### Deep Learning Architectures

Introduction to Machine Learning, Day 4

#### Wintersession 2025 with PICSciE/RC

#### 20 hours of machine learning training

#### Instructors

Sarah-Jane Leslie, Professor of Philosophy and CSML, and NAM Co-Director Julian Gold, DataX Data Scientist, CSML Gage DeZoort, Postdoctoral Research Associate and Lecturer, Physics Simon Park, Graduate Student, Computer Science and PLI Abhishek Panigrahi, Graduate Student, Computer Science and PLI Christian Jespersen, Graduate Student, Astrophysical Sciences Rafael Pastrana, Graduate Student, Architecture Quinn Gallagher, Graduate Student, Chemical and Biological Engineering Holly Johnson, Graduate Student, Electrical and Computer Engineering





Introduction to Machine Learning for Humanists and Social Scientists

A Hands-On Introduction to Machine Learning

Part 1 Part 2

Mon Jan. 13 Tue Jan. 14

10 AM-12 PM 10 AM-12 PM

Part 1
Wed Jan. 15
2-4 PM

Thu Jan. 16 2-4 PM

Part 2

Part 3

Fri Jan. 17 Tue Jan. 21 2-4 PM 2-4 PM

Getting Started with LLMs with Princeton Language and Intelligence

Machine Learning for the Physical Sciences

**Graph Neural** 

**Networks for** 

Your Research

Part 1 Part 2

Wed Jan. 22 Thu Jan. 23 2-4 PM 2-4 PM

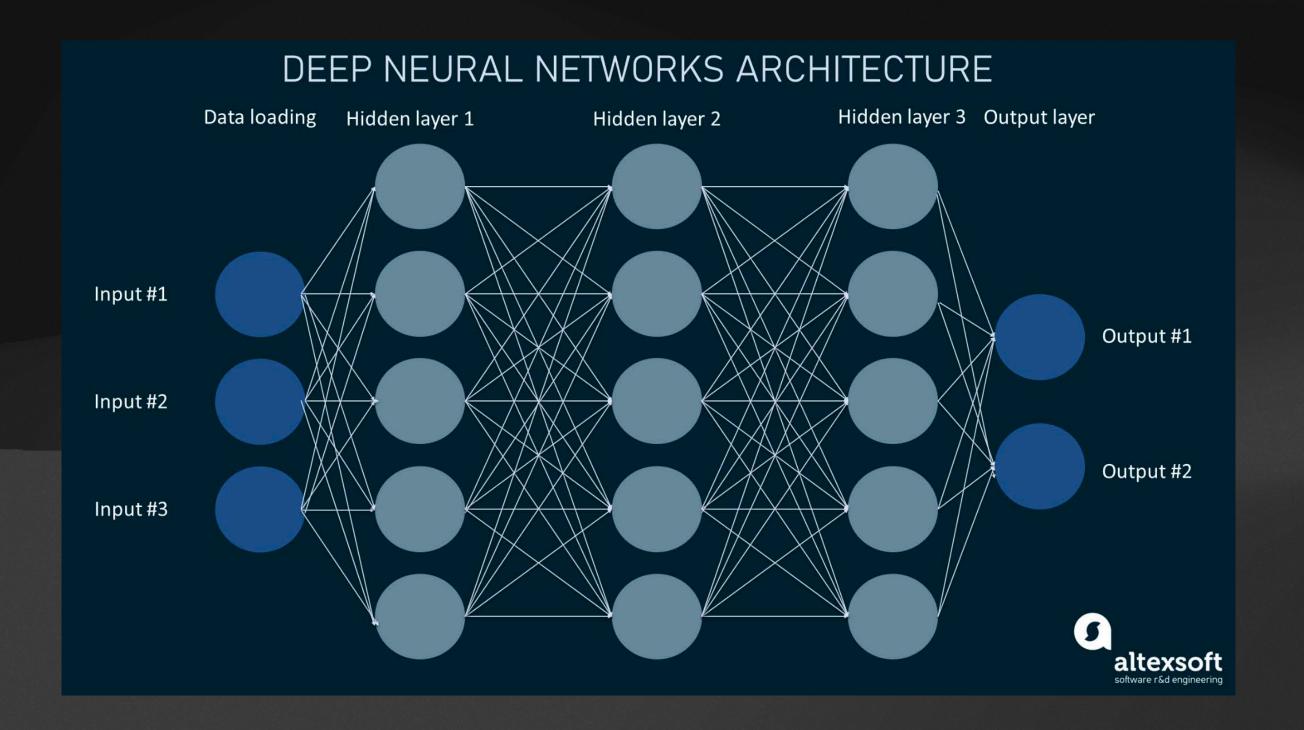






Part 4





Forward pass:

$$z_i^{(\ell+1)} = \sum_{i=1}^{n_{\ell}} W_{ij}^{(\ell+1)} \sigma(z_j^{(\ell)}) + b_i^{(\ell+1)}$$

