Non-linear Models-IV

CS771: Introduction to Machine Learning

Purushottam Kar

Outline of discussion

- Kernel Approximation Methods
- PML with kernels
- Neural networks

Kernel methods can be slow ☹

- Need to work with indirect "dual" representations
- Although finite, these representations blow up with data size
- Prediction requires a full pass over data i.e. $O(dn)$ time
- Will see some techniques to remedy this

The Tale of a Trio of Techniques

- **Post-processing techniques**: learn the kernel SVM (a bit costly), but then make the model cheaper to store and predict
- **Approximate training techniques**: directly learn a kernel SVM model that is cheap to store and predict
- **Kernel approximation techniques**: use a different kernel than the one you wanted to, so that the new kernel mimics the original one but always gives models that are cheap to store and predict
- Kernel approximation is the most successful of the three

Post Processing Techniques

- Learn kernel SVM, support vectors $\{x_{i_j}, \alpha_{i_j}\}$
- Find a *reduced set* of $k \ll \tilde{n}$ support vectors $\{\tilde{x}_{i_1}, \ldots, \tilde{x}_{i_k}\}$ e.g. by using k-means clustering on original support vectors
- Re-compute α values for these reduced set support vectors e.g. by running SVM again on $\{\tilde{x}_{i_1}, \ldots, \tilde{x}_{i_k}\}$
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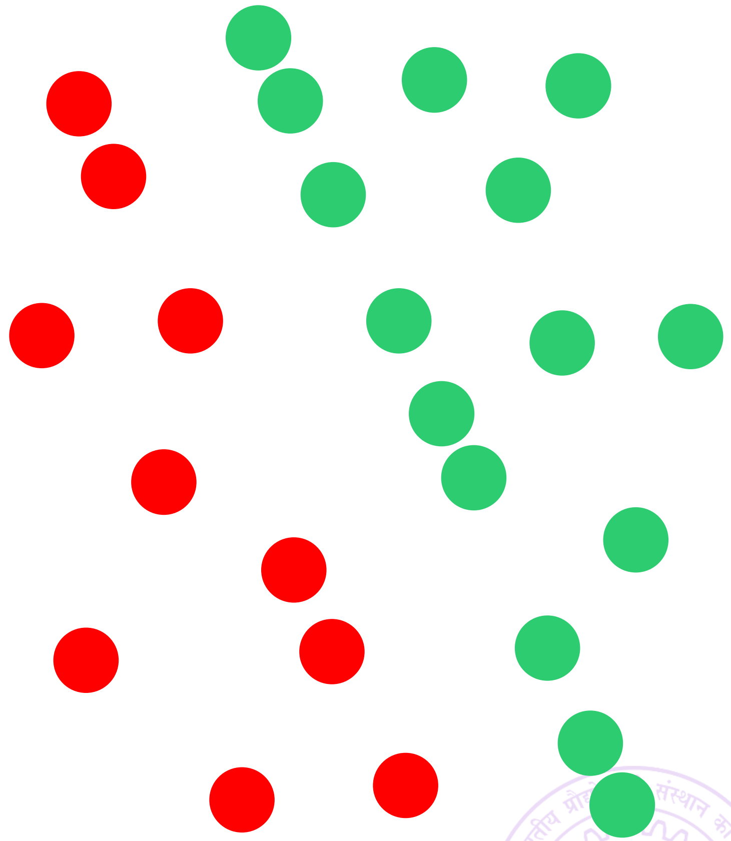

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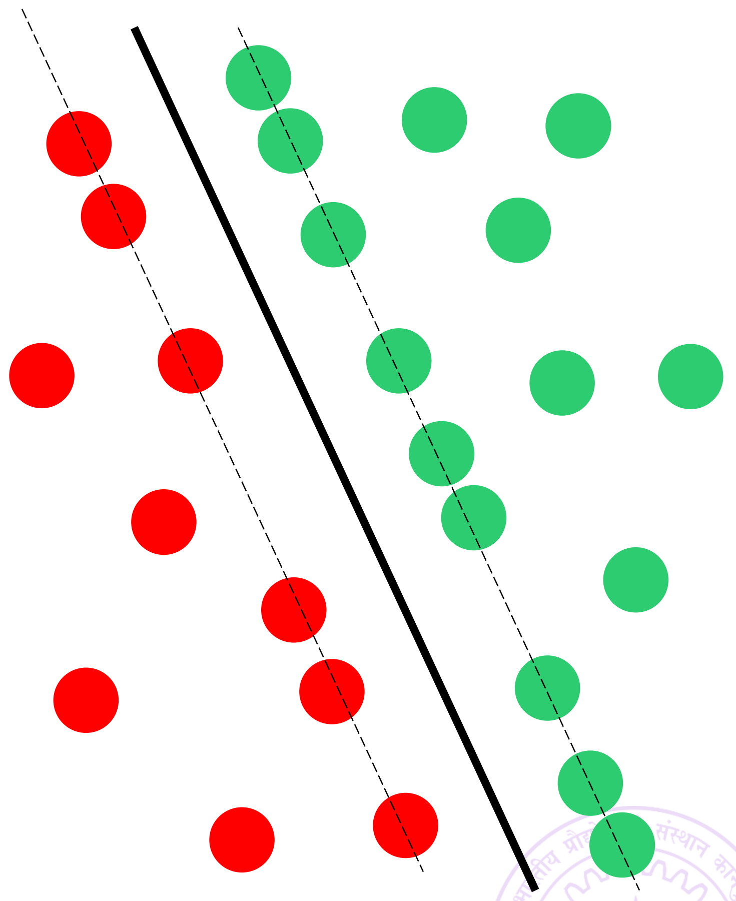

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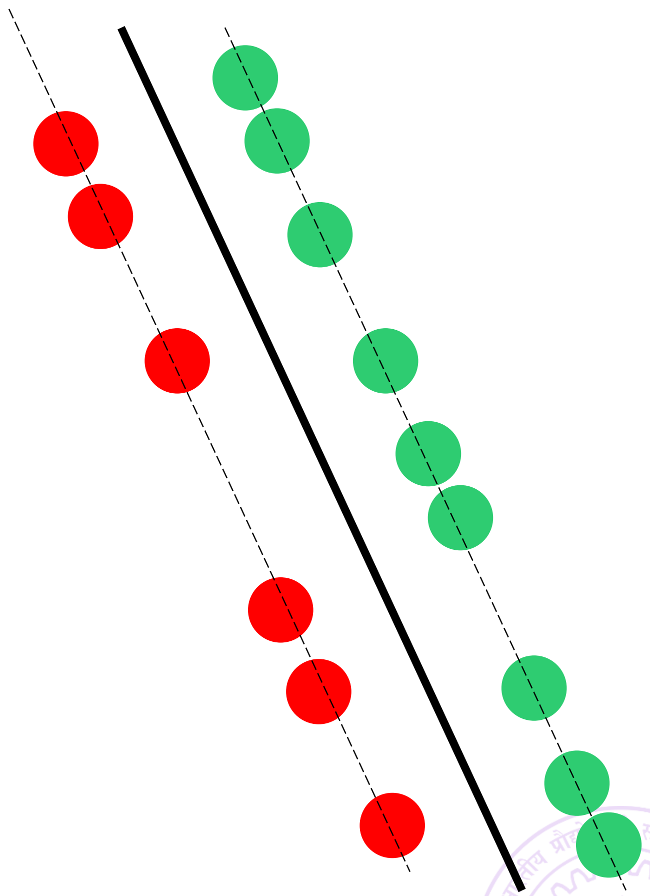

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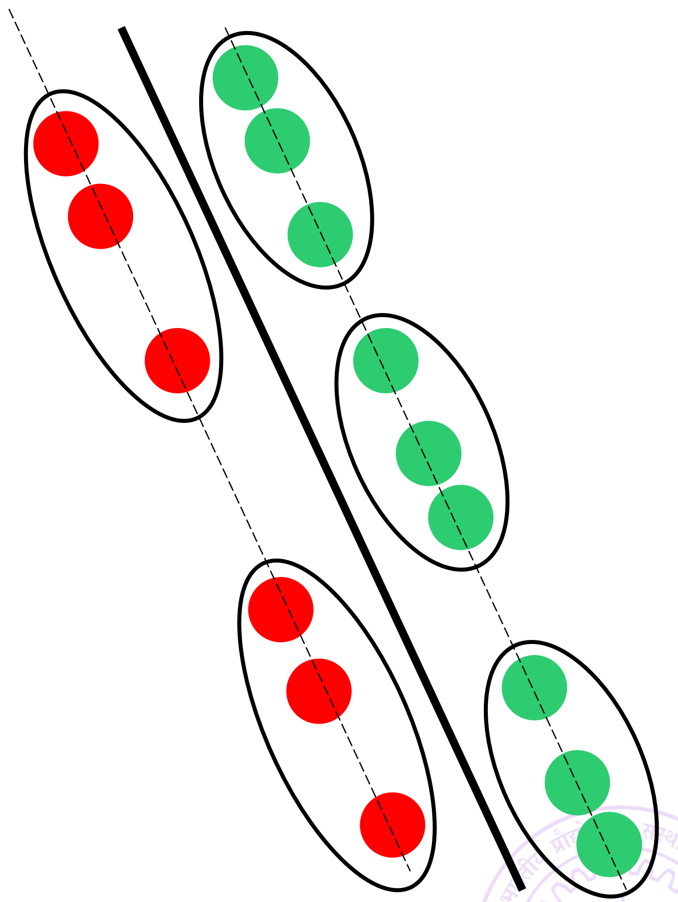

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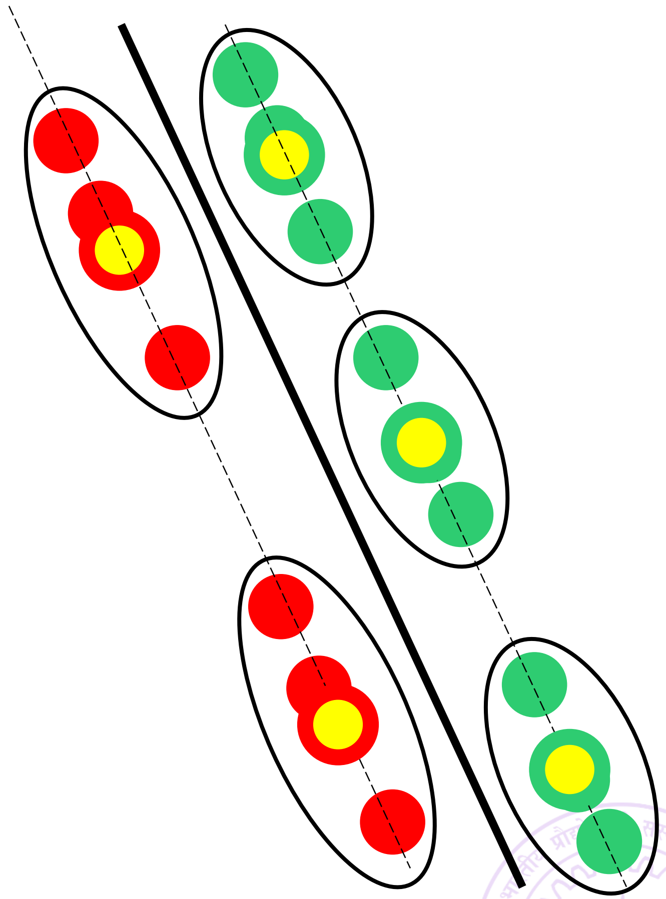

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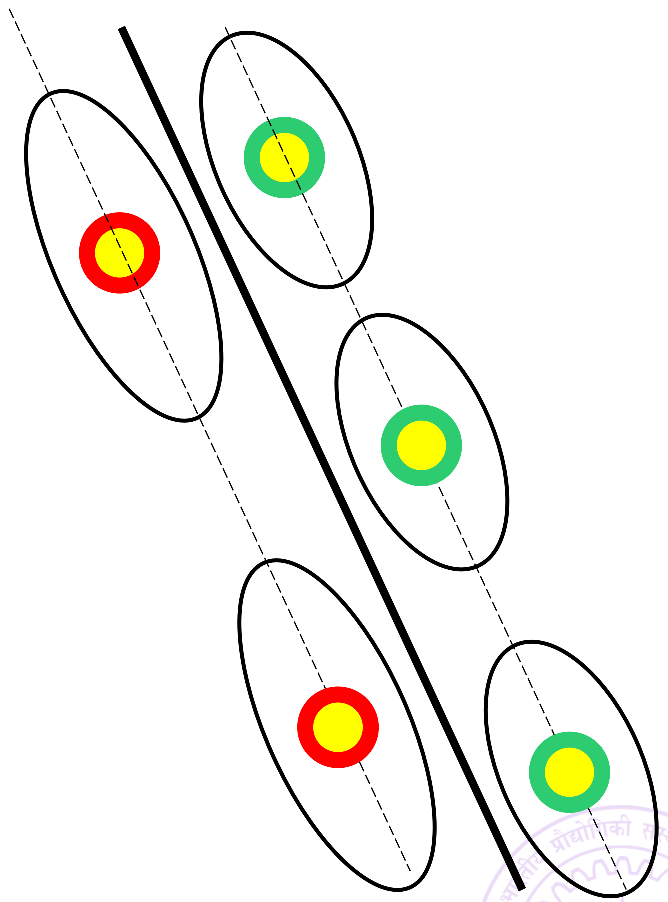

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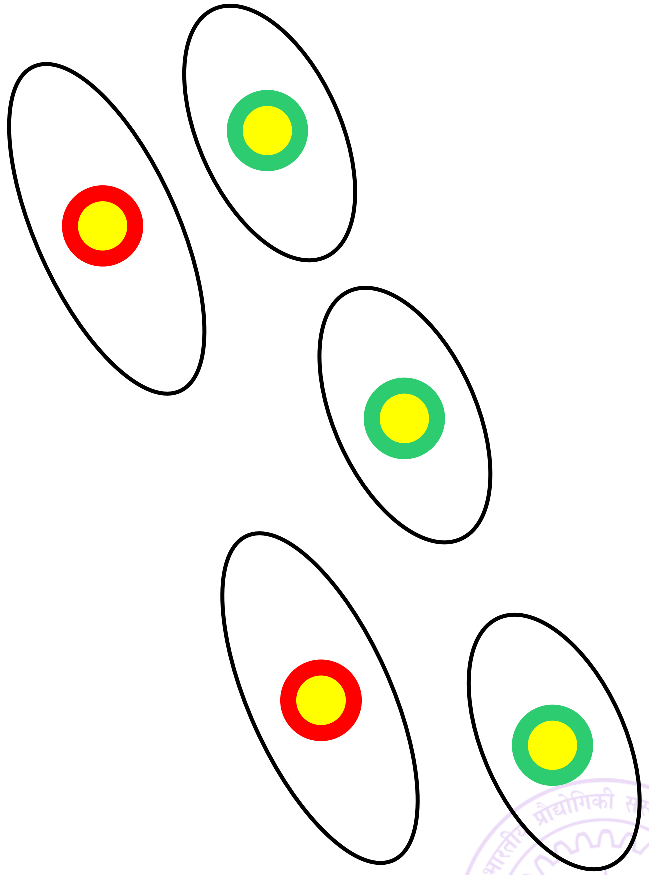

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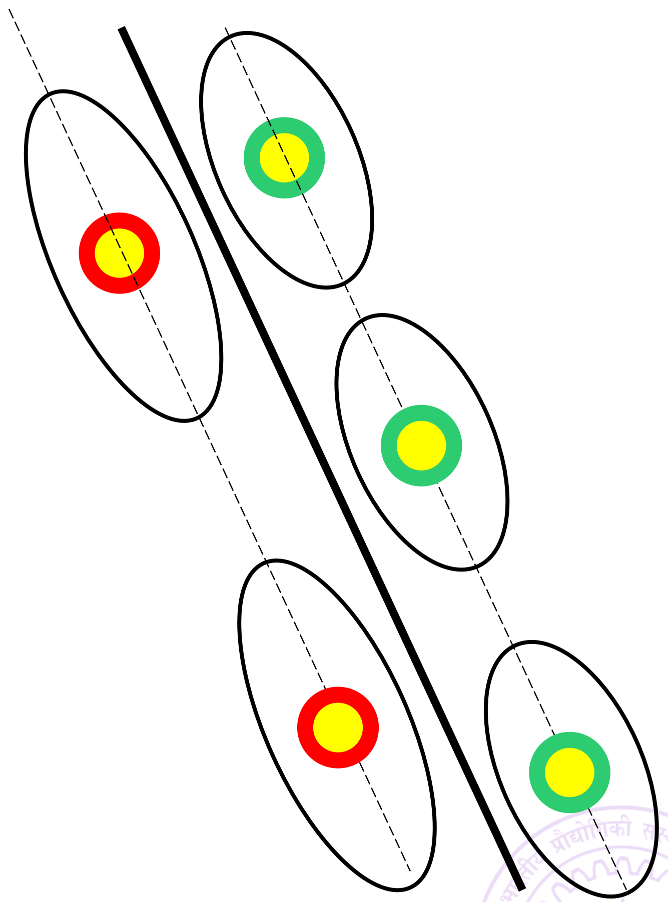

Approximate Training Techniques

- Notice that support vectors are always a subset of training data
- Maybe removing this restriction can reduce their number?
- Learn support vectors as well (not necessarily training points)!
- Learn vectors $\mathbf{z}^1, \ldots, \mathbf{z}^k \in \mathbb{R}^d$ and weights $\alpha_1, \ldots, \alpha_k \in \mathbb{R}$ so that
$$\mathbf{w} = \sum_{i=1}^{k} \alpha_i \cdot \phi_K(\mathbf{z}^i)$$
is a good model (classifier, regressor etc)
- k chosen based on budget (space, time) of application
- $\mathcal{O}(kd)$ storage and $\mathcal{O}(kd)$ time for prediction

- Joachims and Yu. Sparse Kernel SVMs via Cutting-Plane Training, Machine Learning 76(2):179-193, 2009
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ϕ_K is the map for kernel K

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Kernel Approximation

Landmarking

- Given: training set $S = \{x^1, \dots, x^n\}$ and kernel K
- Select $k \ll n$ *landmarks*

$$\hat{S} = \{\hat{x}^1, \dots, \hat{x}^k\} \subset S$$

- Choice may be random or careful (more expensive)
- Use landmarks to create a new k-dim. feature representation

$$\hat{\phi}(x) = \left[K(x, \hat{x}^1), \dots, K\left(x, \hat{x}^k\right)\right]$$

- Now use $\hat{\phi}(x)$ to perform classification, regression, etc
- Can be theoretically shown that if K was nice, so will be $\widehat{K}$
- No agony of high dim-feature map with $\widehat{K}$

- Balcan and Blum. On a Theory of Learning with Similarity Functions, ICML 2006.
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Since k is chosen to be small, so use linear SVM/RR over $\hat{\phi}(x)$ directly

Can think of $\hat{\phi}$ as giving us a new kernel $\widehat{K}(x, y) = \langle \hat{\phi}(x), \hat{\phi}(y) \rangle$

$\mathcal{O}(kd)$ model size and $\mathcal{O}(kd)$ prediction time

Work with non-Mercer kernels too!

