Non-linear Models-V

CS771: Introduction to Machine Learning

Purushottam Kar

Outline of discussion

- More on architecture of neural networks
- Training methods for feedforward networks

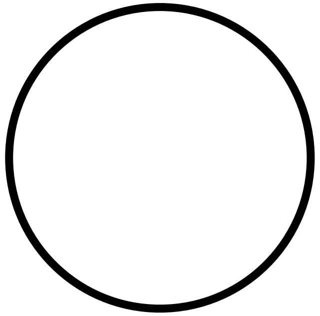
Answering the Fan Mail

- How does the notion of similarity (kernels) over notion of distance?
  - Two sides of the same coin
  - Kernels have nice math properties that algorithms exploit
- Please relate toy examples in Lec 17 to accelerated kernel methods
  - Better idea: download data from https://goo.gl/JXEQjr
  - Create feature maps for Gaussian kernel https://goo.gl/hBsX1E
  - See the magic happen!

Neural Networks

The “neuron” in Neural Networks

The "neuron" in Neural Networks



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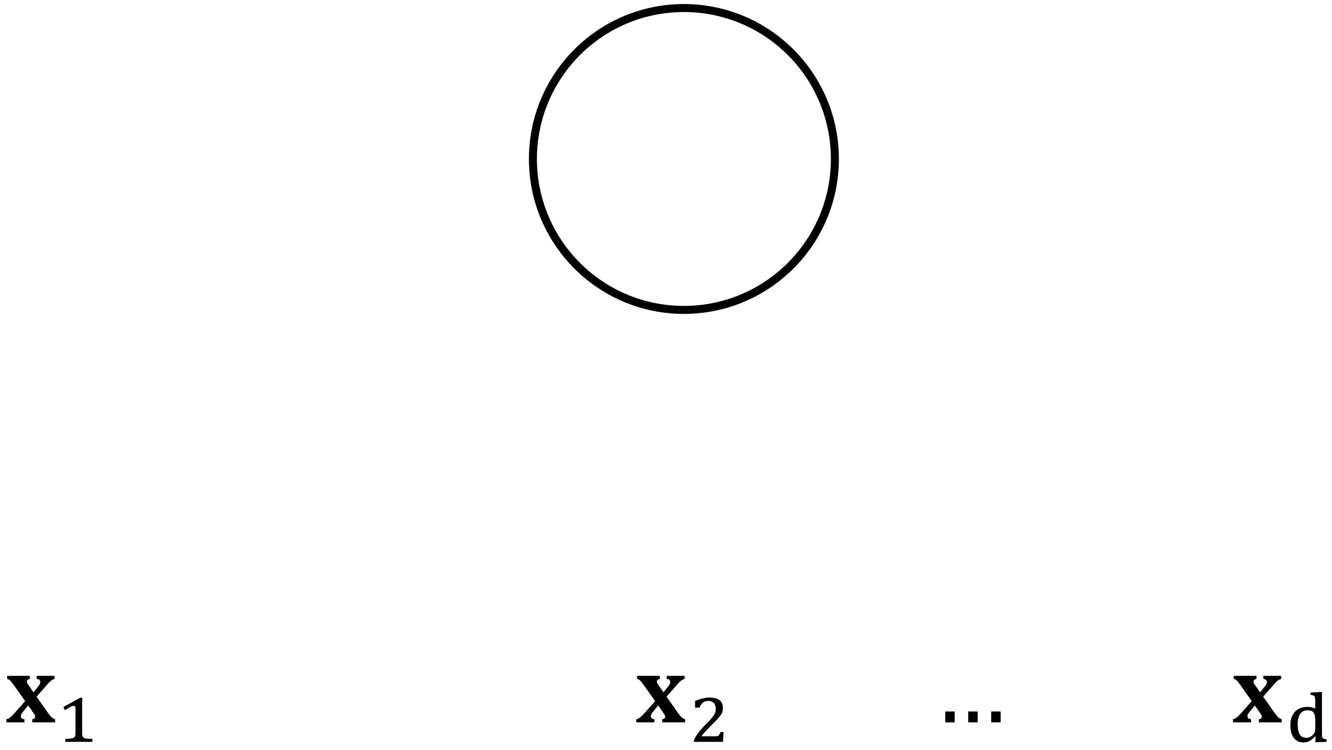

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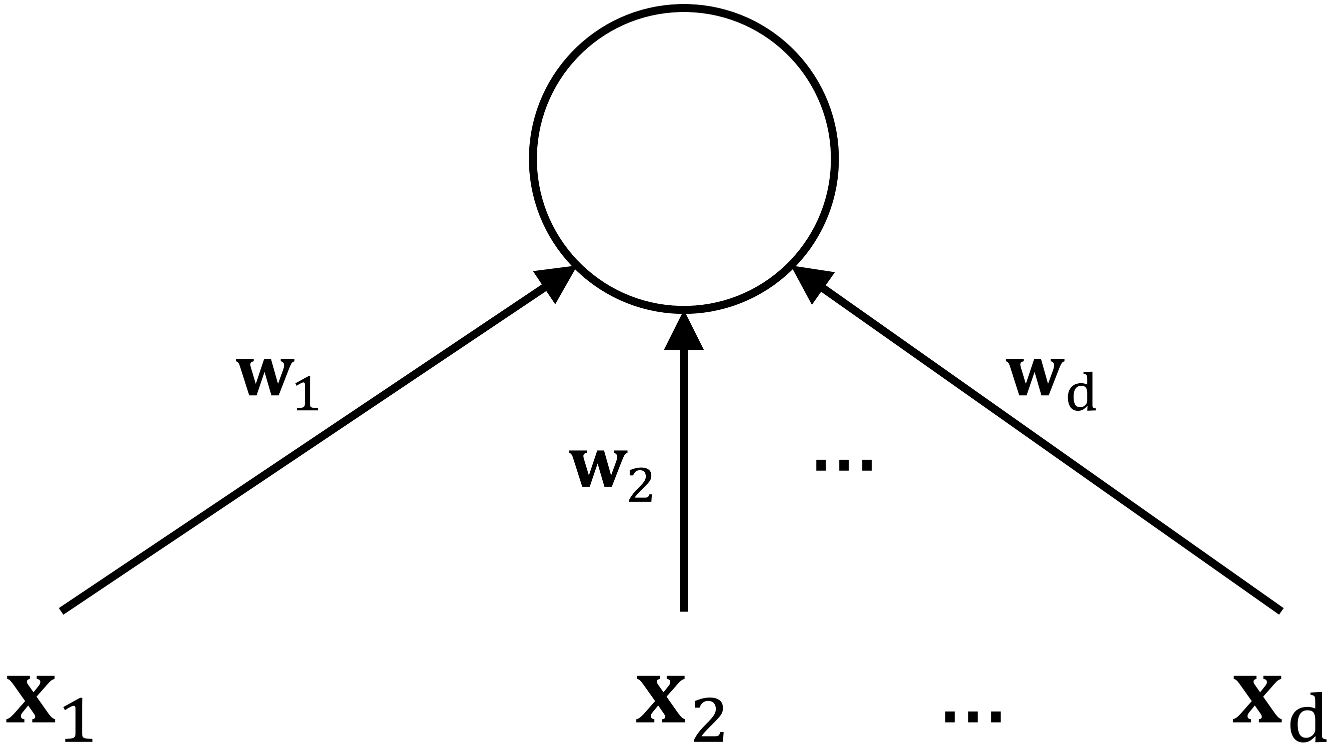

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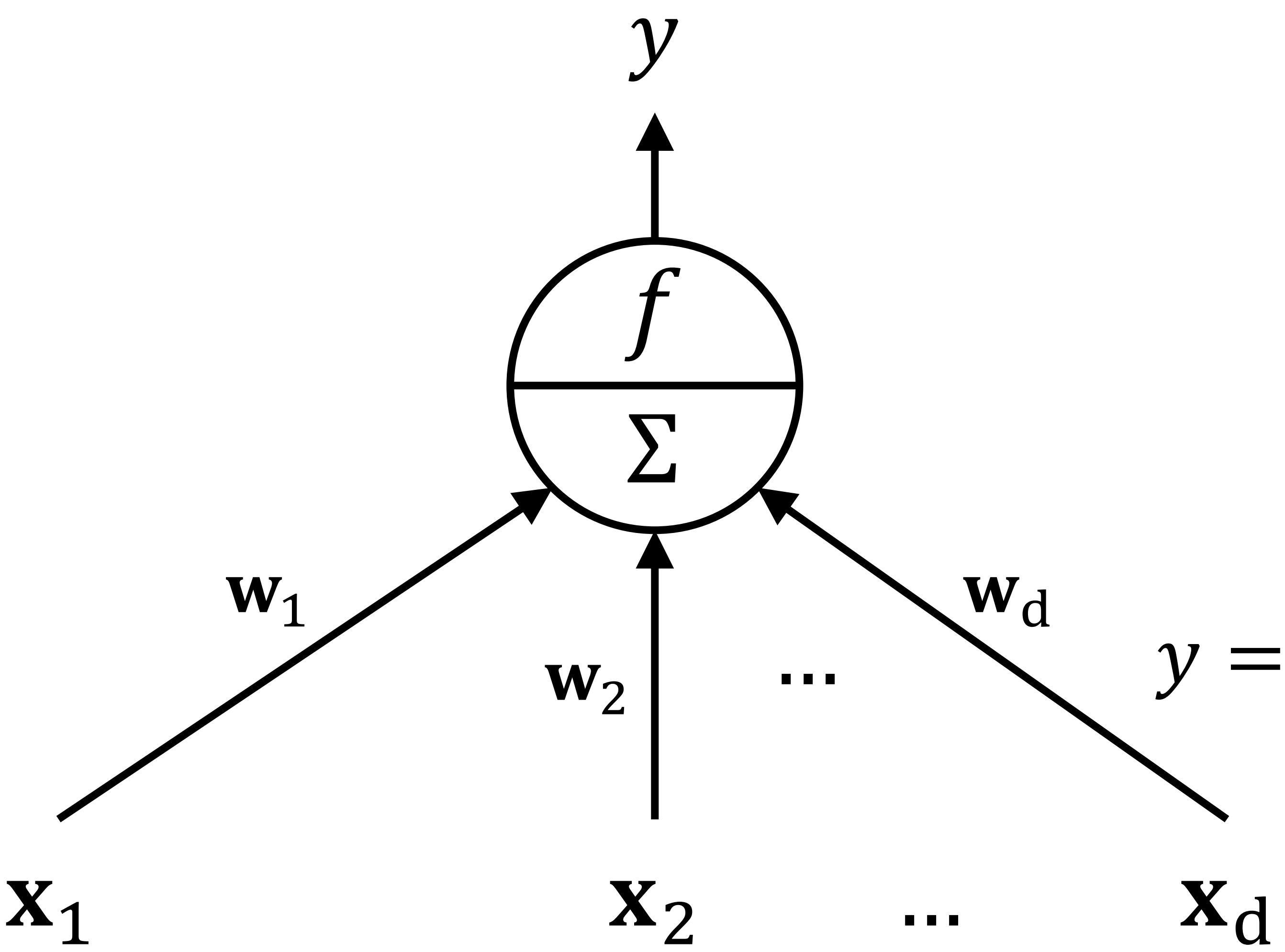

$$y = f\left(\sum_{i=1}^{d} \mathbf{w}_i \cdot \mathbf{x}_i\right)$$

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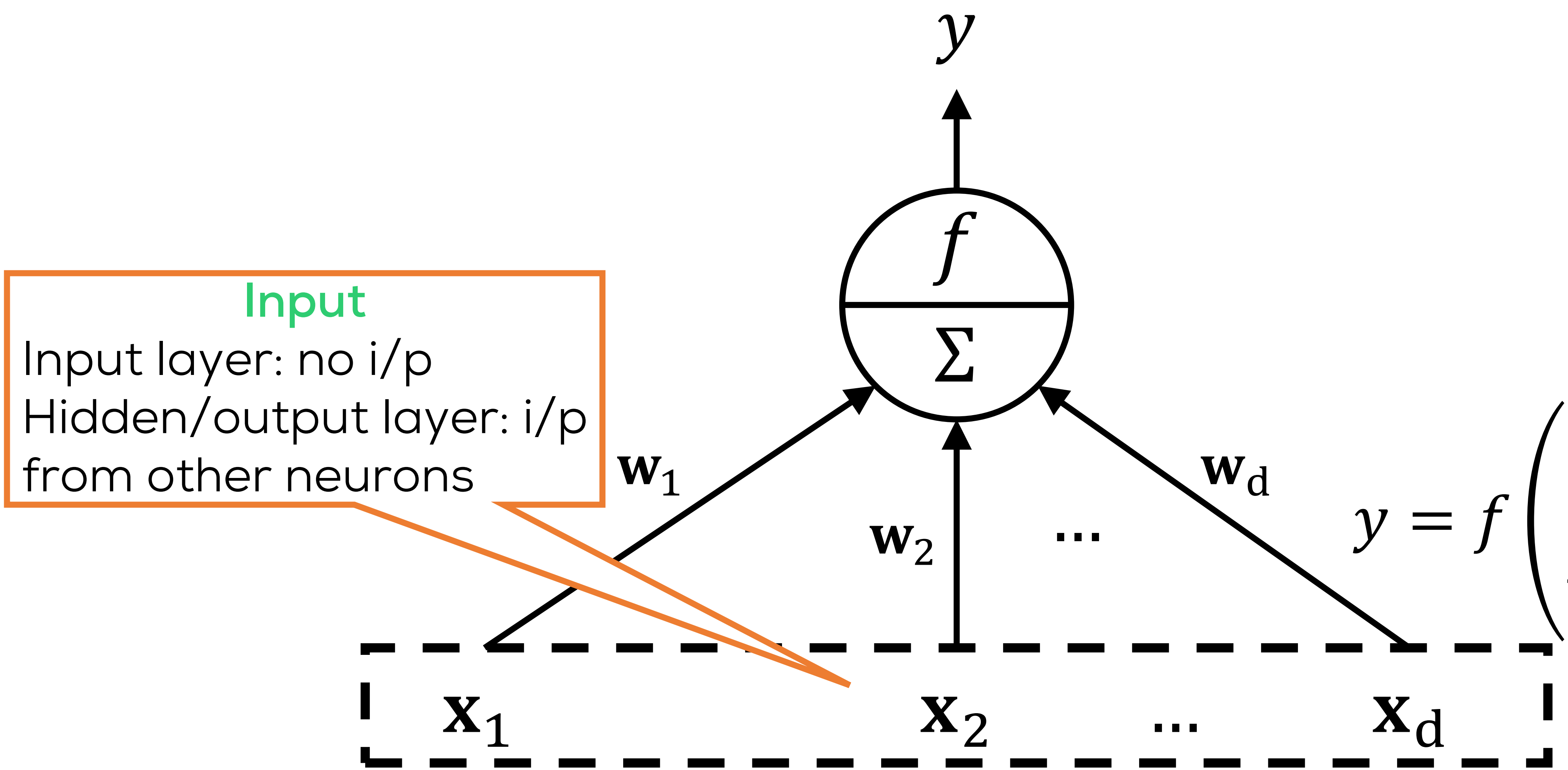

