Generalizations of SAT

- Constraint programming (CP)
  - allows integer variables
  - more operators (besides $\neg, \vee, \wedge$), such as all_different($x_1, \ldots, x_k$).
- Satisfiability modulo theories (SMT)
  - other types of operators,
  - introduces bit vectors, etc.

Non linear optimization

Consider

(OPT)

$$\min f(x)$$
$$\text{s.t. } g_i(x) \leq 0, \text{ for } i=1,\dots,m$$
$$x \in \mathbb{R}^n$$

where f and g_i are functions $\mathbb{R}^n \to \mathbb{R}$, not necessarily linear.

Black-box / oracle model

f and g_i can be any functions, but we can evaluate them and their derivatives at any point $x \in \mathbb{R}^n$.

Theorem: In the absence of further assumptions, (OPT) is unsolvable.

Example: find an optimal solution x^* to

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & x \in \mathbb{R} \end{aligned}$$

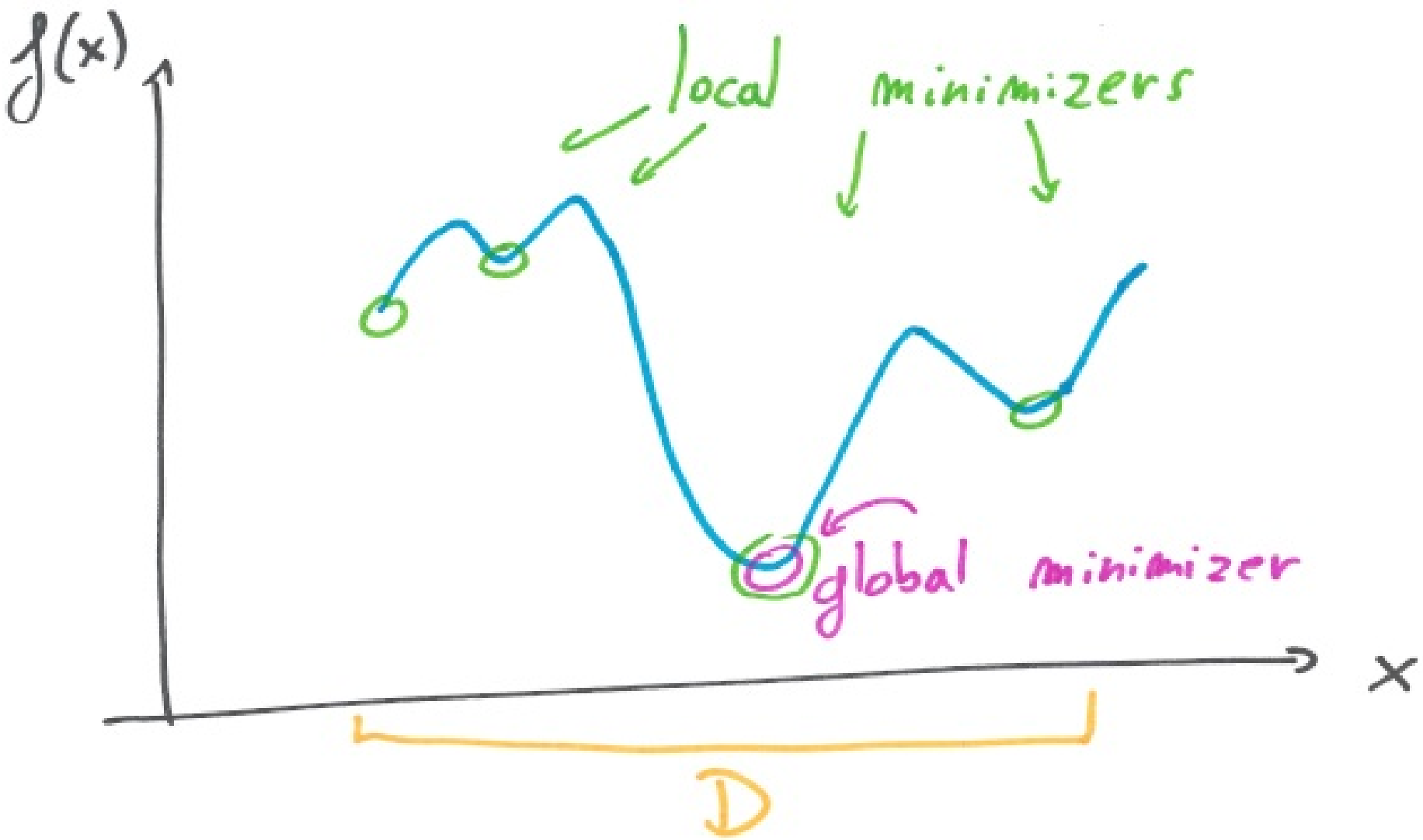
$$f(x) = \begin{cases} 0 & \text{if } x = \lambda \text{ for some } \lambda \in \mathbb{R} \\ 1 & \text{otherwise} \end{cases}$$

