Part 2: Building a Network and Fully-Connected Networks

Mikhail Romanov, Igor Slinko

Dataset

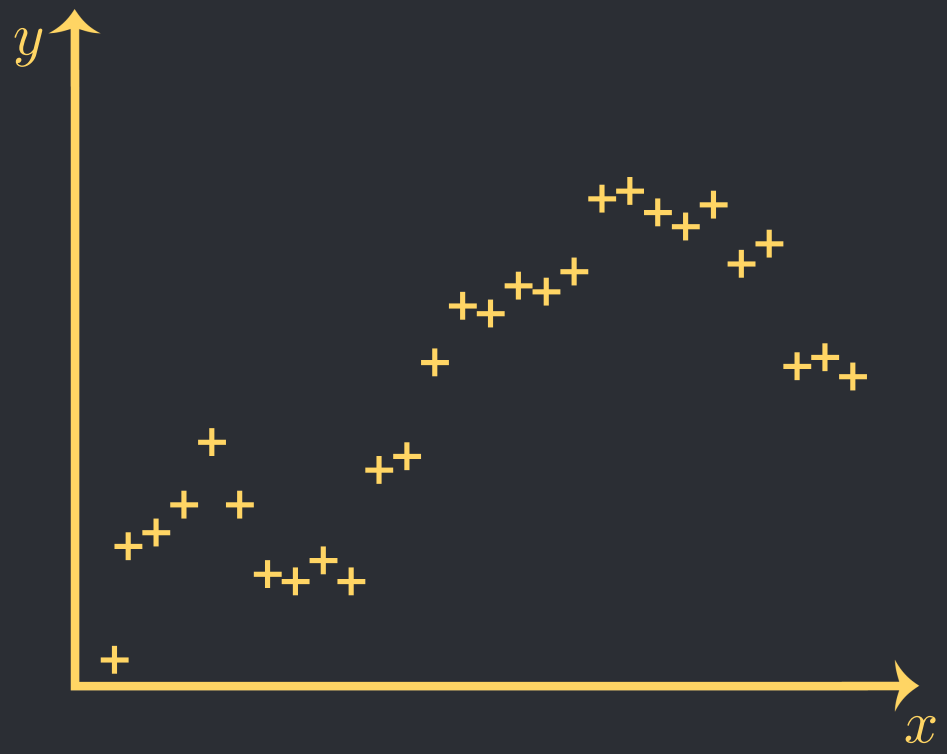
$\mathbf{x}_1$	$\mathbf{y}_1$
$\mathbf{x}_2$	$\mathbf{y}_2$
$\mathbf{x}_3$	$\mathbf{y}_3$
$\mathbf{x}_4$	$\mathbf{y}_4$
$\mathbf{x}_5$	$\mathbf{y}_5$
$\mathbf{x}_6$	$\mathbf{y}_6$
$\dots$	$\dots$
$\mathbf{x}_S$	$\mathbf{y}_S$

Dataset

- Split in three subsets: train, validation, tests

$\mathbf{x}_1$	$\mathbf{y}_1$
$\mathbf{x}_2$	$\mathbf{y}_2$
$\mathbf{x}_3$	$\mathbf{y}_3$
$\mathbf{x}_4$	$\mathbf{y}_4$
$\mathbf{x}_5$	$\mathbf{y}_5$
$\mathbf{x}_6$	$\mathbf{y}_6$
...	...
$\mathbf{x}_S$	$\mathbf{y}_S$

Problem Example: Regression (Data Fitting)



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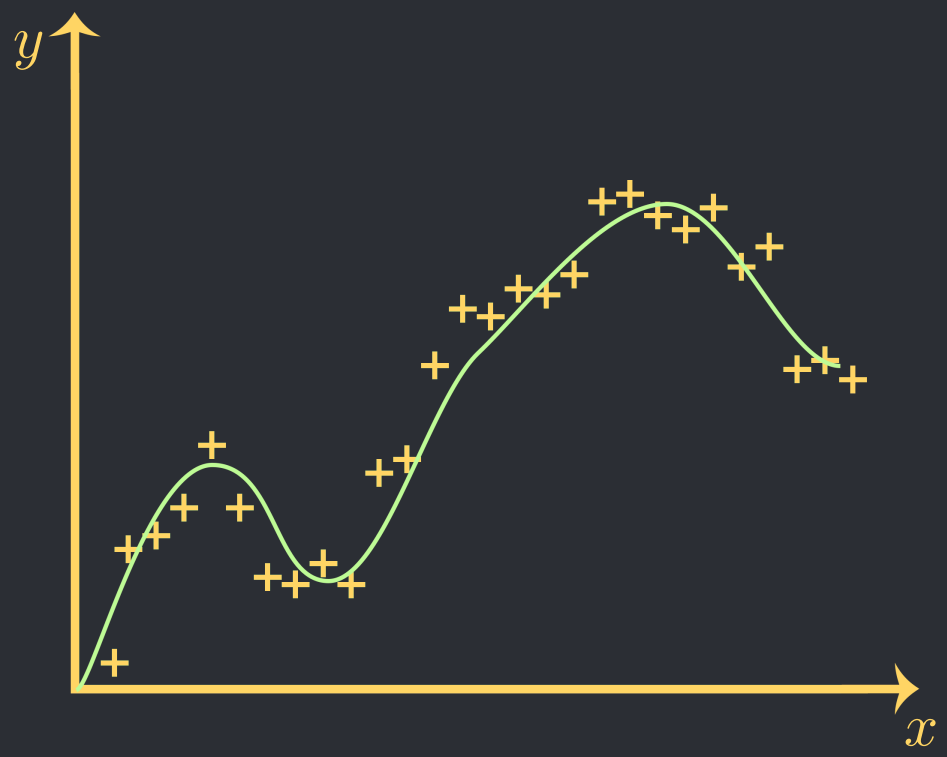
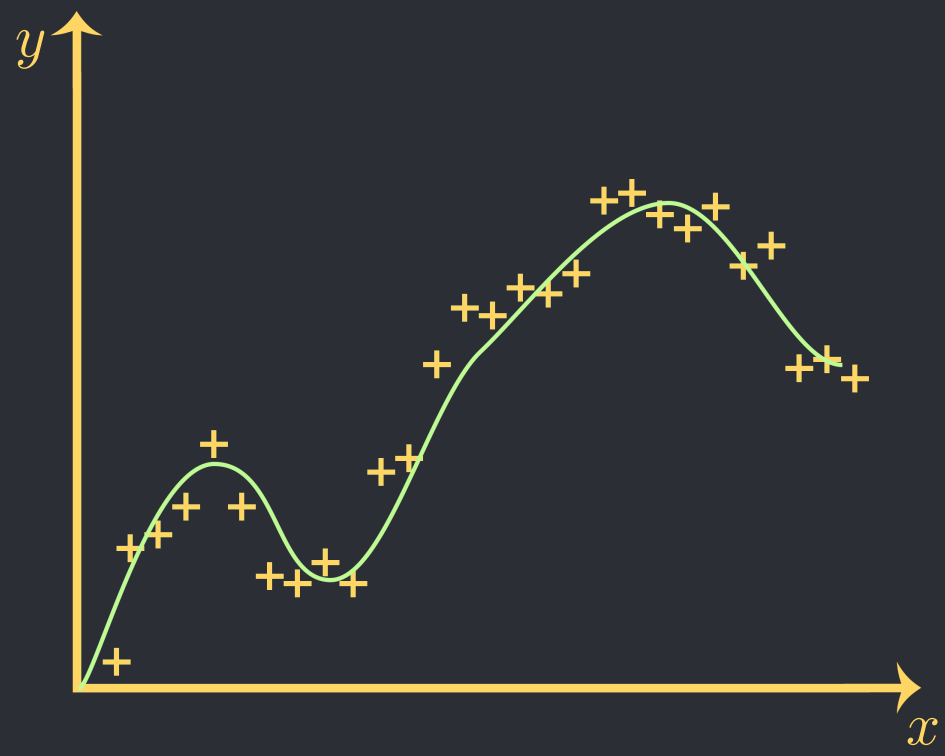


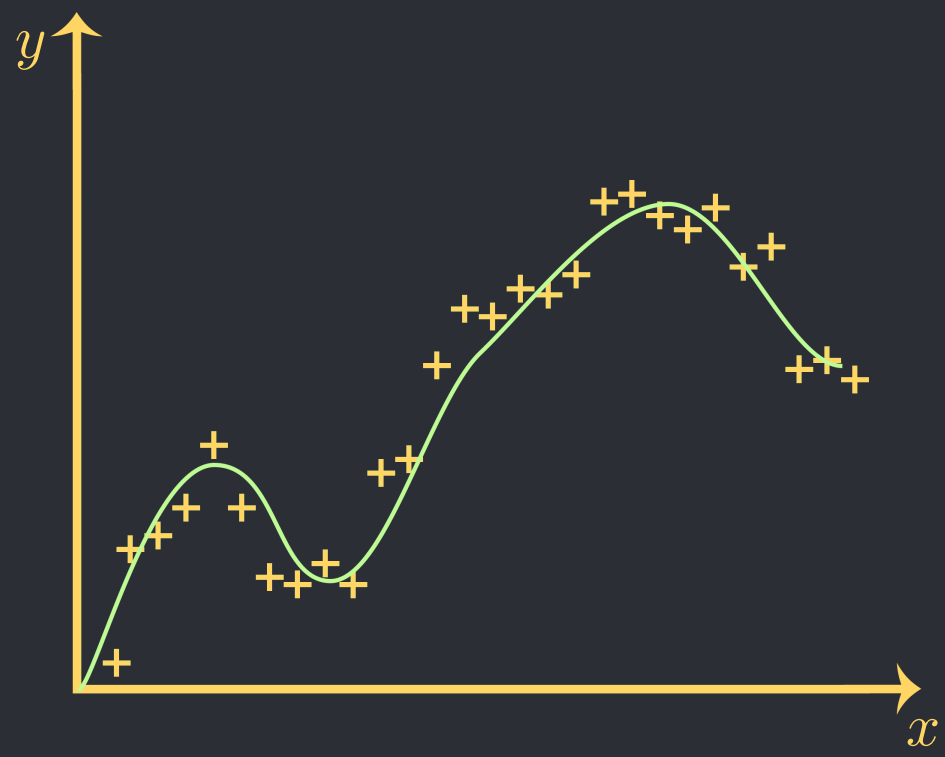
Problem Example: Regression (Data Fitting)

$$\mathbf{y}_s = f(\mathbf{x}_s)$$



Problem Example: Regression (Data Fitting)

$$\mathbf{y}_s = f(\mathbf{x}_s) + \boldsymbol{\varepsilon}_s$$



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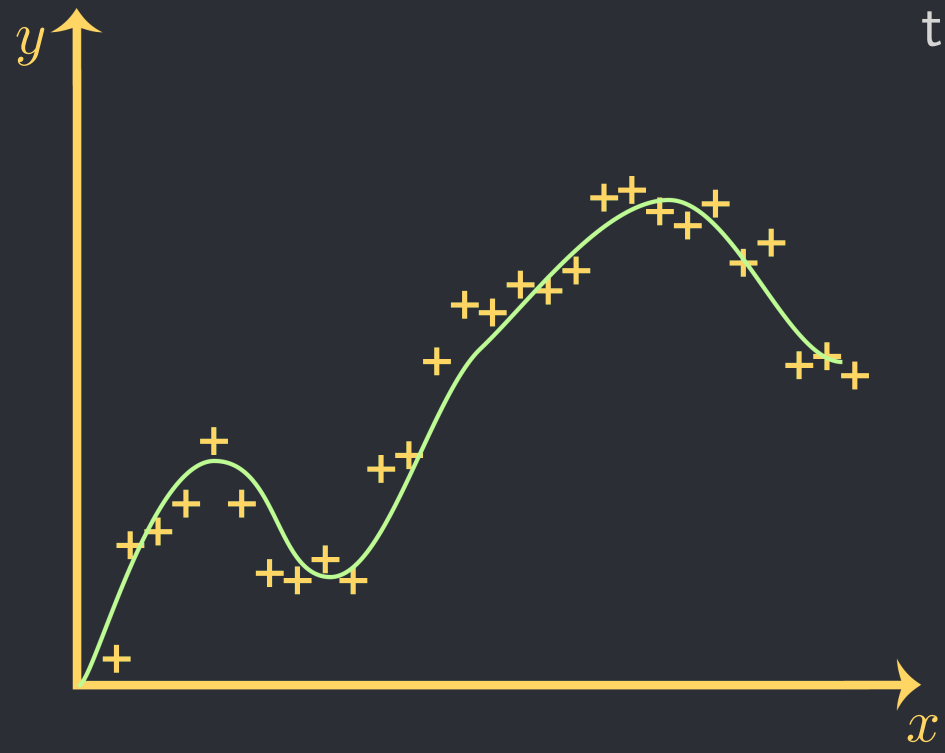

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$f(\mathbf{x}_s)$ – unobservable ground truth function