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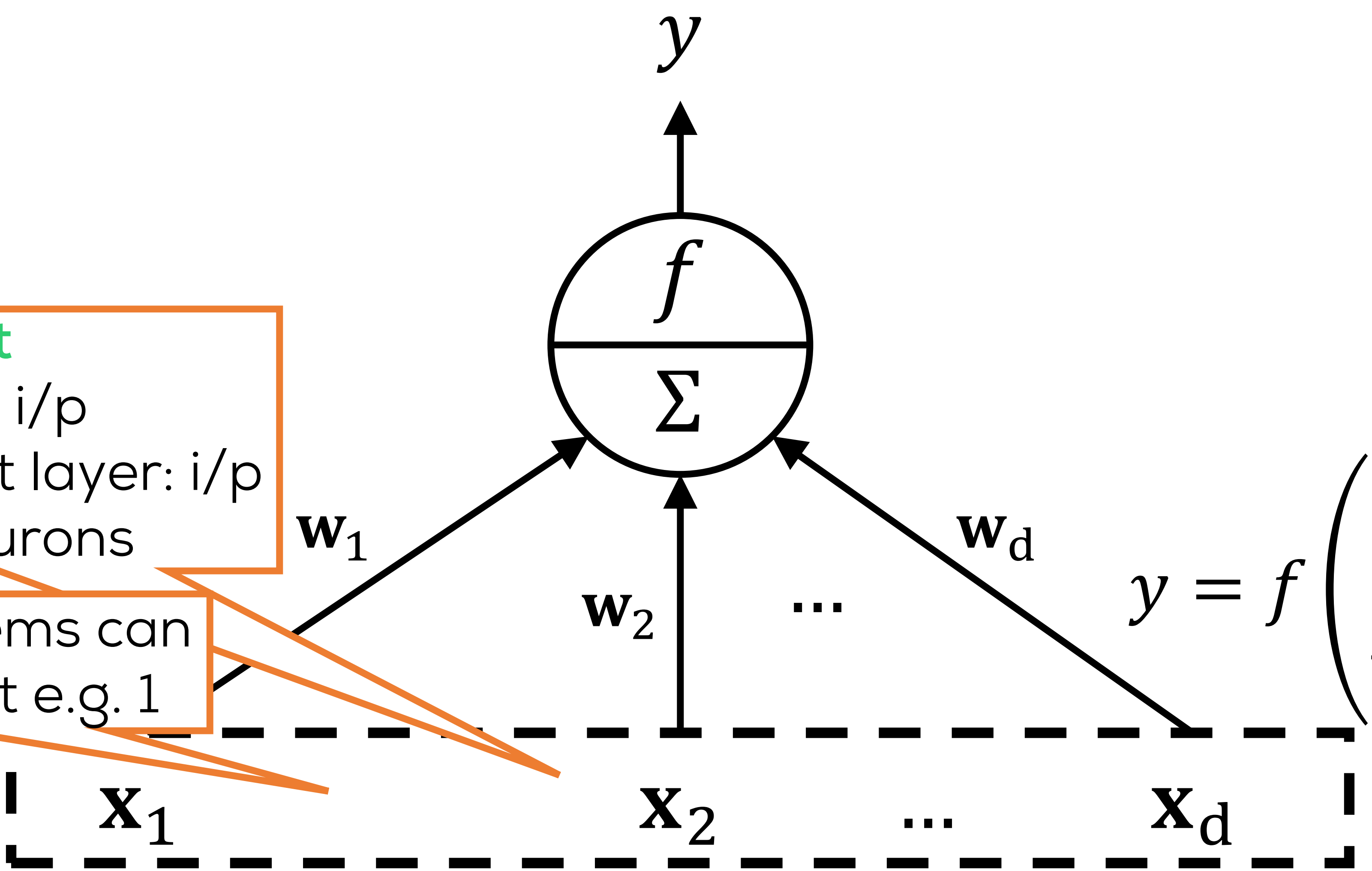

Input
Input layer: no i/p
Hidden/output layer: i/p from other neurons

Some input items can be a constant e.g. 1

$$y = f\left(\sum_{i=1}^{d} \mathbf{w}_i \cdot \mathbf{x}_i\right)$$

The "neuron" in Neural Networks

Activation
Input/output layer: id
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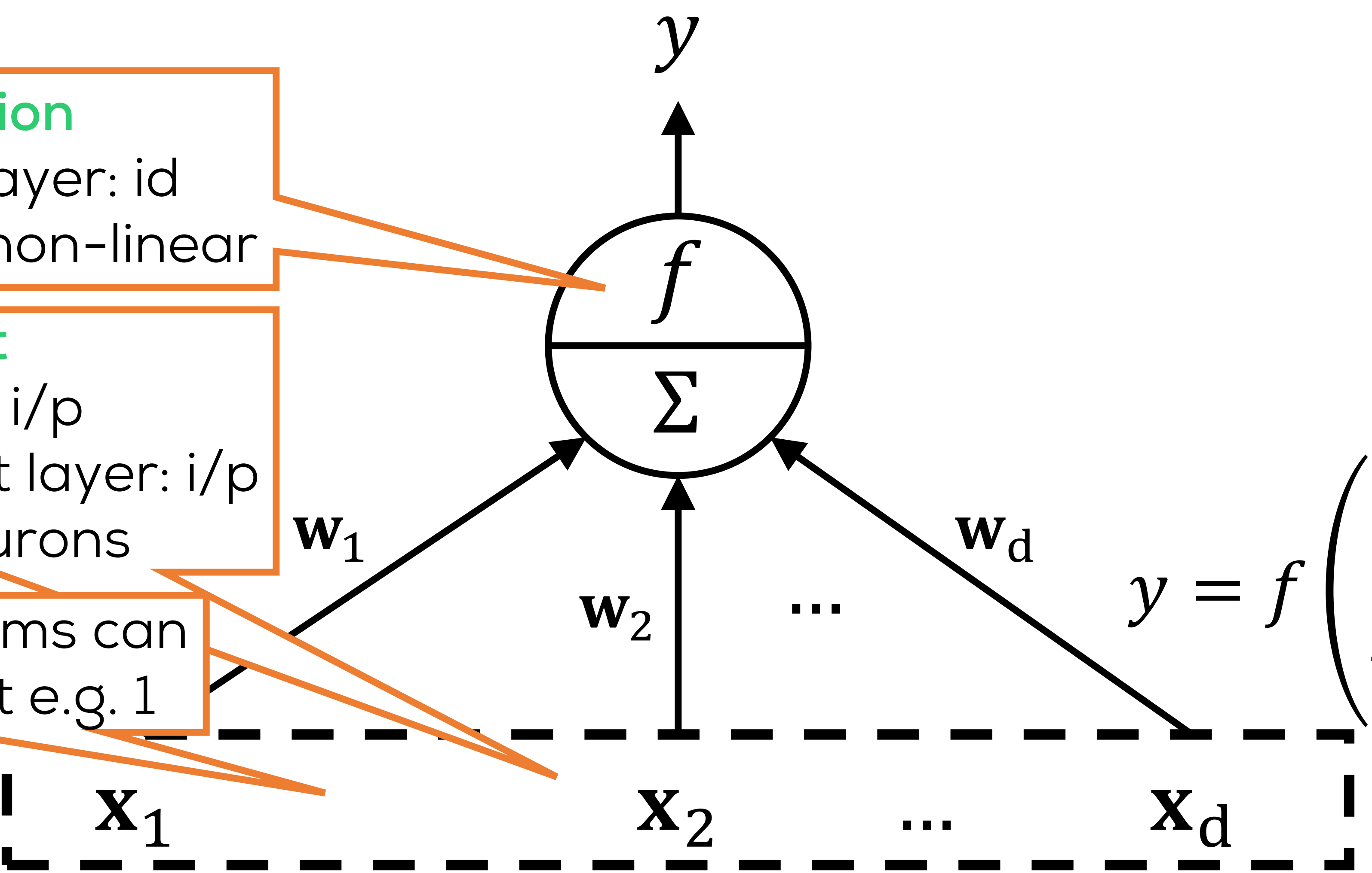

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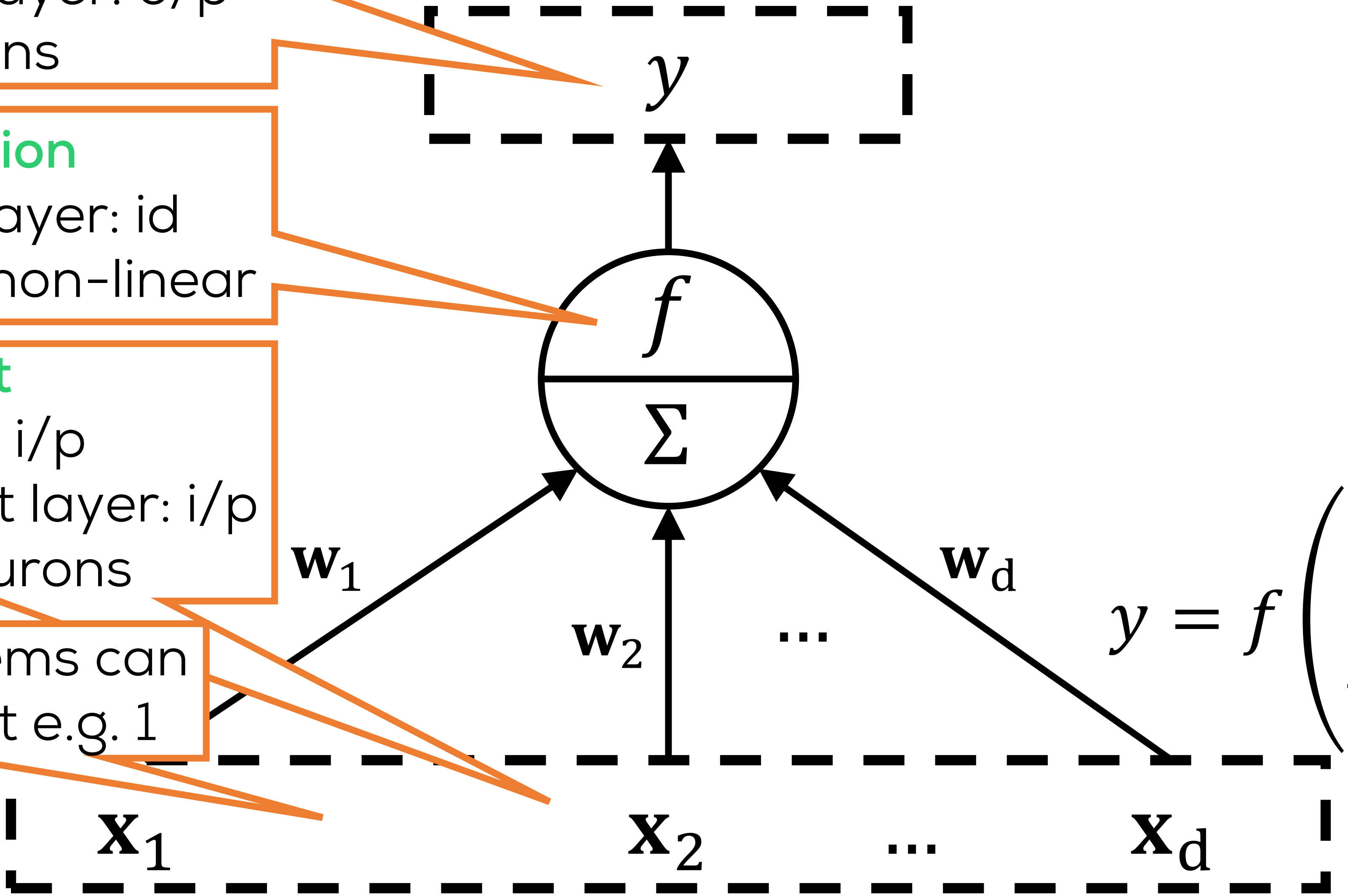

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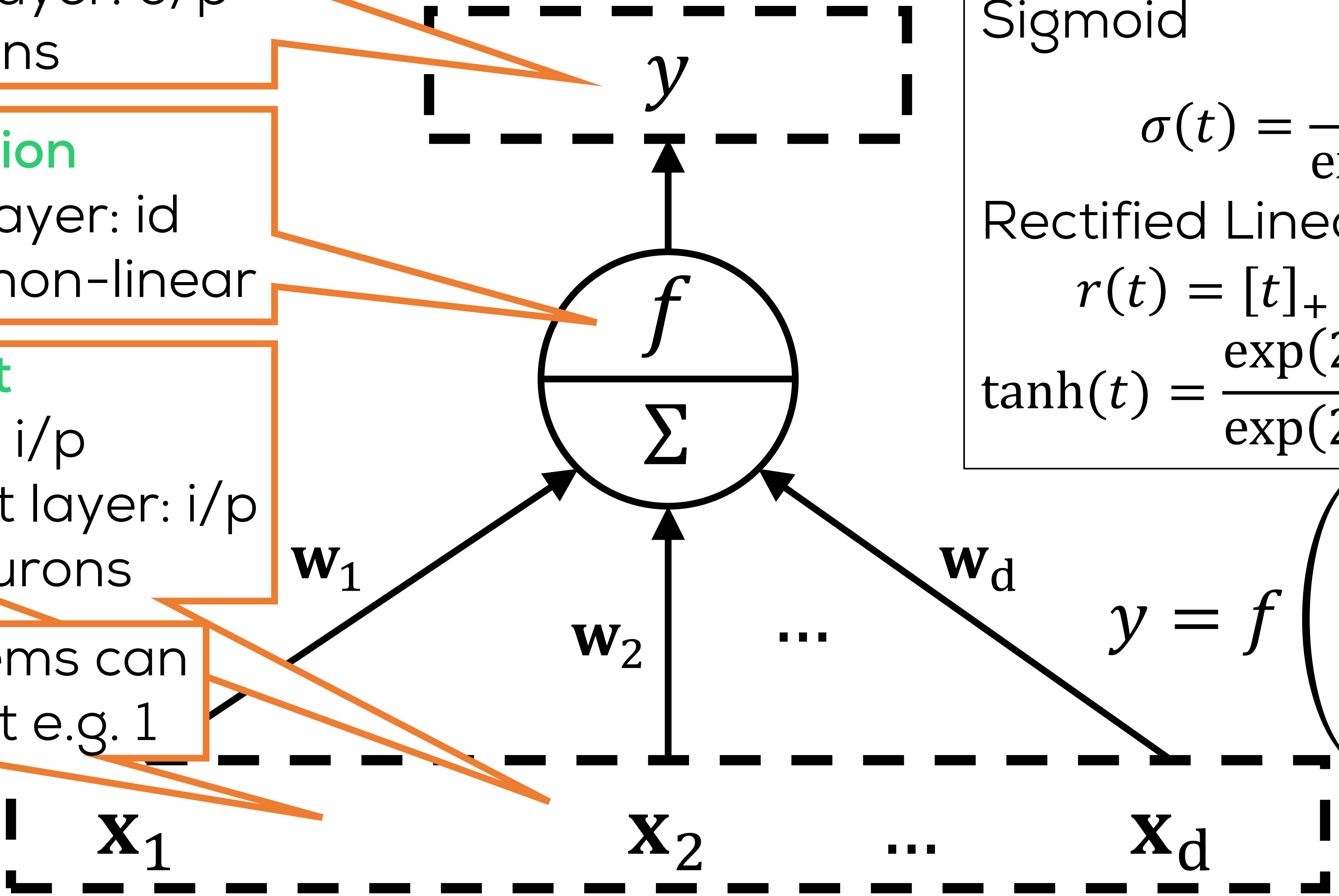

