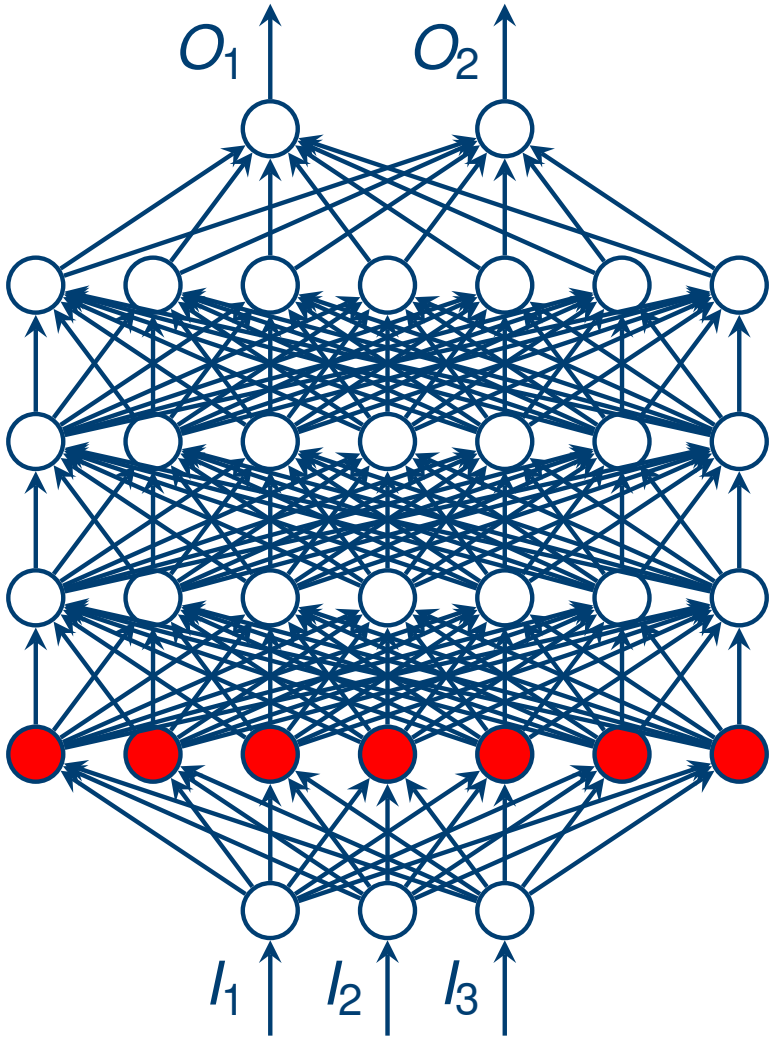


Passing data through the network: *Input*

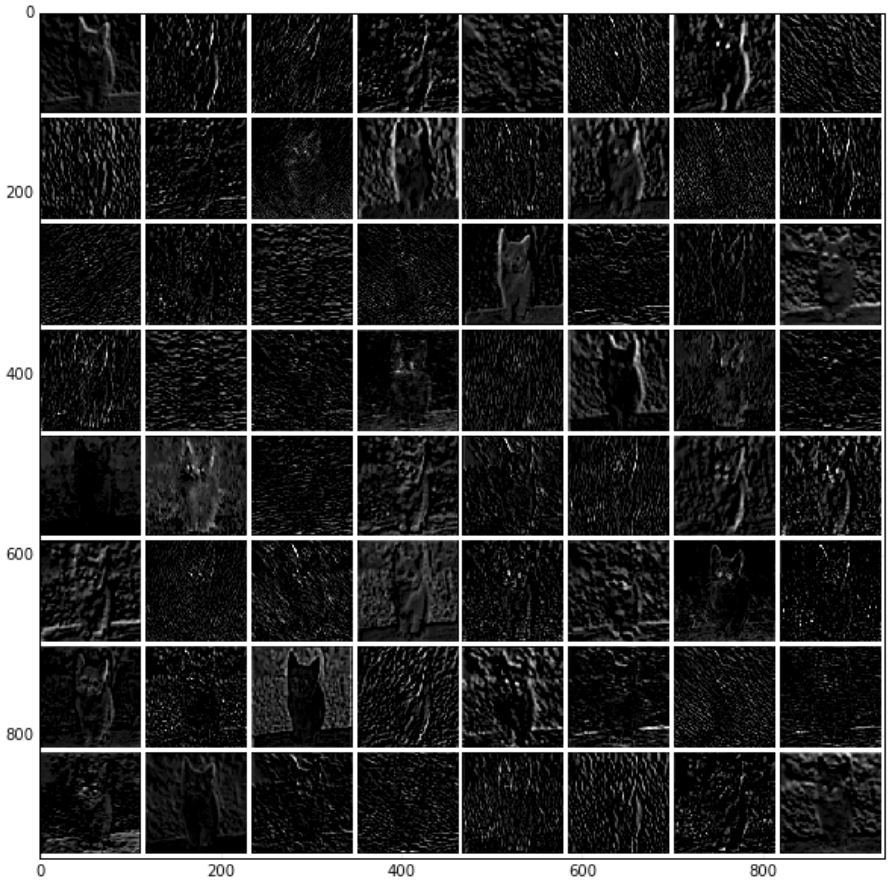


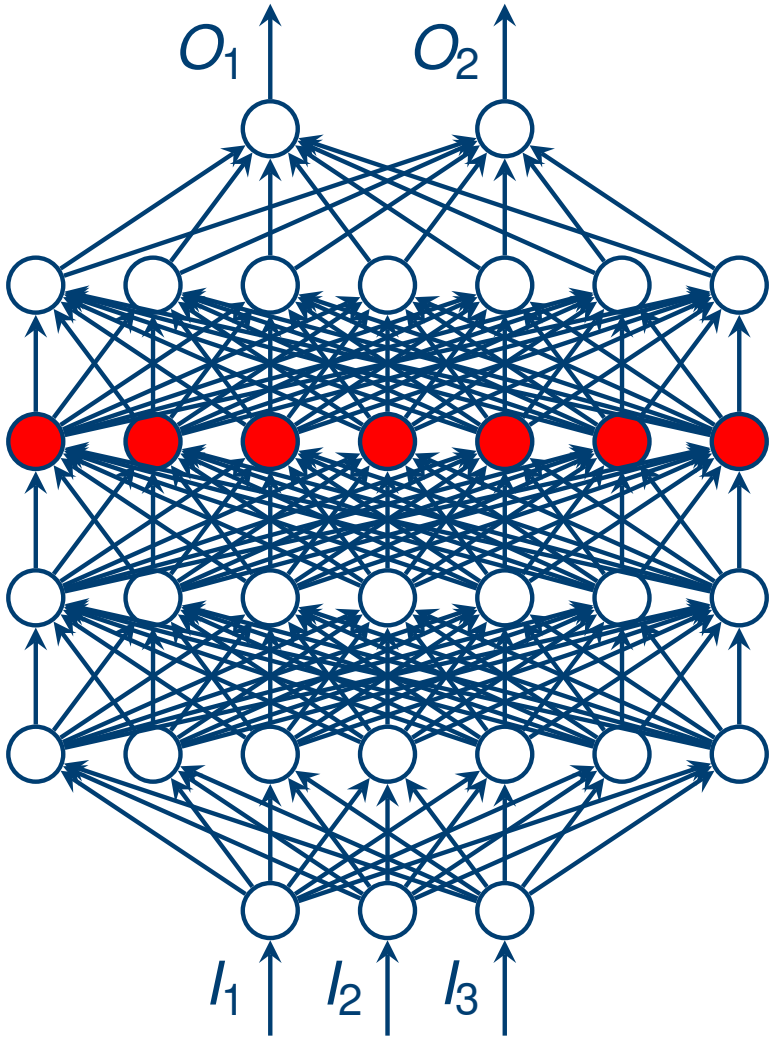
Passing data through the network: *Shallow layer*



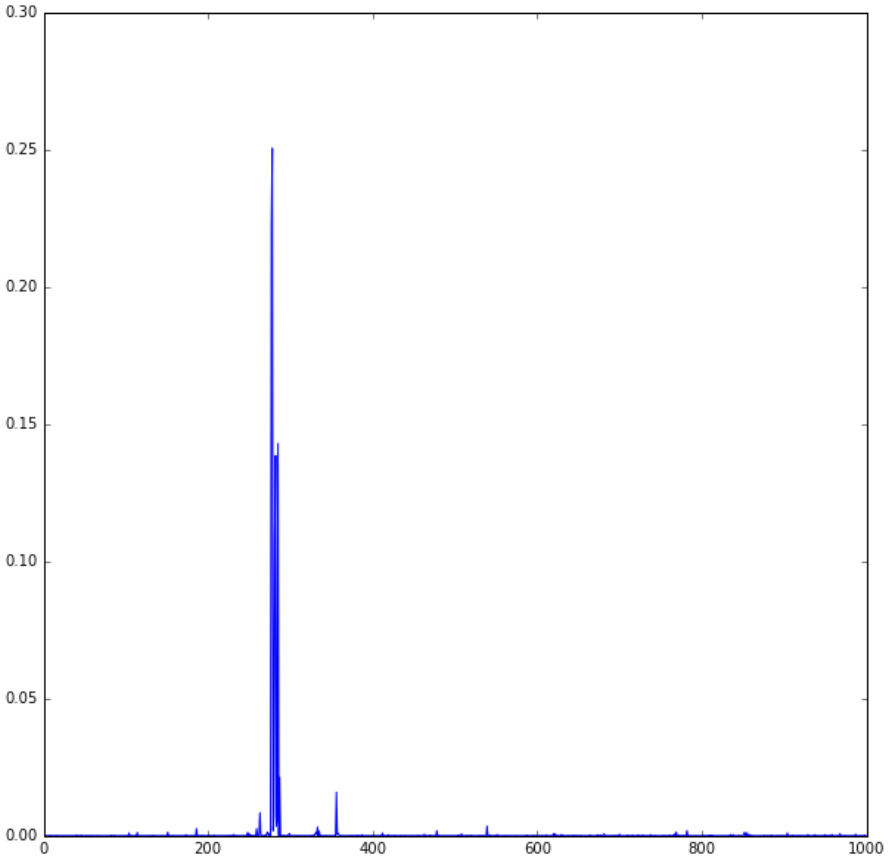


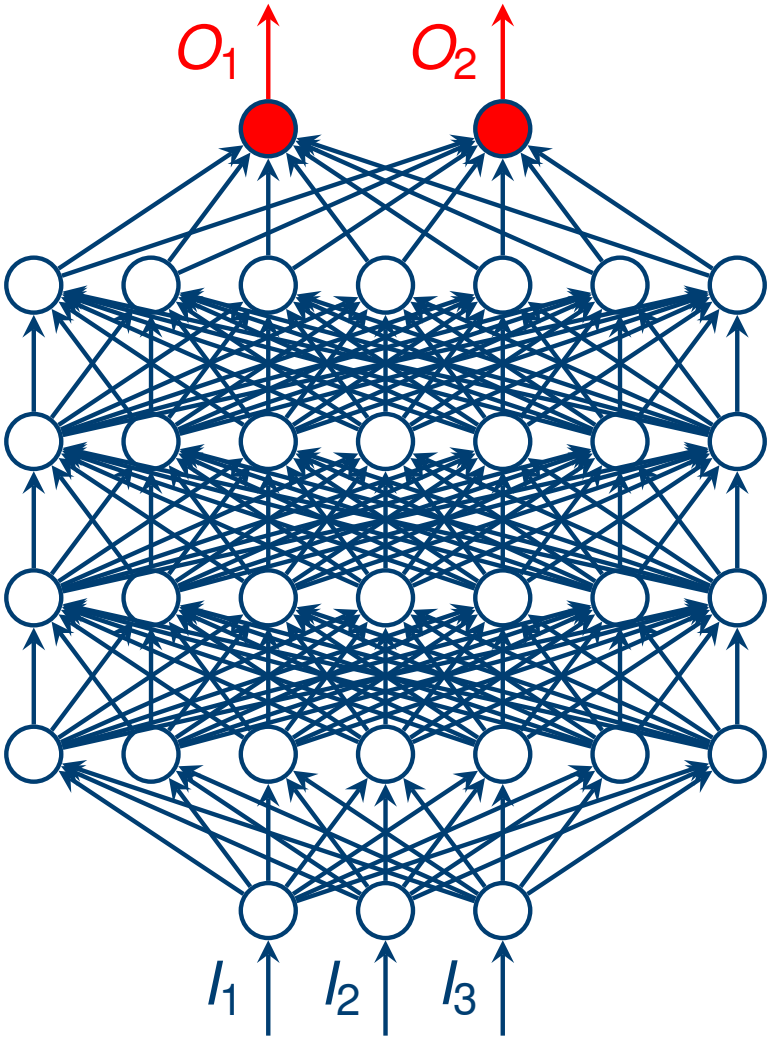
Passing data through the network: *Deep layer*





Passing data through the network: *Output*

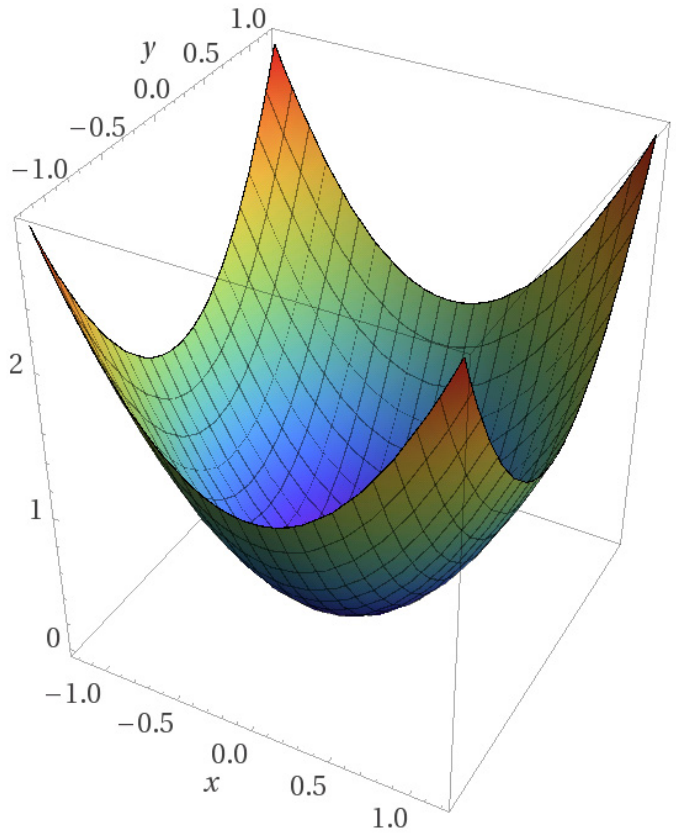


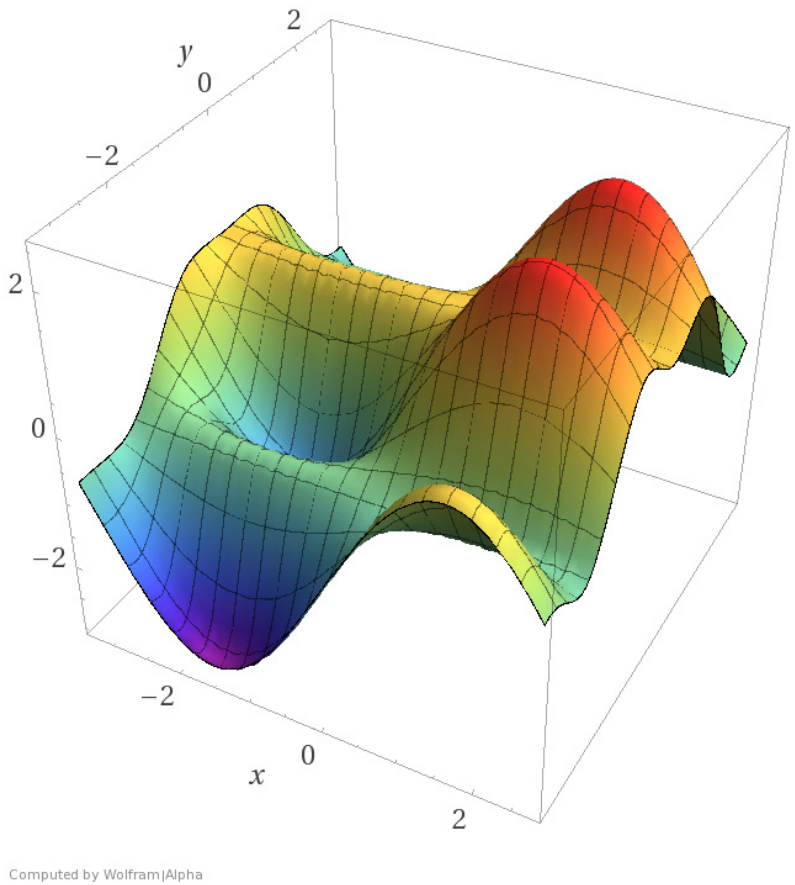


Issues with learning through backpropagation

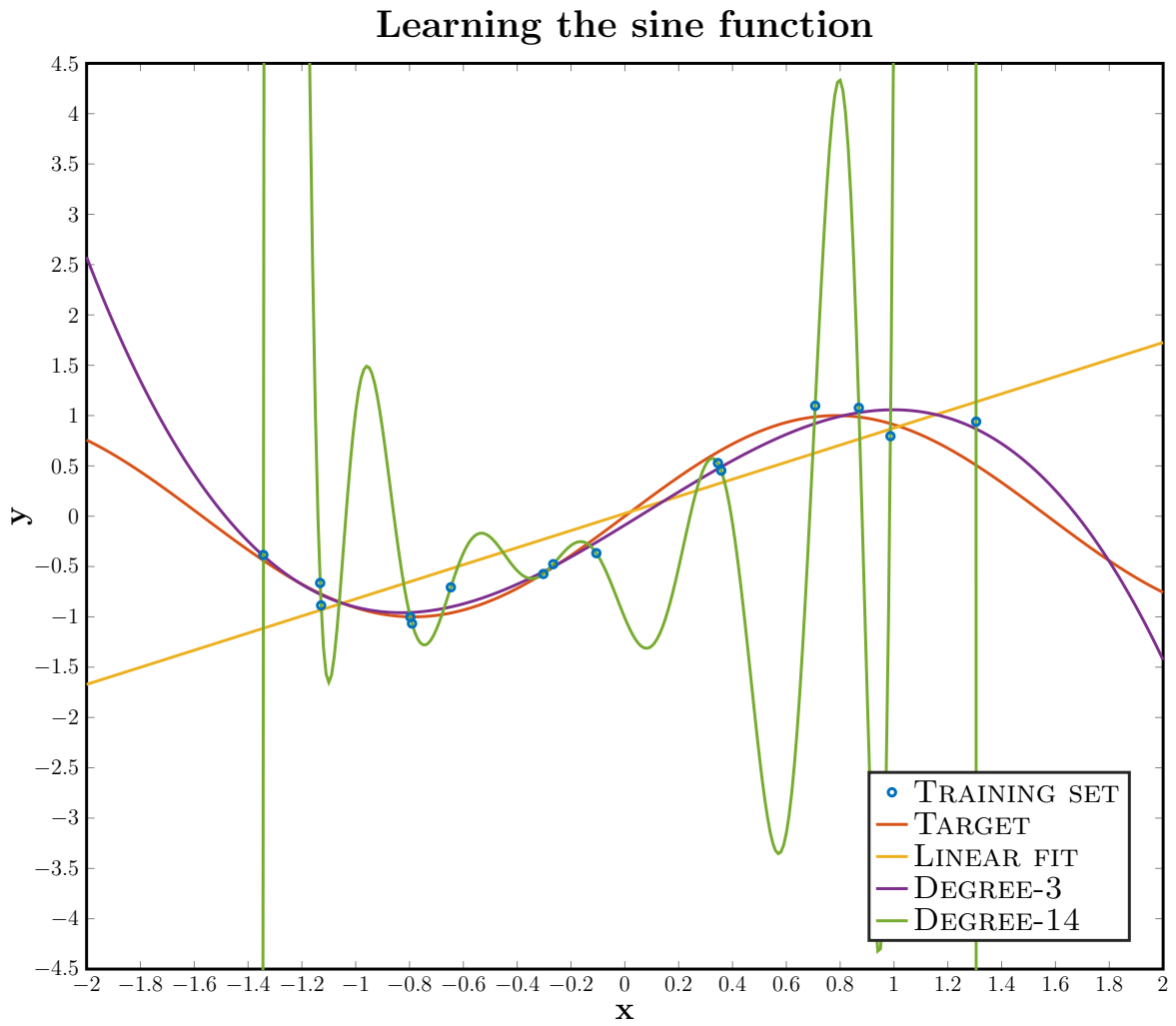
- We will start by analysing a direct way in which unsupervised techniques can aid the kind of supervised learning more common for deep neural networks.
- "Deep learning" was around for decades, but took a long time to become practically usable.
- We'd start with some randomly initialised weights, present our training examples to the network, and. . . the network *wouldn't really learn that well*.

Loss function surfaces





Beware of *overfitting*!



(In)appropriate initialisers

- It has since been determined that *initialisation* plays a **critical** role in neural network training stability.
- Extremely, what happens to error gradients if you initialise the network with *zero weights*? Or randomly sample them with a *huge variance*?
- *Be good to your signals. . .*
- Using an appropriate initialiser can mean the difference between getting *great results* and *not converging at all*!

What can we do?

- Reuse a network that performs great on a much larger dataset, and *fine-tune* (some of) its weights.
  - This is the concept of *transfer learning (week 7)*, and is fundamental to the successes of many deep learning startups. :)
  - Not always possible to do!
- I will now show how we can employ *unsupervised techniques* to determine weights that are "good" for working with our input data (regardless of what the outputs are!).
  - One of the first "success stories" of deep learning!
- In 2010, *Glorot and Bengio* discovered very appropriate parameters for randomly initialising weights (week 5). Unsupervised pre-training is very scarcely used nowadays.

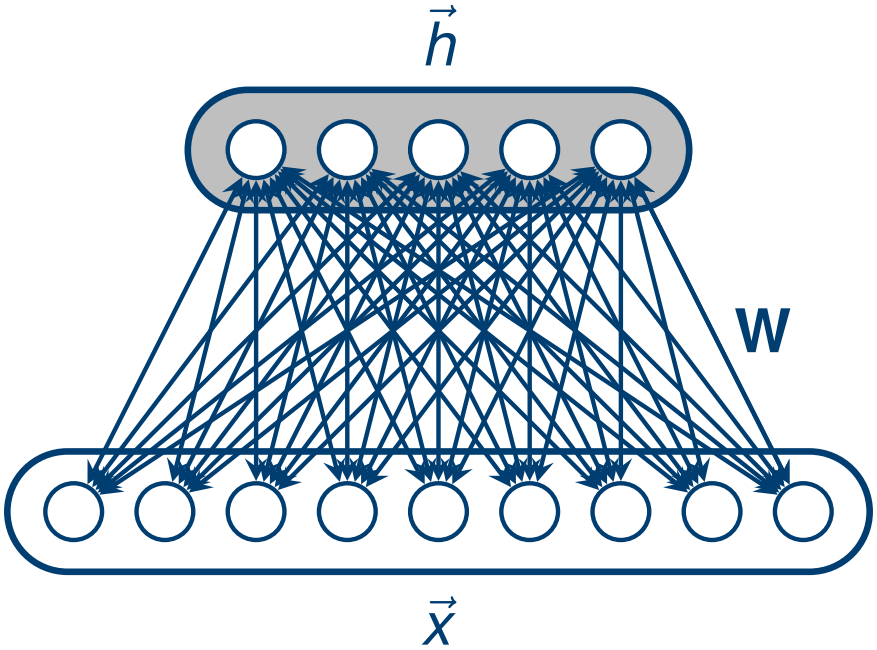
Reconstruction objective

- Assume that we want to initialise a *single-layer fully-connected* neural network, to be trained by backpropagation.
- We will further assume, for simplicity, that the inputs in our training dataset are *binarised* (0/1).
- Without a clear target, we can assume that *a good choice of weights will cause the output to retain most of the information about the input*.
- Therefore, **the weights should be chosen such that we can also use them to *reconstruct* the input given the output**!

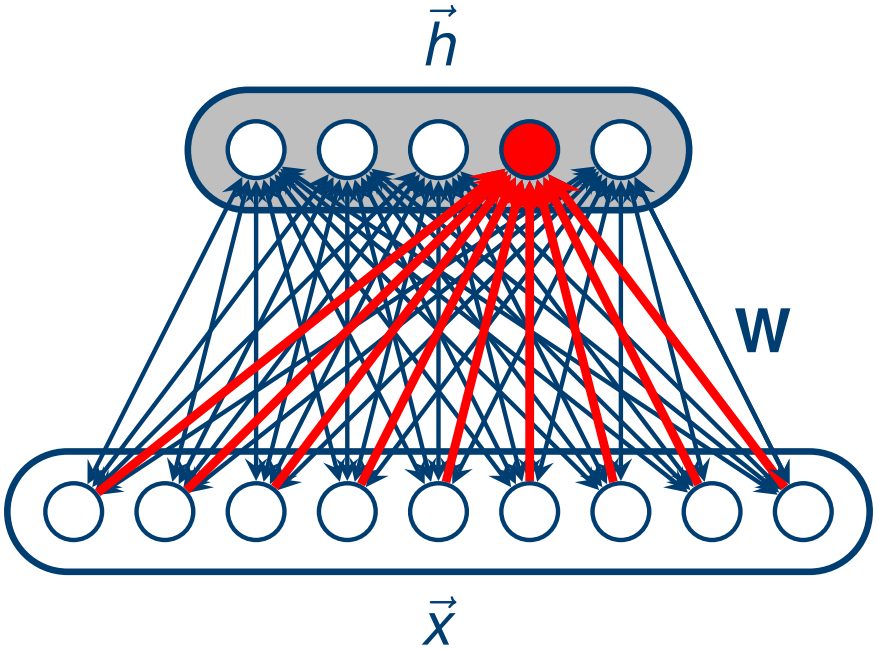
Restricted Boltzmann Machine (RBM)

- A simple unsupervised *stochastic* extractor of binary features, $\vec{h}$, from binary data, $\vec{x}$.
- Parametrised by a weight matrix $\mathbf{W}$ and bias vectors $\vec{a}$ and $\vec{b}$ to transform the data to the feature space, but *also to go back*!
- $\mathbb{P}(h_j = 1|\vec{x}) = \sigma\left((\mathbf{W}\vec{x} + \vec{b})_j\right) = \frac{1}{1+\exp\left(-(\mathbf{W}\vec{x}+\vec{b})_j\right)}$
- $\mathbb{P}(x_i = 1|\vec{h}) = \sigma\left((\mathbf{W}^T\vec{h} + \vec{a})_i\right) = \frac{1}{1+\exp\left(-(\mathbf{W}^T\vec{h}+\vec{a})_i\right)}$
- Trained efficiently using *contrastive divergence* (*Hinton, 2010*). Once trained, can use $\mathbf{W}$ and $\vec{b}$ as initial values for a neural net!