Nystrom Method

- A more careful implementation of landmarking
- **Basic idea**: landmarks may be correlated – decorrelate them
- Recall landmark set $\hat{S}$ of size k gave us a map $\hat{\phi}$ that maps to $\mathbb{R}^k$
- Let $\hat{G} \in \mathbb{R}^{k\times k}$ be Gram matrix over landmark set $\hat{S}$ and let its eigendecomposition be $\hat{G} = U\Lambda U^\top$ where $U = [u^1, \ldots, u^k] \in \mathbb{R}^{k\times k}$ is the matrix of eigenvectors and $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_k)$ be eigenvalues
- Nystrom method defines the similarity between x, y as
$$\hat{\phi}(x)^\top G^\dagger \hat{\phi}(y)$$
- Nystrom features are modified version of landmarking feature $\hat{\phi}$
$$\tilde{\phi}(x) = \sqrt{\Lambda^{-1}}U^\top\hat{\phi}(x)$$
if any $\lambda_i = 0$, remove that eigenvalue from Λ and vector from U

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Pseudoinverse

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Nystrom Method

- The Nystrom feature also gives us a new kernel $\widetilde{K}$
$$\widetilde{K}(x,y) = \tilde{\phi}(x)^\top \tilde{\phi}(y) = \hat{\phi}(x)^\top U \Lambda^{-1} U^\top \hat{\phi}(y)$$
- Note that the Gram matrices corresponding to the landmarking kernels $\widehat{K}$ as well as Nystrom kernel $\widetilde{K}$ are always rank atmost k
- Interesting note: suppose actual kernel K has map $\phi_K(x) \in \mathbb{R}^D$
- Let $\Phi_{\hat{S}} = \left[\phi\left(\hat{x}^i\right)\right]_{i=1,\ldots,k} \in \mathbb{R}^{D \times k}$ where $\hat{S} = \{\hat{x}^1, \ldots, \hat{x}^k\}$ is landmark set
- This means $\hat{\phi}(x) = \Phi_{\hat{S}}^\top \phi_K(x)$ and $\hat{G} = \Phi_{\hat{S}}^\top \Phi_{\hat{S}}$ i.e.
$$\widetilde{K}(x,y) = \phi_K(x)^\top \Phi_{\hat{S}} \left(\Phi_{\hat{S}}^\top \Phi_{\hat{S}}\right)^\dagger \Phi_{\hat{S}}^\top \phi_K(y)$$
- Takes more time $O(k^2 + kd)$ to construct Nystrom feature map
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Decorrelation

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Explicit Feature Constructions

- Realize that high dim. of feature map ϕ_K is root of all problems
- If ϕ_K were small dim. then training, storage, testing much easier
- Given a Mercer kernel $K: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ can we construct $\bar{\phi}: \mathcal{X} \to \mathbb{R}^k$
  - k should not be too large so we can use $\bar{\phi}$ explicitly
  - It should be easy to map $x \mapsto \bar{\phi}(x)$
  - $\bar{\phi}$ should act as an approx feature map for K i.e. for all $x, y \in \mathcal{X}$
$$\langle \bar{\phi}(x), \bar{\phi}(y) \rangle =: \bar{K}(x, y) \approx \mathrm{K}(\mathrm{x}, \mathrm{y}) = \langle \phi_K(x), \phi_K(y) \rangle$$
- Note that landmarking and Nystrom do not seek to ensure that $\hat{K}$ or $\tilde{K}$ values approximate K but $\bar{K}$ should approximate K values
- Why should such $\bar{\phi}$ even exist?

Random Feature Constructions

- Several popular Mercer kernels have a peculiar form

$$K(x,y) = \mathbb{E}_{\omega \sim \mathcal{D}_K}[K_\omega(x,y)]$$

  - ω is an auxiliary variable (depending on the kernel, $\omega \in \mathbb{N}, \mathbb{R}, \mathbb{R}^d$)
  - $\mathcal{D}_K$ is a distribution that depends on kernel K and known to us
  - K_ω is a very "simple" Mercer kernel, ho

$$K_\omega(x,y) = \langle \phi_\omega(x), \phi_\omega$$
$$\phi_\omega : \mathcal{X} \to \mathbb{R}$$

Normalization constant needed to ensure $\langle \bar{\phi}(x), \bar{\phi}(y) \rangle \approx K(\mathrm{x}, \mathrm{y})$

- Sample several $\omega_1, \ldots, \omega_k$ and define the map

$$\bar{\phi} : x \mapsto \frac{1}{\sqrt{k}} \cdot \left[\phi_{\omega_1}(x), \ldots, \phi_{\omega_k}(x)\right] \in \mathbb{R}^k$$

- Can theoretically prove that with high probability

$$\langle \bar{\phi}(x), \bar{\phi}(y) \rangle \approx K(\mathrm{x}, \mathrm{y})$$

Random Feature Constructions

- Gaussian/Laplacian kernels

$$K(\mathbf{x},\mathbf{y}) = \mathbb{E}_{\boldsymbol{\omega}\sim\mathcal{D}_K}[\cos(\boldsymbol{\omega}^\top\mathbf{x})\cos(\boldsymbol{\omega}^\top\mathbf{y})]$$
$$\phi_{\boldsymbol{\omega}}: \mathbf{x} \mapsto \cos(\boldsymbol{\omega}^\top\mathbf{x})$$

  Note that auxiliary variable is a vector here $\boldsymbol{\omega} \in \mathbb{R}^d$

  Rahimi and Recht, Random Features for Large Scale Kernel Machines, NIPS 2007
- Intersection kernel
  Maji and Berg, Max-margin Additive Classifiers for Detect, ICCV 2009.
- Homogeneous kernels
  Vedaldi and Zisserman. Efficient Additive Kernels via Explicit Feature Maps, CVPR 2010
- Polynomial kernels
  K. and Karnick. Random Feature Maps for Dot Product Kernels. AISTATS 2012

Other kernel approximation approaches

- Use decision trees to compute similarity between two points and use that as kernel – extremely fast prediction

  Jose et al. Local Deep Kernel Learning, ICML 2013.

- Learn these kernel approximations in a task-dependent manner

  Perronnin et al. d Yan Liu. Large-scale Image Categorization with Explicit Data embedding, CVPR 2010.

PML with Kernels

Gaussian Processes

Priors and Posteriors

- How can we argue about priors and posteriors in an RKHS $\mathcal{H}_K$?
- Details too advanced (covered in CS772, CS775, CS698X)
- Basic idea: argue about distributions over functions $f\colon \mathcal{X} \to \mathbb{R}$
- Gaussian processes is one such family of distributions
$$f \sim \mathrm{GP}(\mu, K)$$
$\mu\colon \mathcal{X} \to \mathbb{R}$ is the *mean* function and κ is the covariance kernel
- What does it mean to sample a function?
- Think of sampling a very very long vector (imprecise way though)
- Let $|\mathcal{X}| = N < \infty$ with $\mathcal{X} = \{x^1, x^2, \ldots, x^N\}$
- Then can think of $f\colon \mathcal{X} \to \mathbb{R}$ as a vector in $\mathbb{R}^N$
$$f = [f(x^1), \ldots, f(x^N)]$$

Gaussian Processes

- For $|\mathcal{X}| = N < \infty$, we say a function f is sampled from $\mathrm{GP}(\mu, K)$ if
$$f \sim \mathcal{N}(\mu, G)$$
where $\mu \in \mathbb{R}^N$ is mean fn. and $G \in \mathbb{R}^{N\times N}$ with $G_{ij} = K(x^i, x^j)$
- Note that f need not be linear etc, can be very complex
- Gaussian processes popularly use a Gaussian kernel for K
- Note that the Gaussian kernel K forces f to be *smooth* i.e. if two points $x^i, x^j \in \mathcal{X}$ are close i.e. $\left\|x^i - x^j\right\|_2$ is small then functions f that take very different values on these points get low prob.
- **Exercise**: verify this yourself
- Mean function is taken to be zero (unless we have other reasons)

Gaussian Process Regression

- Solve a regression problem $\{x^i, y^i\}_{i=1,\ldots,n}$,$x^i \in \mathcal{X}, y^i \in \mathbb{R}$ and $n \ll N$
- Prior dist. (GP) $f \sim \mathrm{GP}(0, K)$
- Likelihood dist. (Gaussian) $y^i | f \sim \mathcal{N}\left(f\left(x^i\right), \sigma^2\right)$
- Note: GP makes sense even if $\mathcal{X}$ is set of vectors, images, text etc
- Can do regression over vectors, images as we did in kernel RR
- Let $\mathbf{y} = [y^1, \ldots, y^n]^\top \in \mathbb{R}^n$
- Using a very special property of Gaussians we can show
$$\mathbf{y} \sim \mathcal{N}(\mathbf{0}, G_n + \sigma^2 \cdot I_n)$$
where $\mathbf{0} \in \mathbb{R}^n$ and $G_n \in \mathbb{R}^{n \times n}$ is the Gram matrix of training data

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If a vector $\mathbf{v} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$ then $\mathbf{v}_S \sim \mathcal{N}(\mu_S, \Sigma_{S,S})$ $\Sigma_{S,S} \in \mathbb{R}^{|S| \times |S|}$

If a vector $\mathbf{v} \in \mathbb{R}^n$ is distributed according to a Gaussian, then for every subset $S \subset [n]$, the sub-vector $\mathbf{v}_S = [\mathbf{v}_i]_{i \in S} \in \mathbb{R}^{|S|}$ is also a Gaussian vector!

$\mathbf{y}$ is just a subvector of f

Gaussian Process Regression

- So we have $\mathbf{y} \sim \mathcal{N}(\mathbf{0}, G_n + \sigma^2 \cdot I_n)$
- Now a new test point comes along $\tilde{x} \in \mathcal{X}$. Can we predict $\tilde{y}$?
- Let $\tilde{\mathbf{y}} = [\mathbf{y}, \tilde{y}] \in \mathbb{R}^{n+1}$, G_{n+1} be the Gram matrix over $\{x^i\}_{i=1,\dots,n} \cup \tilde{x}$
- Previous slide gives us $\tilde{\mathbf{y}} \sim \mathcal{N}(\mathbf{0}, G_{n+1} + \sigma^2 \cdot I_{n+1})$
- Let $\tilde{\mathbf{g}} = [K(x^1, \tilde{x}), \dots, K(x^n, \tilde{x})]^\top \in \mathbb{R}^n$
- Then we can show that

$$\mathbb{P}\left[\tilde{y} \,\middle|\, \tilde{x}, \{x^i, y^i\}_{i=1,\dots,n}\right] = \mathcal{N}(\tilde{\mu}, \tilde{\sigma}^2)$$
$$\tilde{\mu} = \tilde{\mathbf{g}}^\top (G_n + \sigma^2 \cdot I_n)^{-1} \mathbf{y}$$
$$\tilde{\sigma}^2 = K(\tilde{x}, \tilde{x}) + \sigma^2 - \tilde{\mathbf{g}}^\top (G_n + \sigma^2 \cdot I_n)^{-1} \tilde{\mathbf{g}}$$

Gaussian Process Regression

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$$\mathbb{P}\left[\tilde{y} \,\middle|\, \tilde{x}, \{x^i, y^i\}_{i=1,\ldots,n}\right] = \mathcal{N}(\tilde{\mu}, \tilde{\sigma}^2)$$

$$\tilde{\mu} = \tilde{\mathbf{g}}^\top (G_n + \sigma^2 \cdot I_n)^{-1} \mathbf{y}$$

$$\tilde{\sigma}^2 = K(\tilde{x}, \tilde{x}) + \sigma^2 - \tilde{\mathbf{g}}^\top (G_n + \sigma^2 \cdot I_n)^{-1} \tilde{\mathbf{g}}$$

Predictive posterior

Verify that the mean $\tilde{\mu}$ is nothing but the kernel RR solution!

A few thoughts

- GP regression is a Bayesian counterpart to kernel RR
- Similar cost for storing model, making predictions
- GP gives additional information about variance in prediction just as Bayesian models usually do (ref. Bayesian linear regression)
- Can apply accelerated learning techniques to GPs as well
- Can use GPs to perform kernel dim-redn as well
- Just as we did online MAP, can do online GP as well
- Btw, can do online kernel SVM, online kernel RR as well ☺
- Kernel perceptron is already online

Neural Networks

Disclaimers

- Field is progressing rapidly – newer methods being proposed
- Some of the mentors, even some course students, more experienced with neural networks than the instructor
- Will cover very basics and essentials

Back to Kernels first

- Consider the quadratic kernel $K_{\text{quad}} = (\langle \mathbf{x}^1, \mathbf{x}^2 \rangle + 1)^2$ on $\mathcal{X} = \mathbb{R}^2$
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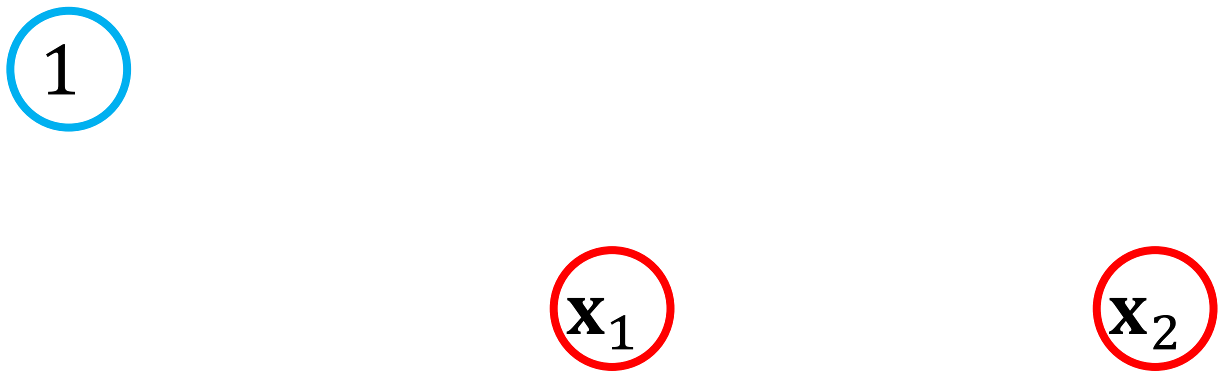

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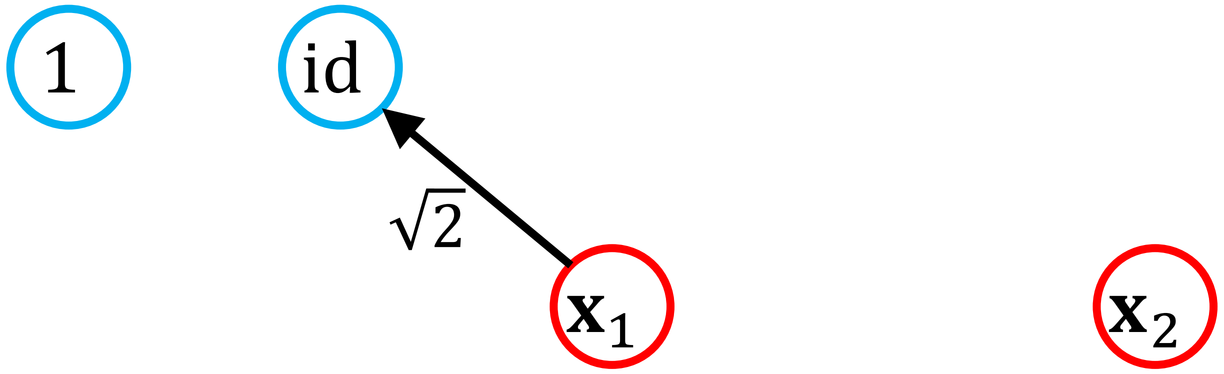

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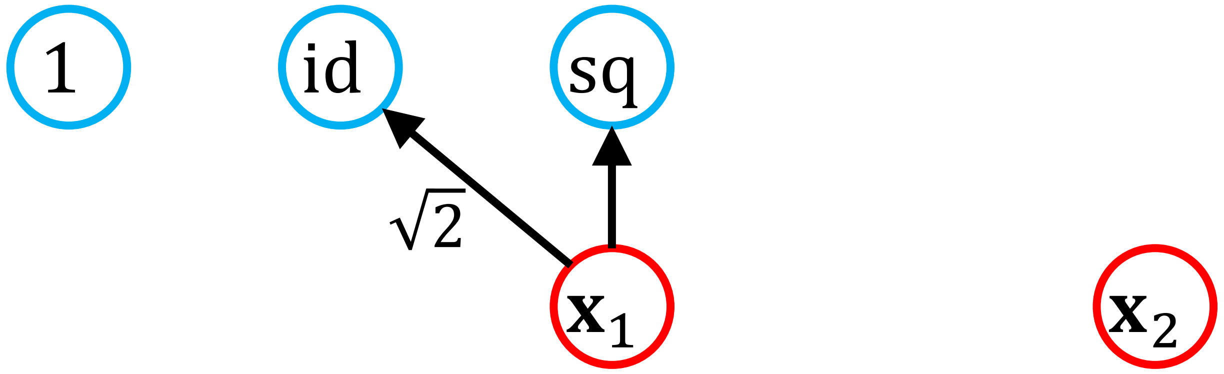

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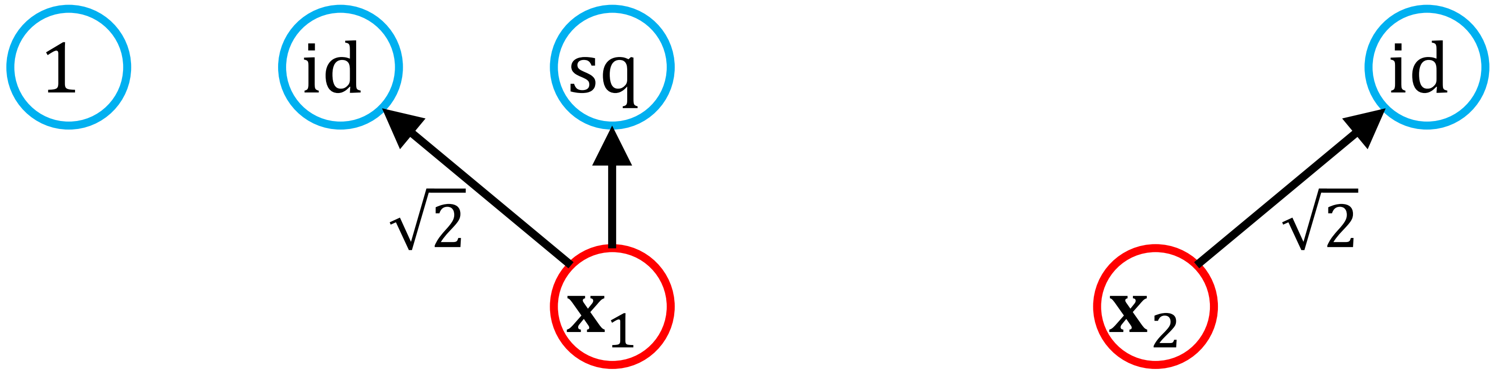

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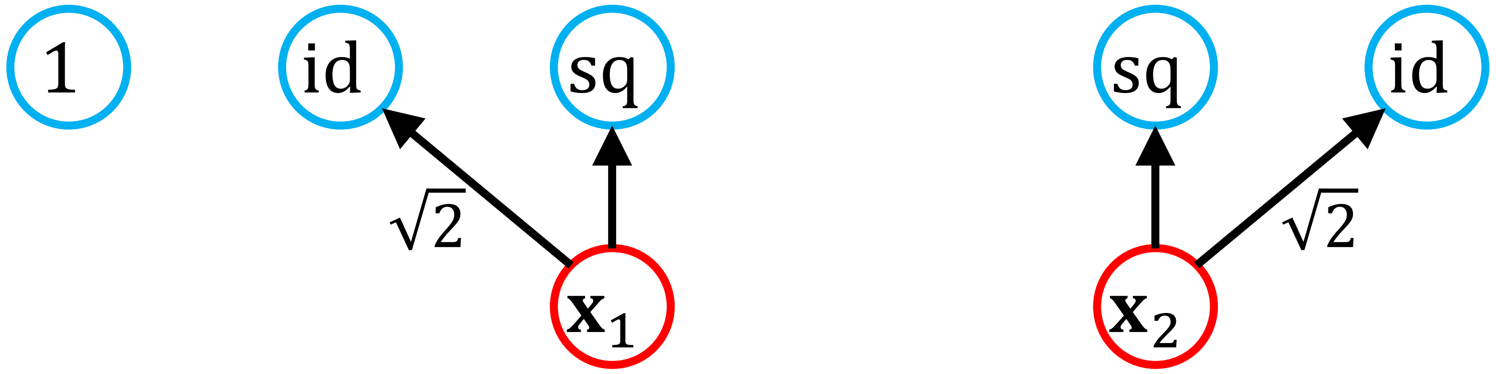

