Non-linear Models-VI

CS771: Introduction to Machine Learning

Purushottam Kar

Answering the Fan Mail

- None this week.
- Assignment 3 is out. Deadline Nov 14, 2359 hrs
- Discussion session this Sunday, Nov 5, 6PM, RM101
- Please submit questions to http://tinyurl.com/ml17-18ads2
- Please submit questions latest by Friday, Nov 3
- Please (re)upload your project proposals to GS by Sun, Nov 5
- Make sure all teammates are linked to the (group) submission

Recap

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

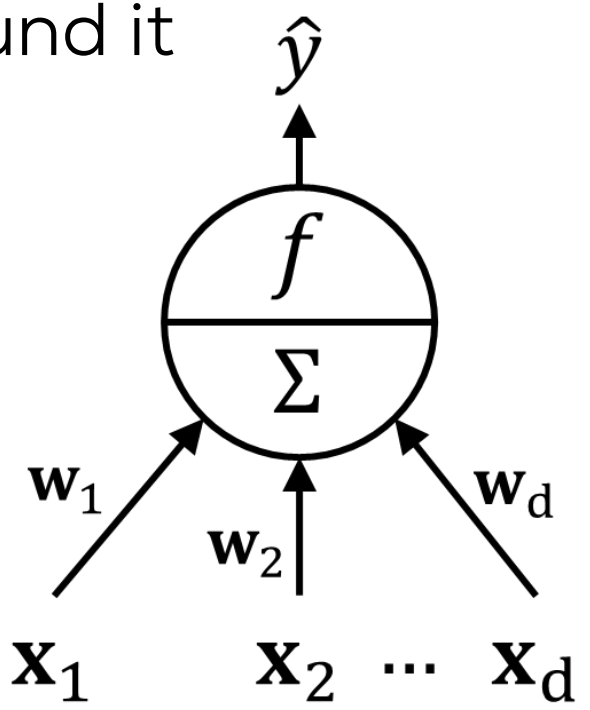
$$(\mathbf{x}^1, y^1), \ldots, (\mathbf{x}^n, y^n), \mathbf{x}^i \in \mathbb{R}^d$$

- … and a loss function

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

- … training a perceptron involves finding

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



Gradient Descent Revisited

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

- 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

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

- 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

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

Choosing a descent direction

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

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Chain rule!

Very small batch sizes usually not used for deep networks

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

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

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?

- 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

$$\eta_t = \arg\min_{\eta \geq 0} F(\mathbf{w}^t - \eta \cdot \mathbf{g}^t)$$

- **Momentum methods**: don't let the procedure take zig-zag routes
  - Nesterov's Accelerated Gradient (NAG)
- **Adaptive step length**: control how much each coordinate of $\mathbf{w}$ gets updated. Slow down coordinates getting too many updates and speed up training along coordinates not getting updated
  - Adagrad, RMSProp, Adam

How to prevent overfitting?

- Add a regularization term L_2/L_1 to the objective

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

- Gradient/step length calculations still easy to perform
- Constraint the weights of the network to satisfy $|\mathbf{w}_i| < r$ for all i