Backward pass:

$$W_{ij}^{(\ell+1)} = W_{ij}^{(\ell)} - \gamma \frac{\partial L}{\partial W_{ij}} \bigg|_{W_{ij}^{(\ell)}}$$

$$b_i^{(\ell+1)} = b_i^{(\ell)} - \gamma \frac{\partial L}{\partial b_i} \Big|_{b_i^{(\ell)}}$$

```
class NeuralNetwork(nn.Module):
   def __init__(self):
        super().__init__()
        self.flatten = nn.Flatten()
        self.linear_relu_stack = nn.Sequential(
            nn.Linear(28*28, 512),
            nn.ReLU(),
            nn.Linear(512, 512),
            nn.ReLU(),
            nn.Linear(512, 10),
   def forward(self, x):
        x = self.flatten(x)
        logits = self.linear_relu_stack(x)
        return logits
```

```
def train_one_epoch(epoch_index, tb_writer):
    running_loss = 0.
   last_loss = 0.
    # Here, we use enumerate(training_loader) instead of
    # iter(training_loader) so that we can track the batch
    # index and do some intra-epoch reporting
    for i, data in enumerate(training_loader):
        # Every data instance is an input + label pair
        inputs, labels = data
        # Zero your gradients for every batch!
        optimizer.zero_grad()
        # Make predictions for this batch
        outputs = model(inputs)
        # Compute the loss and its gradients
        loss = loss_fn(outputs, labels)
        loss.backward()
        # Adjust learning weights
        optimizer.step()
        # Gather data and report
        running_loss += loss.item()
        if i % 1000 == 999:
            last_loss = running_loss / 1000 # loss per batch
            print(' batch {} loss: {}'.format(i + 1, last_loss))