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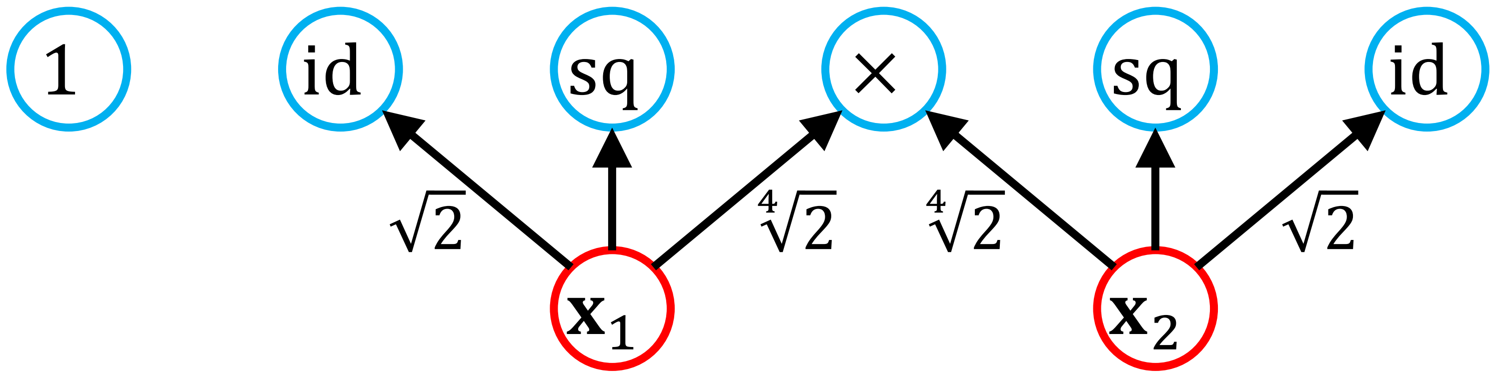

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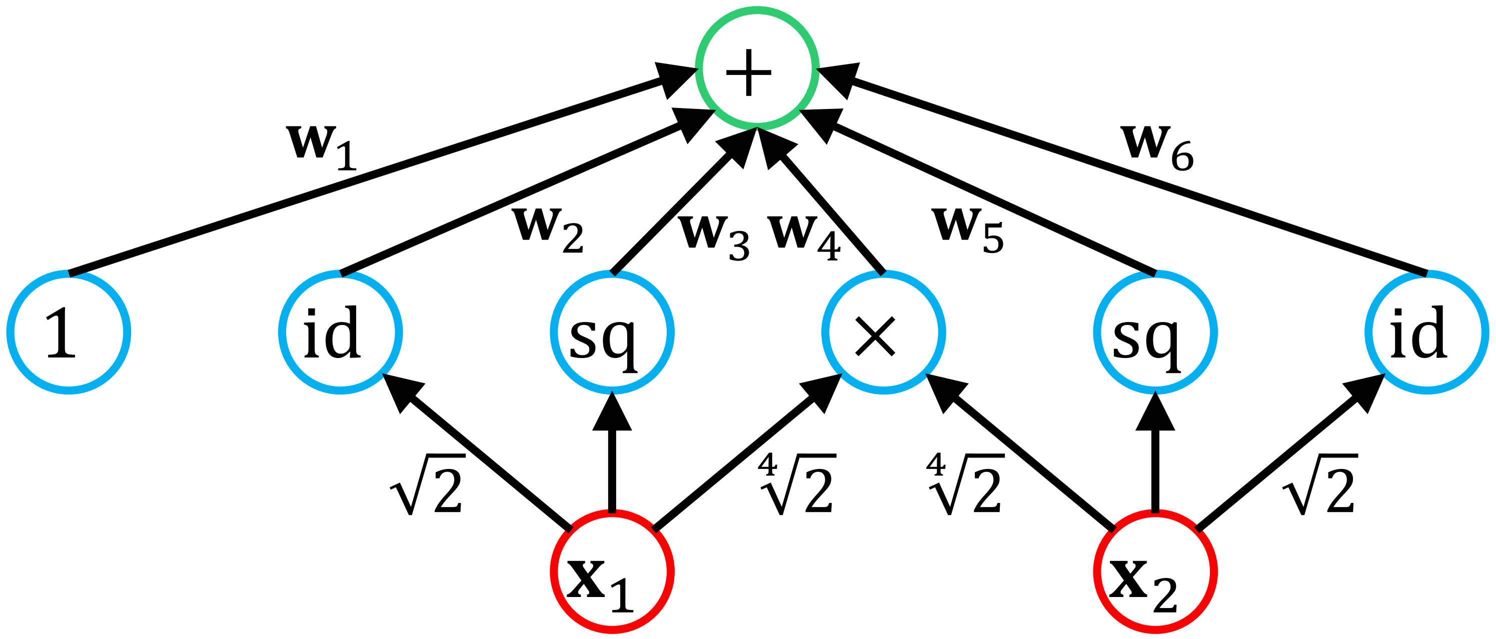

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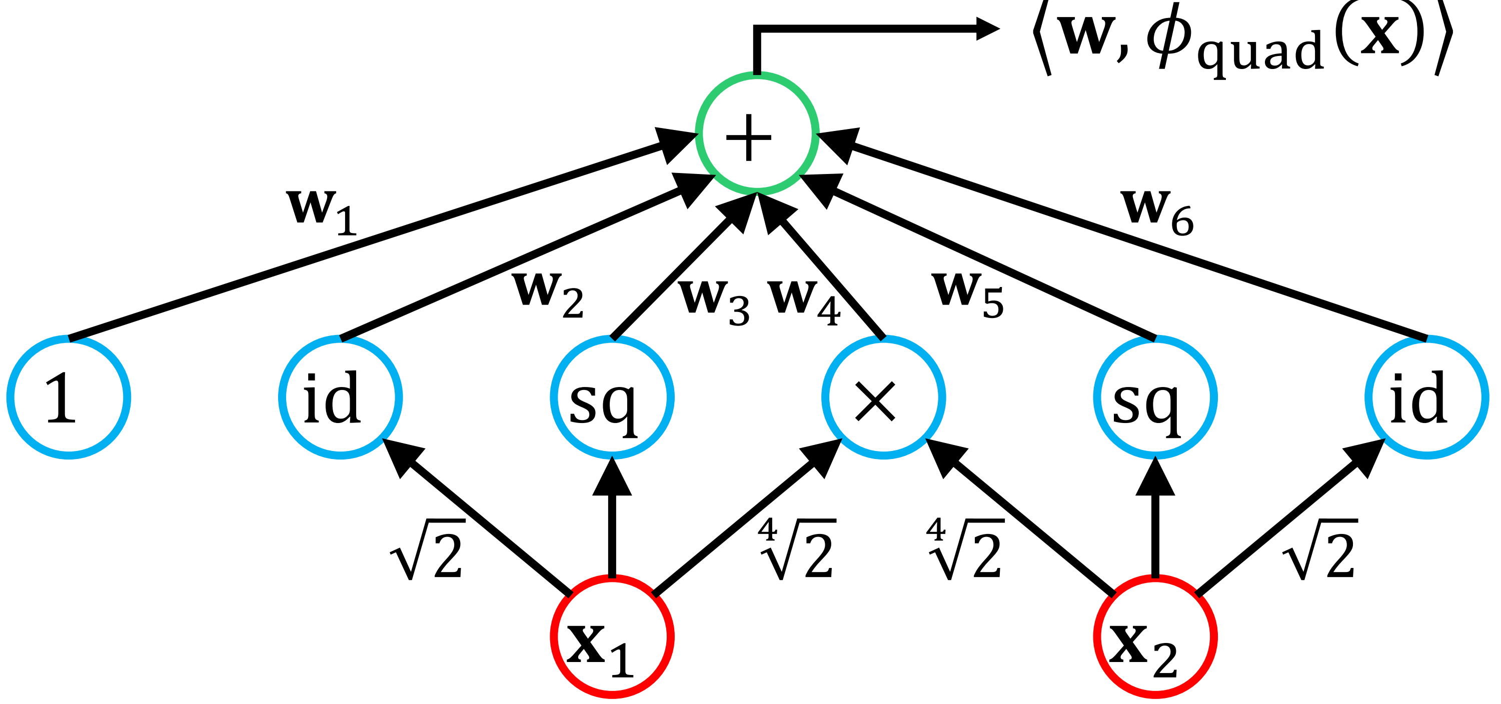

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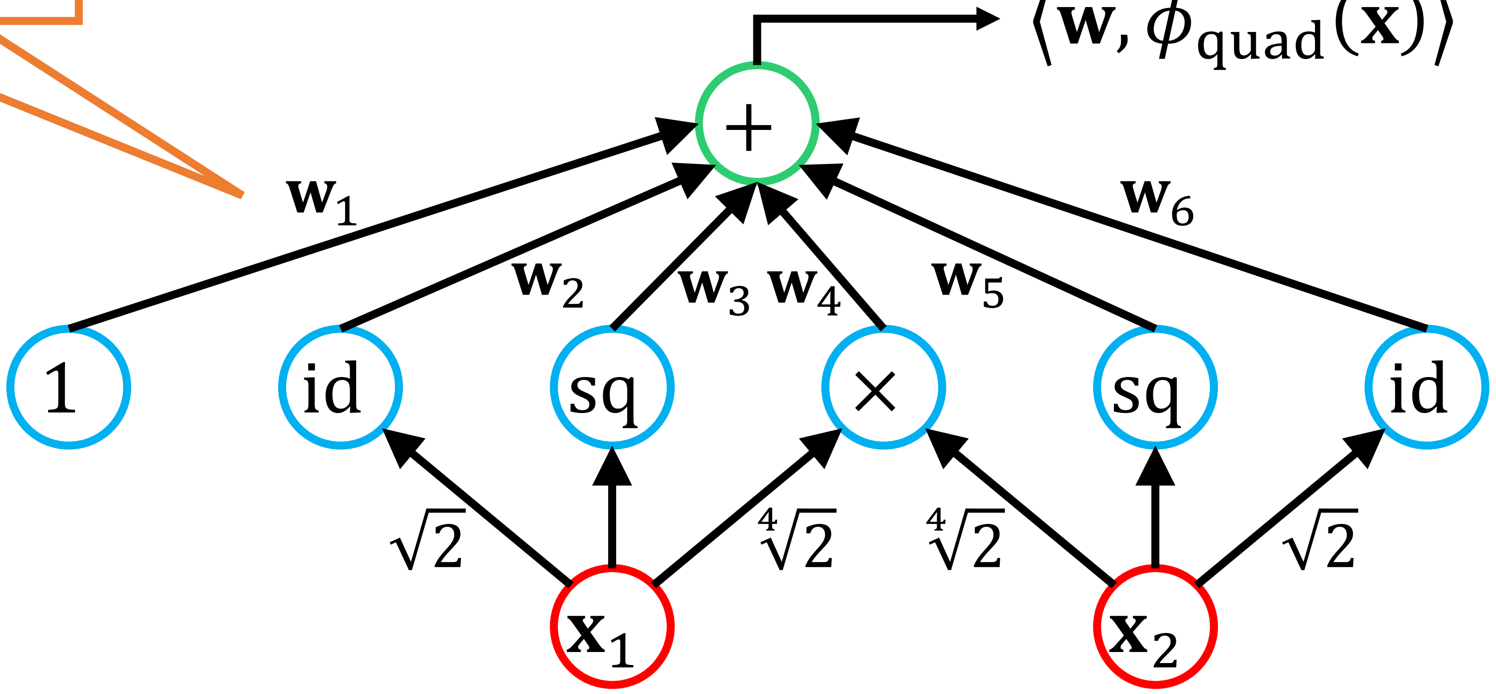

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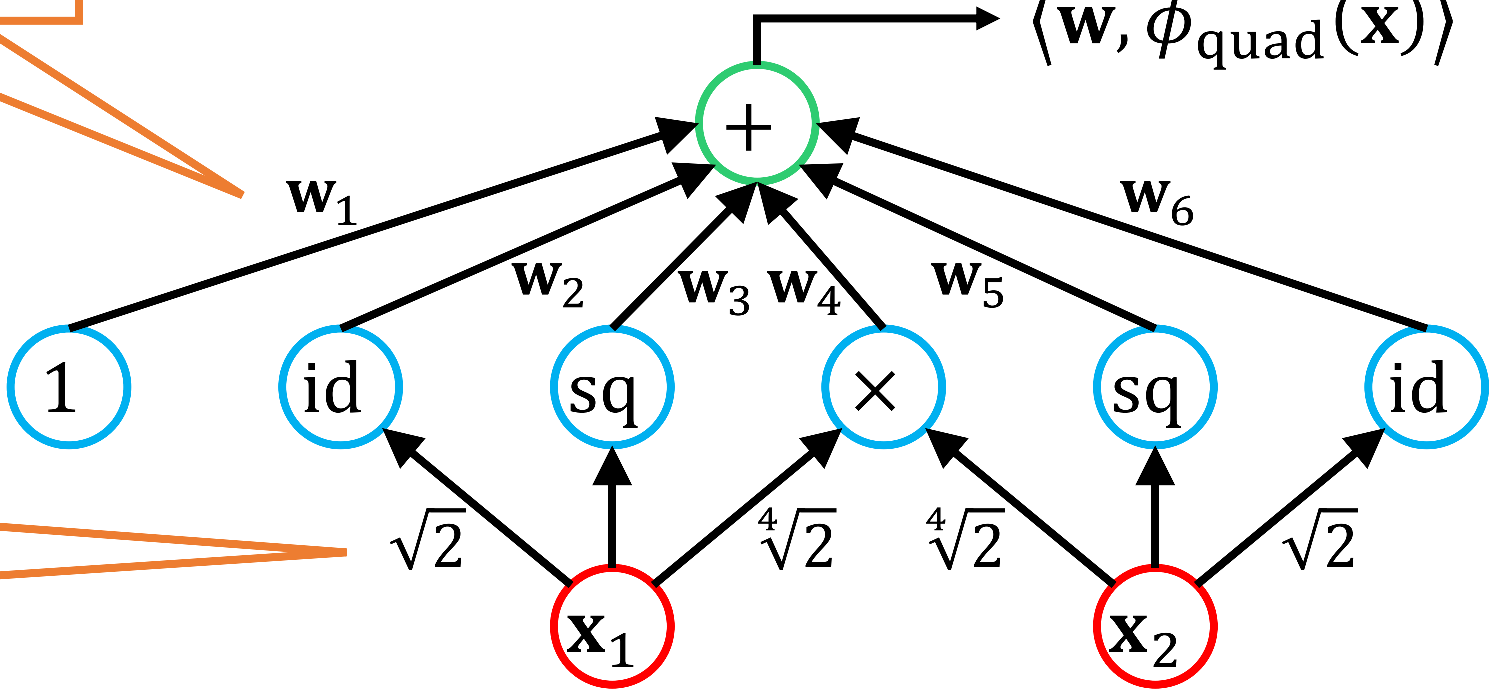

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A 3 layer network

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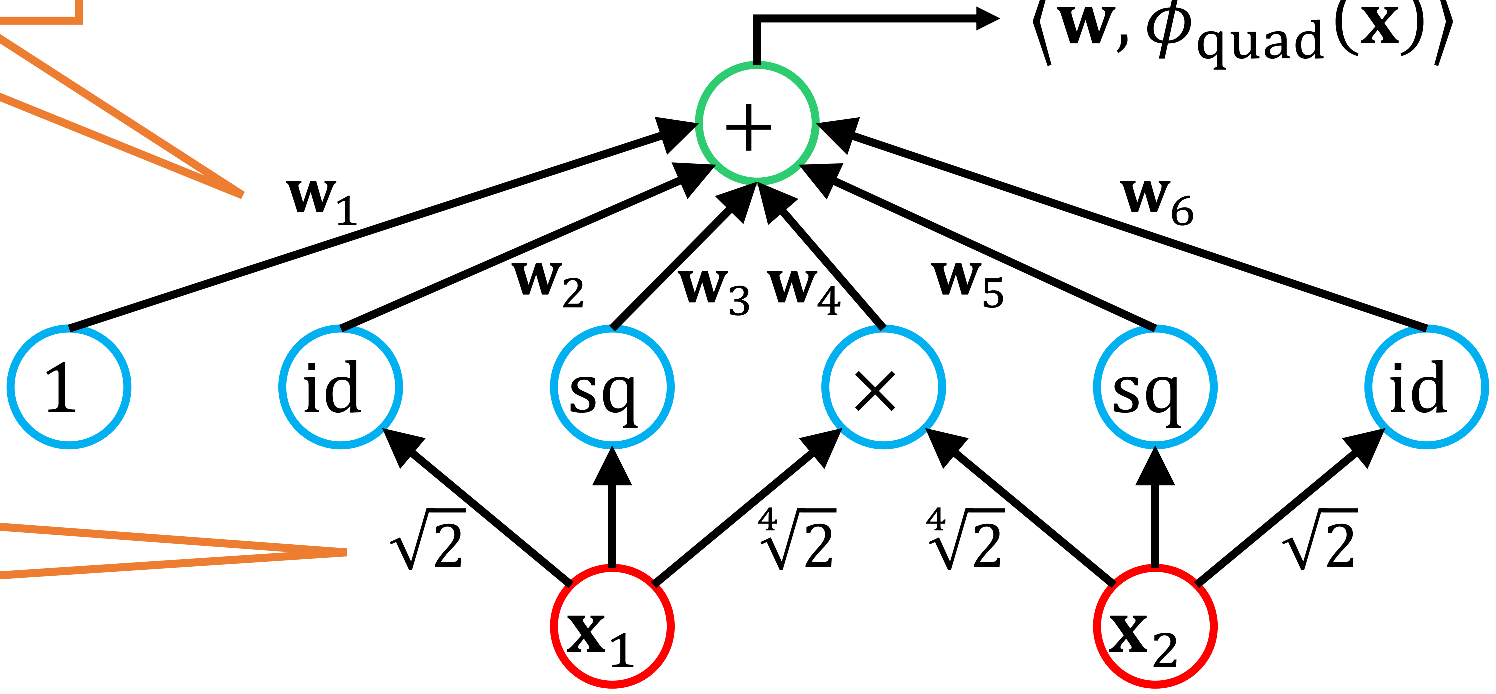

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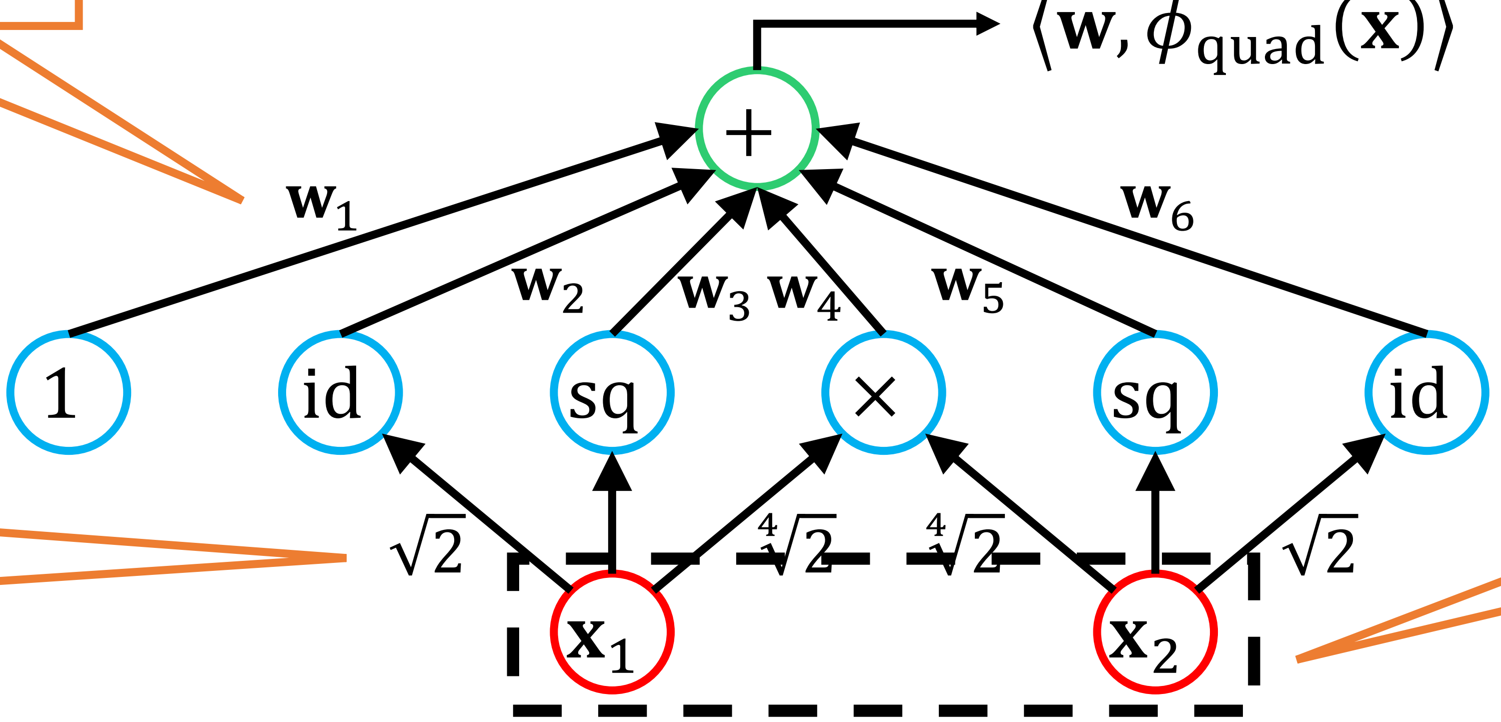
Input layer



