Multi-layer Perceptrons (MLPs)

Multi-layer Perceptrons

An **r-layer perceptron** is a neural network with a graph $G = (U, C)$ that satisfies the following conditions:

(i) $U_{\text{in}} \cap U_{\text{out}} = \emptyset$,

(ii) $U_{\text{hidden}} = U_{\text{hidden}}^{(1)} \cup \cdots \cup U_{\text{hidden}}^{(r-2)}$,

$\forall 1 \leq i < j \leq r-2: \quad U_{\text{hidden}}^{(i)} \cap U_{\text{hidden}}^{(j)} = \emptyset$,

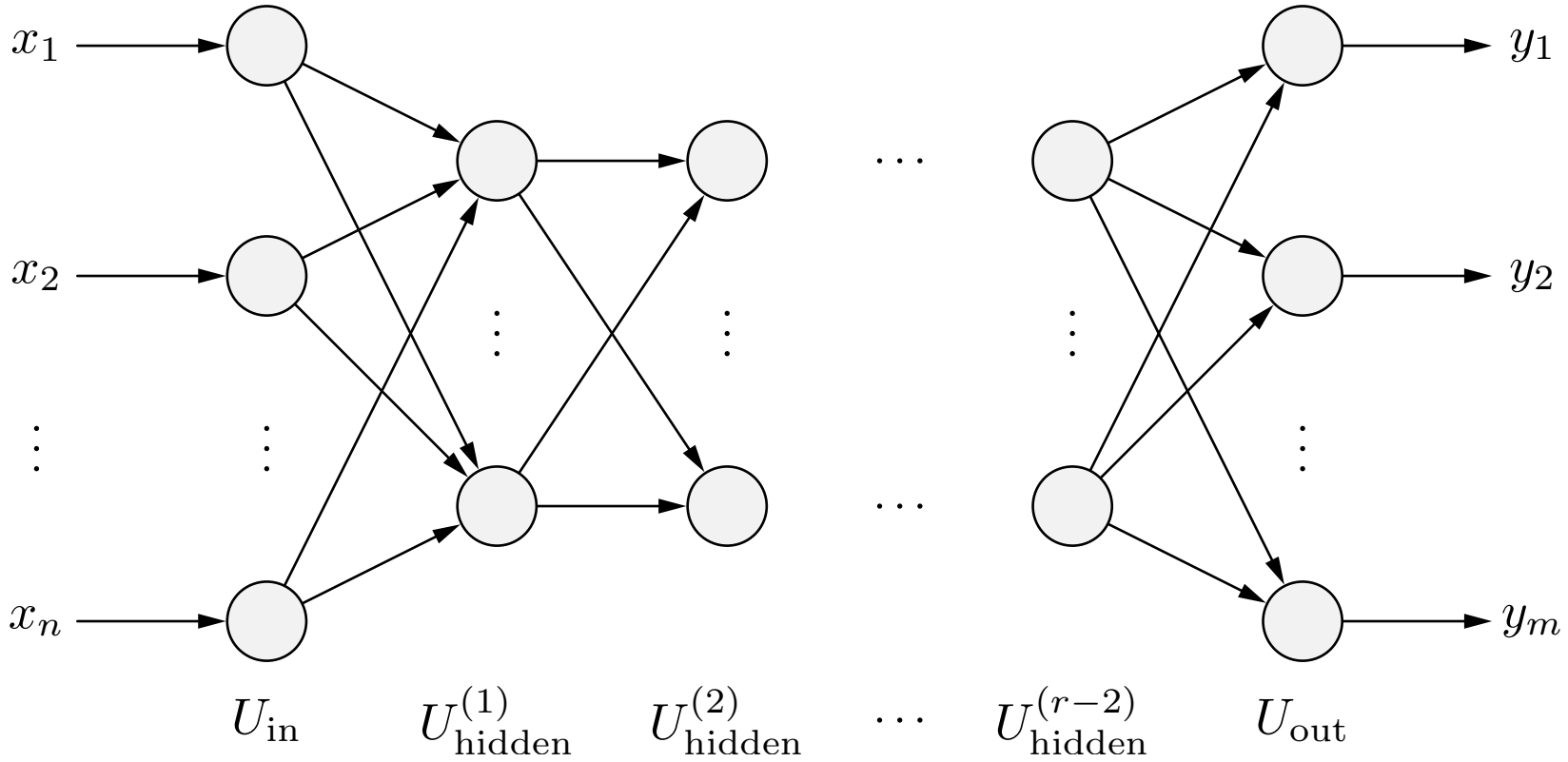
(iii) $C \subseteq \left(U_{\text{in}} \times U_{\text{hidden}}^{(1)}\right) \cup \left(\bigcup_{i=1}^{r-3} U_{\text{hidden}}^{(i)} \times U_{\text{hidden}}^{(i+1)}\right) \cup \left(U_{\text{hidden}}^{(r-2)} \times U_{\text{out}}\right)$

or, if there are no hidden neurons ($r = 2, U_{\text{hidden}} = \emptyset$),

$C \subseteq U_{\text{in}} \times U_{\text{out}}$.

- Feed-forward network with strictly layered structure.

General structure of a multi-layer perceptron



Multi-layer Perceptrons

- The network input function of each hidden neuron and of each output neuron is the **weighted sum** of its inputs, that is,

$$\forall u \in U_{\text{hidden}} \cup U_{\text{out}}: \qquad f_{\text{net}}^{(u)}(\vec{w}_u, \vec{\text{in}}_u) = \vec{w}_u^\top \vec{\text{in}}_u = \sum_{v \in \text{pred}(u)} w_{uv}\, \text{out}_v\,.$$

- The activation function of each hidden neuron is a so-called **sigmoid function**, that is, a monotonically increasing function

$$f : \mathbb{R} \to [0,1] \quad \text{with} \quad \lim_{x \to -\infty} f(x) = 0 \quad \text{and} \quad \lim_{x \to \infty} f(x) = 1.$$

- The activation function of each output neuron is either also a sigmoid function or a **linear function**, that is,

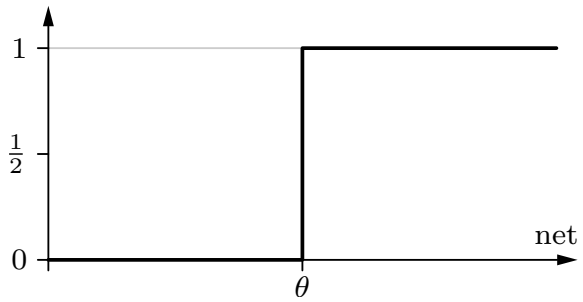
$$f_{\text{act}}(\text{net}, \theta) = \alpha\, \text{net} - \theta.$$

Only the step function is a neurobiologically plausible activation function.

Sigmoid Activation Functions

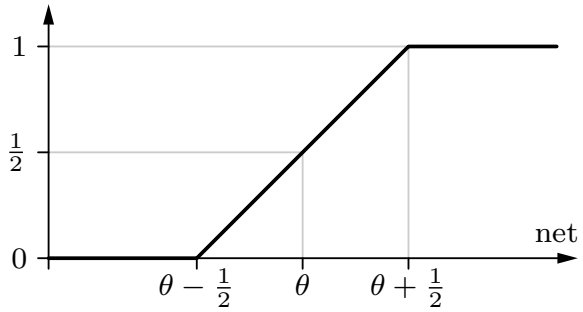
step function:

$$f_{\text{act}}(\text{net}, \theta) = \begin{cases} 1, & \text{if net} \geq \theta, \\ 0, & \text{otherwise.} \end{cases}$$



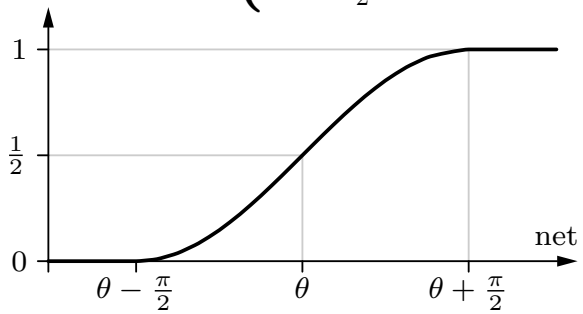
semi-linear function:

$$f_{\text{act}}(\text{net}, \theta) = \begin{cases} 1, & \text{if net} > \theta + \frac{1}{2}, \\ 0, & \text{if net} < \theta - \frac{1}{2}, \\ (\text{net} - \theta) + \frac{1}{2}, & \text{otherwise.} \end{cases}$$



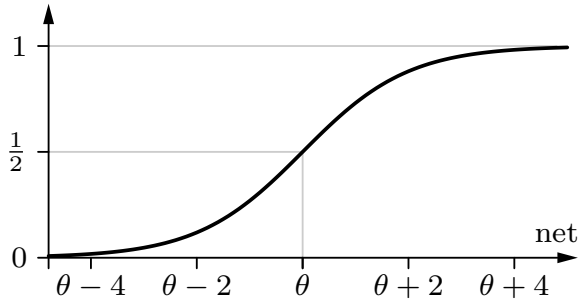
sine until saturation:

$$f_{\text{act}}(\text{net}, \theta) = \begin{cases} 1, & \text{if net} > \theta + \frac{\pi}{2}, \\ 0, & \text{if net} < \theta - \frac{\pi}{2}, \\ \frac{\sin(\text{net} - \theta) + 1}{2}, & \text{otherwise.} \end{cases}$$



logistic function:

$$f_{\text{act}}(\text{net}, \theta) = \frac{1}{1 + e^{-(\text{net} - \theta)}}$$

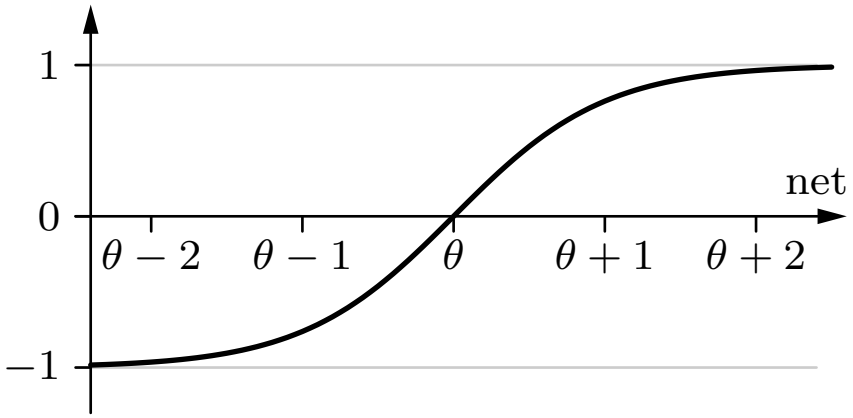


Sigmoid Activation Functions

- All sigmoid functions on the previous slide are **unipolar**, that is, they range from 0 to 1.
- Sometimes **bipolar** sigmoid functions are used (ranging from -1 to $+1$), like the hyperbolic tangent (*tangens hyperbolicus*).

hyperbolic tangent:

$$
\begin{aligned}
f_{\text{act}}(\text{net}, \theta) &= \tanh(\text{net} - \theta) \\
&= \frac{e^{(\text{net}-\theta)} - e^{-(\text{net}-\theta)}}{e^{(\text{net}-\theta)} + e^{-(\text{net}-\theta)}} \\
&= \frac{1 - e^{-2(\text{net}-\theta)}}{1 + e^{-2(\text{net}-\theta)}} \\
&= \frac{2}{1 + e^{-2(\text{net}-\theta)}} - 1
\end{aligned}
$$



Multi-layer Perceptrons: Weight Matrices

Let $U_1 = \{v_1, \ldots, v_m\}$ and $U_2 = \{u_1, \ldots, u_n\}$ be the neurons of two consecutive layers of a multi-layer perceptron.

