NEURAL NETWORKS AND BACKPROPAGATION

Machine Learning for Autonomous Robots

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1. Recap: Linear Regression and Logistic Regression
2. Neural Networks
3. Learning Neural Networks with Backpropagation
4. Automatic Differentiation
5. Summary and applications

Recap

Linear Model

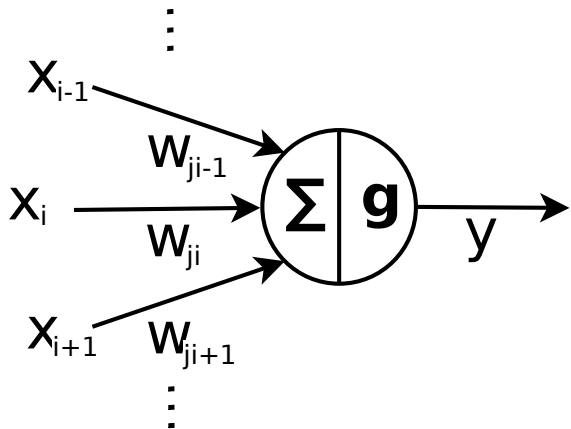


Figure: A linear model computes the **weighted** sum of inputs and optionally applies a non-linear scaling function g.

Multi-dimensional output:

$$\boldsymbol{y} = \boldsymbol{W}\boldsymbol{x}, \quad \boldsymbol{y} \in \mathbb{R}^F, \quad \boldsymbol{x} \in \mathbb{R}^D, \quad \boldsymbol{W} \in \mathbb{R}^{F \times D}$$

Error function (sum of squared errors):

$$E(\boldsymbol{W}) = \frac{1}{2} \sum_n ||\boldsymbol{W}\boldsymbol{x}_n - \boldsymbol{y}_n||^2$$

Gradient:

$$\nabla_{\boldsymbol{W}} E_n(\boldsymbol{W}) = (\boldsymbol{W}\boldsymbol{x}_n - \boldsymbol{y}_n)\boldsymbol{x}_n^T$$

Multi-Class Logistic Regression

Multi-dimensional output (one-hot encoding, softmax):

$$\boldsymbol{y} = g(\boldsymbol{W}\boldsymbol{x}),\ \boldsymbol{y} \in [0,1]^F,\ \boldsymbol{x} \in \mathbb{R}^D,\ \boldsymbol{W} \in \mathbb{R}^{F \times D},\ g_i(t) = \frac{e^{t_i}}{\sum e^{t_j}}$$

Error function (cross-entropy):

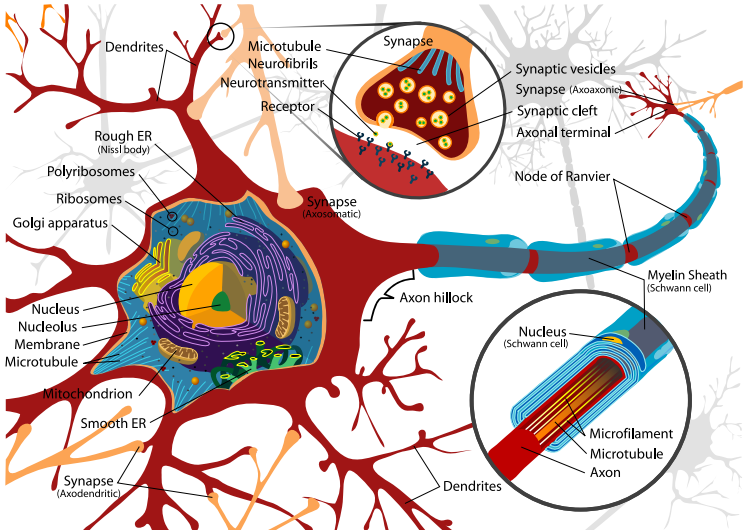
$$E(\boldsymbol{W}) = -\sum_n \sum_f \boldsymbol{y}_{nf} \ln \left(g(\boldsymbol{W}\boldsymbol{x}_n)\right)_f$$

Gradient:

$$\nabla_{\boldsymbol{W}} E_n(\boldsymbol{W}) = \left(g(\boldsymbol{W}\boldsymbol{x}_n) - \boldsymbol{y}_n\right) \boldsymbol{x}_n^T$$