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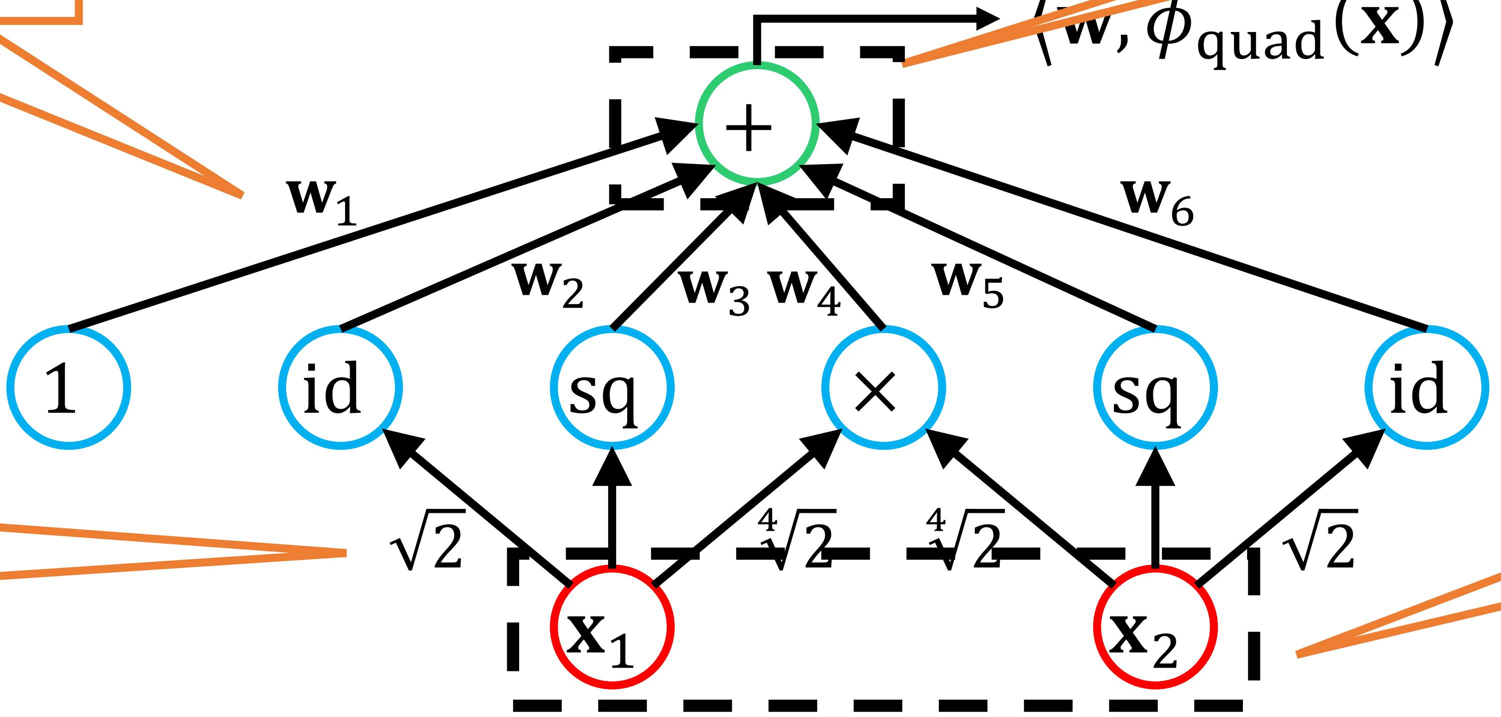
Output layer

But not these weights

Input layer



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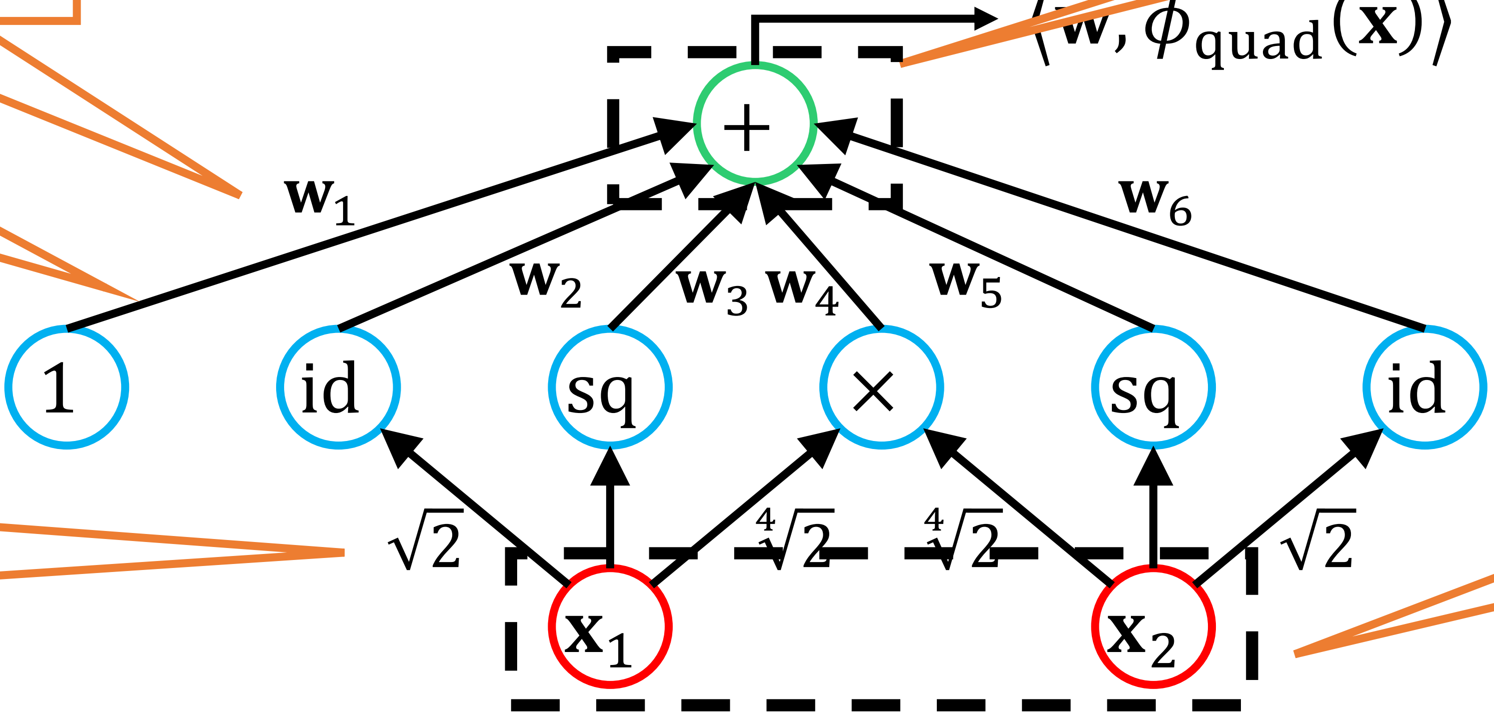
I/O layers are called "visible"

But not these weights

Output layer

Input layer



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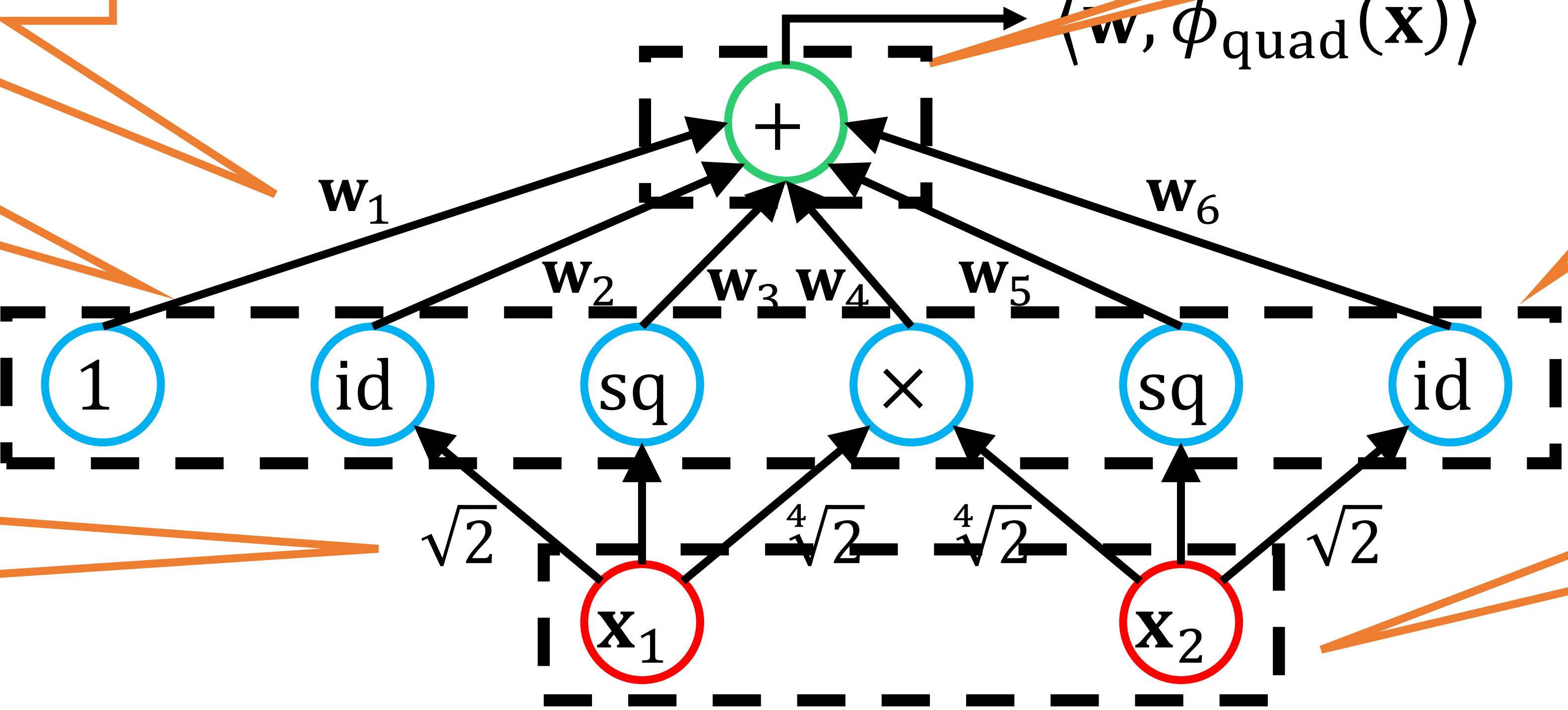
Hidden layer

But not these weights

Input layer



The “neuron” in Neural Networks

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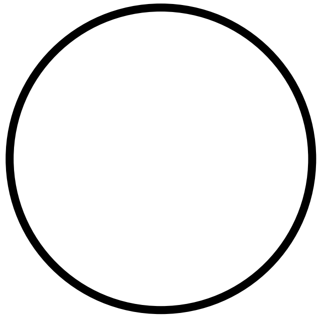

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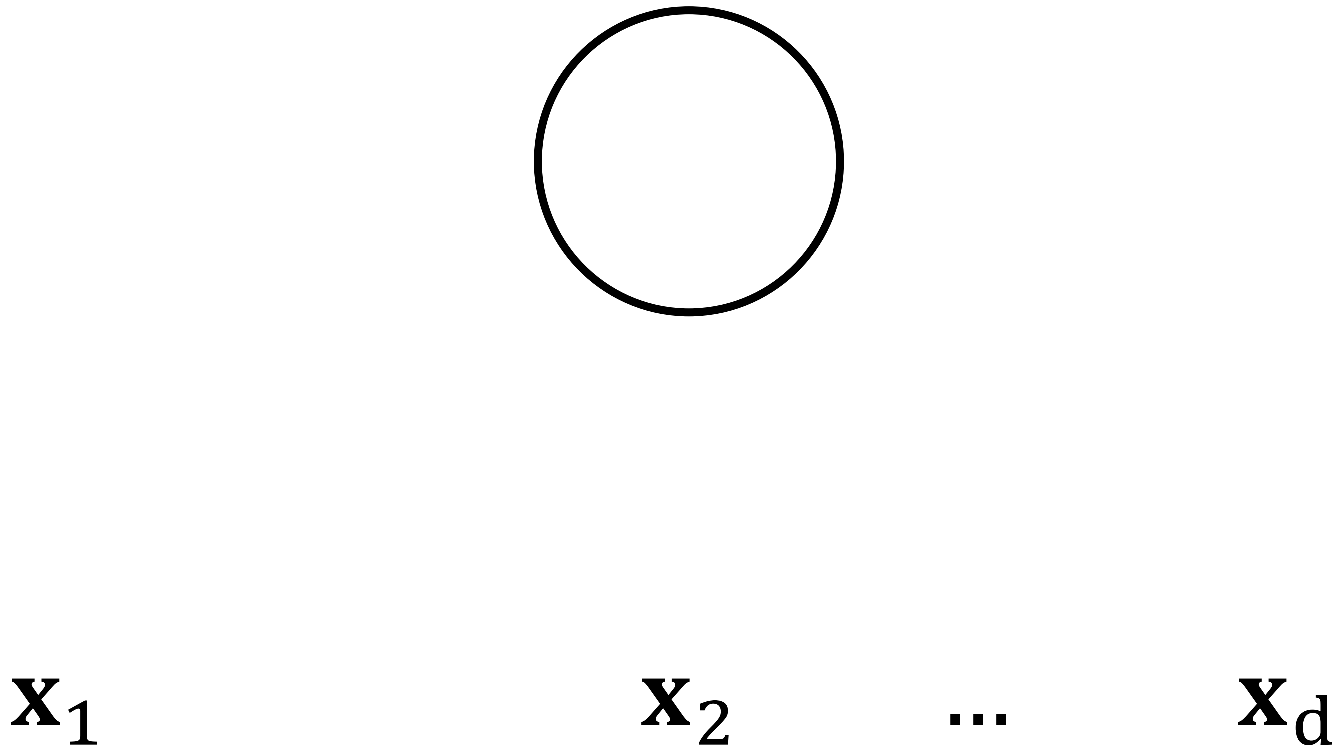

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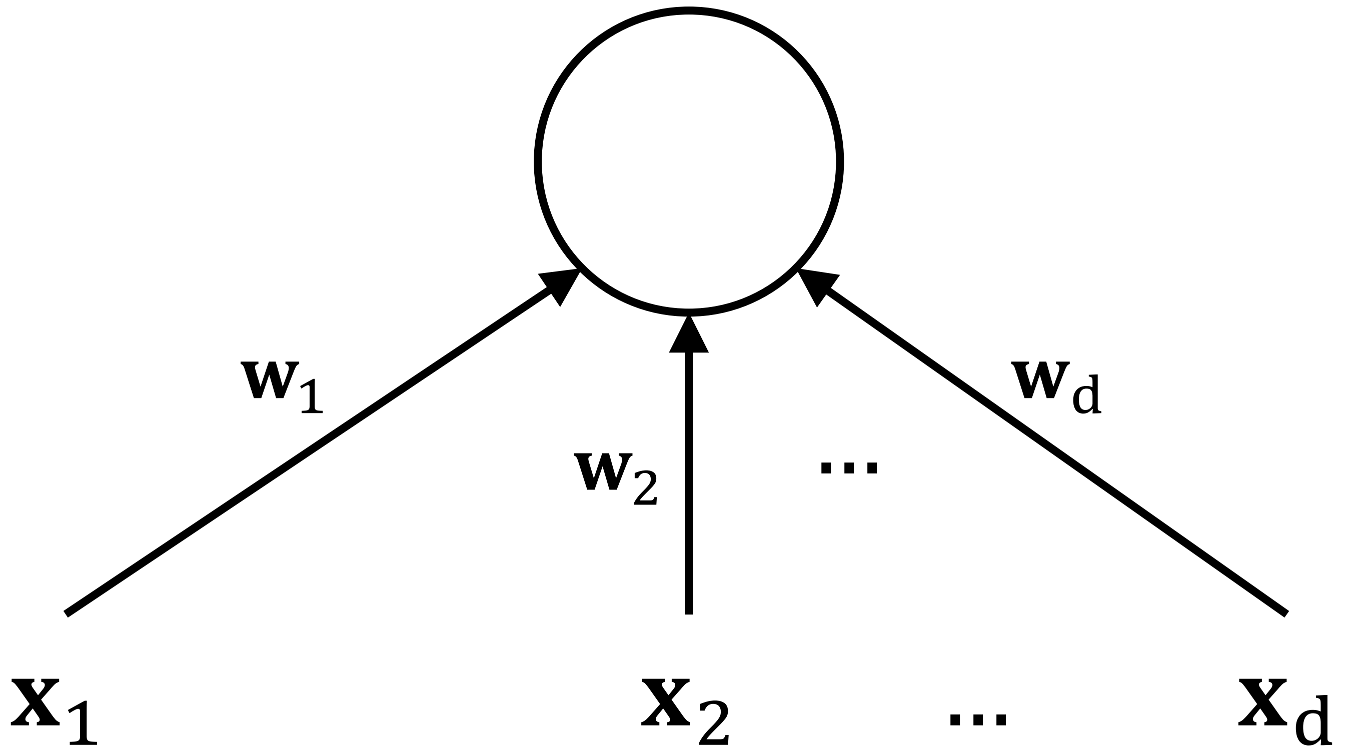

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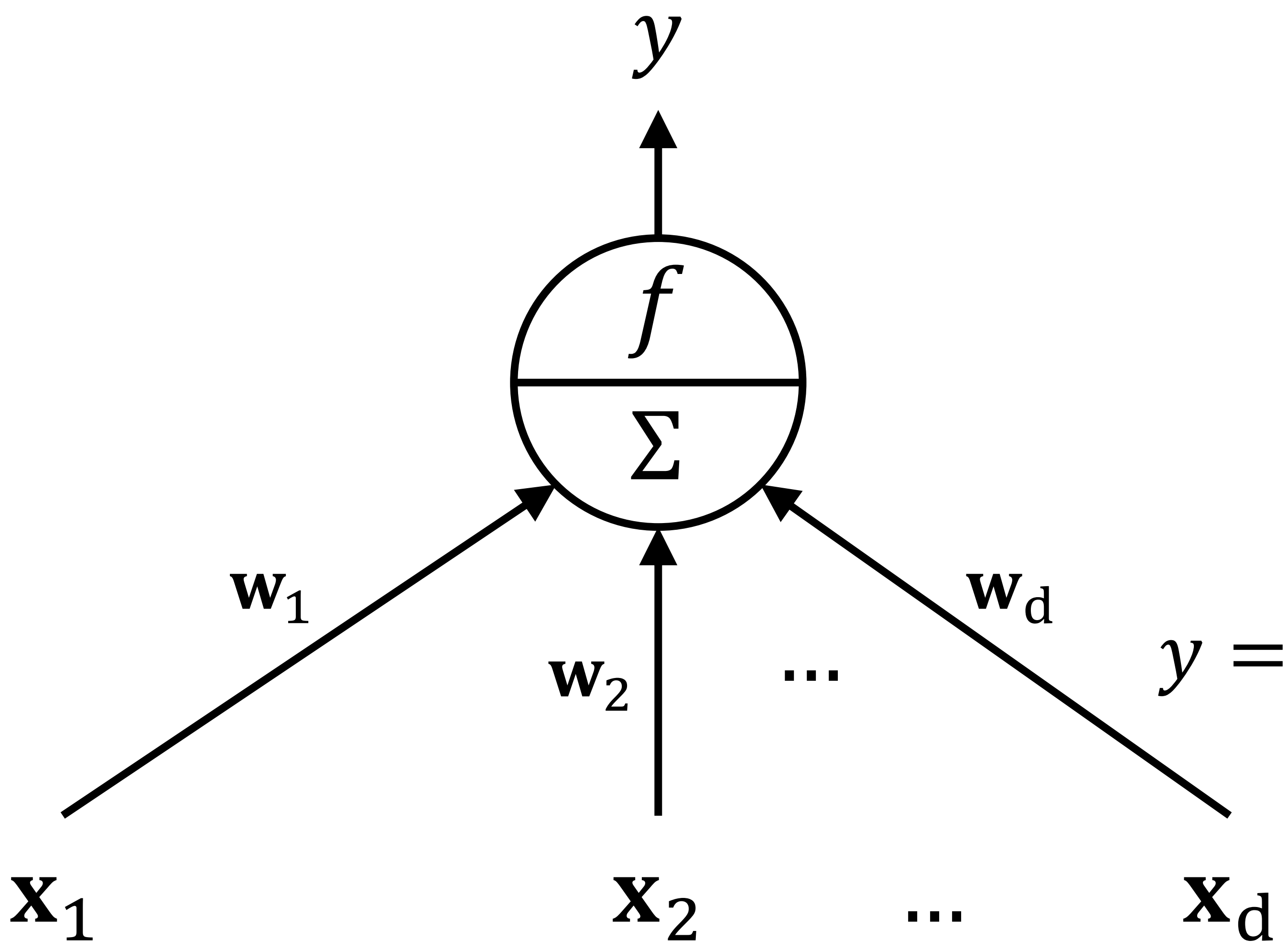