Restricted Boltzmann Machine (RBM)

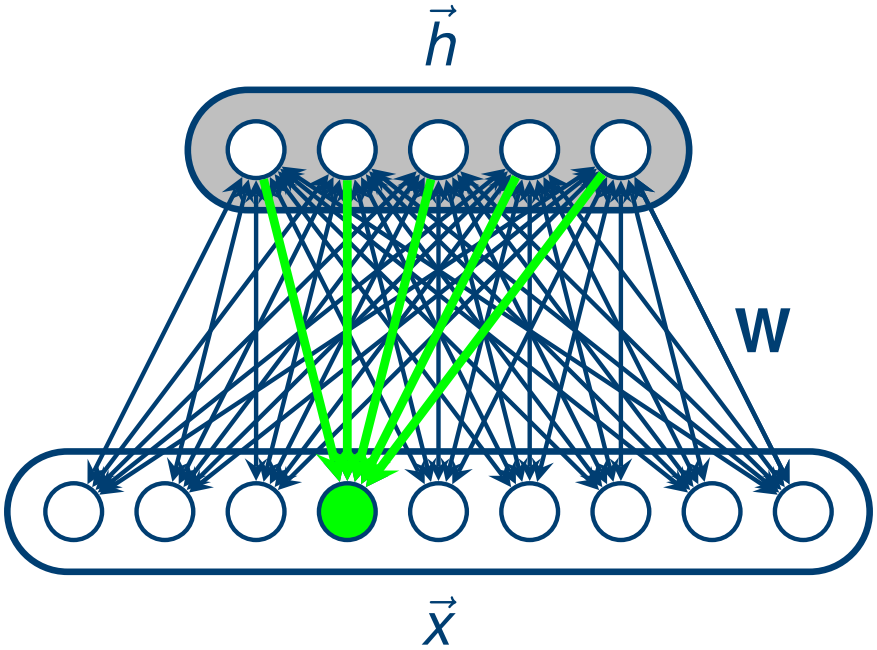


Restricted Boltzmann Machine (RBM)



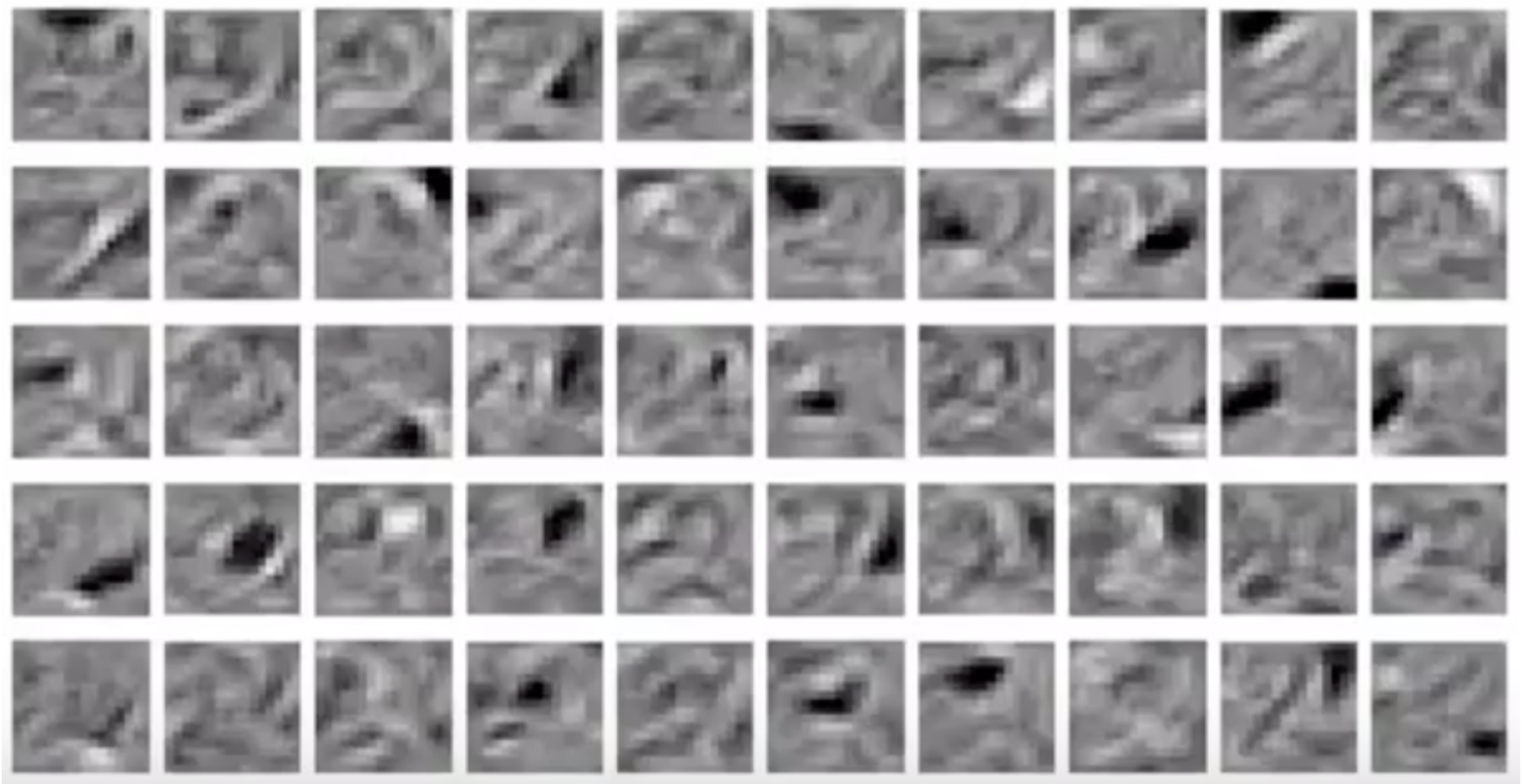
$$\mathbb{P}(h_j = 1|\vec{x}) = \sigma\left((\mathbf{W}\vec{x} + \vec{b})_j\right) = \frac{1}{1 + \exp\left(-(\mathbf{W}\vec{x} + \vec{b})_j\right)}$$

Restricted Boltzmann Machine (RBM)



$$\mathbb{P}(x_i = 1|\vec{h}) = \sigma\left((\mathbf{W}^T\vec{h} + \vec{a})_i\right) = \frac{1}{1 + \exp\left(-(\mathbf{W}^T\vec{h} + \vec{a})_i\right)}$$

RBM feature extraction (MNIST ‘2’ digits)

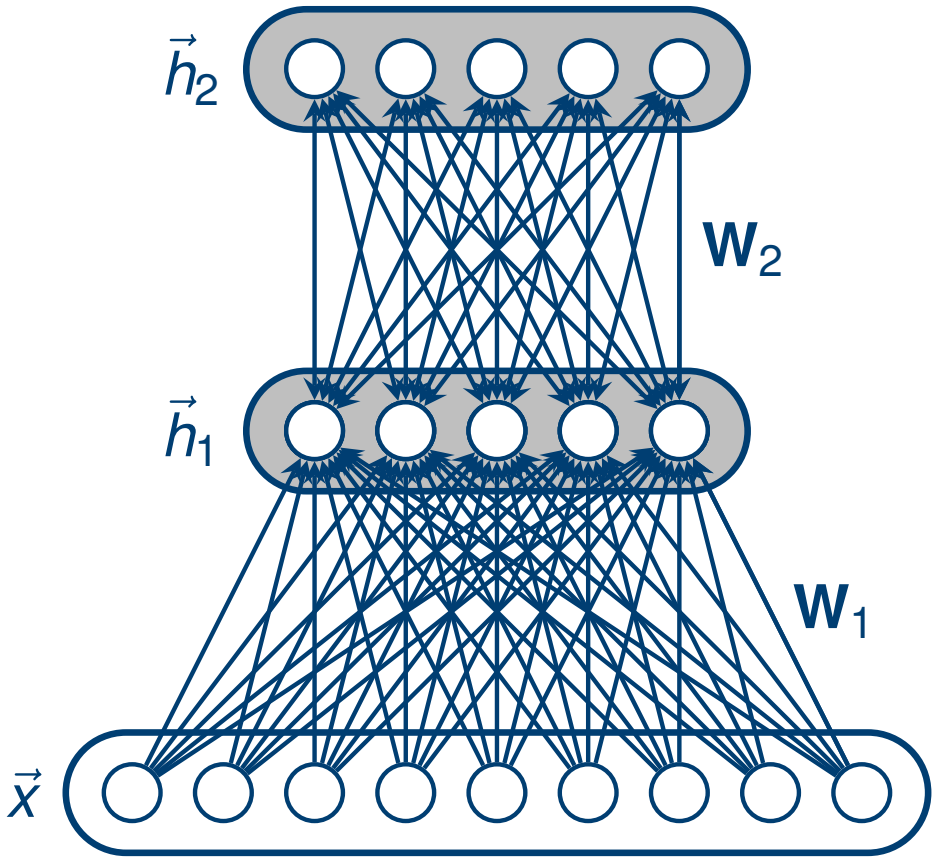


RBM reconstruction

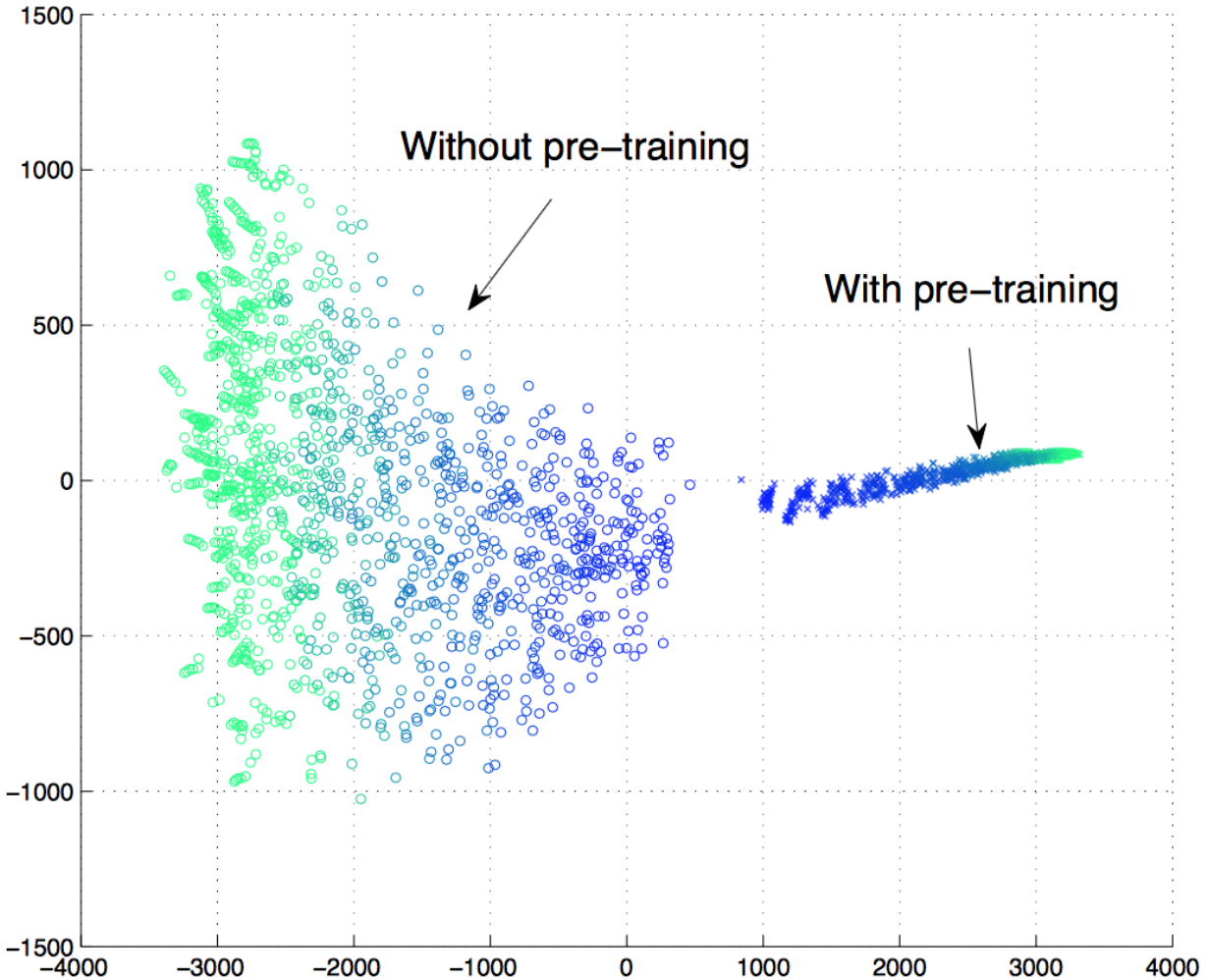
Deep Belief Network (DBN)

- If we want to go deeper, we can *stack additional RBMs*.
- Use the layers trained so far to generate outputs (by sampling or averaging), and use those as inputs for a new RBM. This construction is known as a **deep belief network (DBN)**.
- Can iteratively stack as many layers as we like!

Deep Belief Network (DBN)



Pre-training can help! (*Erhan et al., 2010*)



Dimensionality reduction

- We now focus on the general unsupervised problem of **dimensionality reduction**—finding a way to appropriately *compress* our input into a useful "bottleneck" vector of smaller dimensionality (we often call this algorithm an **encoder**).
- Obvious application to supervised learning: *feeding the output of the bottleneck into a simple classifier* (e.g. k-NN, SVM, logistic regression...), perhaps fine-tuning the encoder as well.
- Fundamentally, dimensionality reduction (along with appropriate *interpretability*) is the **essence** of unsupervised learning—to compress data well, one must first *understand* it!

Reconstruction strikes again

- Once again—in absence of any other information (that would be contained in labels), the best notion of "usefulness" for the bottleneck is **our ability to reconstruct the input from it**.
- Broadly speaking, we aim to specify two transformations:
  - The **encoder** – $enc : \mathcal{X} \to \mathcal{Z}$
  - The **decoder** – $dec : \mathcal{Z} \to \mathcal{X}$

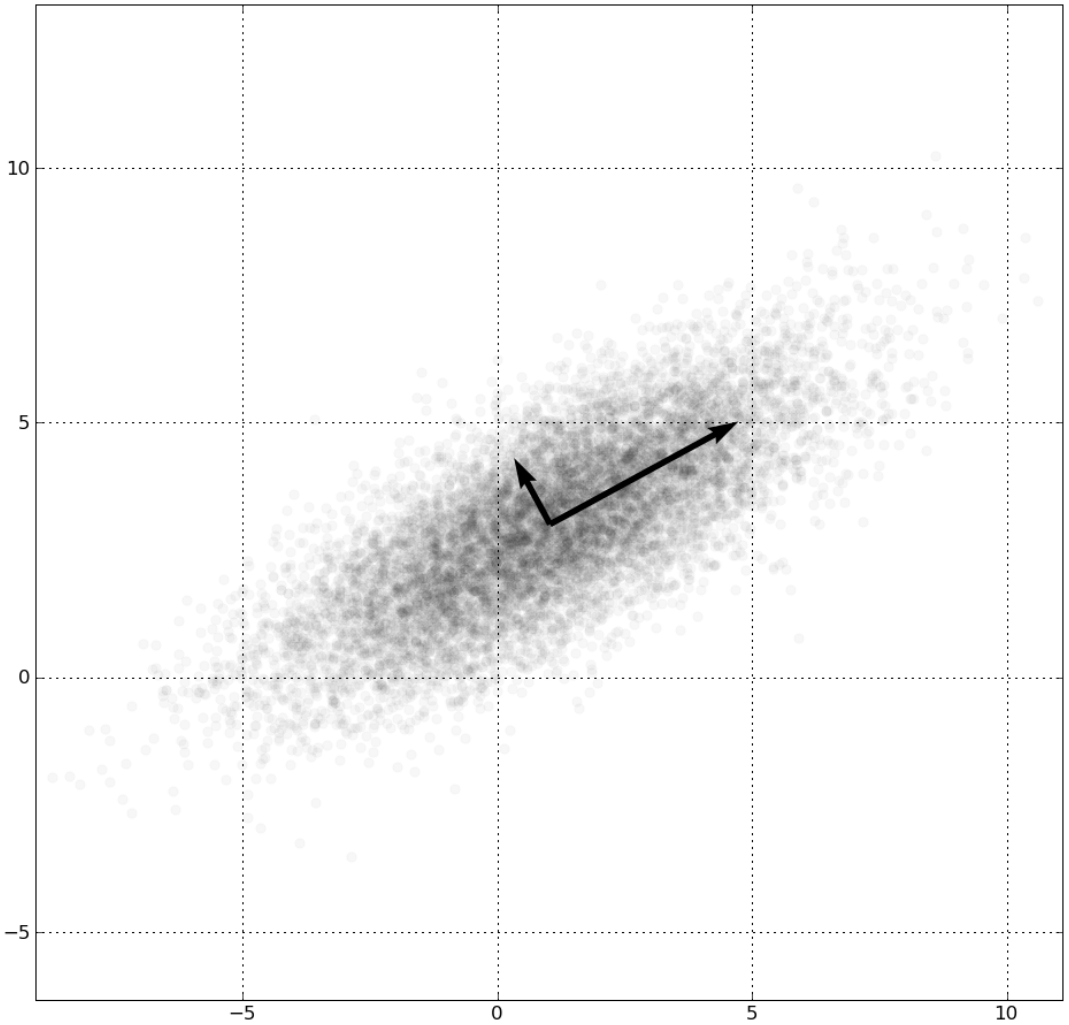
  where $\mathcal{X}$ and $\mathcal{Z}$ are the input and code spaces, respectively (these are often simply $\mathbb{R}^n$ and $\mathbb{R}^m$ with $n > m$).
- Then we seek to find parameters of the encoder/decoder that minimise the *reconstruction loss*:

$$\mathcal{L}(\vec{x}) = \|dec(enc(\vec{x})) - \vec{x}\|^2$$

Principal Component Analysis

- Perhaps the simplest instance of this framework is the **principal component analysis** (PCA) algorithm.
- Encode by *projecting* the n-dimensional data onto a set of m *orthogonal* axes ($n \geq m$).
- To preserve the most information, always choose one of the axes to be the direction in which the dataset *has the highest variance*! Then constrain subsequent ones to be orthogonal...
- Preserve m axes with highest variance.

PCA in action



PCA details

- Since projection onto orthogonal axes is a linear operation, the PCA encoder can be seen as simple matrix multiplication:

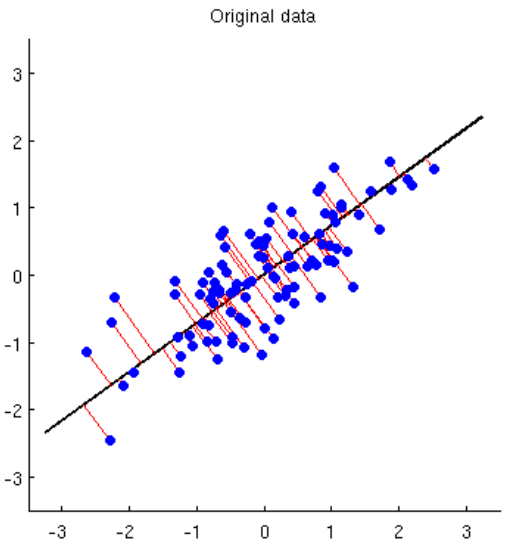
$$enc(\vec{x}) = \mathbf{W}\vec{x}$$

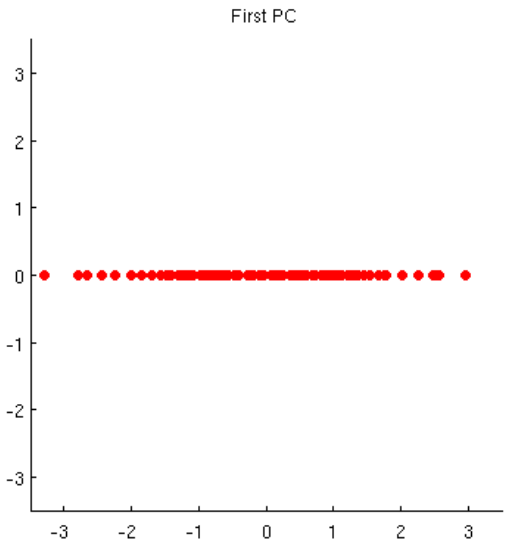
  where $\mathbf{W}$ is of size $m \times n$.
- As this is an *orthogonal* transformation, its inverse (*along retained axes only*) is its matrix's *transpose*:

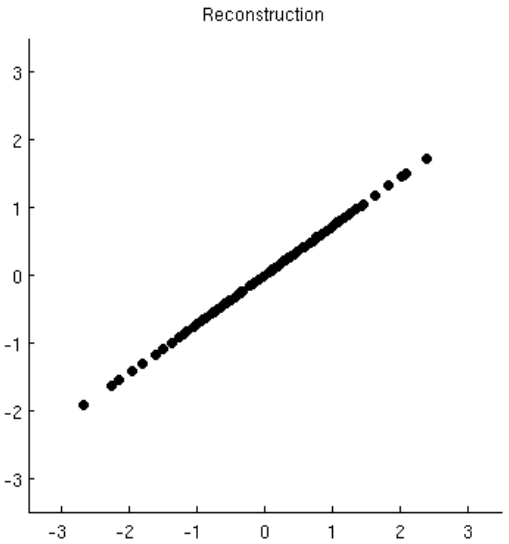
$$dec(\vec{z}) = \mathbf{W}^T\vec{z}$$

- We therefore seek to choose $\mathbf{W}$ to minimise $\|\vec{x} - \mathbf{W}^T\mathbf{W}\vec{x}\|^2$. Can solve this *explicitly* (using eigenvalue analysis)!

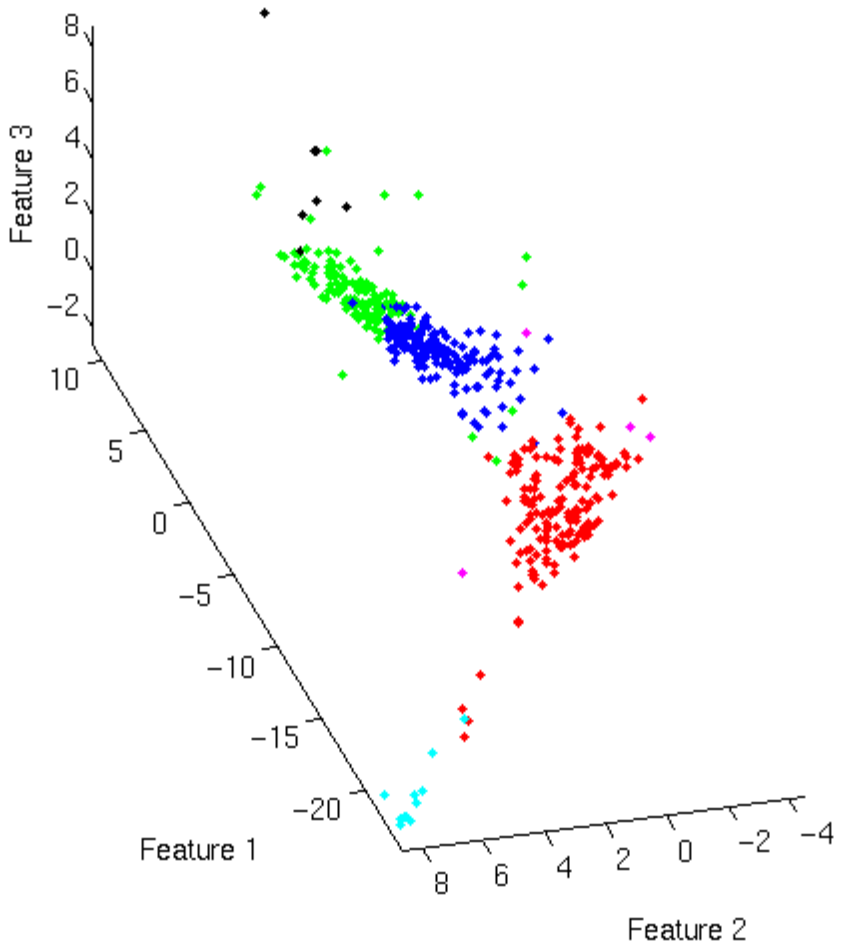
PCA reconstruction



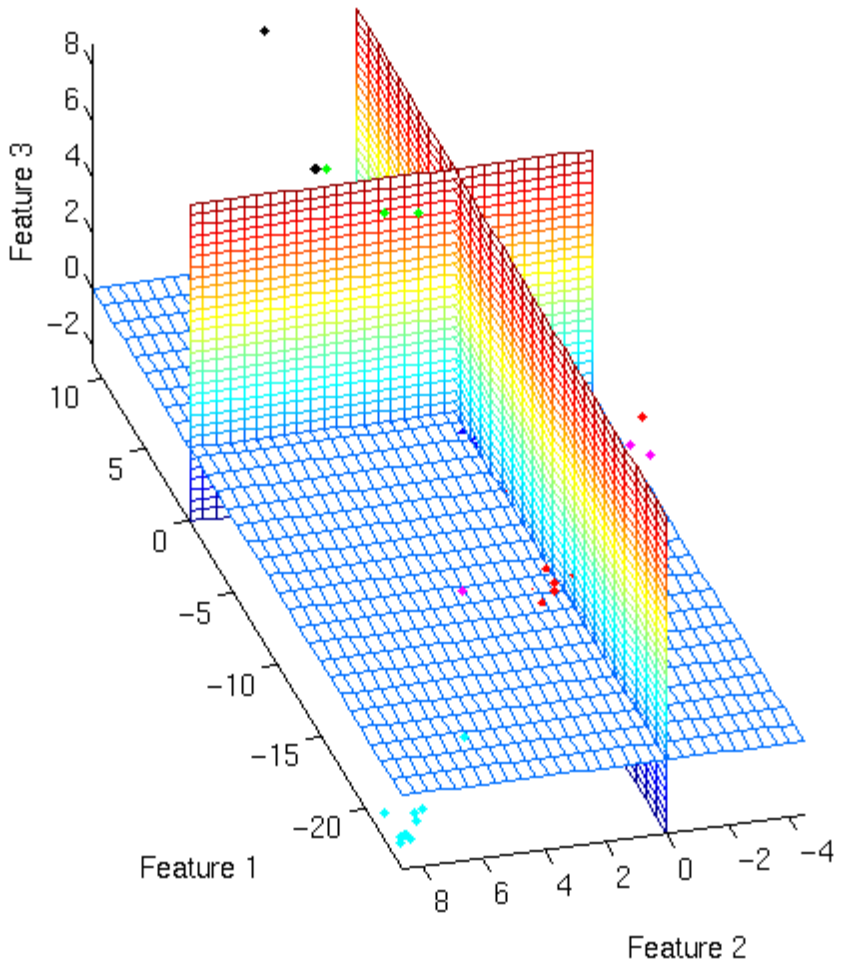




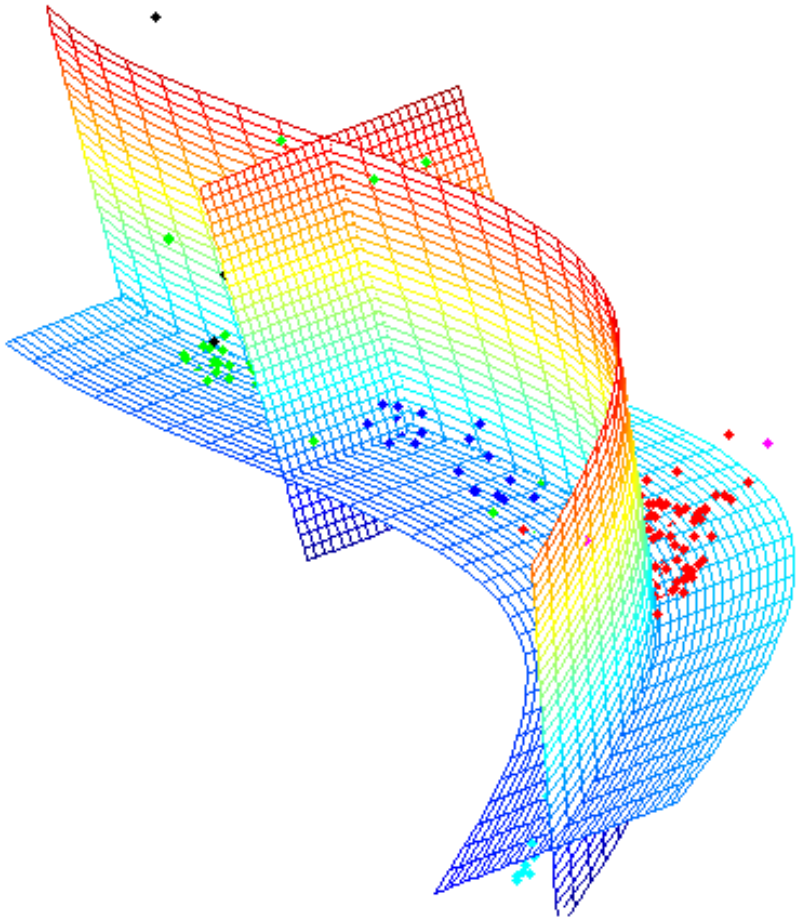
Limitations of PCA



Limitations of PCA



Limitations of PCA



Linear model $\Longrightarrow$ Incapable of capturing *nonlinear manifolds*!