Their connection weights are represented by an $n \times m$ matrix

$$\mathbf{W} = \begin{pmatrix} w_{u_1 v_1} & w_{u_1 v_2} & \ldots & w_{u_1 v_m} \\ w_{u_2 v_1} & w_{u_2 v_2} & \ldots & w_{u_2 v_m} \\ \vdots & \vdots & & \vdots \\ w_{u_n v_1} & w_{u_n v_2} & \ldots & w_{u_n v_m} \end{pmatrix},$$

where $w_{u_i v_j} = 0$ if there is no connection from neuron v_j to neuron u_i.

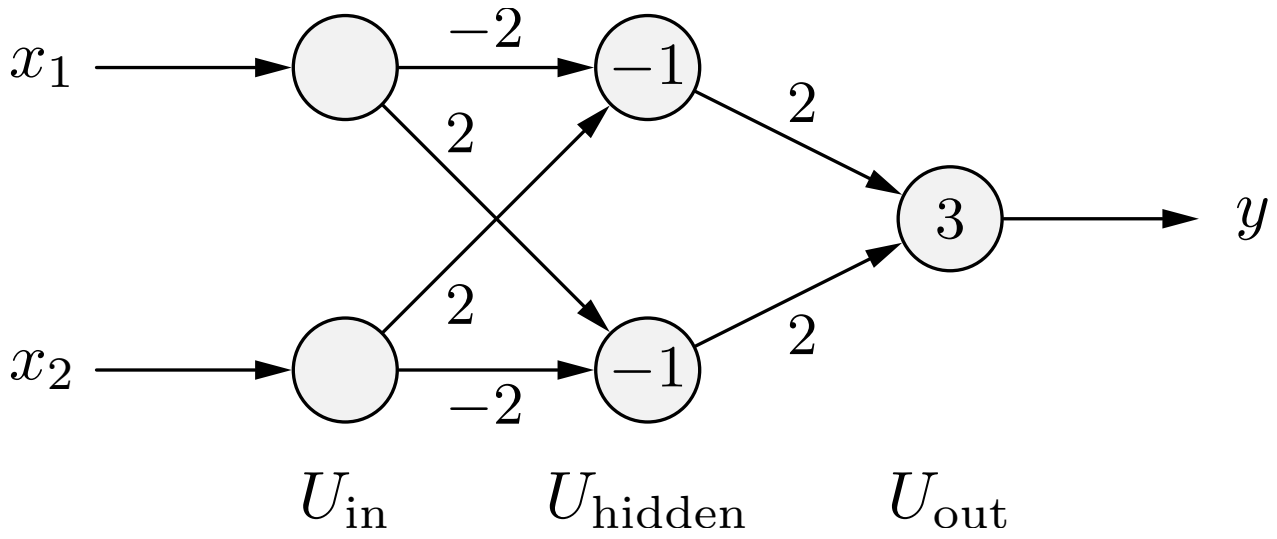
Advantage: The computation of the network input can be written as

$$\vec{\text{net}}_{U_2} = \mathbf{W} \cdot \vec{\text{in}}_{U_2} = \mathbf{W} \cdot \vec{\text{out}}_{U_1}$$

where $\vec{\text{net}}_{U_2} = (\text{net}_{u_1}, \ldots, \text{net}_{u_n})^\top$ and $\vec{\text{in}}_{U_2} = \vec{\text{out}}_{U_1} = (\text{out}_{v_1}, \ldots, \text{out}_{v_m})^\top$.

Multi-layer Perceptrons: Biimplication

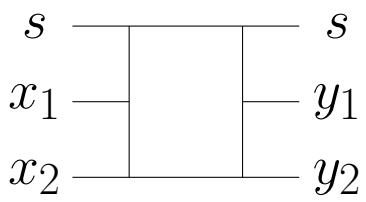
Solving the biimplication problem with a multi-layer perceptron.

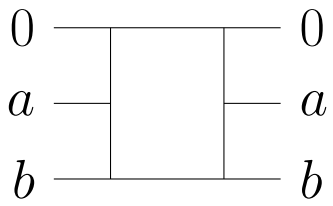


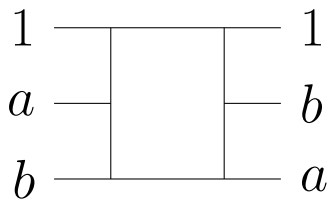
Note the additional input neurons compared to the TLU solution.

$$\mathbf{W}_1 = \begin{pmatrix} -2 & 2 \\ 2 & -2 \end{pmatrix} \quad \text{and} \quad \mathbf{W}_2 = \begin{pmatrix} 2 & 2 \end{pmatrix}$$

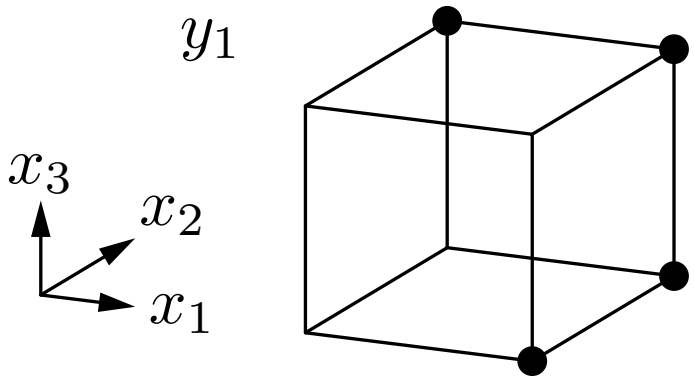
Multi-layer Perceptrons: Fredkin Gate

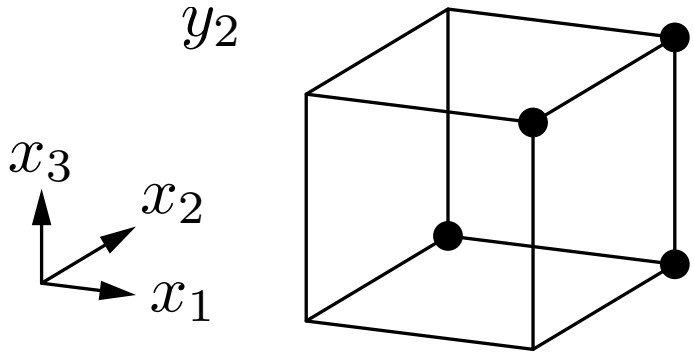






s	0	0	0	0	1	1	1	1
x_1	0	0	1	1	0	0	1	1
x_2	0	1	0	1	0	1	0	1
y_1	0	0	1	1	0	1	0	1
y_2	0	1	0	1	0	0	1	1





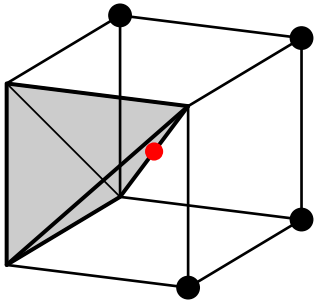
Multi-layer Perceptrons: Fredkin Gate

- The **Fredkin gate** (after Edward Fredkin *1934) or **controlled swap gate** (CSWAP) is a computational circuit that is used in **conservative logic** and **reversible computing**.
- Conservative logic is a model of computation that explicitly reflects the physical properties of computation, like the reversibility of the dynamical laws and the conservation of certain quantities (e.g. energy) [Fredkin and Toffoli 1982].
- The Fredkin gate is **reversible** in the sense that the inputs can be computed as functions of the outputs in the same way in which the outputs can be computed as functions of the inputs (no information loss, no entropy gain).
- The Fredkin gate is **universal** in the sense that all Boolean functions can be computed using only Fredkin gates.
- Note that both outputs, y_1 and y_2 are **not linearly separable**, because the convex hull of the points mapped to 0 and the convex hull of the points mapped to 1 share the point in the center of the cube.

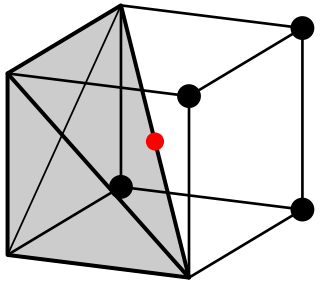
Reminder: Convex Hull Theorem

Theorem: Two sets of points in a Euclidean space are **linearly separable** if and only if their convex hulls are disjoint (that is, have no point in common).

