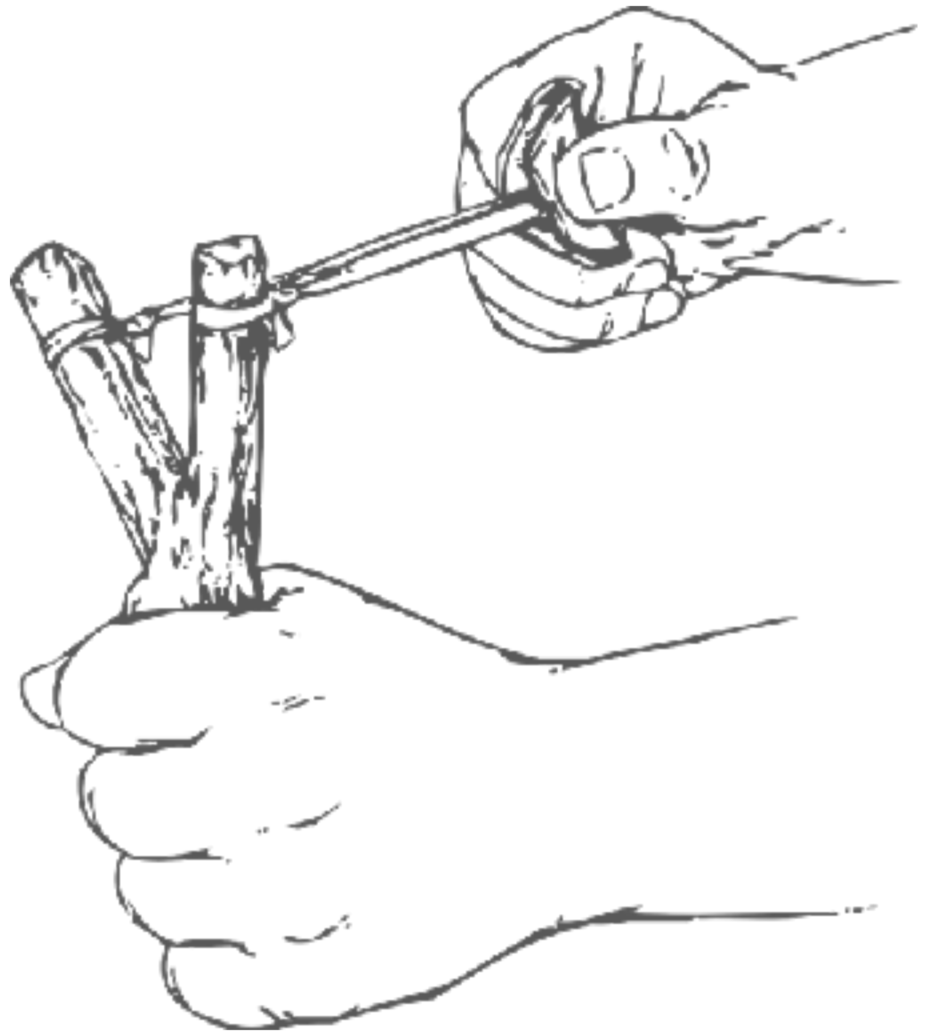
Understanding Large Language Models

Carsten Eickhoff, Michael Franke and Polina Tsvilodub

Session 02: PyTorch, Optimization, ANNs, LMs & RNNs

Main learning goals



1. PyTorch
   - simple optmization problems with stochastic gradient descent (SGD)
   - basic usage of nn.Module and Dataset classes
2. Optimization (via Backpropagation)
   - basic concepts: loss function, gradients, brackpropagation, SGD
   - anatomy of update step & training loop (in PyTorch)
3. Artificial Neural Networks (specifically: Multi-Layer Perceptrons)
   - definitions of ANNs & MLPs, mathematical notation in matrix-vector form
   - concepts: weights & biases (slopes & intercepts), activation (function), hidden layers, score, prediction (sample, probability)
4. Language Models
   - definition of (autoregressive) language models, loss functions, decoding
5. Recurrent Neural Networks
   - definition & example (character-level RNN for surname generation)

PyTorch

Key features

- high-level framework for ML
  - especially for artificial neural networks
- efficient tensor algebra
  - ability to run on GPUs
- pre-defined building blocks for ANNs
  - standard layers, data handling etc.
- automatic differentiation
  - enables efficient optimization

```
nTrainingSteps= 10000
for i in range(nTrainingSteps):
    pred =  torch.distributions.Normal(loc=location,
                                           scale=1.0)
    loss = -torch.sum(prediction.log_prob(trainData))
    loss.backward()
    if (i+1) % 500 == 0:
        opt.step()
        opt.zero_grad()
```


Patzke et al. (2019) “PyTorch: An Imperative Style, High-Performance Deep Learning Library”

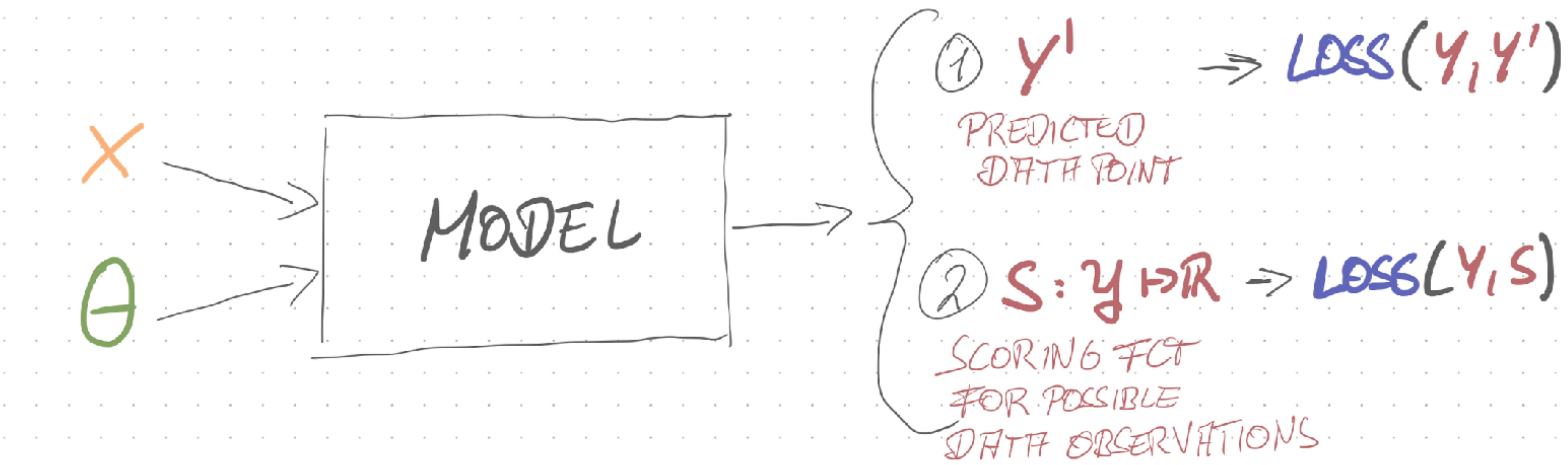
demo
PyTorch

demo 01: PyTorch essentials

Optimizatio
n

Models, parameters, predictions & loss

DATA : $\langle X, Y \rangle$ MODEL: $F_\theta : X \mapsto Y$

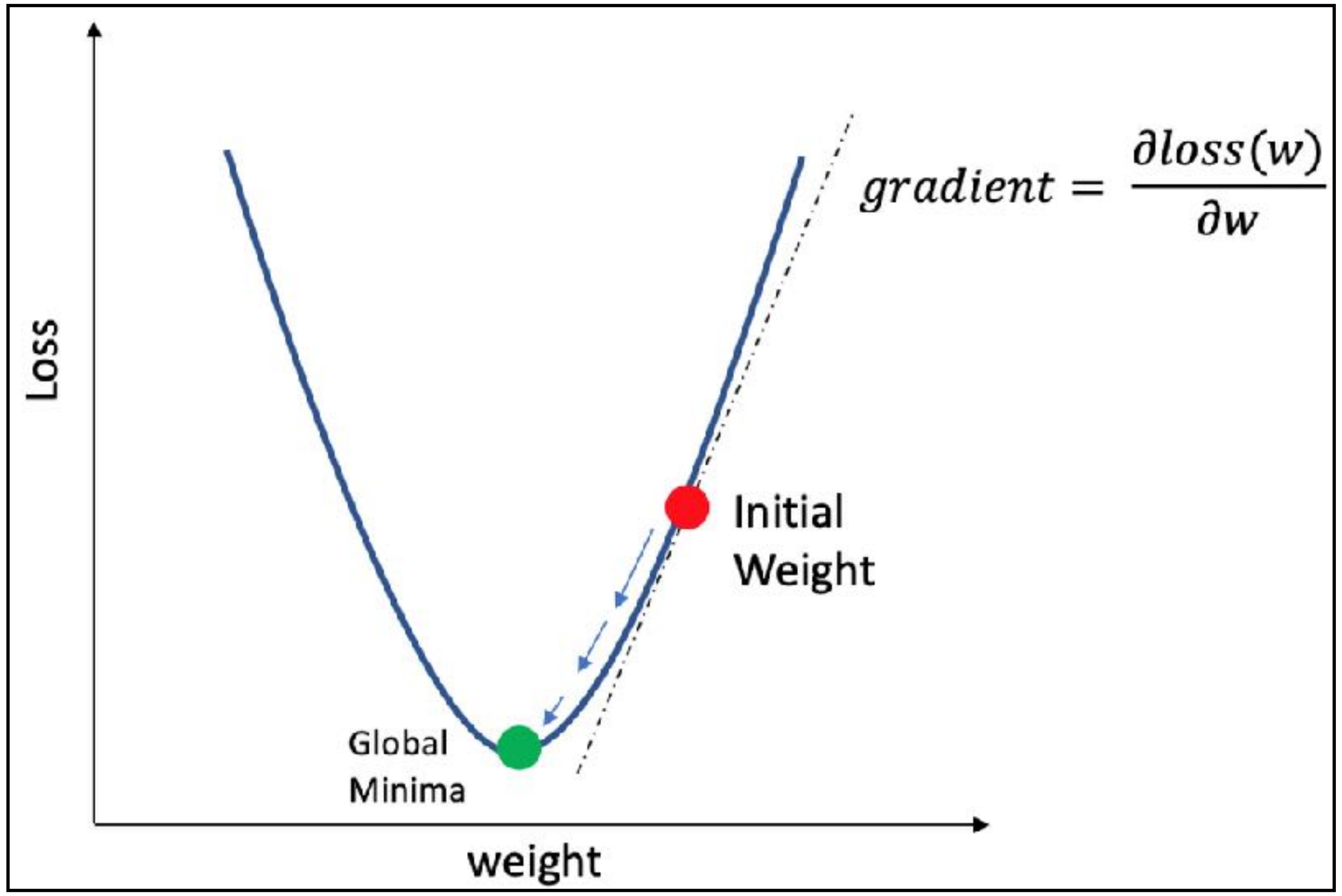


Optimization
for probabilistic models

- given:
  - data $D = \langle X, Y \rangle$
  - probabilistic model $M\colon \Theta, X \to \Delta(Y)$
  - loss function $L\colon \Theta, X, Y \to \mathbb{R}$
    - most commonly used is negative log likelihood:

      $$L\left(\theta, x, y\right) = -\log P_{M(\theta,x)}\left(y\right)$$
- find parameters that minimize loss for data:

  $$\hat{\theta} = \arg\max_{\theta \in \Theta} = \sum_{x \in X, y \in Y} L\left(\theta, x, y\right)$$