           tb_x = epoch_index * len(training_loader) + i + 1
            tb_writer.add_scalar('Loss/train', last_loss, tb_x)
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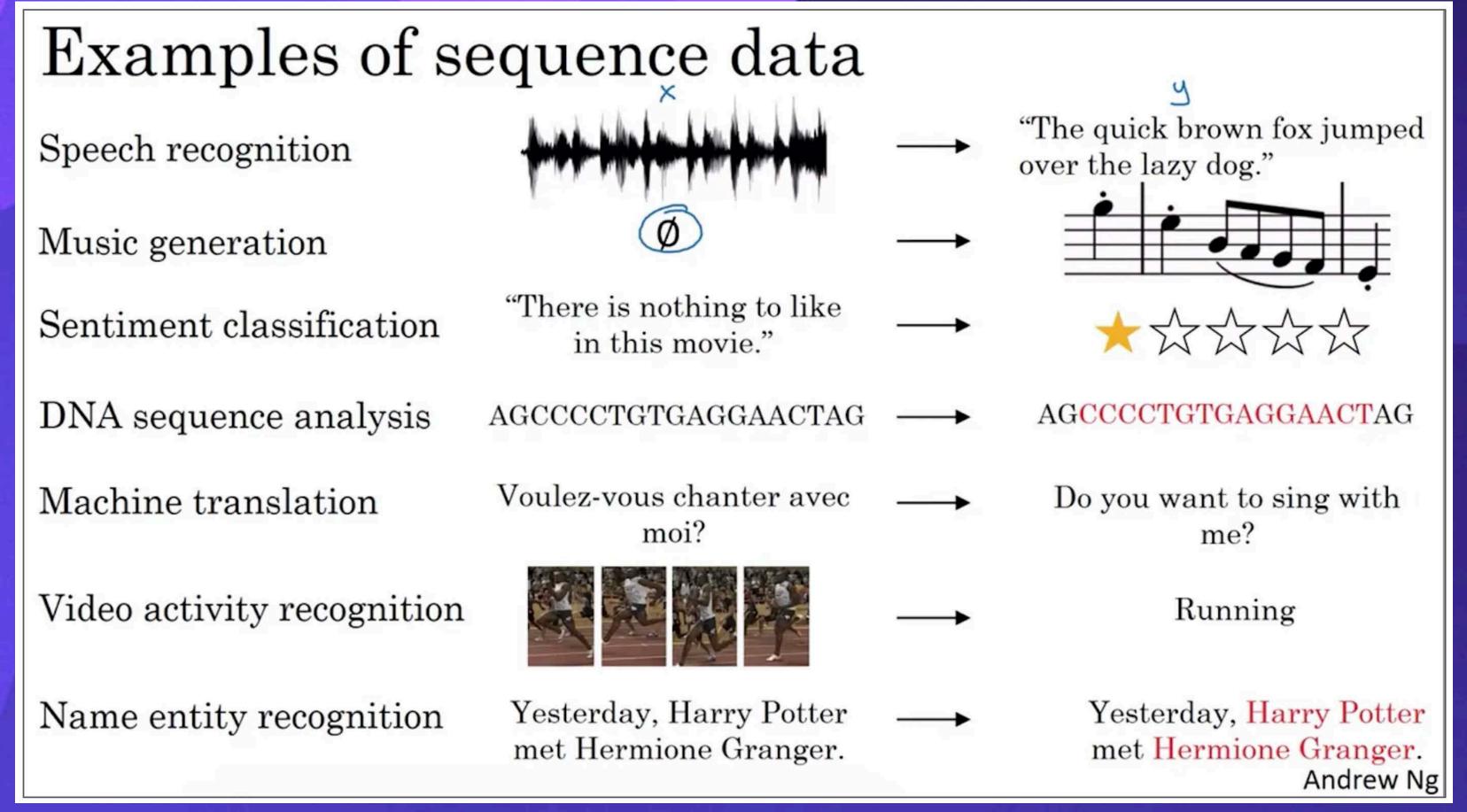
$$W_{ij}^{(\ell+1)} = W_{ij}^{(\ell)} - \gamma \frac{\partial L}{\partial W_{ij}} \Big|_{W_{ij}^{(\ell)}} \qquad b_i^{(\ell+1)} = b_i^{(\ell)} - \gamma \frac{\partial L}{\partial b_i} \Big|_{b_i^{(\ell)}}$$

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# Beyond Simple DNNs Survey of Deep Learning Architectures

- Deep NN (DNN) ←→ Feed-Forward NN (FFNN) ←→ Fully-Connected NN (FCNN)
- Many other architectures exist:
  - Recurrent NNs (RNNs): process sequential data
  - Convolutional NNs (CNNs): process data on a grid