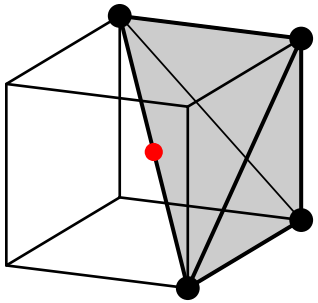
Both outputs y_1 and y_2 of a Fredkin gate are not linearly separable:



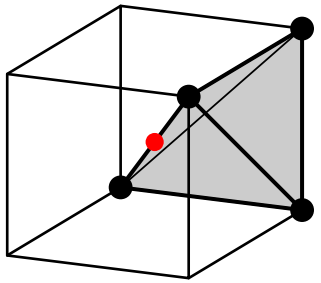
Convex hull of points with $y_1 = 0$



Convex hull of points with $y_2 = 0$



Convex hull of points with $y_1 = 1$

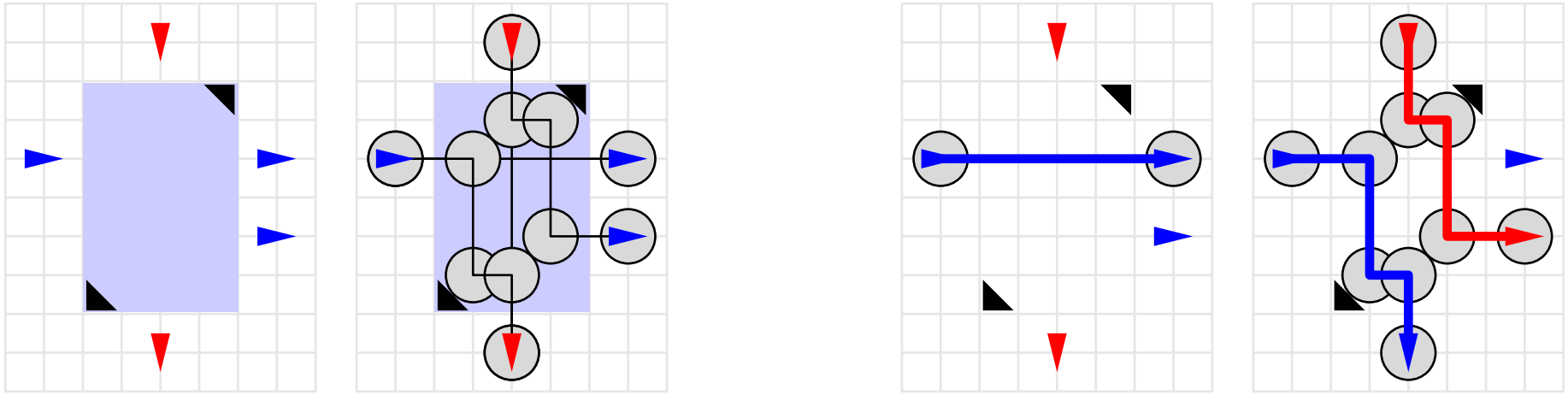


Convex hull of points with $y_2 = 1$

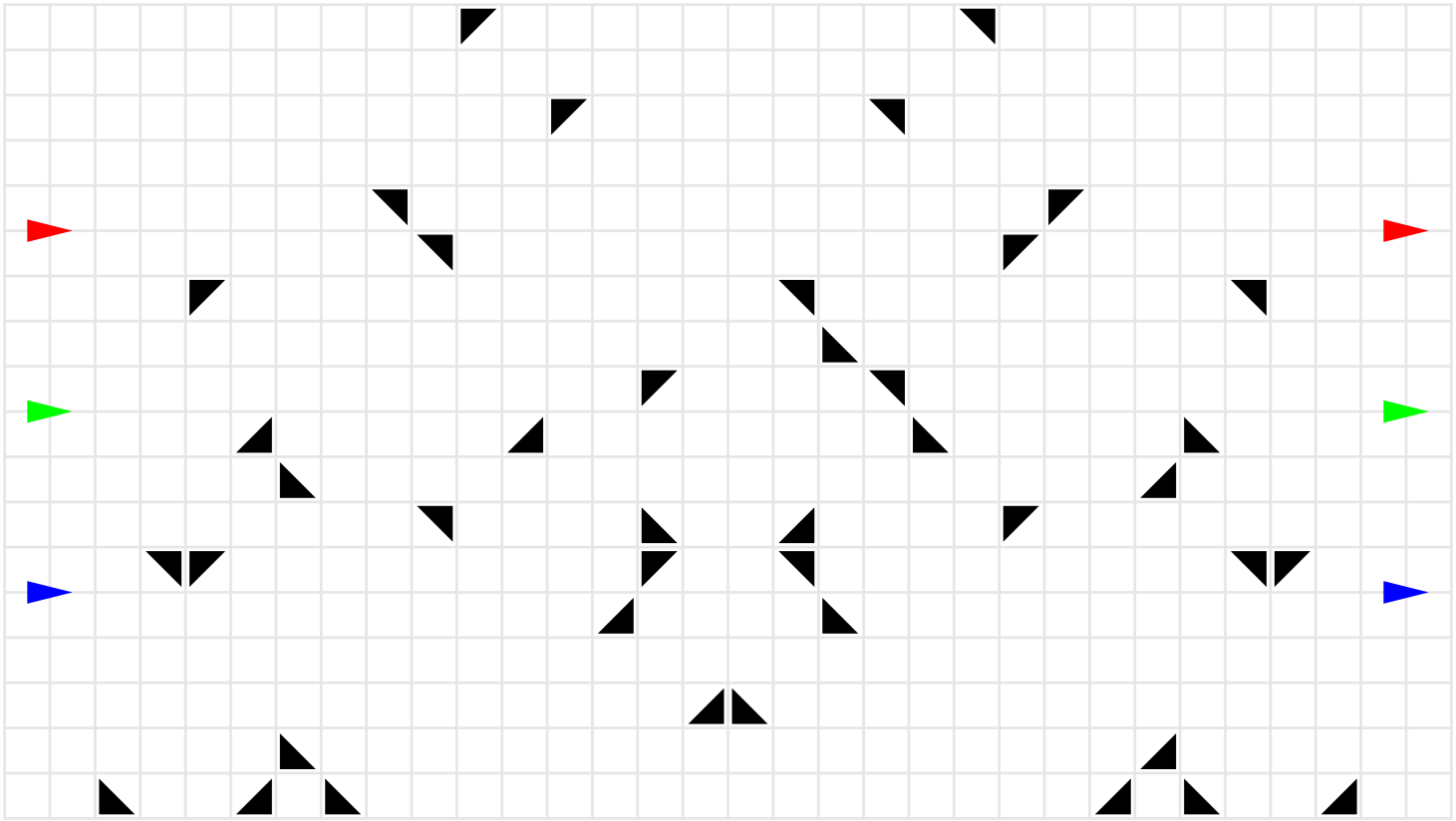
Excursion: Billiard Ball Computer

- A **billiard-ball computer** (a.k.a. **conservative logic circuit**) is an idealized model of a reversible mechanical computer that simulates the computations of circuits by the movements of spherical billiard balls in a frictionless environment [Fredkin and Toffoli 1982].

Switch (control output location of an input ball by another ball;
equivalent to an AND gate in its second/lower output):