Neural Networks

Natural Neuron



Artificial Neuron

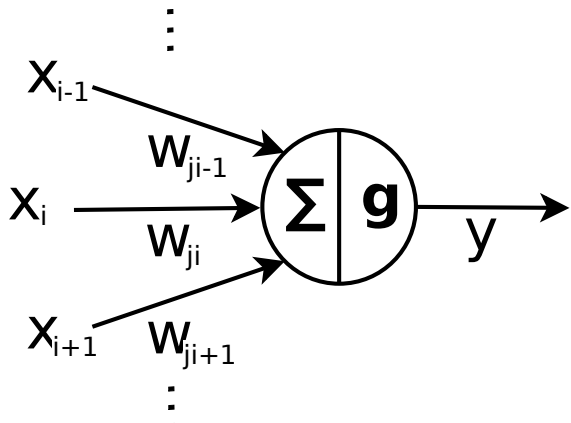


Figure: An artificial neuron computes the **weighted** sum of inputs and applies a non-linear activation function g.

Artificial Neuron

The **output** y_j of a neuron node is calculated by taking the sum of all signals x_i weighted by a **connection strength** w_{ji} and transforming the sum by the **activation function** g.

$$y_j = g\left(\sum_i^n w_{ji} x_i\right)$$

We can compute the outputs of multiple neurons that have the same inputs with

$$\boldsymbol{y} = g\left(\boldsymbol{W}\boldsymbol{x}\right) .$$

Does that remind you of something?

Artificial Neural Network (ANN)

- ANNs are **interconnected assemblies** of computational **nodes** which are loosely based on the animal **neuron**.
- The computational ability of the neural network is encoded in the inter-unit connection strengths (**weights**).
- A neural network has **input** and **output nodes** which receive and give out signals to the environment, respectively.
- All other nodes are called **hidden nodes**.

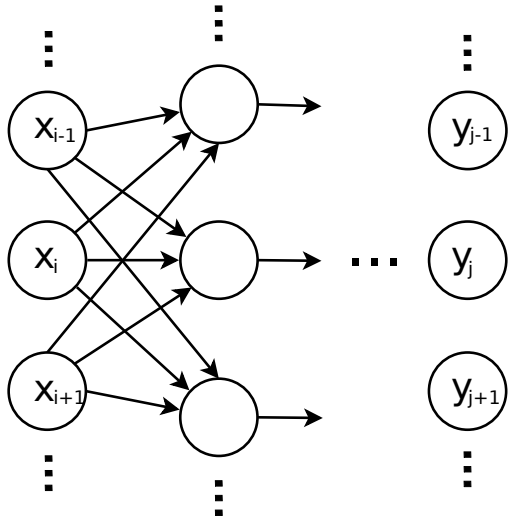


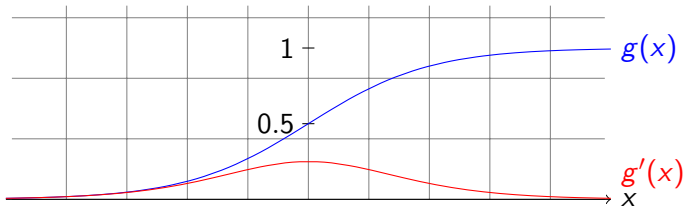
Figure: Where are the input nodes, output nodes and hidden nodes?

Activation Functions

Most commonly used activation functions:

- identity function $g(a) = a$
- rectified linear unit: $g(a) = a$ if $a > 0$, else 0
- leaky rectified linear unit: $g(a) = a$ if $a > 0$, else ϵa
- sigmoid functions:
  - logistic sigmoid $g(a) = \frac{1}{1+\exp(-a)} \in [0, 1]$
  - hyperbolic tangent: $g(a) = \tanh(a) \in [-1, 1]$

Logistic Sigmoid



$$g(x) = \frac{1}{1 + e^{-x}}$$
$$g'(x) = g(x)(1 - g(x))$$

Architecture

The architecture of a neural network plays an important role for its behavior.