  - Graph Neural Networks (GNNs): process data on a graph / attention
  - Generative Models: produce new data
  - ... and more!

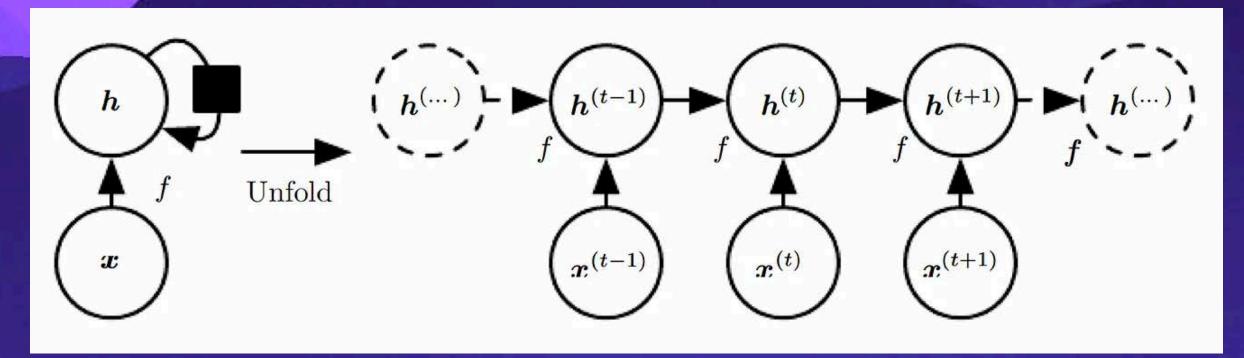
## Recurrent Neural Networks Designed to Process Sequential Data



### Recurrent Neural Networks Basic Idea

- Time-indexed inputs:  $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \dots, \mathbf{X}^{(T)}$
- Parameter sharing: apply the same set of learnable weights to all values of the time index
- Given a set of learnable parameters  $\theta$ , the hidden units in many RNNs are calculated via.  $\mathbf{h}^{(t)} = f(\mathbf{h}^{(t-1)}, \mathbf{x}^{(t)}; \theta)$

Image from Deep Learning by Goodfellow et al.



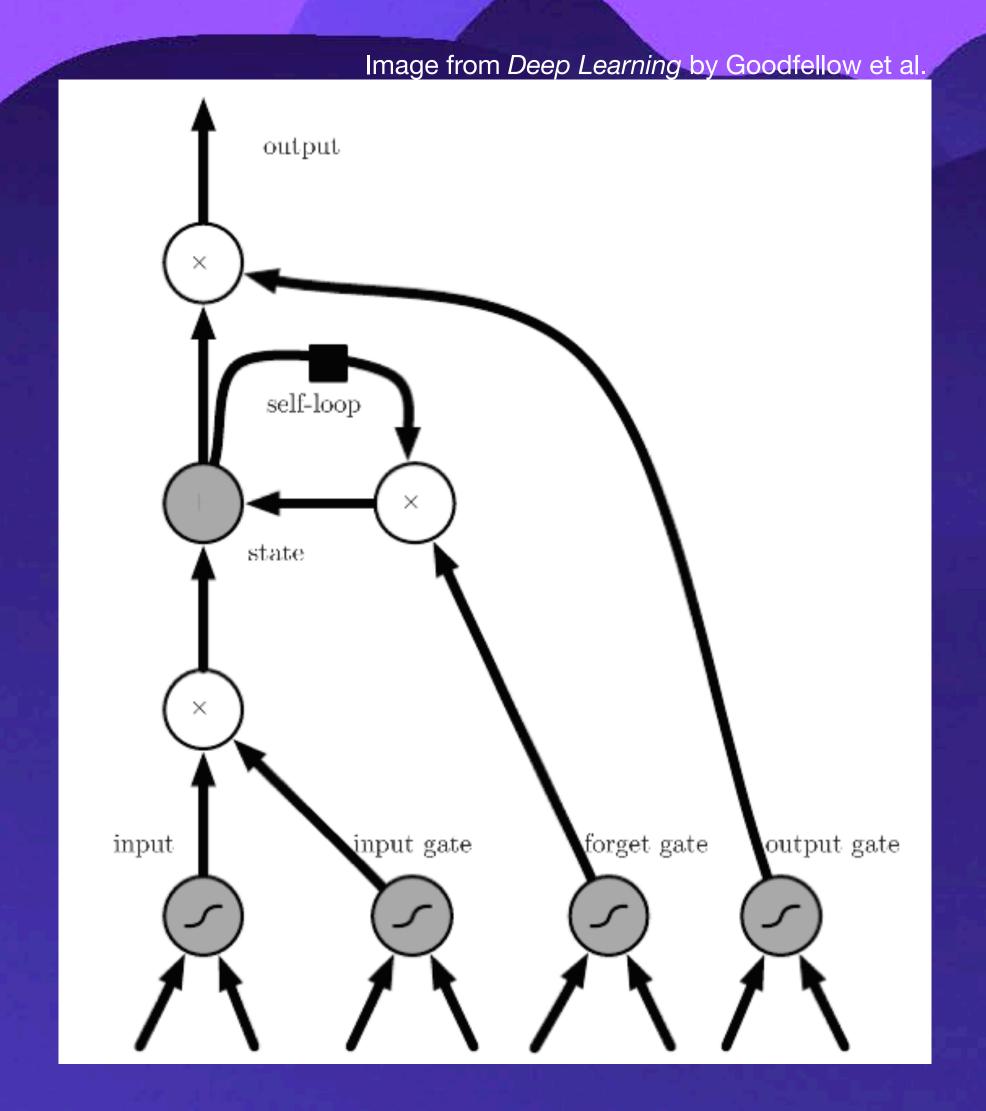