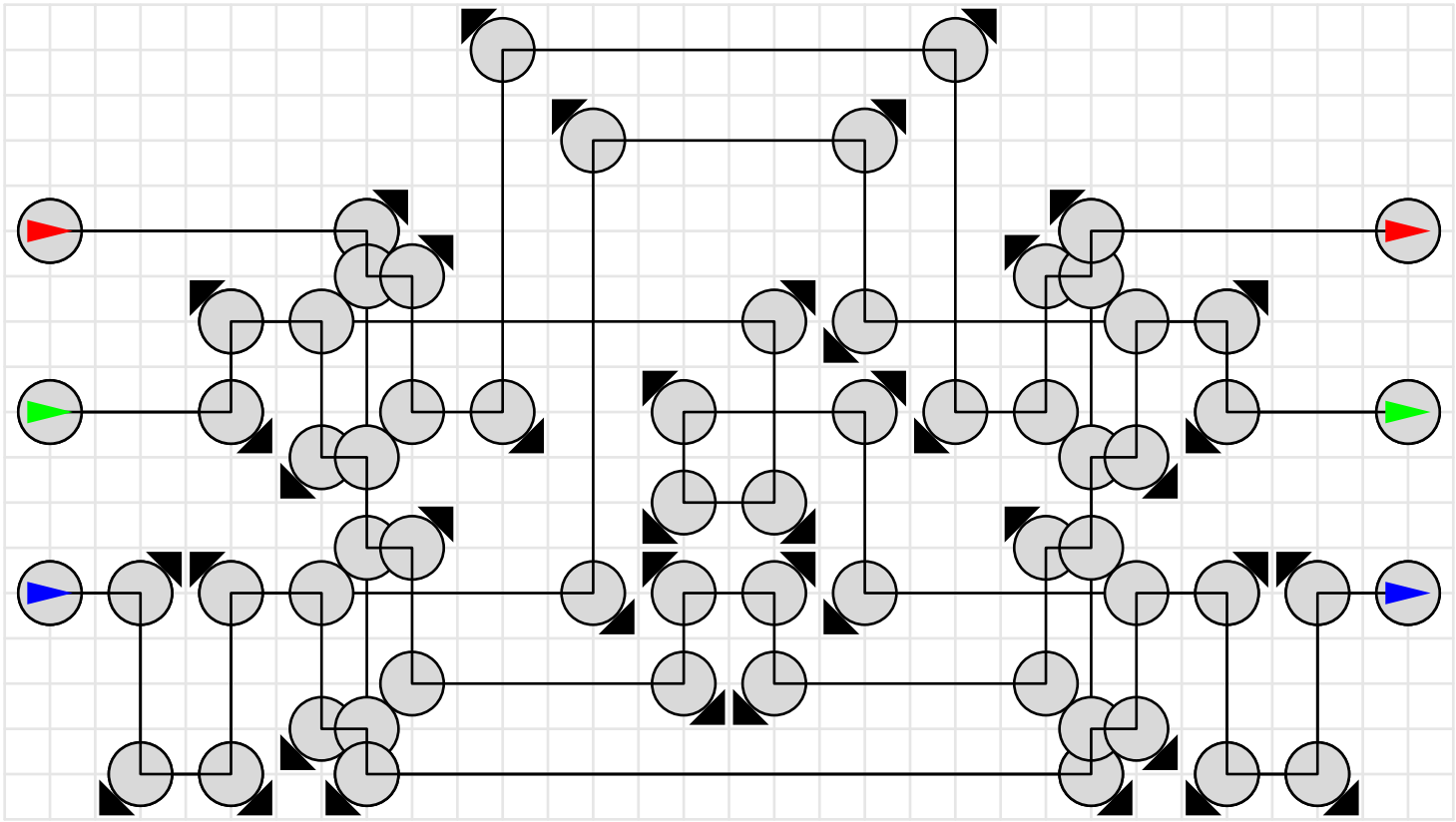


Excursion: The (Negated) Fredkin Gate



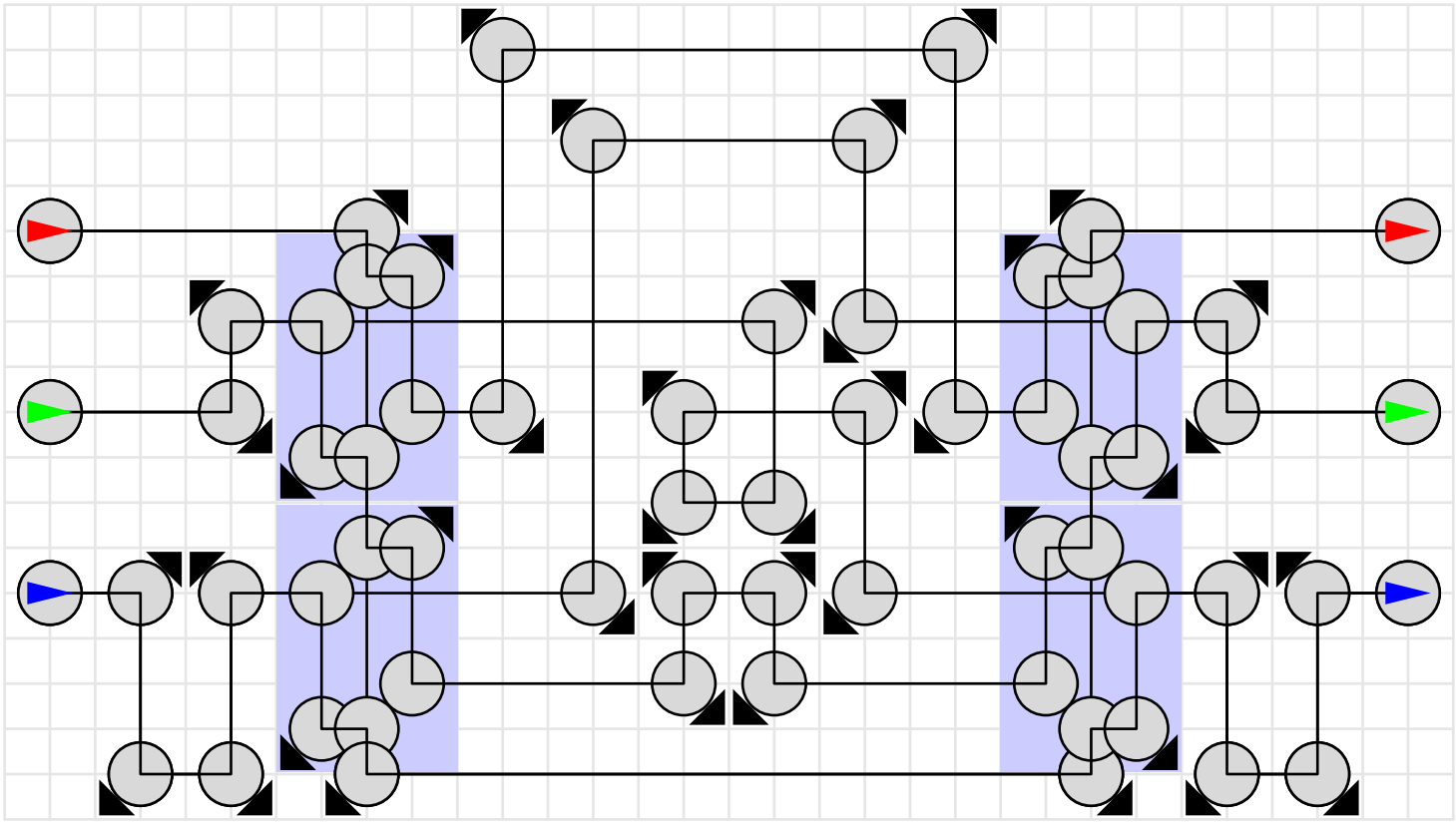
- Only reflectors (black) and inputs/outputs (color) shown.
- Meaning of switch variable is negated compared to value table on previous slide: 0 switches inputs, 1 passes them through.

Excursion: The (Negated) Fredkin Gate



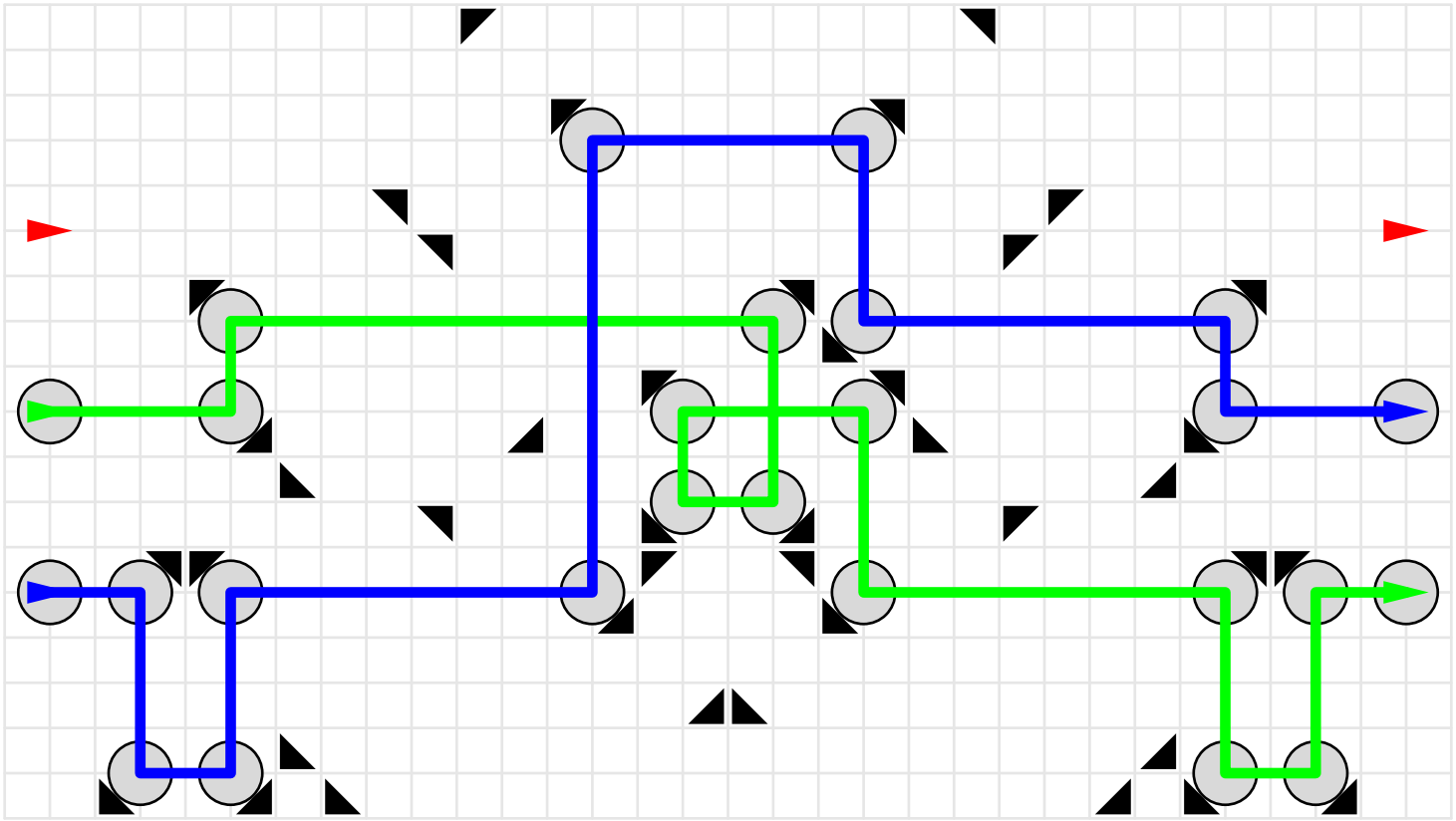
- All possible paths of billiard-balls through this gate are shown.
  Inputs/outputs are in color; red: switch, green: x_1/y_1, blue: x_2/y_2.
- Billiard-balls are shown in places where their trajectories may change direction.

Excursion: The (Negated) Fredkin Gate



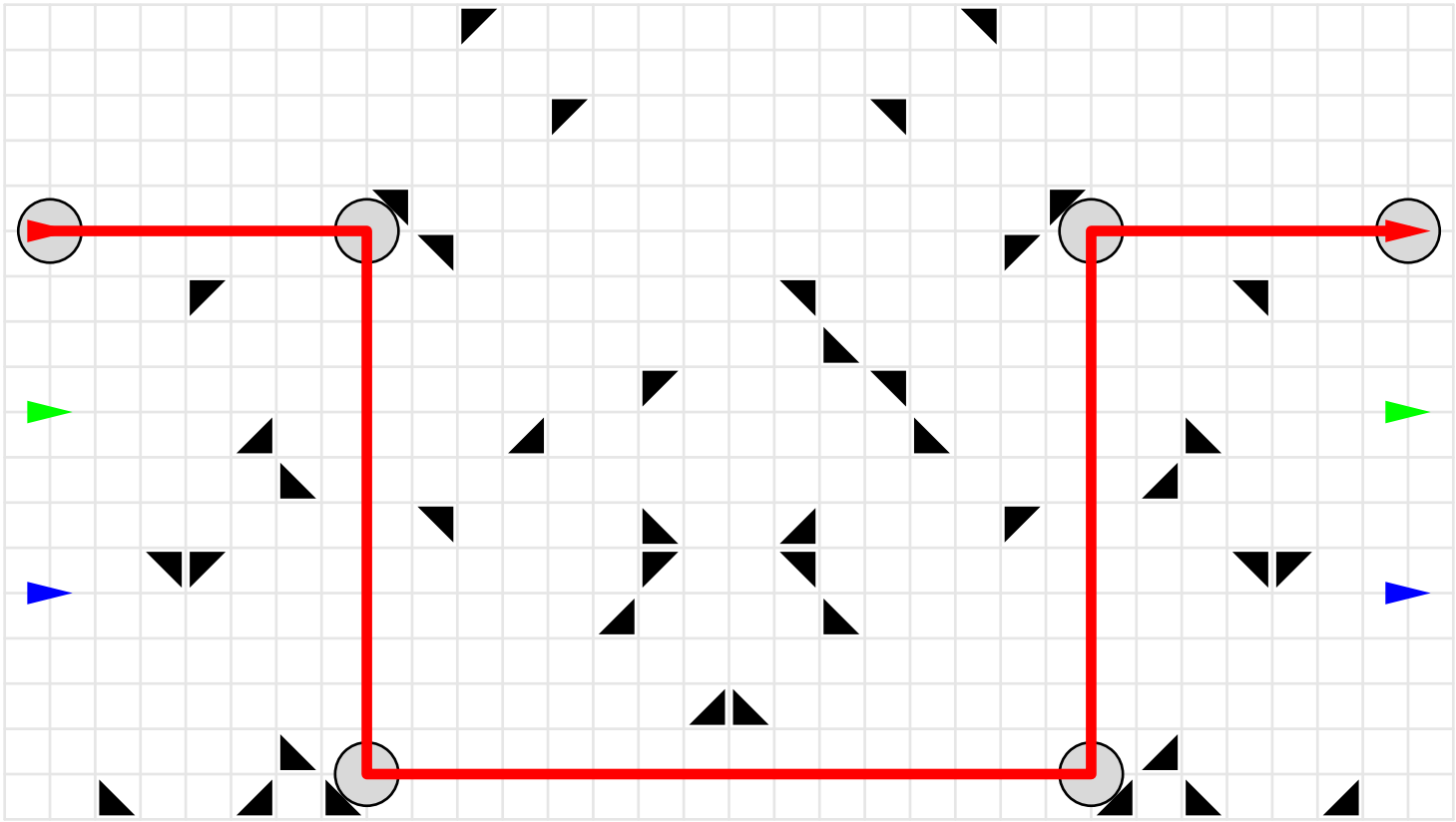
- This Fredkin gate implementation contains four switches (shown in light blue).
- The other parts serve the purpose to equate the travel times of the balls through the gate.