- **number** of neurons
- **pattern of connectivity** (most neural nets are organized in layers: input layer, hidden layer(s) and output layer)
- **feedforward**: directed acyclic graphs
- **recurrent**: recurrent connection from upper layer to a lower layer, or recurrent connection from the same neuron, results in *complex time-dependent dynamics* (deutsch: rückläufig)

Multilayer Neural Network

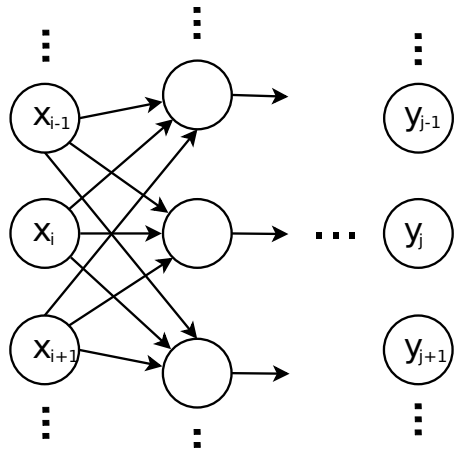
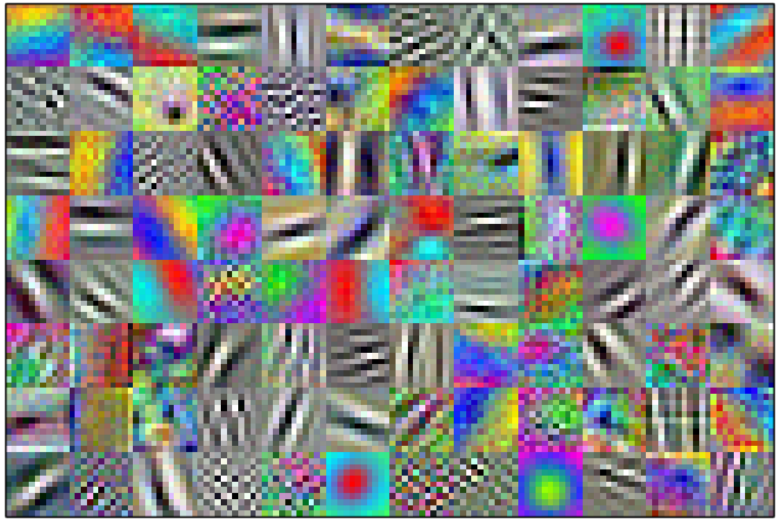


Figure: Neurons of successive layers are fully connected.

Weight Visualizations

Weight Visualizations



http://sklearn-theano.github.io/images/plot_overfeat_layer1_filters_002.png

Backpropagation

Supervised Learning

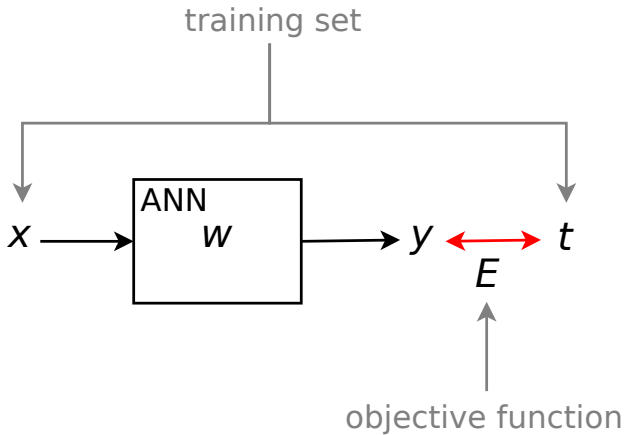


Figure: Weights are updated **iteratively** using the discrepancy between the **desired output** $\boldsymbol{t}$ and the **output given by the network for a given input pattern** $\boldsymbol{x}$.

Weight Update

The weights are modified, e.g. using **gradient descent**

$$w_{ji}(t+1) = w_{ji}(t) - \alpha \Delta w_{ji}(t) \qquad 0 < \alpha \leq 1\,,$$

where

- $w_{ji}(t)$ and $w_{ji}(t+1)$ is the weight of input i for neuron j before and after modification, respectively,
- and α is the learning rate

How can we compute $\Delta w_{ji}(t)$?