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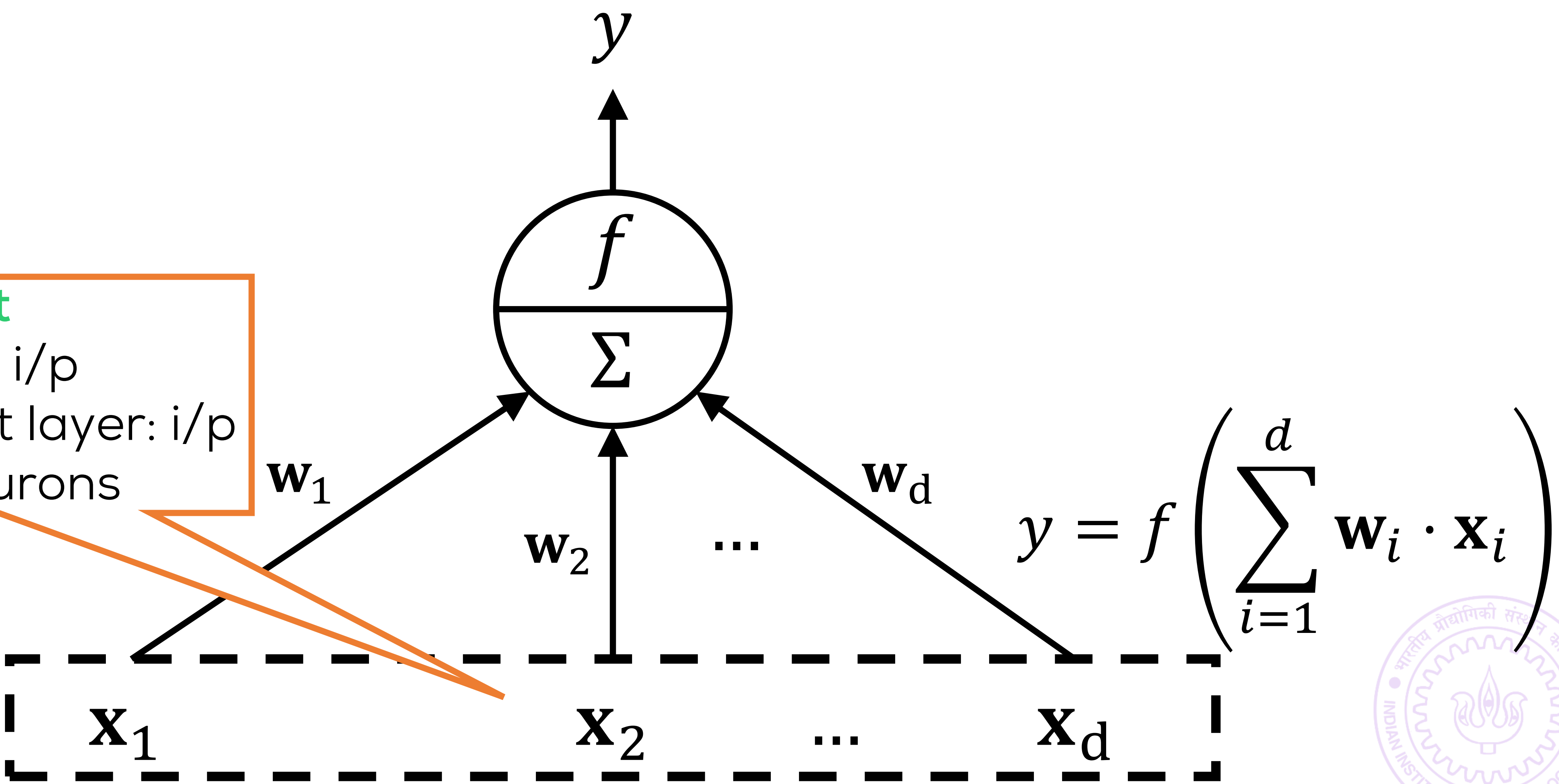

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Input

Input layer: no i/p

Hidden/output layer: i/p from other neurons

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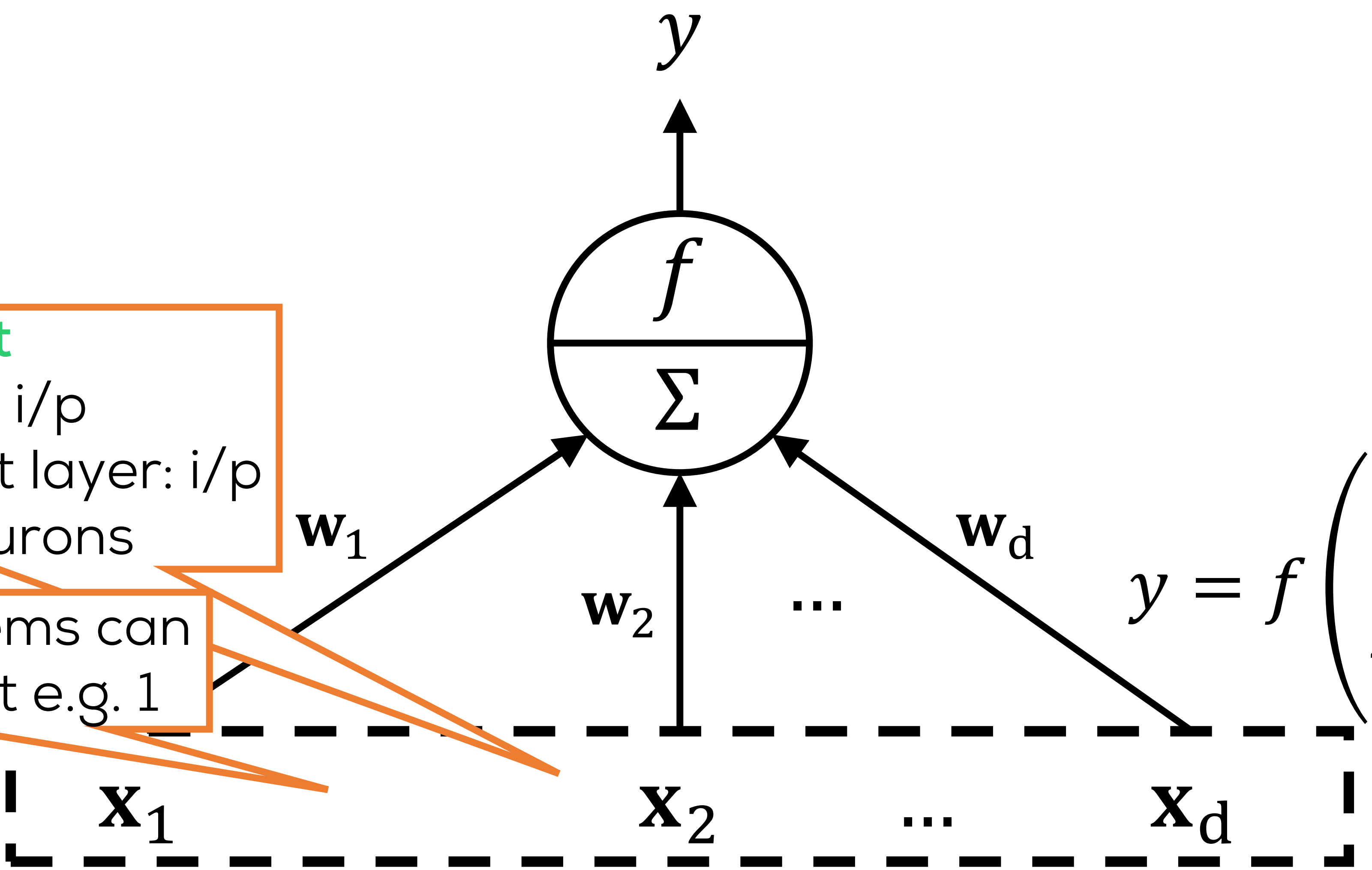

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Some input items can be a constant e.g. 1

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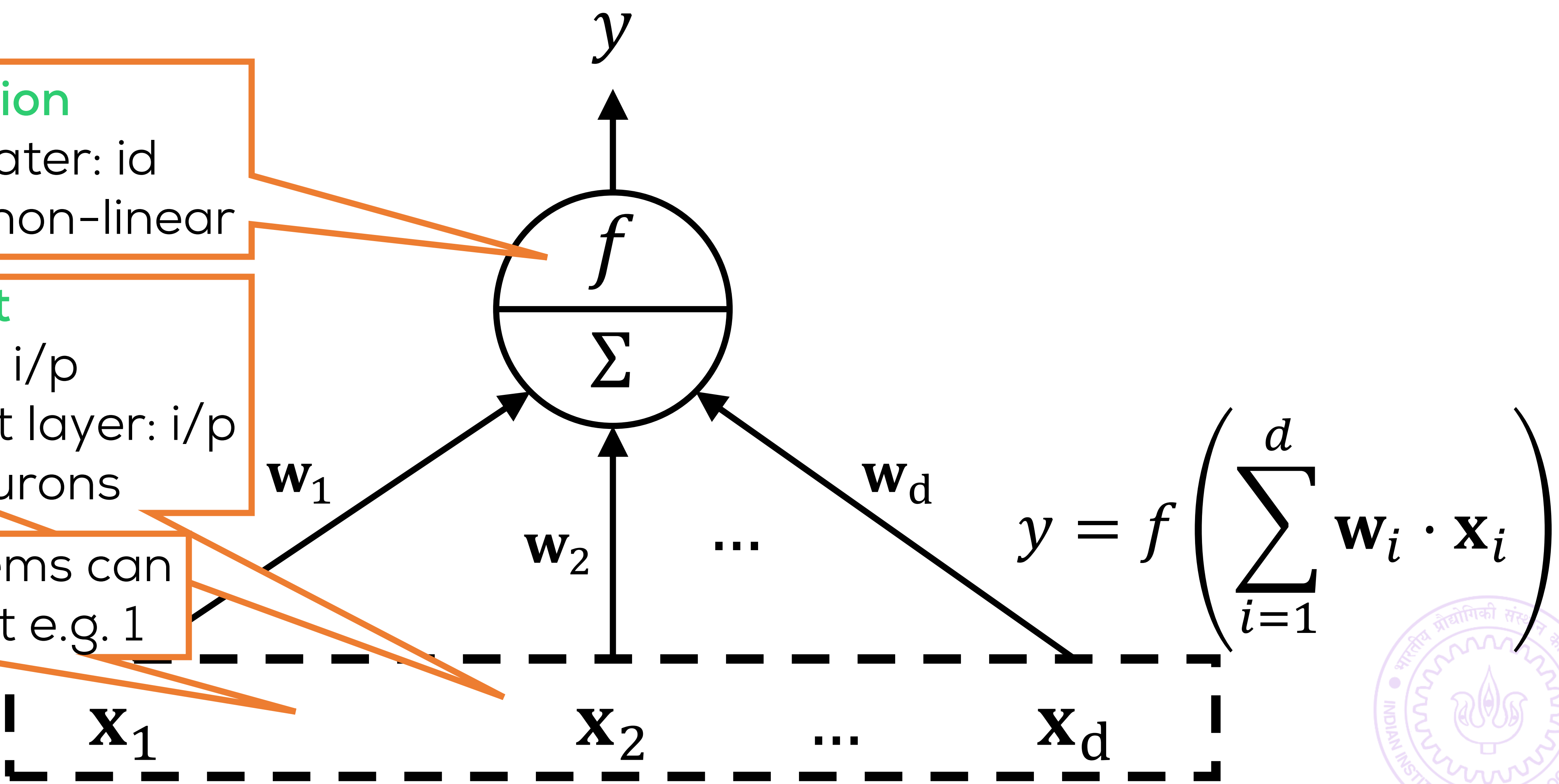

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Activation
Input/output later: id
Hidden layer: non-linear

Input
Input layer: no i/p
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Some input items can be a constant e.g. 1

The "..." in Neural Networks

Output
Output layer: final o/p
Input/hidden layer: o/p to other neurons

Activation
Input/output later: id
Hidden layer: non-linear

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

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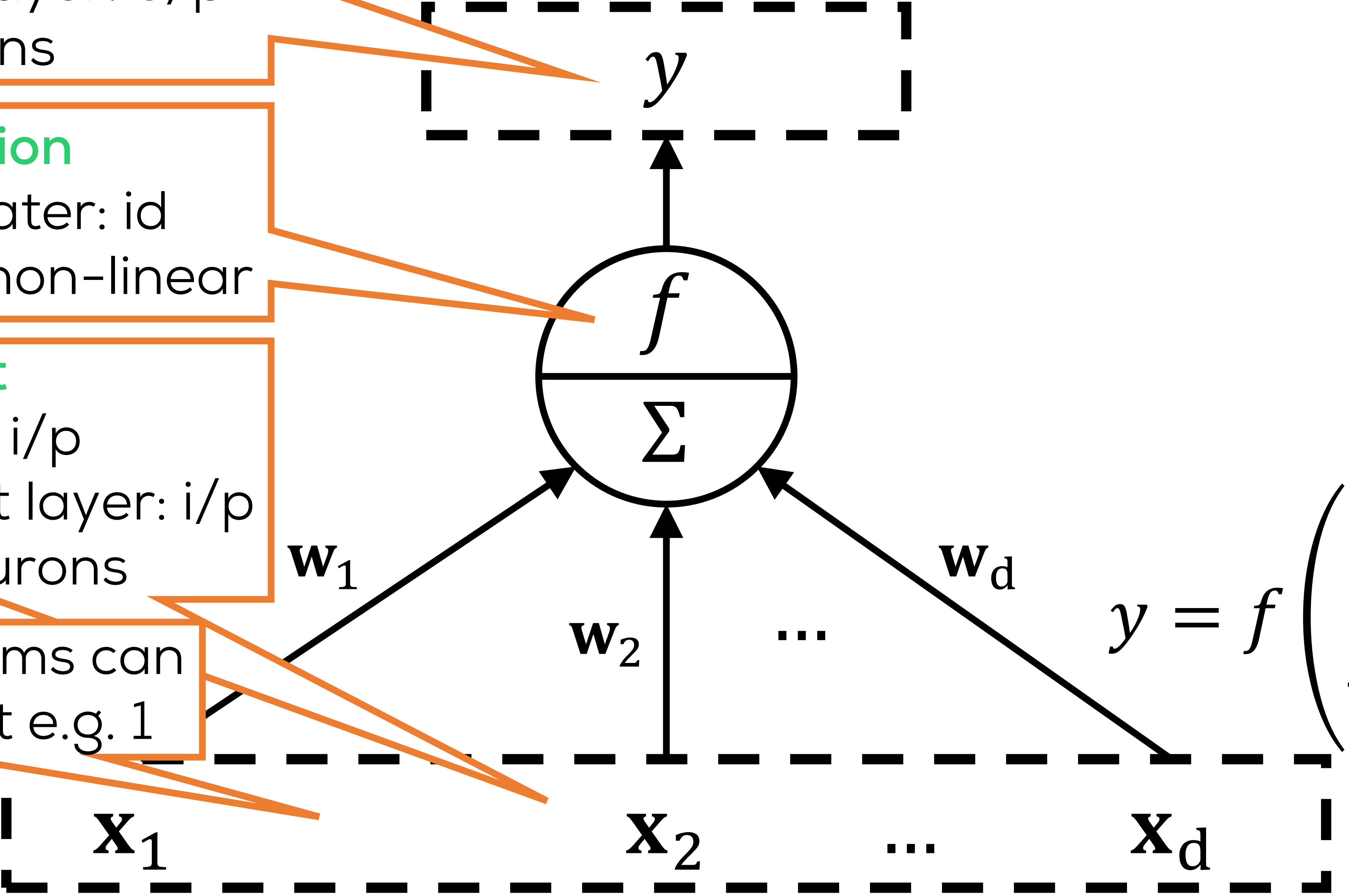

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n Neural Networks

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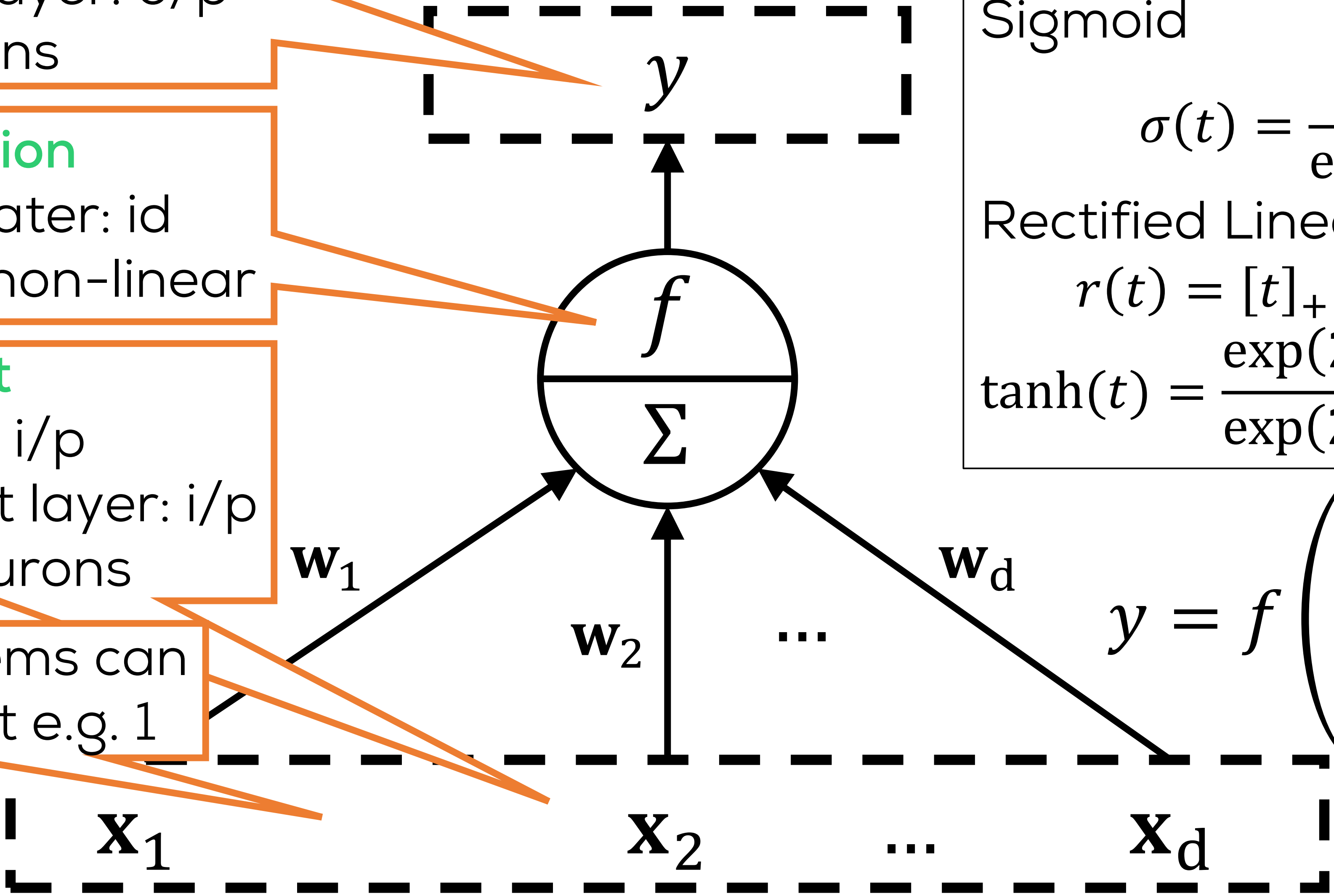