Excursion: The (Negated) Fredkin Gate



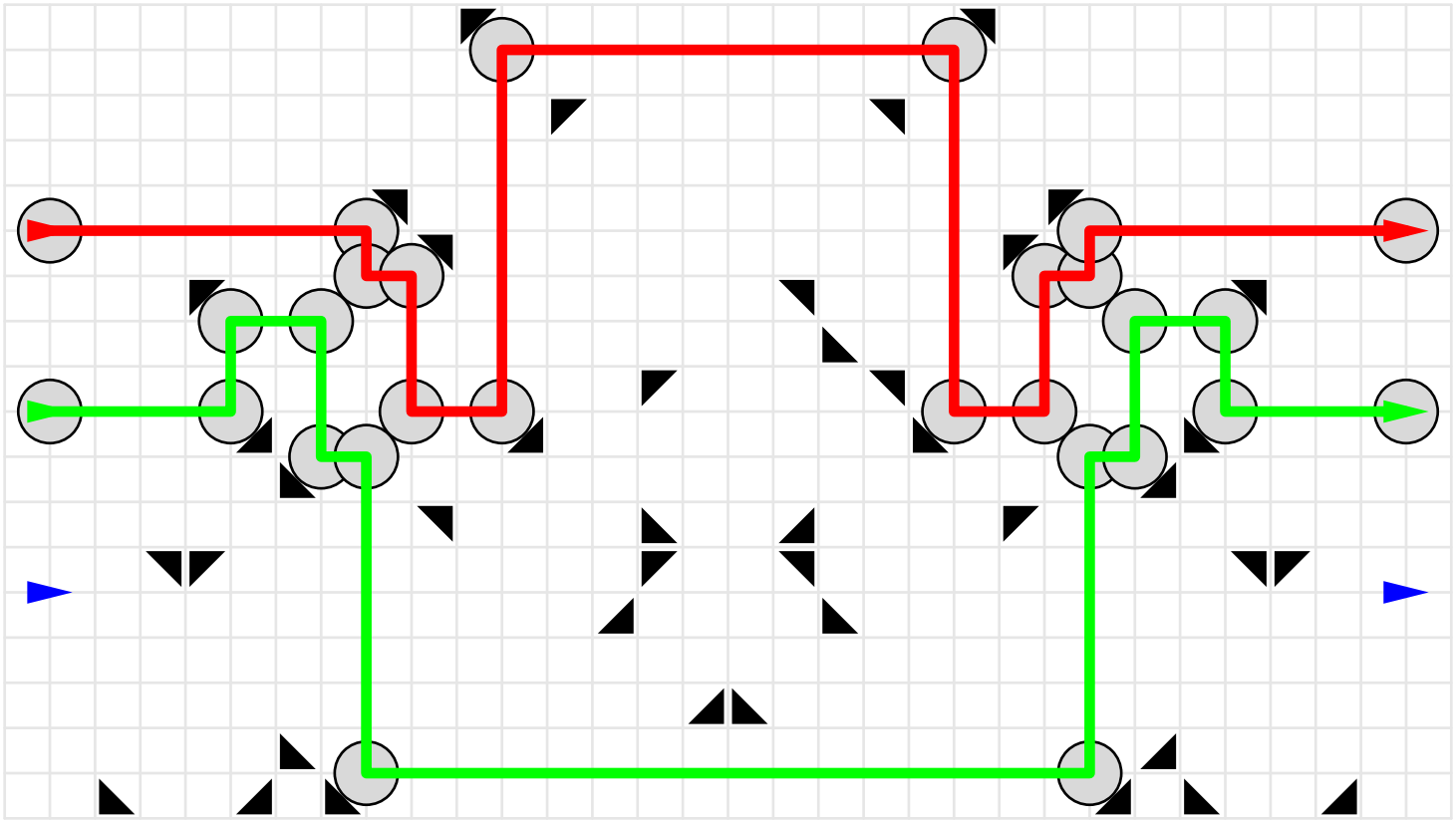
- Reminder: in this implementation the meaning of the switch variable is negated.
- Switch is zero (no ball enters at red arrow):
  blue and green balls switch to the other output.

Excursion: The (Negated) Fredkin Gate



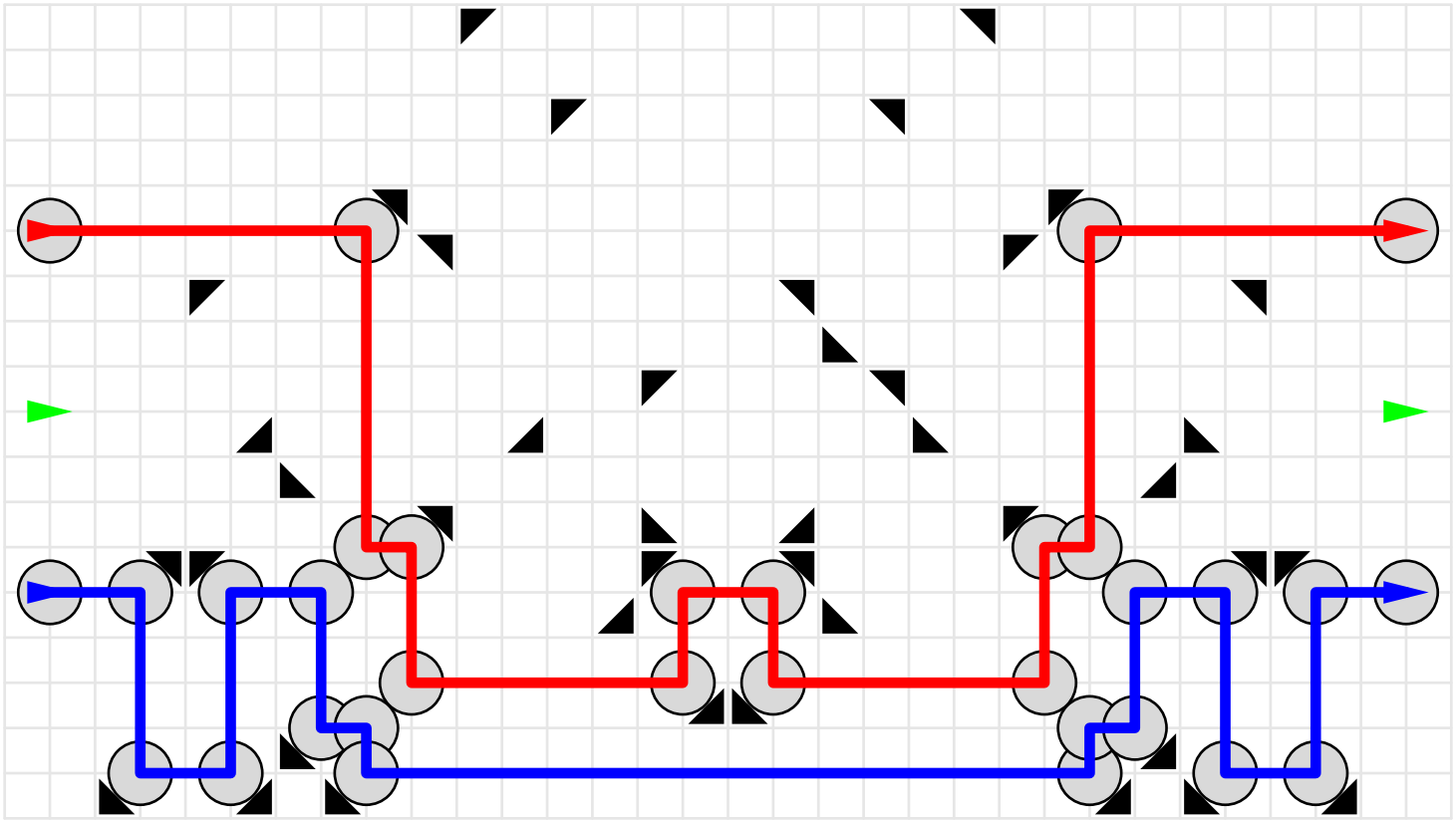
- If a ball is entered at the switch input, it is passed through.
- Since there are no other inputs, the other outputs remain 0 (no ball in, no ball out).

Excursion: The (Negated) Fredkin Gate



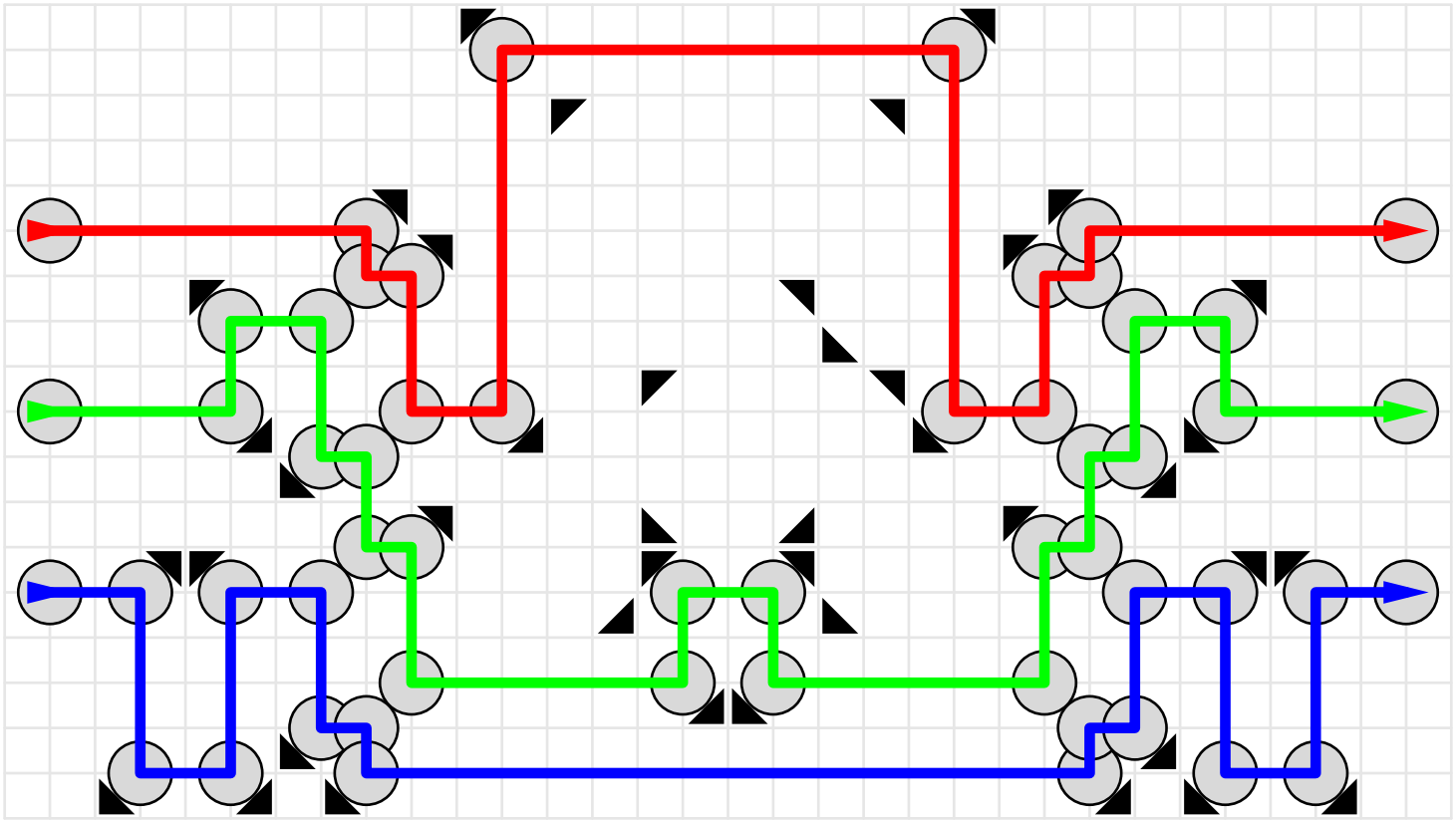
- A ball is entered at the switch input and passed through.
- A ball entered at the first input x_1 is also passed through to output y_1. (Note the symmetry of the trajectories.)