- **Backpropagation** is a method to compute the gradient of the error function E with respect to the weights $\boldsymbol{w}$ of a neural net

$$\nabla_{\boldsymbol{w}} E = \begin{pmatrix} \vdots \\ \frac{\partial E}{\partial w_{ji}} \\ \vdots \end{pmatrix}.$$

- The gradient can be used in the update equation (here: written with vectors)

$$\boldsymbol{w}(t+1) = \boldsymbol{w}(t) - \alpha \Delta \boldsymbol{w}(t) \qquad 0 < \alpha \leq 1, \quad \Delta \boldsymbol{w}(t) = \nabla_{\boldsymbol{w}(t)} E$$

Objective Function

- We seek to minimize the total error E over all patterns in the training set given by (the index n labels the patterns)

$$E = \sum_n E^n.$$

- Let us assume that the error function E^n is a function of network outputs $y_1, \ldots, y_F$,

$$E^n = E^n(y_1, \ldots, y_F)\,.$$

- Our goal is to find a procedure (error back-propagation) for evaluating the derivative of the error function with respect to the weights of the network.

Forward Propagation

- Each neuron j in a neural net computes a weighted sum

$$a_j = \sum_i w_{ji} x_i,$$

  where x_i is the i-th input, which is connected to neuron j and w_{ji} is the weight associated with that connection.
- The output of neuron j denoted by y_j is obtained by

$$y_j = g(a_j).$$

- In the next layer, the output y_j of the previous layer will be written as x_i and the output of the last layer will be the output of the neural net.

Artificial Neuron

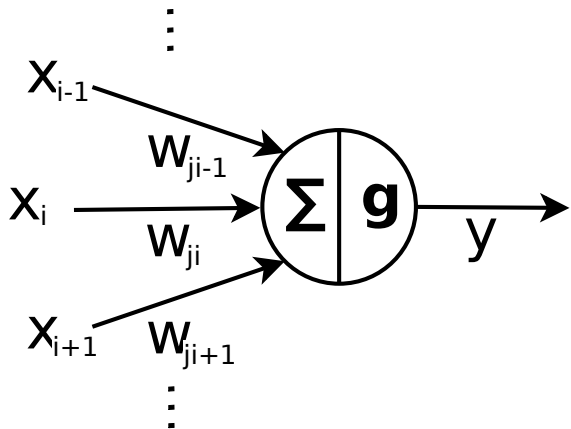


Figure: An artificial neuron computes the **weighted** sum of inputs and applies a non-linear scaling function g.

Tools (Differentiation Rules)

- Sum rule:

$$(f + g)' = f' + g'$$

- Chain rule:

$$(f \circ g)' = (f' \circ g) \cdot g'$$

$$\frac{\partial f}{\partial x} = \sum_y \frac{\partial f}{\partial y} \frac{\partial y}{\partial x}$$

- Product rule:

$$(f \cdot g)' = f' \cdot g + f \cdot g'$$

Notation

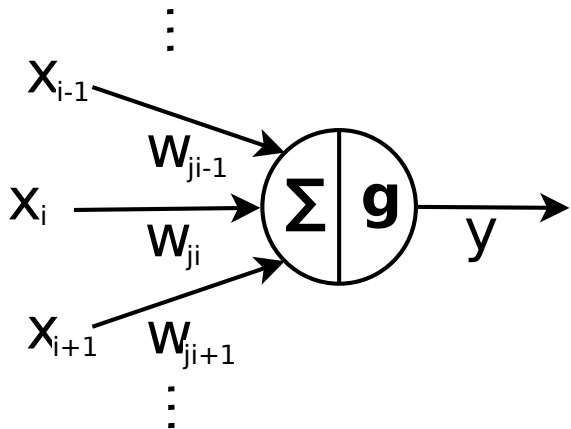


Figure: i refers to an input and j refers to the corresponding neuron. Note that in the next layer the output of neuron j might be called input with index i.