This problem is equivalent to "guess λ", $\lambda \in \mathbb{R}$.

Definition Consider $f: D \to \mathbb{R}$.

The point $x^* \in D$ is

- a global minimizer (optimal solution) if $f(x^*) \leq f(x)$, $\forall x \in D$.
- a local minimizer if $\exists\ \delta > 0$ $f(x^*) \leq f(x)$, $\forall x \in D : \|x - x^*\| < \delta$


f(x)
local
minimizers
global
minimizer
x
D

Definition Let $f \in \mathbb{R}^n \to \mathbb{R}$ be differentiable function. Its **gradient** $\nabla f \in \mathbb{R}^n \to \mathbb{R}^n$ is given by

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x) \end{bmatrix}$$

Example Let $f(x) = x_1^2 + 2x_2^2 - 3x_1x_2 + x_1$

Then $\nabla f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x) \\ \frac{\partial f}{\partial x_2}(x) \end{bmatrix} = \begin{bmatrix} 2x_1 - 3x_2 + 1 \\ 4x_2 - 3x_1 \end{bmatrix}$

What are the values of f and ∇f at $x = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$?

$$f\left(\begin{bmatrix} 2 \\ 1 \end{bmatrix}\right) = 2^2 + 2.1^2 - 3.2.1 + 2 = 2$$

$$\nabla f\left(\begin{bmatrix} 2 \\ 1 \end{bmatrix}\right) = \begin{bmatrix} 2.2 - 3.1 + 1 \\ 4.1 - 3.2 \end{bmatrix} = \begin{bmatrix} 2 \\ -2 \end{bmatrix}$$

Assumption: f is differentiable and its derivatives are continuous.

Theorem: If $p^k \cdot \nabla f(x^k) < 0$, then there exists $\alpha^k > 0$ such that

$$f(x^k + \alpha^k p^k) < f(x^k)$$

Theorem: If $p^k = -\dfrac{\nabla f(x^k)}{\|\nabla f(x^k)\|}$, then there exists $\alpha^k > 0$ such that

$$f(x^k + \alpha^k p^k) = \min \{ f(x) : \|x - x^k\| \leq \alpha^k \}$$

Note: If x^k is a local minimizer, $\nabla f(x^k) = 0$. (But $\nabla f(x^k) = 0 \not\Rightarrow x^k$ is a local minimizer)

Note: Choosing always $p^k = -\frac{\nabla f(x^k)}{\|\nabla f(x^k)\|}$ yields "steepest descent".

⇒ Algorithm to find local minimizers for unconstrained problems.

Gradient descent

Choose any $x^0 \in \mathbb{R}^n$

for $k = 0, 1, 2, \ldots$

choose search direction $p^k \in \mathbb{R}^n$:

- $\|p^k\| = 1$, and
- $p^k \cdot \nabla f(x^k) < 0$

choose step length $\alpha^k > 0$

let $x^{k+1} = x^k + \alpha^k p^k$

Classification / labelling problem

We are given a training set:

many input vectors $x^j \in [0,1]^n$,

already labelled into k categories.

Find "good" labels to more vectors of $[0,1]^n$.