Common “activation” fns f

Sigmoid

$$\sigma(t) = \frac{\exp(t)}{\exp(t)+1}$$

Rectified Linear Unit (ReLU)

$$r(t) = [t]_+ = \max(t, 0)$$

$$\tanh(t) = \frac{\exp(2t)-1}{\exp(2t)+1}$$

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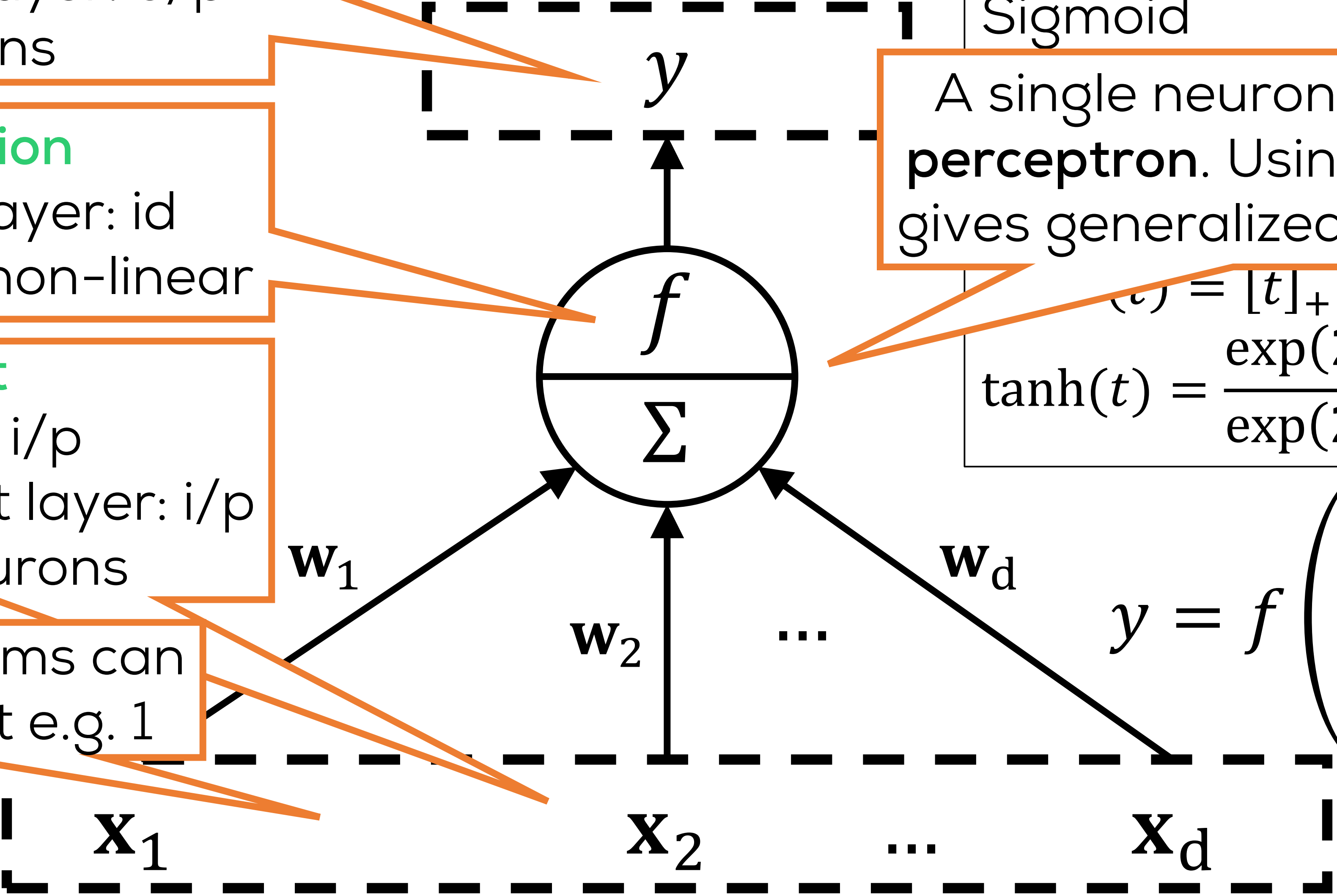

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A single neuron also called a **perceptron**. Using non-linear f gives generalized linear models

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Output layer: final o/p
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Sometimes output layer is given a non-id activation. Matter of convention

Common “activation” fns f

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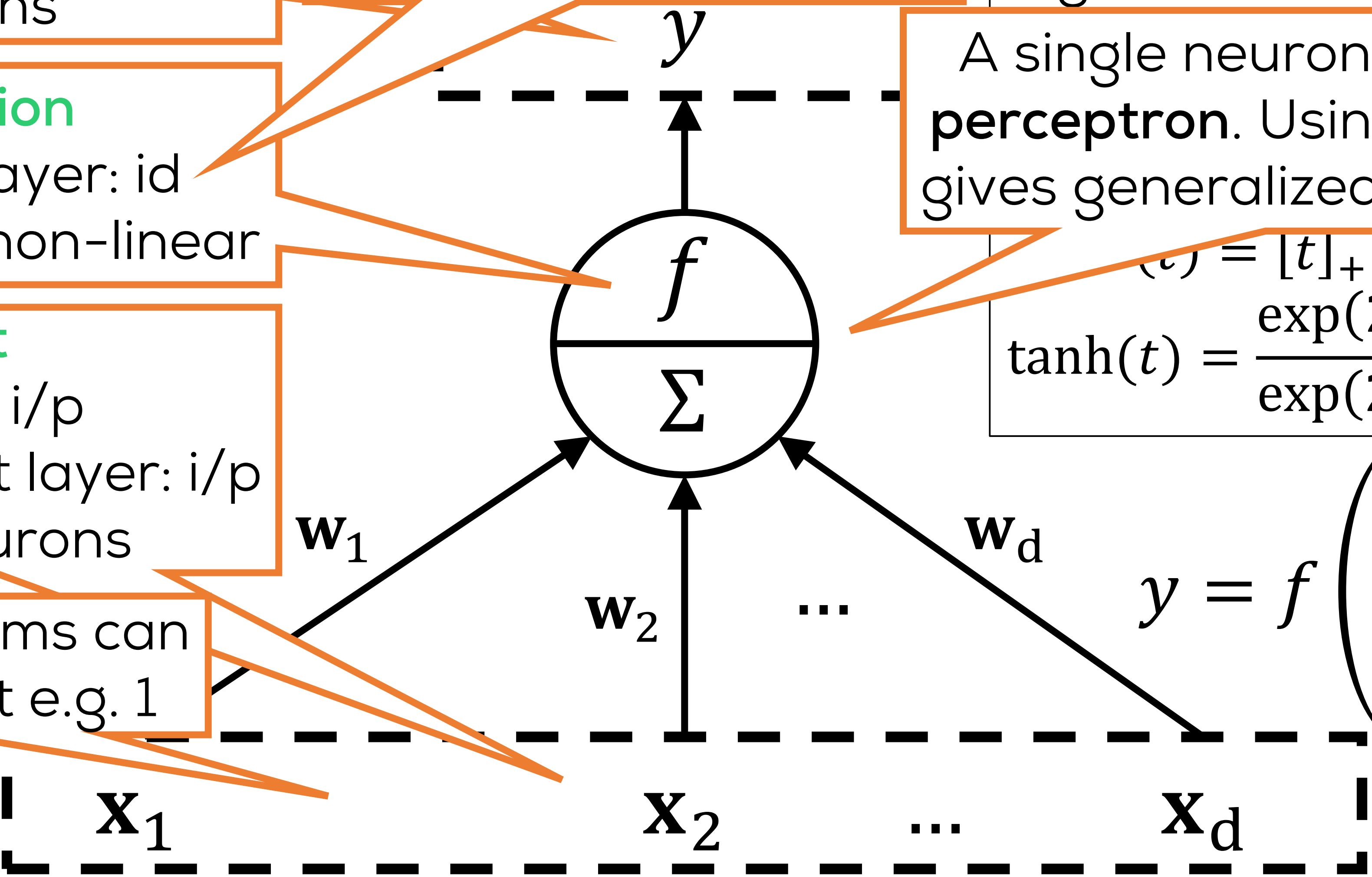

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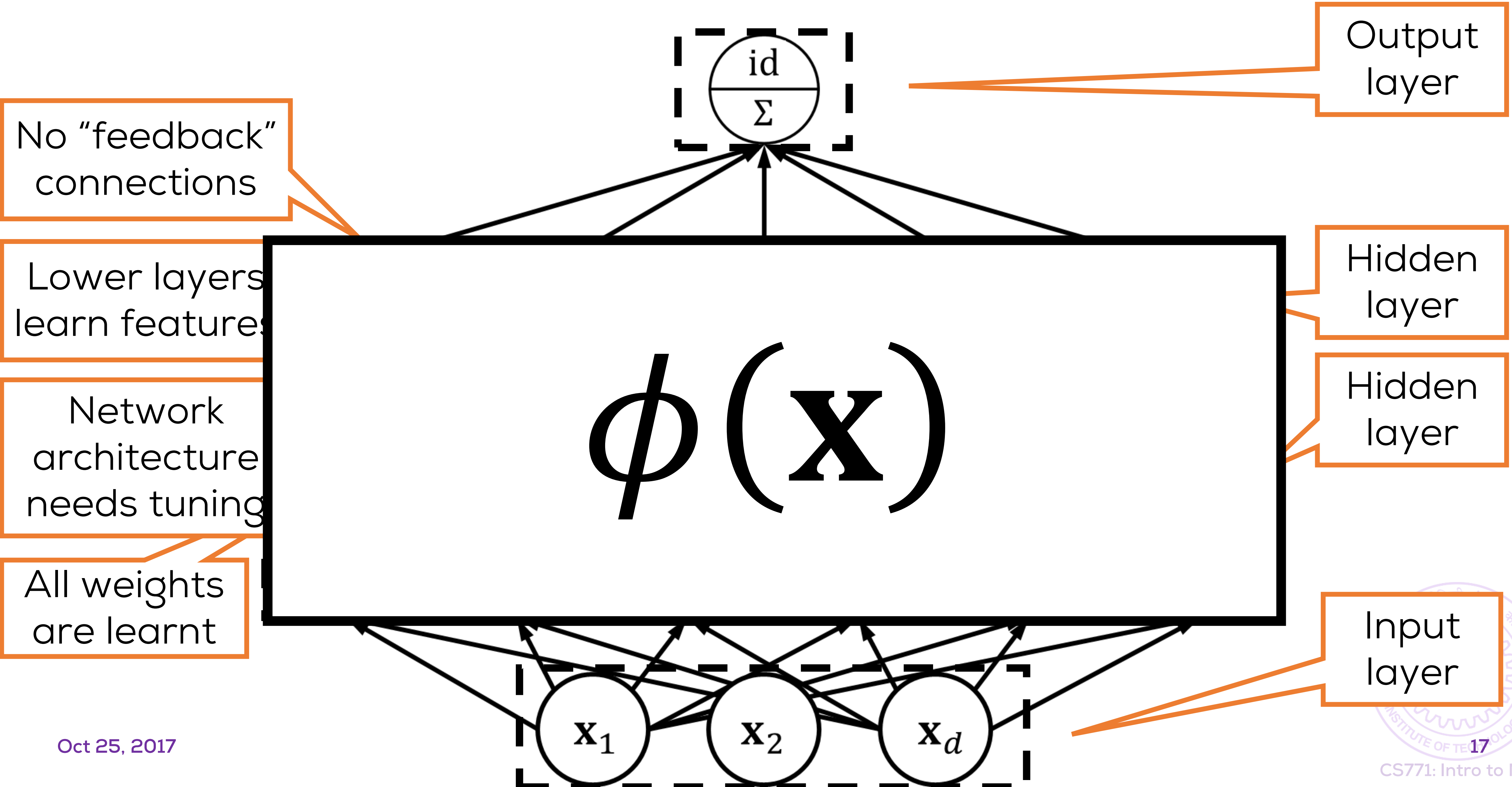
Feedforward Neural Network