Gradient

- The partial derivative of E^n with respect to w_{ji} is

$$\frac{\partial E^n}{\partial w_{ji}} = \frac{\partial E^n}{\partial a_j} \frac{\partial a_j}{\partial w_{ji}} .$$

- It is obvious that

$$\frac{\partial a_j}{\partial w_{ji}} = \frac{\partial \sum_{i'} w_{ji'} x_{i'}}{\partial w_{ji}} = x_i .$$

- By *forward propagation*, we can calculate x_i.
- The quantity $\frac{\partial E^n}{\partial a_j}$ is replaced by the symbol δ_j so that

$$\frac{\partial E^n}{\partial w_{ji}} = \delta_j x_i .$$

Deltas (Hidden Neurons)

- For a hidden neuron i, we derive an equation that represents δ_i in terms of δ_j's of neurons j **to which it sends its output**.
- We **back-propagate** the δ_j's for the network.

$$\delta_i = \frac{\partial E^n}{\partial a_i} = \sum_j \frac{\partial E^n}{\partial a_j} \frac{\partial a_j}{\partial a_i} = \sum_j \delta_j \frac{\partial a_j}{\partial a_i} .$$

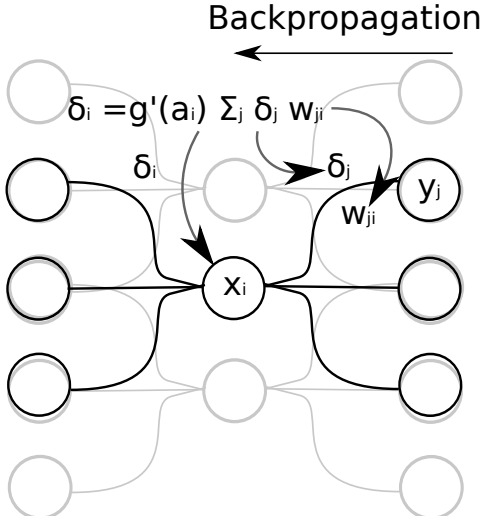
- We know that $a_j = \sum_{i'} w_{ji'} \underline{x_{i'}} = \sum_{i'} w_{ji'} \underline{g(a_{i'})}$. It follows that

$$\frac{\partial a_j}{\partial a_i} = g'(a_i) w_{ji} .$$

- The equation for the back-propagation is thus given by

$$\delta_i = \sum_j \delta_j g'(a_i) w_{ji} = g'(a_i) \sum_j \delta_j w_{ji} .$$

Deltas (Hidden Neurons)



Deltas (Output Neurons)

- For an output neuron k,

$$\delta_k = \frac{\partial E^n}{\partial a_k} = \frac{\partial E^n}{\partial y_k}\frac{\partial y_k}{\partial a_k} = \frac{\partial E^n}{\partial y_k} g'(a_k)$$

- Let as assume that the activation function of the output neurons is linear and is given by $g(a) = a$. **Since $g'(a_k) = 1$, we get**

$$\delta_k = \frac{\partial E^n}{\partial y_k}\,.$$

Deltas (Output Neurons)

- Assuming a sum of squared error function

$$E^n = \frac{1}{2}\sum_{k=1}^{c}(y_k - t_k^n)^2\,,$$

  we get

$$\delta_k = \frac{\partial E^n}{\partial y_k} = y_k - t_k^n\,.$$

- We see that δ_k represents in this case an error for the output units.

Summary (Backpropagation)

Error back-propagation for evaluating the derivative of E^n:

1. For a given input, do forward propagation: $a_j = \sum_i w_{ji} x_i, \quad y_j = g(a_j)$.
2. Compute the $\delta_k = y_k - t_k^n$ for each output neuron.
3. Back propagate the δ's using $\delta_i = g'(a_i) \sum_j \delta_j w_{ji}$ to obtain δ_i for each hidden neuron in the network.
4. Apply $\frac{\partial E^n}{\partial w_{ji}} = \delta_j x_i$ to calculate the required derivatives.