Neural network: A (trained) neural network (NN) provides a function $F(x) \in \mathbb{R}^n \to \mathbb{R}^k$, such that if $x \in [0,1]^n$ is an input vector, then the largest component

$$k' = \underset{j}{\operatorname{argmax}} \{ (F(x))_j \}$$

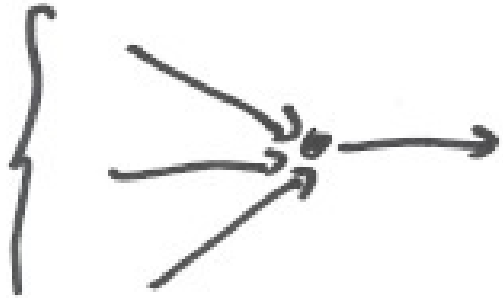
of $F(x)$ is the predicted category.

example: If $x = \begin{bmatrix} 0.3 \\ 0.5 \end{bmatrix}$ and

$F(x) = \begin{bmatrix} 0.1 \\ 0.9 \\ 0.2 \\ 0.2 \end{bmatrix}$, then the predicted category for x is 2.

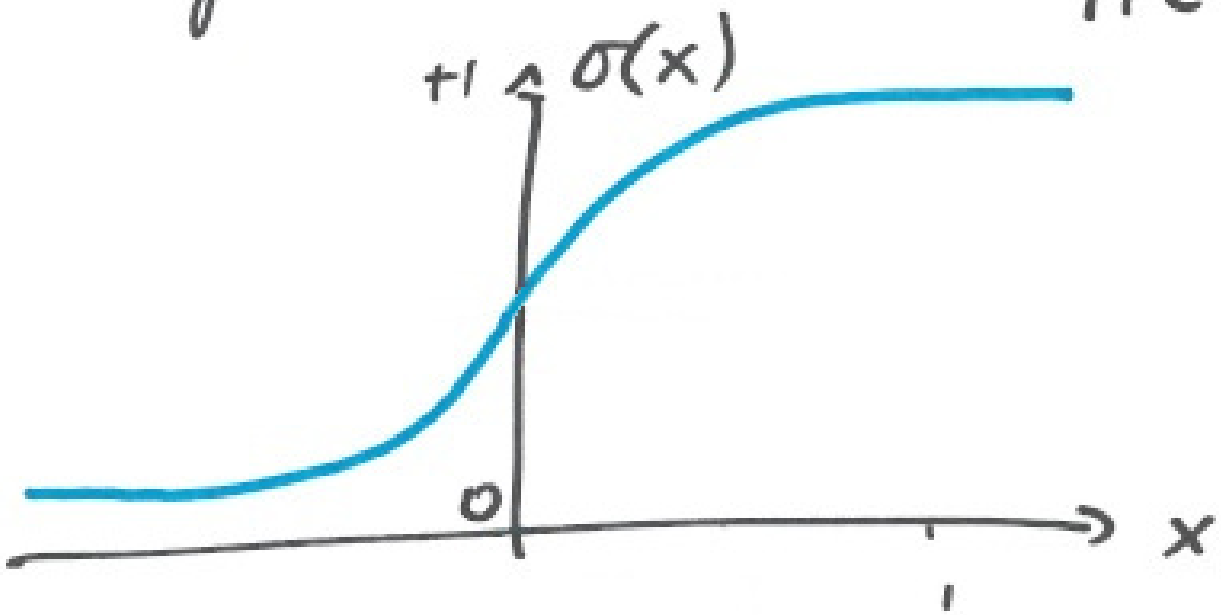
1. Given a NN, how do we compute $F(x)$?
2. How do we get a NN to be a good classifier.