Alternative perspective

- It should be simple to relate the operations of PCA to those of a *two-layer fully-connected neural network without activations*!
- This would allow us to work in exactly the same scenario, but train using *backpropagation*!

$$\vec{z} = enc(\vec{x}) = \mathbf{W}_1\vec{x} + \vec{b}_1$$

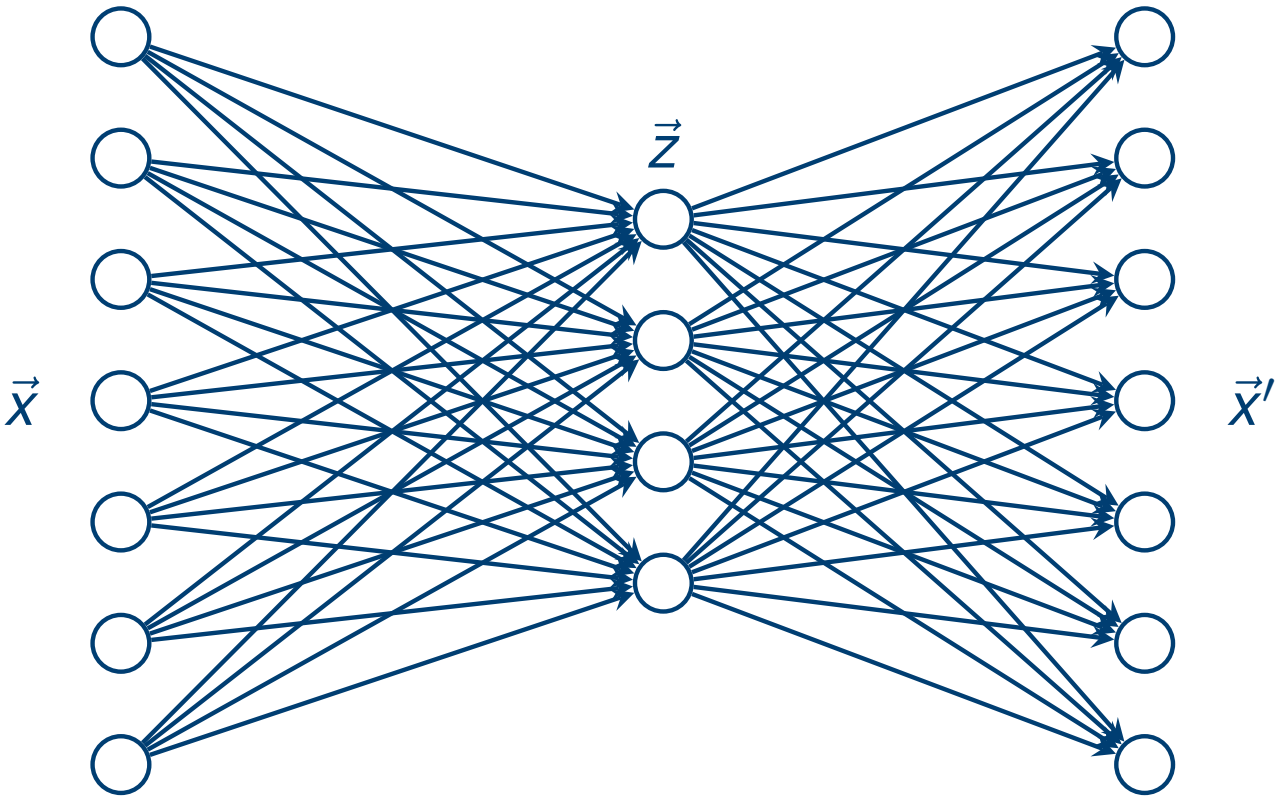
$$\vec{x}' = dec(\vec{z}) = \mathbf{W}_2\vec{z} + \vec{b}_2$$

- Once again, we optimise the *reconstruction loss*

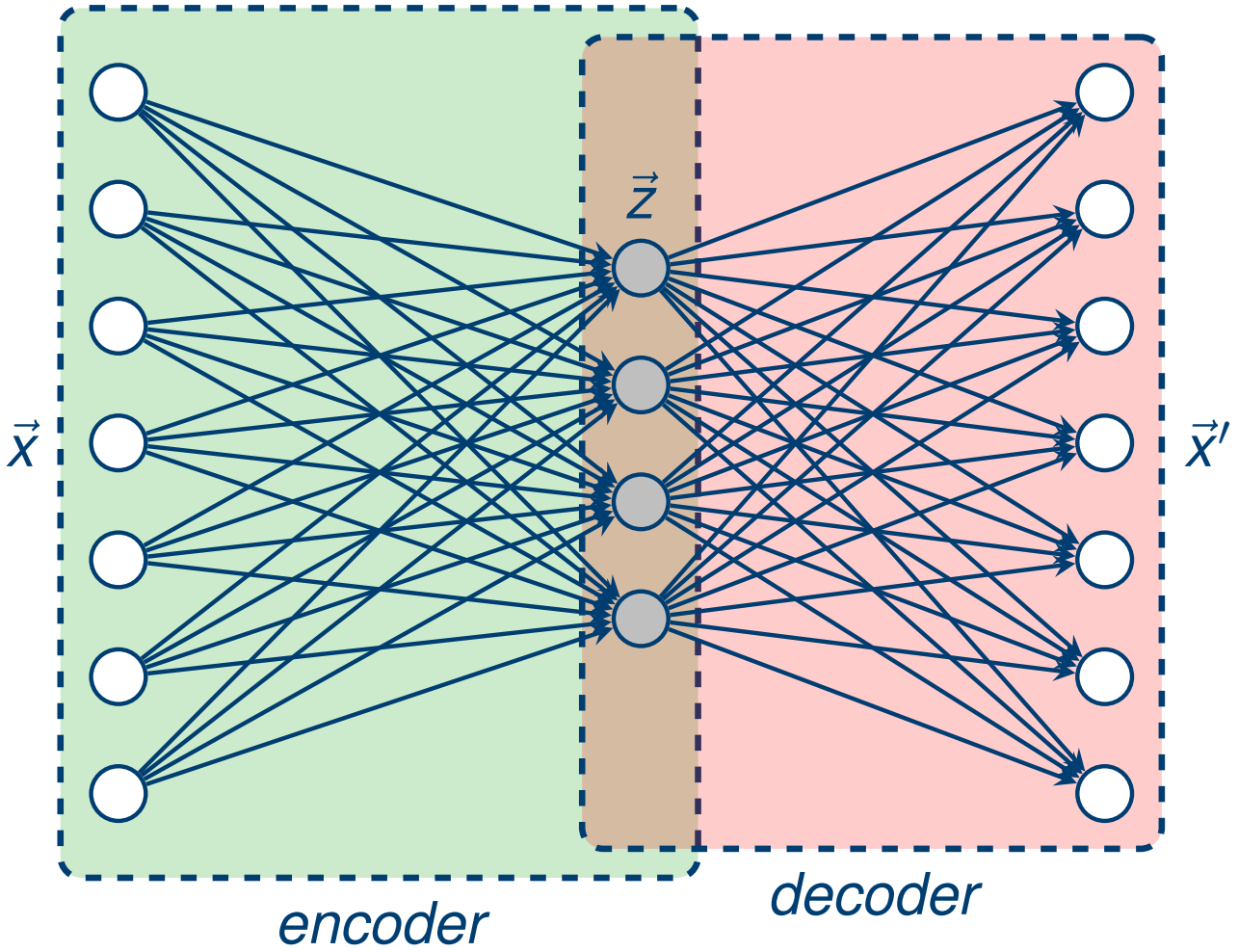
$$\mathcal{L}(\vec{x}') = \|\vec{x}' - \vec{x}\|^2$$

- We have just built our first **autoencoder**!

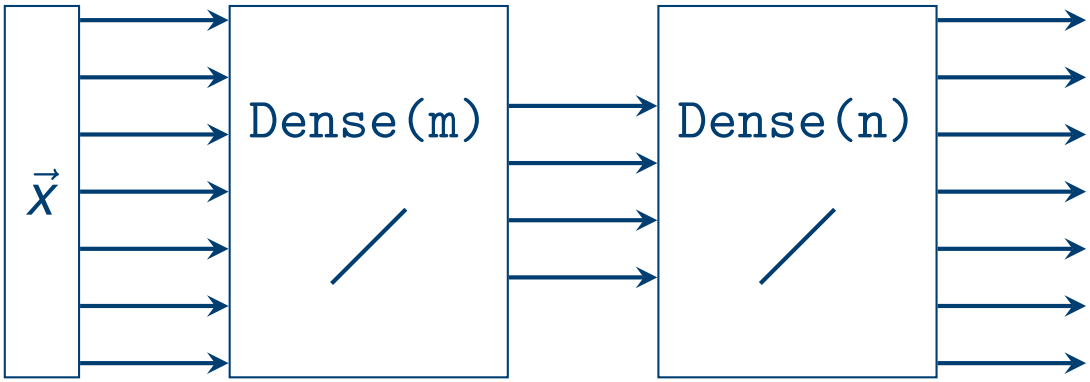
Autoencoder



Autoencoder



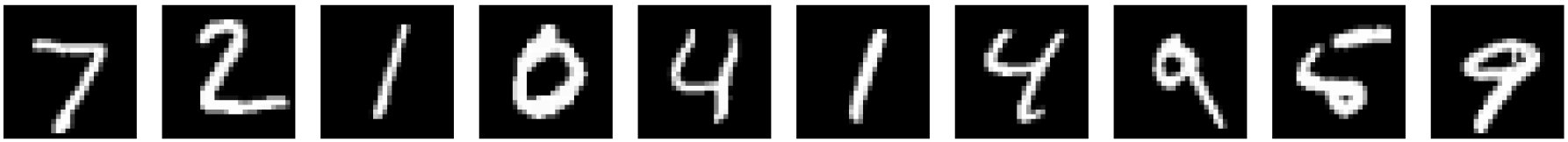
Autoencoder in Keras



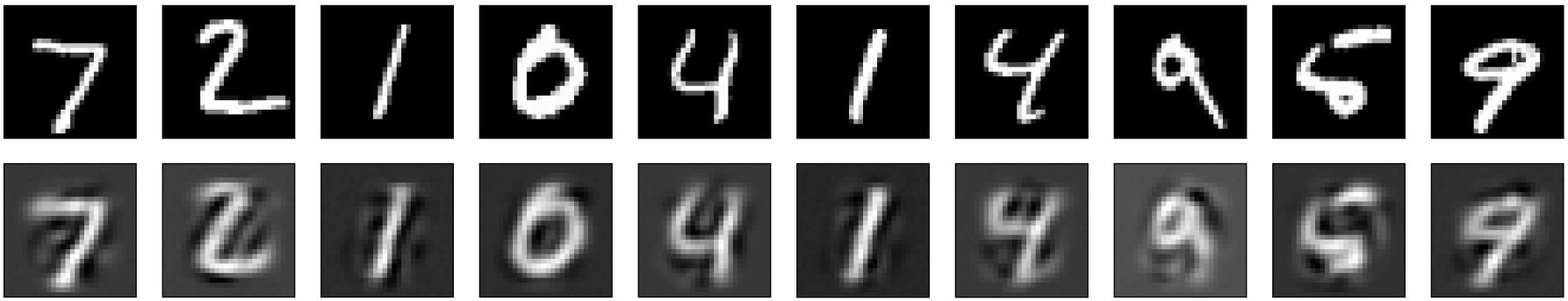
Keras code (for MNIST):

```
x = Input(shape=(784,))
z = Dense(32)(x)
y = Dense(784)(z)
```

Autoencoder performance on MNIST



Autoencoder performance on MNIST



Going deeper. . .

- Thus far, our autoencoder was only capable of the same kind of expressivity as PCA.
  - More so, it was doing so *inefficiently* compared to PCA!
- However, enabling training by backpropagation means that we can now introduce *depth* and *nonlinearity* into the model!
- This should allow us to capture complex nonlinear manifolds more accurately. . .

Deep autoencoders

- We will introduce an additional layer of depth, ReLU activations, and use *logistic sigmoid* units to reconstruct the image (closer to 1 $\sim$ whiter).

$$\vec{z} = enc(\vec{x}) = ReLU\left(\mathbf{W}_2 ReLU\left(\mathbf{W}_1\vec{x} + \vec{b}_1\right) + \vec{b}_2\right)$$

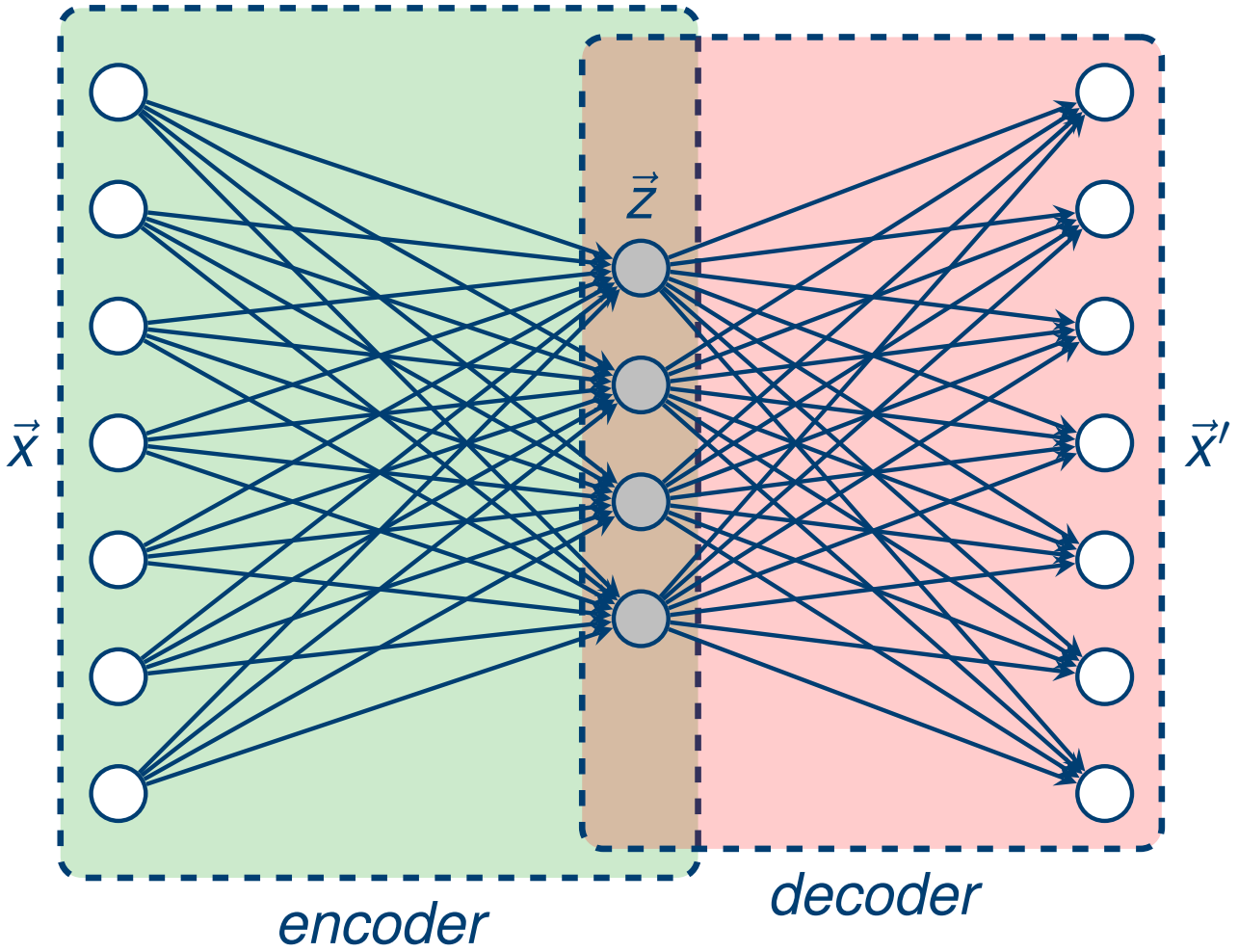
$$\vec{x}' = dec(\vec{z}) = \sigma\left(\mathbf{W}_4 ReLU\left(\mathbf{W}_3\vec{z} + \vec{b}_3\right) + \vec{b}_4\right)$$

- Now we can interpret the output as the probability of each pixel being white—can use *cross-entropy* as the reconstruction loss!

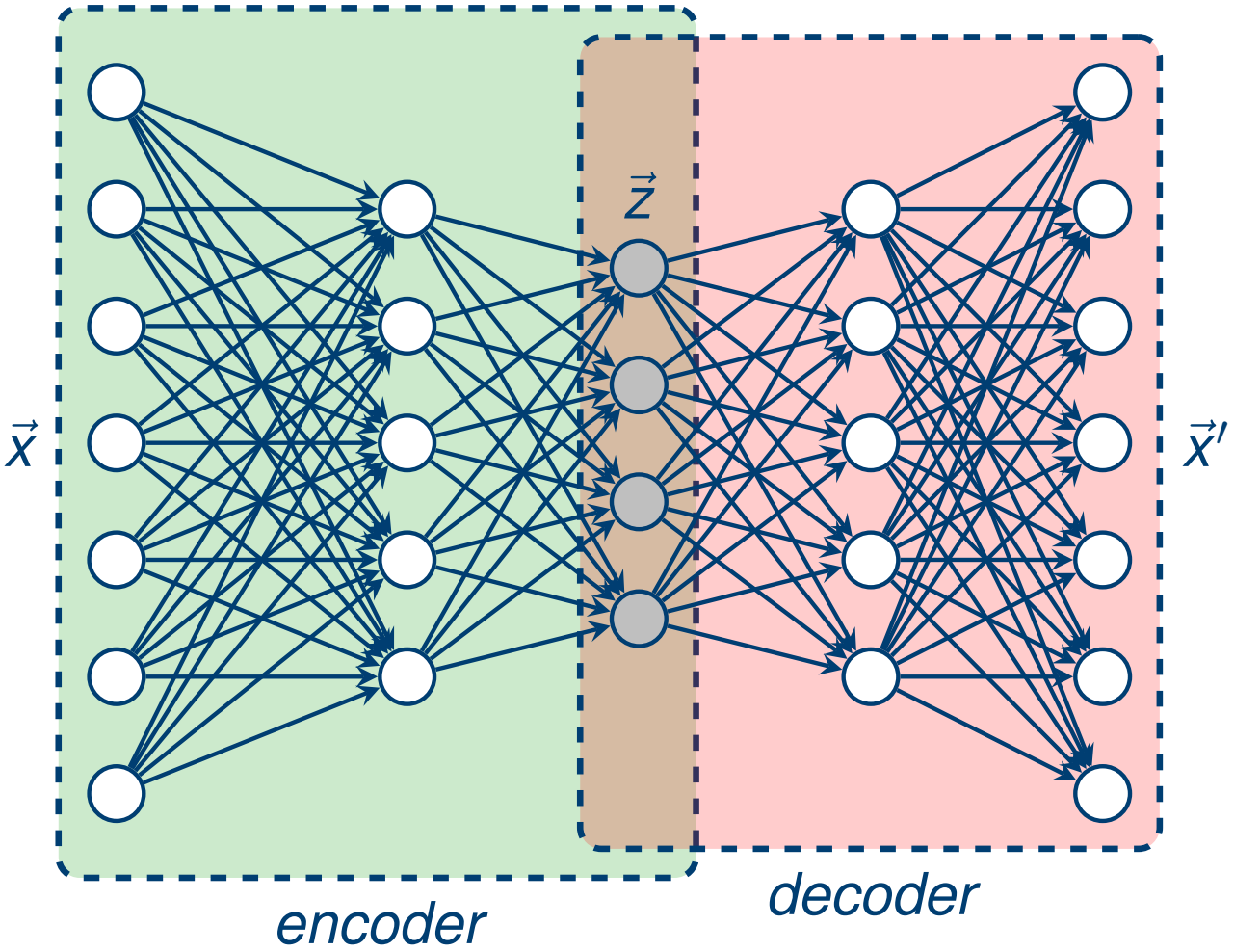
$$\mathcal{L}(\vec{x}') = -\sum_{i=1}^{n} x_i \log x_i' + (1 - x_i)\log(1 - x_i')$$

- We now have a **deep autoencoder**!

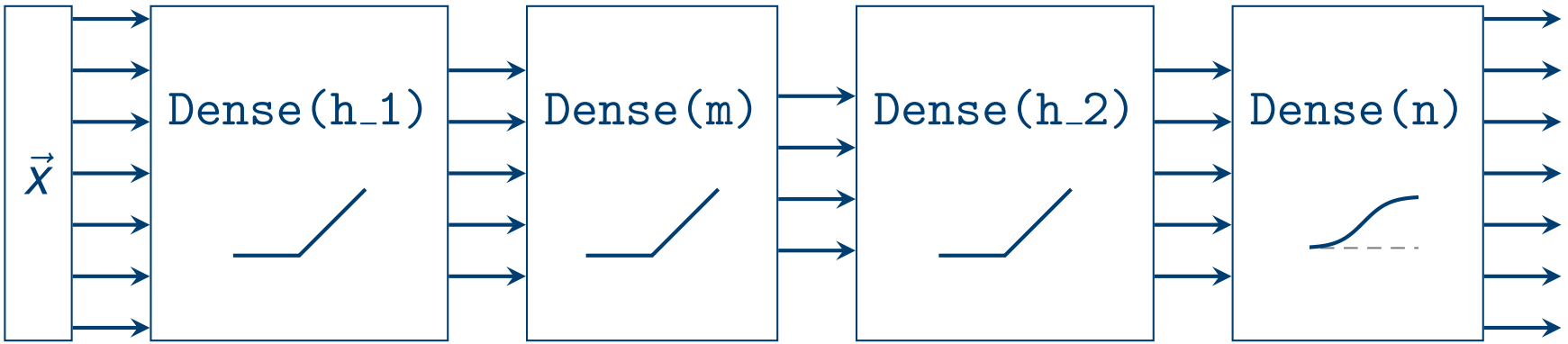
From autoencoders. . .