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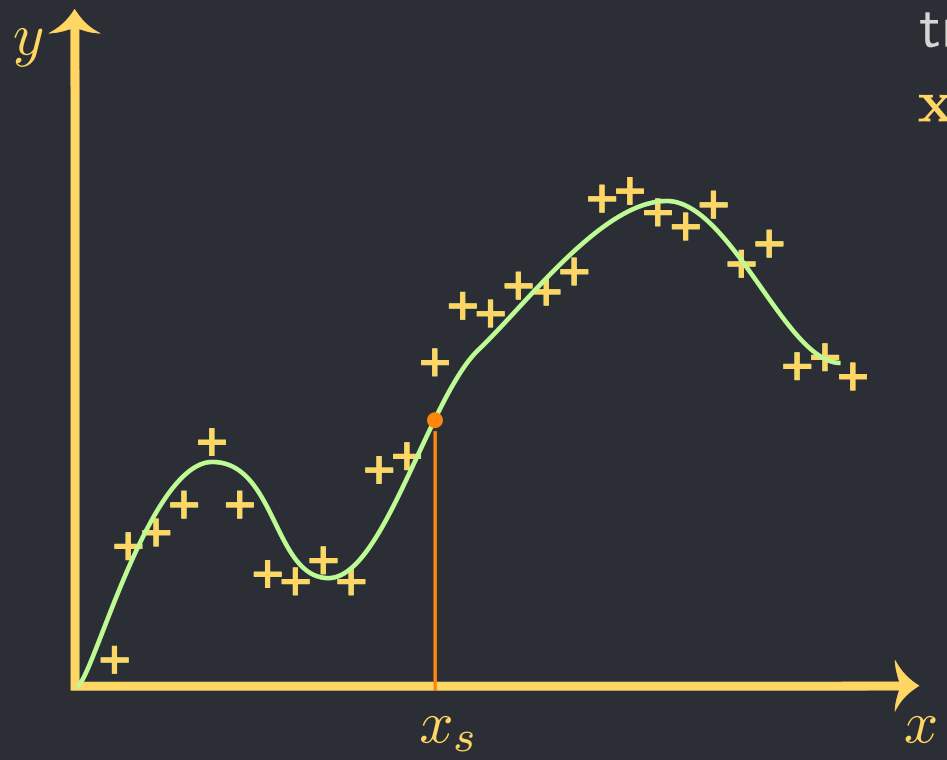

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$\mathbf{x}_s$ – measurement conditions

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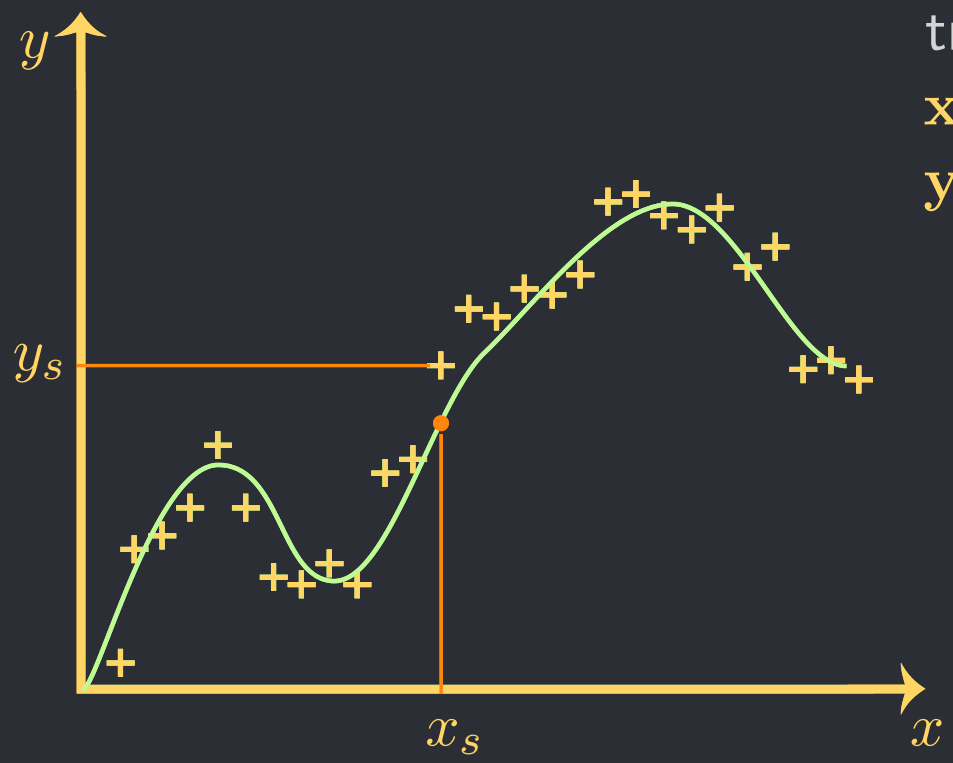

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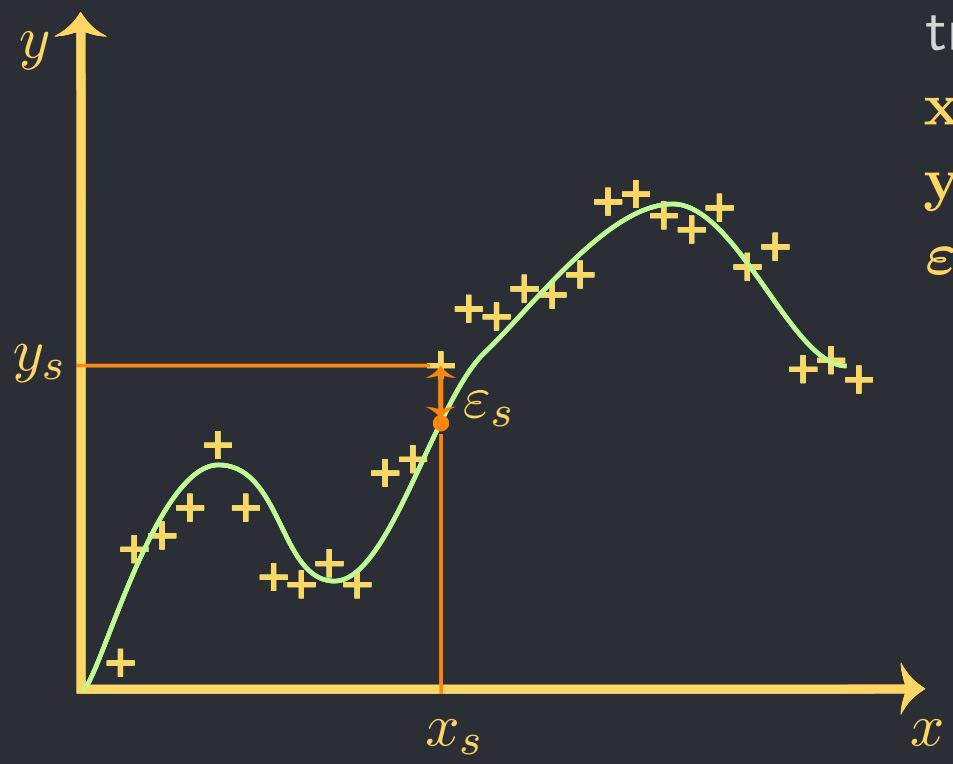

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$\mathbf{y}_s$ – measured value

$\boldsymbol{\varepsilon}_s$ – noise

Starter Kit

Starter Kit

- Neural Network Architecture

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- Loss Function

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- Loss Function
- Numerical Optimization Method

Starter Kit

- Neural Network Architecture
- Loss Function
- Numerical Optimization Method
- Metrics

Neural Network

x_s

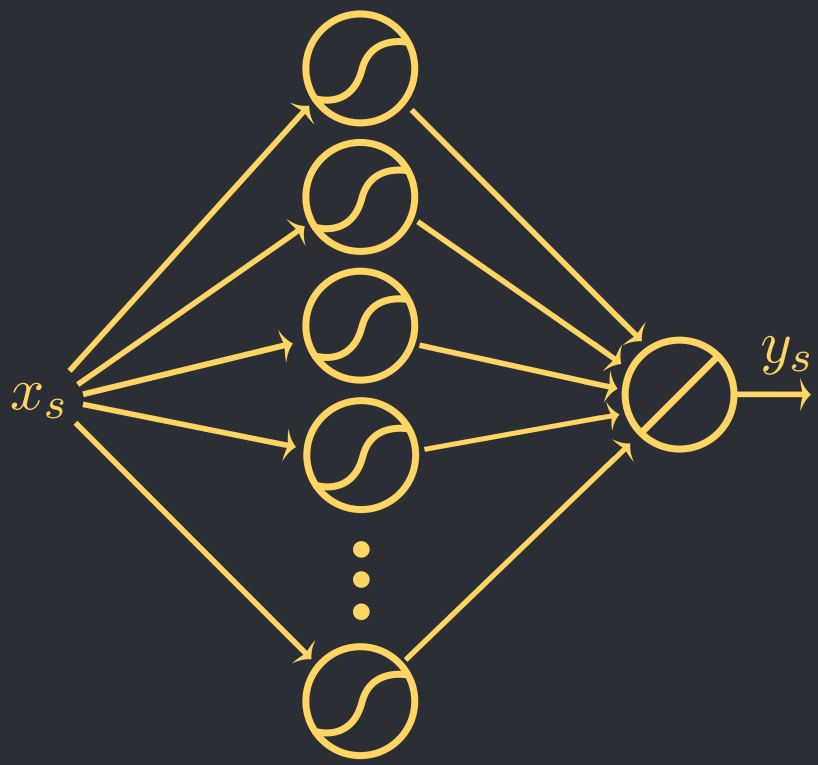
Neural Network

x_s

Neural Network

x_s

Neural Network



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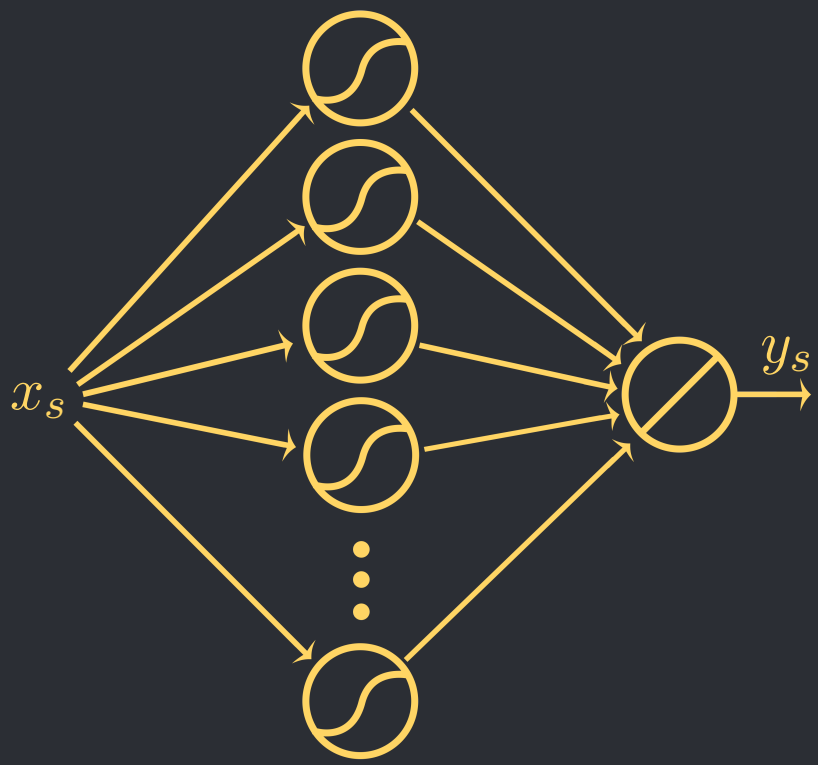

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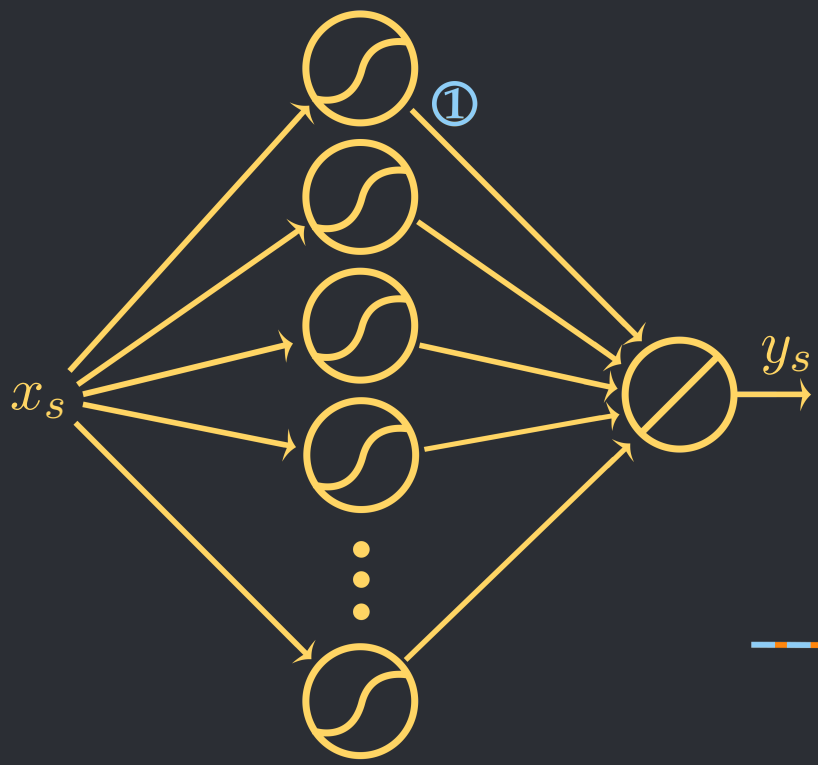