The derivative for the total error can be obtained using

$$\frac{\partial E}{\partial w_{ji}} = \sum_n \frac{\partial E^n}{\partial w_{ji}} .$$

Batch vs. Stochastic

For training the network the weights of the network are modified using

$$w_{ji} = w_{ji} - \alpha \Delta w_{ji} \qquad 0 < \alpha \leq 1\,,$$

For **online learning** (stochastic gradient descent) we choose

$$\Delta w_{ji} = \frac{\partial E^n}{\partial w_{ji}}$$

For **batch learning** (gradient descent) we choose

$$\Delta w_{ji} = \frac{\partial E}{\partial w_{ji}}\,.$$

Automatic Differentiation

Types of Differentiation

We can distinguish

- Symbolic differentiation
  - symbolic expression of gradient for all possible inputs
  - cannot compute derivative of complex control flows (branching, loops, recursion)
- Numeric differentiation
  - approximation of gradient for specific input
  - computationally expensive for large number of variables
- Automatic differentiation (AD)
  - evaluation of gradient for specific input

Automatic Differentiation

We can distinguish

- Forward mode / forward accumulation mode / tangent linear mode
  - implementation: dual numbers, single pass
  - better for multivariate functions with many outputs
  - worse for functions with large number of arguments
- Reverse mode / reverse accumulation mode
  - implementation: generalized backpropagation, two phases
  - better for functions with large number of arguments
  - worse for multivariate functions with many outputs

More details: `http://jmlr.org/papers/v18/17-468.html`

Dual Numbers

A dual number has the form

$$v + \dot{v}\epsilon,$$

where

- $v, \dot{v} \in \mathbb{R}$
- $\epsilon^2 = 0$ and $\epsilon \neq 0$

Basic operations:

- Addition: $(1 + 2\epsilon) + (3 + 4\epsilon) = 4 + 6\epsilon$
- Subtraction: $(1 + 2\epsilon) - (3 + 4\epsilon) = -2 - 2\epsilon$
- Multiplication: $(1 + 2\epsilon) \cdot (3 + 4\epsilon) = 3 + 6\epsilon + 4\epsilon + \underbrace{8\epsilon^2}_{0} = 3 + 10\epsilon$

Differentiation with Dual numbers

$$f(x) = x^2 + 2x + 3$$

What is $f'(x)$?

$$f'(x) = 2x + 2$$

For example, $f'(3) = 8$, $f'(-2) = -2$

$$\begin{aligned} f(3+\epsilon) &= (3+\epsilon)^2 + 2(3+\epsilon) + 3 \\ &= 9 + 6\epsilon + 6 + 2\epsilon + 3 \\ &= 18 + \underline{8\epsilon} \end{aligned}$$

$$\begin{aligned} f(-2+\epsilon) &= (-2+\epsilon)^2 + 2(-2+\epsilon) + 3 \\ &= 4 - 4\epsilon - 4 + 2\epsilon + 3 \\ &= 3\underline{-2\epsilon} \end{aligned}$$

Summary and applications

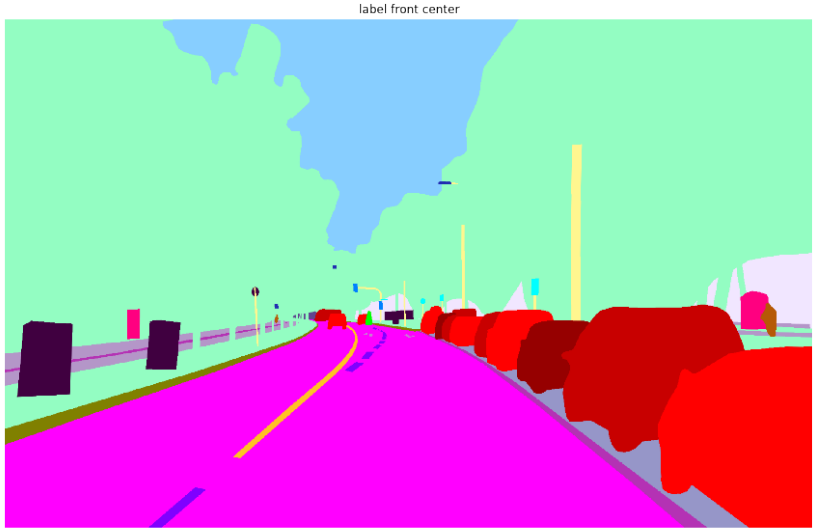
- Recap: linear regression and logistic regression
- Very loose motivation by natural neurons
- Different activation functions
- We often use a layer structure
- Derivation of backpropagation
- Backpropagation is automatic differentiation