. . . to *deep* autoencoders



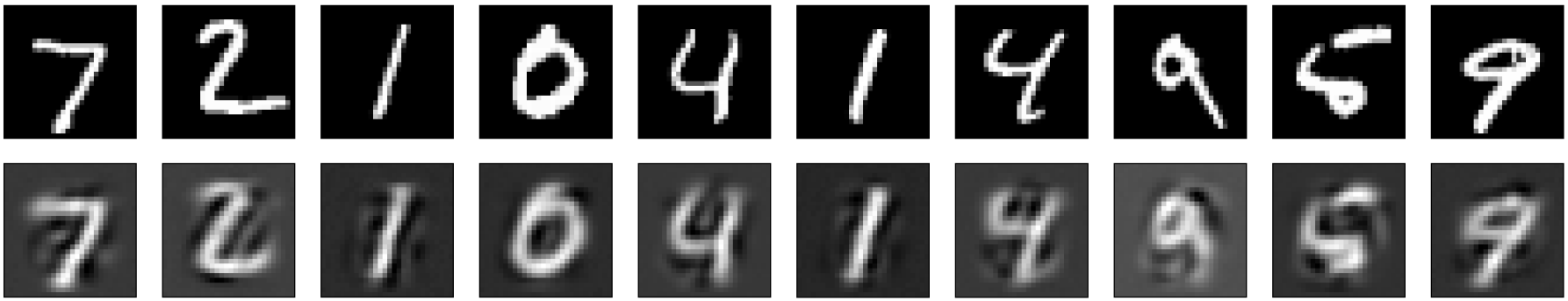
Deep autoencoder in Keras



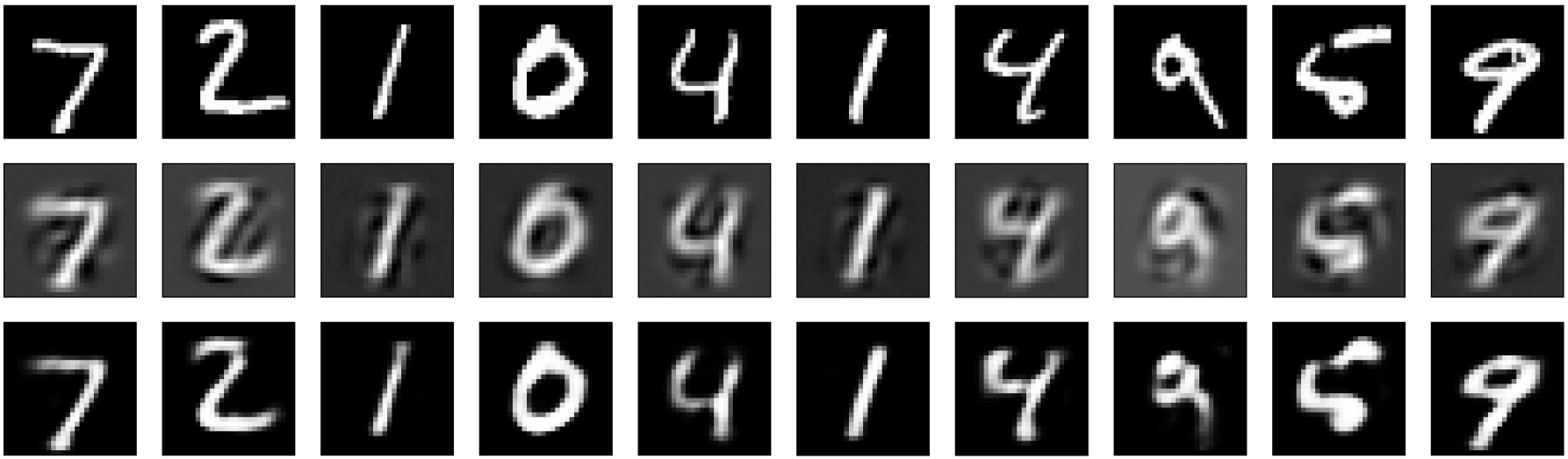
Keras code (for MNIST):

```
x = Input(shape=(784,))
h_1 = Dense(128, activation='relu')(x)
z = Dense(32, activation='relu')(h_1)
h_2 = Dense(128, activation='relu')(z)
y = Dense(784, activation='sigmoid')(h_2)
```

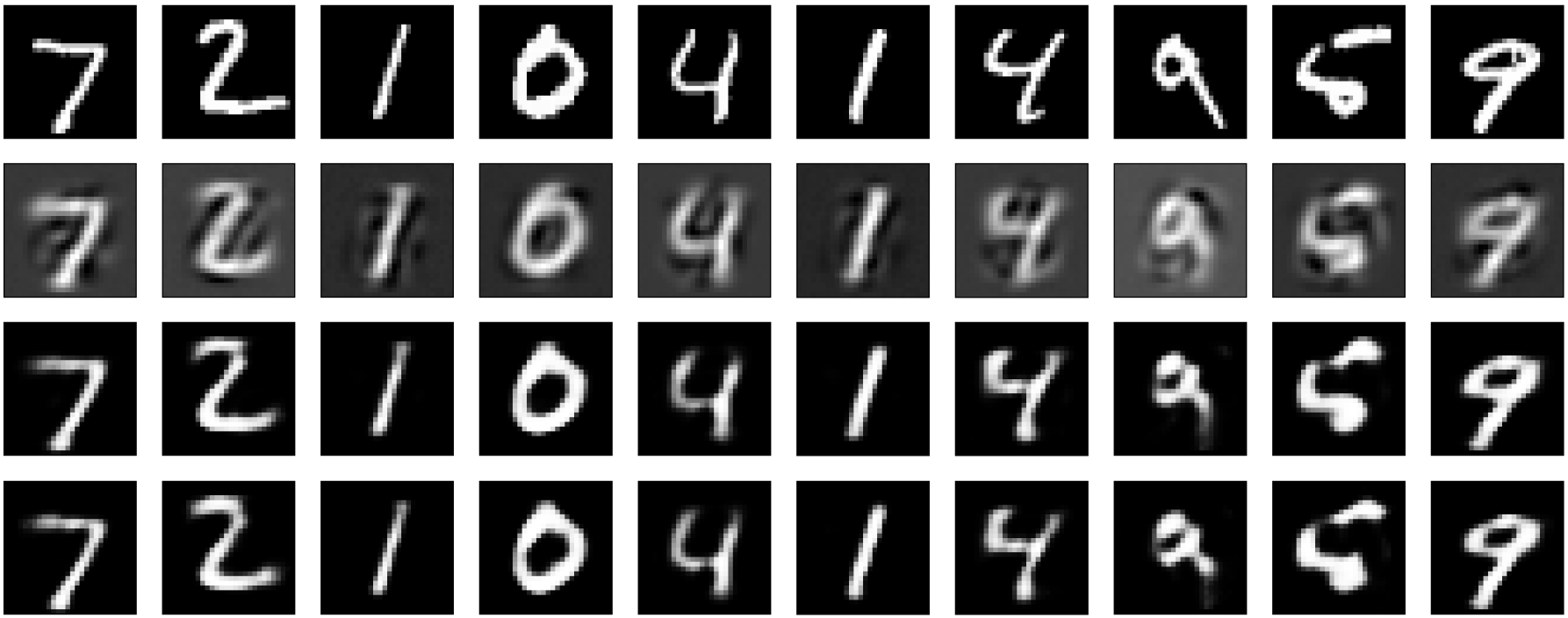
Deep autoencoder performance on MNIST



Deep autoencoder performance on MNIST



Deep(er) autoencoder performance on MNIST



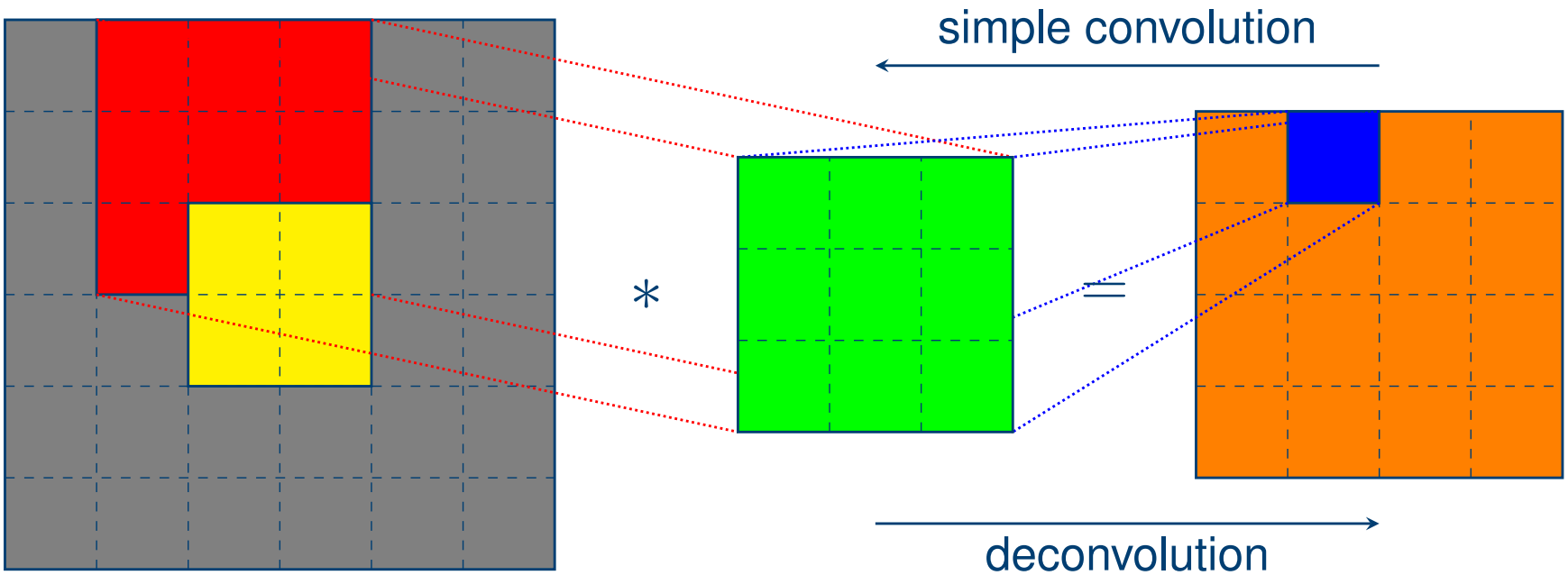
Reintroducing convolutional layers

- But. . . we've been working with **images** all this time! Didn't I say that fully-connected layers are bad for images?
- They are indeed—MNIST is small ($28 \times 28 \times 1$). We can't go much further with only fully-connected layers.
- Luckily, inserting convolutional and pooling layers into autoencoders is not a major issue.
- **How do we *decode*** (especially from a *downsampled* image)?

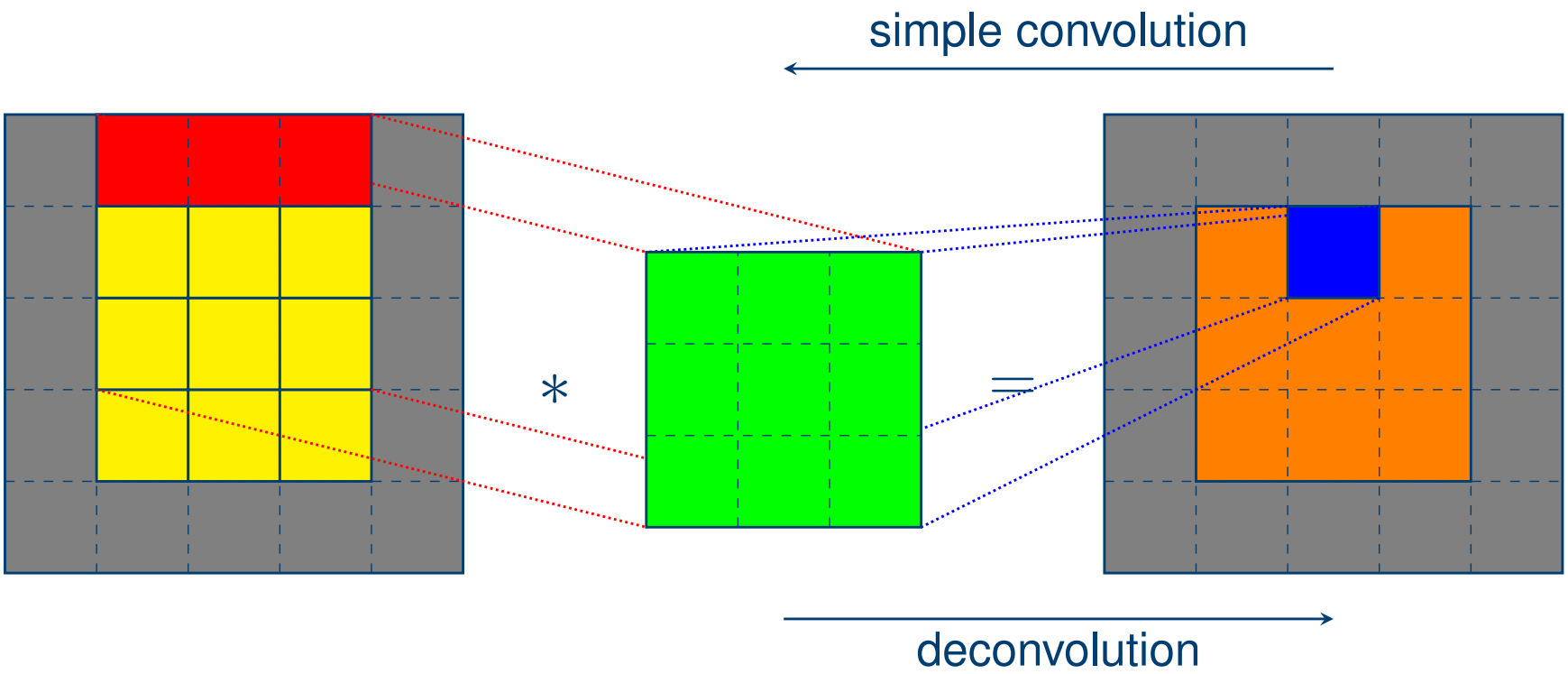
Towards the *deconvolutional* layer

- Essentially, we want to transform the *output* of a convolution into something of the shape of its *input*, while maintaining the desired connectivity patterns.
- Luckily (and perhaps surprisingly), *the backpropagation update of a convolutional layer is **itself a convolution***!
  - Details omitted, to follow in week 3 (but illustrations incoming)!
- This means that we can carefully craft a (potentially *strided*) convolutional layer that will behave like a "target" convolutional layer in the backwards direction!
- This forms the basis of the **deconvolutional** layer, which is extremely useful across a variety of applications of deep learning to computer vision!

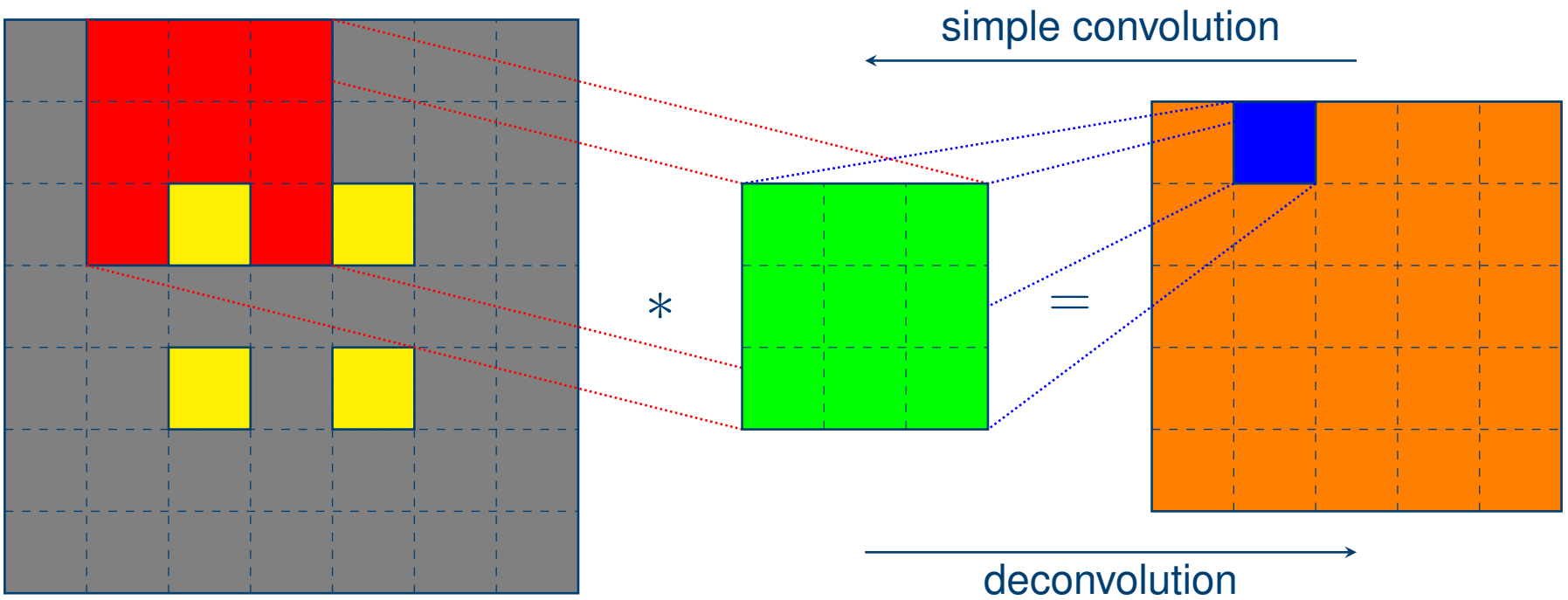
Deconvolution



Deconvolution



Deconvolution



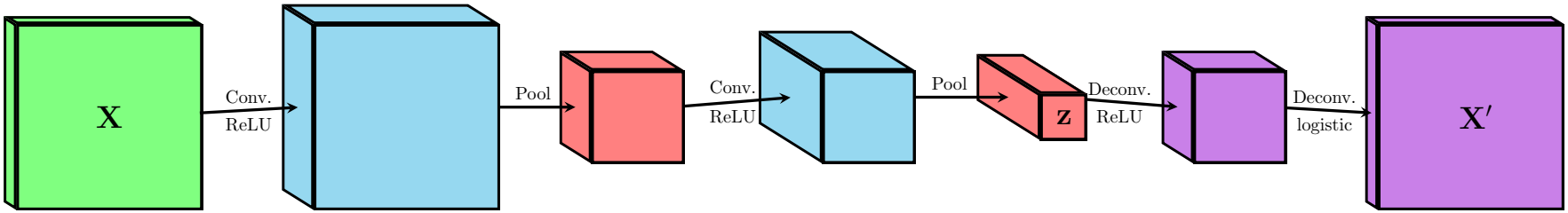
Convolutional autoencoder

- Now we stack convolutional and pooling layers in the encoder, and deconvolutional layers in the decoder. All other details remain unchanged.

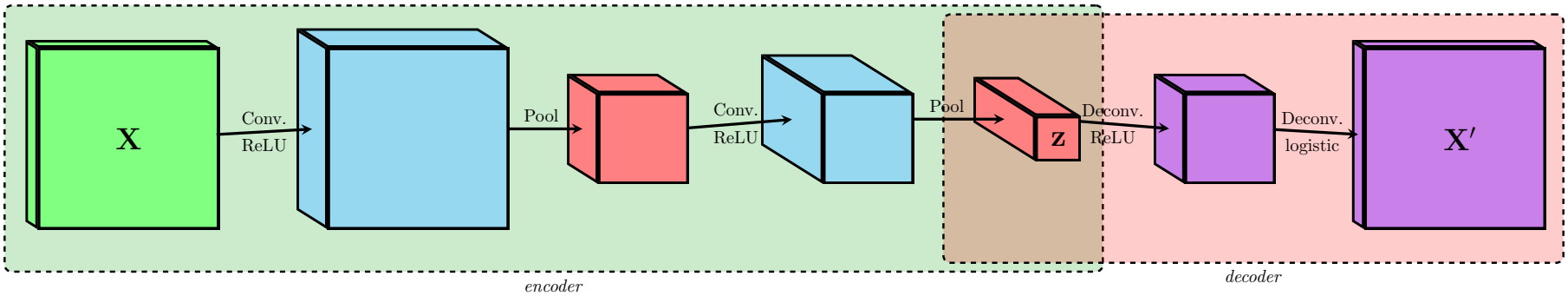
$$\begin{aligned}\mathbf{z} &= enc(\mathbf{X}) \\ &= Pool\left(ReLU\left(Conv\left(Pool\left(ReLU\left(Conv(\mathbf{X}, \mathbf{K}_1\right)\right)\right), \mathbf{K}_2\right)\right)\right)\end{aligned}$$

$$\mathbf{X}' = dec(\mathbf{z}) = \sigma\left(Deconv\left(ReLU\left(Deconv(\mathbf{z}, \mathbf{K}_3\right)\right), \mathbf{K}_4\right)\right)$$

Convolutional autoencoder (CAE)



Convolutional autoencoder (CAE)



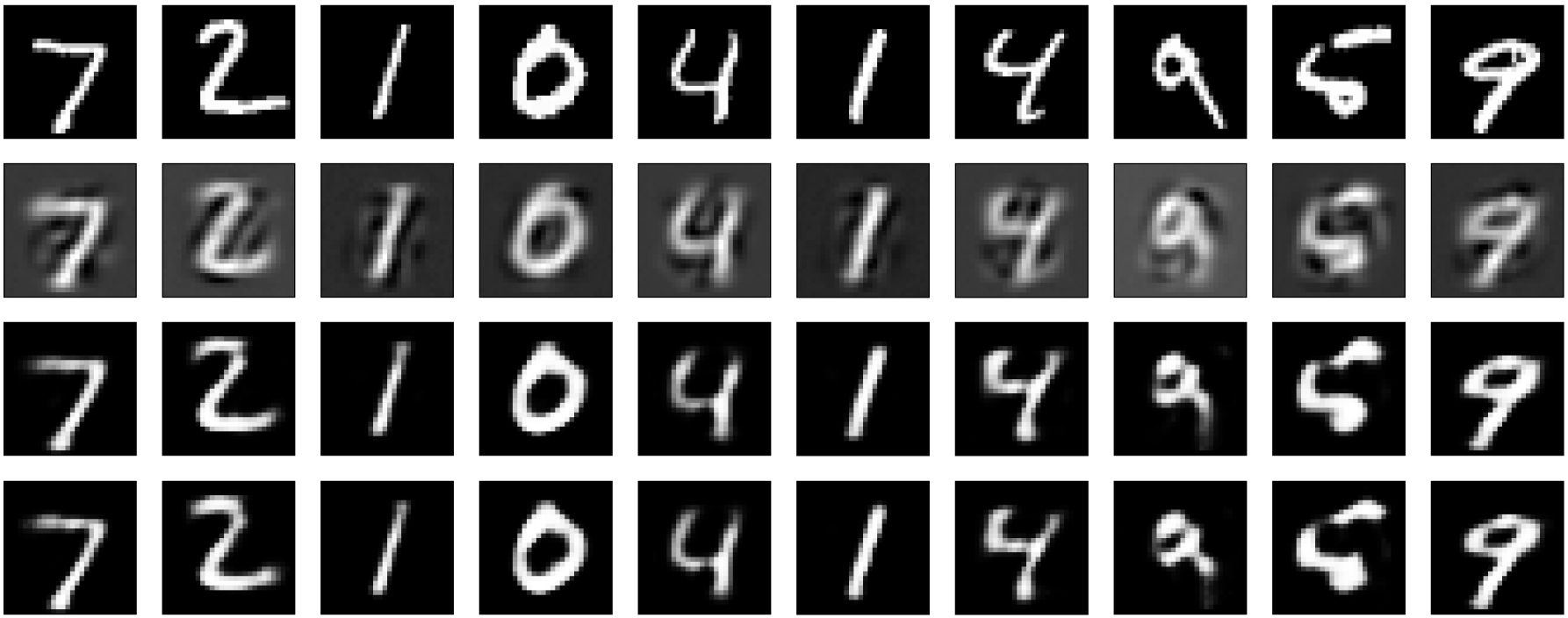
Convolutional autoencoder in Keras: Encoder

```
x = Input(shape=(28, 28, 1))
x_up = ZeroPadding2D((2, 2))(x)
h_1 = Conv2D(16, (3, 3), padding='same',
activation='relu')(x_up)
p_1 = MaxPooling2D((2, 2))(h_1)
h_2 = Conv2D(8, (3, 3), padding='same',
activation='relu')(p_1)
p_2 = MaxPooling2D((2, 2))(h_2)
h_3 = Conv2D(8, (3, 3), padding='same',
activation='relu')(p_2)
z = MaxPooling2D((2, 2))(h_3)
```

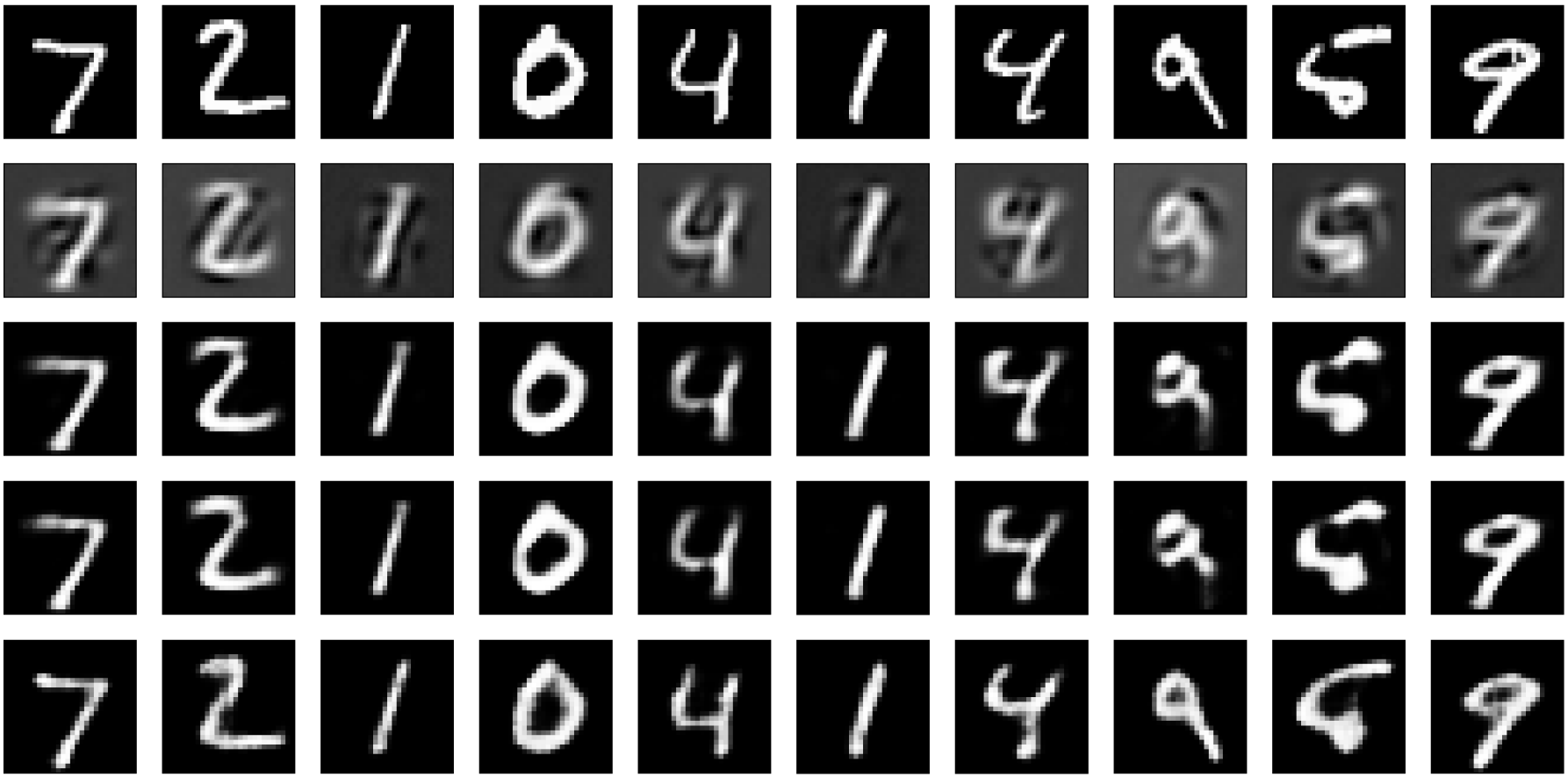
Convolutional autoencoder in Keras: Decoder

```
h_4 = Conv2DTranspose(8, (3, 3), padding='same',
strides=(2, 2), activation='relu')(z)
h_5 = Conv2DTranspose(16, (3, 3), padding='same',
strides=(2, 2), activation='relu')(h_4)
y_up = Conv2DTranspose(1, (3, 3), padding='same',
strides=(2, 2), activation='sigmoid')(h_5)
y = Cropping2D((2, 2))(y_up)
```