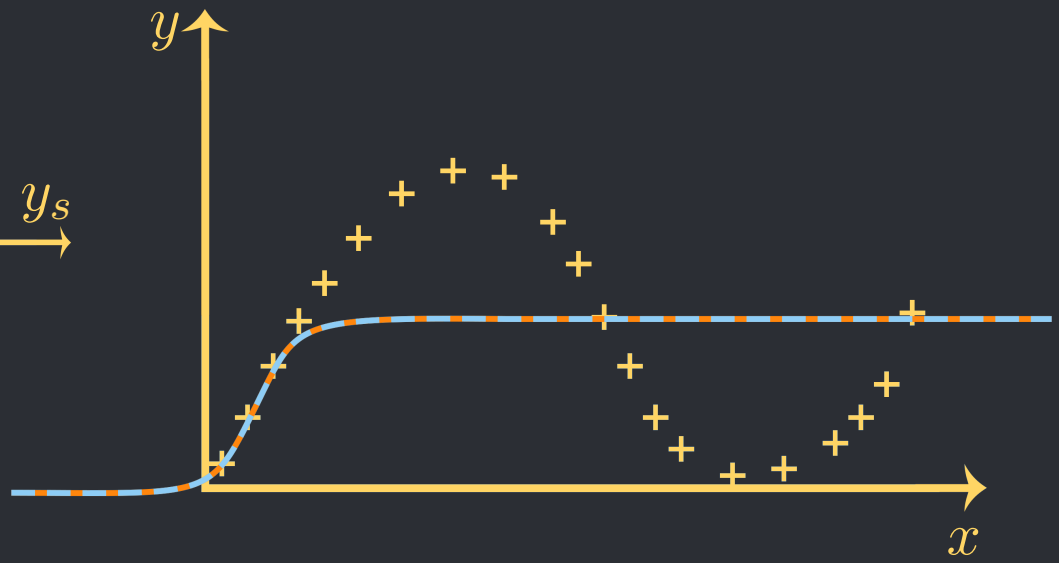

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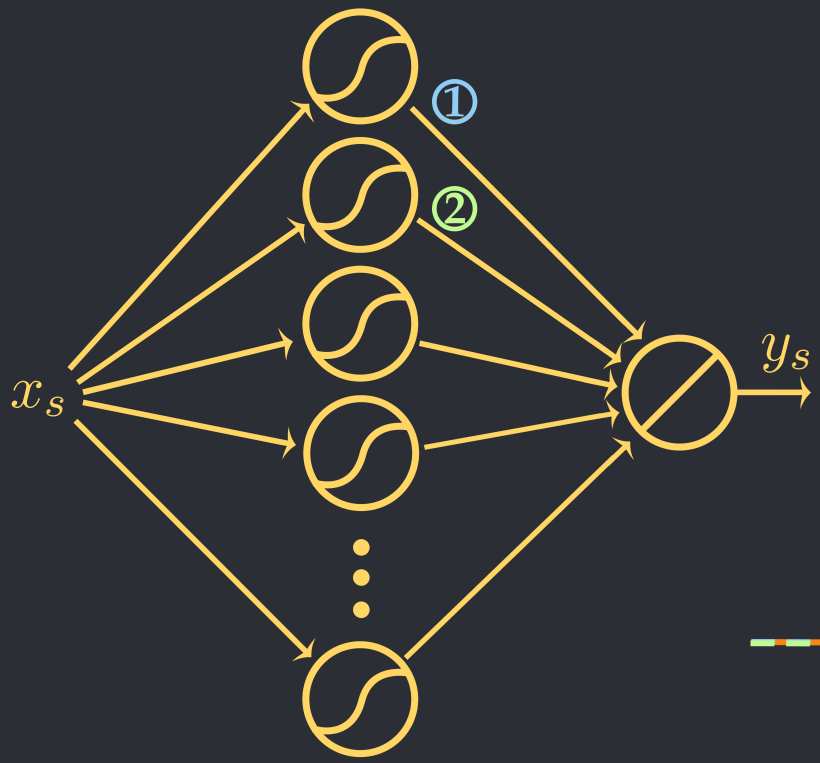

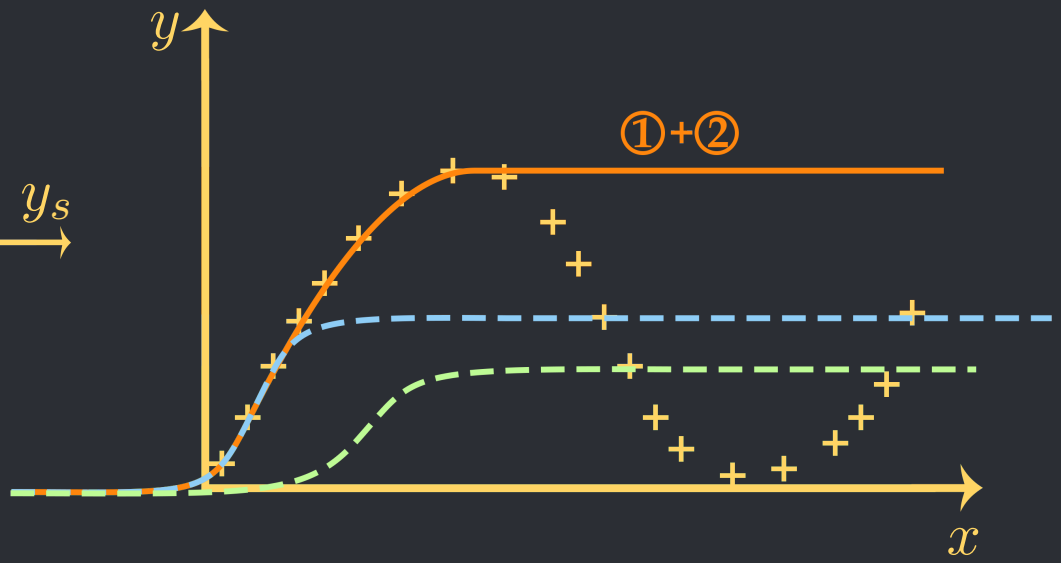

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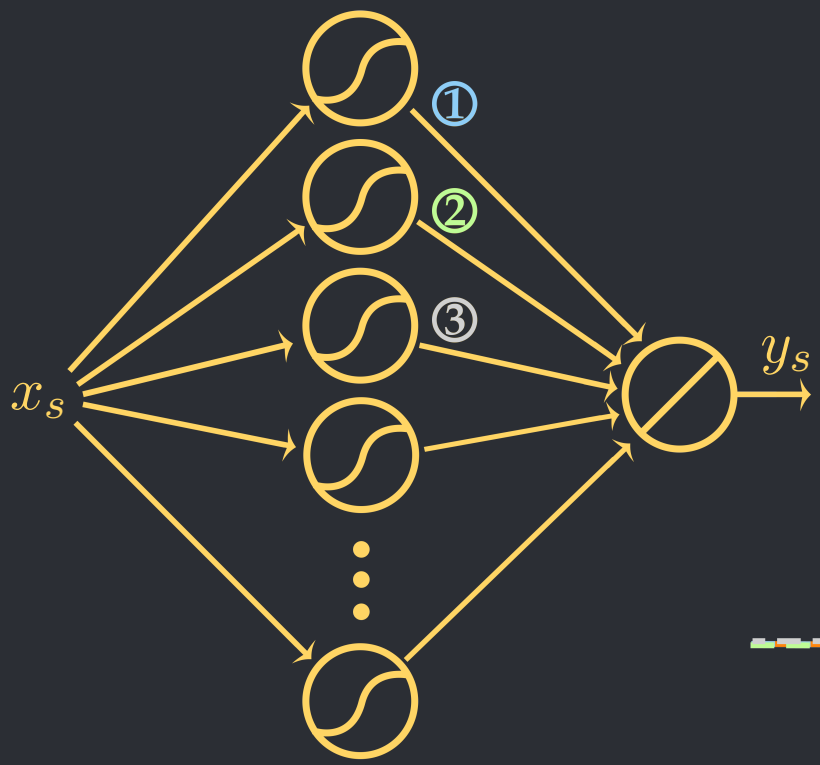

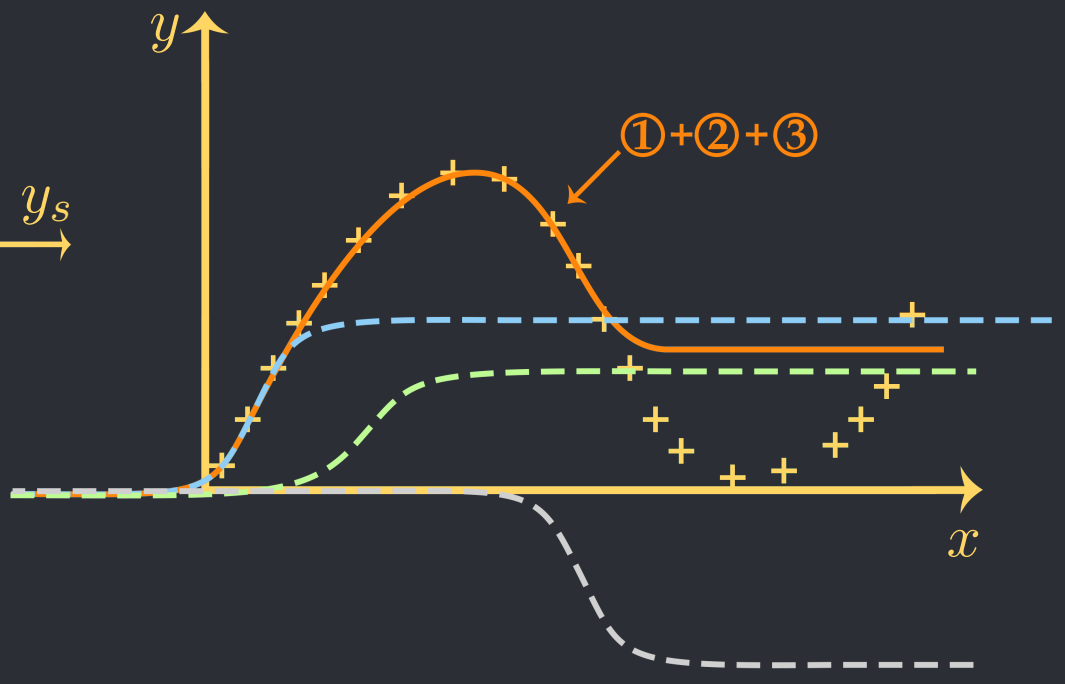

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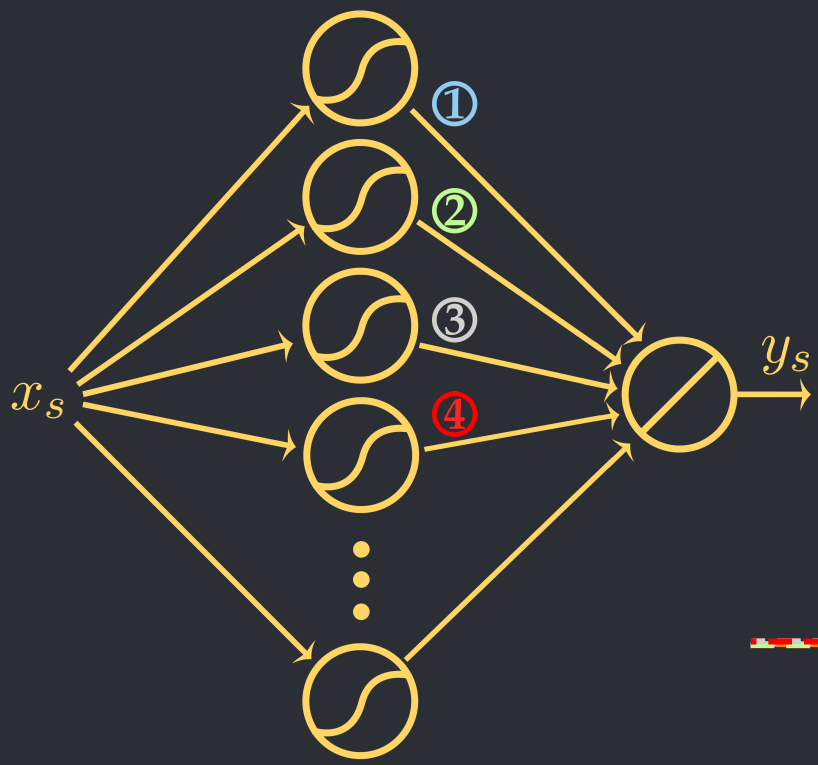