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

- 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

$$\mathbf{w}_i = \mathbf{w}_j$$

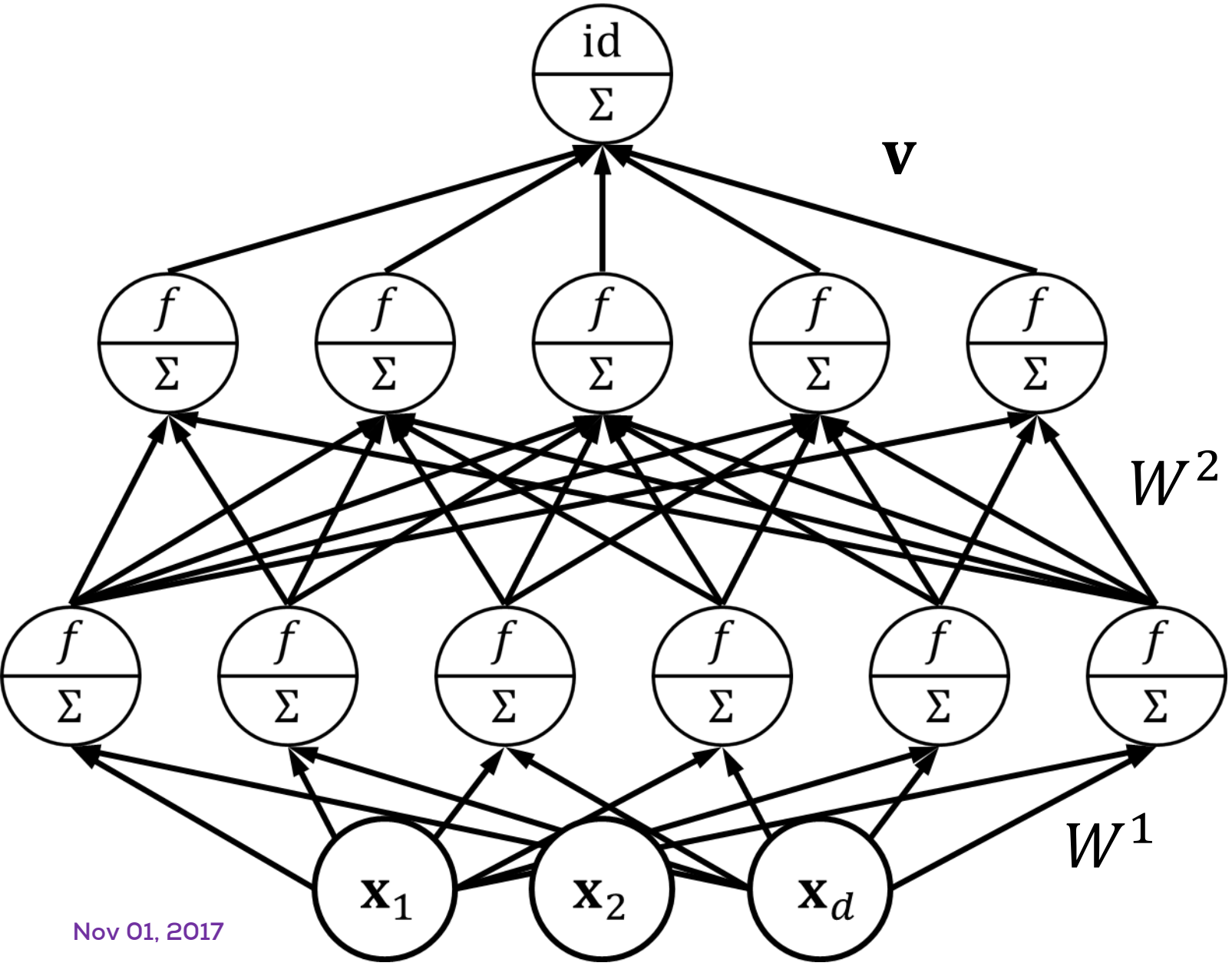
- Sparse recovery – constrain, say at least 10% weights to be zero

$$\|\mathbf{w}\|_0 \leq k \ll d$$

- Dropout – will see in a short while!