Convolutional autoencoder performance on MNIST

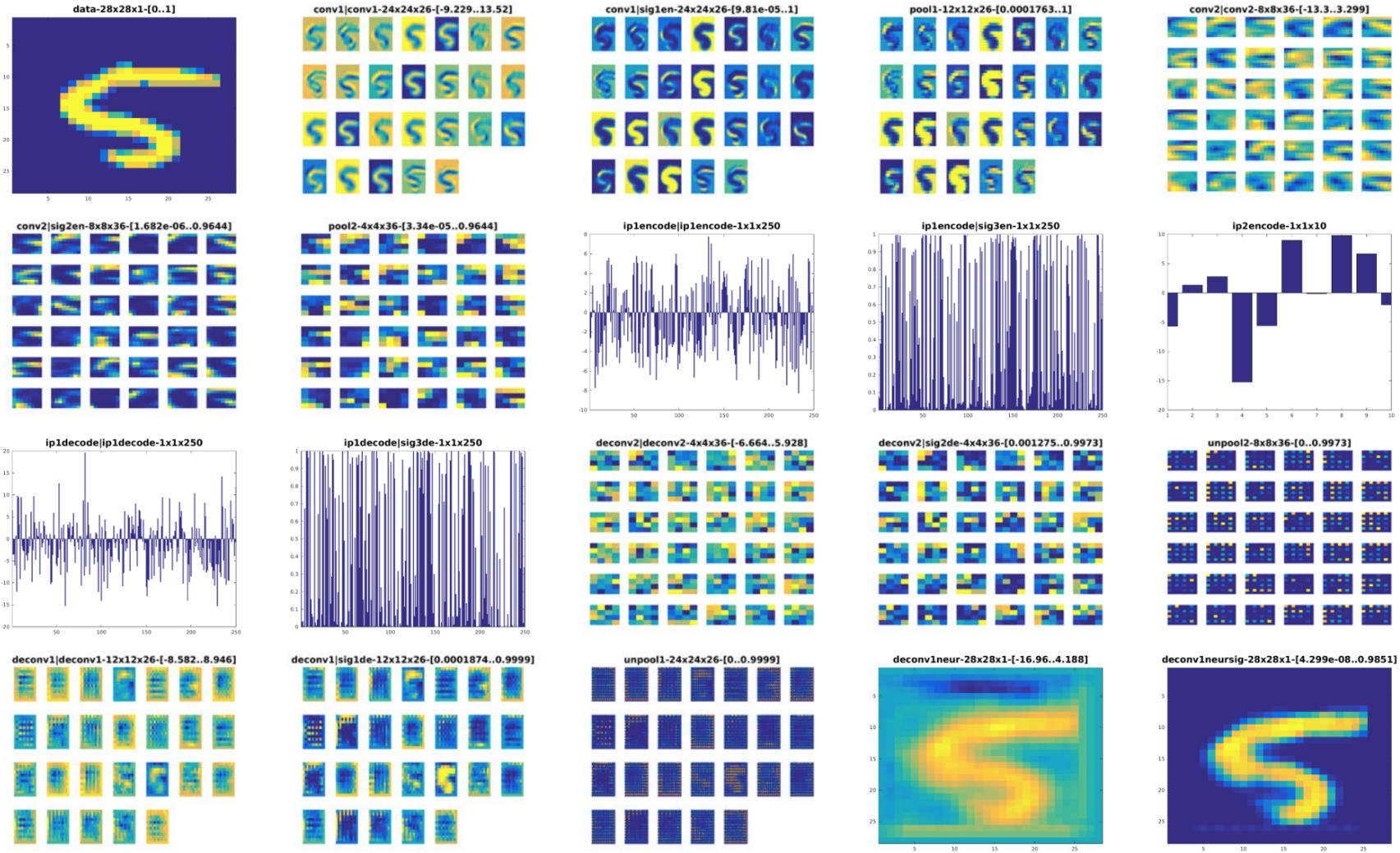


Convolutional autoencoder performance on MNIST

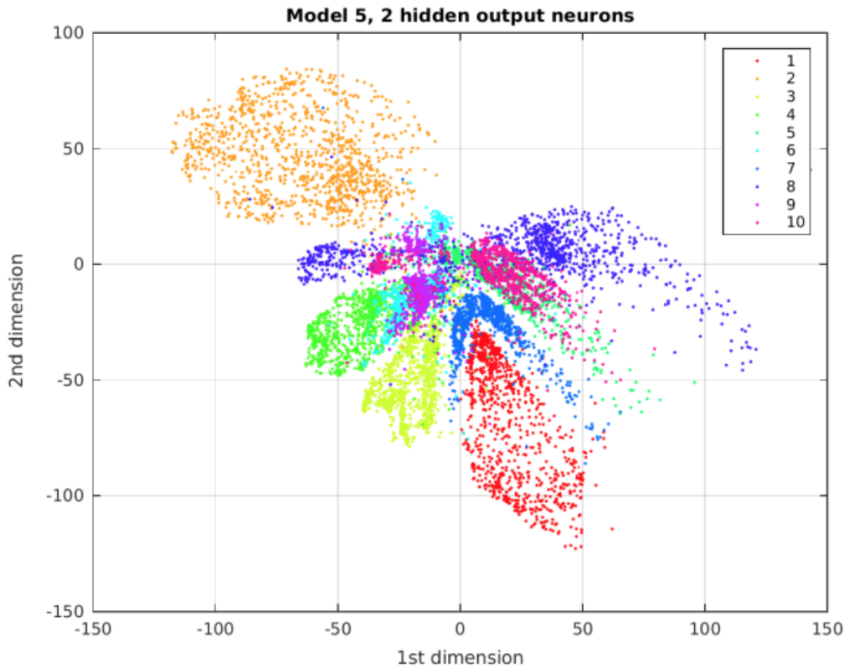


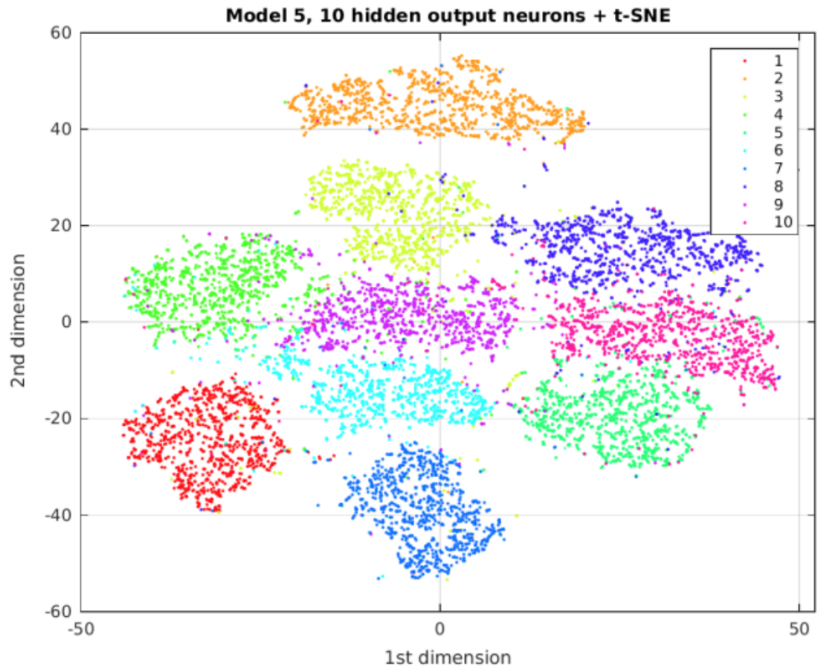
*with **significantly** fewer parameters (∼3K vs. ∼220K)!*

Intermediate layers (*Turchenko et al., 2017*)



The code is *discriminative* (*Turchenko et al., 2017*)





Applying autoencoders to eliminating noise

- One popular application of autoencoders is **denoising**.
- Namely, we may wish to be able to reconstruct our input while simultaneously *eliminating any noise present within it*!
- This comes from several motivations:
  - Real-world data *is* often noisy;
  - Combatting overfitting the training data;
  - *Learning more robust representations*!

Denoising autoencoder

- Constructing a **denoising autoencoder** (of any kind!) requires modifying two aspects of the framework.
- Firstly, the input data $\vec{x}$ is *corrupted* by a corruption process (for images, this could be e.g. injecting Gaussian noise):

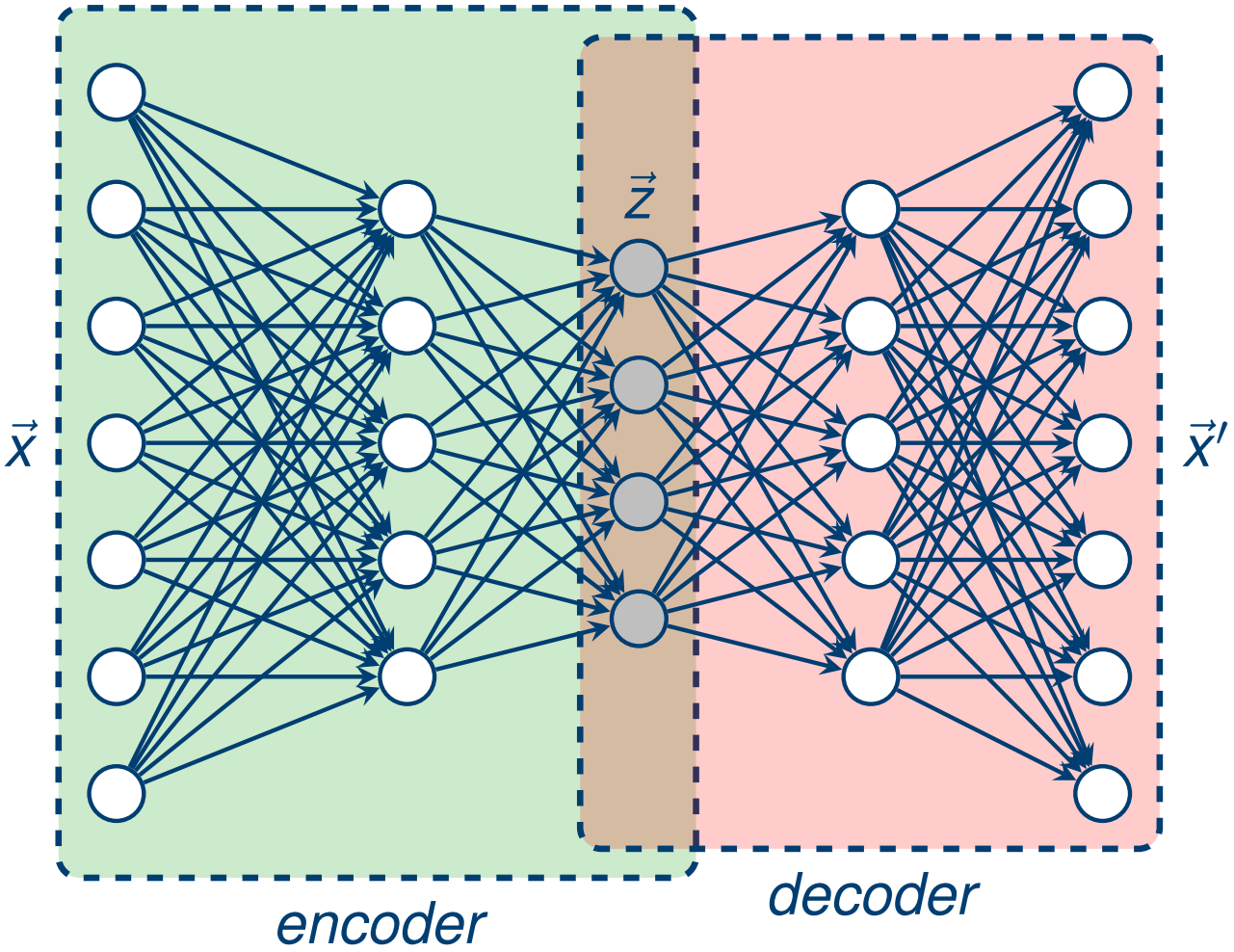
$$\tilde{\vec{x}} = corrupt(\vec{x})$$

- Then, the network is judged on how well it reconstructs the *original input* from the *corrupted input*:

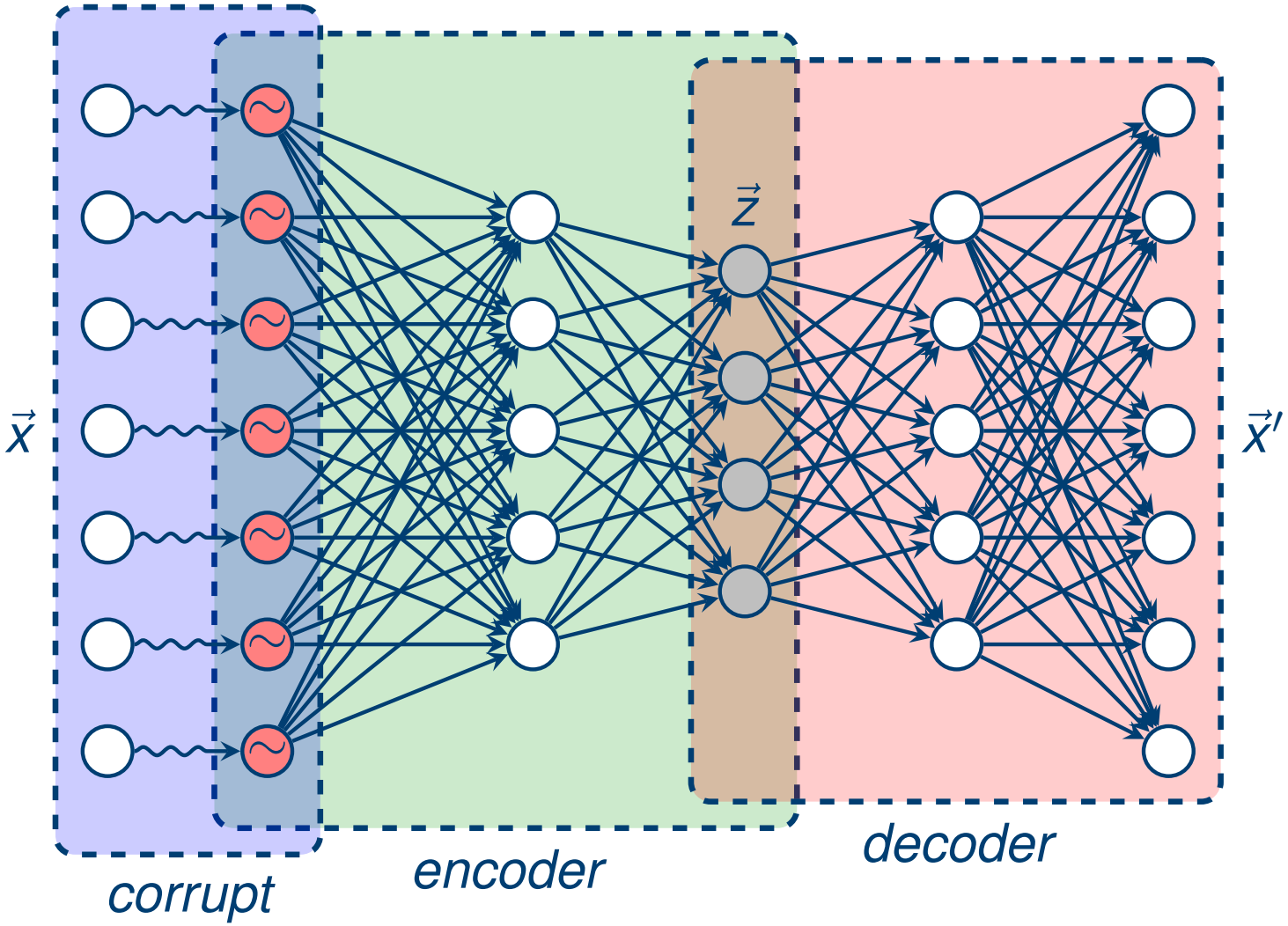
$$\mathcal{L}(\vec{x}) = \|dec(enc(corrupt(\vec{x}))) - \vec{x}\|^2$$

(similarly if cross-entropy is used)

Denoising autoencoder (DAE)



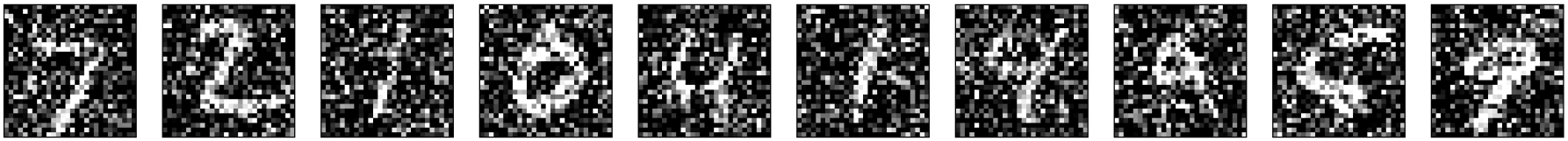
Denoising autoencoder (DAE)



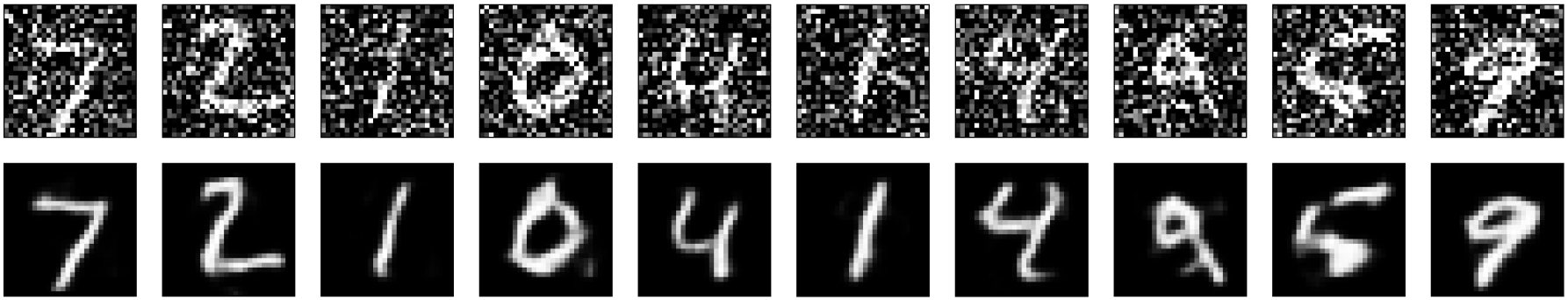
Denoising convolutional autoencoder in Keras

```
x = Input(shape=(28, 28, 1))
x_c = GaussianNoise(0.5)(x)
h_1 = Conv2D(32, (3, 3), padding='same',
activation='relu')(x_c)
p_1 = MaxPooling2D((2, 2))(h_1)
h_2 = Conv2D(32, (3, 3), padding='same',
activation='relu')(p_1)
z = MaxPooling2D((2, 2))(h_2)
h_3 = Conv2DTranspose(32, (3, 3), padding='same',
strides=(2, 2), activation='relu')(z)
y = Conv2DTranspose(1, (3, 3), padding='same',
strides=(2, 2), activation='sigmoid')(h_3)
```

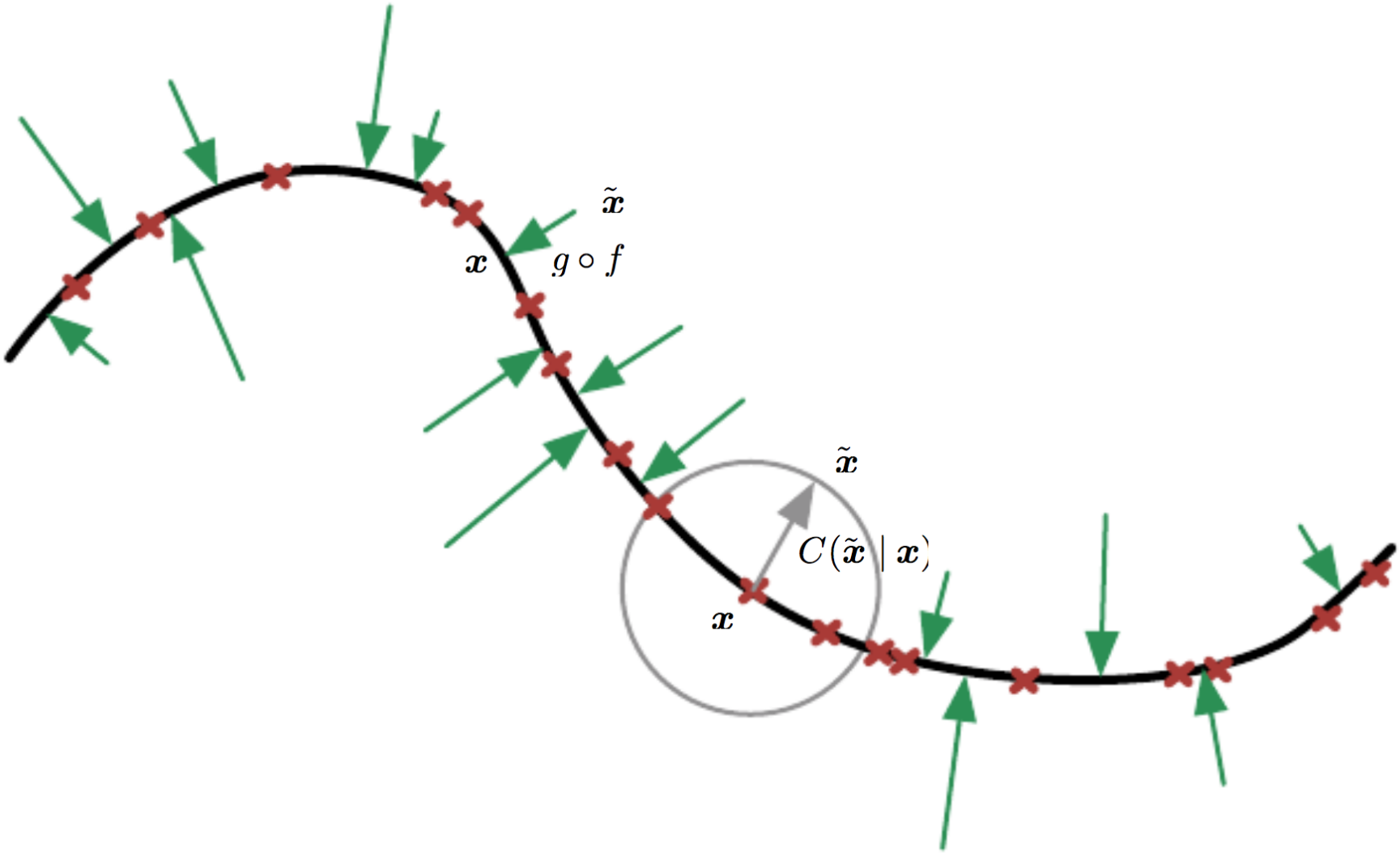
Denoising autoencoder performance on MNIST



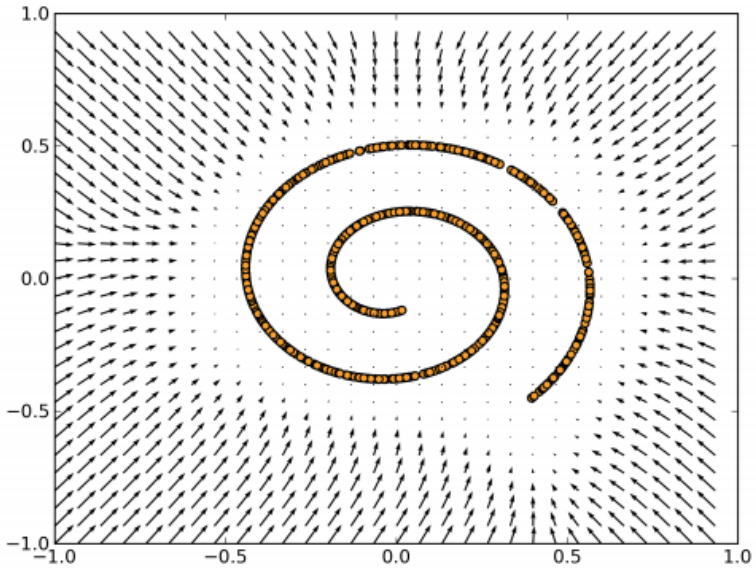
Denoising autoencoder performance on MNIST



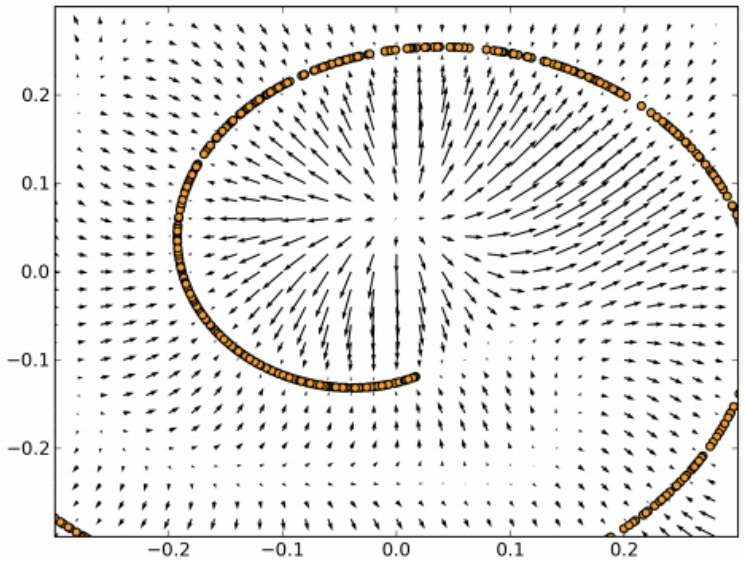
Robust representations! (*Goodfellow et al., 2016*)



Robust representations! (*Alain and Bengio, 2014*)



(a) $r(x) - x$ vector field, acting as sink, zoomed out

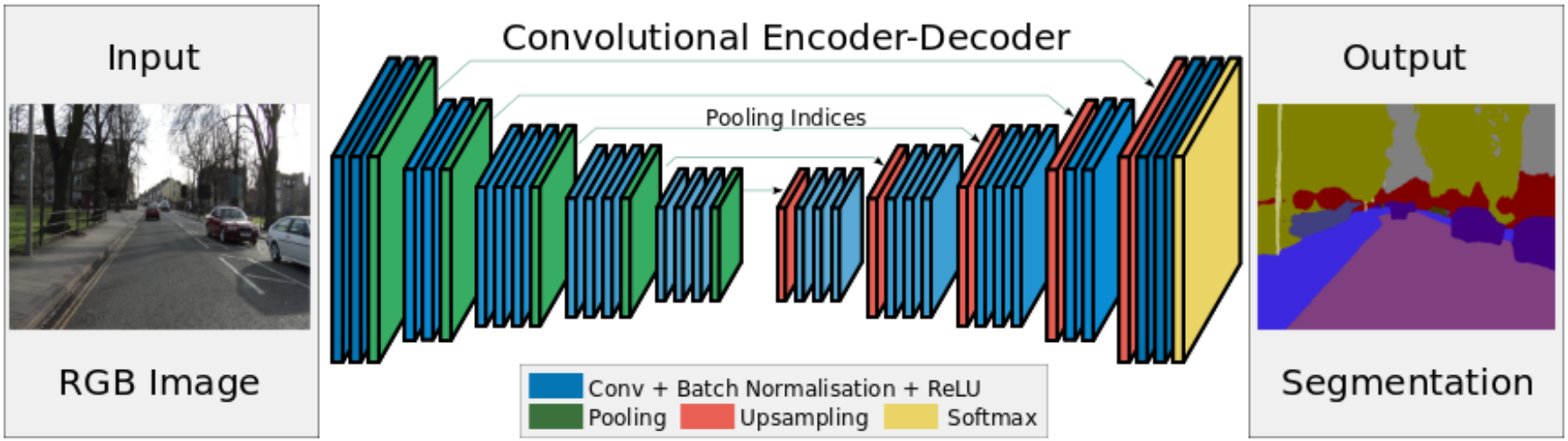


(b) $r(x) - x$ vector field, close-up

Aside: encoder-decoder architectures

- Strictly speaking, a denoising autoencoder is not performing **auto**encoding, i.e. it's not trying to reconstruct its exact input.
- We can generalise this idea further, to make our network have a similar structure to an autoencoder, but actually perform some useful *transformation* on the input!
- This gives rise to **encoder-decoder architectures**, which are now used across the board for tasks such as segmentation.

An encoder-decoder architecture for segmentation



SegNet (*Kendall et al., 2015*)

Generative modelling returns

- To conclude our exploration of autoencoders, we will focus our attention on *generative models*.
- The autoencoder architectures covered so far will do a good job at learning an appropriate dimensionality reduction of inputs similar to our training set's.
- But what does this *tell us* about the underlying properties of the data? Can we plug in arbitrary codes $\vec{z}$ into the decoder and expect useful results?