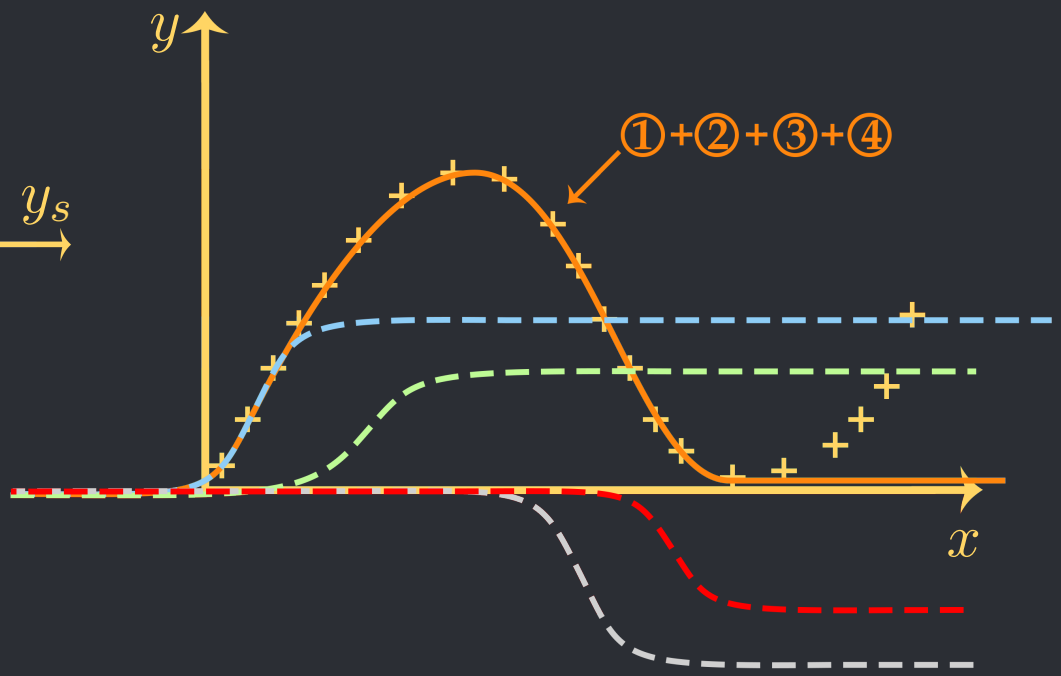

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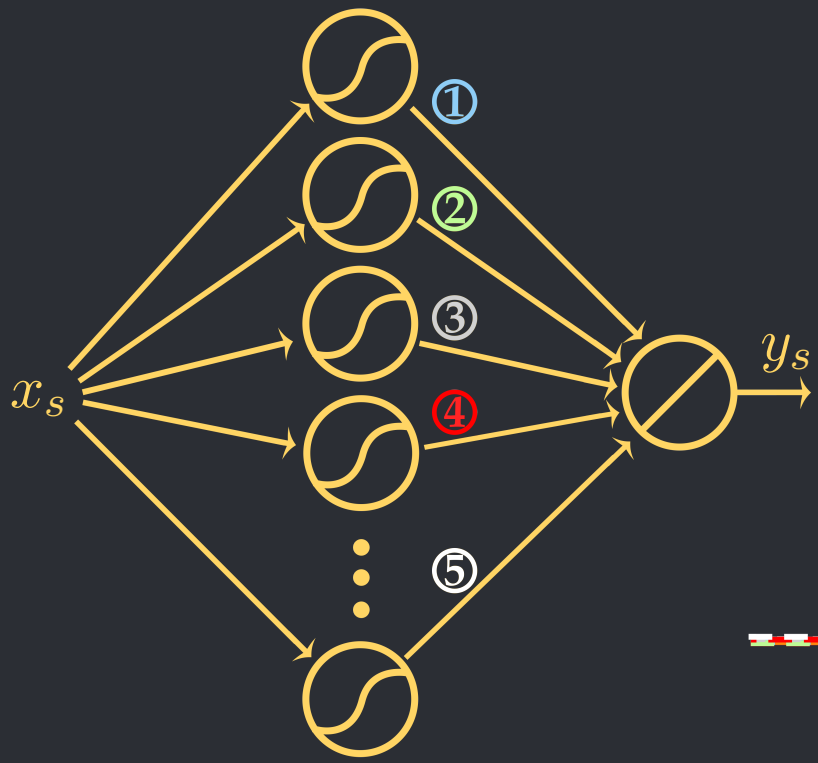

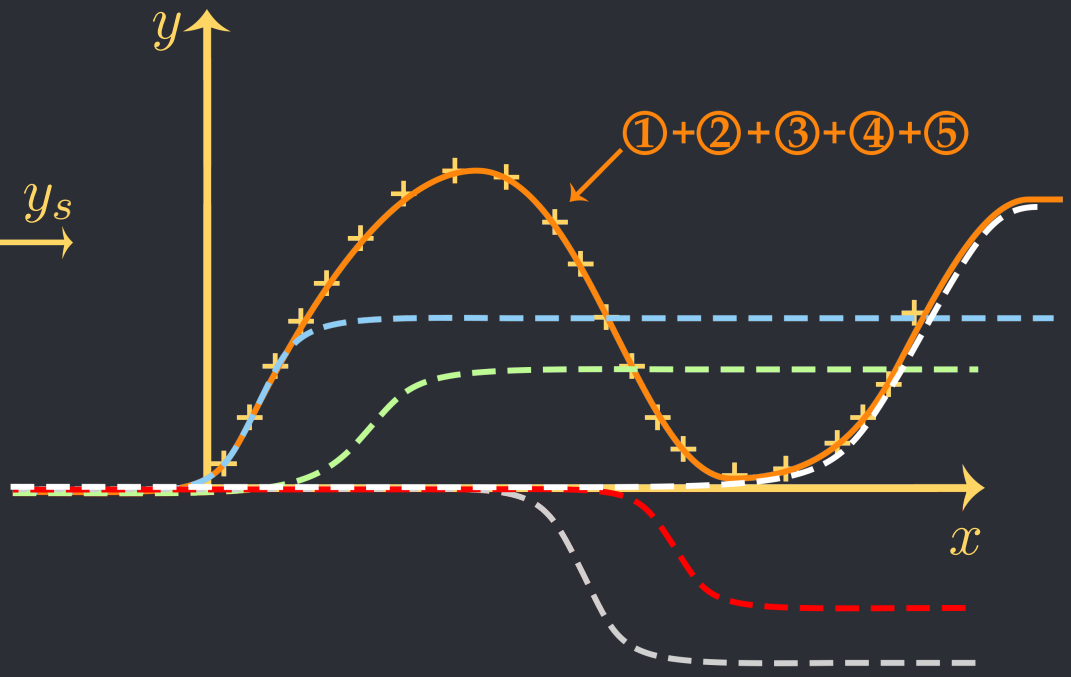

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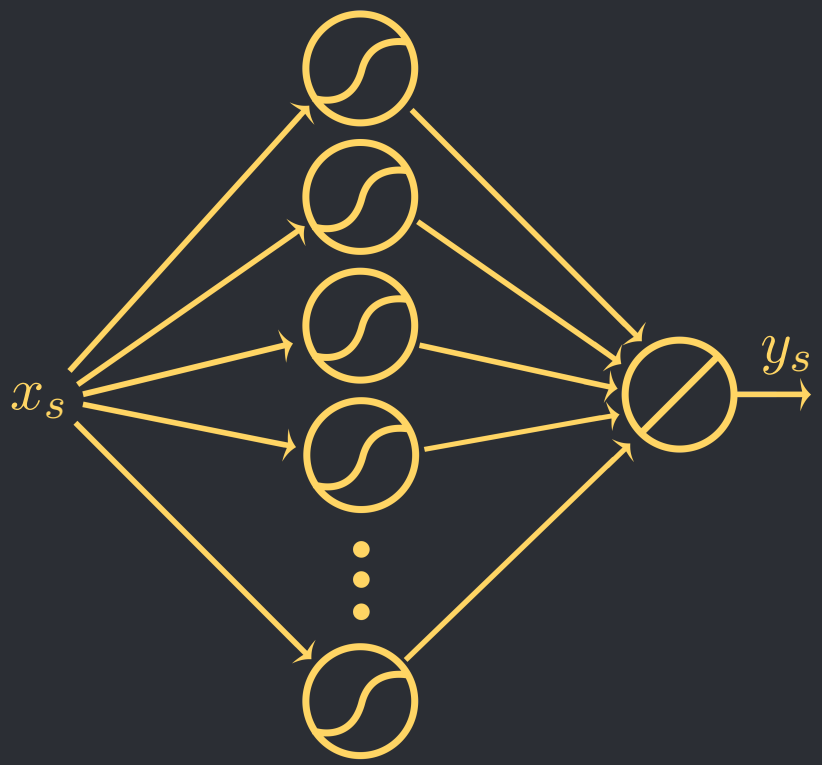
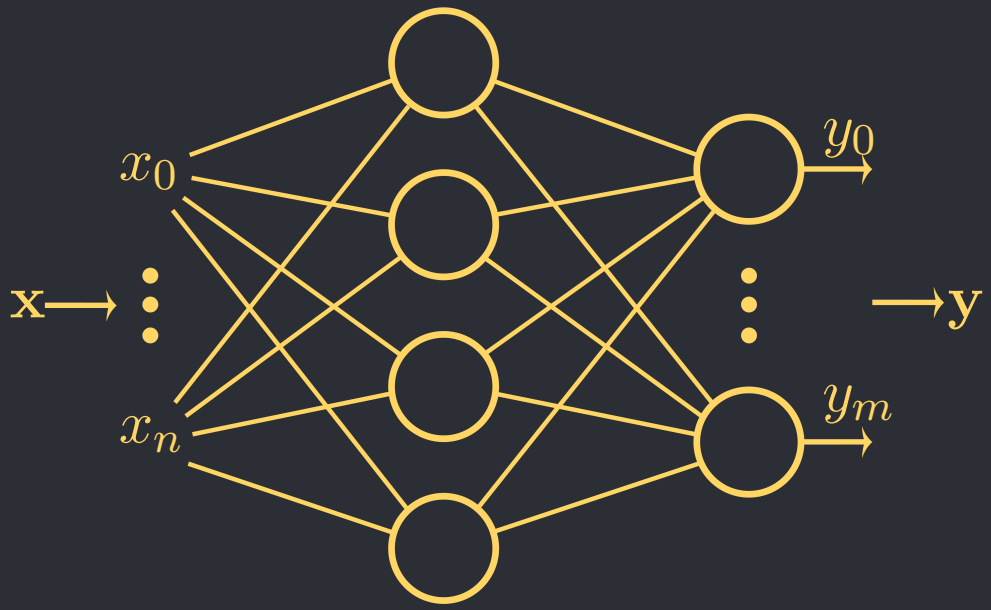
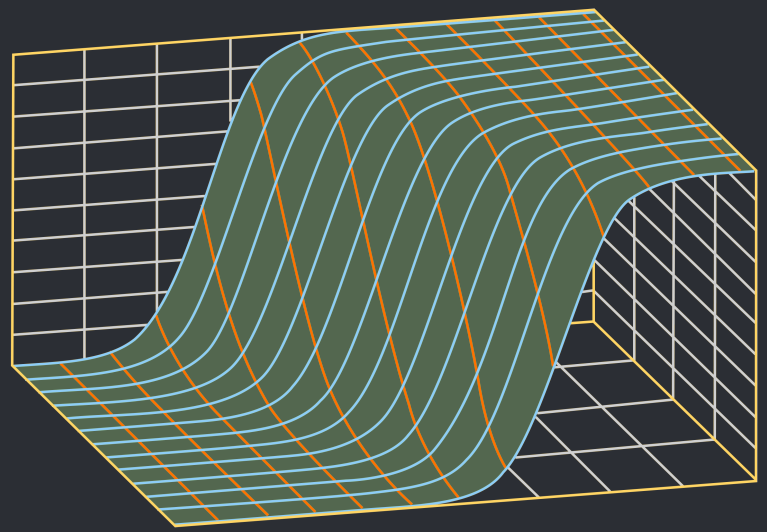


Using a linear combination of sigmoids it is possible to approximate with any accuracy any bounded function with limited amount of discontinuities.

Neural Network





Loss function

Consider one of the simpliest loss functions:
Mean Squared Error (MSE) for our problem.

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Network output

Target values

Metrics

- It is possible to use any function as a metric, including the loss functions
- Examples: precision, recall, ROC AUC, top N
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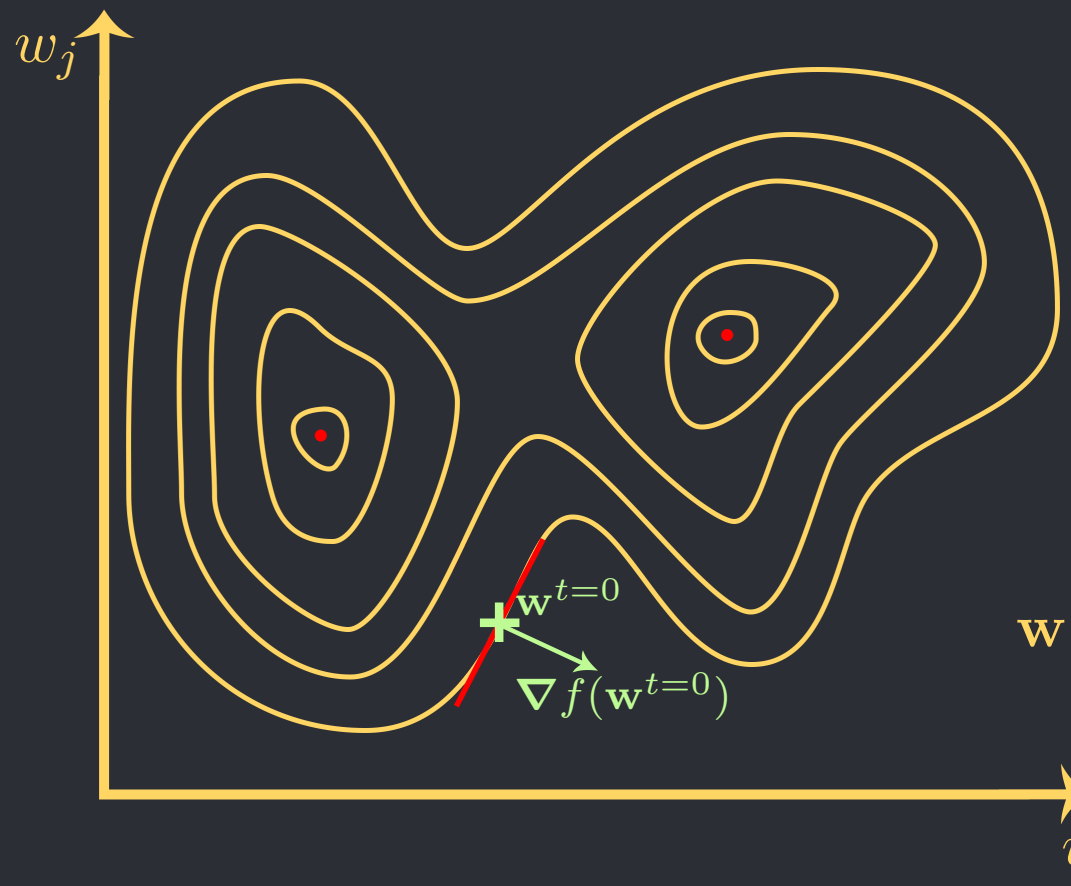
$$Acc_\varepsilon = \frac{1}{S}\sum_{s=1}^{S}[|y_s - \widetilde{y}_s| < \varepsilon]$$

Tuning the Parameters: Gradient Descent

All the weights of the network - $\mathbf{w}$

$$\begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_i \\ w_{P-1} \end{bmatrix}$$

