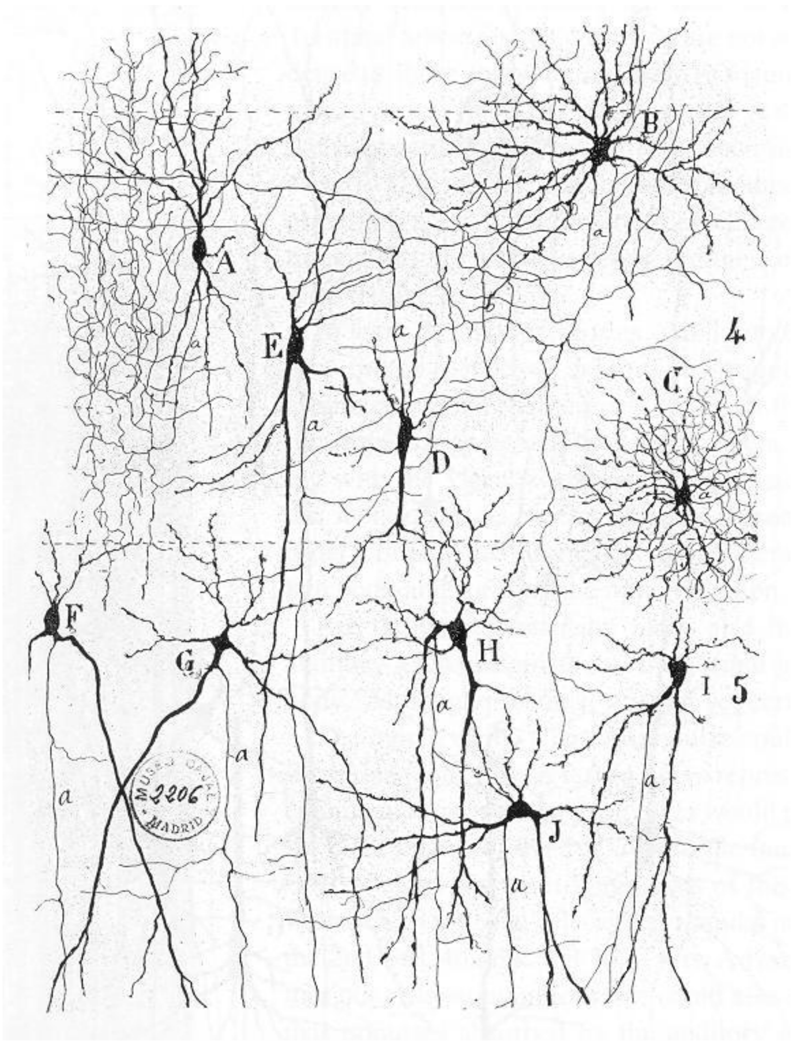
# Neural Networks

- Inspired by biology
- Better picture: nested linear algebra functions, fully parametrized
- Layers: Differentiable functions on previous intermediate results with free parameters for training
- Deep learning: more layers




## Key ingredients

- Non-linear function
- Linear model
  - w: some weights
  - b: bias

$$g(\mathbf{X})$$
$$\hat{y} = \mathbf{w}g(\mathbf{X}) + \mathbf{b}$$

## Universal Approximation Theorem

Given enough layers and width, any function can be represented.

# Layer types



**Convolution layer**: includes a fixed neighborhood

- Weighted combination of close entries, fixed weights

**Pooling layer**: reduce dimensionality

- Aggregate (typically max) values

**Dense layer**: general use

Input

$$\sigma(\mathbf{W}\mathbf{x}) + \mathbf{b}$$

Activation function    Weights    Bias

# Layer ingredients



**Activation function**
- Differentiable
- Non-linear
- Hyperparameter
- Common: rectified linear unit (ReLU) = max(0, x)

**Weights**
- Matrix, free parameters
- Shape determines dimensionality of output

**Bias**
- Vector, free parameters

Input

$$\sigma(\mathbf{W}\mathbf{x}) + \mathbf{b}$$

Activation function Weights Bias

# Layers with are no layers



**Hidden layer**: anything the result of which is not inspected by the user

**Activation layer**: Explicit application of the activation function

**Dropout layer**: stochastic method of ignoring features to reduce overfitting

**Input layer**: tensor of input features

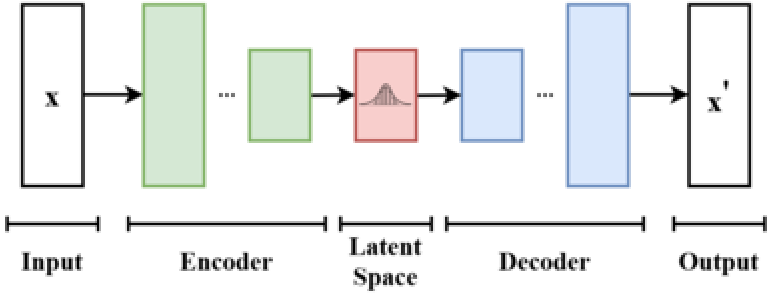
**Output layer**: tensor (often vector) of observables or probabilities

# Latent space



Implicitly learned representation
- Other methods: require features
- NN: implicitly find one at the cost of complexity and data

Use cases
- Generate more similar systems / elements of similar properties



# Common types of networks



**Graph neural network (GNN):** Input is a graph

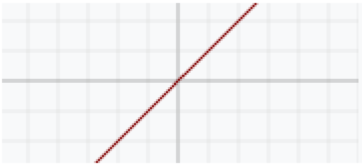
**Convolutional neural network (CNN):** Uses at least one convolution, often for image-like data

**Autoencoder:** small layer somewhere in the network (everything before: encoder, everything after: decoder)

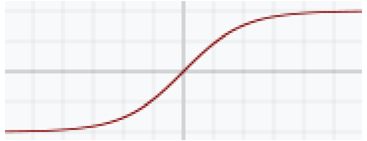
# Common types of activation functions



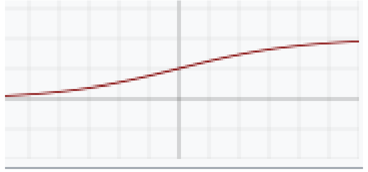
Step



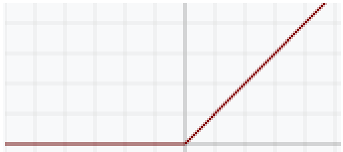
Tanh



Logistic



Rectified Linear Unit (ReLU)



**Vanishing gradient**
Is the function almost constant anywhere?

**Cost**
Can be evaluated quickly?

**Normalisation**
Is there a finite output domain?

**Differentiable**
Otherwise hard to optimize

# **Summary** Neural networks



- Chained, heavily parametrized functions
- Applied in order („layers“)
- Implictly find a representation
- Somewhat intransparent
- Need to be trained iteratively