Neural Networks as Feature Learners

Zeiler, M. D. and Fergus, R. ECCV 2014

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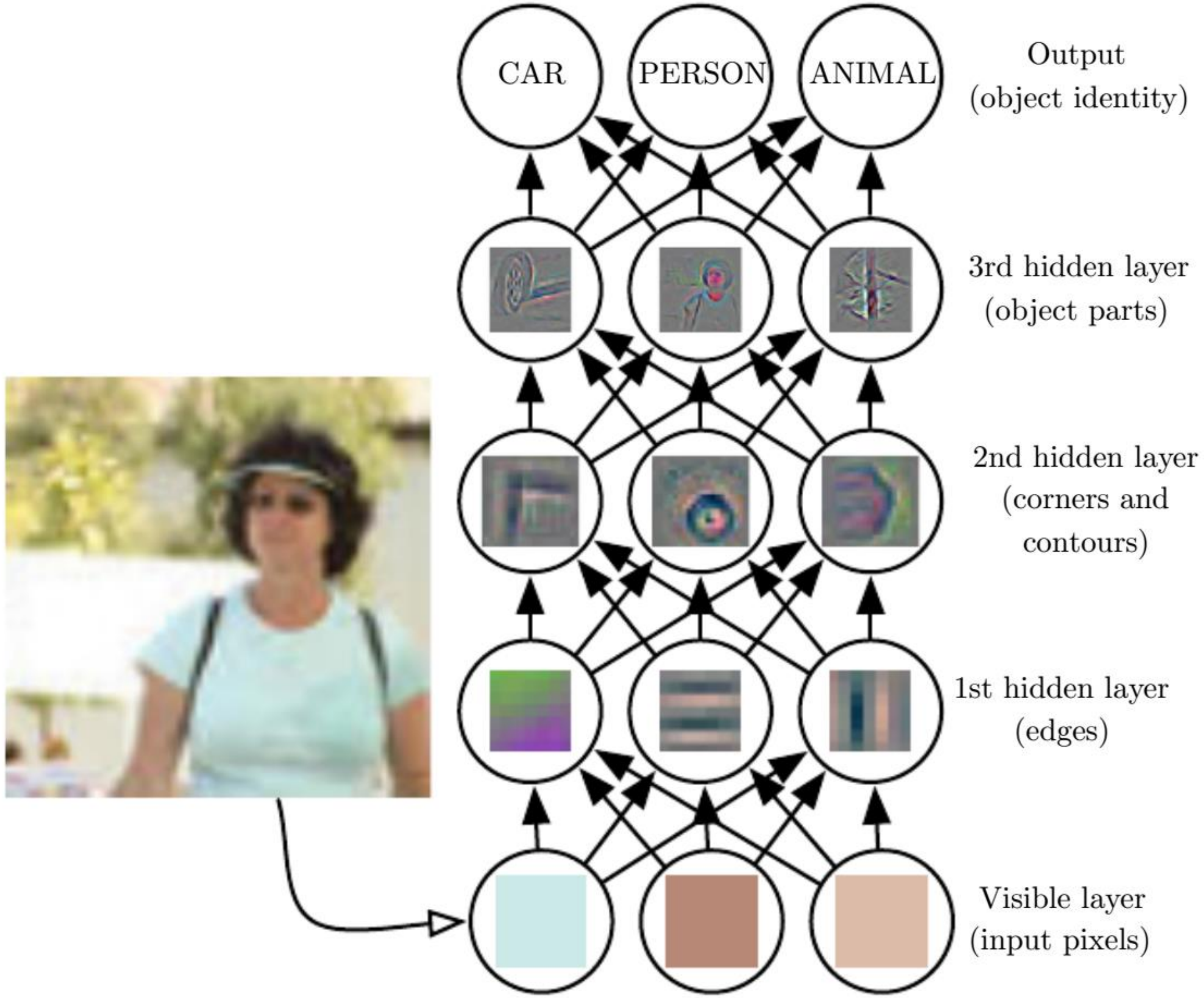

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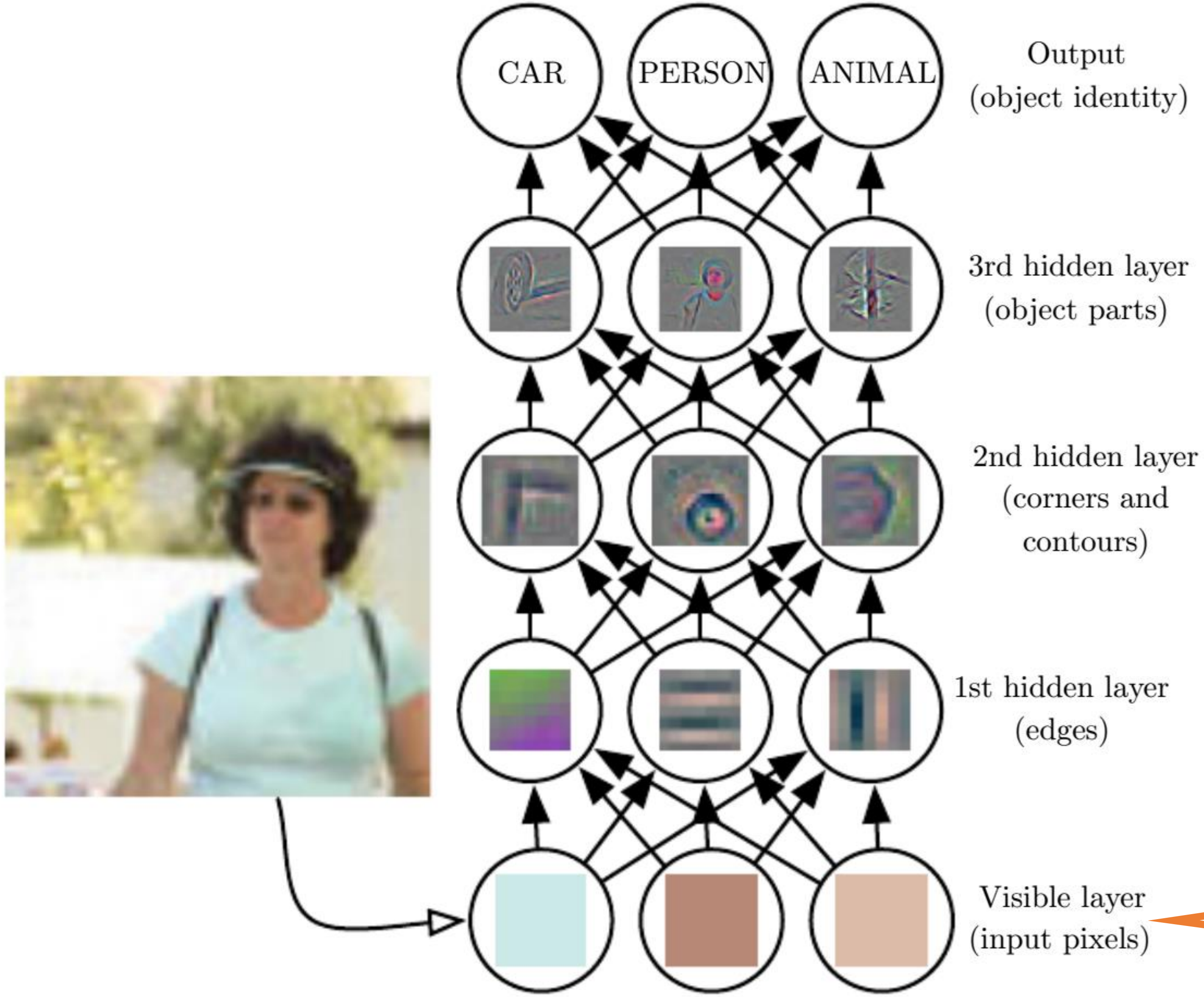

Input layer received with data i.e. “visible”

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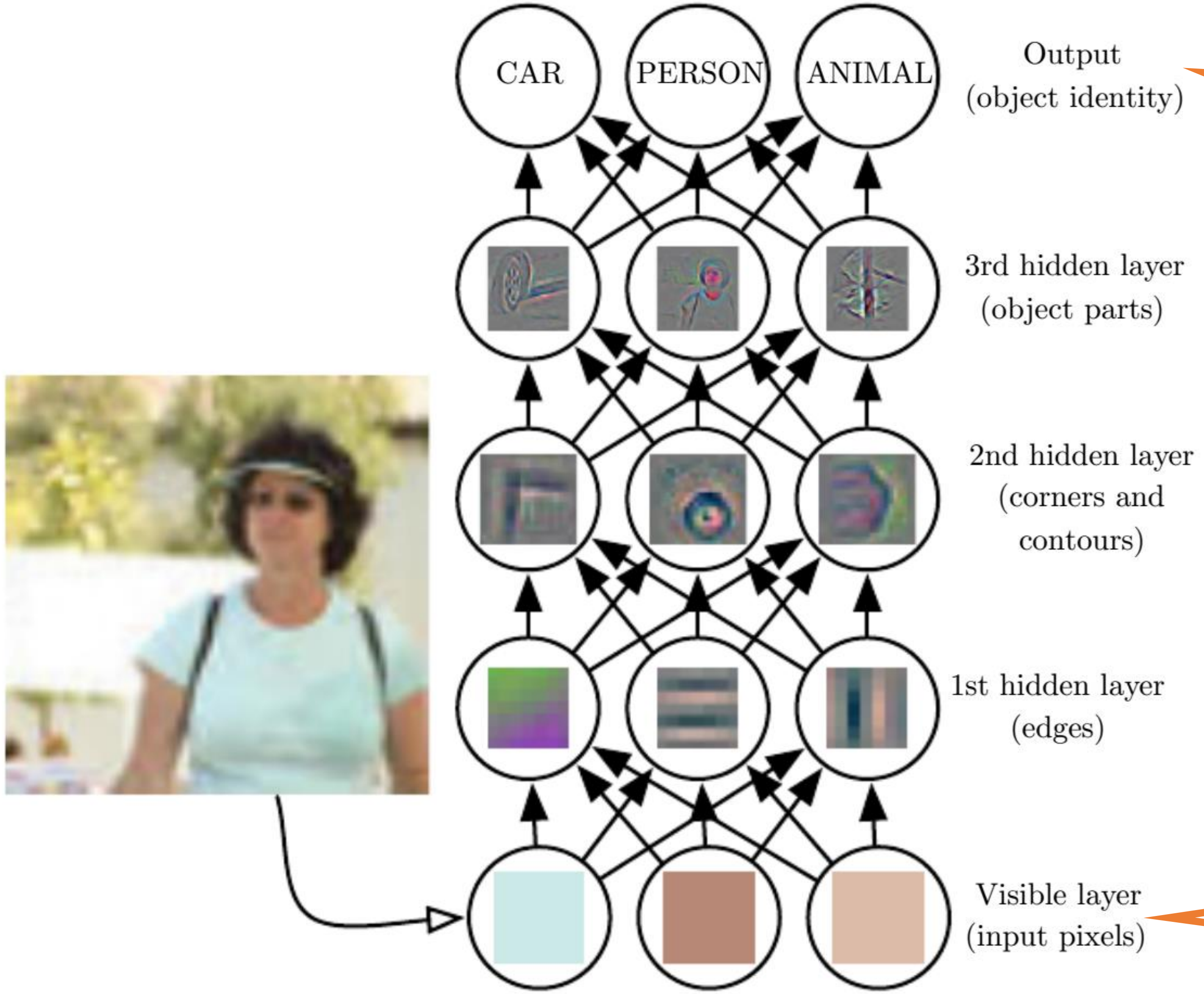

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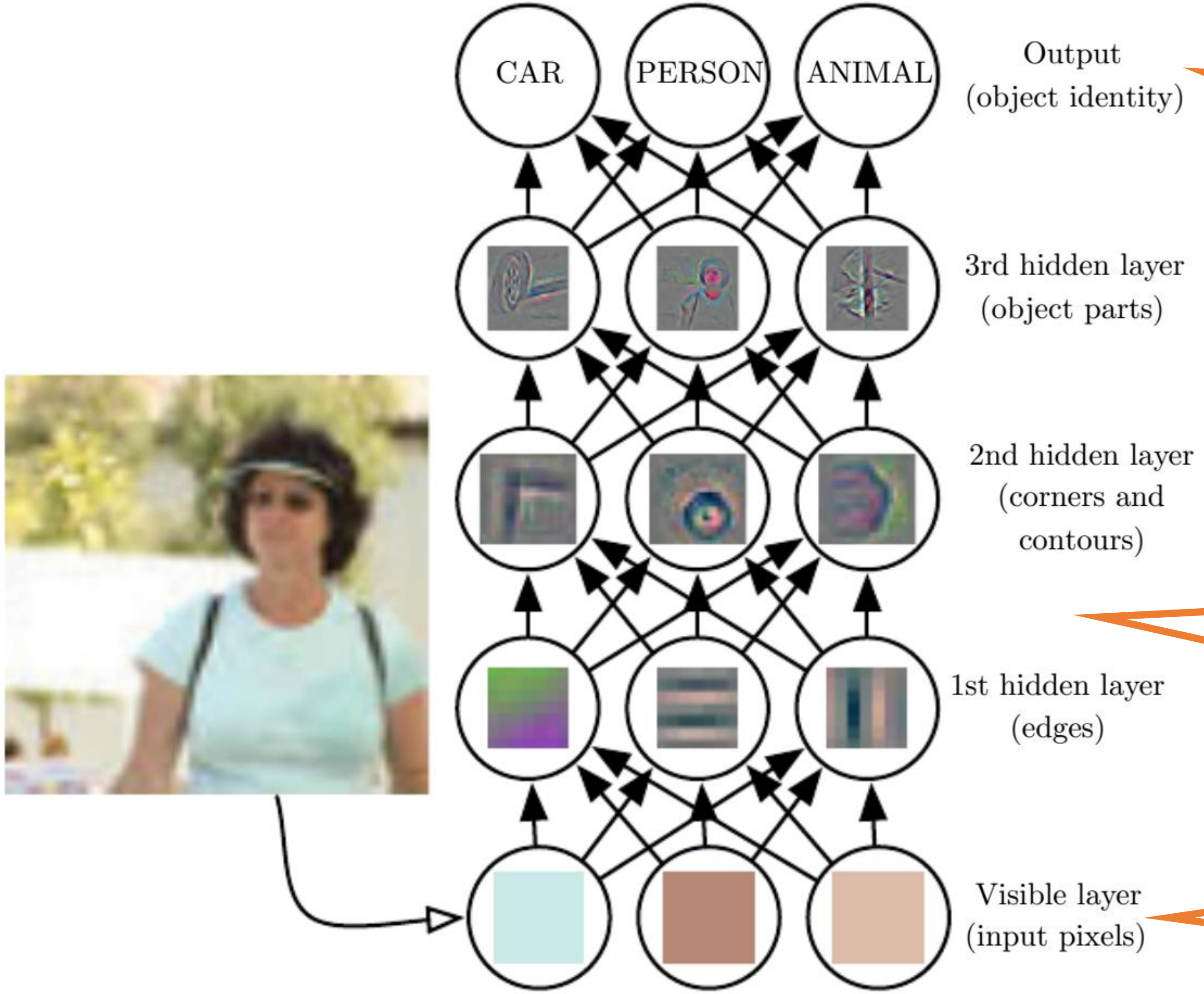

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Hidden layer compute latent representations "hidden" from data