Tuning the Parameters: Gradient Descent



$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_{P-1} \end{bmatrix} \qquad \nabla f = \begin{bmatrix} \frac{\partial f}{\partial w_0} \\ \frac{\partial f}{\partial w_1} \\ \vdots \\ \frac{\partial f}{\partial w_{P-1}} \end{bmatrix}$$

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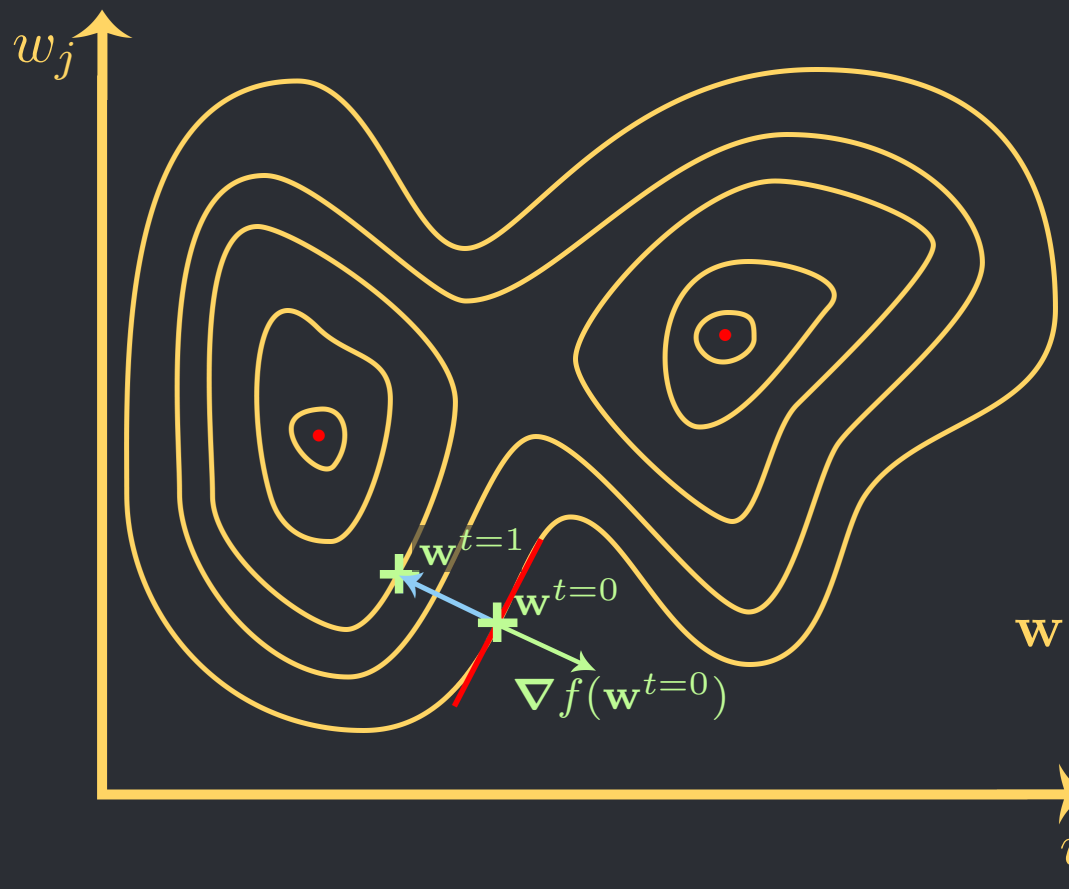
$$\mathbf{w}^{t=0}$$

$$\mathbf{w}^{t=1} = \mathbf{w}^{t=0} - \alpha \boldsymbol{\nabla} f(\mathbf{w}^{t=0})$$



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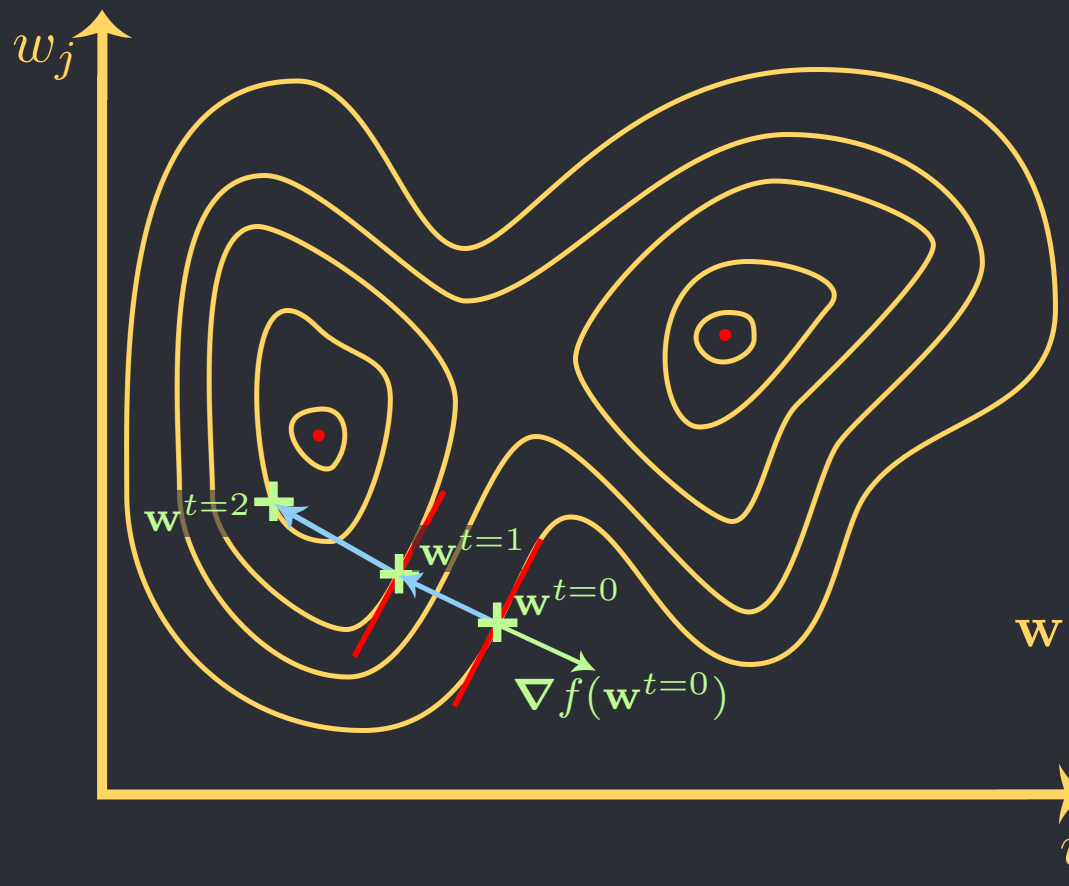

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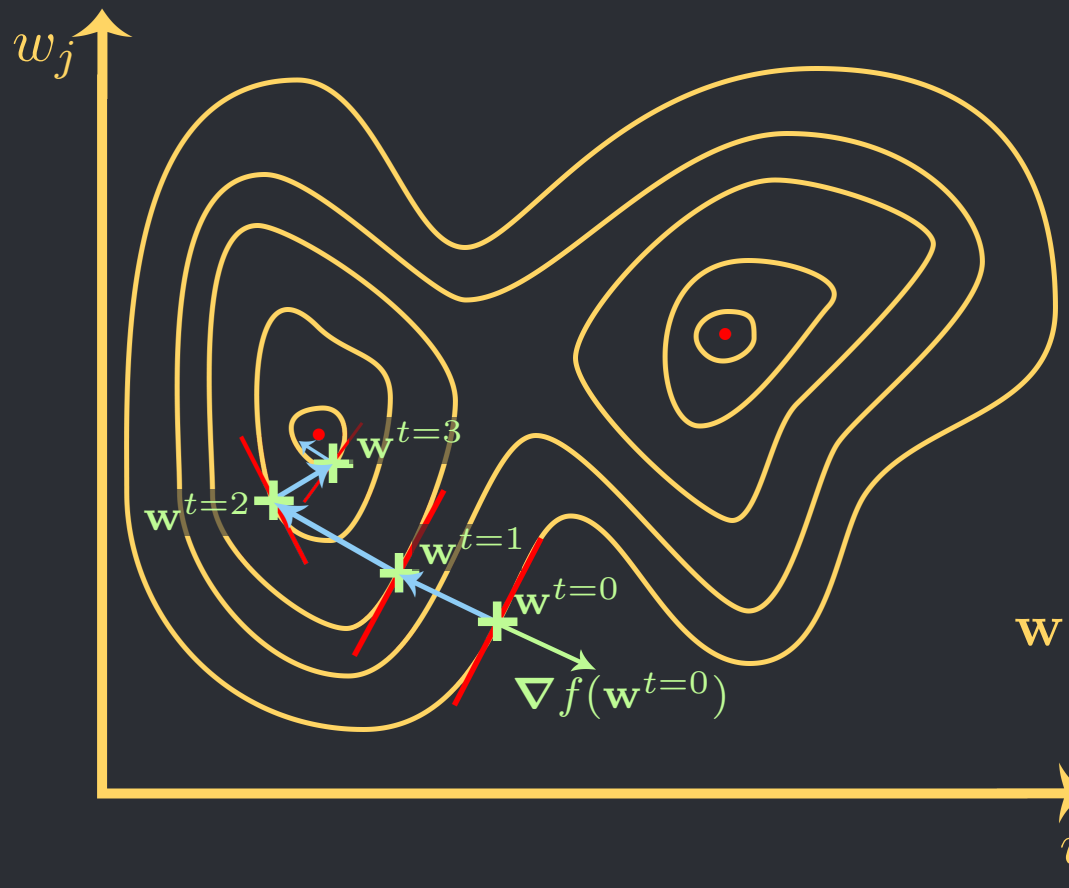

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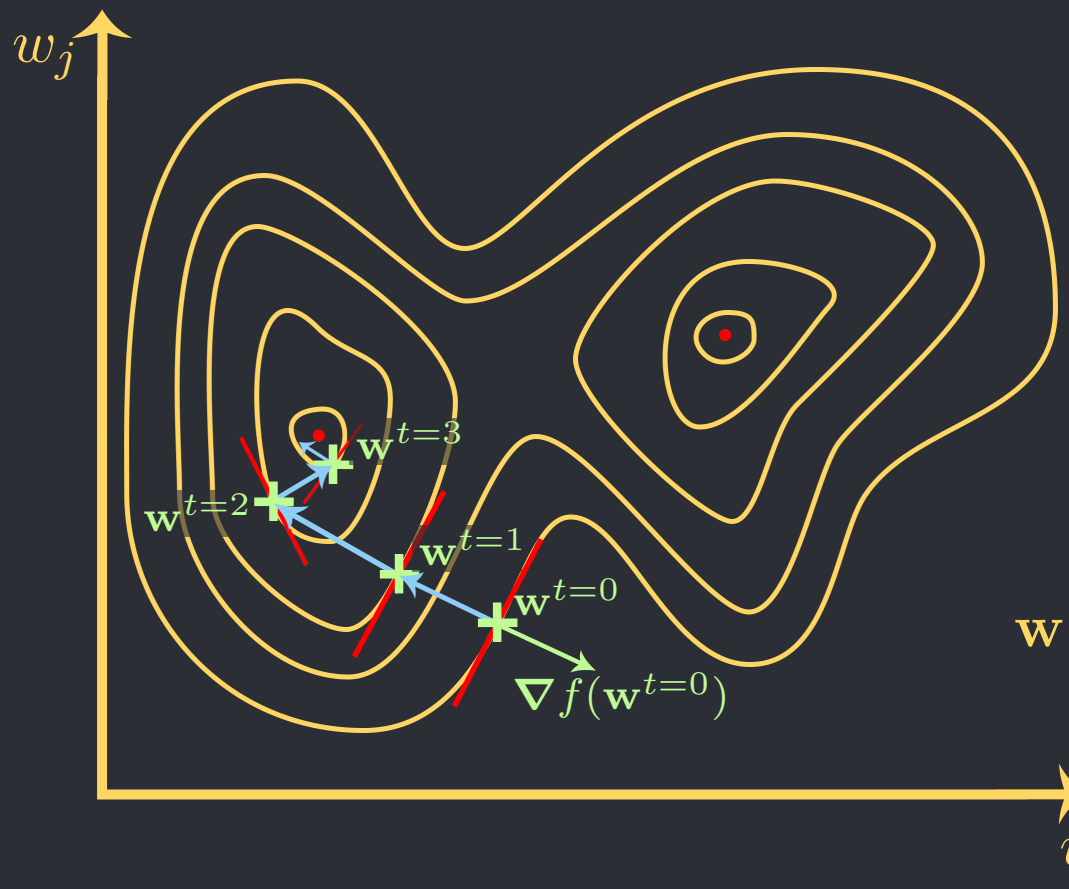

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$$\dots$$
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Tuning the Network: Gradient of a Loss Function

To be able to perform a Gradient Descent, we need a differentiable loss function

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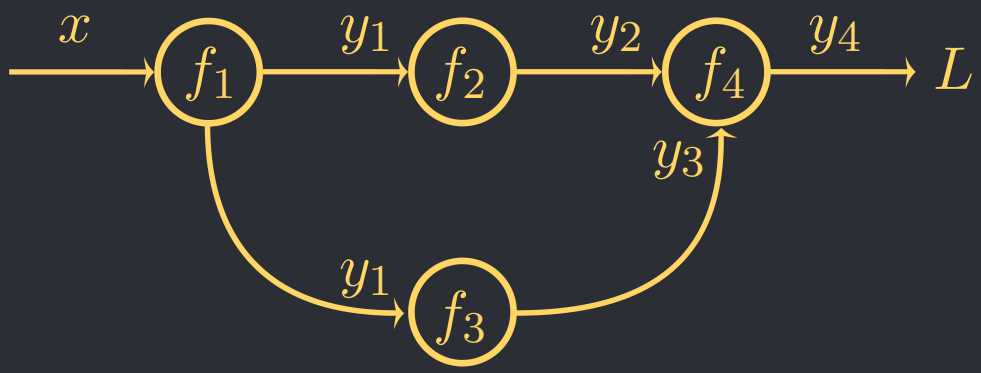
$$\frac{\partial}{\partial \widetilde{y}_s} MSE = -\frac{2}{S}(y_s - \widetilde{y}_s)$$