Generative modelling

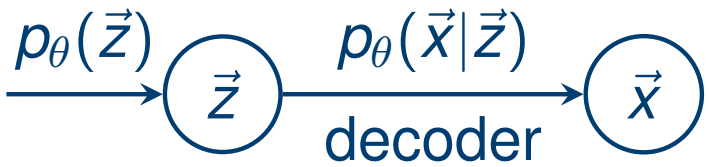
“What I cannot create, I do not understand.” —Richard Feynman

A probabilistic generative framework

- We will think of the code, $\vec{z}$, as an object that captures the essential properties of our input data, $\vec{x}$.
- We can make it easy to generate new, useful, codes—namely, we can engineer the *prior* distribution of codes $\mathbb{P}(\vec{z})$ to be a "tractable" probability distribution (such as a $\mathcal{N}(\vec{0}, \mathbf{I})$, the unit Gaussian).
- Once we have the code, generating data implies sampling the probability distribution $\mathbb{P}(\vec{x}|\vec{z})$. This can also be designed to be tractable (e.g. a learnt decoder neural network).
- This allows us to generate new data points!

A probabilistic generative framework

- Let's assume that the code prior $\mathbb{P}(\vec{z})$ and the generating distribution $\mathbb{P}(\vec{x}|\vec{z})$ are both parametrised by θ (these could be, say, the weights of a neural network).
- We will denote the prior by $p_\theta(\vec{z})$ and the generating distribution by $p_\theta(\vec{x}|\vec{z})$ to make this explicit.
- What do we have so far?



Learning the generative framework

- Note that, having specified $p_\theta(\vec{z})$ and $p_\theta(\vec{x}|\vec{z})$, we can also derive an expression for $\mathbb{P}(\vec{x}) = p_\theta(\vec{x})$!
- This roughly corresponds to: "how likely is it that our model will generate $\vec{x}$?" and sounds like a great objective to maximise!
- We could train our model to maximise $p_\theta(\vec{x})$ over all the samples $\vec{x}$ in our training set.

Maximising the *evidence*

- Unfortunately, computing this quantity (sometimes called the *evidence*) requires *integrating over all possible codes*:

$$p_\theta(\vec{x}) = \mathbb{P}(\vec{x}) = \int_{\vec{z}\in\mathcal{Z}} \mathbb{P}(\vec{x},\vec{z})\,\mathrm{d}\vec{z} = \int_{\vec{z}\in\mathcal{Z}} p_\theta(\vec{x}|\vec{z})p_\theta(\vec{z})\,\mathrm{d}\vec{z}$$

  and this is intractable in all except the simplest of cases!

- We could try approximating it using *Monte Carlo* methods, but this does not scale for large datasets and large networks.

- It is possible to make this objective work—and we will see how! For now, we need to address an even more serious issue...

Performing inference

- For *inference* purposes, we also would very much like to be able to *attach codes* to known inputs $\vec{x}$.
- This would allow us to use the code for other purposes, such as *dimensionality reduction*, obtaining new inputs similar to $\vec{x}$ (e.g. for *data augmentation*) by modifying the code, etc.
- This involves sampling codes from the *posterior distribution* $\mathbb{P}(\vec{z}|\vec{x})$, and is almost always **insanely hard**!

Why is the posterior *so hard*?

- At a glance, it might seem like we could use Bayes' theorem to help us evaluate the posterior:

$$p_\theta(\vec{z}|\vec{x}) = \mathbb{P}(\vec{z}|\vec{x}) = \frac{\mathbb{P}(\vec{x}|\vec{z})\mathbb{P}(\vec{z})}{\mathbb{P}(\vec{x})} = \frac{p_\theta(\vec{x}|\vec{z})p_\theta(\vec{z})}{p_\theta(\vec{x})}$$

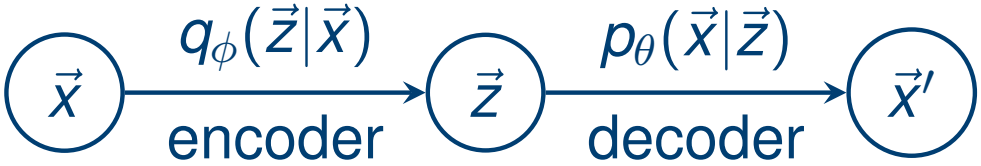
- However, the pesky *evidence* reappears in the denominator :(and this time we need to *sample* from something involving it, not just evaluate it...

Variational inference

- This issue is circumvented by employing **variational inference**.
- We accept that the posterior is hard, and rather than explicitly sampling it, we choose to sample from something *simpler*.
- Generally, we choose to approximate the posterior with a *recognition model*, $q_\phi(\vec{z}|\vec{x})$, parametrised by ϕ. Typically, this will also be a neural network, with ϕ being its weights!
- The parameters ϕ should be selected to make $q_\phi(\vec{z}|\vec{x})$ as close to the true posterior $p_\theta(\vec{z}|\vec{x})$ as possible!

Variational autoencoder (*Kingma & Welling, 2015*)

- Our model of the world now looks like this:



- Looks like an *autoencoder*, doesn't it?
- Indeed—when p_θ and q_ϕ are specified by neural networks, this is the general setup of a **variational autoencoder** (VAE).
- The loss function is now a bit more complicated. . .

Towards a VAE loss

- As discussed, a VAE has **two objectives** that need to be *simultaneously satisfied*. For a training example, $\vec{x}$:
  - We want to make our *decoder* highly likely to generate this example—this implies **maximising**

$$\boxed{\log p_\theta(\vec{x})}$$

  - Simultaneously, we would like our *encoder* to not stray too far from the *true posterior* $p_\theta(\vec{z}|\vec{x})$. This implies **minimising**

$$\boxed{D_{KL}\left(q_\phi(\vec{z}|\vec{x})\|p_\theta(\vec{z}|\vec{x})\right)}$$

    where D_{KL} is the Kullback-Leibler (KL) divergence:

$$D_{KL}(q(x)\|p(x)) = \int_{x\in\mathcal{X}} q(x)\log\frac{q(x)}{p(x)}\mathrm{d}x$$

The evidence lower bound

- Combined, these objectives give us the **evidence lower bound** (ELBO), which our network needs to maximise:

$$ELBO(\theta, \phi) = \log p_\theta(\vec{x}) - D_{KL}\left(q_\phi(\vec{z}|\vec{x}) \| p_\theta(\vec{z}|\vec{x})\right)$$

- The troublesome posterior $p_\theta(\vec{z}|\vec{x})$ is **still** here...
- Luckily, we can rewrite ELBO in a form that *completely eliminates the posterior*!

$$ELBO(\theta, \phi) = \underbrace{\mathbb{E}_{\vec{z}\sim q_\phi(\vec{z}|\vec{x})}[\log p_\theta(\vec{x}|\vec{z})]}_{\text{Reconstruction accuracy}} - \underbrace{D_{KL}(q_\phi(\vec{z}|\vec{x}) \| p_\theta(\vec{z}))}_{\text{Regularisation}}$$

Derivation to follow in the next two slides—likely omitted.

ELBO derivation

Recall: $ELBO(\theta, \phi) = \log p_\theta(\vec{x}) - D_{KL}\left(q_\phi(\vec{z}|\vec{x}) \| p_\theta(\vec{z}|\vec{x})\right)$

$$
\begin{aligned}
\log p_\theta(\vec{x}) &= \int_{\vec{z}\in\mathcal{Z}} q_\phi(\vec{z}|\vec{x}) \log p_\theta(\vec{x}) \, \mathrm{d}\vec{z} \\
&= \int_{\vec{z}\in\mathcal{Z}} q_\phi(\vec{z}|\vec{x}) \log \frac{p_\theta(\vec{x},\vec{z})}{p_\theta(\vec{z}|\vec{x})} \, \mathrm{d}\vec{z} \\
&= \int_{\vec{z}\in\mathcal{Z}} q_\phi(\vec{z}|\vec{x}) \log \frac{p_\theta(\vec{x},\vec{z})}{q_\phi(\vec{z}|\vec{x})} \frac{q_\phi(\vec{z}|\vec{x})}{p_\theta(\vec{z}|\vec{x})} \, \mathrm{d}\vec{z} \\
&= \int_{\vec{z}\in\mathcal{Z}} q_\phi(\vec{z}|\vec{x}) \log \frac{p_\theta(\vec{x},\vec{z})}{q_\phi(\vec{z}|\vec{x})} \, \mathrm{d}\vec{z} + \int_{\vec{z}\in\mathcal{Z}} q_\phi(\vec{z}|\vec{x}) \log \frac{q_\phi(\vec{z}|\vec{x})}{p_\theta(\vec{z}|\vec{x})} \, \mathrm{d}\vec{z} \\
&= \int_{\vec{z}\in\mathcal{Z}} q_\phi(\vec{z}|\vec{x}) \log \frac{p_\theta(\vec{x},\vec{z})}{q_\phi(\vec{z}|\vec{x})} \, \mathrm{d}\vec{z} + D_{KL}(q_\phi(\vec{z}|\vec{x}) \| p_\theta(\vec{z}|\vec{x}))
\end{aligned}
$$

Looks like we can cancel out the term containing the posterior! :)

ELBO derivation

Recall: $ELBO(\theta, \phi) = \log p_\theta(\vec{x}) - D_{KL}\left(q_\phi(\vec{z}|\vec{x}) \| p_\theta(\vec{z}|\vec{x})\right)$

$$\log p_\theta(\vec{x}) = \int_{\vec{z}\in\mathcal{Z}} q_\phi(\vec{z}|\vec{x}) \log \frac{p_\theta(\vec{x},\vec{z})}{q_\phi(\vec{z}|\vec{x})}\, \mathrm{d}\vec{z} + D_{KL}(q_\phi(\vec{z}|\vec{x}) \| p_\theta(\vec{z}|\vec{x}))$$

Finally,

$$\begin{aligned}
ELBO(\theta,\phi) &= \int_{\vec{z}\in\mathcal{Z}} q_\phi(\vec{z}|\vec{x}) \log \frac{p_\theta(\vec{x},\vec{z})}{q_\phi(\vec{z}|\vec{x})}\, \mathrm{d}\vec{z} \\
&= \int_{\vec{z}\in\mathcal{Z}} q_\phi(\vec{z}|\vec{x}) \log \frac{p_\theta(\vec{x}|\vec{z})p_\theta(\vec{z})}{q_\phi(\vec{z}|\vec{x})}\, \mathrm{d}\vec{z} \\
&= \int_{\vec{z}\in\mathcal{Z}} q_\phi(\vec{z}|\vec{x}) \log p_\theta(\vec{x}|\vec{z})\, \mathrm{d}\vec{z} - \int_{\vec{z}\in\mathcal{Z}} q_\phi(\vec{z}|\vec{x}) \log \frac{q_\phi(\vec{z}|\vec{x})}{p_\theta(\vec{z})} \mathrm{d}\vec{z} \\
&= \boxed{\mathbb{E}_{\vec{z}\sim q_\phi(\vec{z}|\vec{x})}[\log p_\theta(\vec{x}|\vec{z})] - D_{KL}(q_\phi(\vec{z}\|\vec{x}) \| p_\theta(\vec{z}))}
\end{aligned}$$

The ELBO function—analysed

$$ELBO(\theta, \phi) = \underbrace{\mathbb{E}_{\vec{z} \sim q_\phi(\vec{z}|\vec{x})}[\log p_\theta(\vec{x}|\vec{z})]}_{\text{Reconstruction accuracy}} - \underbrace{D_{KL}(q_\phi(\vec{z}|\vec{x}) || p_\theta(\vec{z}))}_{\text{Regularisation}}$$

- The first term can be interpreted as the usual *autoencoder reconstruction loss*—given input $\vec{x}$, use the encoder to sample a code $\vec{z}$ from $q_\phi(\vec{z}|\vec{x})$, then use the decoder to compute $p_\theta(\vec{x}|\vec{z})$. We want to maximise this value!
- Minimising the second term forces the distribution of generated codes to remain close to the prior—prevents the network from "cheating" (by, e.g., assigning distant codes to every example)!

Practical choice of $p_\theta(\vec{x}|\vec{z})$

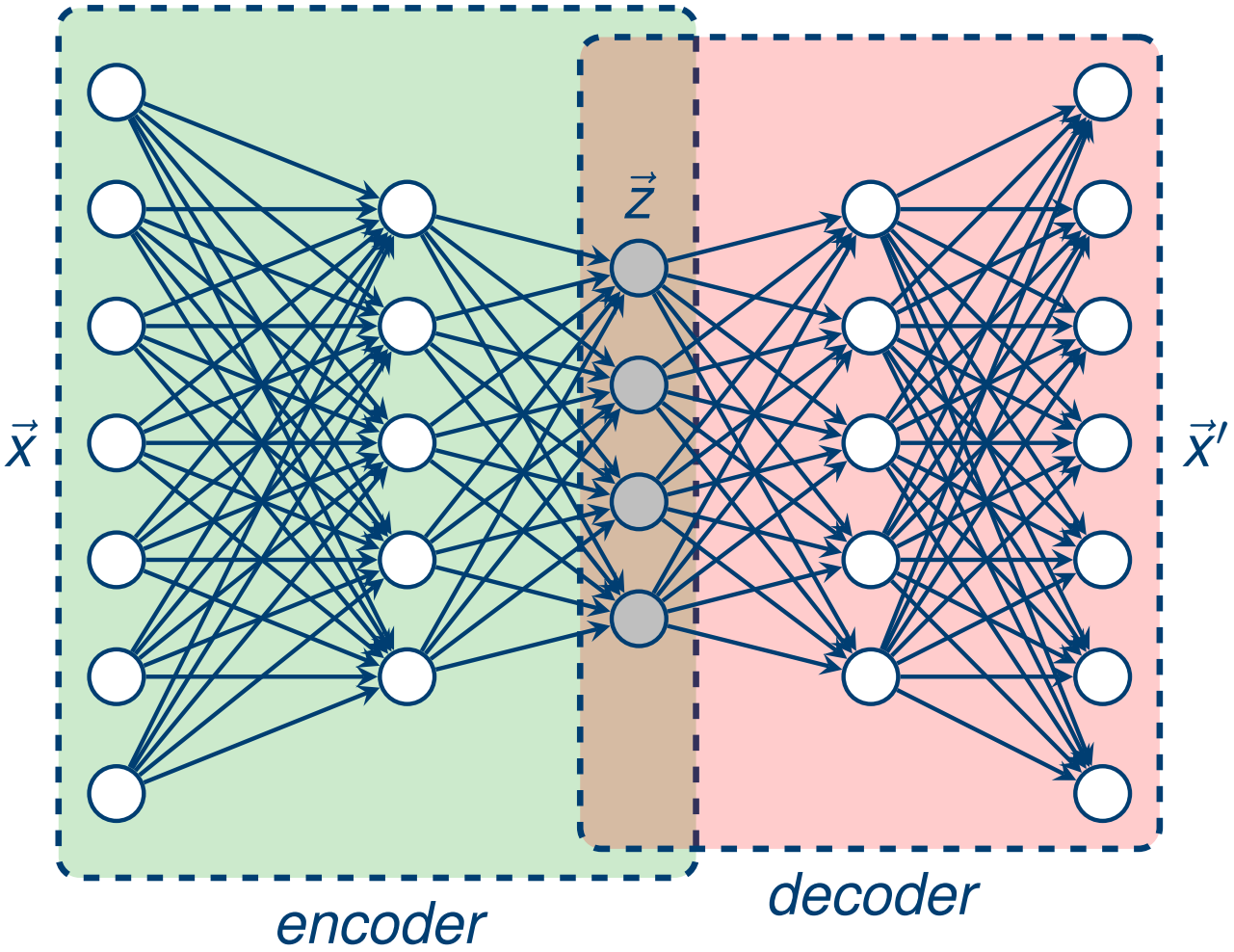
- Now I will present a specific example of a VAE implementation (which is also most common).
- Our decoder will generate samples $\vec{x}'$ coming from a Gaussian distribution, where each component is sampled independently with standard deviation one.
- Essentially, $p_\theta(\vec{x}|\vec{z}) = \mathcal{N}(\vec{\mu}, \mathbf{I})$.
- For computing the mean sample $\vec{\mu}$, we will utilise a neural network (with weights θ) of exactly the same kind as before—with **logistic output units**.
- We can then use the cross-entropy of the encoder input $\vec{x}$ and $\vec{\mu}$ as the reconstruction loss (just as before).

Practical choice of $q_\phi(\vec{z}|\vec{x})$

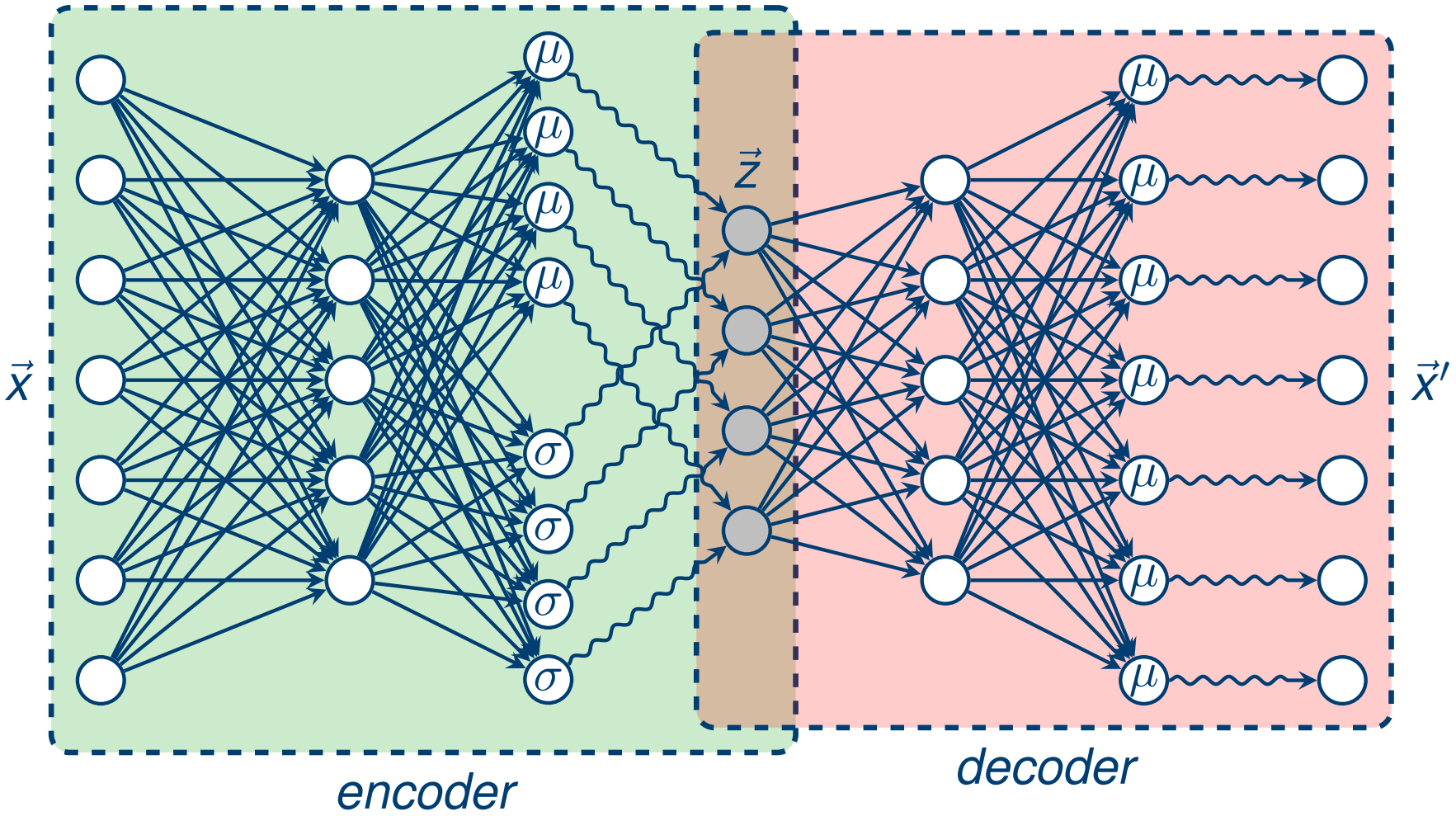
- For the encoder, we will use m Gaussian distributions to generate each of the m elements of the code.
- The parameters of these distributions $(\vec{\mu}, \vec{\sigma})$ are computed by a neural network (with weights ϕ and **linear output units**). This implies $q_\phi(\vec{z}|\vec{x}) = \mathcal{N}(\vec{\mu}, diag(\vec{\sigma}^2))$.
- If we use the prior $p_\theta(\vec{z}) = \mathcal{N}(\vec{0}, \mathbf{I})$, then the regularisation term has an expression we can easily work with!

$$-D_{KL}(\mathcal{N}(\vec{\mu}, diag(\vec{\sigma}^2))\|\mathcal{N}(\vec{0}, \mathbf{I})) = \sum_{j=1}^{m} 1 + \log \sigma_j^2 - \mu_j^2 - \sigma_j^2$$

Variational autoencoder (VAE)



Variational autoencoder (VAE)



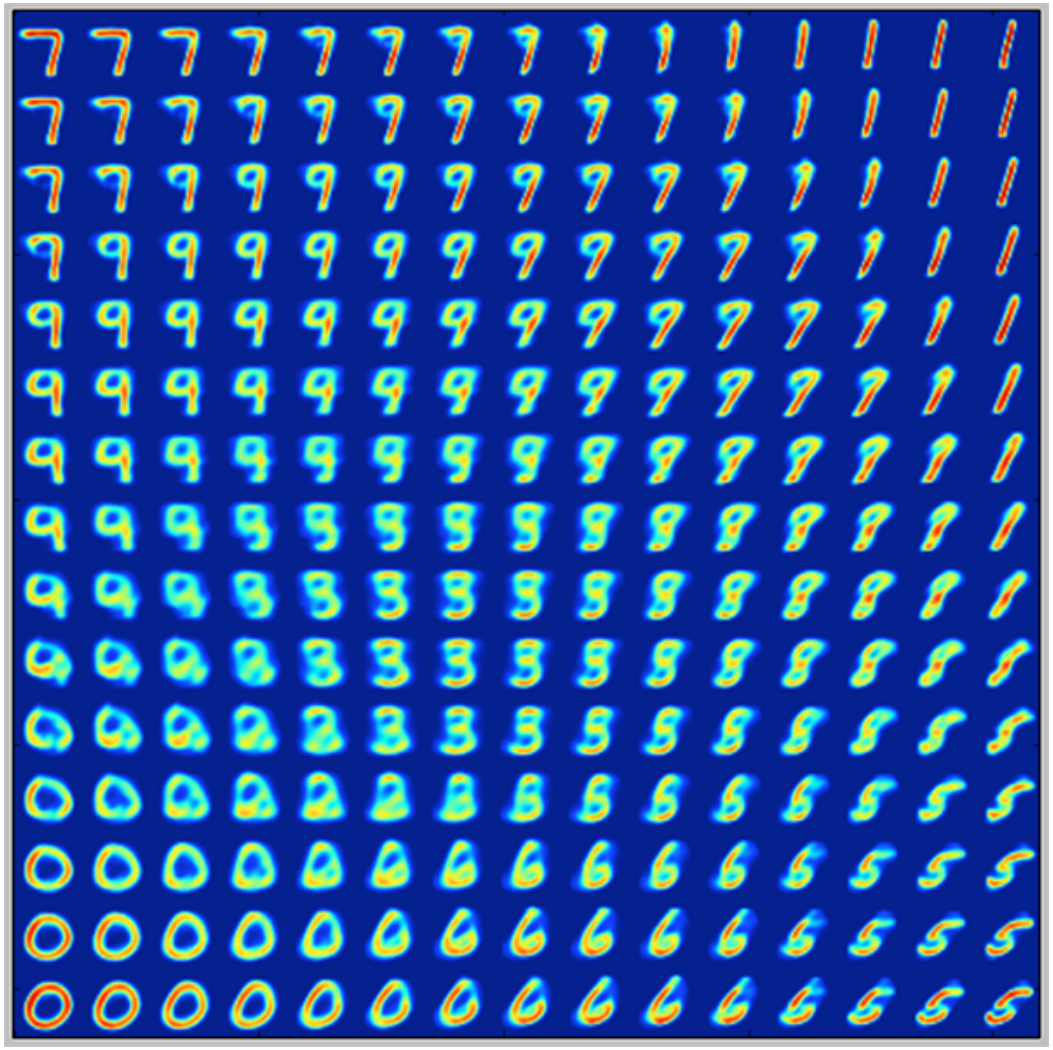
Reparametrisation trick

- Naïvely plugging in the sampling operation into the encoder *will not work*, because the sampling operation **has no gradient**!
- To make it work, we can instead sample upfront $\vec{\varepsilon} \sim \mathcal{N}(\vec{0}, \mathbf{I})$, feed it as an *external input*, and transform appropriately:

$$\vec{z} = \vec{\mu} + \vec{\varepsilon} \odot \vec{\sigma}$$

```
def sampling(args):
    z_mean, z_log_var = args
    epsilon = K.random_normal(shape=(batch_size, m),
                              mean=0., stddev=1.)
    return z_mean + K.exp(z_log_var) * epsilon
z = Lambda(sampling)([z_mean, z_log_var])
```

Generative power of VAEs on MNIST ($m = 2$)

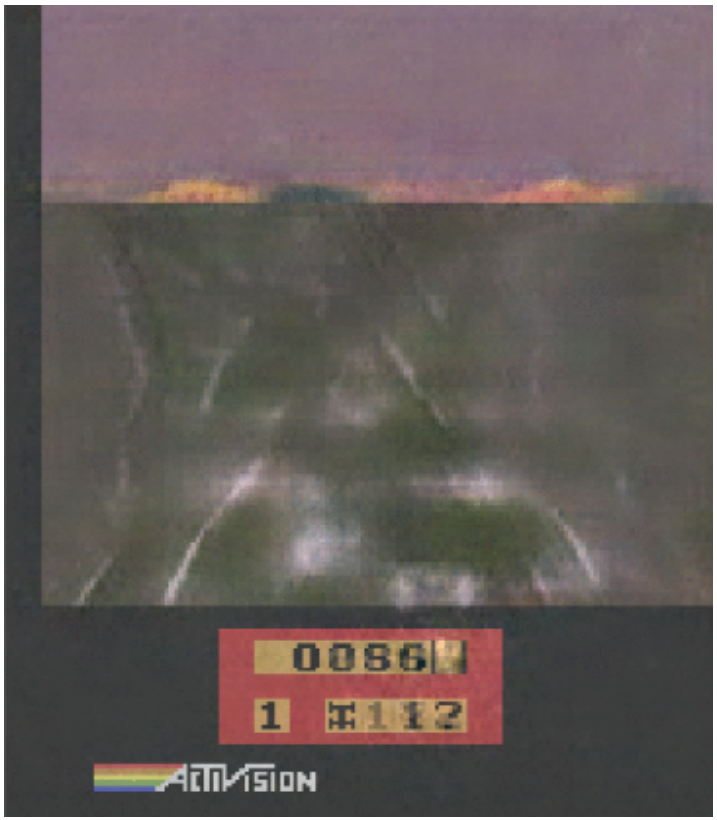


Using VAEs to generate fake faces

https://youtu.be/XNZIN7Jh3Sg

Combatting *entanglement*

Can we *make sense* of what the code **represents**?
What happens if we *shift* one of the code elements slightly?