Excursion: The (Negated) Fredkin Gate



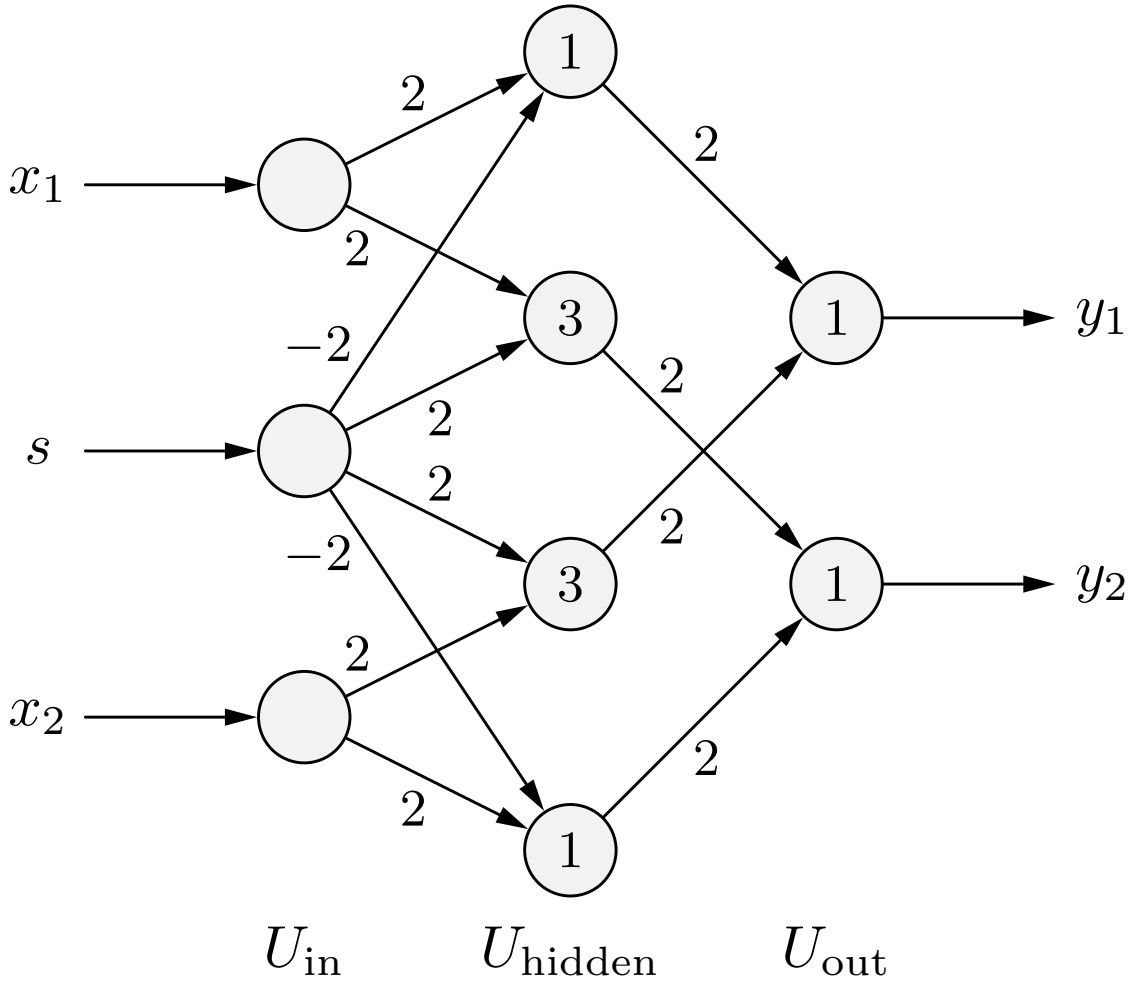
- A ball is entered at the switch input and passed through.
- A ball entered at the second input x_2 is also passed through to output y_2. (Note the symmetry of the trajectories.)

Excursion: The (Negated) Fredkin Gate



- A ball is entered at the switch input and passed through.
- Ball entered at both inputs x_1 and x_2 and are also passed through to the outputs y_1 and y_2. (Note the symmetry of the trajectories.)

Multi-layer Perceptrons: Fredkin Gate



$$\mathbf{W}_1 = \begin{pmatrix} 2 & -2 & 0 \\ 2 & 2 & 0 \\ 0 & 2 & 2 \\ 0 & -2 & 2 \end{pmatrix}$$

$$\mathbf{W}_2 = \begin{pmatrix} 2 & 0 & 2 & 0 \\ 0 & 2 & 0 & 2 \end{pmatrix}$$

Why Non-linear Activation Functions?

With weight matrices we have for two consecutive layers U_1 and U_2

$$\vec{\text{net}}_{U_2} = \mathbf{W} \cdot \vec{\text{in}}_{U_2} = \mathbf{W} \cdot \vec{\text{out}}_{U_1}.$$

If the activation functions are linear, that is,

$$f_{\text{act}}(\text{net}, \theta) = \alpha \, \text{net} - \theta.$$

the activations of the neurons in the layer U_2 can be computed as

$$\vec{\text{act}}_{U_2} = \mathbf{D}_{\text{act}} \cdot \vec{\text{net}}_{U_2} - \vec{\theta},$$

where

- $\vec{\text{act}}_{U_2} = (\text{act}_{u_1}, \ldots, \text{act}_{u_n})^\top$ is the activation vector,
- $\mathbf{D}_{\text{act}}$ is an $n \times n$ diagonal matrix of the factors α_{u_i}, $i = 1, \ldots, n$, and
- $\vec{\theta} = (\theta_{u_1}, \ldots, \theta_{u_n})^\top$ is a bias vector.

Why Non-linear Activation Functions?

If the output function is also linear, it is analogously

$$\vec{\text{out}}_{U_2} = \mathbf{D}_{\text{out}} \cdot \vec{\text{act}}_{U_2} - \vec{\xi},$$

where

- $\vec{\text{out}}_{U_2} = (\text{out}_{u_1}, \ldots, \text{out}_{u_n})^\top$ is the output vector,
- $\mathbf{D}_{\text{out}}$ is again an $n \times n$ diagonal matrix of factors, and
- $\vec{\xi} = (\xi_{u_1}, \ldots, \xi_{u_n})^\top$ a bias vector.

Combining these computations we get

$$\vec{\text{out}}_{U_2} = \mathbf{D}_{\text{out}} \cdot \left(\mathbf{D}_{\text{act}} \cdot \left(\mathbf{W} \cdot \vec{\text{out}}_{U_1} \right) - \vec{\theta} \right) - \vec{\xi}$$

and thus

$$\vec{\text{out}}_{U_2} = \mathbf{A}_{12} \cdot \vec{\text{out}}_{U_1} + \vec{b}_{12}$$

with an $n \times m$ matrix $\mathbf{A}_{12}$ and an n-dimensional vector $\vec{b}_{12}$.

Why Non-linear Activation Functions?

Therefore we have

$$\vec{\text{out}}_{U_2} = \mathbf{A}_{12} \cdot \vec{\text{out}}_{U_1} + \vec{b}_{12}$$

and

$$\vec{\text{out}}_{U_3} = \mathbf{A}_{23} \cdot \vec{\text{out}}_{U_2} + \vec{b}_{23}$$

for the computations of two consecutive layers U_2 and U_3.

These two computations can be combined into

$$\vec{\text{out}}_{U_3} = \mathbf{A}_{13} \cdot \vec{\text{out}}_{U_1} + \vec{b}_{13},$$

where $\mathbf{A}_{13} = \mathbf{A}_{23} \cdot \mathbf{A}_{12}$ and $\vec{b}_{13} = \mathbf{A}_{23} \cdot \vec{b}_{12} + \vec{b}_{23}$.

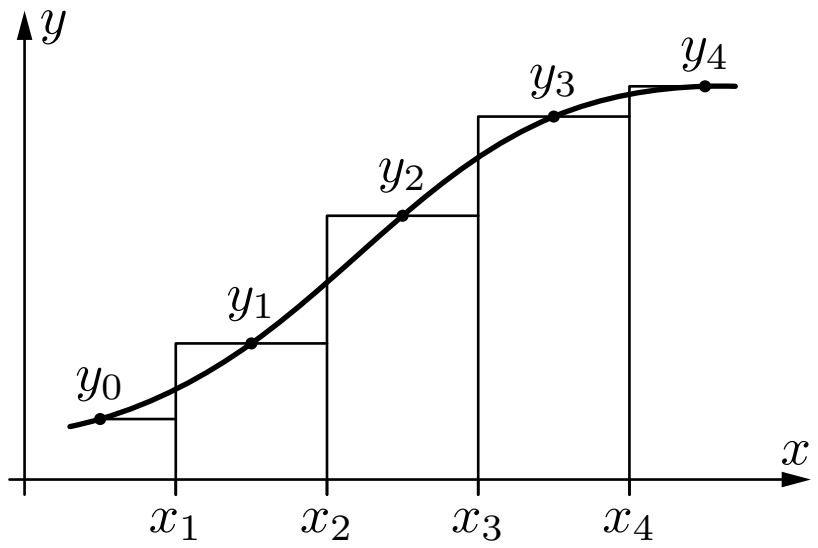
Result: With linear activation and output functions any multi-layer perceptron can be reduced to a two-layer perceptron.