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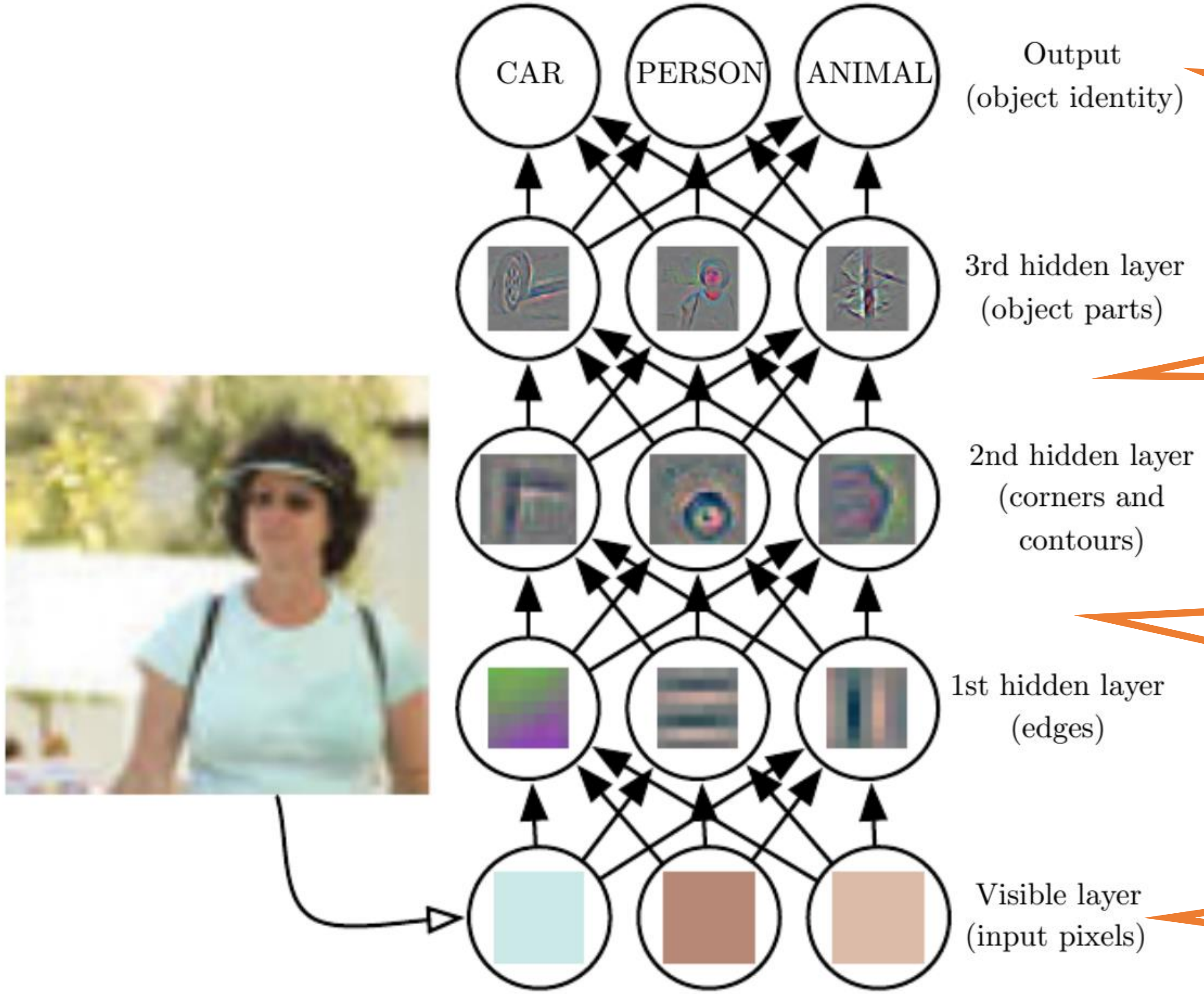

Output layer received with data i.e. "visible"

Greatly simplify learning task

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Activation/link functions

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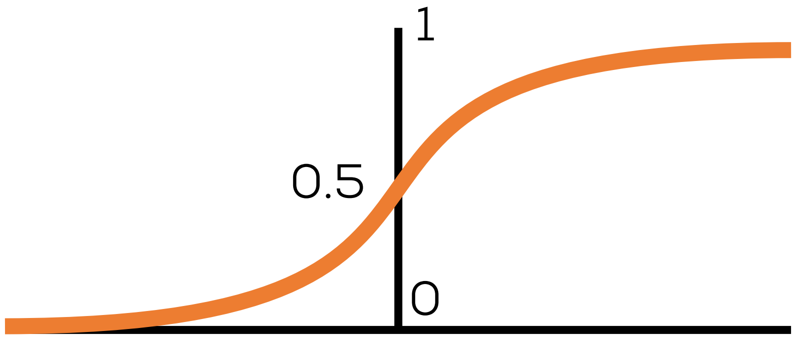

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Sigmoid

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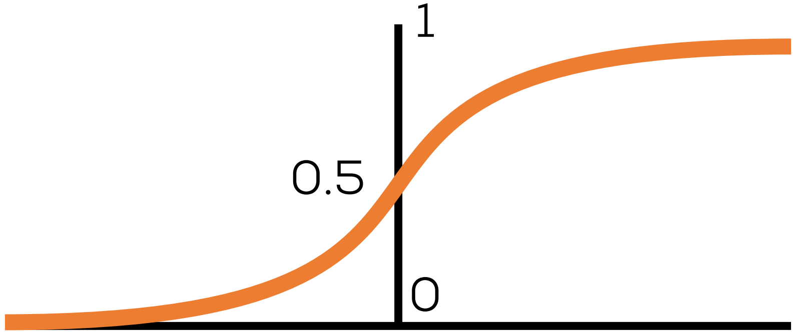

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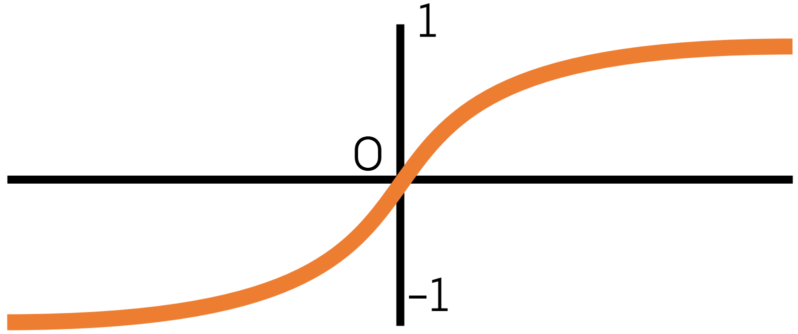

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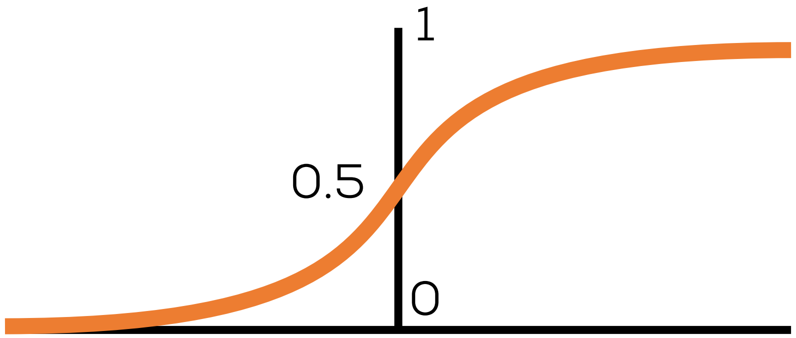
Hyperbolic Tangent

Activation/link functions



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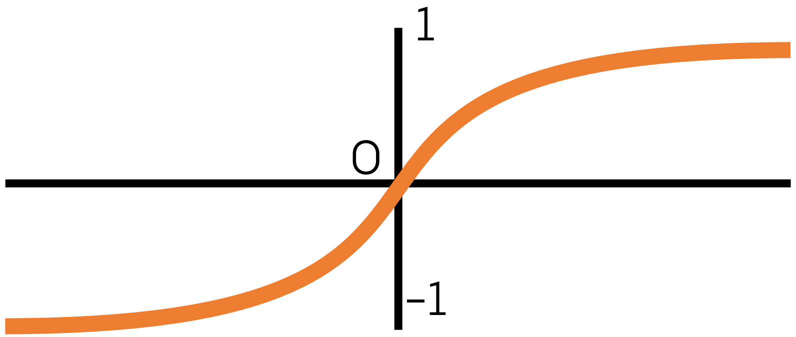

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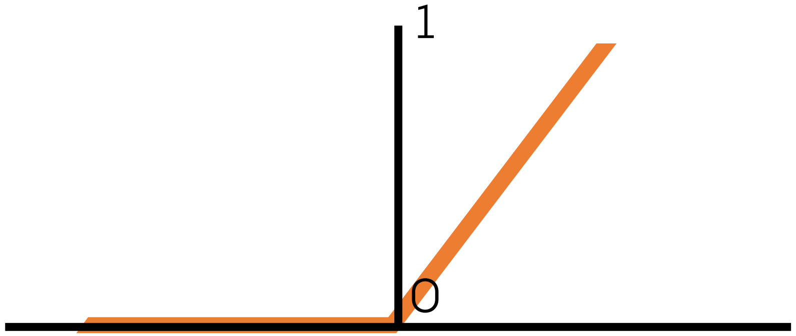

$$f(t) = \max(t, 0)$$

Rectified Linear Unit (ReLU)

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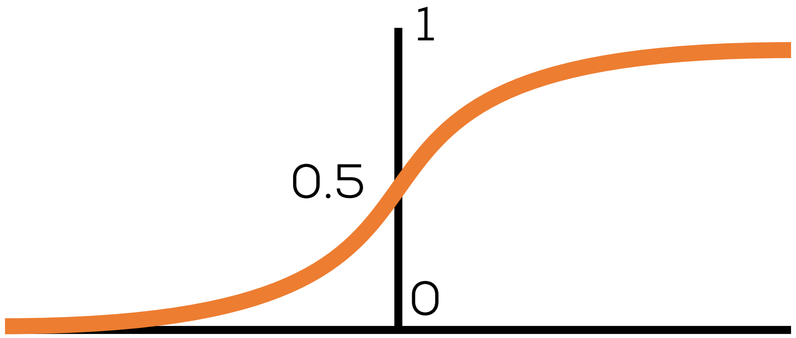

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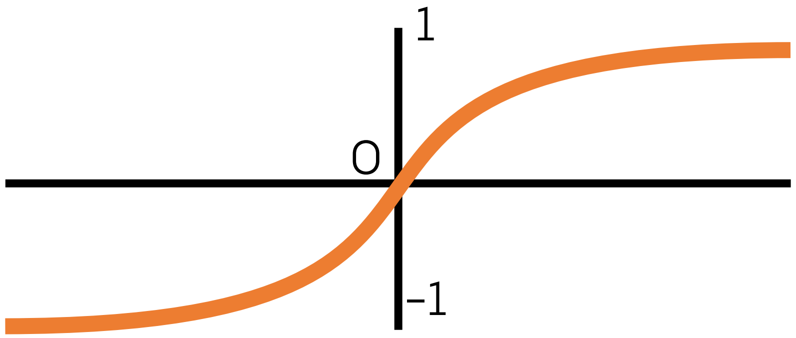

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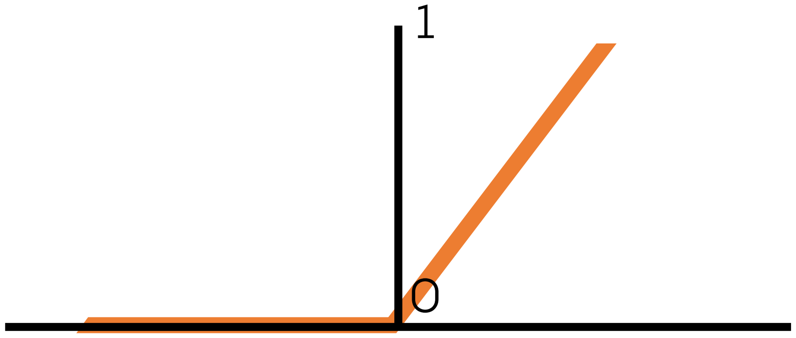

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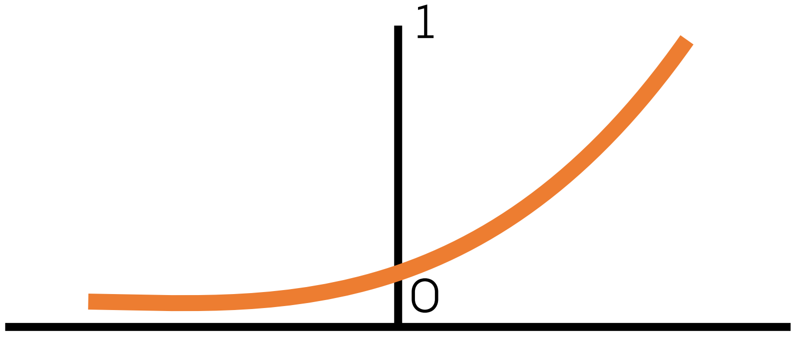

$$f(t) = \log(1+\exp(t))$$

Softplus

Multi-output Networks

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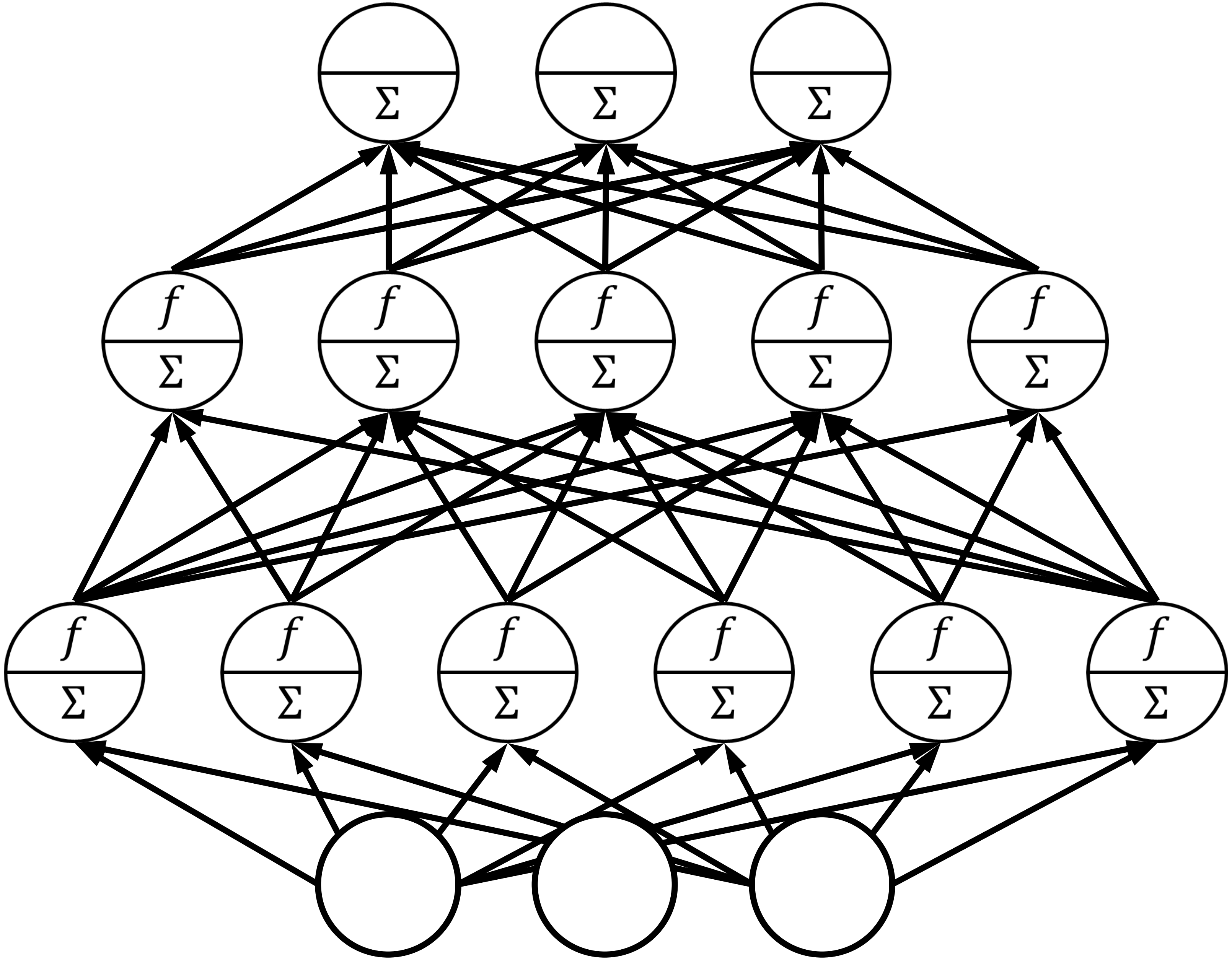