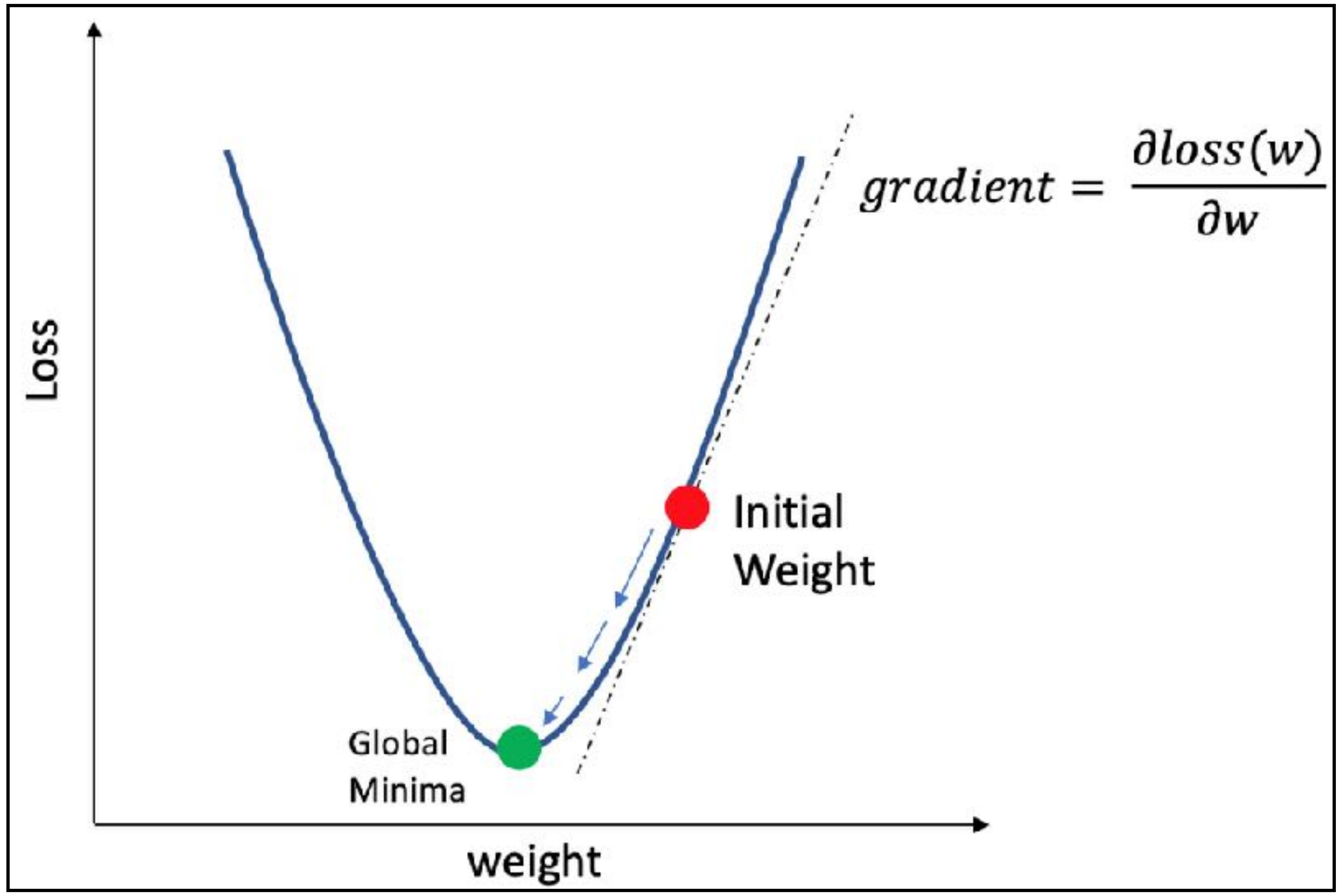
Stochastic gradient descent

input : γ (lr), θ_0 (params), $f(\theta)$ (objective), λ (weight decay),
μ (momentum), τ (dampening), *nesterov*, *maximize*

for $t = 1$ **to** $\ldots$ **do**
  $g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$
  if $\lambda \neq 0$
    $g_t \leftarrow g_t + \lambda \theta_{t-1}$
  if $\mu \neq 0$
    if $t > 1$
      $\mathbf{b}_t \leftarrow \mu \mathbf{b}_{t-1} + (1 - \tau) g_t$
    else
      $\mathbf{b}_t \leftarrow g_t$
    if *nesterov*
      $g_t \leftarrow g_t + \mu \mathbf{b}_t$
    else
      $g_t \leftarrow \mathbf{b}_t$
  if *maximize*
    $\theta_t \leftarrow \theta_{t-1} + \gamma g_t$
  else
    $\theta_t \leftarrow \theta_{t-1} - \gamma g_t$

return $\boldsymbol{\theta_t}$

from PyTorch Documentation of SGD



from this paper

Stochastic gradient descent

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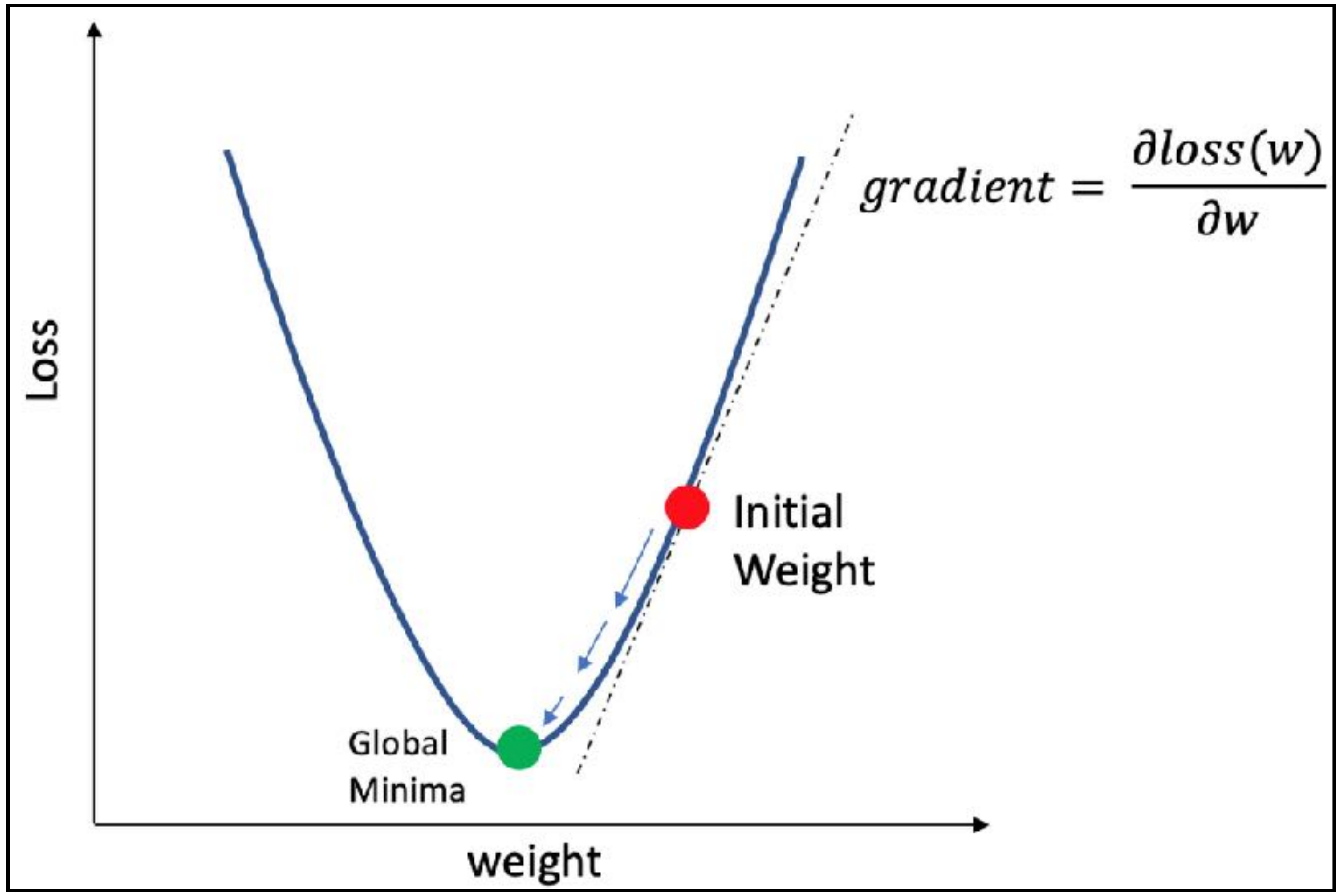
---