Multi-layer Perceptrons: Function Approximation

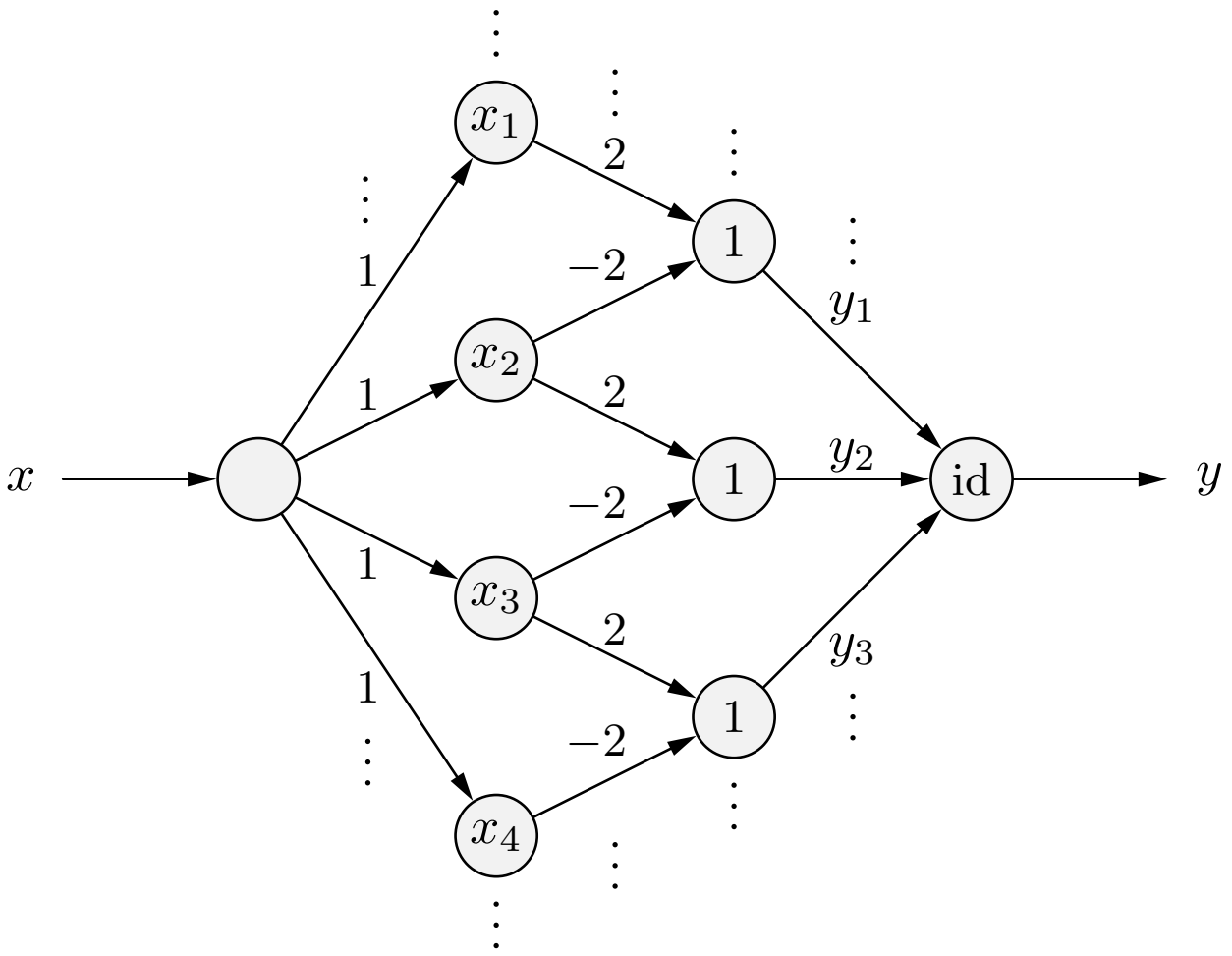
- Up to now: representing and learning Boolean functions $f : \{0,1\}^n \to \{0,1\}$.
- Now: representing and learning real-valued functions $f : \mathbb{R}^n \to \mathbb{R}$.

General idea of function approximation:

- Approximate a given function by a step function.
- Construct a neural network that computes the step function.



Multi-layer Perceptrons: Function Approximation

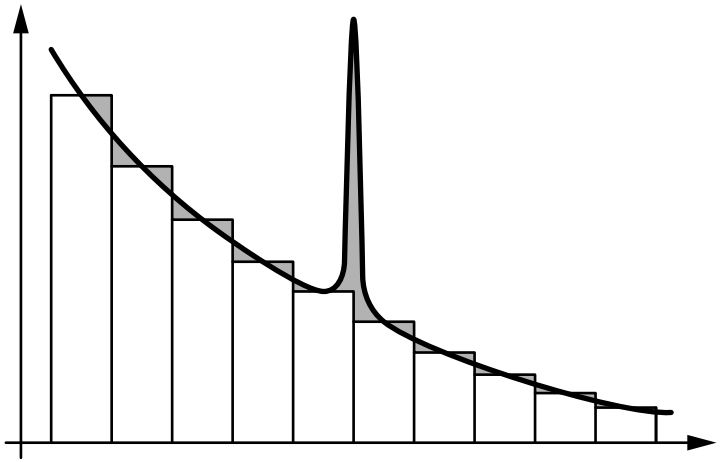


A neural network that computes the step function shown on the preceding slide.
According to the input value only one step is active at any time.
The output neuron has the identity as its activation and output functions.

Multi-layer Perceptrons: Function Approximation

Theorem: Any Riemann-integrable function can be approximated with arbitrary accuracy by a four-layer perceptron.

- But: Error is measured as the **area** between the functions.



- More sophisticated mathematical examination allows a stronger assertion: With a three-layer perceptron any continuous function can be approximated with arbitrary accuracy (error: maximum function value difference).

Multi-layer Perceptrons as Universal Approximators

Universal Approximation Theorem [Hornik 1991]:

Let $\varphi(\cdot)$ be a continuous, bounded and nonconstant function,
let X denote an arbitrary compact subset of $\mathbb{R}^m$, and
let $C(X)$ denote the space of continuous functions on X.

Given any function $f \in C(X)$ and $\varepsilon > 0$, there exists an integer N, real constants $v_i, \theta_i \in \mathbb{R}$ and real vectors $\vec{w}_i \in \mathbb{R}^m$, $i = 1, \ldots, N$, such that we may define

$$F(\vec{x}) = \sum_{i=1}^{N} v_i \, \varphi\Big(\vec{w}_i^{\top} \vec{x} - \theta_i\Big)$$

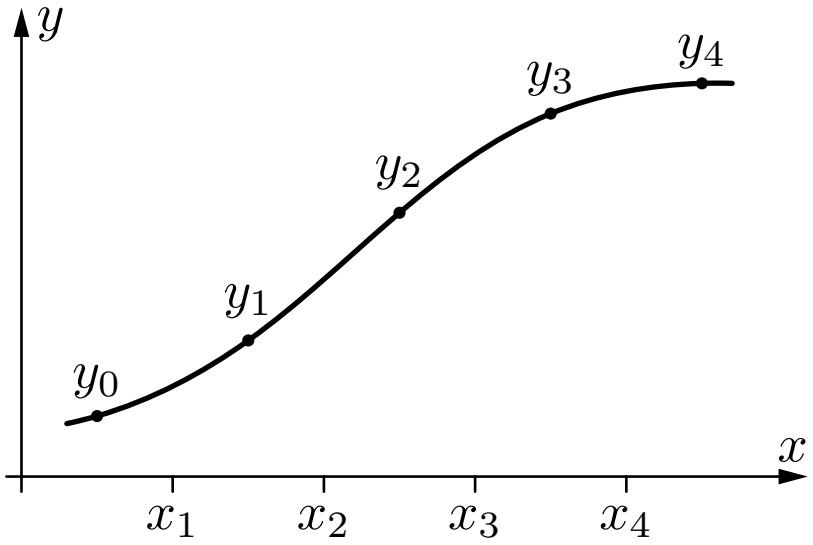
as an approximate realization of the function f where f is independent of φ. That is,

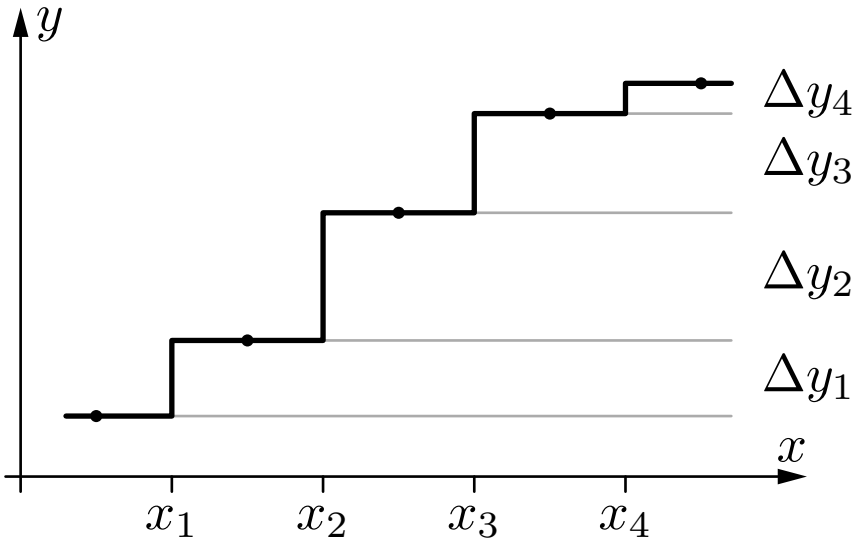
$$|F(\vec{x}) - f(\vec{x})| < \varepsilon$$

for all $\vec{x} \in X$. In other words, functions of the form $F(\vec{x})$ are dense in $C(X)$.

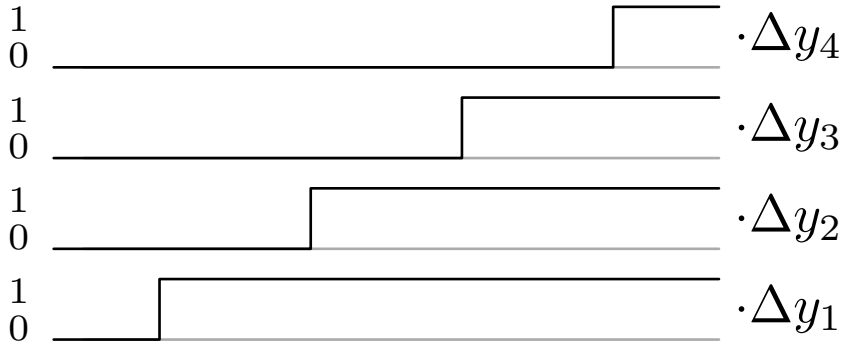
Note that it is *not* the shape of the activation function, but the layered structure of the feedforward network that renders multi-layer perceptrons universal approximators.