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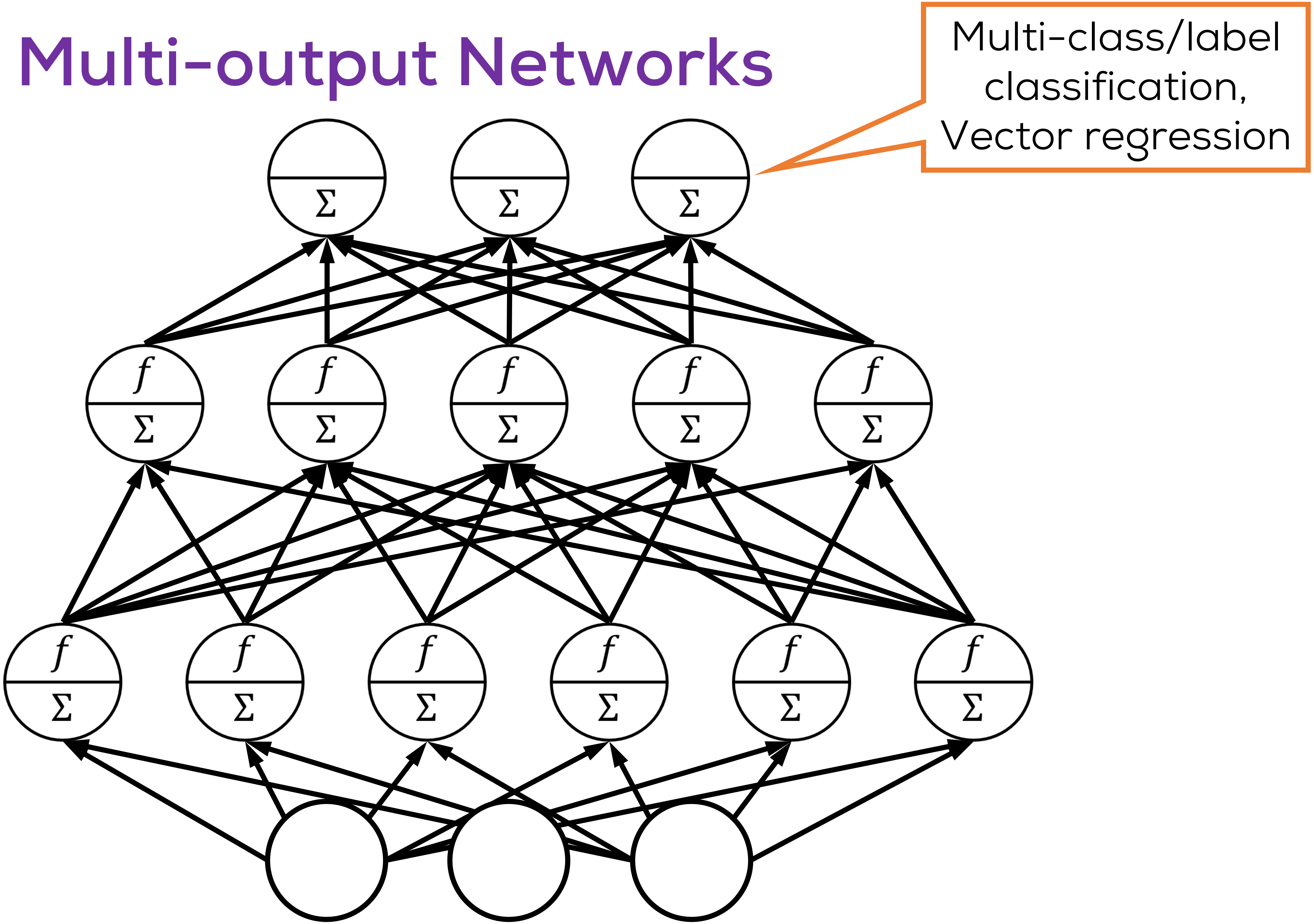

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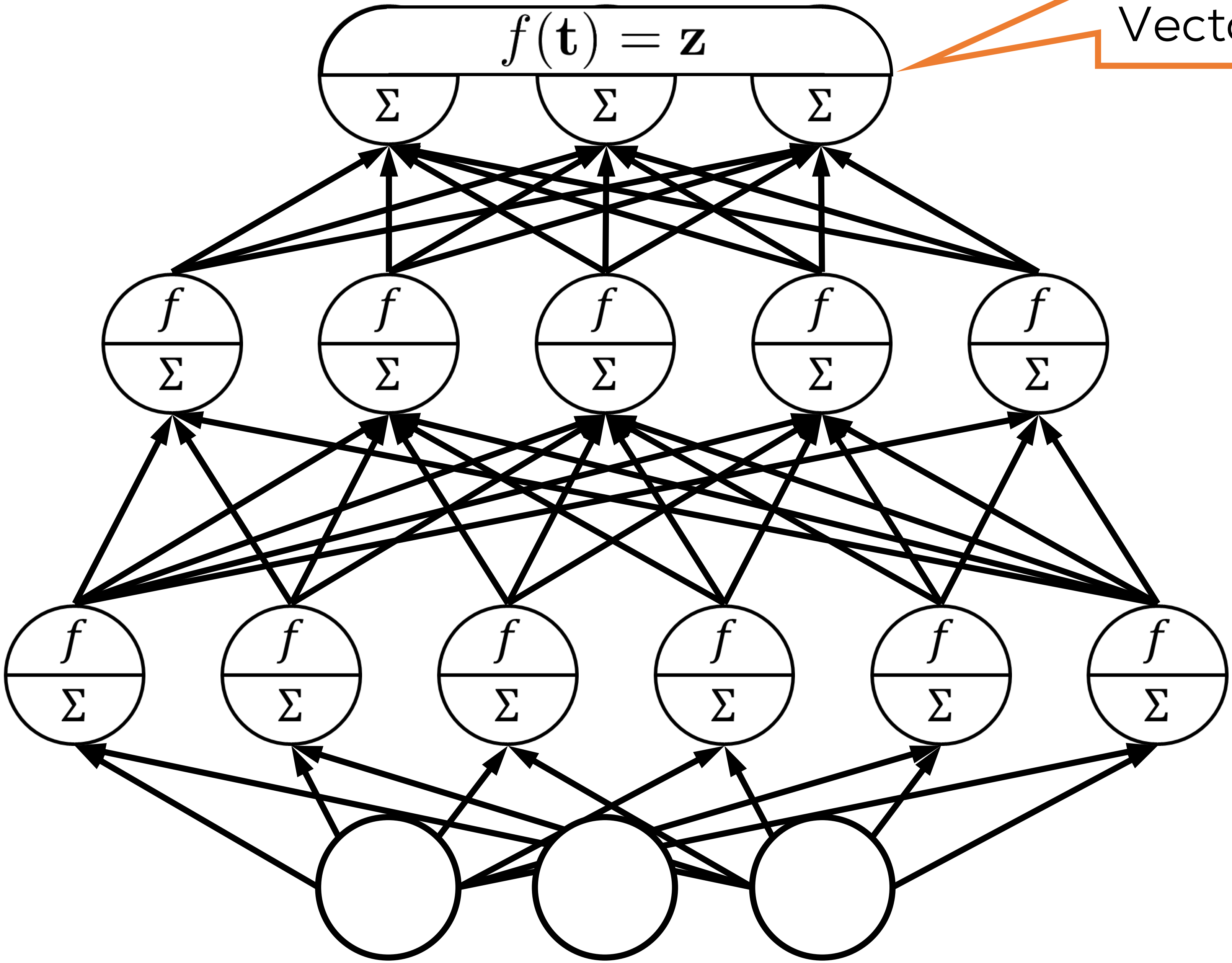
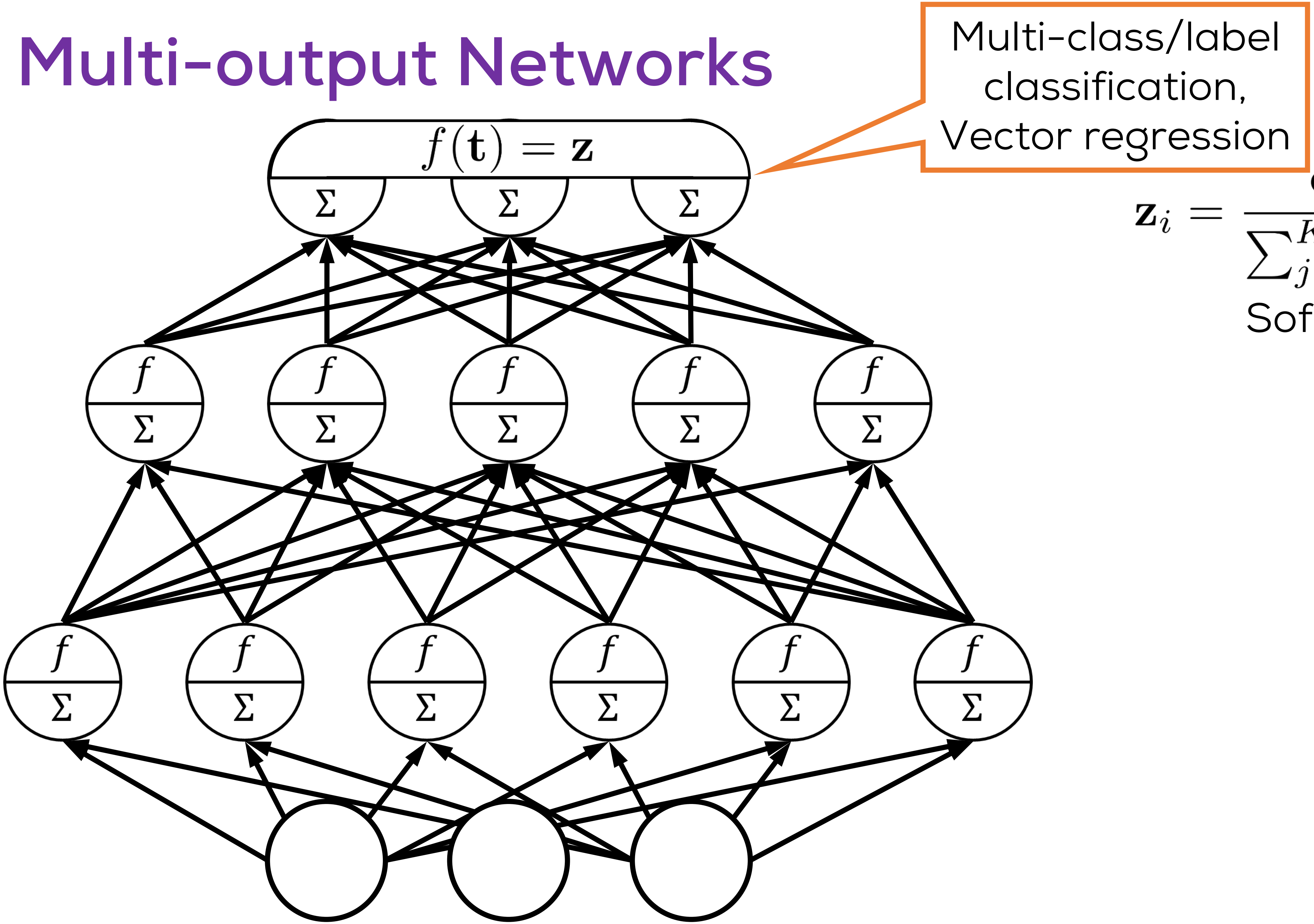