return $\theta_\mathbf{t}$

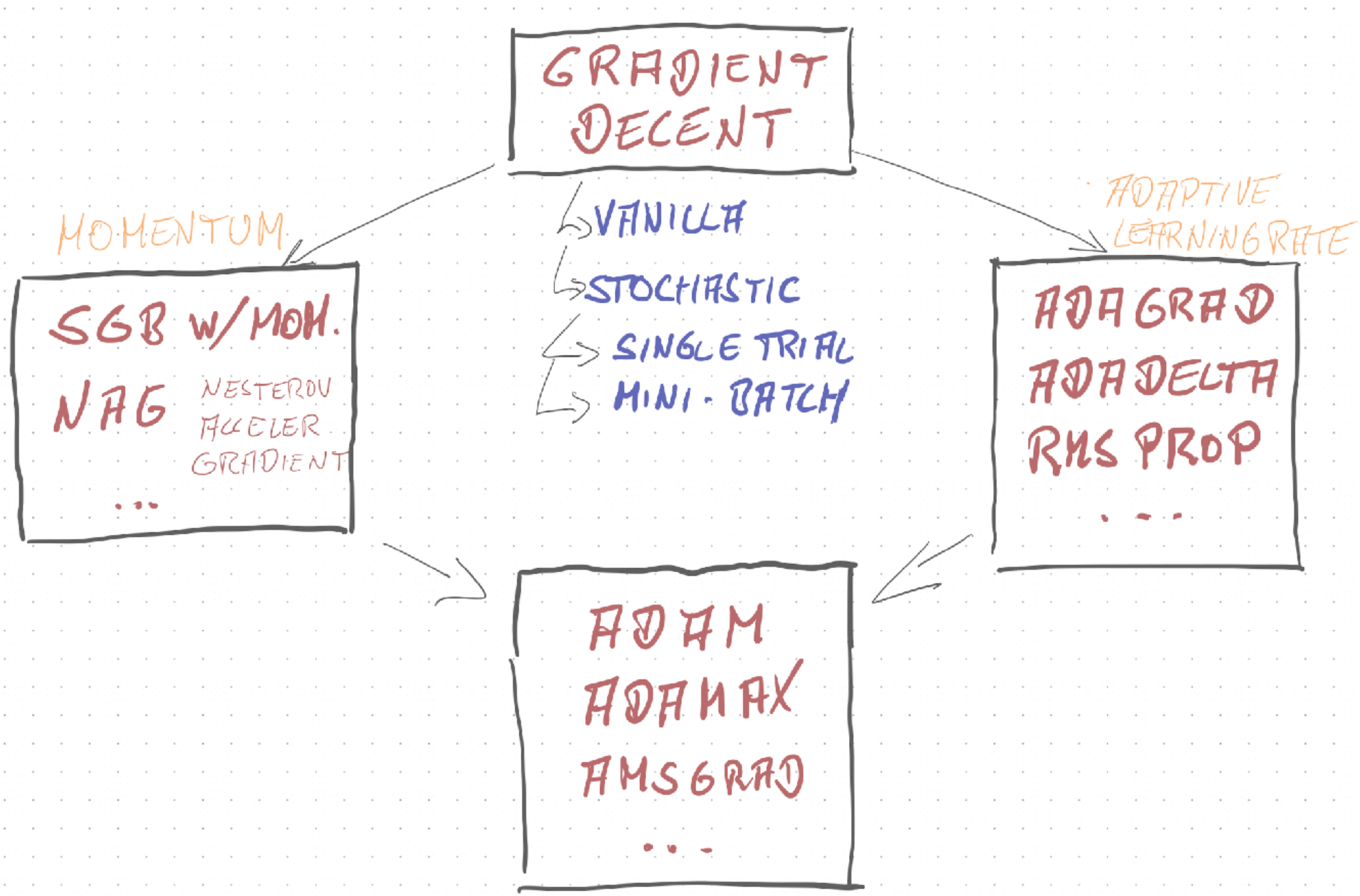
---

from PyTorch Documentation of SGD



from this paper

Common optimization algorithms



Anatomy of a training step

CSP-Subheading

1. compute predictions
   - what do we predict in the current state?
2. compute the loss
   - how good is this prediction (for the training data)?
3. backpropagate the error
   - in which direction would we need to change the relevant parameters to make the prediction better?
4. update the parameters
   - change the parameters (to a certain degree, the so-called learning rate) in the direction that should make them better
5. zero the gradients
   - reset the information about “which direction to tune” for the next training step