Computing the Gradients: Chain Rule

We know a derivative of the Loss Function. How to compute the derivatives of the Loss Function over the all the parameters of the network?



$$L\Big(f_4\Big(f_2\big(f_1(x)\big),\ f_3\big(f_1(x)\big)\Big)\Big)$$

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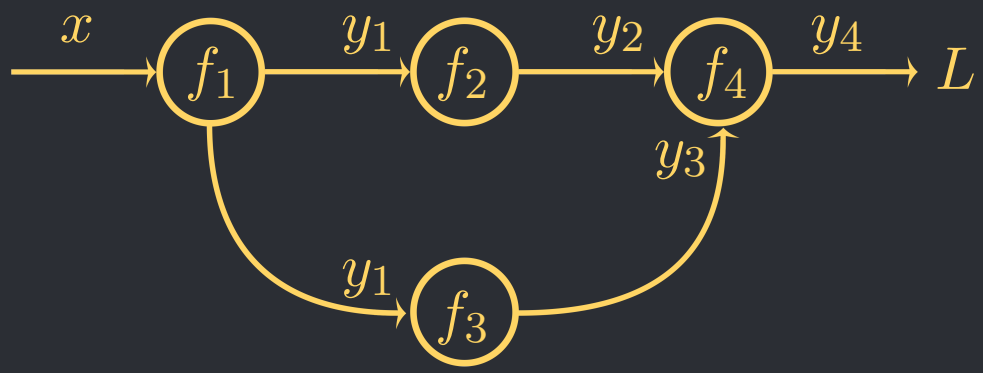

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Правило дифференцирования:

$$\frac{\partial f\big(g(x)\big)}{\partial x} = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial x}$$

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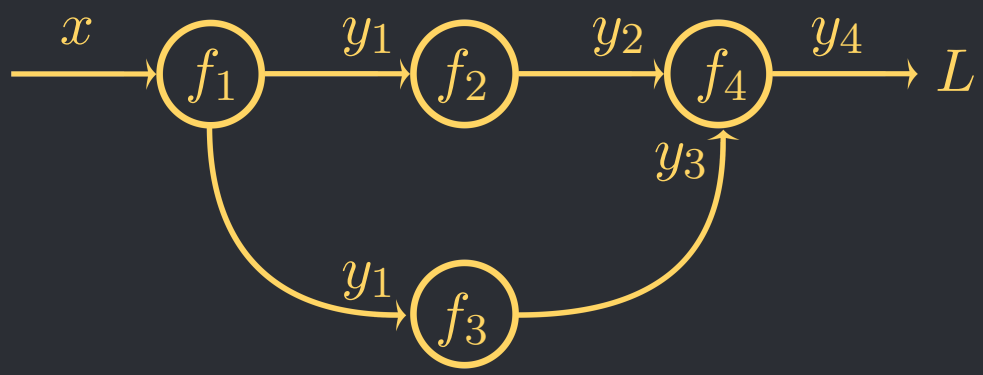

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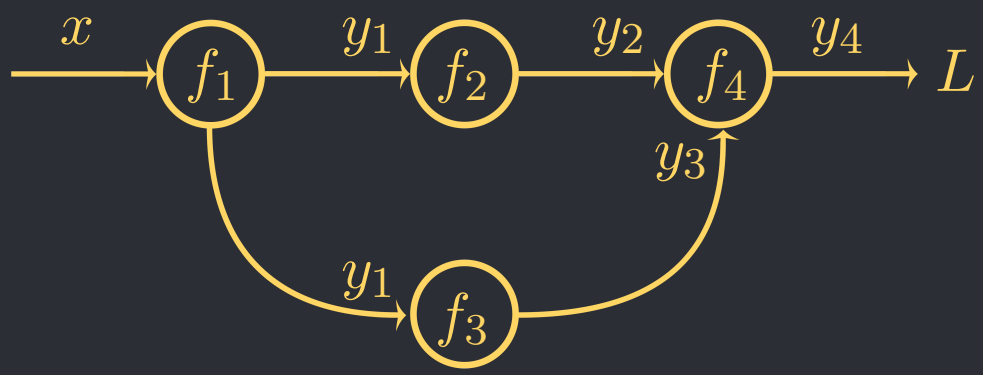

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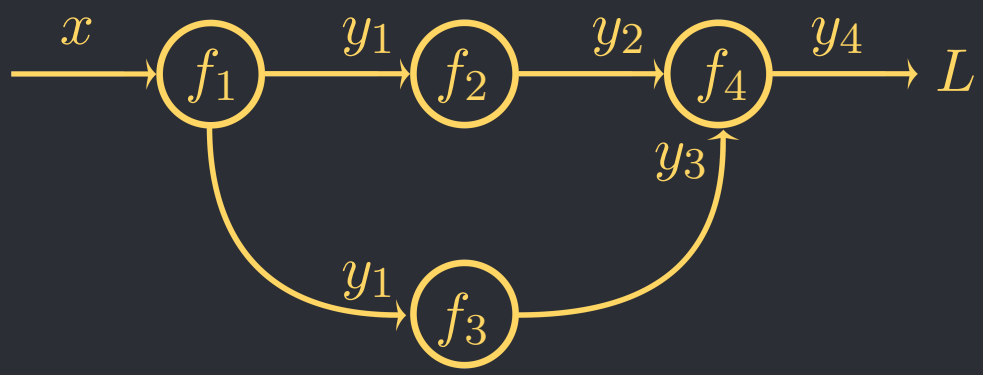

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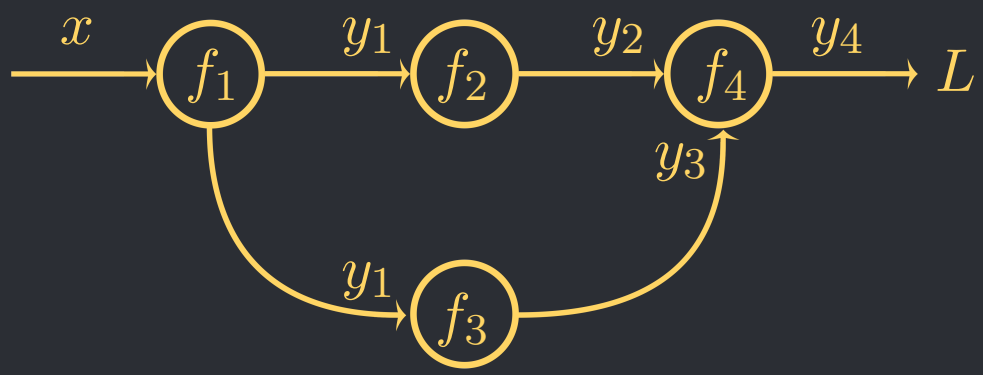

$$L\Big(f_4\Big(f_2\big(f_1(x)\big),\ f_3\big(f_1(x)\big)\Big)\Big)$$

Правило дифференцирования:

$$\frac{\partial f\big(g(x)\big)}{\partial x} = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial x}$$

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial y_4} \cdot \frac{\partial f_4}{\partial y_2} \cdot \frac{\partial f_2}{\partial w_2}$$

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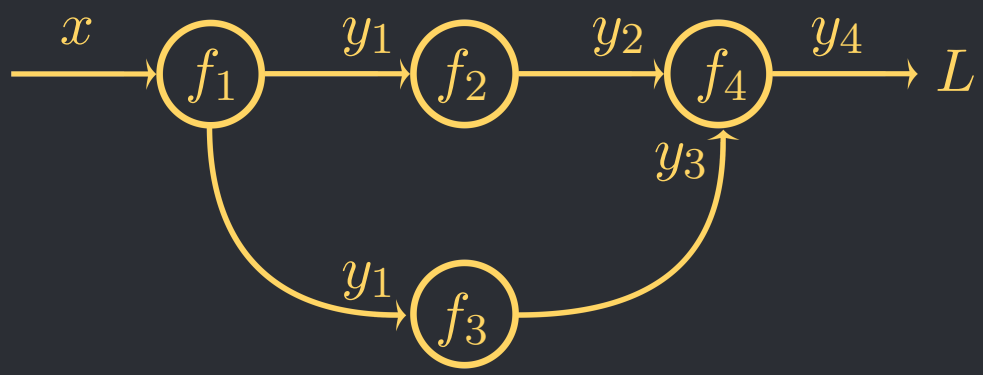

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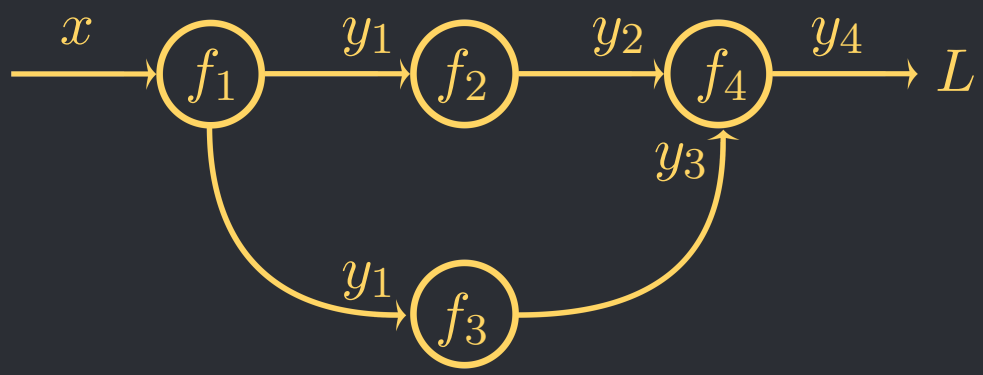

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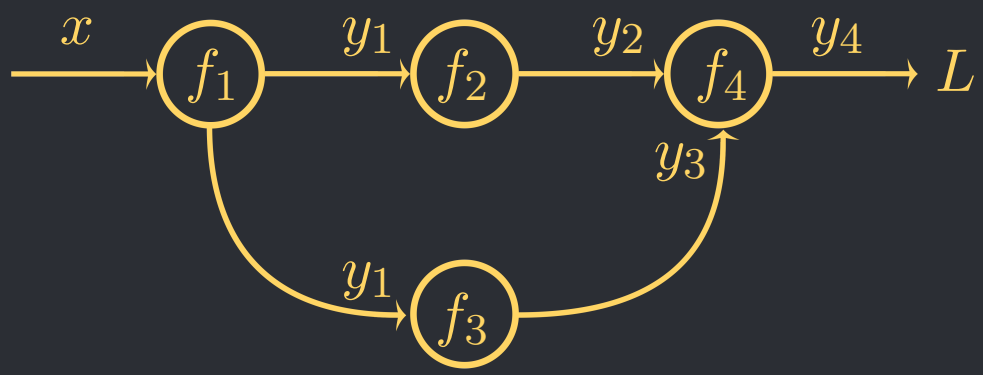

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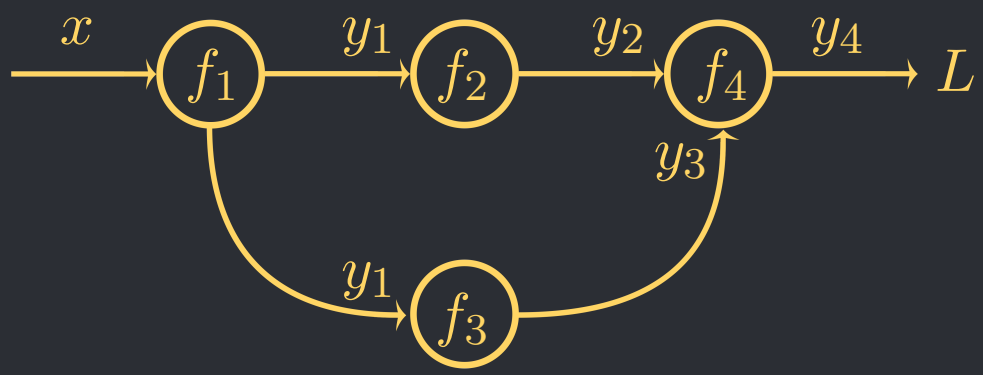

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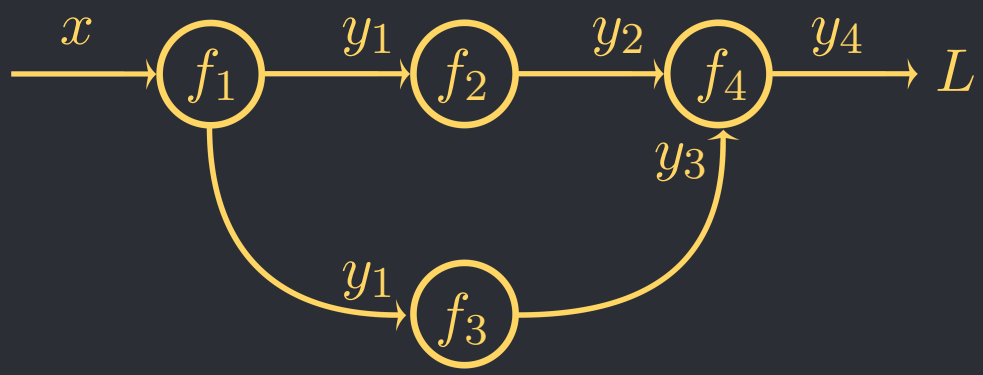