Tackling the black box problem

- Neural networks have achieved state-of-the-art results across a variety of domains, but *interpreting* their exact mode of operation remains difficult.
- For some domains (e.g. autonomous vehicles or medicine), **interpretability is key**!
- Autoencoders typically suffer from the **entanglement** problem—each code element encodes "a little bit of everything" about the output! Shifting one code element ends up blurring the entire result. . .
- Making sense of entangled codes is **hard**!

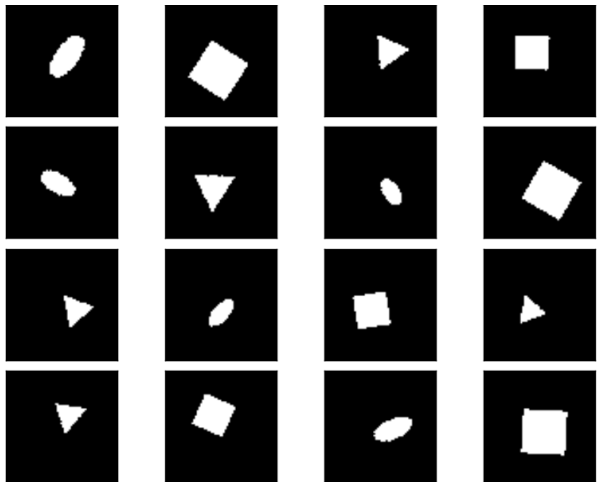
Disentangled VAE (*Higgins et al., 2016*)

- Disentanglement parameter $\beta \geq 0$ – controls the relative importance of the reconstruction accuracy and the regularisation error.
  - Scales the pressure put on $q_\phi(\vec{z}|\vec{x})$ to approximate $p_\theta(\vec{z})$:

$$\mathcal{L}(\theta, \phi) = \mathbb{E}_{\vec{z} \sim q_\phi(\vec{z}|\vec{x})}[\log p_\theta(\vec{x}|\vec{z})] - \beta D_{KL}(q_\phi(\vec{z}|\vec{x}) \| p_\theta(\vec{z}))$$

- Under some *continuity* assumptions in the training data, this model is capable of learning to **disentangle** its representations (for large enough β)!
- (Recall: in our case, $p_\theta(\vec{z}) = \mathcal{N}(\vec{0}, \mathbf{I})$—so the prior has *no covariance* between code elements!)

Example Toy Problem (*Peychev et al., unpublished*)

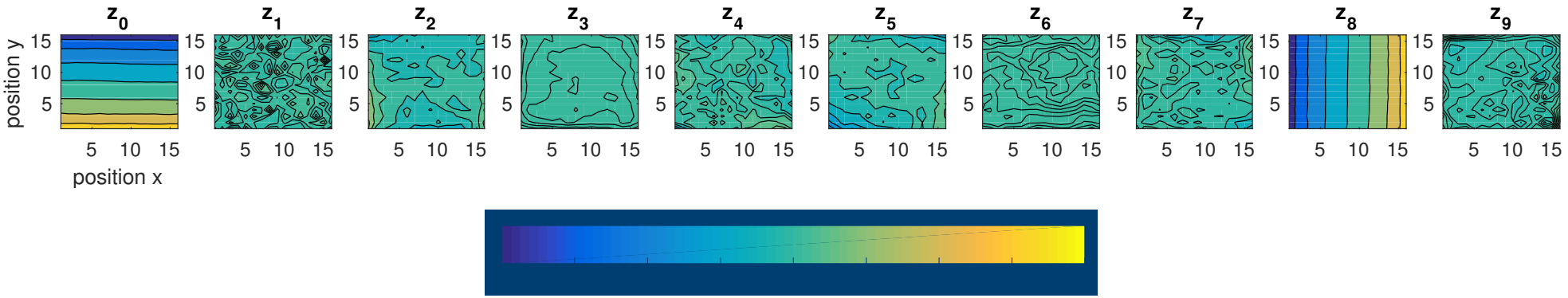


267,021 synthetically generated binary images in total (size: 64 x 64) after removing duplicates. Input generative factors:

- Shape (ellipse, square, triangle)
- Position X and Y (16 values each)
- Scale (6 values)
- Rotation (60 values over the $[0; \pi]$ range)

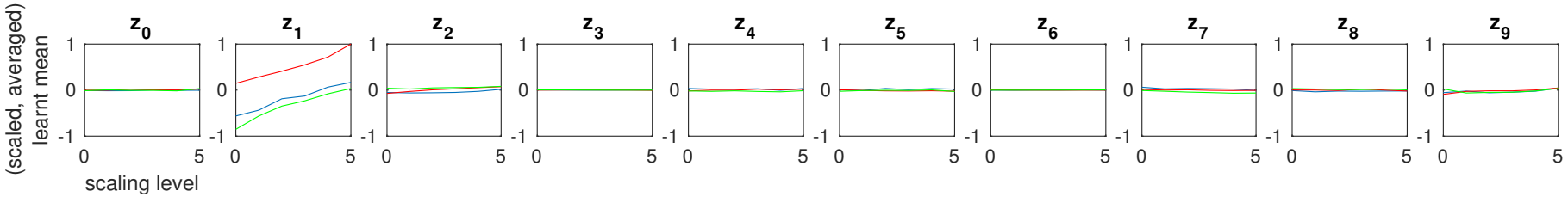
Results ($\beta = 4$)

Learnt means of each code element z_i as a function of all 16x16 **locations**, averaged across objects, rotations and scales.

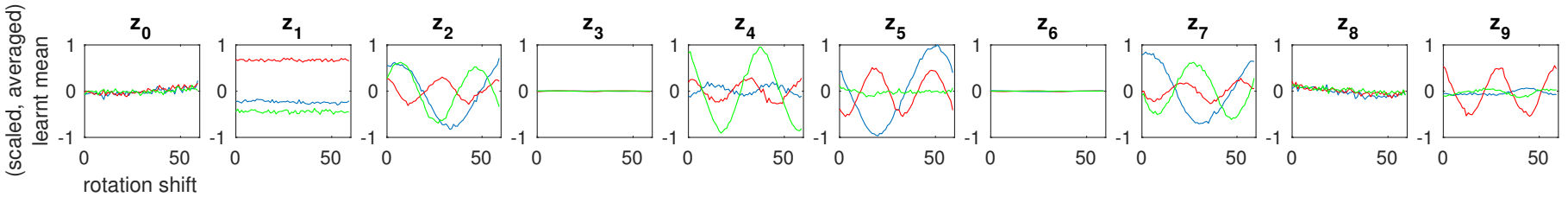


Results ($\beta = 4$)

Learnt means of each code element z_i as a function of the **scale** factor, averaged across rotations and positions.



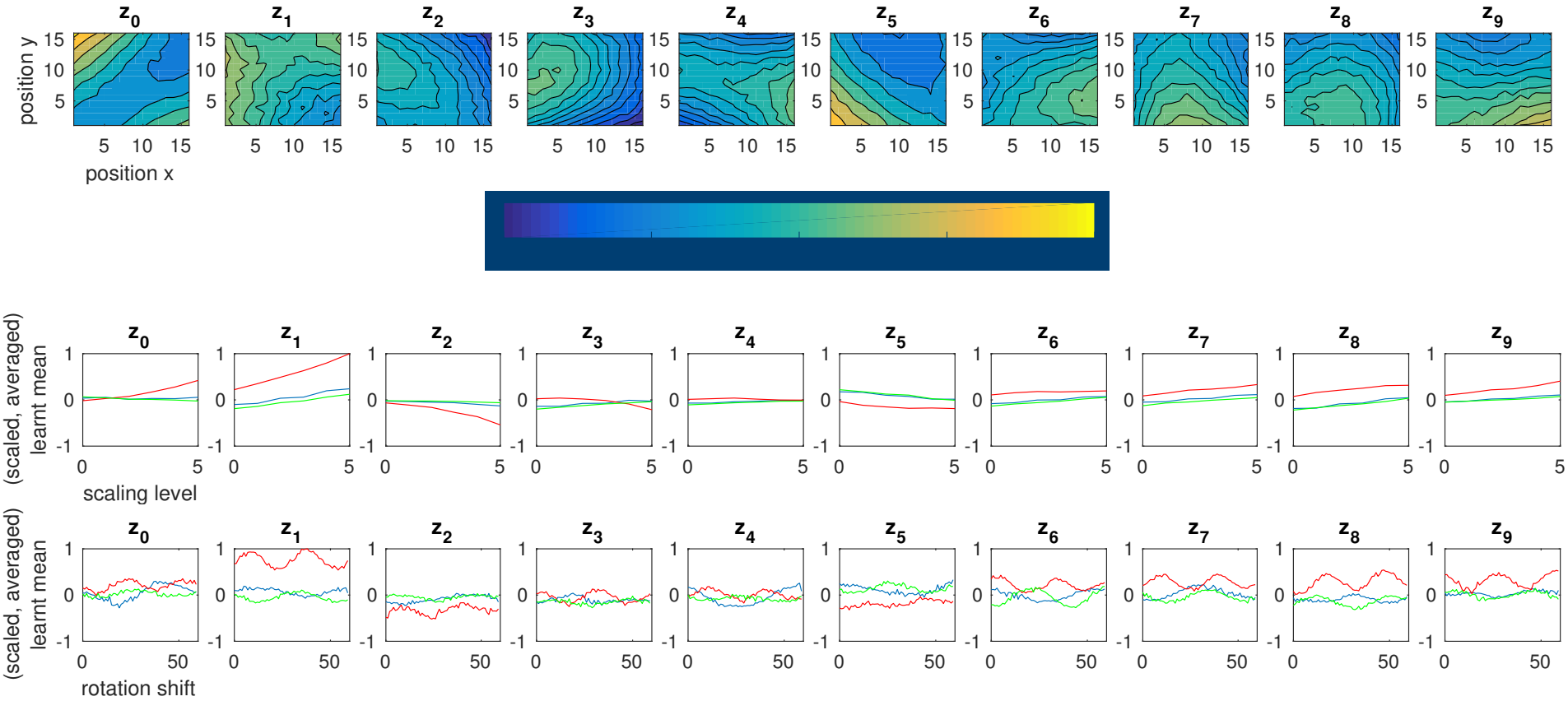
Learnt means of each code element z_i as a function of the **rotation** factor, averaged across scales and positions.



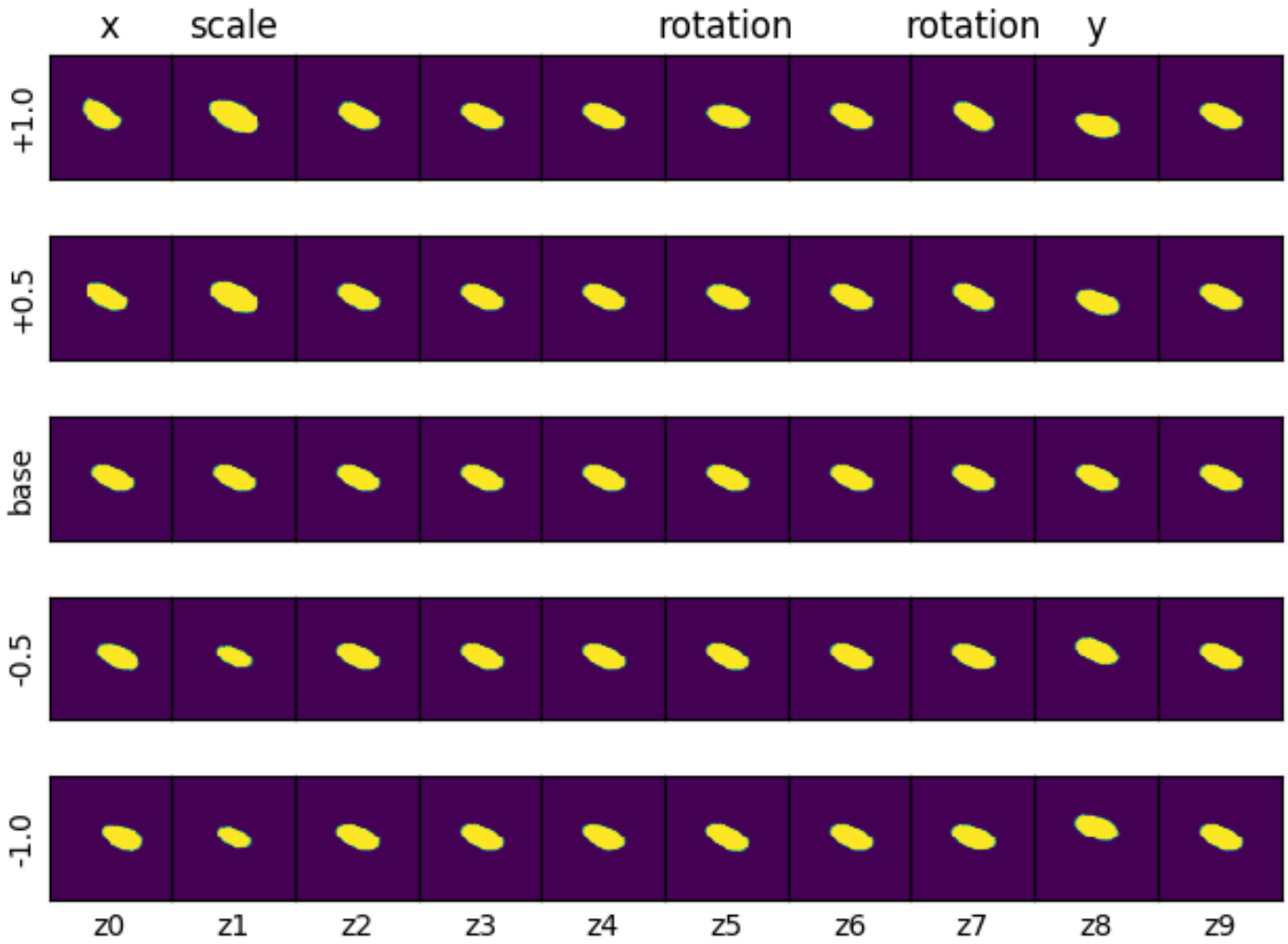
The colours correspond to **shapes** (ellipse, square, triangle).

Results ($\beta = 0$)

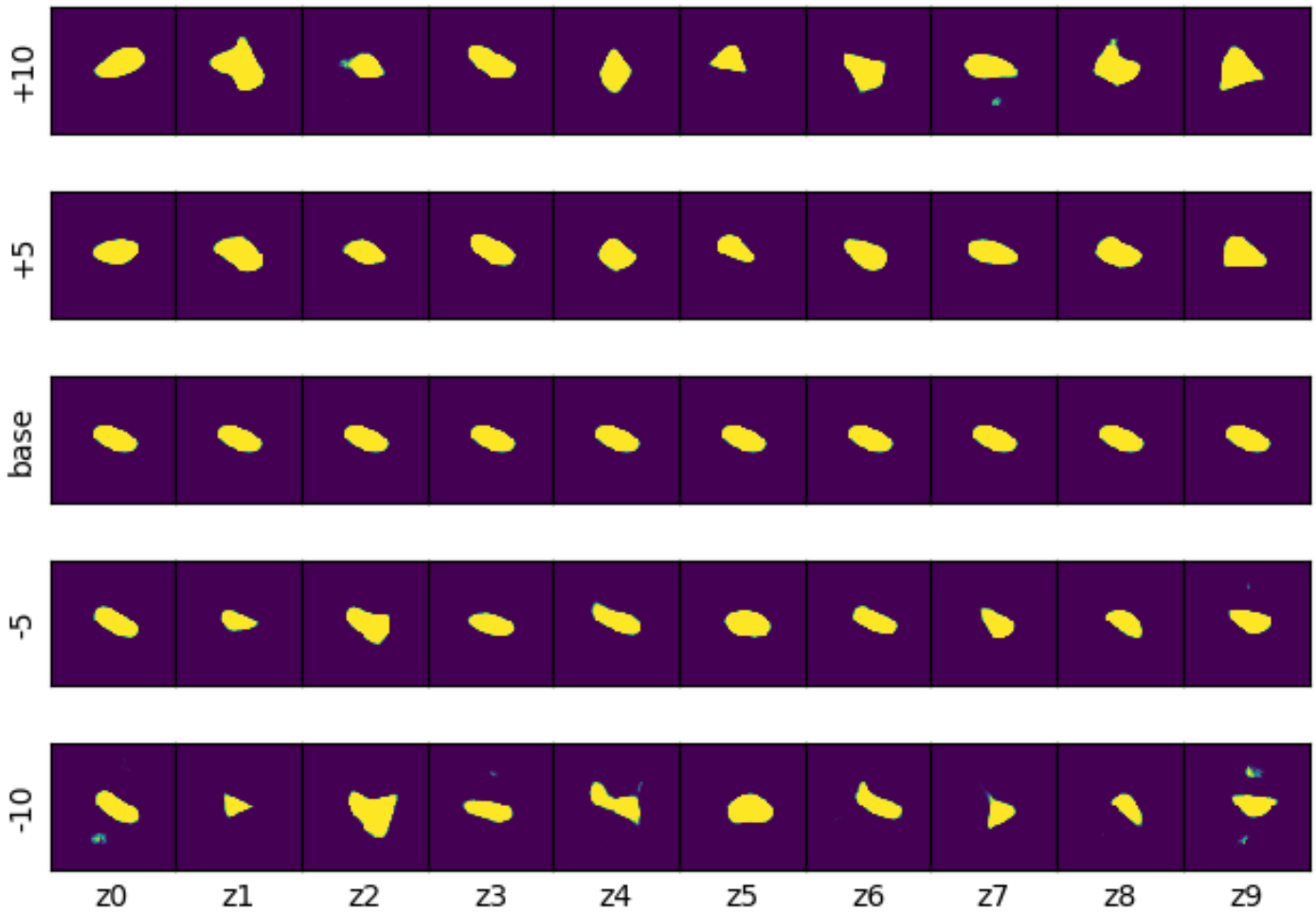
- This autoencoder learns an **entangled** representation.



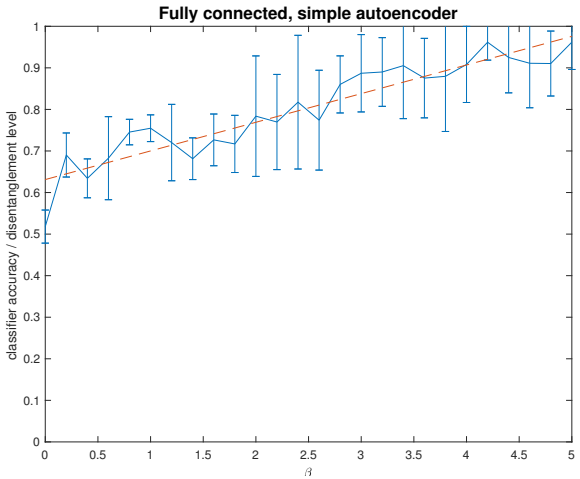
Shifting the code ($\beta = 4$)

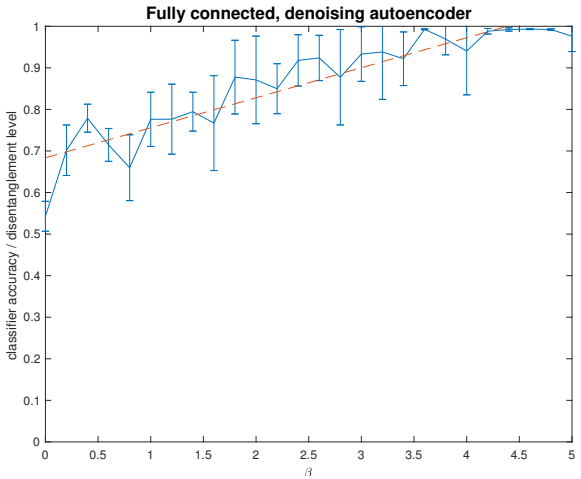


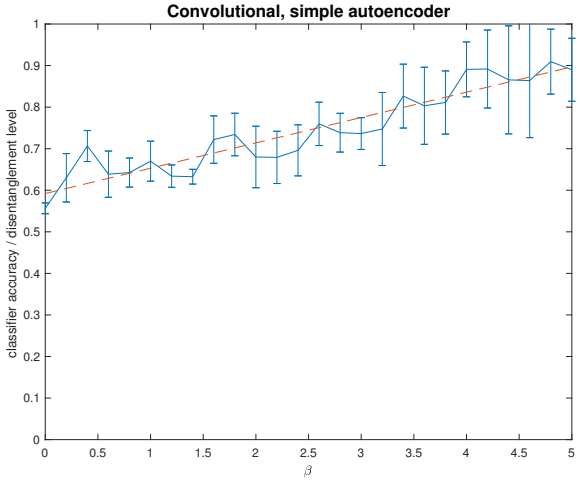
Shifting the code ($\beta = 0$)

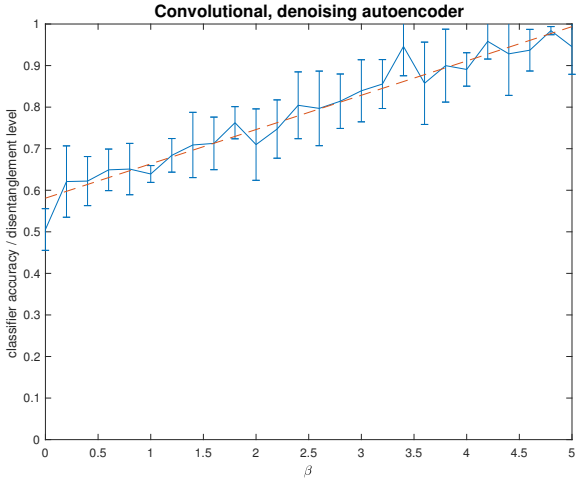


Disentanglement as a function of β





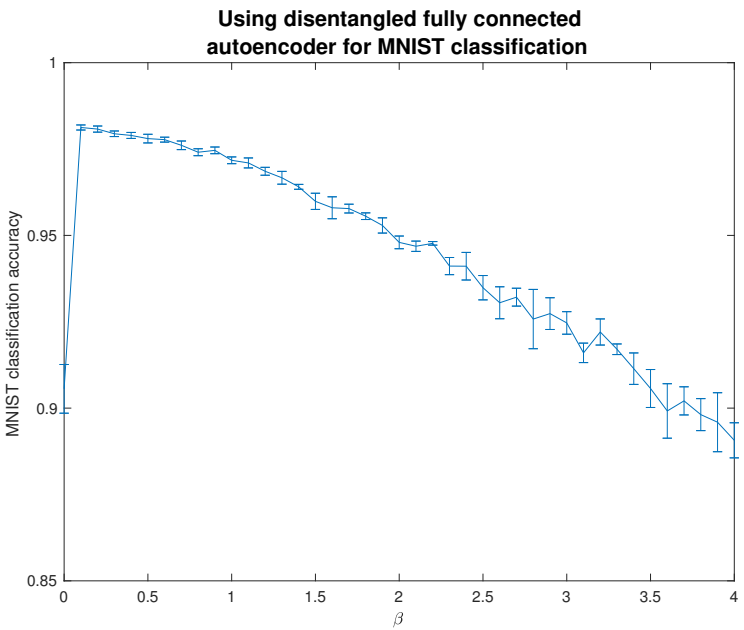


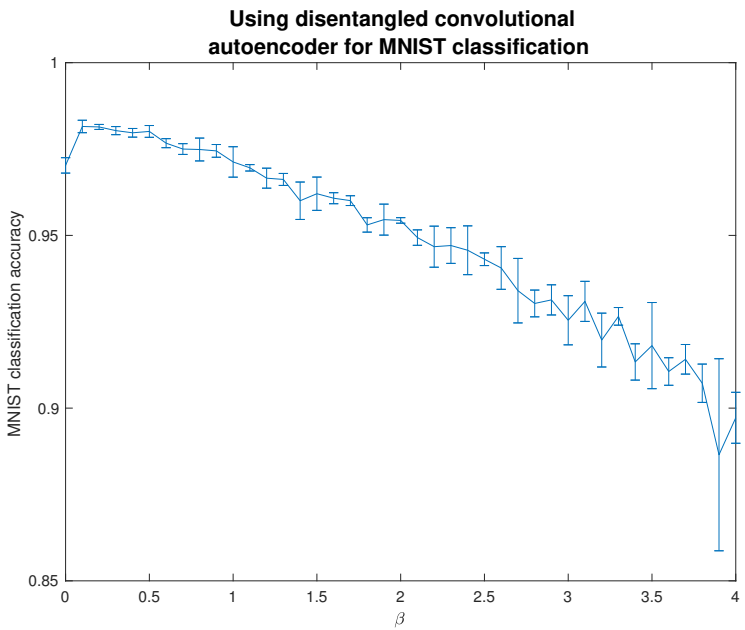


UCL

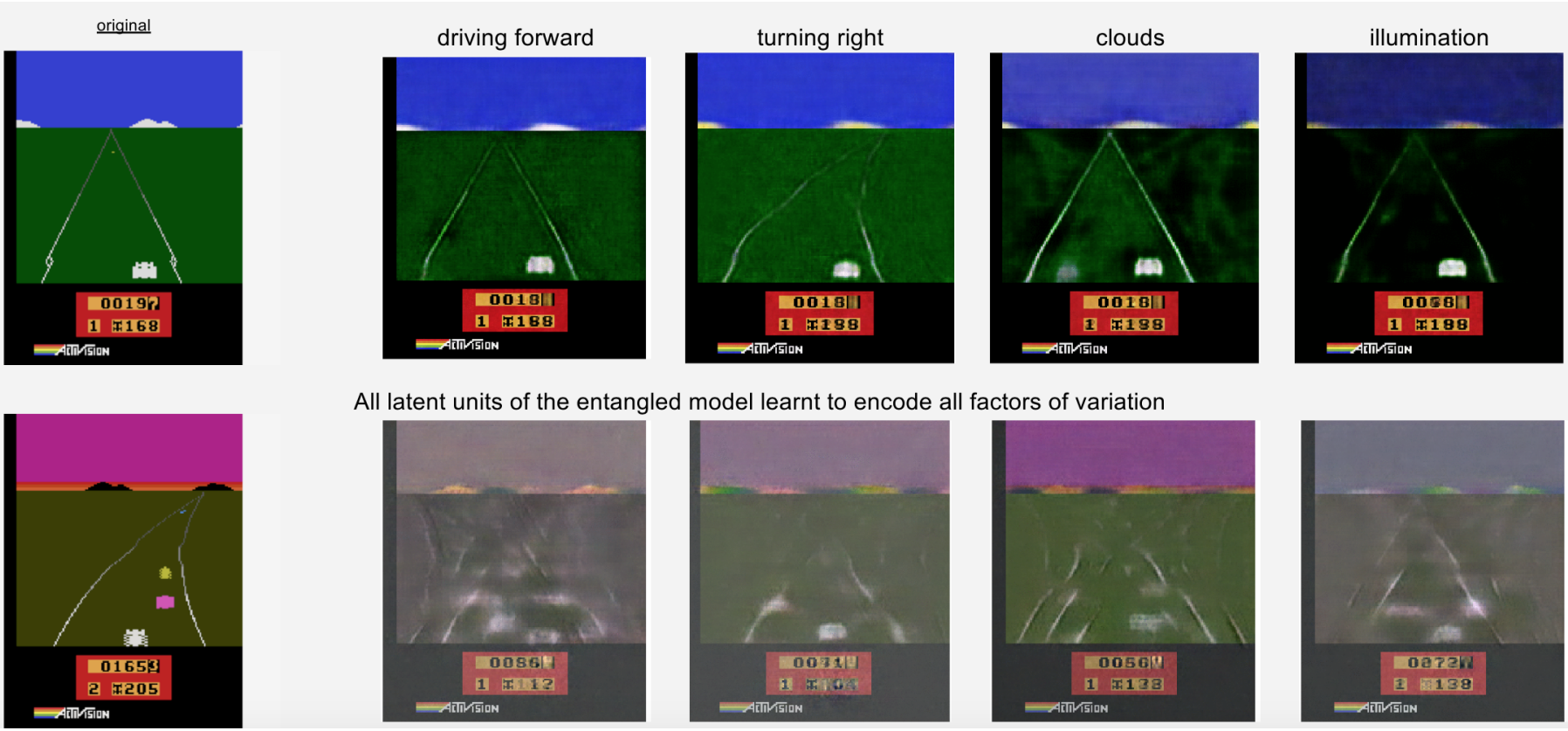
Classification with disentangled VAEs

- Using the VAE's code to classify on MNIST – does not explicitly satisfy the required assumptions made for the disentangled autoencoder to be successful, but tradeoffs evident.