RNN with no outputs; information is processed sequentially, taking into account both  $\mathbf{x}^{(t)}$  and  $h^{(t-1)}$  but applying the same function  $f(\cdot;\theta)$  at each tilmestep

Long Short-Term Memory (LSTM)

An Upgraded RNN Module

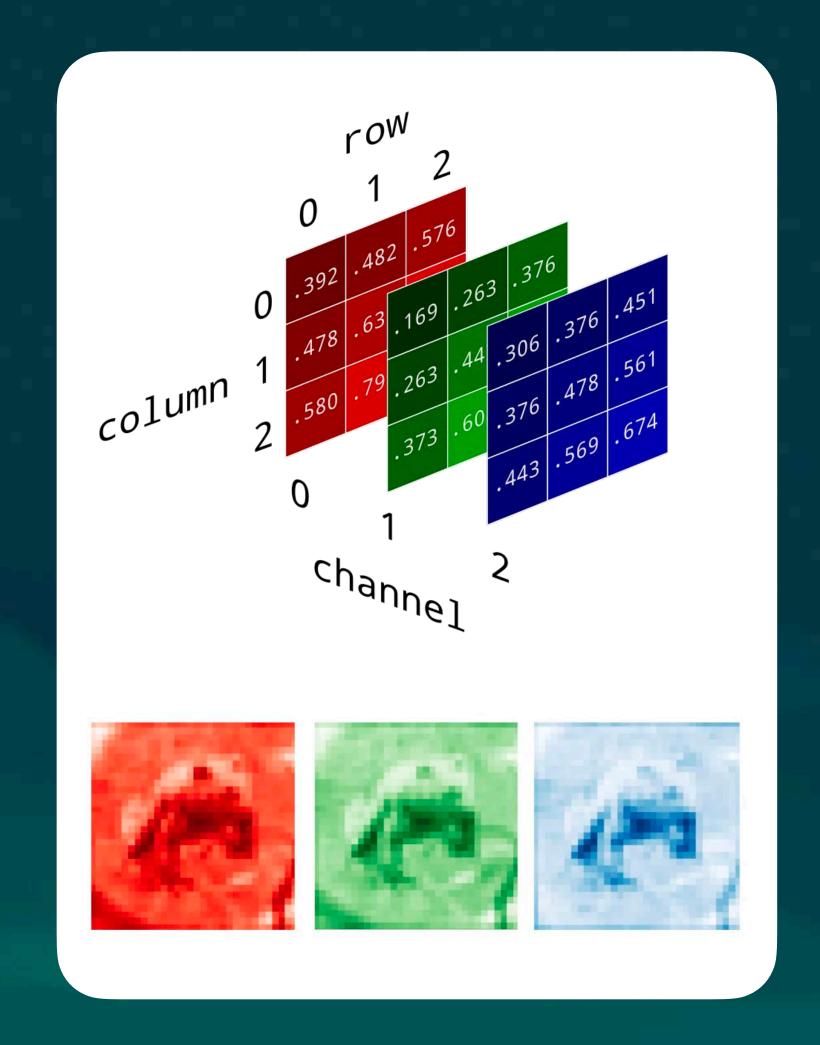
 RNNs are finicky to train; they often suffer from exploding/vanishing gradients

- This has motivated the development of more advanced RNNs like LSTMs
- The LSTM is a recurrent "cell" that is applied to all timesteps equally



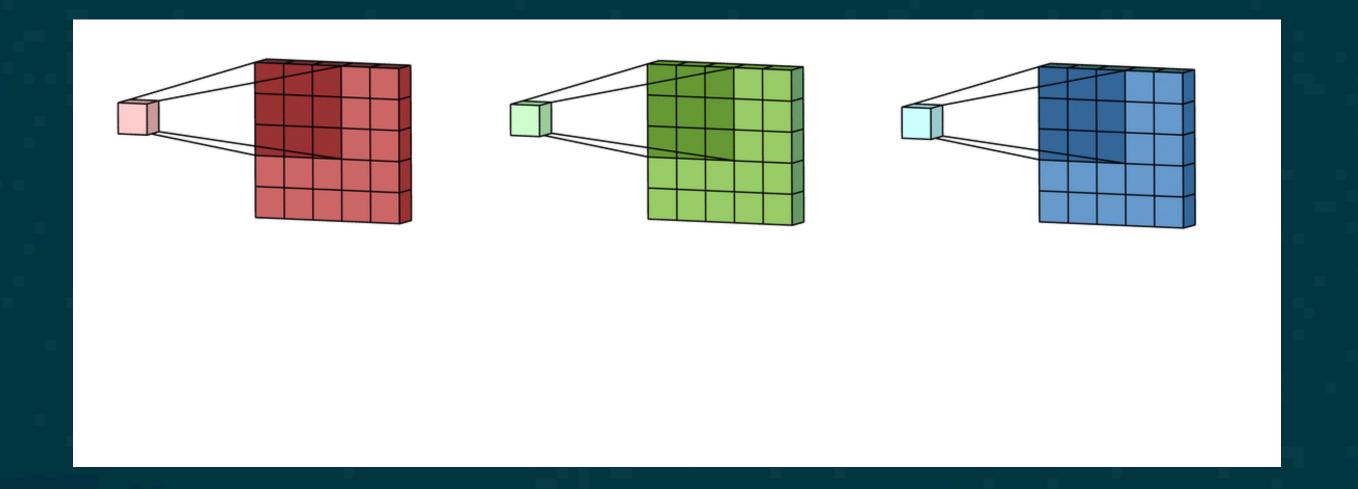
### Convolutional Neural Networks (CNNs)

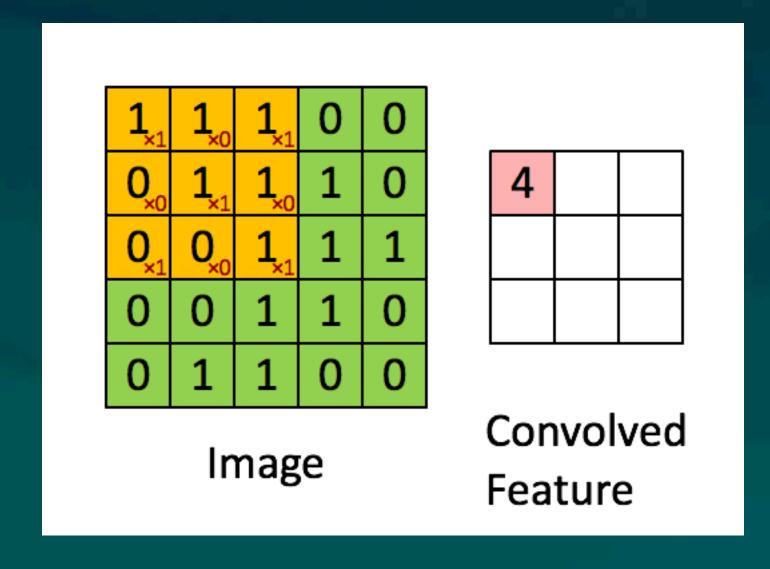
- Deep learning applied to images (data on a grid)
  - For square images, inputs are  $I \in \mathbb{R}^{n_{\text{pixels}} \times n_{\text{pixels}} \times n_{\text{features}}}$



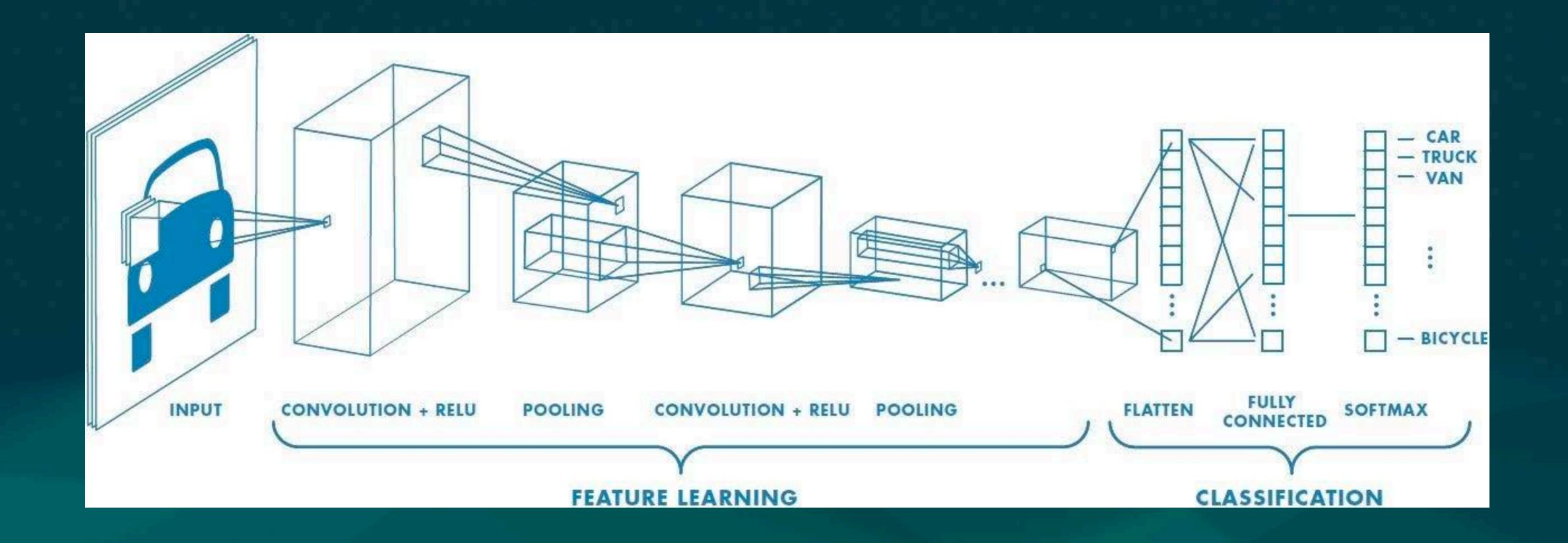