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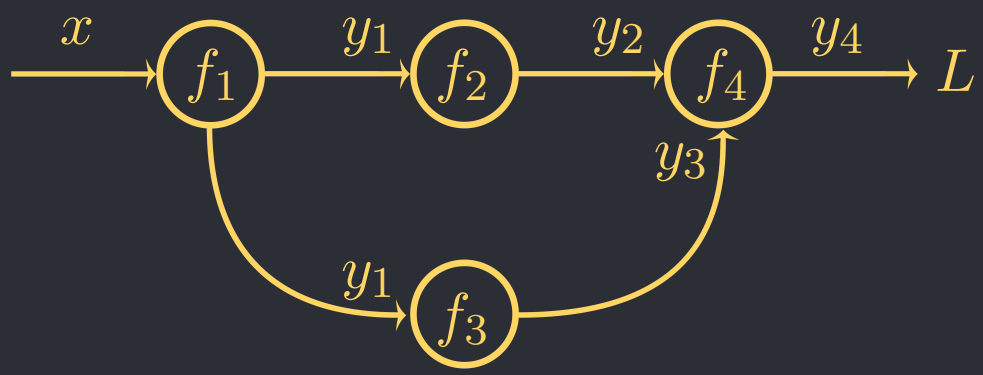

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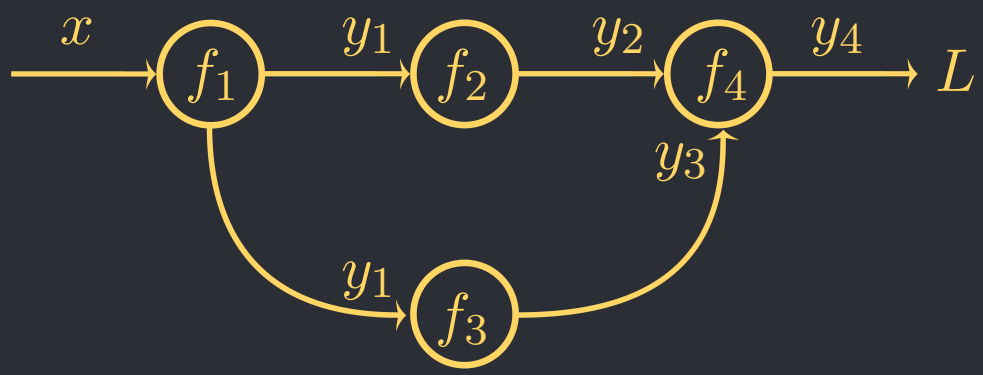

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Example: Logistic Regression

Linear classification algorithm:

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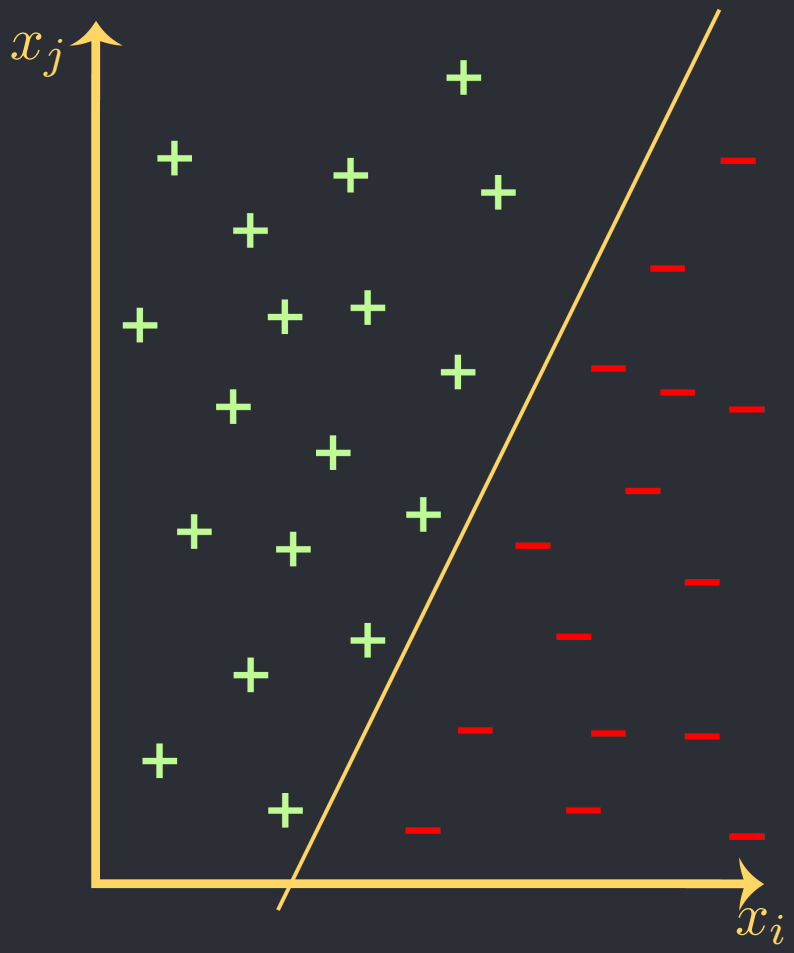

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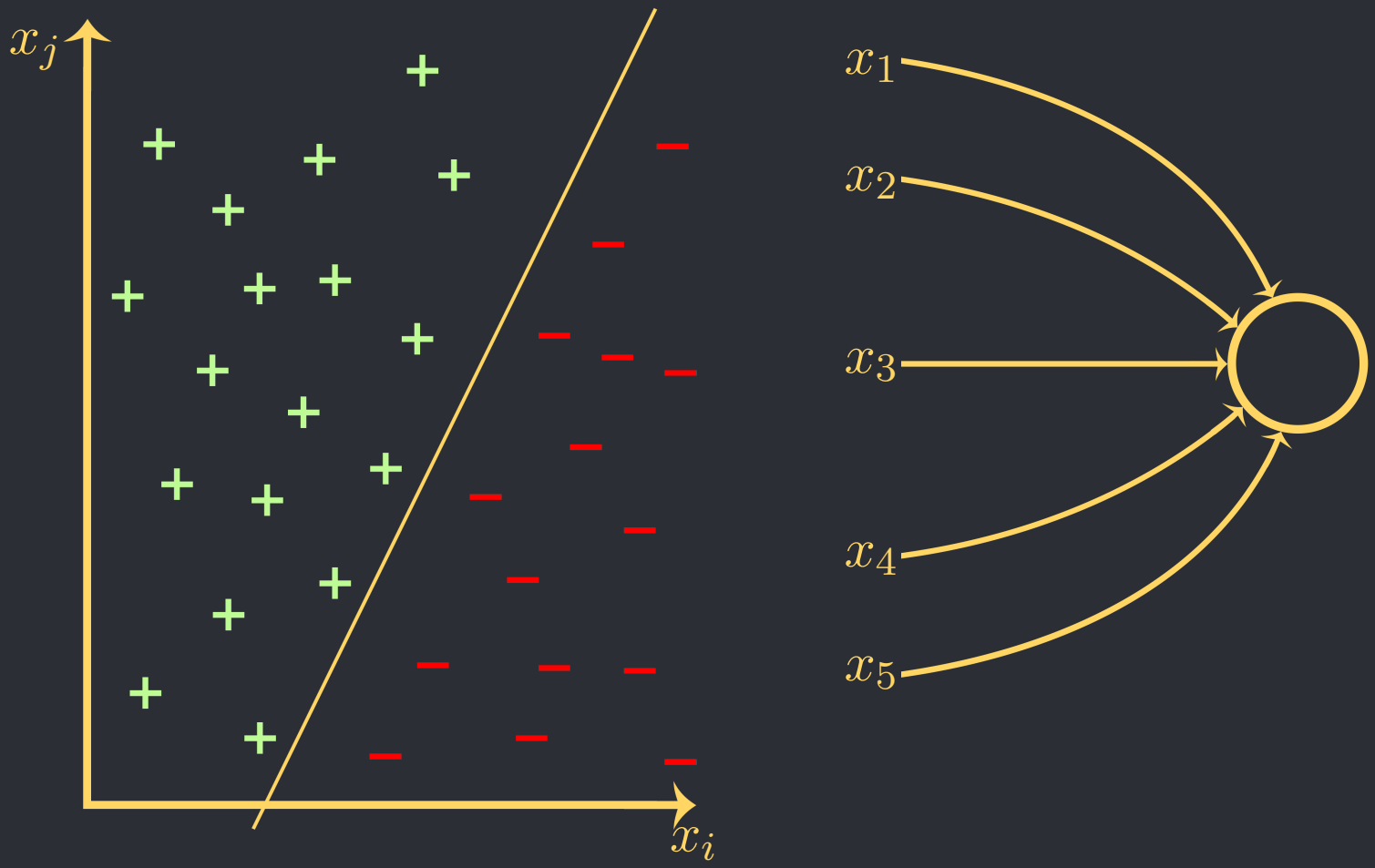

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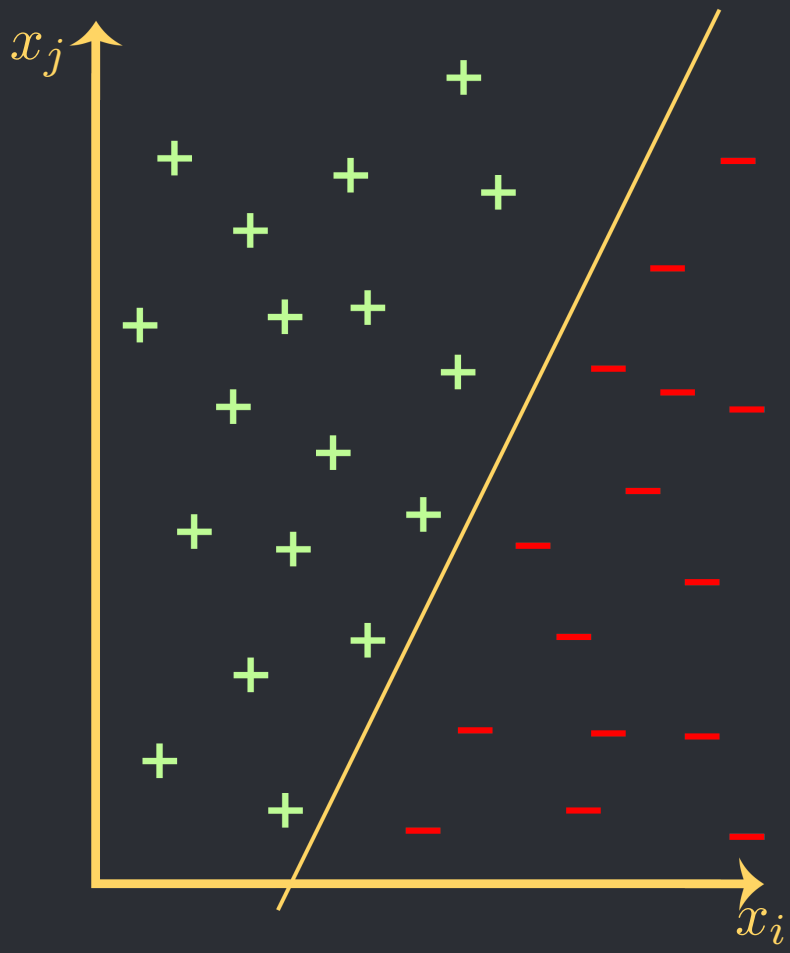