Disentangling Atari (*Higgins et al., 2016*)



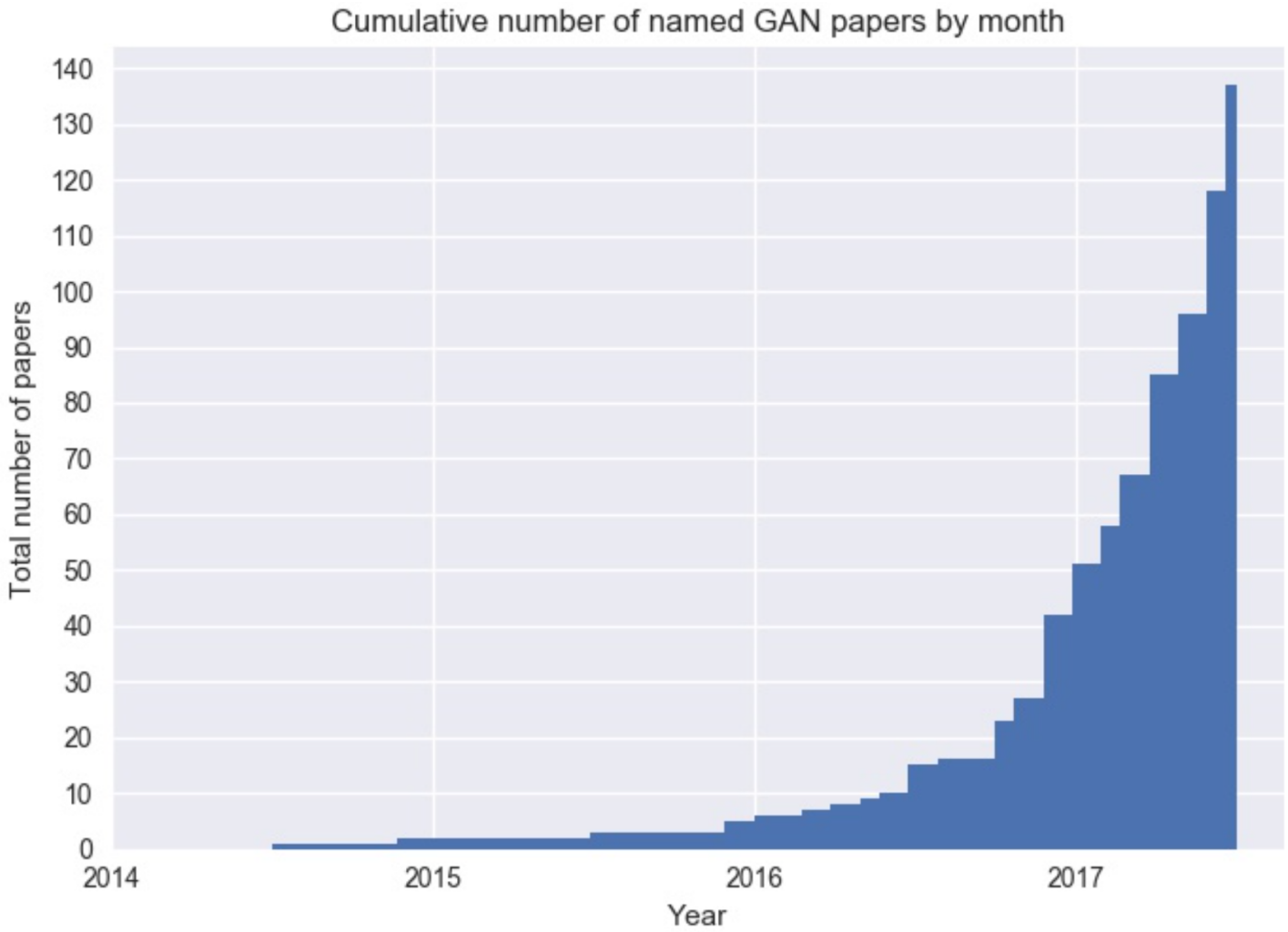
http://tinyurl.com/jgbyzke

Generative Adversarial Networks

- We will conclude with a brief overview of a bleeding-edge generative modelling approach—one of the most popular ideas to hit deep learning in the past decade.

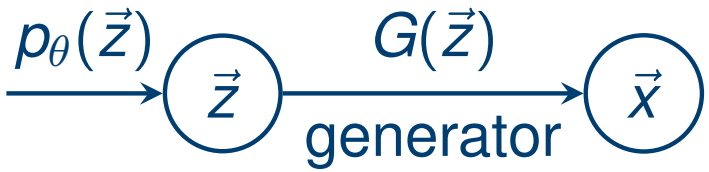
- *"The most important one, in my opinion, is adversarial training (also called GAN for **Generative Adversarial Networks**). This, and the variations that are now being proposed is the most interesting idea in the last 10 years in ML, in my opinion."*
  —Yann LeCun

GANs are **everywhere**



A probabilistic generative framework, revisited

- Recall the basic generative framework from before...



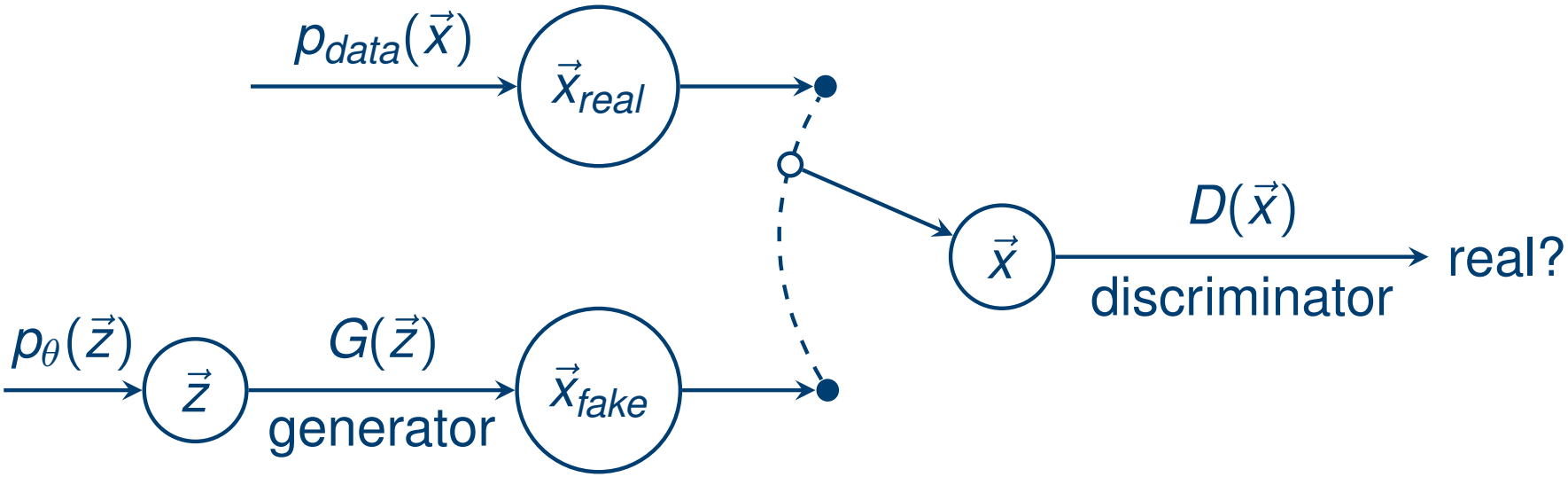
(**N.B.** $p_\theta(\vec{x}|\vec{z})$ is replaced by $G(\vec{z})$, and is *deterministic*!)

- What we **really** want to do is make the distribution of this generator *approach* the **true data distribution**, $p_{data}(\vec{x})$.
- With VAEs, we used the *KL-divergence* as an objective for enforcing one distribution to approach another.
  - Tractable only if we **know** our target distribution!
  - But we only have empirical samples from $p_{data}(\vec{x})$...

Simplifying the distributions

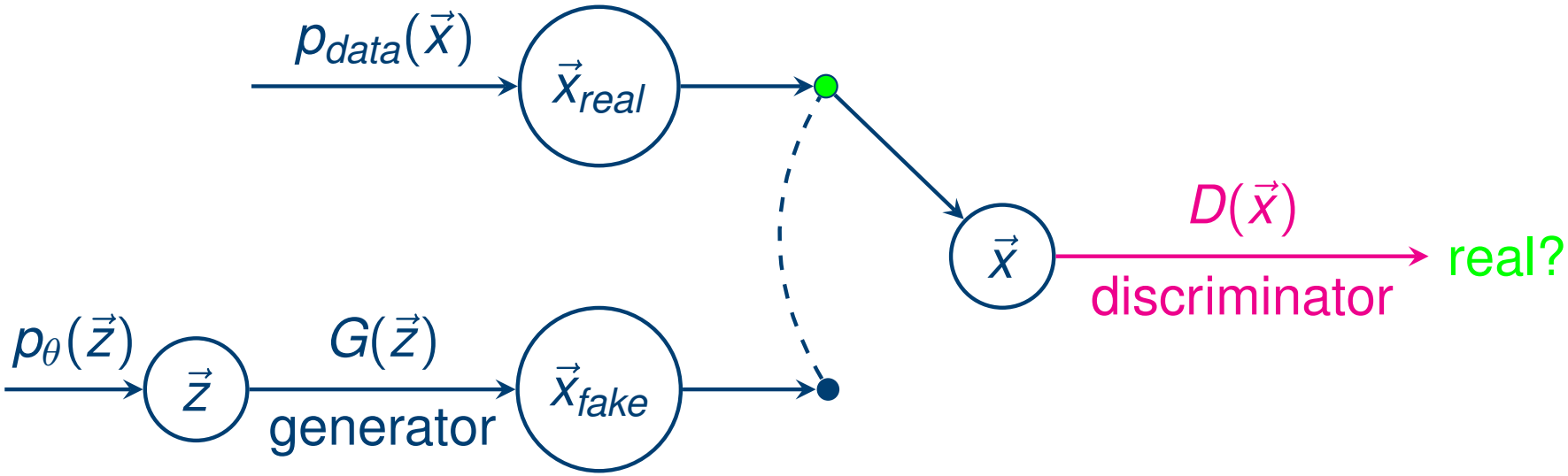
- Looking over full data distributions (e.g. individual image pixels) is *hard*.
- We can utilise a *neural network* to extract underlying features from inputs of these two distributions, and examine those.
- If these features are "good enough", the network should be capable of *telling the two distributions apart*!
- Call this network the **discriminator**, $D(\vec{x})$.
- Essentially, a *binary classifier*, telling whether $\vec{x}$ came from $p_{data}(\vec{x})$ or $G(\vec{z})$. **N.B.** The discriminator effectively **specifies the *loss function*** we're optimising!

The GAN framework



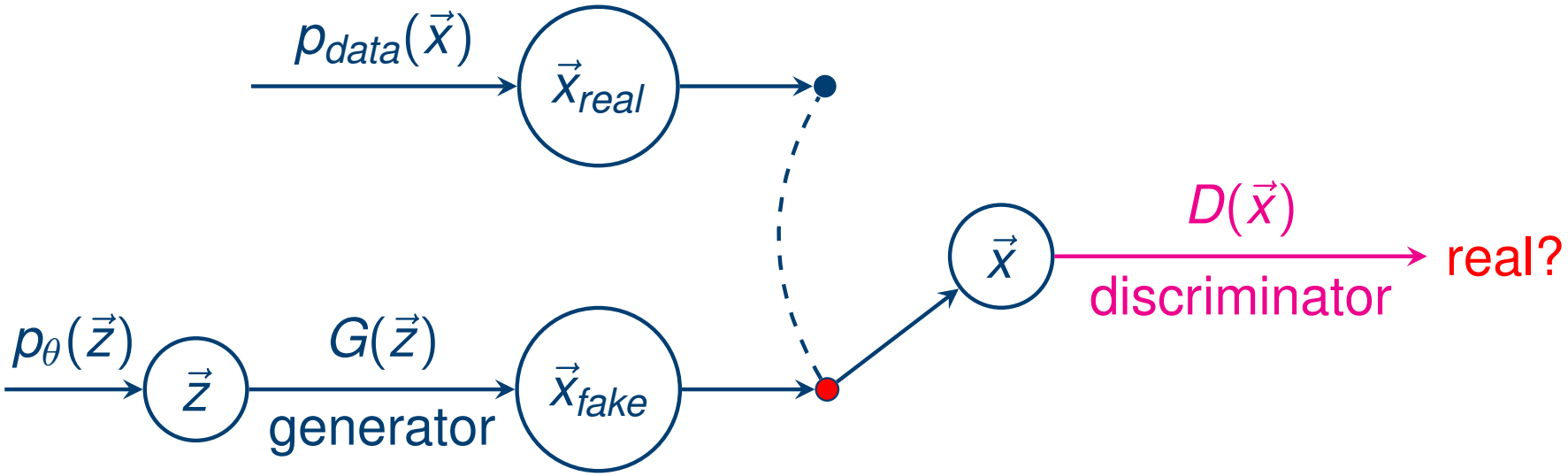
Two neural networks *playing a game*. . .
Alternate updating their weights; hopefully they *improve* together!

The GAN framework—update step 1



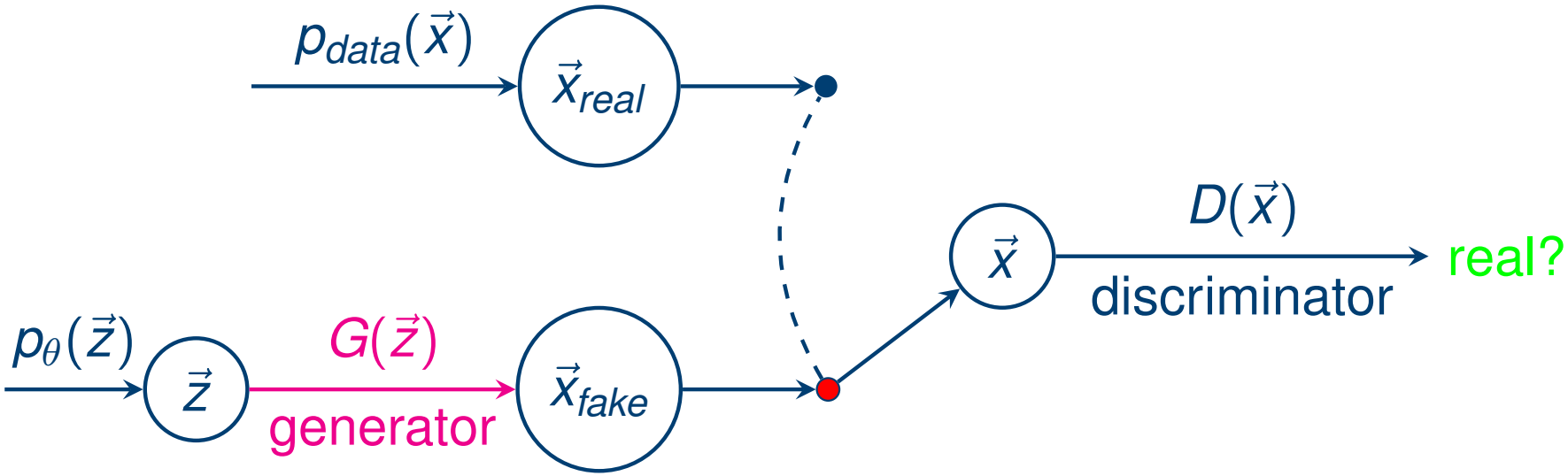
Train discriminator to maximise probability of '**real**' on real data.

The GAN framework—update step 2



Train discriminator to maximise probability of **'fake'** on fake data.

The GAN framework—update step 3



Train generator to maximise probability of **'real'** on fake data.

The desired final outcome

$$\min_G \max_D V(D, G) = \mathbb{E}_{\vec{x} \sim p_{data}(\vec{x})}[\log D(\vec{x})] + \mathbb{E}_{\vec{z} \sim p_\theta(\vec{z})}[\log(1 - D(G(\vec{z})))]$$

- Assuming everything goes well, concluding the training process we obtain **two** very useful networks!
  - The **generator**, $G(\vec{z})$, becomes capable of generating extremely useful examples, which can then be used for *data augmentation*.
  - The **discriminator**, $D(\vec{x})$, becomes a high-quality **feature extractor** from data, which can then be used for the usual supervised learning tasks.
- The exact *update rule* we use in the above scenarios will depend on the **distance metric** between $p_{data}(\vec{x})$ and $G(\vec{z})$ that we seek to optimise.

Two potential distance metrics

- The Jensen-Shannon (JS) divergence, D_{JS}:

$$D_{JS}(q(x)\|p(x)) = \frac{1}{2}D_{KL}(q(x)\|m(x)) + \frac{1}{2}D_{KL}(p(x)\|m(x))$$

  where $m(x) = \frac{1}{2}(p(x) + q(x))$
  - Optimised in the original GAN paper (*Goodfellow et al., 2014*), *assuming optimal discriminator*.
  - Therefore, want the discriminator to be *very good*.
  - However, suffers from vanishing gradients when discriminator is *too good* (making the generator **stop improving**). Tradeoffs?!

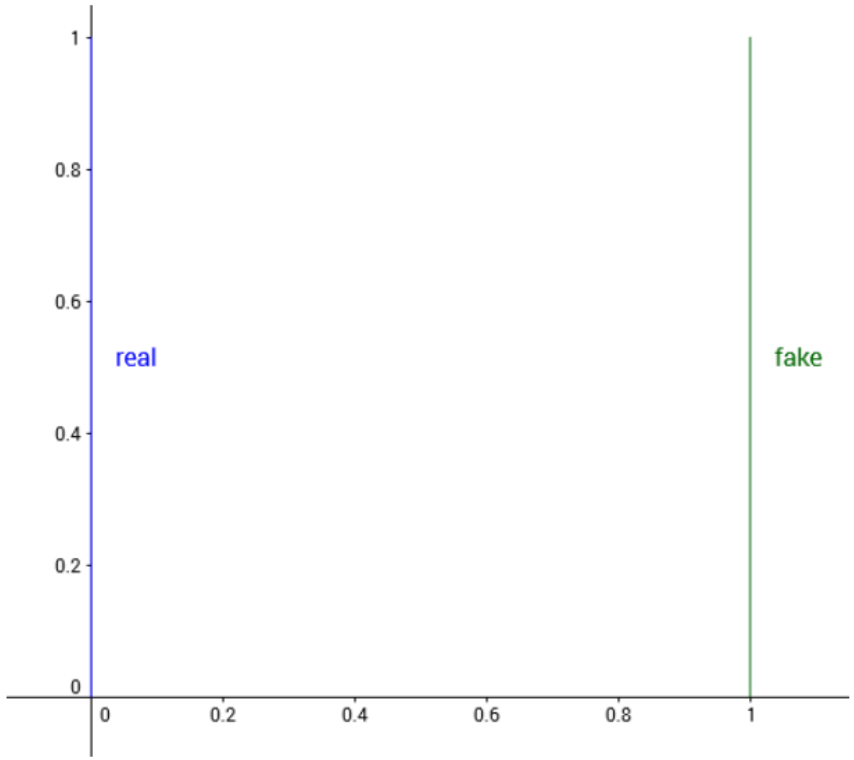
Two potential distance metrics

- The Wasserstein/Earth Mover (EM) distance, W:

$$W(p(x), q(x)) = \inf_{\gamma \in \Pi(p,q)} \mathbb{E}_{(x,y)\sim\gamma}[\|x - y\|]$$

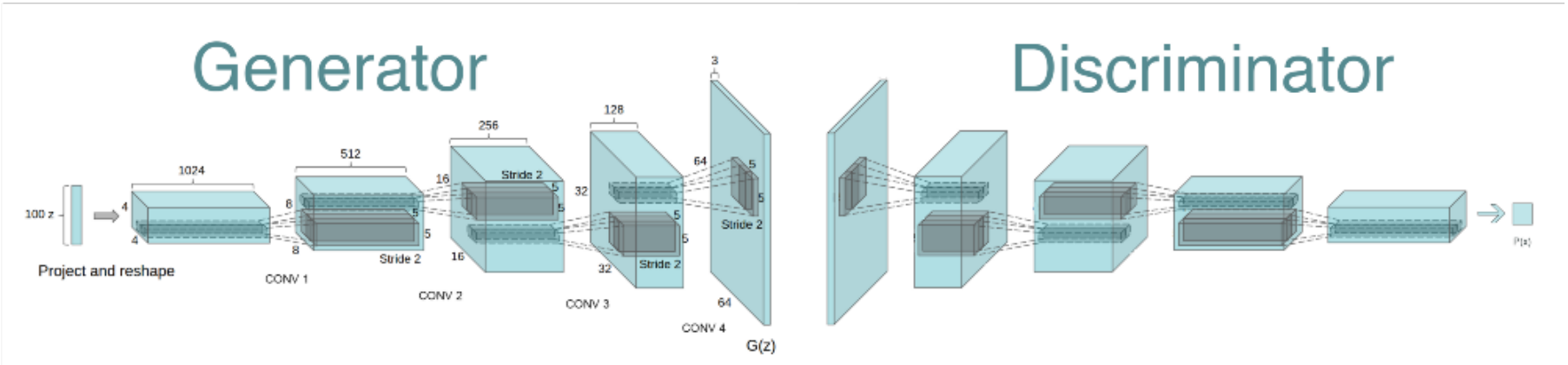
  - Takes into account the underlying geometry of the distributions
  - Indicates the cost of transforming p into q under an "optimal transport plan".
  - Intractable in this form (but various interesting developments)!

Aside: Why Wasserstein is desirable



KL-divergence is $+\infty$, JS-divergence is a constant ($\log 2$),
Wasserstein distance is equal to the distance between the lines!

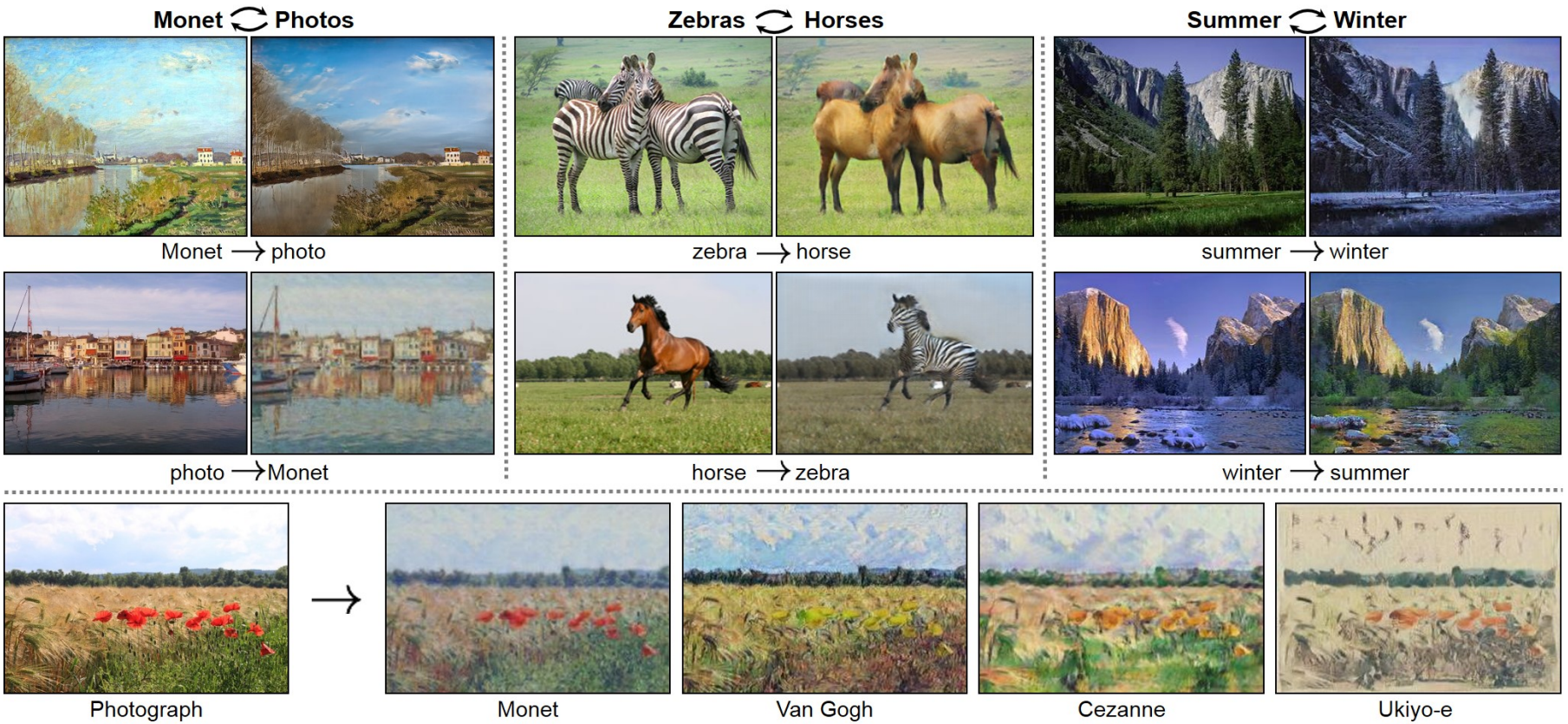
A deep convolutional GAN (*Radford et al., 2015*)



Architectures like this allow us to create some really interesting applications with image distributions. . .

Generating fake celebrities (*Hjelm et al., 2017*)

Domain transfer: *CycleGAN* (*Zhu et al., 2017*)



https://junyanz.github.io/CycleGAN/

An overview of historical deep learning ideas

- Initially, we needed to extract hand-crafted features before applying a machine learning model to them.
  - **Deep neural networks** can perform feature extraction by themselves.
- Then, we needed to select a hand-crafted loss function to optimise.
  - **GANs** use a neural network (the *discriminator*) to compute a customised loss!
- We need to figure out a correct way to perform the optimisation of the loss function.
  - **Learn how to learn**?

Thank you!

Questions?

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Special thanks:
Momchil Peychev (*University of Cambridge*)
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Reading material:
‘Deep Learning’, Chapter 13 (PCA)
‘Deep Learning’, Chapter 14 (AEs, DAEs)
‘Deep Learning’, Chapter 20 (RBMs, DBNs, VAEs, GANs)