Multi-layer Perceptrons: Function Approximation

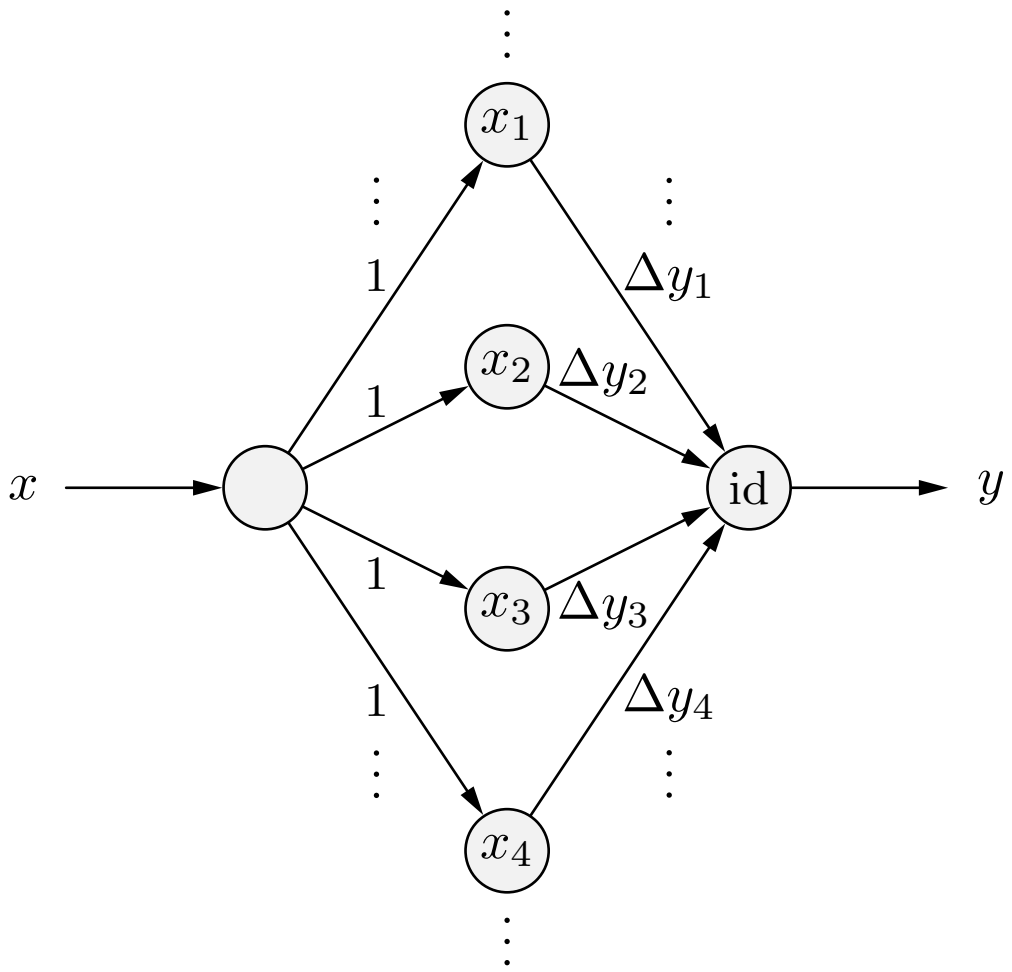




By using relative step heights one layer can be saved.

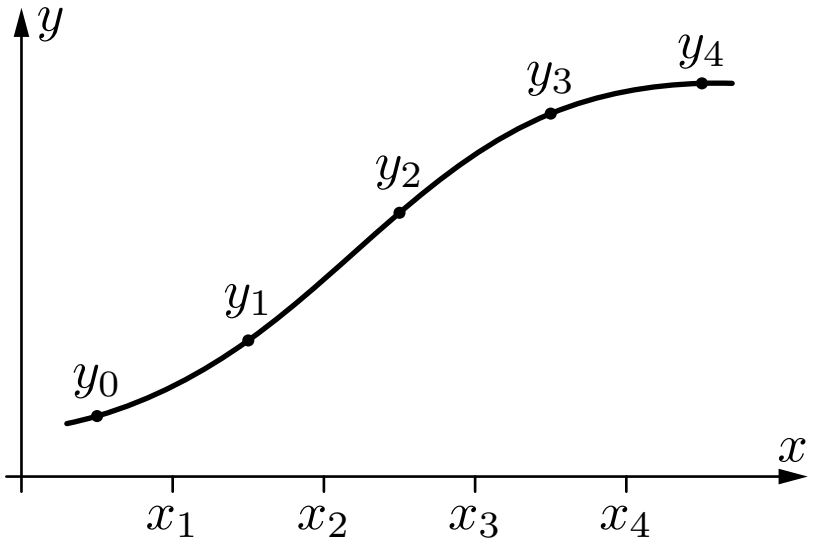


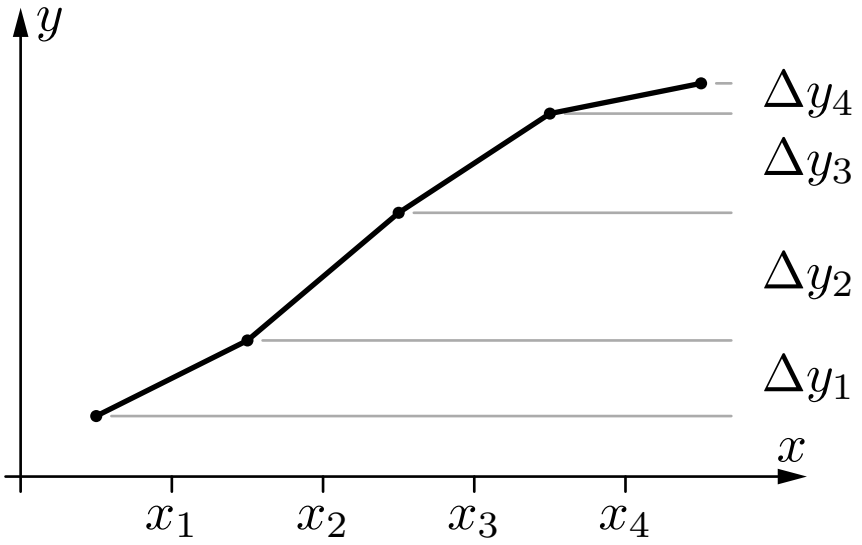
Multi-layer Perceptrons: Function Approximation



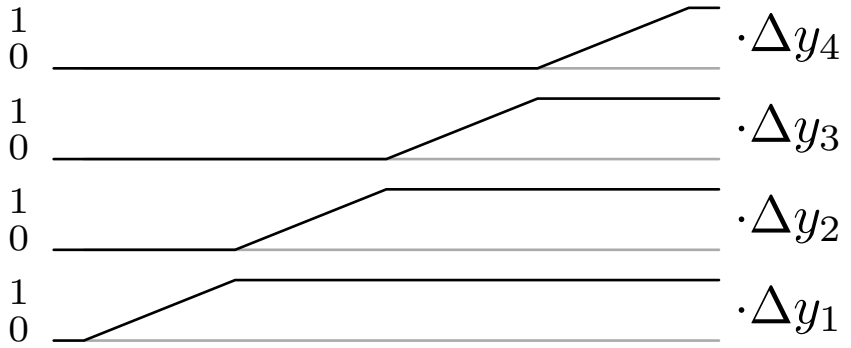
A neural network that computes the step function shown on the preceding slide. The output neuron has the identity as its activation and output functions.

Multi-layer Perceptrons: Function Approximation

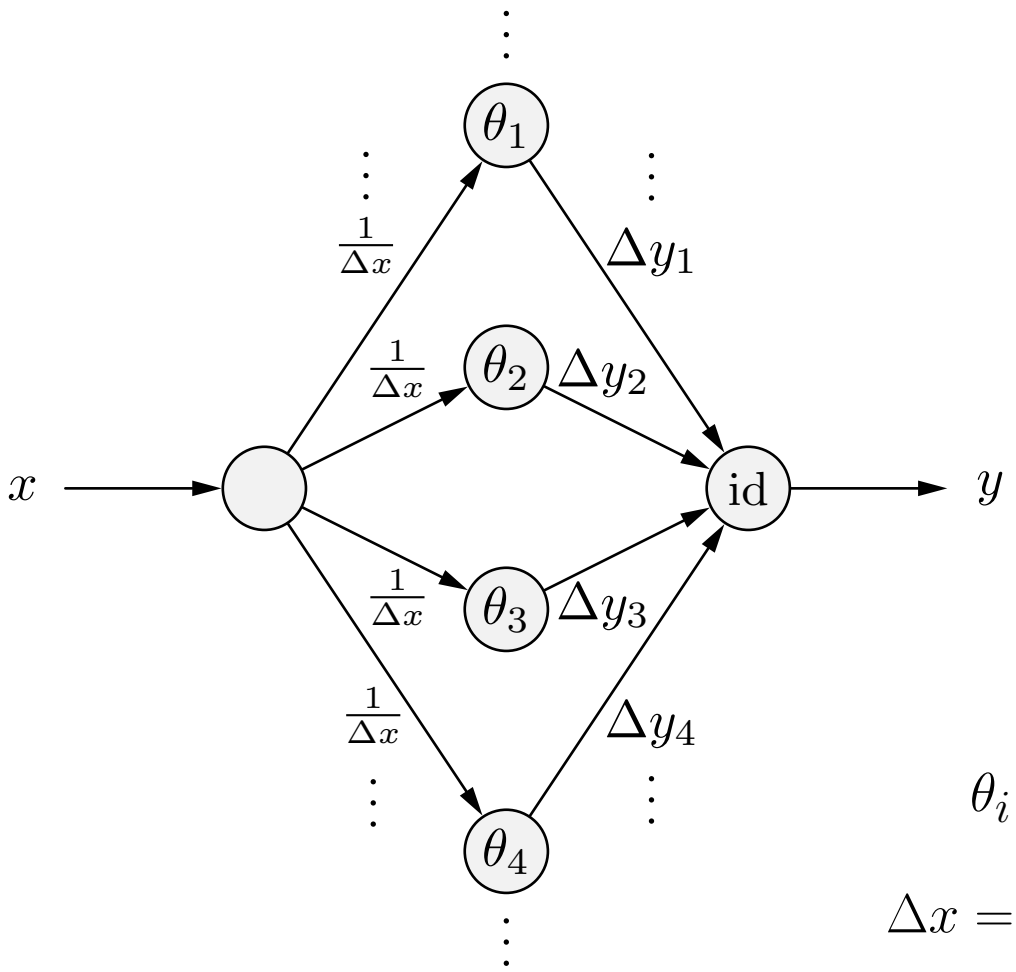




By using semi-linear functions the approximation can be improved.



Multi-layer Perceptrons: Function Approximation



$$\theta_i = \frac{x_i}{\Delta x}$$

$$\Delta x = x_{i+1} - x_i$$

A neural network that computes the step function shown on the preceding slide. The output neuron has the identity as its activation and output functions.