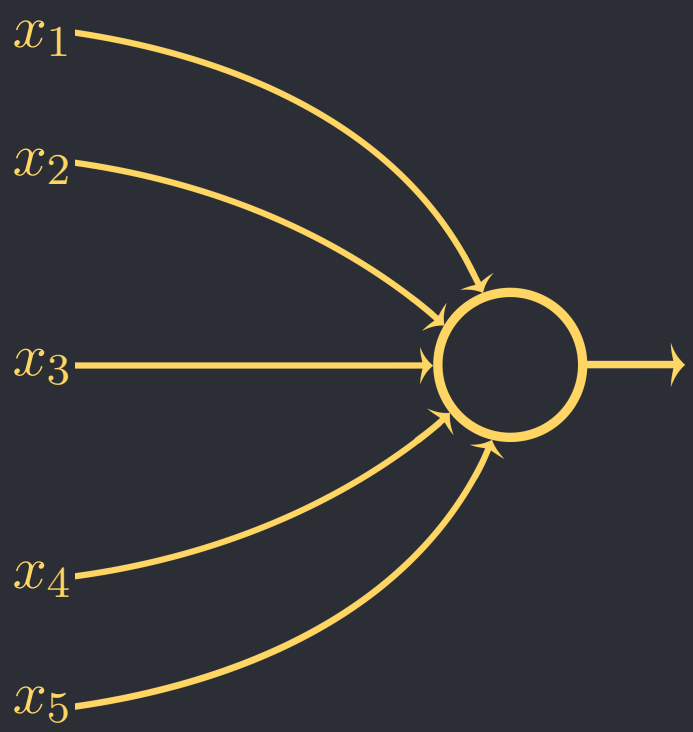

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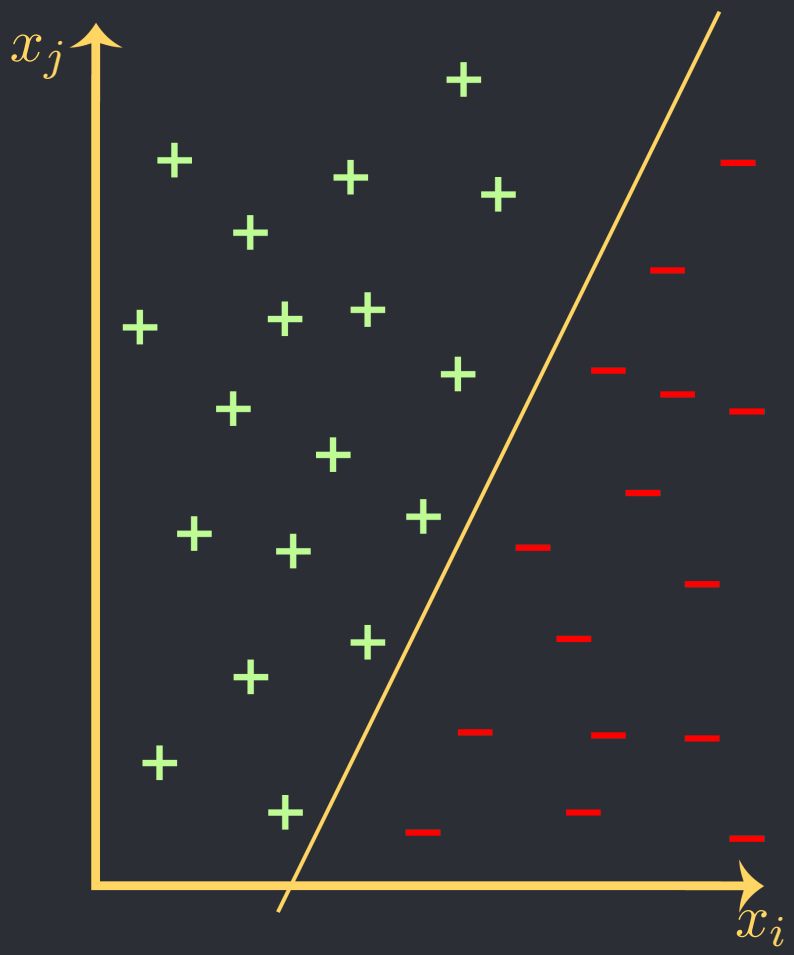
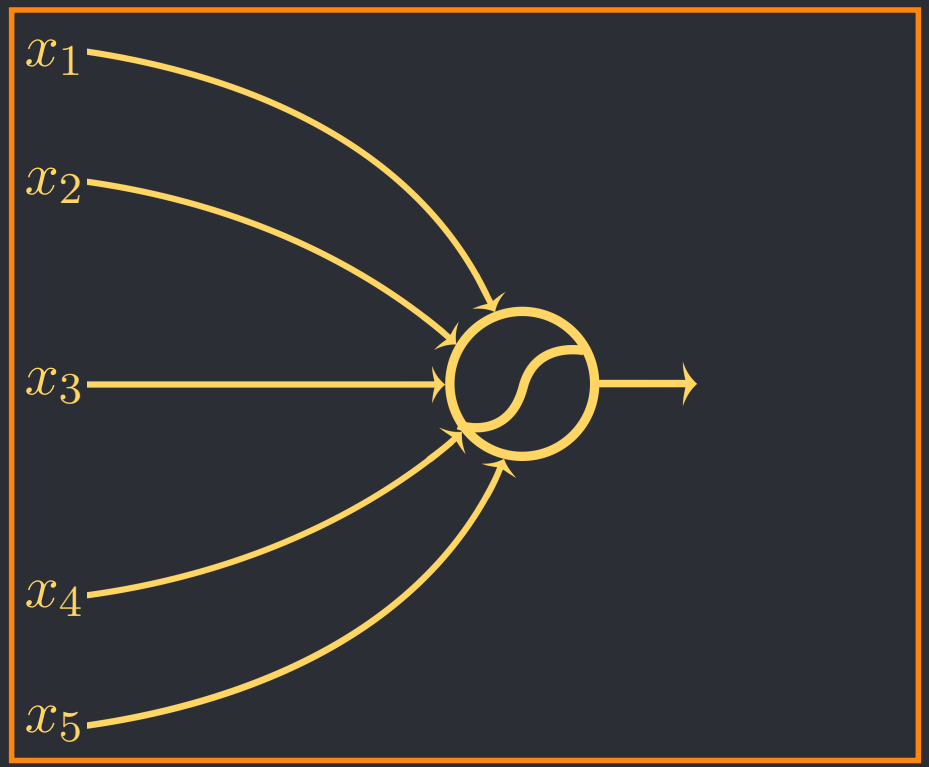


Architecture



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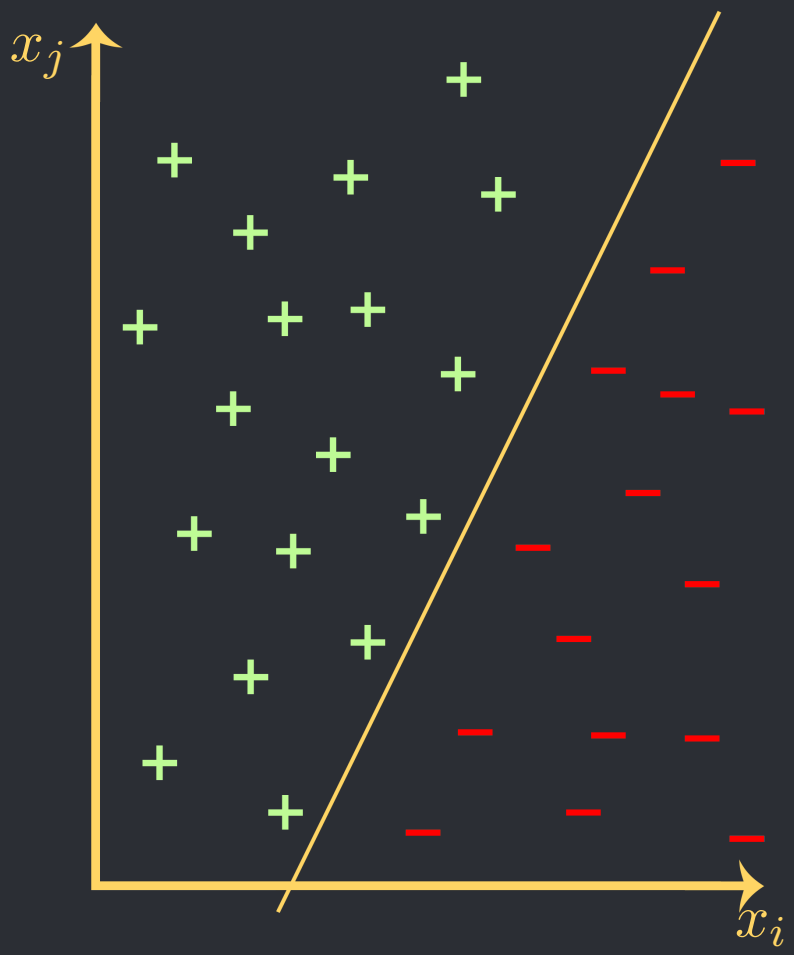

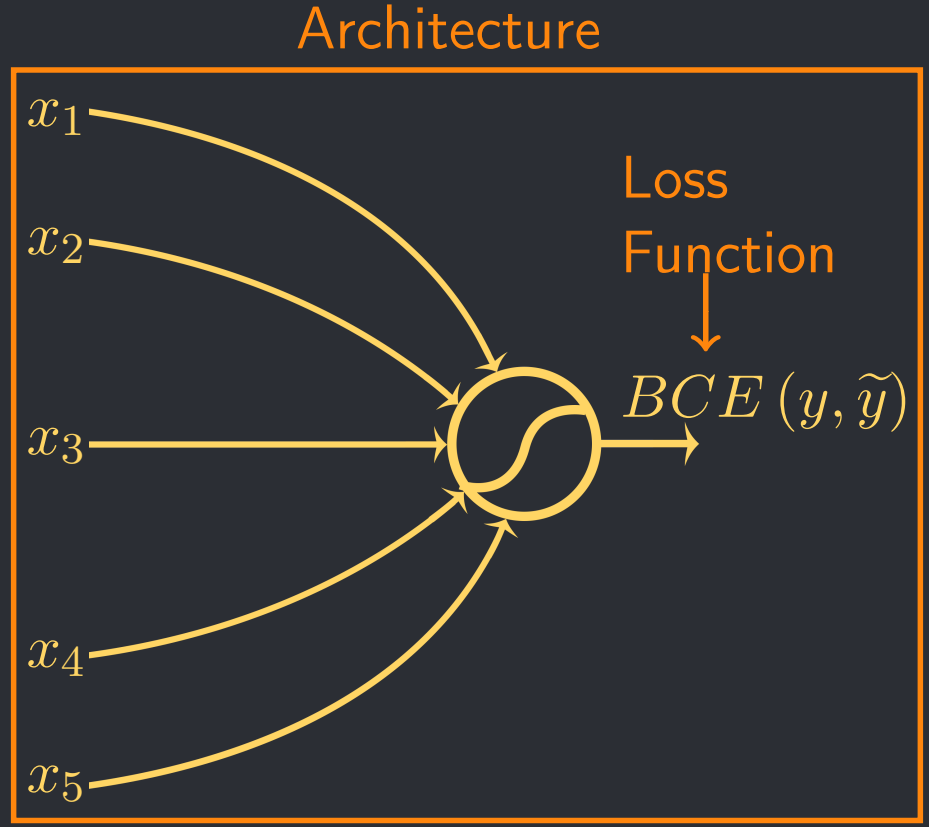

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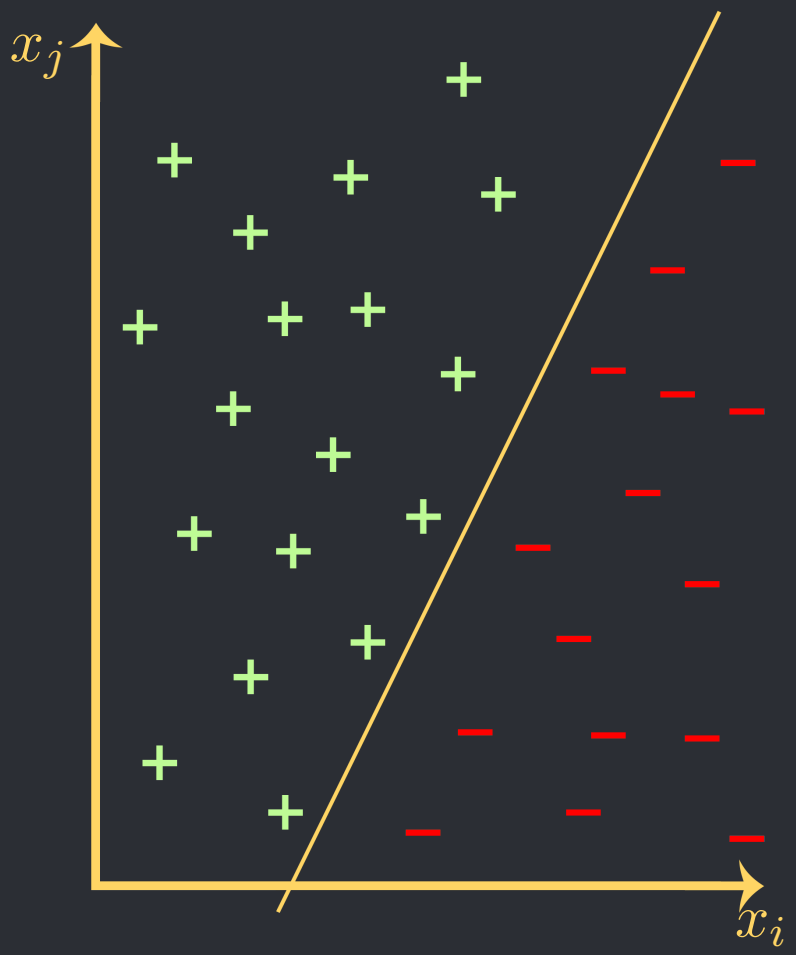

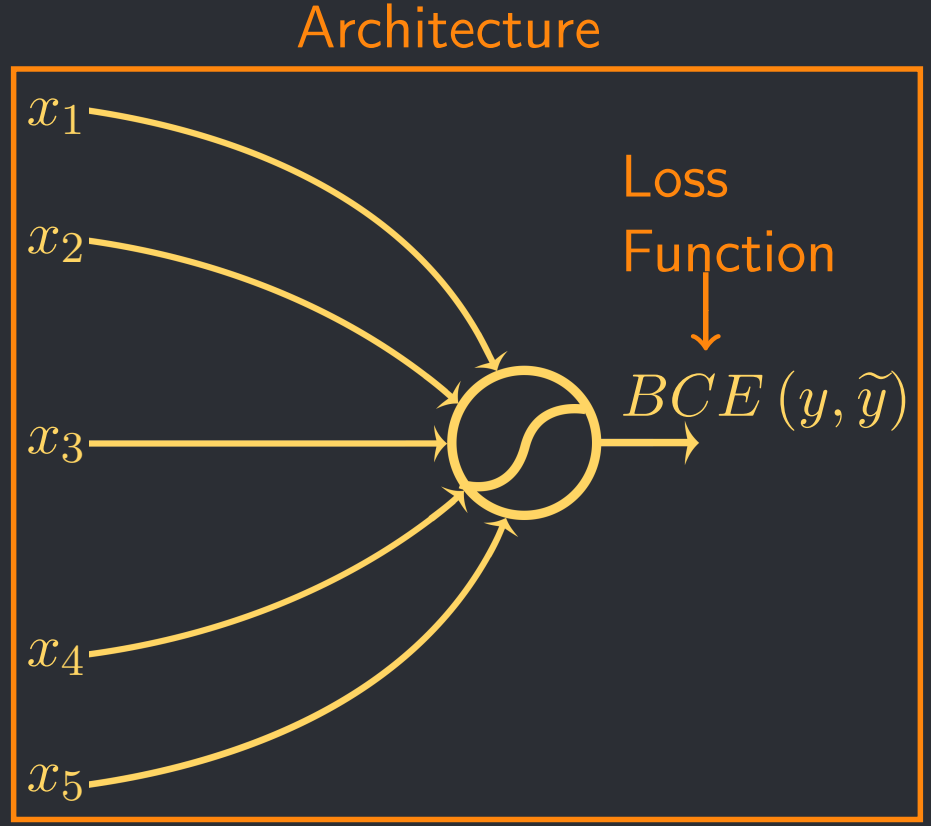

Optimization – stochastic gradient descent

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