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Common "activation" fns f

Sigmoid

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

Rectified Linear Unit (ReLU)

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

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

Th“ ”n Neural Networks

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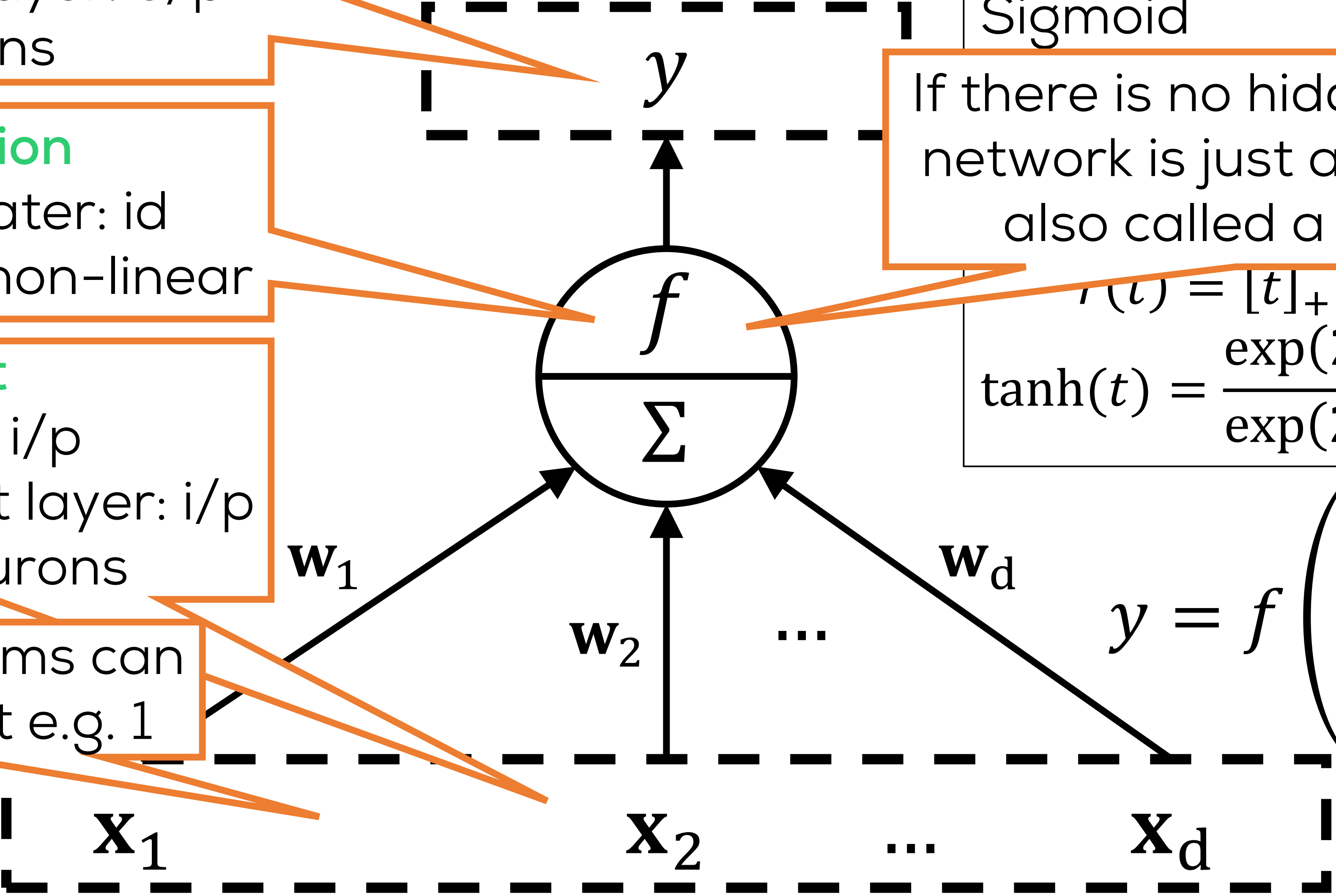

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Common “activation” fns f
Sigmoid

If there is no hidden layer then network is just a linear model, also called a **percepton**

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

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

Output
Output layer: final o/p
Input/hidden layer: o/p to other neurons

Sometimes output layer is given a non-id activation. Matter of convention

Common “activation” fns f
Sigmoid

If there is no hidden layer then network is just a linear model, also called a **percepton**

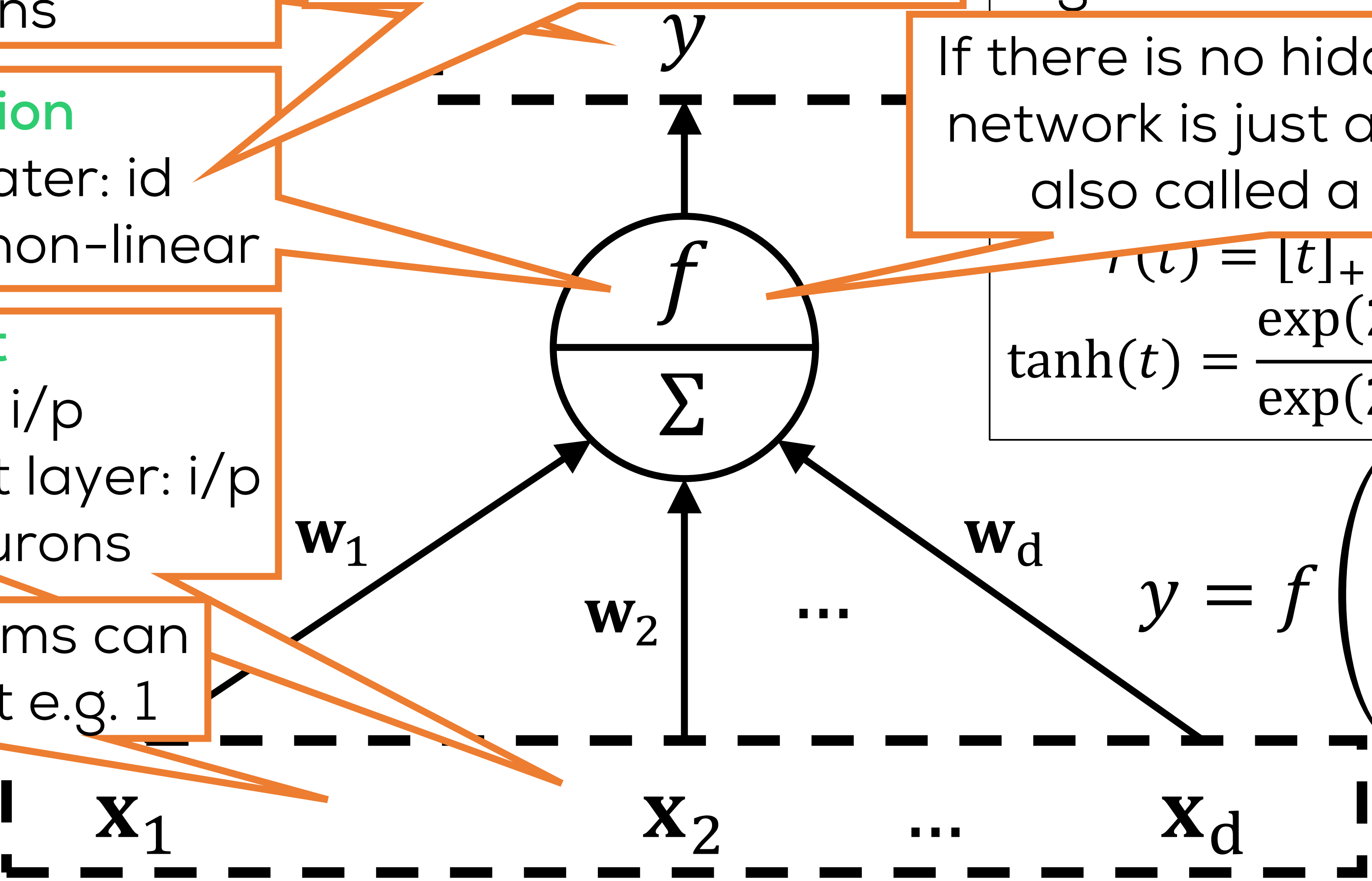
Activation
Input/output later: id
Hidden layer: non-linear

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

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

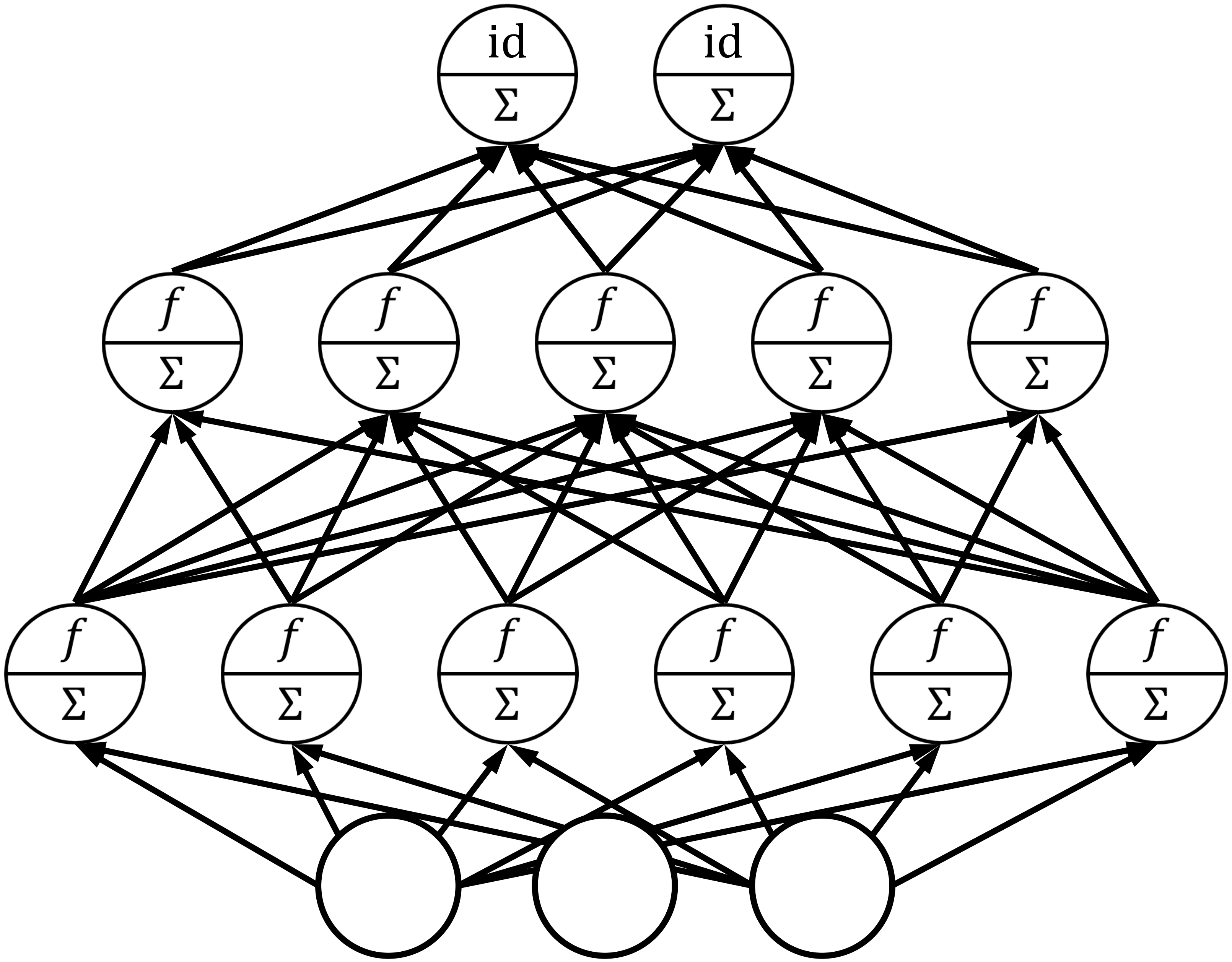
Input
Input layer: no i/p
Hidden/output layer: i/p from other neurons

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

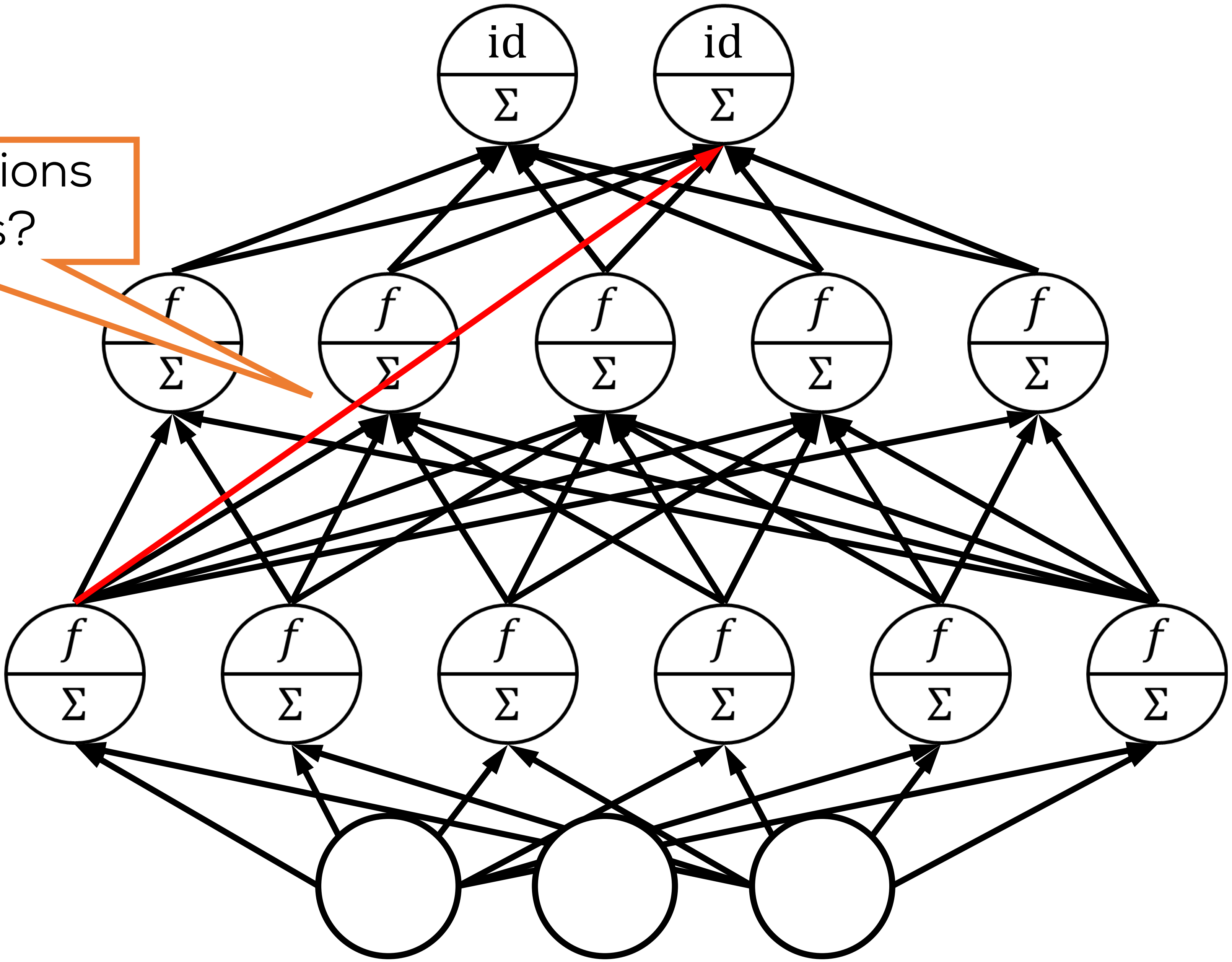


$$y = f\left(\sum_{i=1}^{d} \mathbf{w}_i \cdot \mathbf{x}_i\right)$$

A Feedforward Network

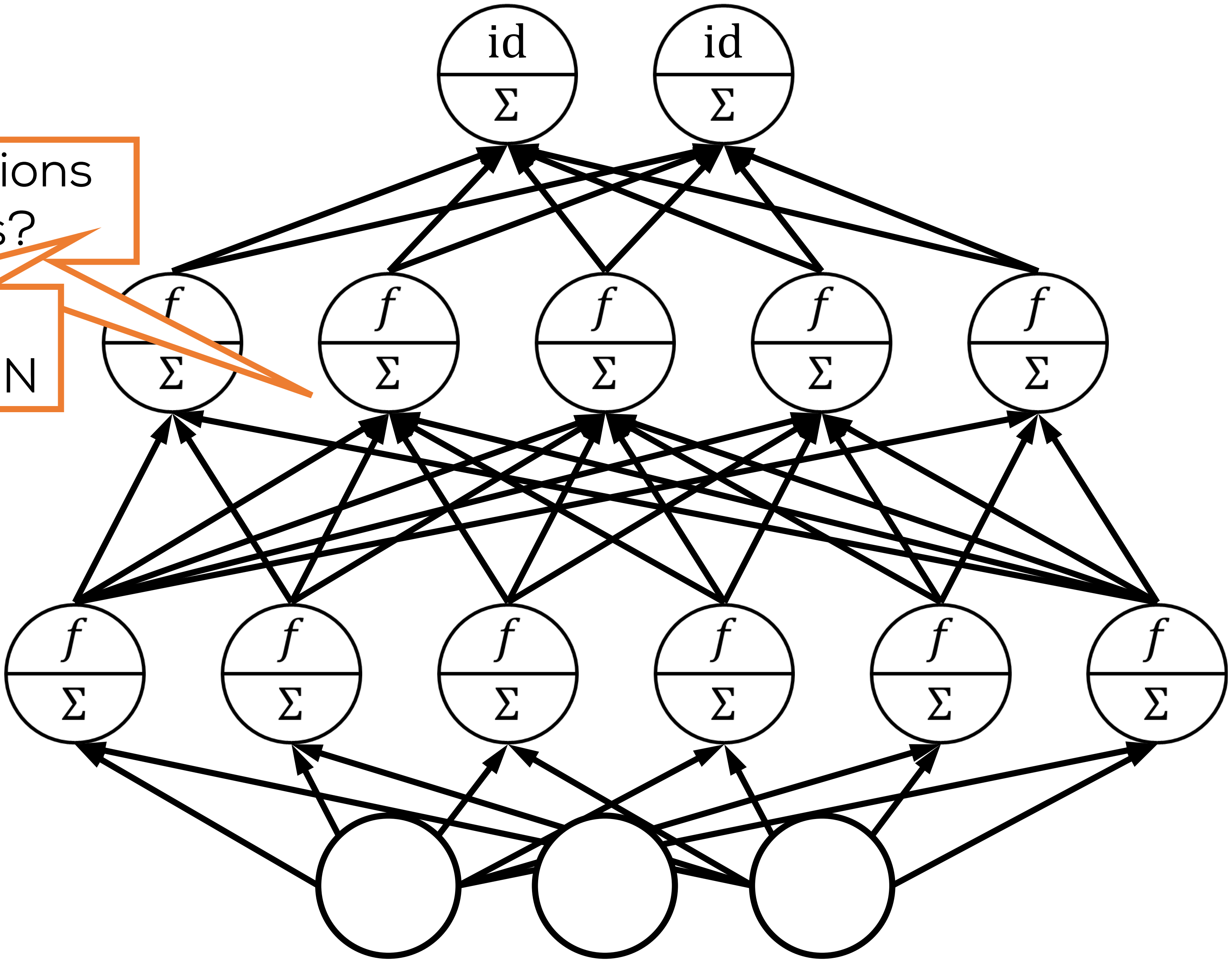


A Feedforward Network



Can I connections jump layers?