Multi-class/label classification, Vector regression

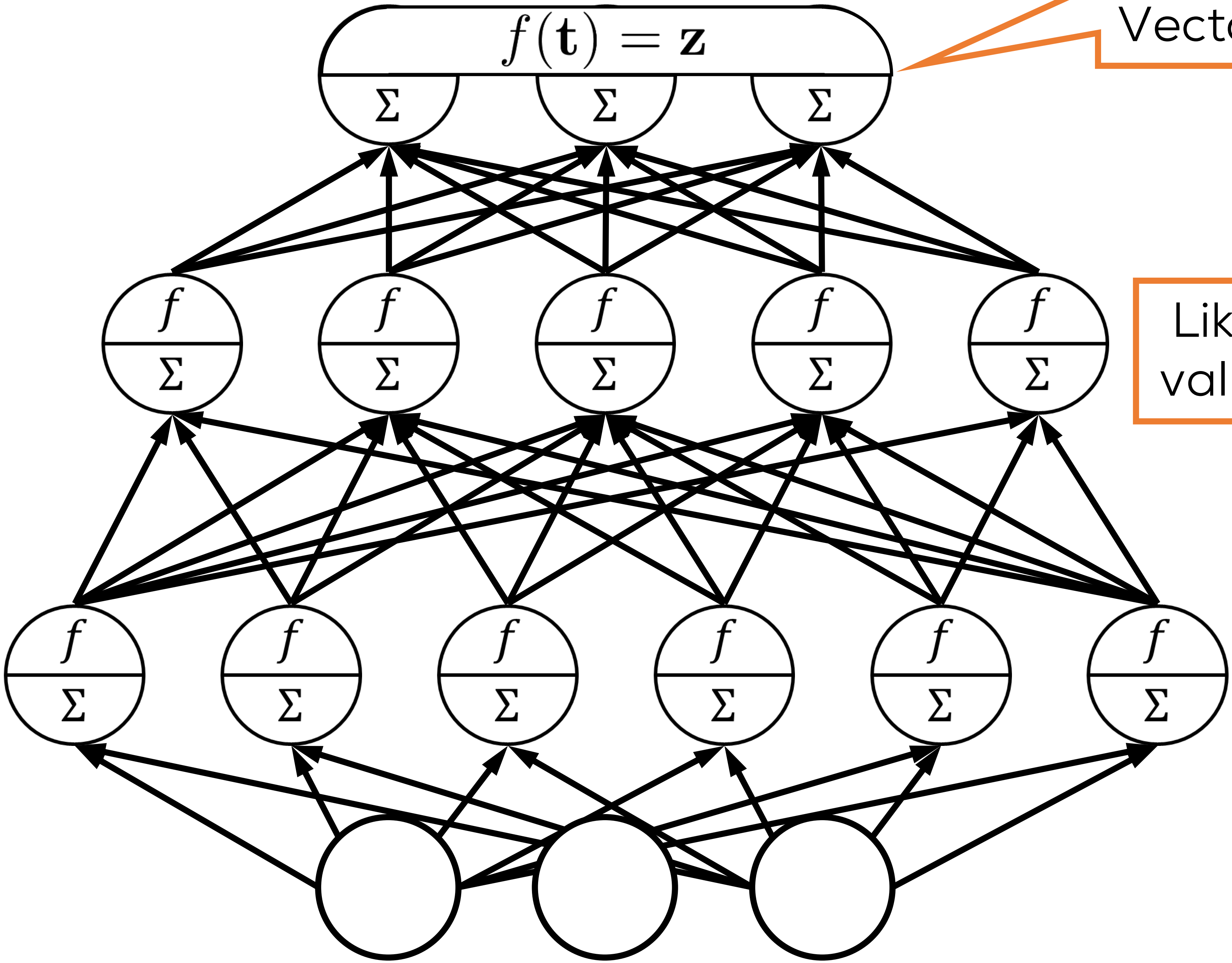
Multi-output Networks



$$\mathbf{z}_i = \frac{\exp(\mathbf{t}_i)}{\sum_{j=1}^{K} \exp(\mathbf{t}_j)}$$

Softmax

Multi-output Networks



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Like sigmoid, converts real values to probability values

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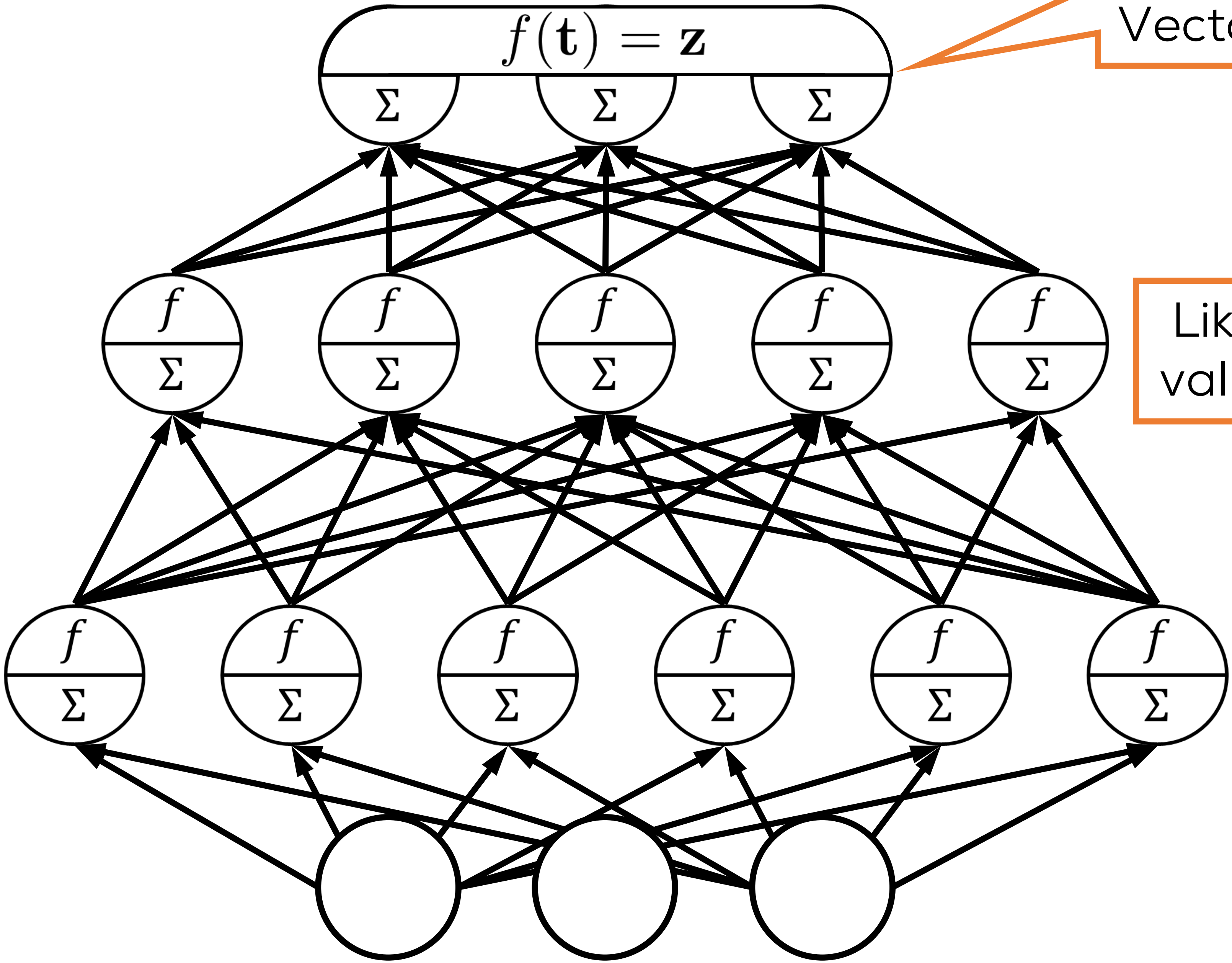

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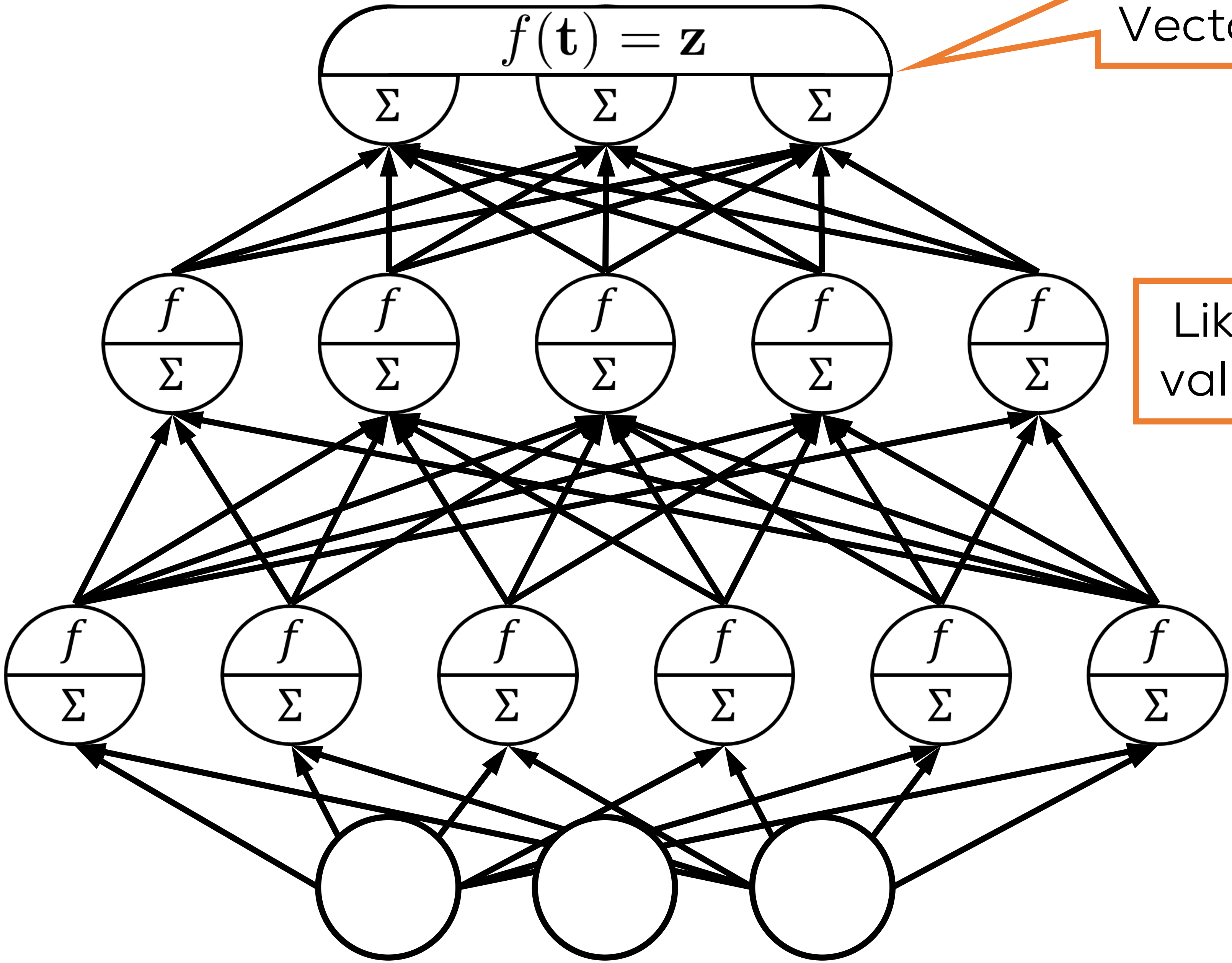

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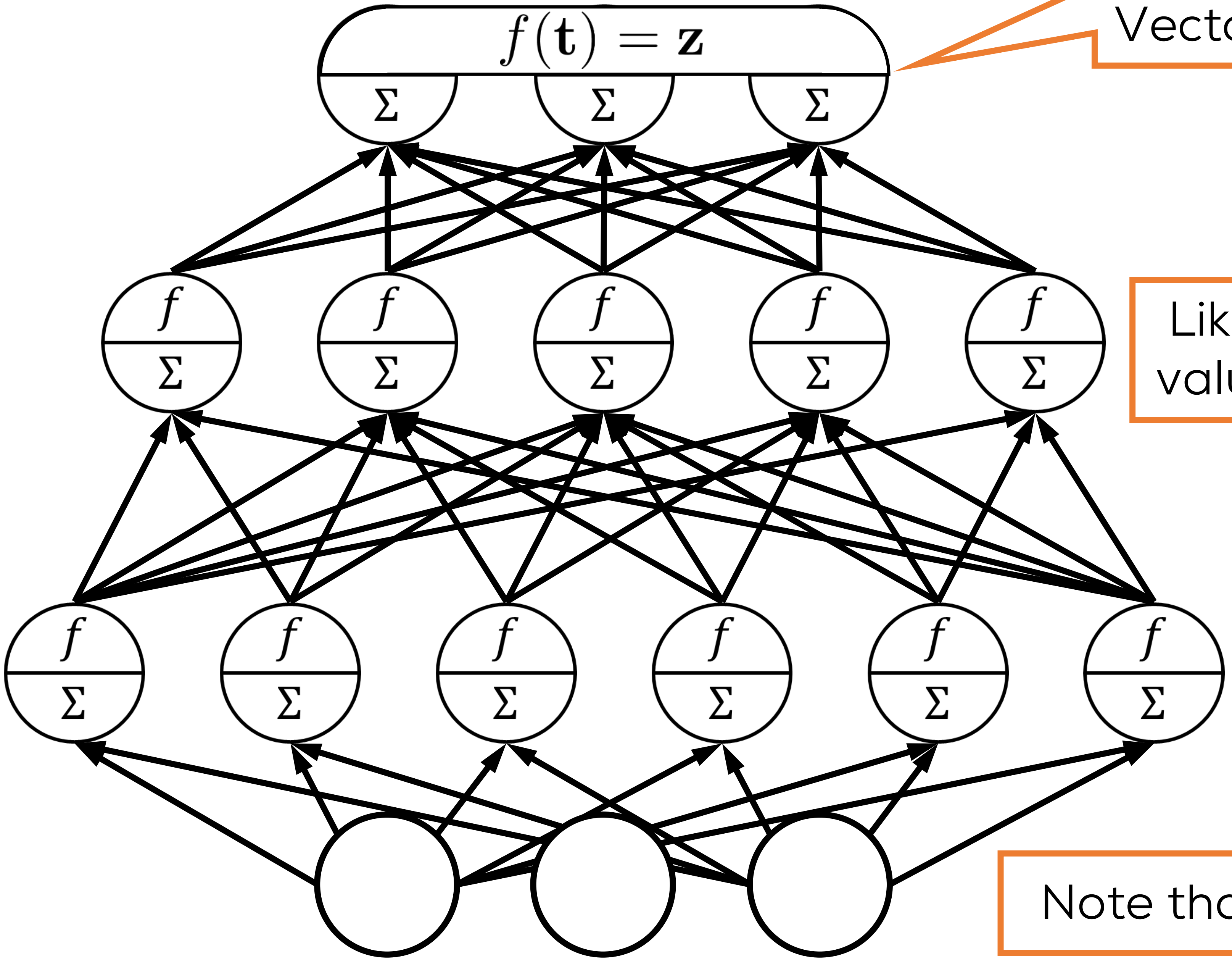

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Note that $\mathrm{f_{SM}}(\mathbf{t}) = \mathrm{f_{SM}}(\tilde{\mathbf{t}})$