One neuron



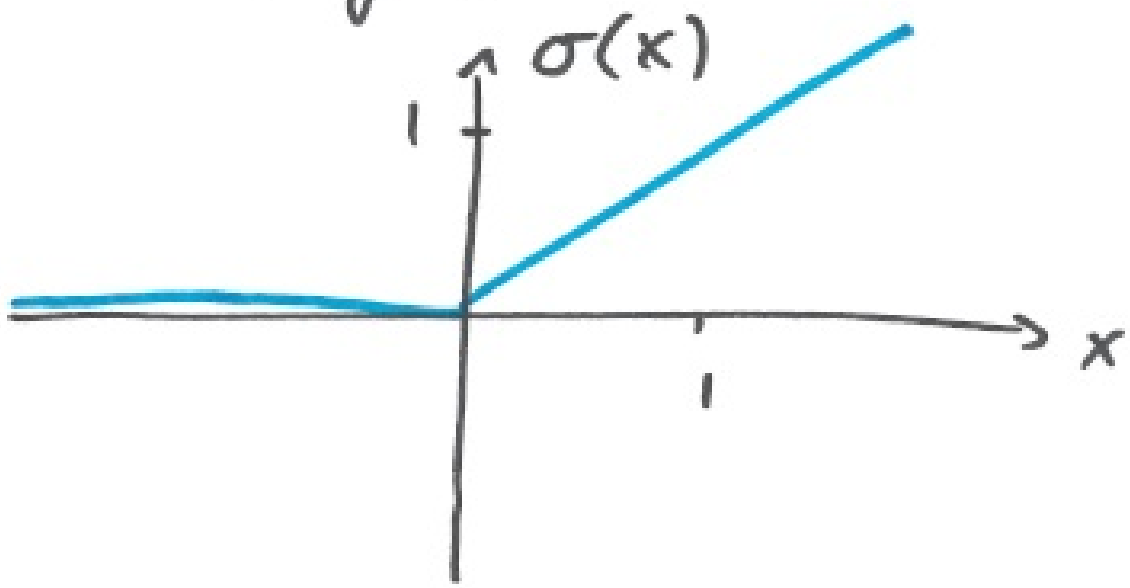
Typical choice of σ:

- Sigmoid function : $\sigma(x) = \frac{1}{1+e^{-x}}$

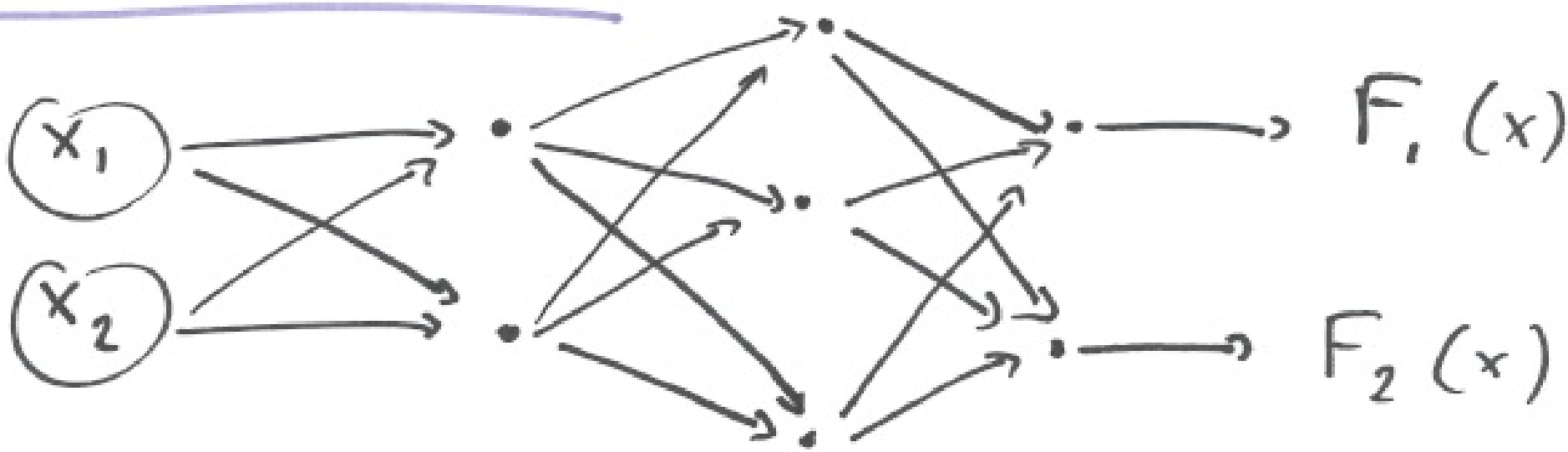


- rectified linear unit (ReLU):

$$\sigma = \begin{cases} 0 & , \text{if } x \leq 0 \\ x & , \text{if } x > 0 \end{cases}$$



A neural network:



- the neural graph is fixed
- the σ function is fixed
- what can change is the linear combination of inputs in each neuron

$$y = \sigma(w^T x + b)$$