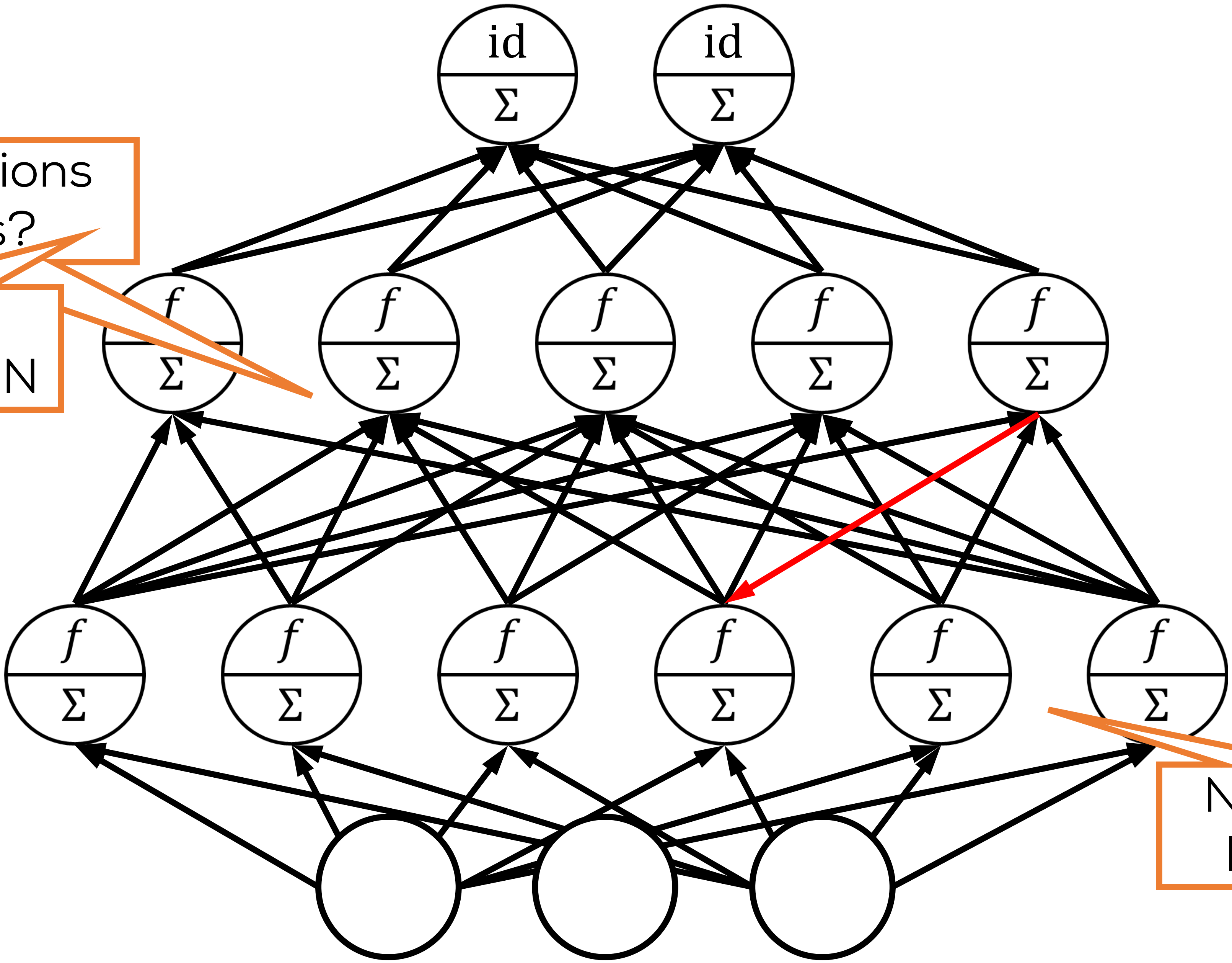
A Feedforward Network



Can I connections jump layers?

Not in a feedforward NN

A Feedforward Network

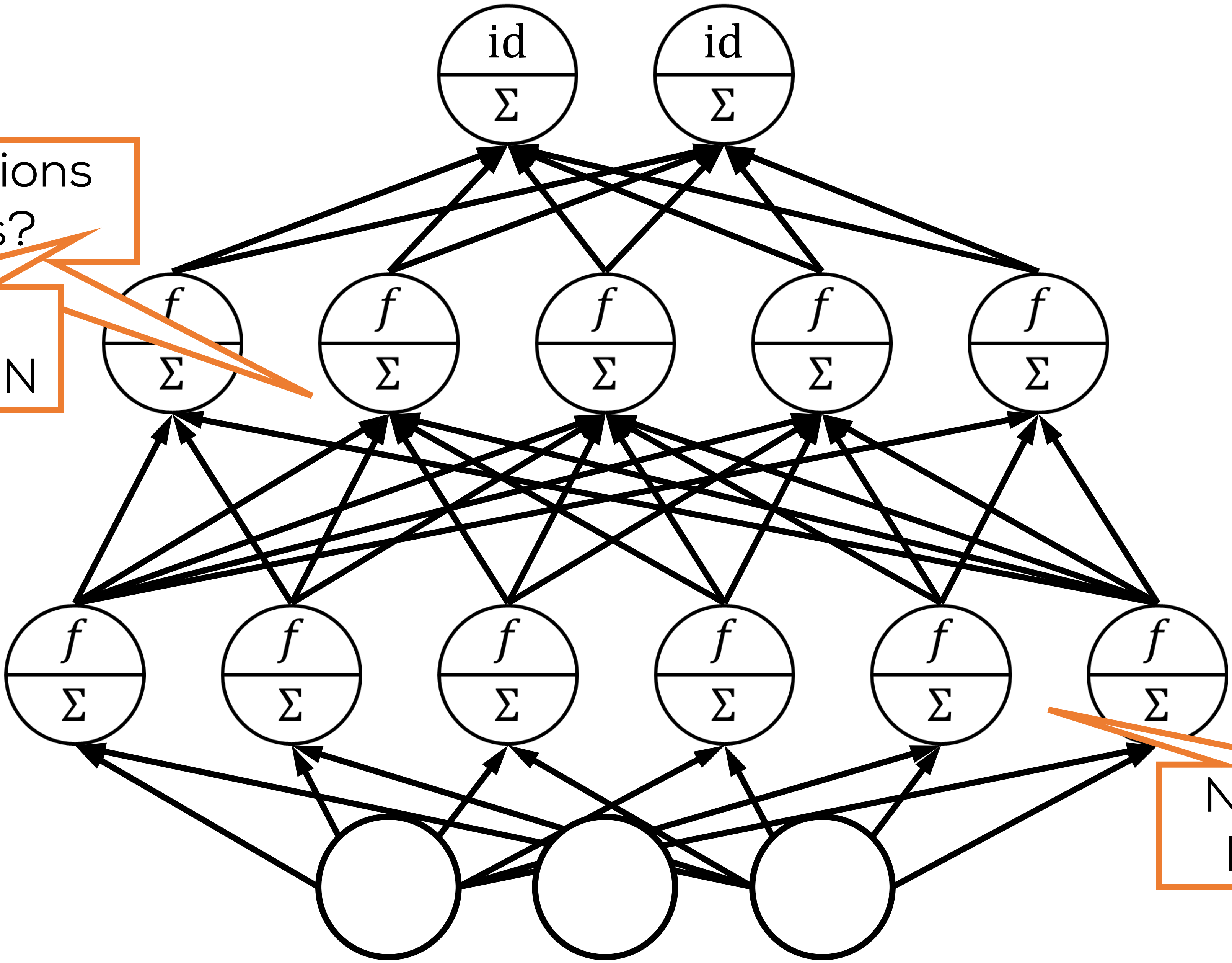


Can I connections jump layers?

Not in a feedforward NN

No "reverse" links either

A Feedforward Network



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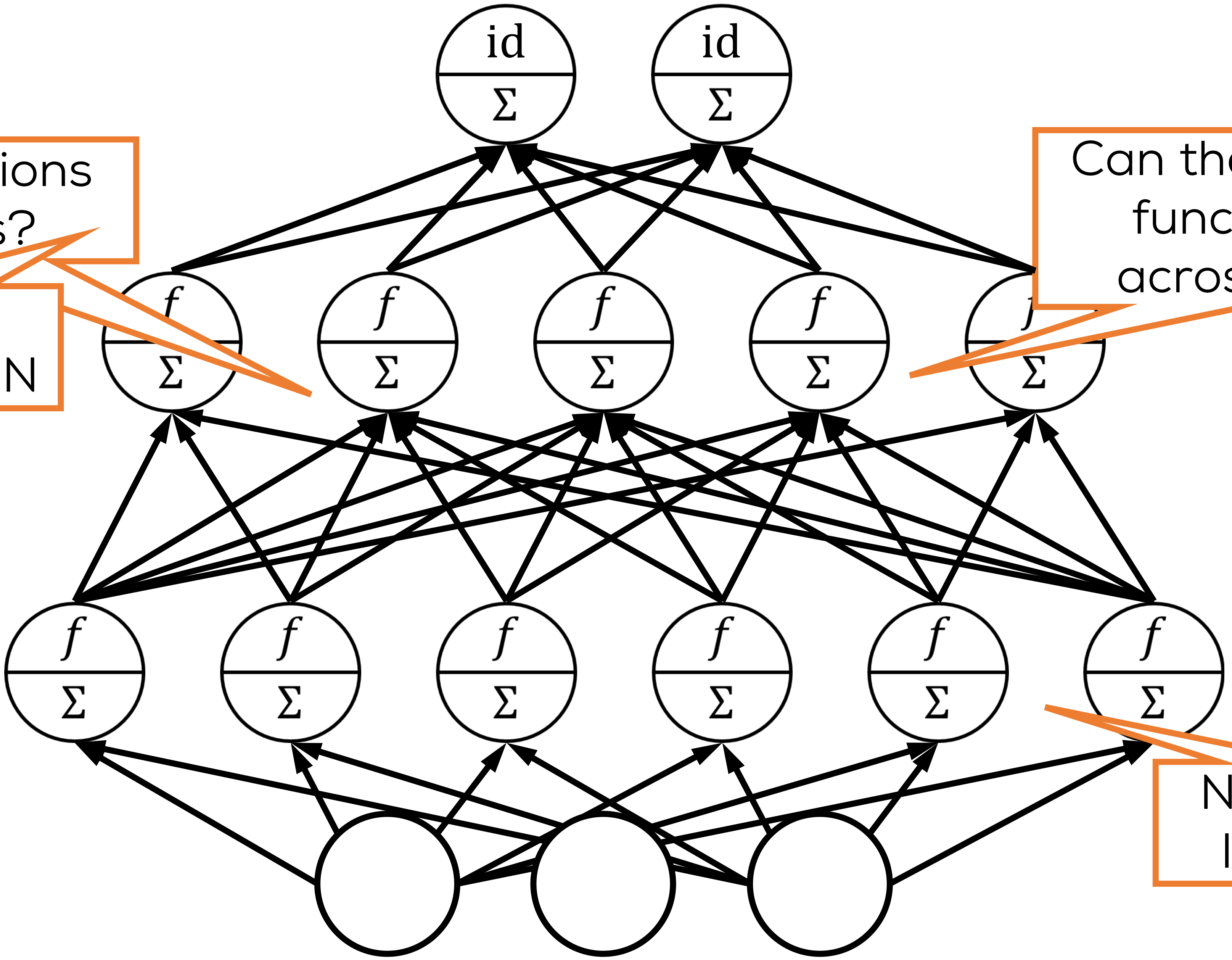
A Feedforward Network



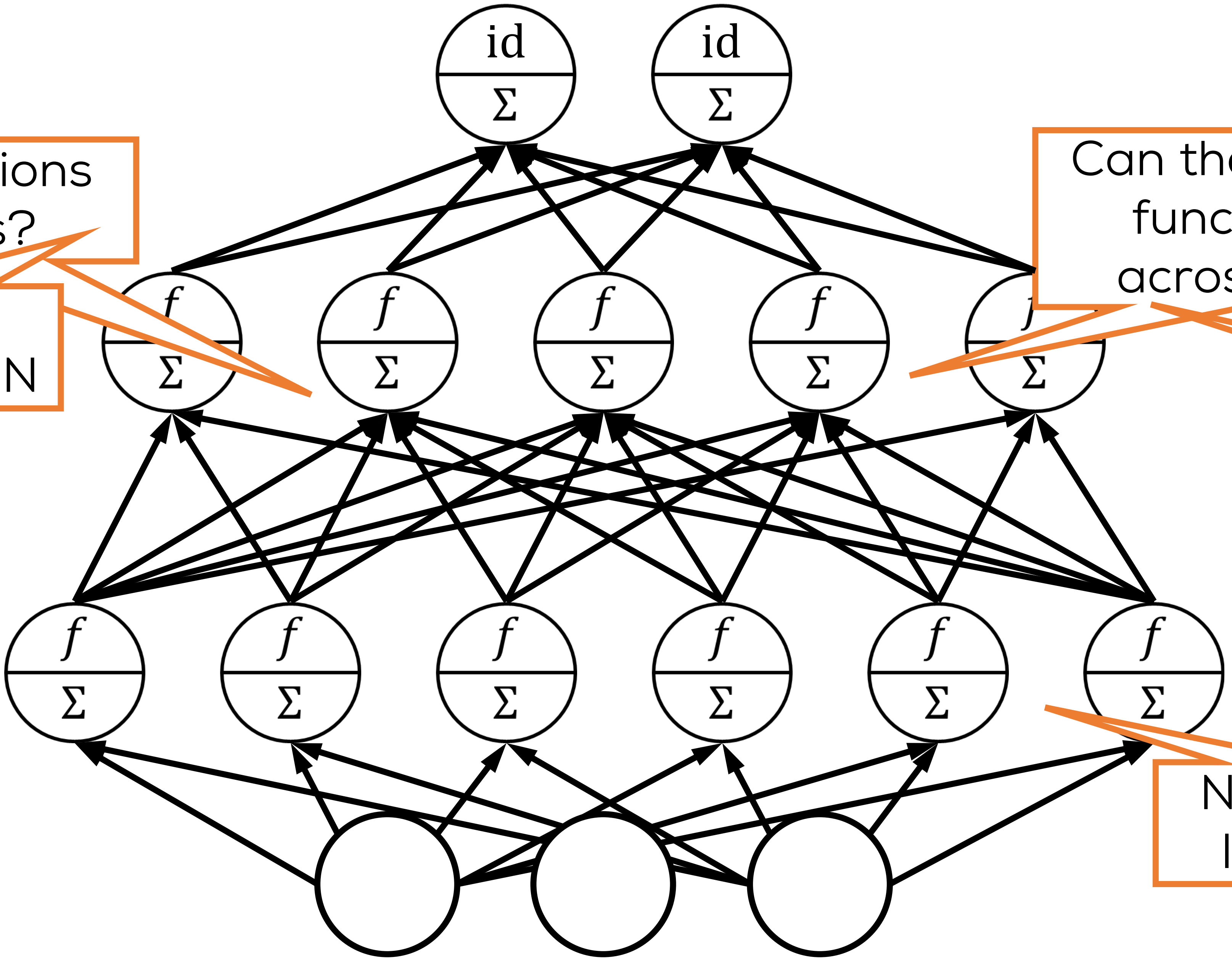
Can I connections jump layers?

Not in a feedforward NN

Can the activation function vary across layers?

No "reverse" links either

A Feedforward Network



Can I connections jump layers?

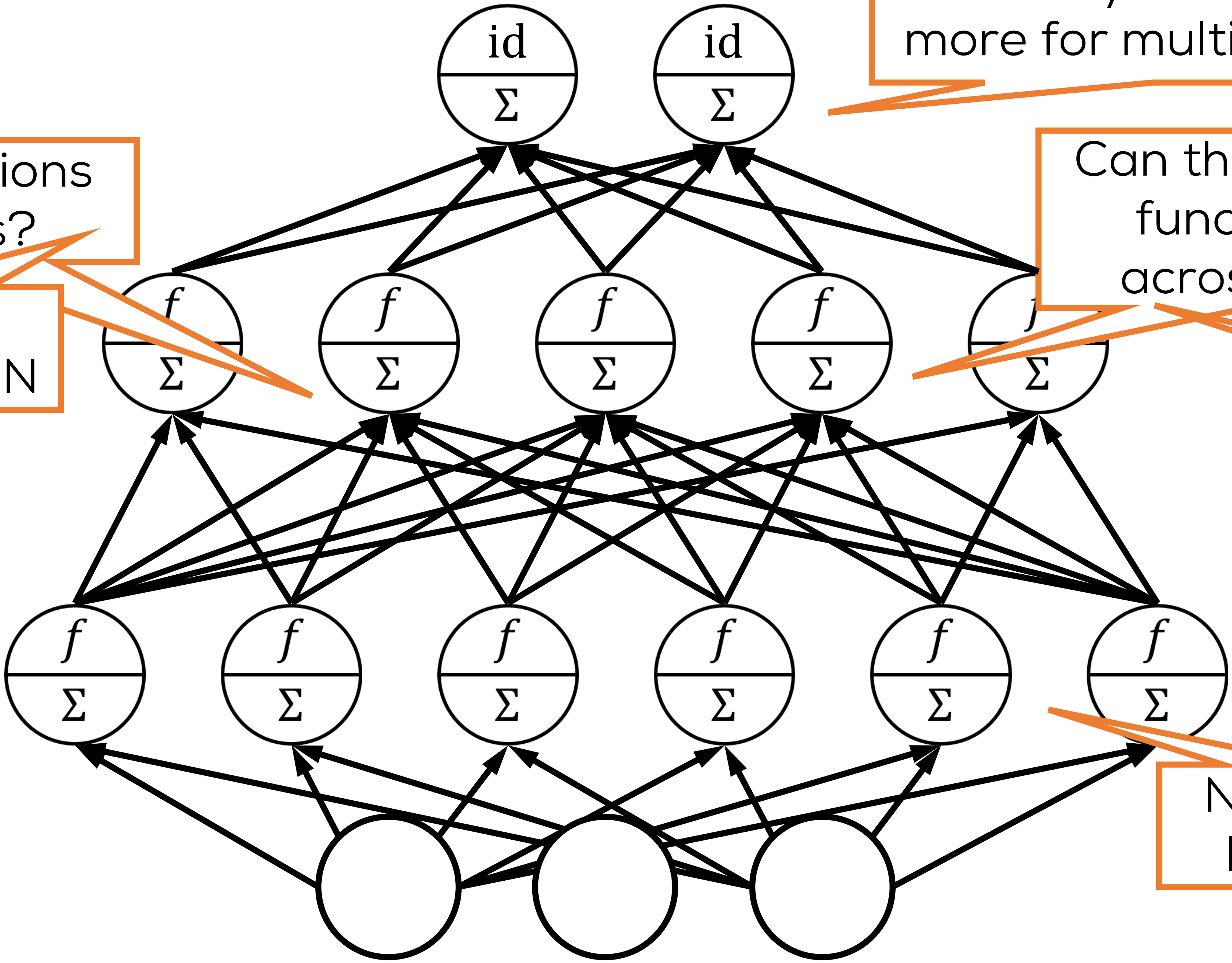
Not in a feedforward NN

Can the activation function vary across layers?

Yes. Wait for CNNs

No "reverse" links either

A Feedforward Network



One output node needed for binary classfn, regresn, more for multi-label/class

Can I connections jump layers?