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    loss.backward()
    if (i+1) % 500 == 0:
        opt.step()
        opt.zero_grad()
```

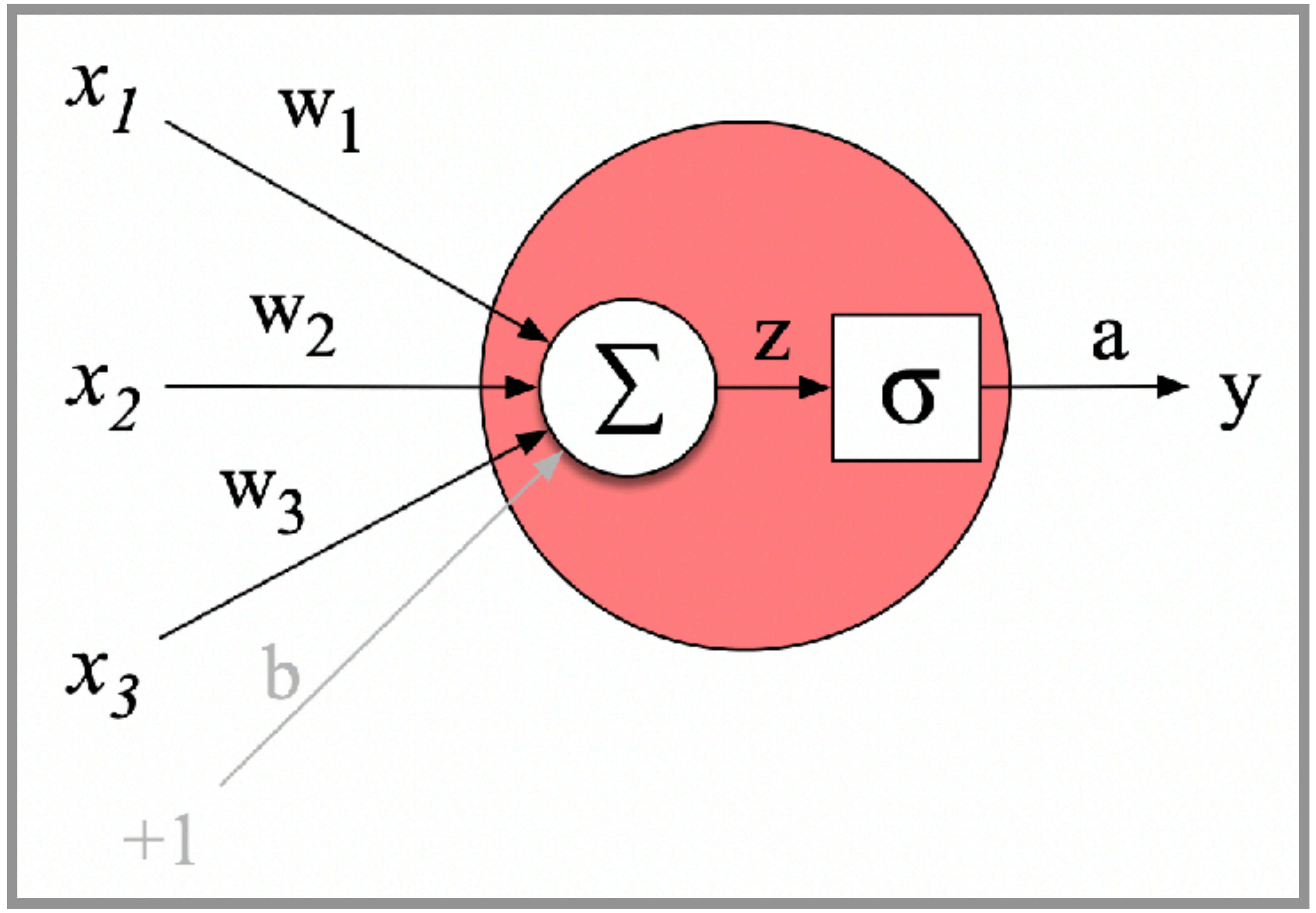
demo
optimization

demo 02: Maximum Likelihood Estimation (in PyTorch)

Artificial Neural Networks

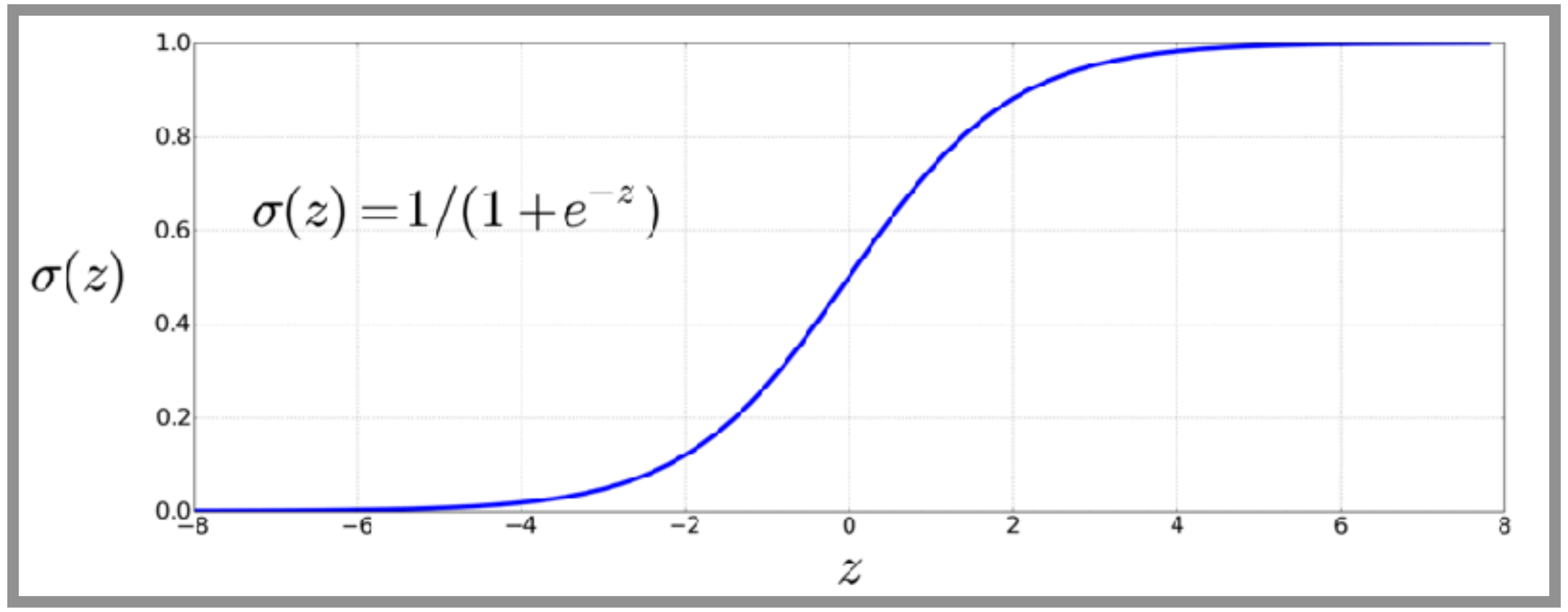
Units neurons

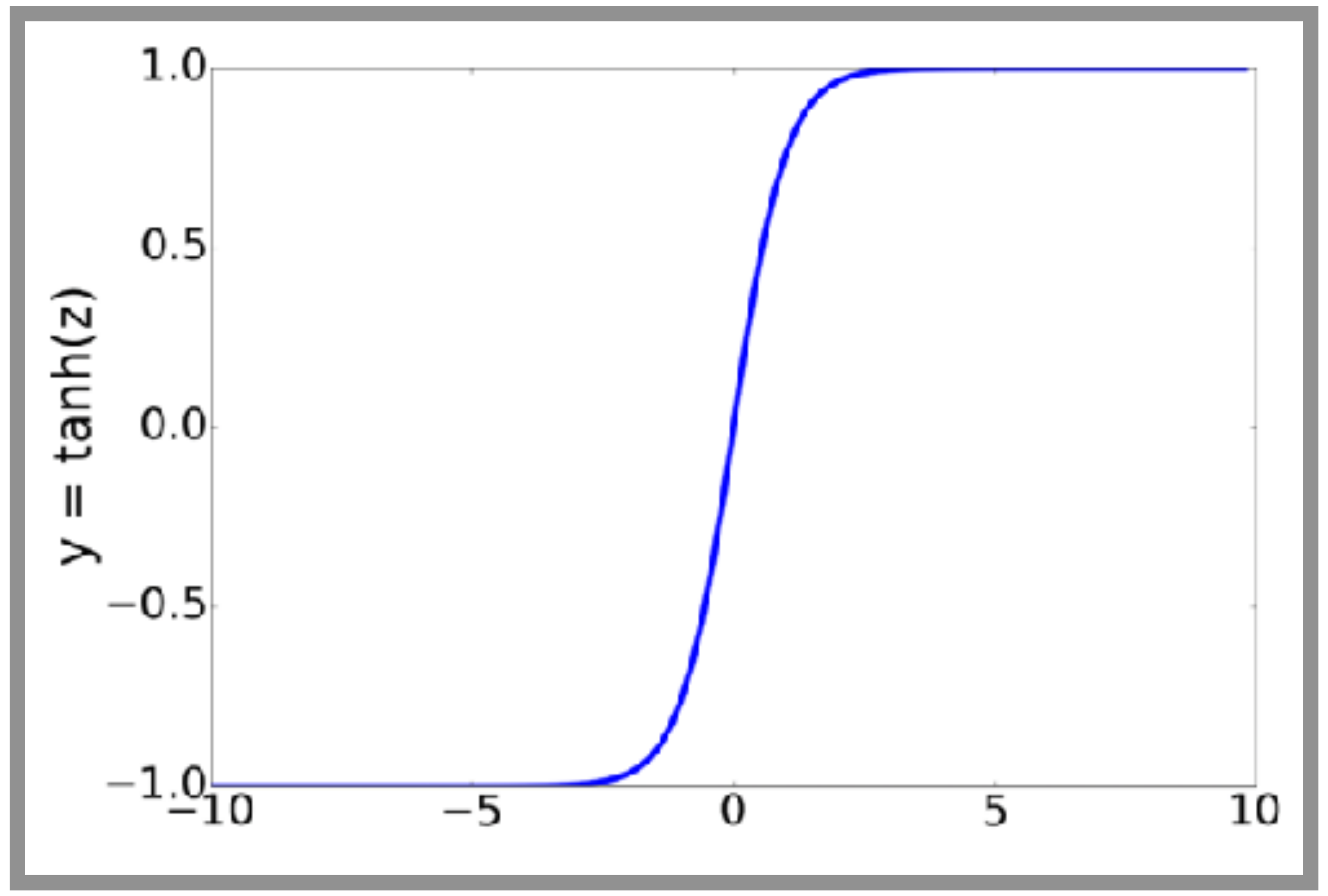
- input vector:
  $\mathbf{x} = [x_1, \ldots, x_n]^\intercal$
- weight vector:
  $\mathbf{w} = [w_1, \ldots, w_n]^\intercal$
- bias:
  b
- score:
  $$z = b + \sum_{j=1}^{n} w_j x_j = b + \mathbf{w} \cdot \mathbf{x}$$
- activation level:
  - $a = f(z)$, where f is the **activation function**

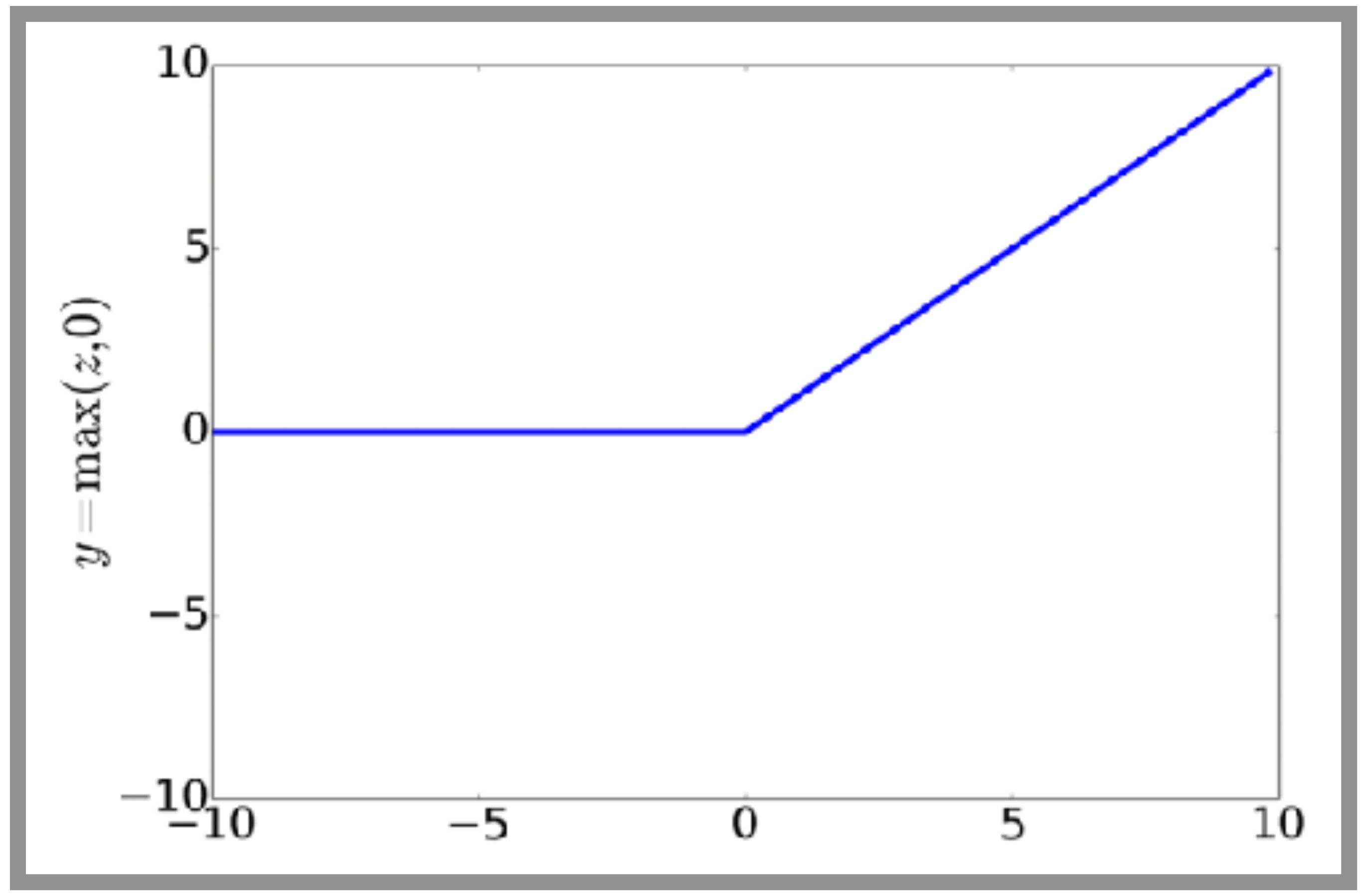


Common activation functions

- perceptron:
  $f(z) = \delta_{z>0}$
- sigmoid:
  $$f(z) = \sigma(z) = \frac{1}{1 + \exp(-z)}$$
- hyperbolic tangent:
  $$f(z) = \tanh(z) = \frac{\exp(z) - \exp(-z)}{\exp(z) + \exp(-z)}$$
- rectified linear unit:
  $f(z) = \mathrm{ReLU}(z) = \max(z,0)$

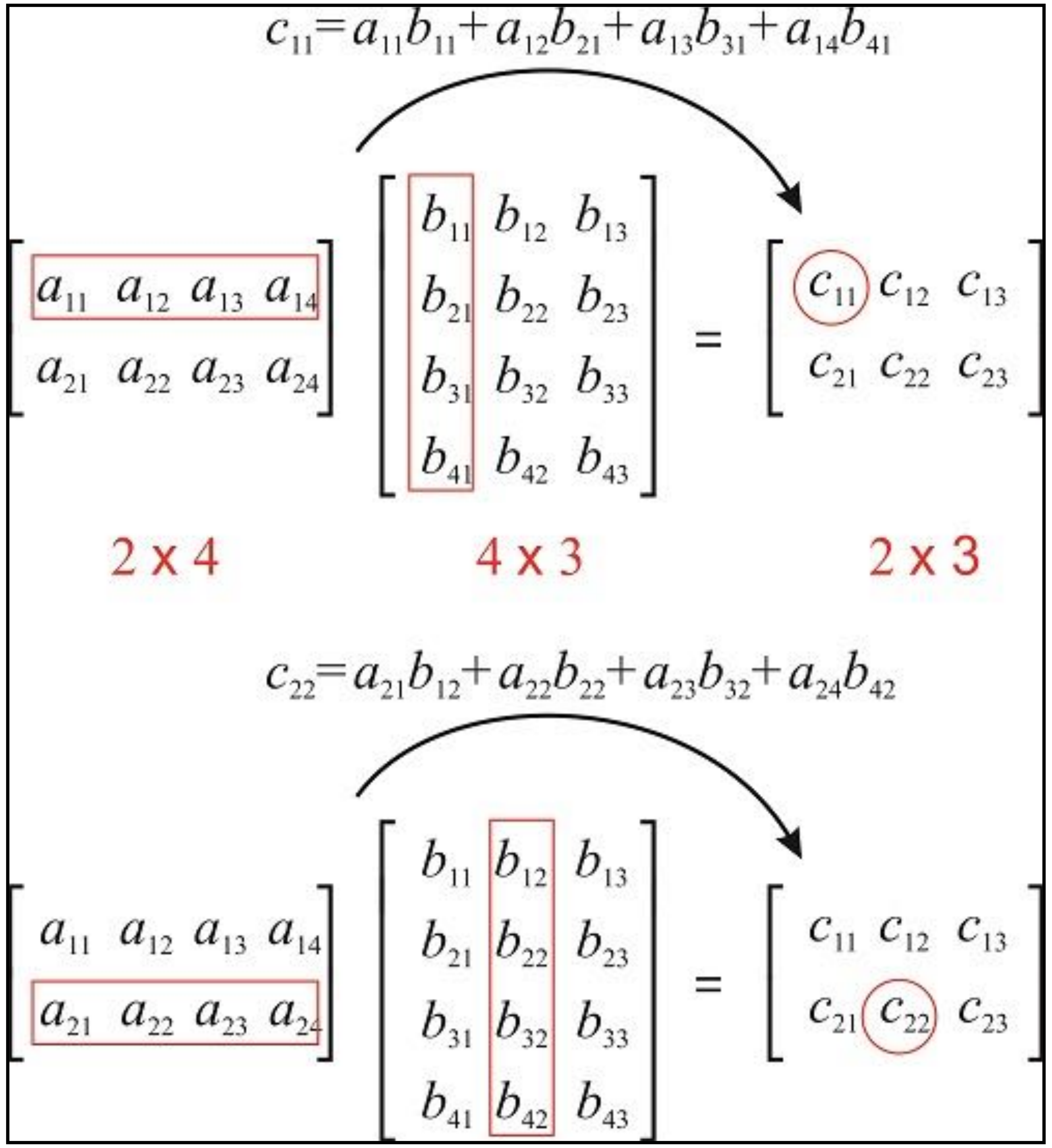






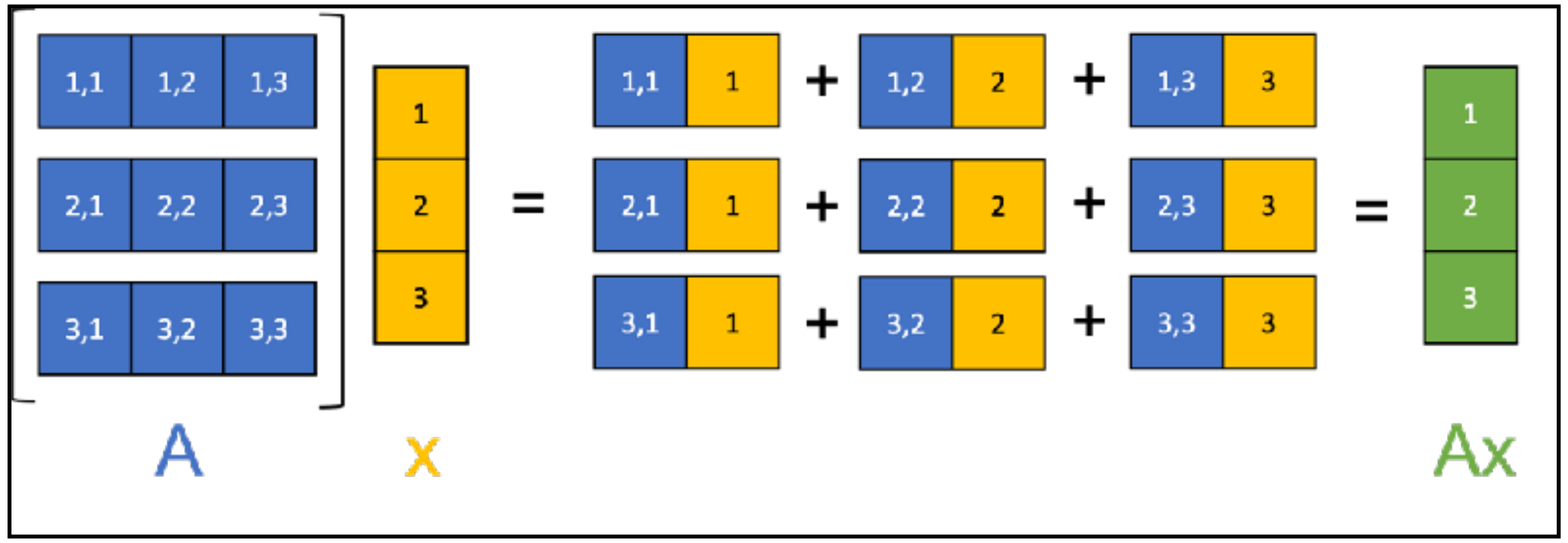
Matrix multiplication

recap



Matrix-vector multiplication

recap



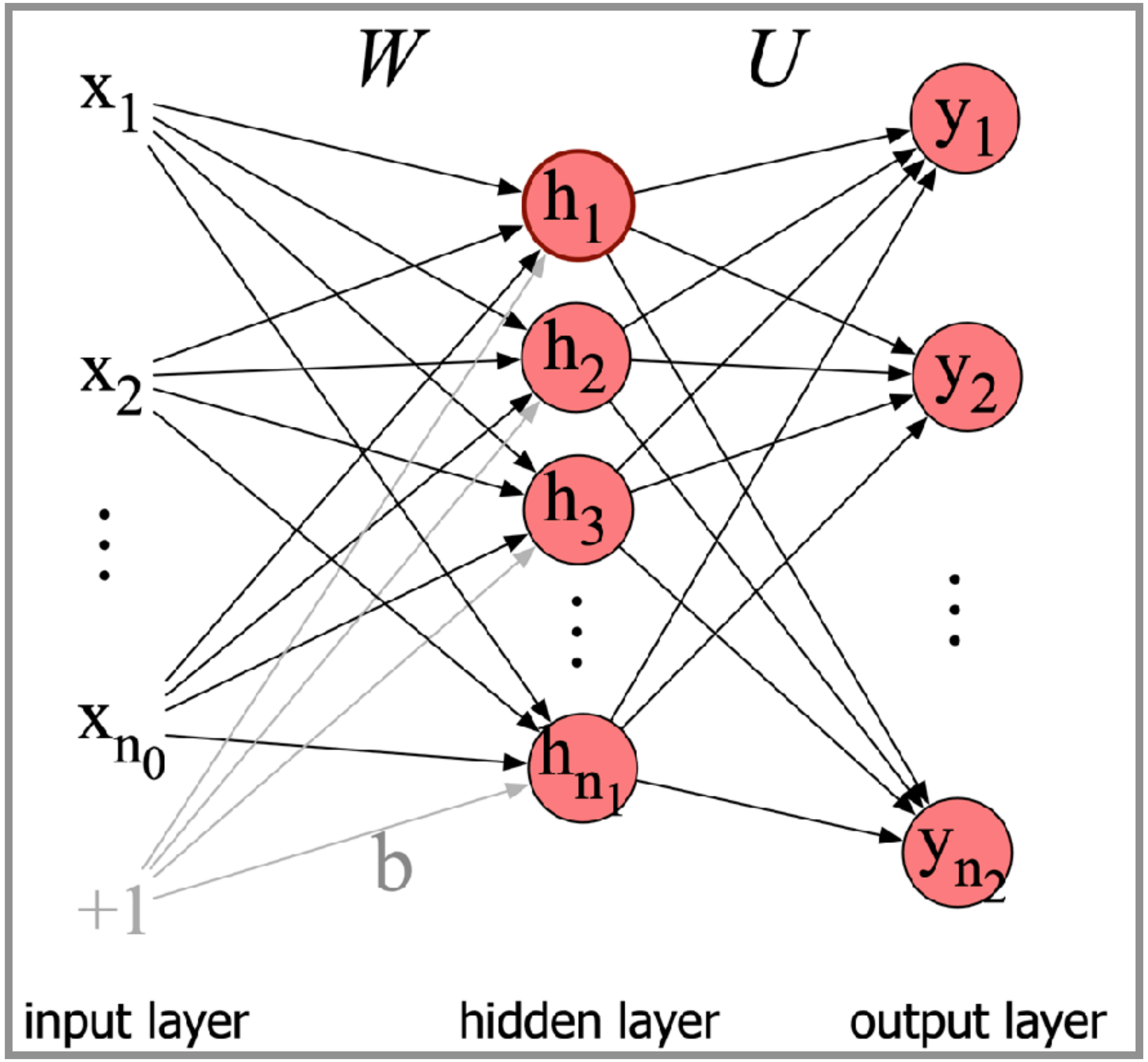
- think of matrix $\mathbf{A}$ with dimensions (n, m) as a **linear mapping** $f_{\mathbf{A}}: \mathbb{R}^n \to \mathbb{R}^m$ from vectors of length m to vectors for length n, so that with $\mathbf{x} = [x_1, \ldots, x_m]$:

$$f_{\mathbf{A}}(\mathbf{x}) = \mathbf{A}\mathbf{x}$$

Feed-forward neural network

one layer

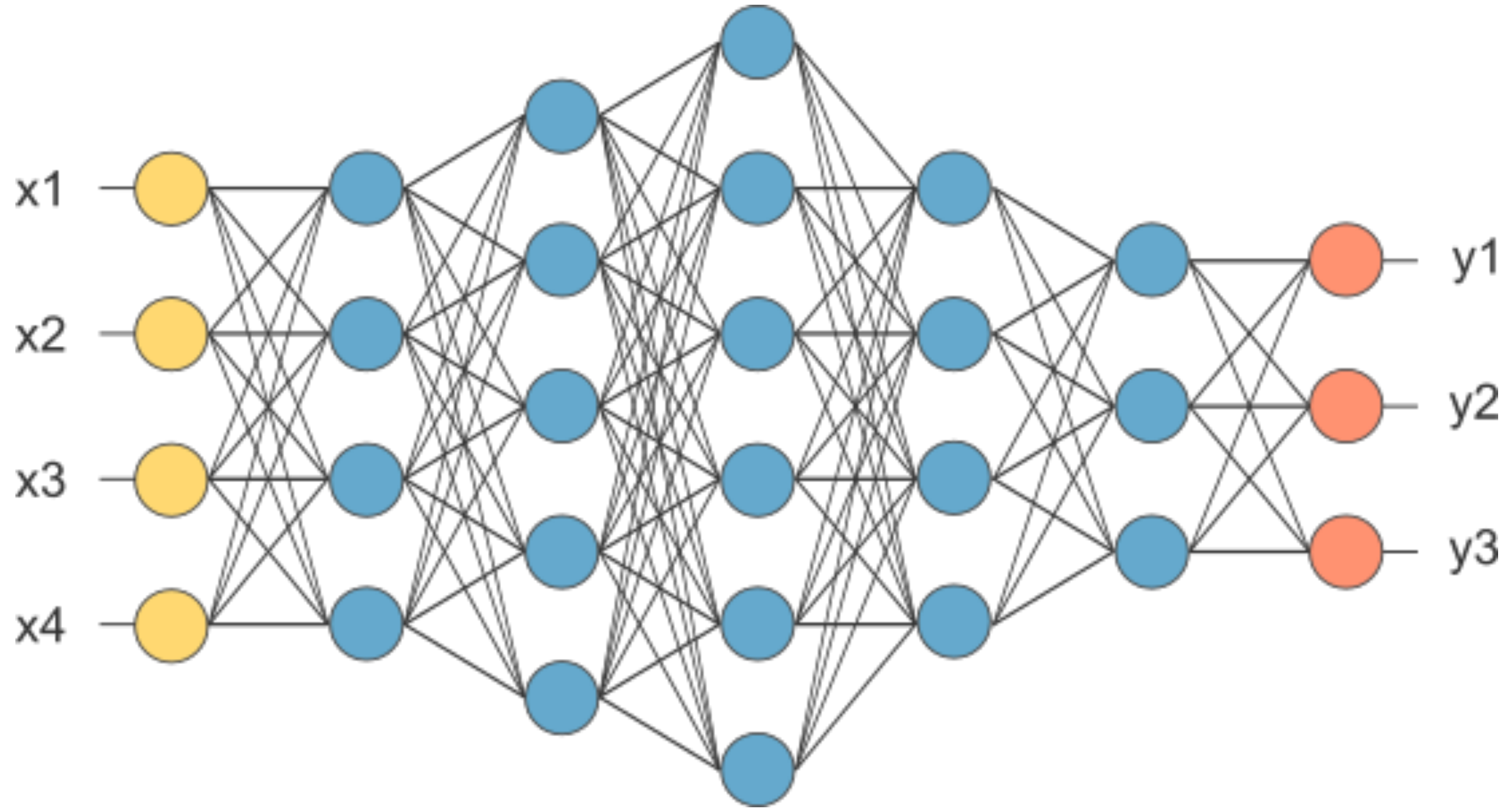
- input:
  $\mathbf{x} = [x_1, \ldots, x_{n_x}]^T$
- weight matrix:
  $\mathbf{W} \in \mathbb{R}^{n_k \times n_x}$
- bias vector:
  $\mathbf{b} = [b_1, \ldots, b_{n_k}]^T$
- activation vector hidden layer:
  $\mathbf{h} = f(\mathbf{Wx} + \mathbf{b})$, with $f \in \{\sigma, \text{tanh}, \ldots\}$
- weight matrix:
  $\mathbf{U} \in \mathbb{R}^{n_y \times n_k}$
- prediction vector:
  $\mathbf{y} = g(\mathbf{Uh})$, with $g \in \{\sigma, \text{soft-max}, \ldots\}$



Feed-forward neural network

multi-layer perceptron

- anchoring in input:
  $\mathbf{a}^{[0]} = \mathbf{x} = [x_1, \ldots, x_{n_x}]^T$
- activation at layer n:
  $\mathbf{a}^{[n]} = f^{[n]}\left(\mathbf{W}^{[n]}\mathbf{a}^{[n-1]} + \mathbf{b}^{[n]}\right)$
  - with $f^{[n]} \in \{\sigma, \text{tanh}, \ldots\}$ if n is a hidden layer, or
  - with $f^{[n]} \in \{\sigma, \text{soft-max}, \ldots\}$ if n is the output layer



demo

MLP

demo 03: Multi-Layer Perceptron for Non-Linear Regression

Language Models

Language model

high-level definition

- let $\mathscr{V}$ be a (finite) **vocabulary**, a set of tokens
  - tokens can be characters, sub-words, phrases, …
- let $w_{1:n} = \langle w_1, \ldots, w_n \rangle$ be a finite sequence of tokens
  - it is still common to use w (reminiscent of "words") for tokens
- let S be a the set of all (finite) sequences of tokens
- let X be a set of input conditions
  - e.g., images, text in a different language …
- a **language model** LM is function that assigns to each input X a probability distribution over S, given parameters $\theta \in \Theta$:

  $$LM_\theta \ : \ \ X \mapsto \Delta(S)$$

  - if there is only one input in set X, the LM is just a probability distribution over all sequences of words
  - LMs originally meant to capture the true occurrence frequency
  - a **neural language model** is an LM realized as a neural network
  - in the following we skip the dependence on X

Language model

left-to-right / autoregressive / causal model

- a **causal language model** is defined as a function that maps an initial token sequence to a next-token distribution:

  $$LM \;:\; w_{1:n} \mapsto \Delta(\mathscr{V})$$

  - we write $P_{LM}(w_{n+1} \mid w_{1:n})$ for the **next-token probability**
  - the **surprisal** of w_{n+1} after sequence $w_{1:n}$ is $-\log\left(P_{LM}(w_{n+1} \mid w_{1:n})\right)$
- the **sequence probability** follows from the chain rule:

  $$P_{LM}(w_{1:n}) = \prod_{i=1}^{n} P_{LM}(w_i \mid w_{1:i-1})$$
- measures of **goodness of fit** for observed sequence $w_{1:n}$:
  - **perplexity**:

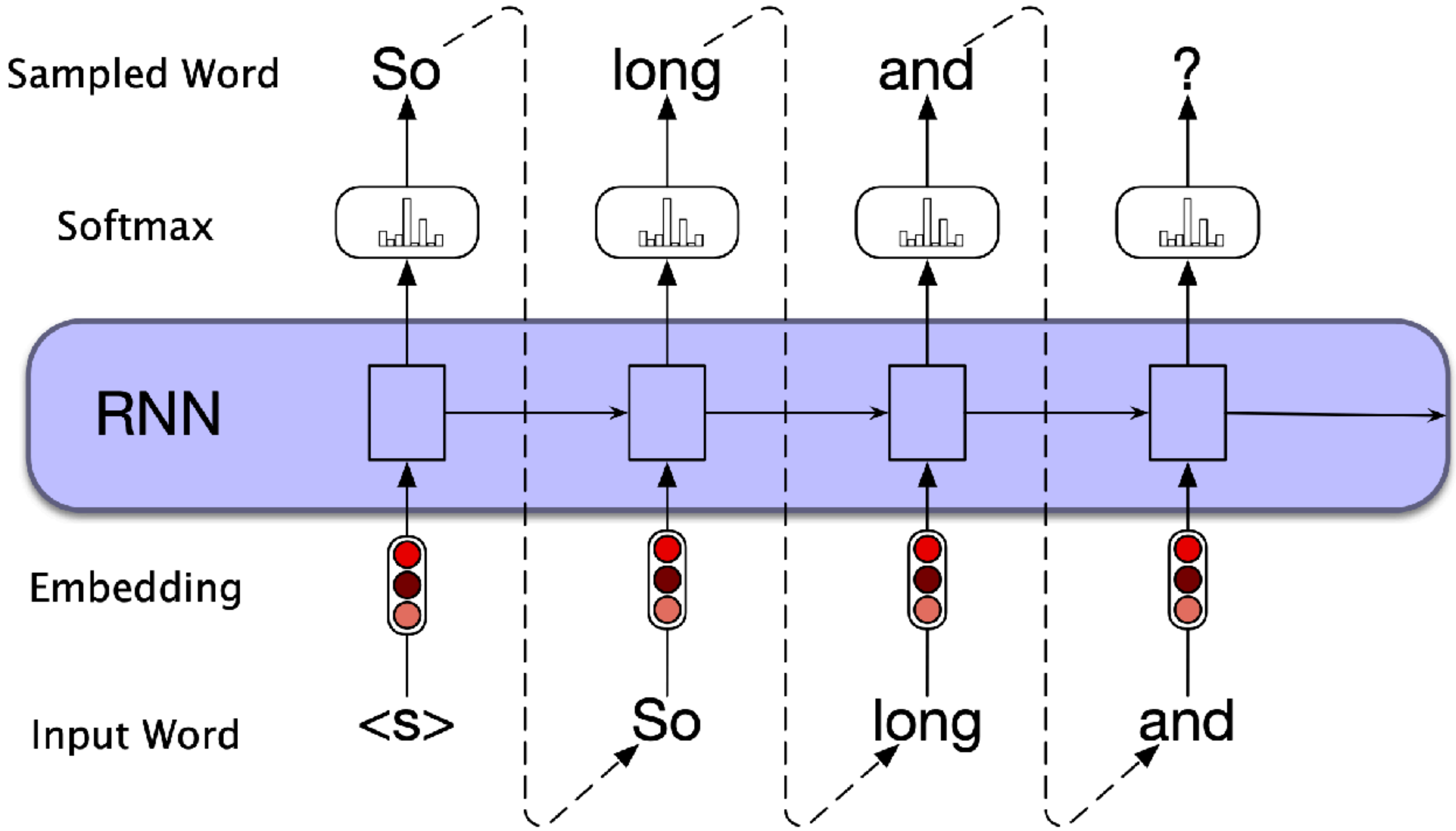
    $$\mathrm{PP}_{LM}(w_{1:n}) = P_{LM}(w_{1:n})^{-\frac{1}{n}}$$
  - **average surprisal**:

    $$\text{Avg-Surprisal}_{LM}(w_{1:n}) = -\frac{1}{n}\log P_{LM}(w_{1:n})$$

$$\log \mathrm{PP}_M(w_{1:n}) = \text{Avg-Surprisal}_M(w_{1:n})$$

Autoregressive generation

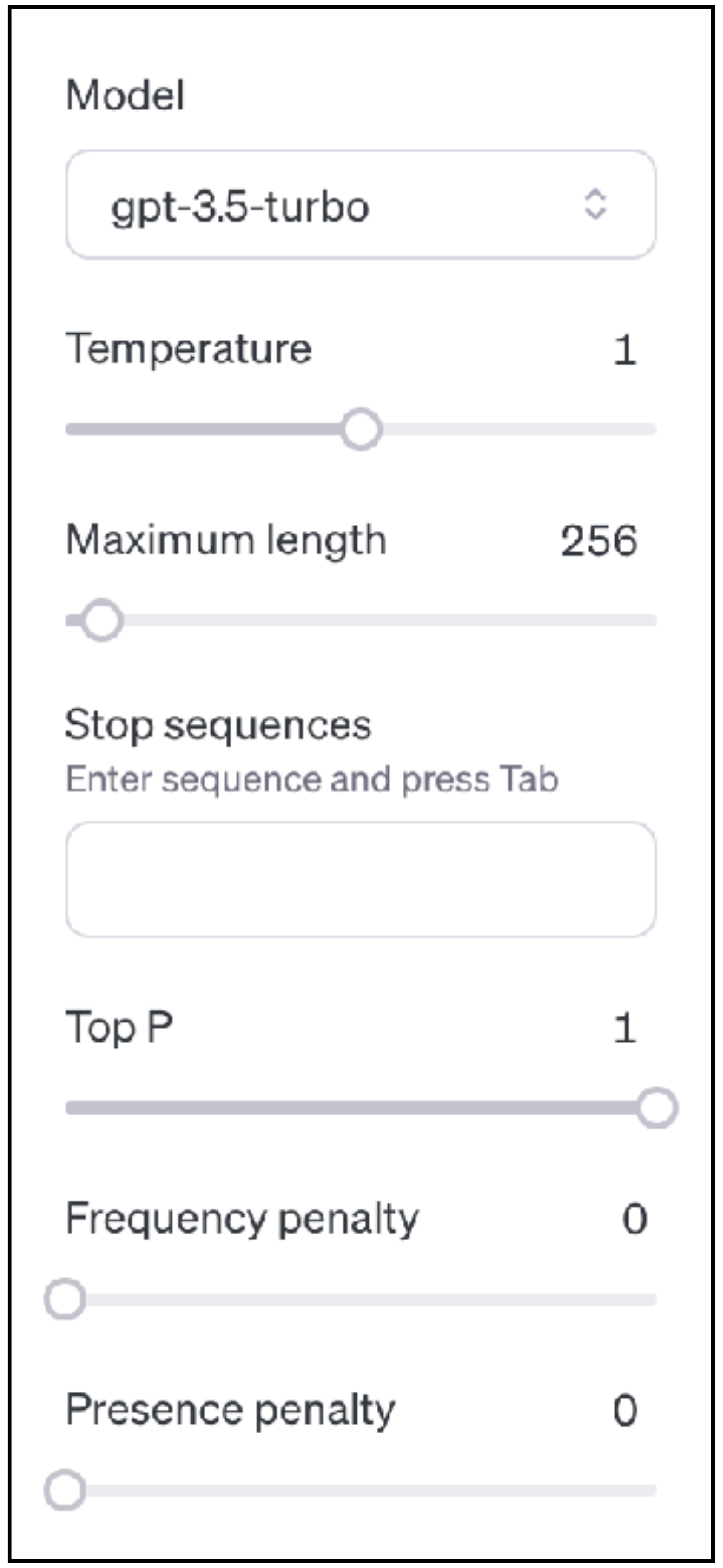
left-to-right / causal model



Predictions from different decoding schemes

based on next-token probability $P(w_{i+1} \mid w_{1:i})$

- **pure sampling**
  - next token is sampled from NTP distribution: $w_{i+1} \sim P(\cdot \mid w_{1:i})$
- **greedy decoding**
  - next token is the one with the highest NTP: $w_{i+1} = \arg\max_{w'} P(w' \mid w_{1:i})$
- **softmax sampling**
  - next token is sampled from softmax of NTP distribution: $w_{i+1} \sim SM_{\alpha}\left(P(\cdot \mid w_{1:i})\right)$
- **top-k sampling**
  - next token is sampled from NTP distribution after restricting to the k most likely words
- **top-p sampling**
  - next token is sampled from NTP distribution after restricting to the smallest set of the most likely tokens which together comprise at least NTP p
- **beam search**
  - frequently use, if relevant we will cover it later

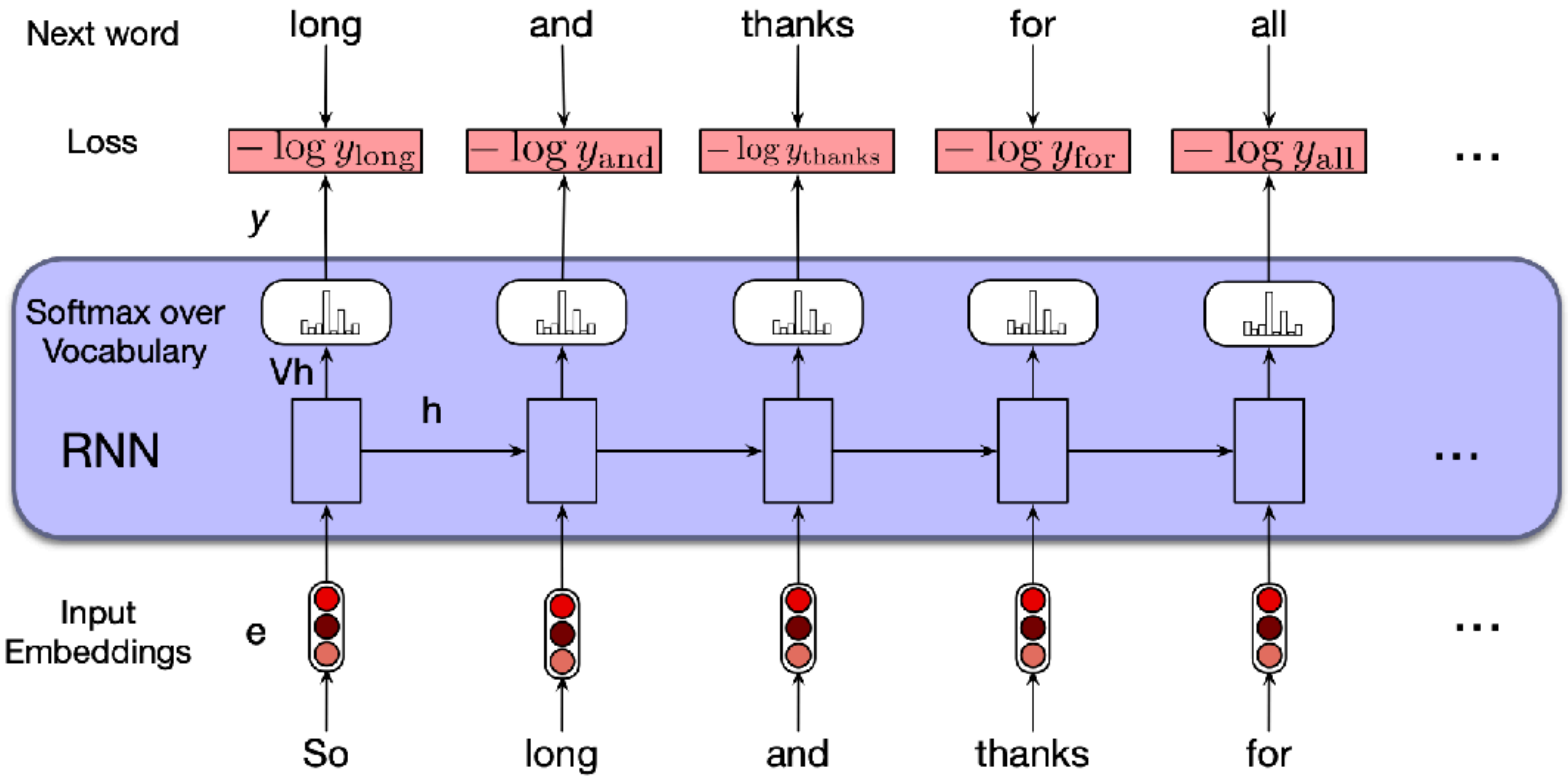


from OpenAI's Playground

Training RNNs

using teacher forcing & next-word surprisal

- teacher forcing
  - predict each next token given the preceding input (not the model-generated sequence)
- next-work surprisal
  - loss function is (average) next-token surprisal



Excursion: Different training regimes

- **teacher forcing**
  - LM is fed true word sequence
  - training signal is next-word assigned to true word
- **autoregressive training** (aka free-running mode)
  - LM autoregressively generates a sequence
  - training signal is next-word probability assigned to true word