Object Detection

For example:

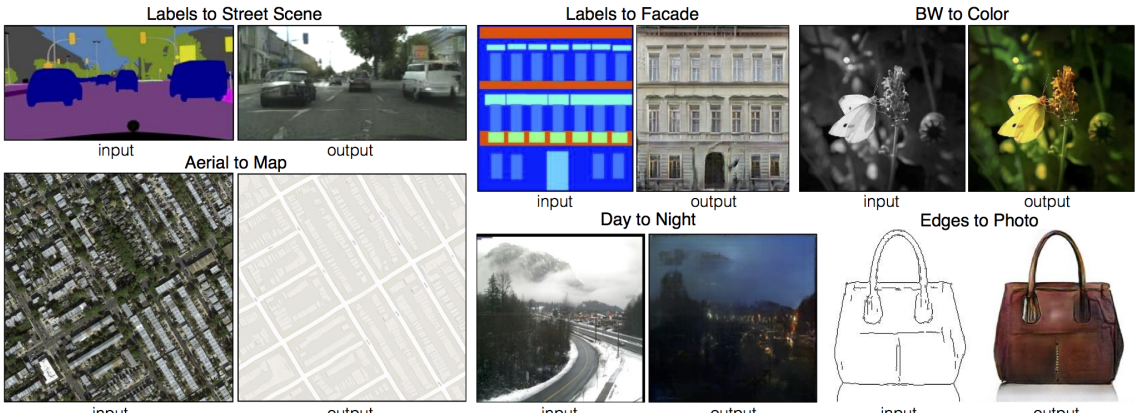
https://github.com/facebookresearch/detectron2

Semantic Segmentation



Dataset: `http://www.a2d2.audi`

Image Enhancement



Translation

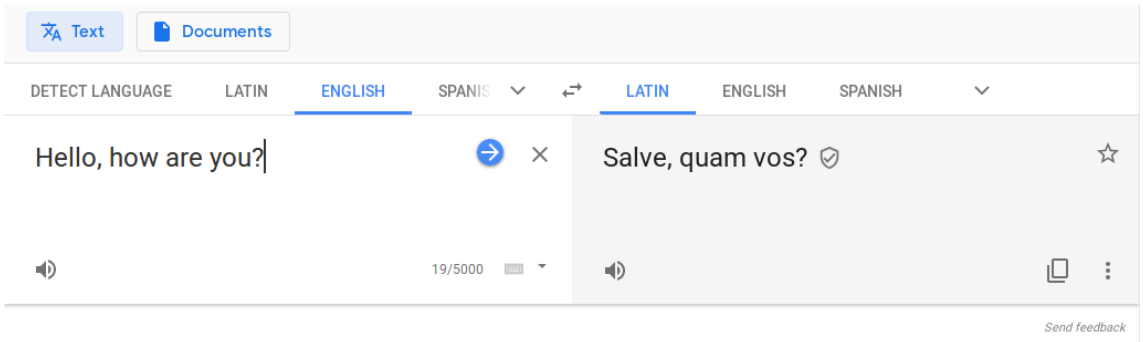


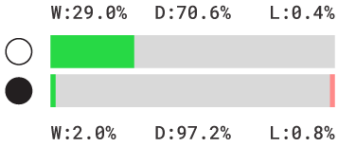
Image Captioning

a group of giraffes standing in a grassy area

Playing Board Games

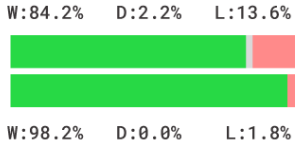
Chess

AlphaZero vs. Stockfish

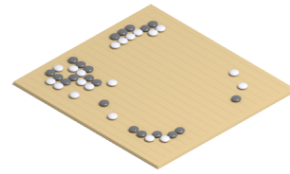


Shogi

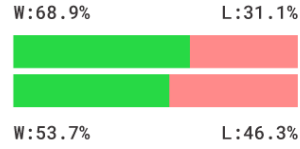
AlphaZero vs. Elmo



Go



AlphaZero vs. AG0



Playing Computer Games

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Thank You!
Please feel free to ask questions in the forums.