### Convolutional Neural Networks (CNNs)

- Very similar approach to DNNs (non-sequential inputs, feedforward approach), except now we use convolutional layers
  - Convolution: filter is convolved (weighted sum with learnable weights) with the input image
  - Again, parameter sharing!



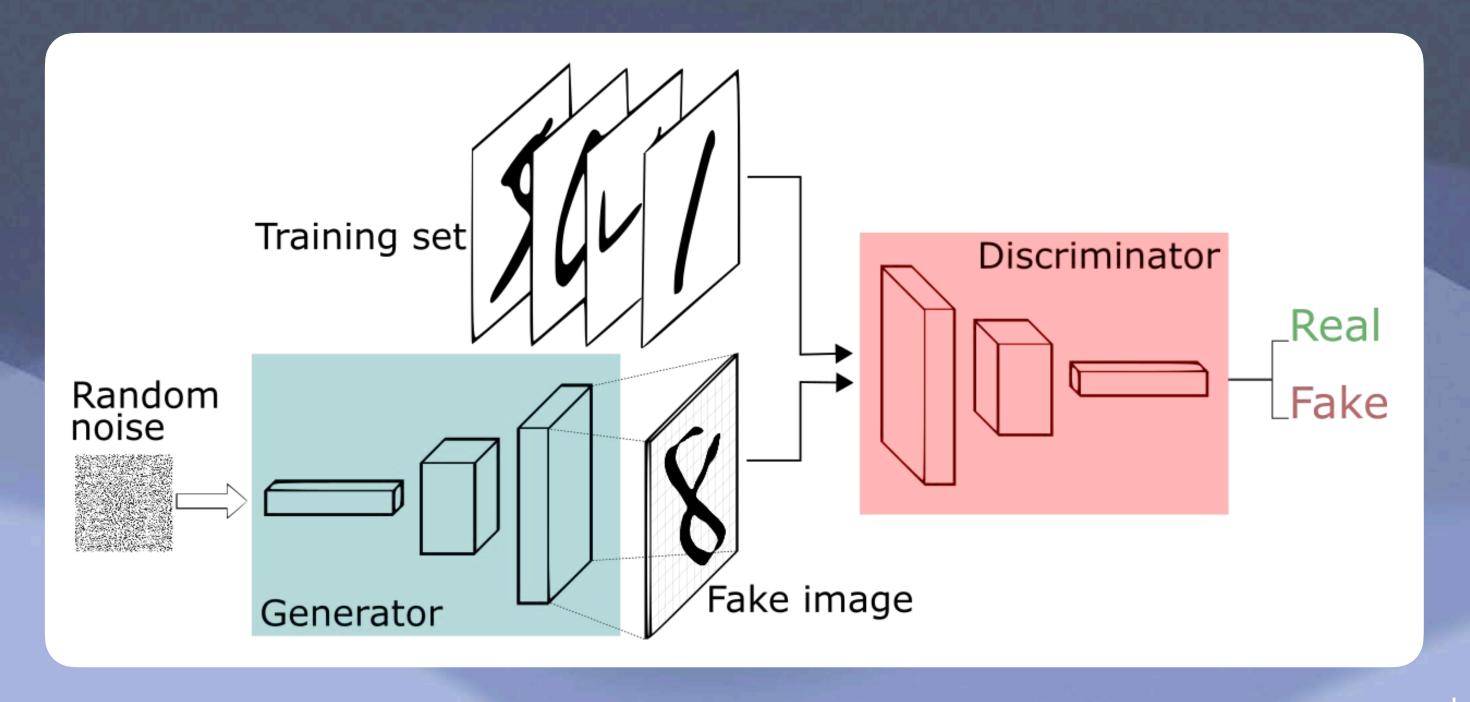


### Convolutional Neural Networks (CNNs)



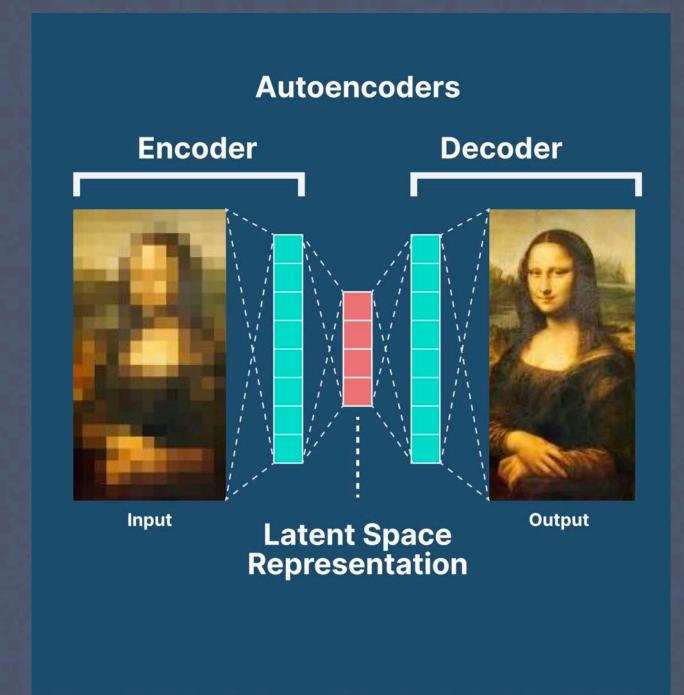
# Generative Adversarial Networks (GANs) Survey of Deep Learning Architectures

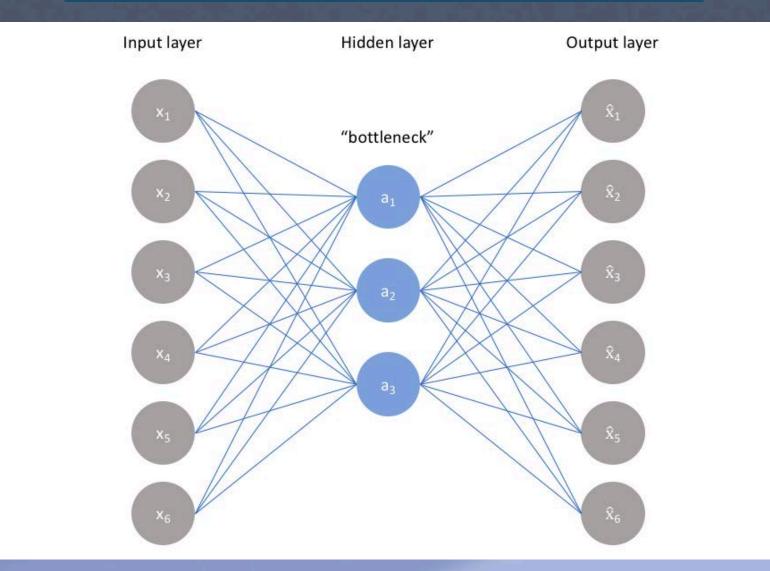
- "Generative" Al: use ML to create new images, sounds, etc.
- GANs: two agents (the generator and the discriminator) are given competing tasks:



# Autoencoders Learning Efficient Codings

- Autoencoders are used to produce compressed data representations
  - Encoder: produces a lower-dimensional (compressed) "latent" representation of the input data
  - Decoder: given the compressed representation, reconstruct the original data
- Decoded representations typically less noisy,
- Uses: efficient encoding, image denoting, generative modeling, anomaly detection





https://www.v7labs.com/blog/autoencoders-guide#:~:text=An%20autoencoder%20is%20an%20unsupervised,even%20generation%20of%20image%20data.

### Variational Autoencoder (VAEs)

#### Generative Modeling via Autoencoders

- Generate realistic images from random noise
  - Encoder: predict means and standard deviations of a probability distribution over the latent features
  - Decoder: given a random sample from the latent distributions, produce the corresponding output