- **curriculum learning** (aka scheduled sampling)
  - combine teacher-forced and autoregressive training
  - start with mostly teacher forcing, then increase amount of autoregressive training
- **professor forcing**
  - combines teacher forcing with adversarial training
  - generative adversarial network GAN is trained to discriminate (autoregressive) predictions from actual data
  - LM is trained to minimized this discriminability
- **decoding-based**
  - use prediction function (decoding scheme) to optimize based on *actual* output

Plain causal LMs in a nutshel

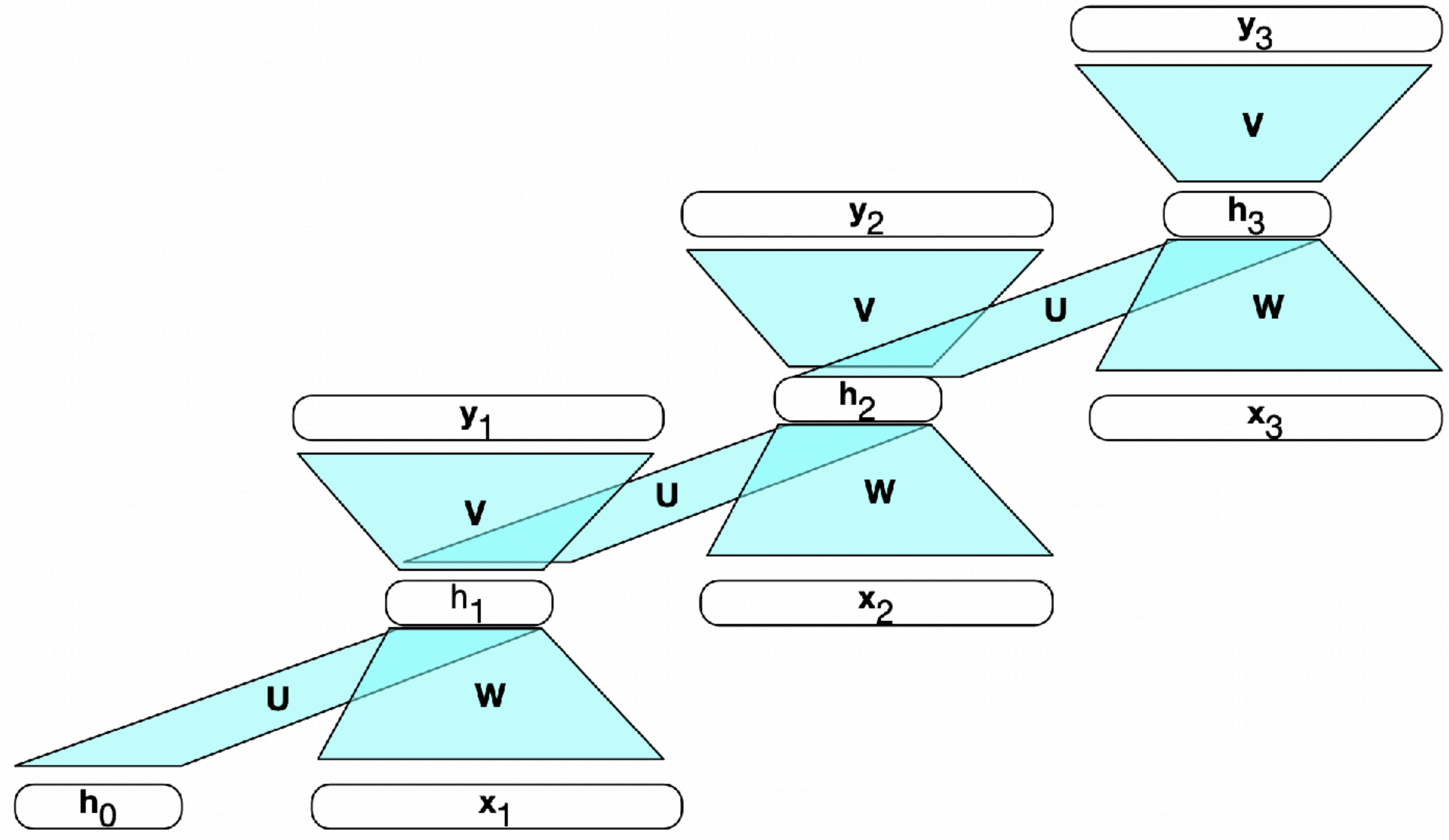
- **definition**
  - sequence probabilities given by product of next-word probabilities
- **training**
  - minimize next-word surprisal
- **prediction**
  - sample auto regressively, using next-word probabilities
- **evaluation**
  - perplexity or average surprisal
- **consistent def-train-pred-eval scheme**

Dirty reality

- **definition**
  - usually only implicit, often unclear
  - task-dependent
- **training**
  - usually based on next-word surprisal
  - other (mixed) **training regimes** exist
- **prediction**
  - whole battery of **decoding strategies**
- **evaluation**
  - baseline: perplexity or average surprisal
  - additional measure of text quality
- **possibly inconsistent**

Recurrent Neural Networks

Recurrent neural networks

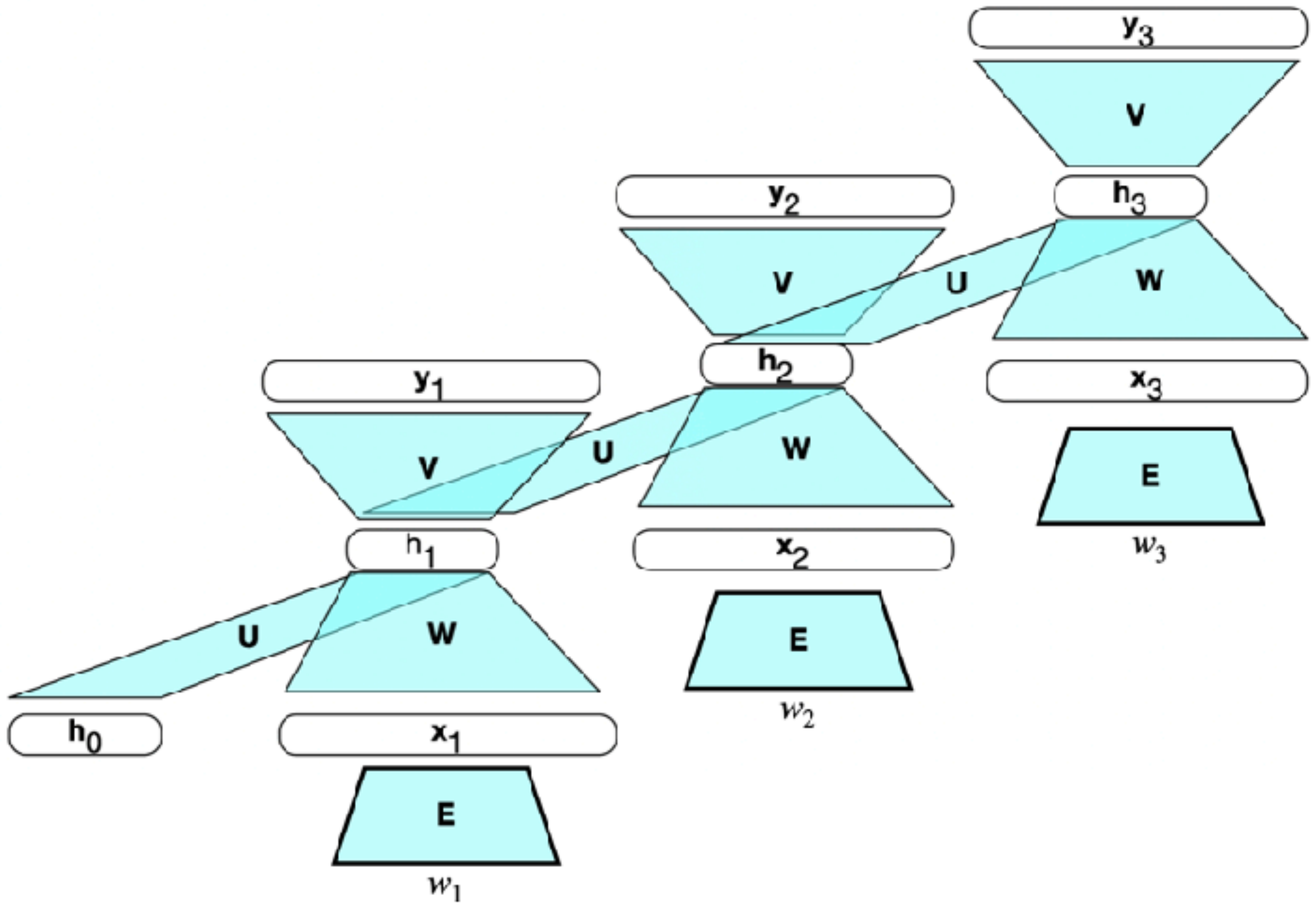


RNN-based language model

one of many similar architectures

- dimensions:
  - n_V : # of tokens in vocabulary
  - n_h : # units in hidden layer
  - n_x : length of input $\mathbf{x}$ (token embedding)
- what is what?
  - $\mathbf{w}_t \in \mathbb{R}^{n_V}$: one-hot vector representing token $\mathbf{w}_t$
  - $\mathbf{x}_t \in \mathbb{R}^{n_x}$: word embedding of token $\mathbf{w}_t$
  - $\mathbf{h}_t \in \mathbb{R}^{n_h}$: hidden layer activation at time t (with $\mathbf{h}_0 = 0$)
  - $\mathbf{y}_t \in \Delta(\mathscr{V})$: probability distribution over tokens