Not in a feedforward NN

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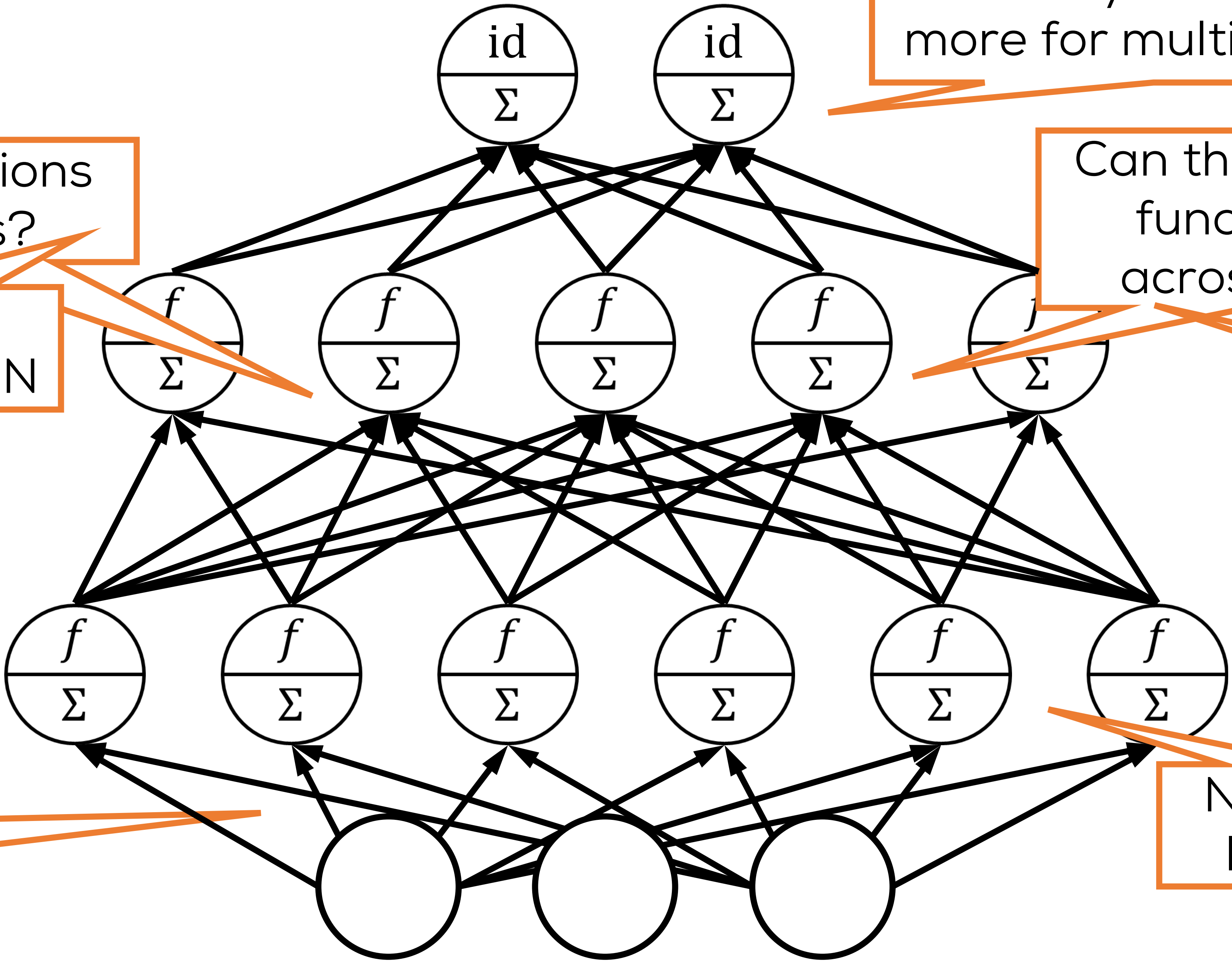
A Feedforward Network



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Can I connections jump layers?

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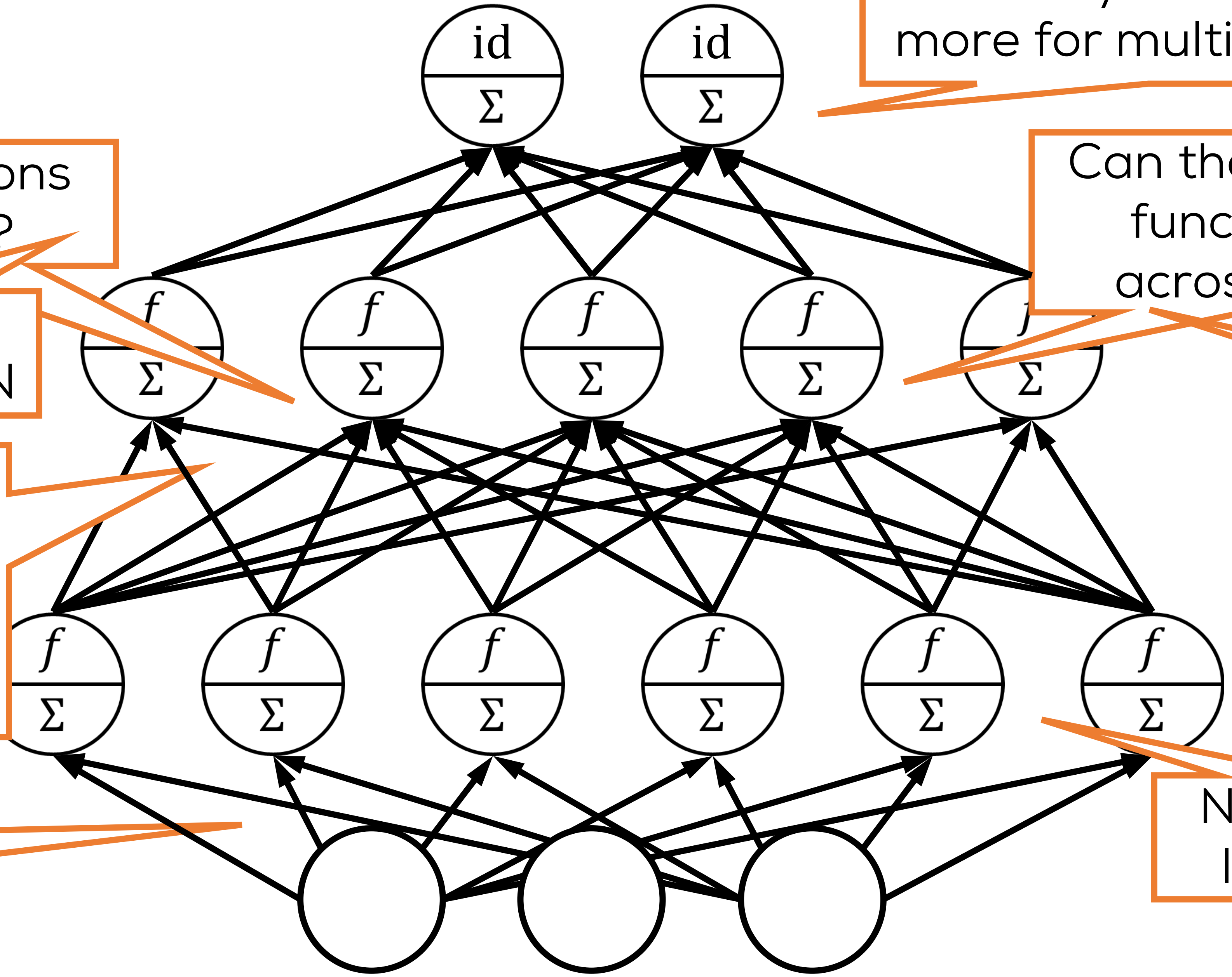
Can the activation function vary across layers?

Yes. Wait for CNNs

All weights are learnt

No "reverse" links either

A Feedforward Network



One output node needed for binary classfn, regresn, more for multi-label/class

Can I connections jump layers?

Not in a feedforward NN

Can the activation function vary across layers?

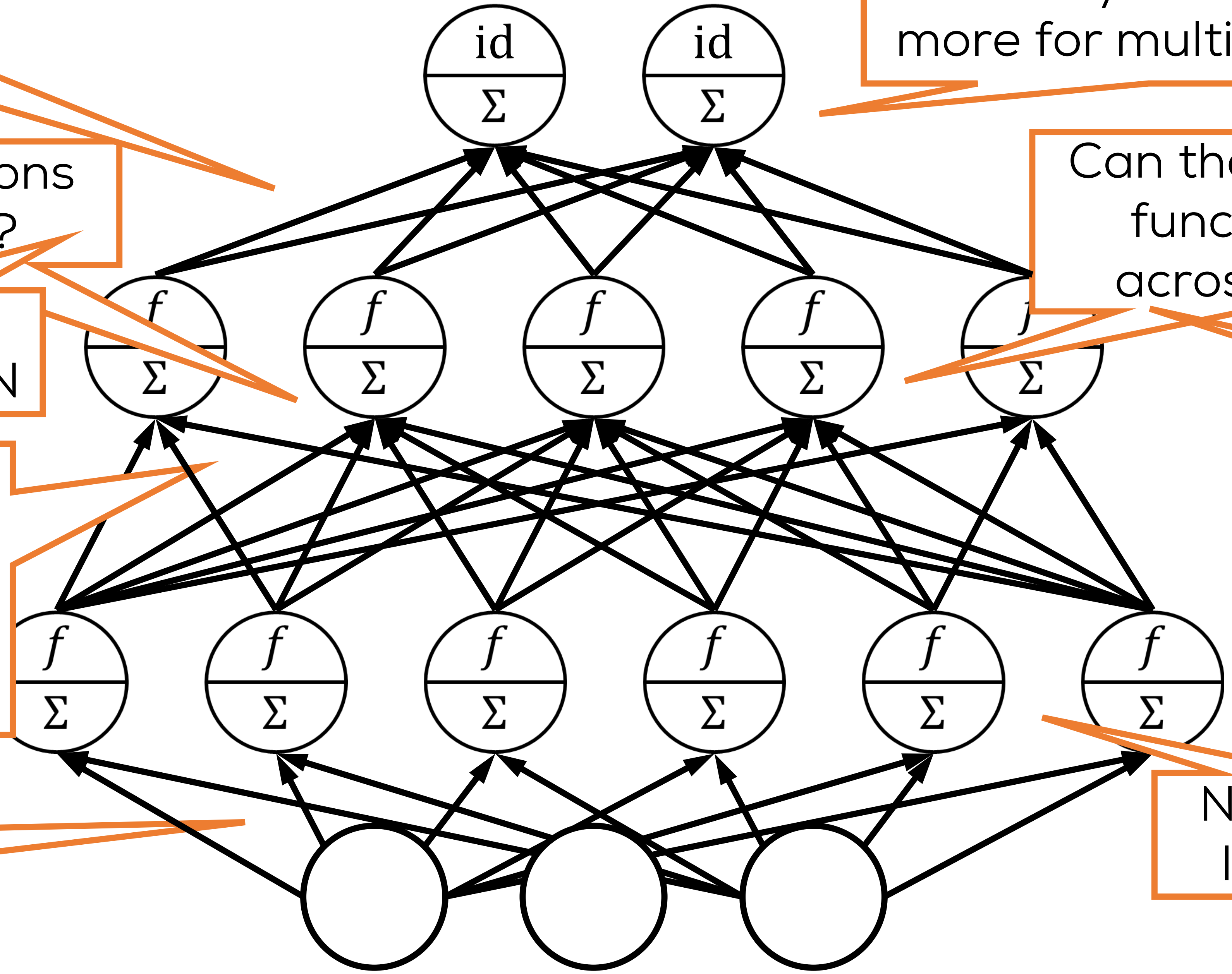
Yes. Wait for CNNs

Connections b/w layers is usually "dense" – all pairs are connected

All weights are learnt

No "reverse" links either

A Feedforward Network



Multi-layered **perceptron**

Can I connections jump layers?

Not in a feedforward NN

Connections b/w layers is usually “dense” – all pairs are connected

All weights are learnt

One output node needed for binary classfn, regresn, more for multi-label/class

Can the activation function vary across layers?

Yes. Wait for CNNs

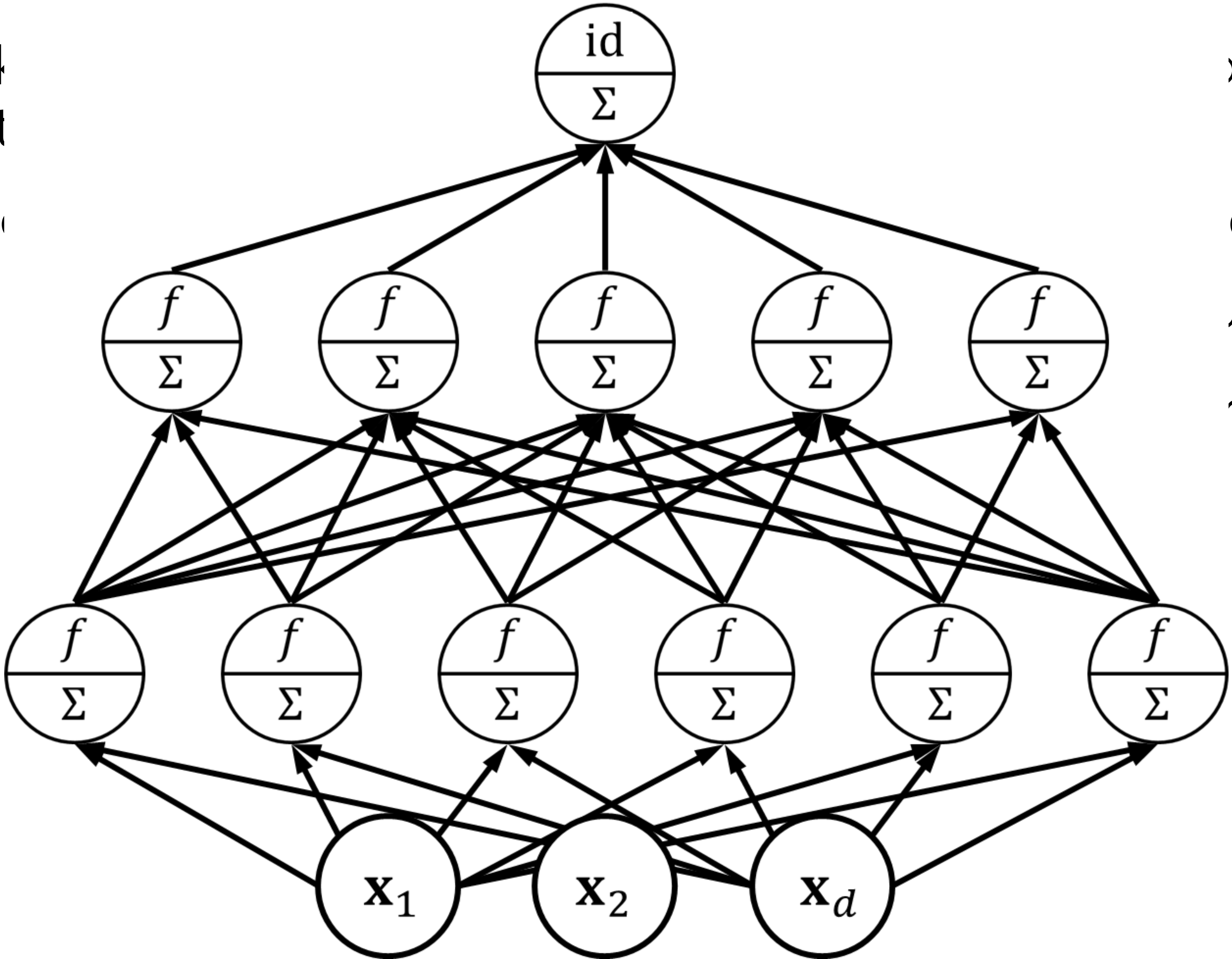
No “reverse” links either

A few thoughts

- Just as in kernel slide, lower layers can be interpreted as working very hard to compute useful and informative features
- Last layer exploits all this hard work to learn a good model $y = \sum_{i=1}^{k_l} \mathbf{w}_i \cdot \phi(\mathbf{x}_i)$, k_l = #nodes in layer previous to output layer
- Note: output is linear in the features computed by lower layers

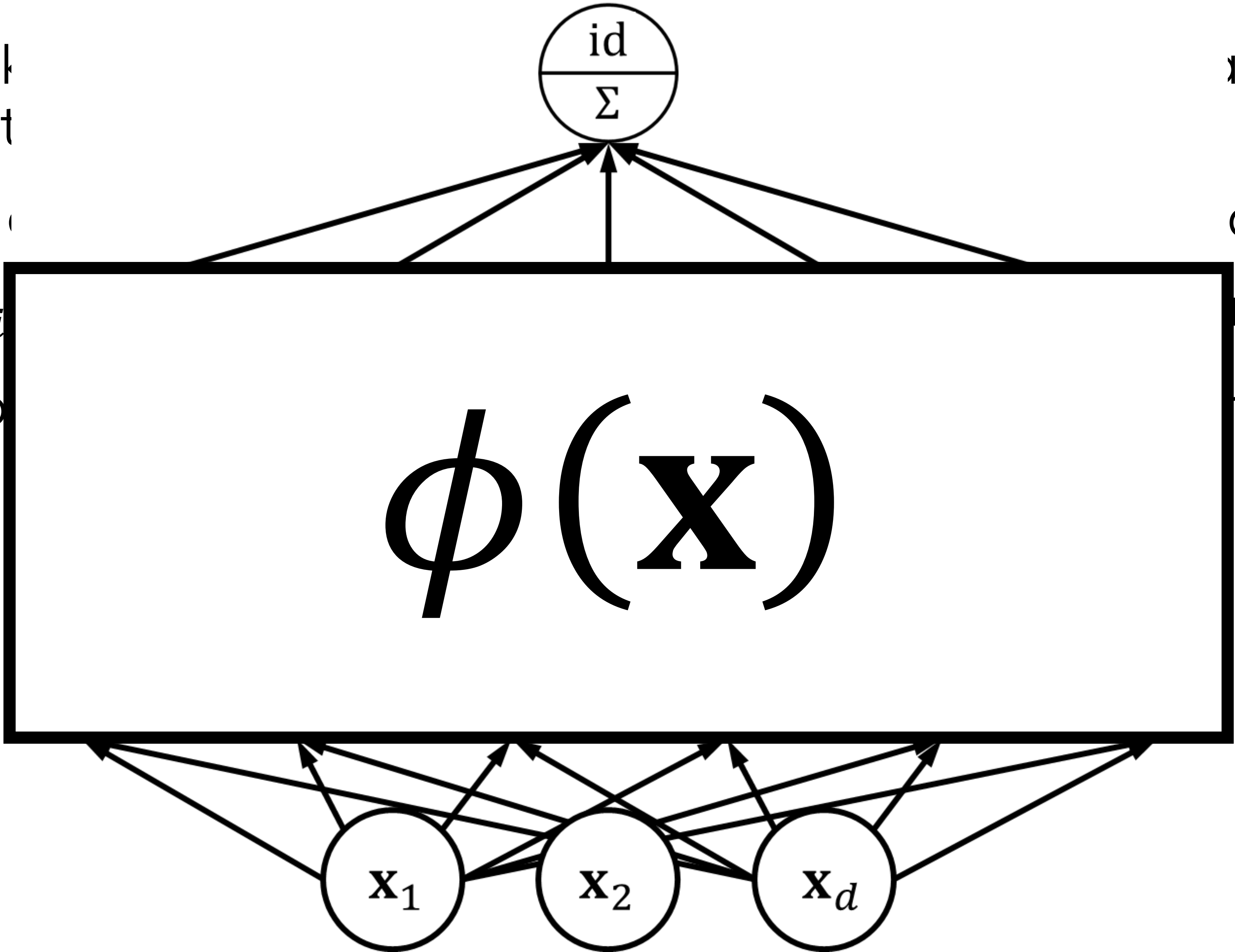
A few thoughts

- Just as in k as working
  very hard t
- Last layer del
  $y = \sum_{i=1}^{k_l} \mathbf{w}_i$ ut layer
- Note: outp layers



A few thoughts

- Just as in k ... as working very hard t
- Last layer ... del $y = \sum_{i=1}^{k_l} \mathbf{w}_i$ ... t layer
- Note: outp ... r layers



A few thoughts

- Just as in kernel slide, lower layers can be interpreted as working very hard to compute useful and informative features
- Last layer exploits all this hard work to learn a good model
  $y = \sum_{i=1}^{k_l} \mathbf{w}_i \cdot \phi(\mathbf{x}_i)$, k_l = #nodes in layer previous to output layer
- Note: output is linear in the features computed by lower layers
- Can have any no. of layers, any no. of nodes in each layer
- Having a linear activation function is useless since the entire network will then just learn a linear function in input
- ReLU networks always learn piecewise linear functions
- Try proving the above two results by induction on number of hidden layers (base case – no hidden layer) as an exercise

A few thoughts

- Kernel models work with a vast (often infinite) set of features. NN methods try to learn a small set of features from data itself
- Features are non-linear in kernels as well as NNs
- Why can't I have the nice operations of product, squaring, identity as "activation functions" as in the kernel slide?
- A variant called *Sum-product Networks* (SPN) does exactly this
- Neural networks are also *universal*
- A neural network with a single hidden layer with infinitely many nodes or else infinitely many layers each with finitely many nodes can learn any function of the input (details technical)
- Next class: how NNs are trained

Please give your Feedback

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