Loss/Cost Functions

- Squared loss

$$\ell_{\text{LS}}(\hat{y}, y) = (\hat{y} - y)^2$$

- Absolute difference

$$\ell_{\text{ABS}}(\hat{y}, y) = |\hat{y} - y|$$

- Negative log-likelihood loss

$$y \in [K], \hat{\mathbf{y}} = f_{\text{SM}}(\mathbf{t}), \mathbf{t} \in \mathbb{R}^K$$
$$\ell_{\text{NLL}}(\hat{\mathbf{y}}, y) = -\log\left(\hat{\mathbf{y}}_y\right)$$

- Cross-entropy

$$\ell_{\text{CE}}(\hat{y}, y) = y \cdot \log \hat{y} + (1 - y) \cdot \log(1 - \hat{y})$$

- Hinge loss

$$\ell_{\text{Hinge}}(\hat{y}, y) = [1 - y\hat{y}]_+$$

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LS used with identity/ReLU activation

Sigmoid/softmax flatten out quickly so LS doesn't work

NLL, CE used with sigmoid/softmax activations

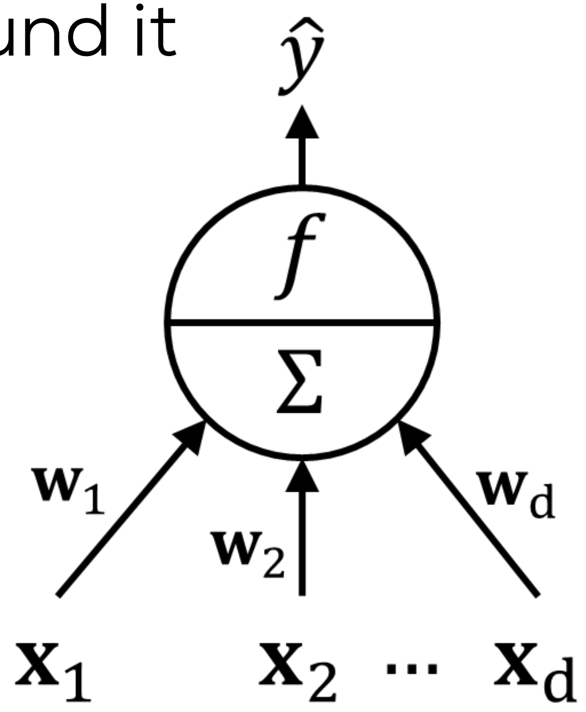
CE/Hinge usually used when $y \in \{0,1\}$ is binary

Training a Perceptron

The Generalized Perceptron

- Simply a linear model will a wrapper thrown around it
- Makes predictions as

$$\hat{y} = f(\langle \mathbf{w}, \mathbf{x} \rangle)$$



- Given lots of data points

$$(\mathbf{x}^1, y^1), \ldots, (\mathbf{x}^n, y^n), \mathbf{x}^i \in \mathbb{R}^d$$

- … and a loss function

$$\ell \colon \mathbb{R} \times \mathbb{R} \to \mathbb{R}_+$$

- … training a perceptron involves finding

$$\arg\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_i^n \ell\left(f\left(\langle \mathbf{w}, \mathbf{x}^i \rangle\right), y^i\right) =: \arg\min_{\mathbf{w} \in \mathbb{R}^d} F(\mathbf{w})$$

Gradient Descent Revisited

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GRADIENT DESCENT

1. Initialize $\mathbf{w}^0$
2. For $t = 1, 2, \ldots$
   1. Obtain a descent direction $\mathbf{g}^t$
   2. Update $\mathbf{w}^{t+1} \leftarrow \mathbf{w}^t - \eta_t \cdot \mathbf{g}^t$
3. Repeat until convergence

Gradient Descent Revisited

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- How to find a descent direction?
- How to choose a step length?
- How to detect convergence?
- How to avoid overfitting?

Have to be more careful than earlier since now, problems are not nicely behaved

Choosing a descent direction

- Batch gradient

$$\mathbf{g}^t = \nabla F(\mathbf{w}^t) = \frac{1}{n}\sum_{i=1}^{n} \ell'\left(f\left(\left\langle \mathbf{w}^t, \mathbf{x}^i \right\rangle\right), y^i\right) \cdot f'\left(\left\langle \mathbf{w}^t, \mathbf{x}^i \right\rangle\right) \cdot \mathbf{x}^i$$

- Mini-batch gradient: choose a mini-batch $I_1^t, I_2^t, \ldots, I_B^t \sim [n]$

$$\mathbf{g}^t = \frac{1}{B}\sum_{j=1}^{B} \ell'\left(f\left(\left\langle \mathbf{w}^t, \mathbf{x}^{I_j^t} \right\rangle\right), y^i\right) \cdot f'\left(\left\langle \mathbf{w}^t, \mathbf{x}^{I_j^t} \right\rangle\right) \cdot \mathbf{x}^{I_j^t}$$

- Newton's method

$$\mathbf{g}^t = \left(\nabla^2 F(\mathbf{w}^t)\right)^{-1} \nabla F(\mathbf{w}^t)$$

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Chain rule!

Very small batch sizes usually not used for deep networks

- Mini-batch gradient: choose a mini-batch $I_1^t, I_2^t, \ldots, I_B^t \sim [n]$

$$\mathbf{g}^t = \frac{1}{B}\sum_{j=1}^{B} \ell'\left(f\left(\left\langle \mathbf{w}^t, \mathbf{x}^{I_j^t} \right\rangle\right), y^i\right) \cdot f'\left(\left\langle \mathbf{w}^t, \mathbf{x}^{I_j^t} \right\rangle\right) \cdot \mathbf{x}^{I_j^t}$$

For a NN with E edges, $\mathcal{O}(E^3)$ time per iteration!

- Newton's method

$$\mathbf{g}^t = \left(\nabla^2 F(\mathbf{w}^t)\right)^{-1} \nabla F(\mathbf{w}^t)$$

Expensive! $\mathcal{O}(d^3)$ time per iteration

How to detect convergence

- Tolerance technique
  - For a predecided tolerance value ϵ, if $F(\mathbf{w}^t) < \epsilon$, stop
- Zero-th order technique
  - If function value has not changed too much between iterations, stop!

$$|F(\mathbf{w}^{t+1}) - F(\mathbf{w}^t)| < \tau$$

- First order technique
  - If gradient is too "small" $\|\nabla F(\mathbf{w}^t)\|_2 < \delta$, stop!
- Primal dual
  - If primal and dual objective values are close, stop
  - Does not work every where – reliable for convex problems

How to decide step length?

- Simply rule of thumb – naïve but fast
  Choose $\eta_t \to 0$ (diminishing) and $\sum \eta_t \to \infty$ (infinite travel)
- Example $\eta_t = C/\sqrt{t}$ or $\eta_t = C/t$ for some $C > 0$
- Line search – super careful but expensive
$$\eta_t = \arg\min_{\eta \geq 0} F(\mathbf{w}^t - \eta \cdot \mathbf{g}^t)$$
- Can we do something more adaptive?
- Can we let each coordinate of $\mathbf{w}$ get its own step length?
- $\mathbf{w}^{t+1} \leftarrow \mathbf{w}^t - \eta \cdot H^{-1}\mathbf{g}^t$ where $H = \mathrm{diag}(h_1, h_2, \ldots, h_d)$
- Wait … this looks like the Newton method!
- Indeed this is an approximate Newton method – wait a bit!

Momentum Methods

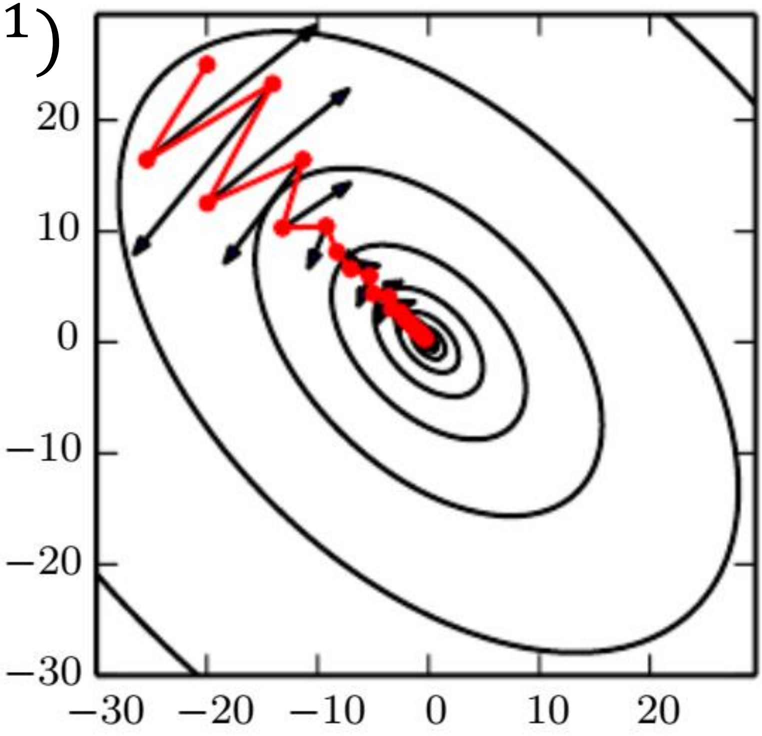
- Introduce a velocity term to push GD along, avoid oscillations

$$\mathbf{v}^t = \gamma \cdot \mathbf{v}^{t-1} + \eta \cdot \nabla F(\mathbf{w}^t)$$
$$\mathbf{w}^{t+1} \leftarrow \mathbf{w}^t - \mathbf{v}^t$$

- **Nesterov's accelerated gradient (NAG)**
- Does a "look-ahead"

$$\mathbf{v}^t = \gamma \cdot \mathbf{v}^{t-1} + \eta \cdot \nabla F(\mathbf{w}^t - \eta \cdot \mathbf{v}^{t-1})$$
$$\mathbf{w}^{t+1} \leftarrow \mathbf{w}^t - \mathbf{v}^t$$

- For "smooth" convex problems, NAG ensures ϵ-convergence in just $\mathcal{O}(1/\epsilon)$ steps
  hence the name "accelerated" gradient
- Don't have very deep insights why it works 😐



Adaptive Learning Rates

$$\mathbf{w}^{t+1} \leftarrow \mathbf{w}^t - \eta \cdot (H^t)^{-1}\mathbf{g}^t$$
$$H^t = \mathrm{diag}(h_1^t, h_2^t, \ldots, h_d^t)$$

- Adagrad (Duchi et al. 2011)

$$h_i^t = \sqrt{\epsilon + \sum_{\tau=1}^{t} \left(\mathbf{g}_i^\tau\right)^2}$$

- Note that if all coordinates get roughly similar gradients then we have $h_i^t \approx t$ and Adagrad behaves as if we had set $\eta_t \approx \eta/t$
- However, if some coordinate getting updated very vigorously, $|\mathbf{g}_i^\tau| \gg 0$ for all τ, Adagrad slows it down a bit
- If some coordinate is static $\mathbf{g}_i^\tau \equiv 0$ for all τ, then $h_i^t = \epsilon$, no effect

Adaptive Learning Rates

$$\mathbf{w}^{t+1} \leftarrow \mathbf{w}^{t} - \eta \cdot (H^{t})^{-1}\mathbf{g}^{t}$$
$$H^{t} = \mathrm{diag}(h_1^t, h_2^t, \ldots, h_d^t)$$

- RMSProp (Hinton 2012)

$$h_i^t = \sqrt{\epsilon + v_i^t}$$

$$v_i^t = \gamma \cdot v_i^{t-1} + (1-\gamma) \cdot \left(\mathbf{g}_i^t\right)^2$$

- Adagrad can be too aggressive in forcing step sizes down
- RMSProp has better performance in non-convex settings
- Hinton suggests $\gamma \approx 0.9$
- May be combined with NAG as well!

Adaptive Learning Rates

$$\mathbf{w}^{t+1} \leftarrow \mathbf{w}^t - \eta \cdot (H^t)^{-1}\mathbf{u}^t$$
$$H^t = \mathrm{diag}(h_1^t, h_2^t, \dots, h_d^t)$$

- Adam (Kingma and Ba 2014)

$$h_i^t = \sqrt{\epsilon + v_i^t}$$
$$\mathbf{u}^t = \gamma_1 \cdot \mathbf{u}^{t-1} + (1-\gamma_1) \cdot \mathbf{g}^t$$
$$v_i^t = \gamma_2 \cdot v_i^{t-1} + (1-\gamma_2) \cdot \left(\mathbf{g}_i^t\right)^2$$

- Keeps track of past gradients as well as squared gradients
- Actually does a bias correction step before using $\mathbf{u}^t$ and H^t
- Details can be found in Deep Learning textbook

How to prevent overfitting?

- Add a regularization term L_2/L_1 to the objective

$$\arg\min_{\mathbf{w}\in\mathbb{R}^d} F(\mathbf{w}) + \lambda \cdot \|\mathbf{w}\|_2^2$$

- Gradients calculations change very slightly
- Constraint the weights of the network to satisfy $|\mathbf{w}_i| < r$

$$\arg\min_{\|\mathbf{w}\|_\infty < r} F(\mathbf{w})$$

- Sometimes gradient coordinates are also *clipped* this way
- Noise injection in output
  - For binary classification $y^i = 0 \rightarrow y^i = \epsilon$, $y^i = 1 \rightarrow y^i = 1 - \epsilon$
  - For regression problems, $y^i \rightarrow y^i + \epsilon^i$, where $\epsilon^i \sim \mathcal{N}(0, \sigma^2)$
  - Can be shown to be equivalent to regularization in nice cases

How to prevent overfitting?

- Early stopping – return model with best validation set performance rather than best training set performance
- Can use many of these strategies in combination
- Parameter sharing – add constraints of the form
$$\mathbf{w}_i = \mathbf{w}_j$$
- Sparse recovery – constrain, say at least 10% weights to be zero
$$\|\mathbf{w}\|_0 \leq k \ll d$$
- Dropout
  - Effectively trains on multiple sparse networks in parallel
  - While executing a GD update, randomly remove edges or entire nodes from network so they do not participate
  - Can be shown to be equivalent to L_2 reg. in nice settings

Other techniques used to train NNs

- Pre-training
- Batch normalization
- Curriculum learning
- Pre-training
- Conjugate gradient descent
- Normalized gradient descent
- Approximate Newton method L-BFGS
- Some of these developed earlier for convex opt. problems
- Some we have discussed earlier in context of linear models
  Coordinate descent, Model averaging (Ruppert-Polyak method)

Nice discussion in the Deep Learning book

Up Next

- Training multi-layered perceptrons - backpropagation
- Autoencoders
- RNNs
- CNNs
- GANs
- Cannot go into too many details but will cover basics ☺

Please give your Feedback

http://tinyurl.com/ml17-18afb