  - $f \in \{\sigma, \tanh, \dots\}$: activation function (as usual)
  - $\mathbf{U} \in \mathbb{R}^{n_h \times n_h}$: mapping hidden-to-hidden
  - $\mathbf{V} \in \mathbb{R}^{n_V \times n_h}$: mapping hidden-to-word
  - $\mathbf{E} \in \mathbb{R}^{n_x \times n_V}$: mapping word-to-embedding
  - $\mathbf{W} \in \mathbb{R}^{n_h \times n_x}$: mapping embedding-to-hidden

- definition (forward pass):
  - $\mathbf{x}_t = \mathbf{E}\mathbf{w}_t$
  - $\mathbf{h}_t = f\left[\mathbf{U}\mathbf{h}_t + \mathbf{W}\mathbf{x}_t\right]$
  - $\mathbf{y}_t = \text{softmax}(\mathbf{V}\mathbf{h}_t)$



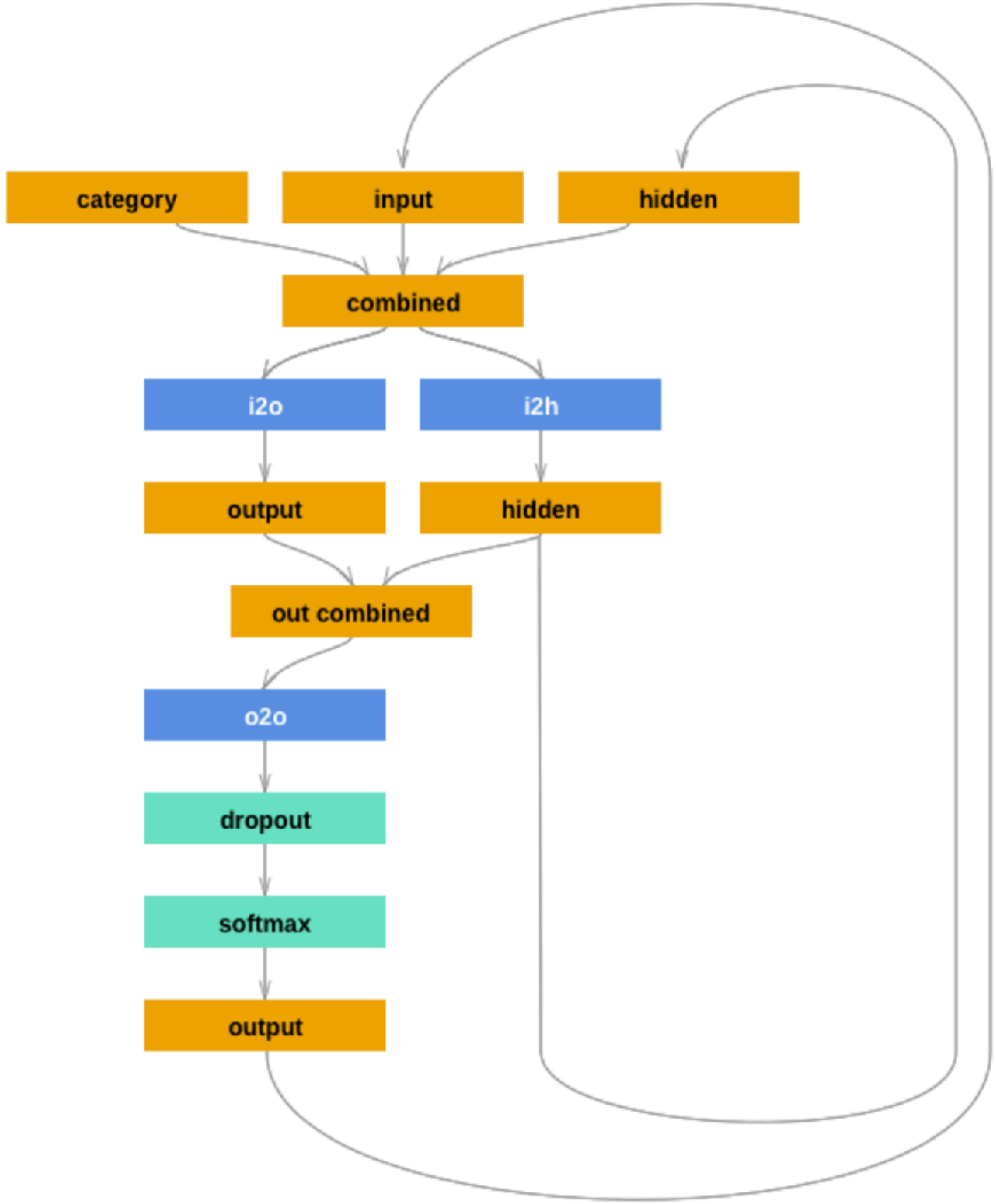
based on Jurafsky & Martin "NLP" book draft

Custom RNN

```
class RNN(nn.Module):
    def __init__(self, input_size, hidden_size, output_size):
        super(RNN, self).__init__()
        self.hidden_size = hidden_size
        self.i2h = nn.Linear(n_categories + input_size + hidden_size,
                             hidden_size)
        self.i2o = nn.Linear(n_categories + input_size + hidden_size,
                             output_size)
        self.o2o = nn.Linear(hidden_size + output_size,
                             output_size)
        self.dropout = nn.Dropout(0.1)
        self.softmax = nn.LogSoftmax(dim=1)

    def forward(self, category, input, hidden):
        input_combined = torch.cat((category, input, hidden), 1)
        hidden = self.i2h(input_combined)
        output = self.i2o(input_combined)
        output_combined = torch.cat((hidden, output), 1)
        output = self.o2o(output_combined)
        output = self.dropout(output)
        output = self.softmax(output)
        return output, hidden

    def initHidden(self):
        return torch.zeros(1, self.hidden_size)
```



demo

RNN

demo 04: Recurrent Neural Network for Character-Level Surname Prediction

Homework for next week

- solve exercises in worksheets from section 2
  - just for yourself; no submission, no grading
- ask questions
  - moodle, tutorial, class