Multilayer Perceptron

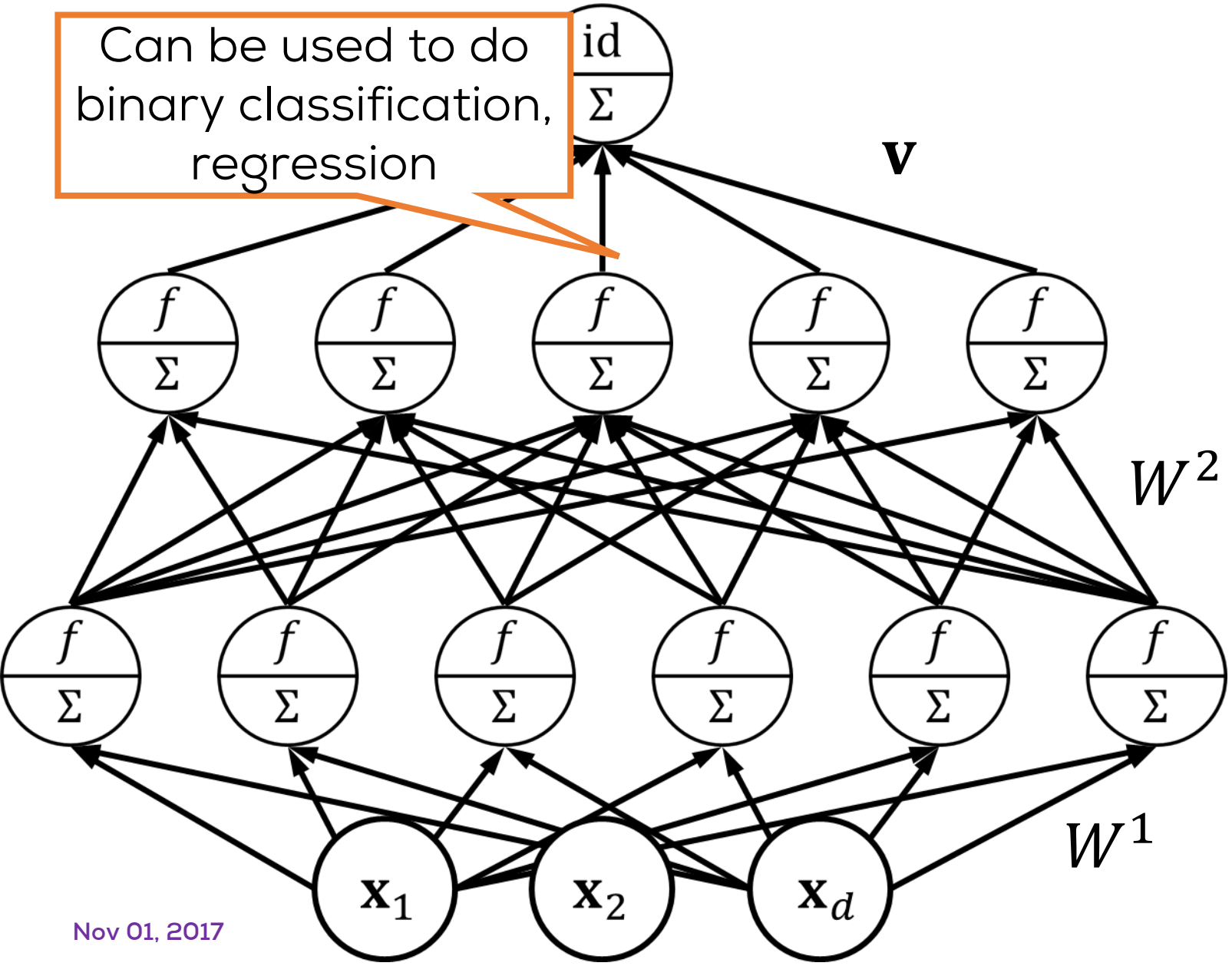
Feedforward Neural Network



- d inputs, L hidden layers
- k_l nodes in l-th layer
- $W^l \in \mathbb{R}^{k_{l-1} \times k_l}$ weights from layer $l-1$ to l
- $\mathbf{v} \in \mathbb{R}^{k_L}$ weights from layer L to output node
- $\mathbf{h}^l \in \mathbb{R}^{k_l}$ o/p by layer l
- $\hat{y}$ output of the network
- $\mathbf{h}^l = f\left(\left(W^l\right)^\top \mathbf{h}^{l-1}\right)$
- $f(\mathbf{u}) = [f(\mathbf{u}_1), \ldots, f(\mathbf{u}_k)]$
- $\hat{y} = \langle \mathbf{v}, \mathbf{h}^L \rangle$

Feedforward Neural Network

Can be used to do binary classification, regression



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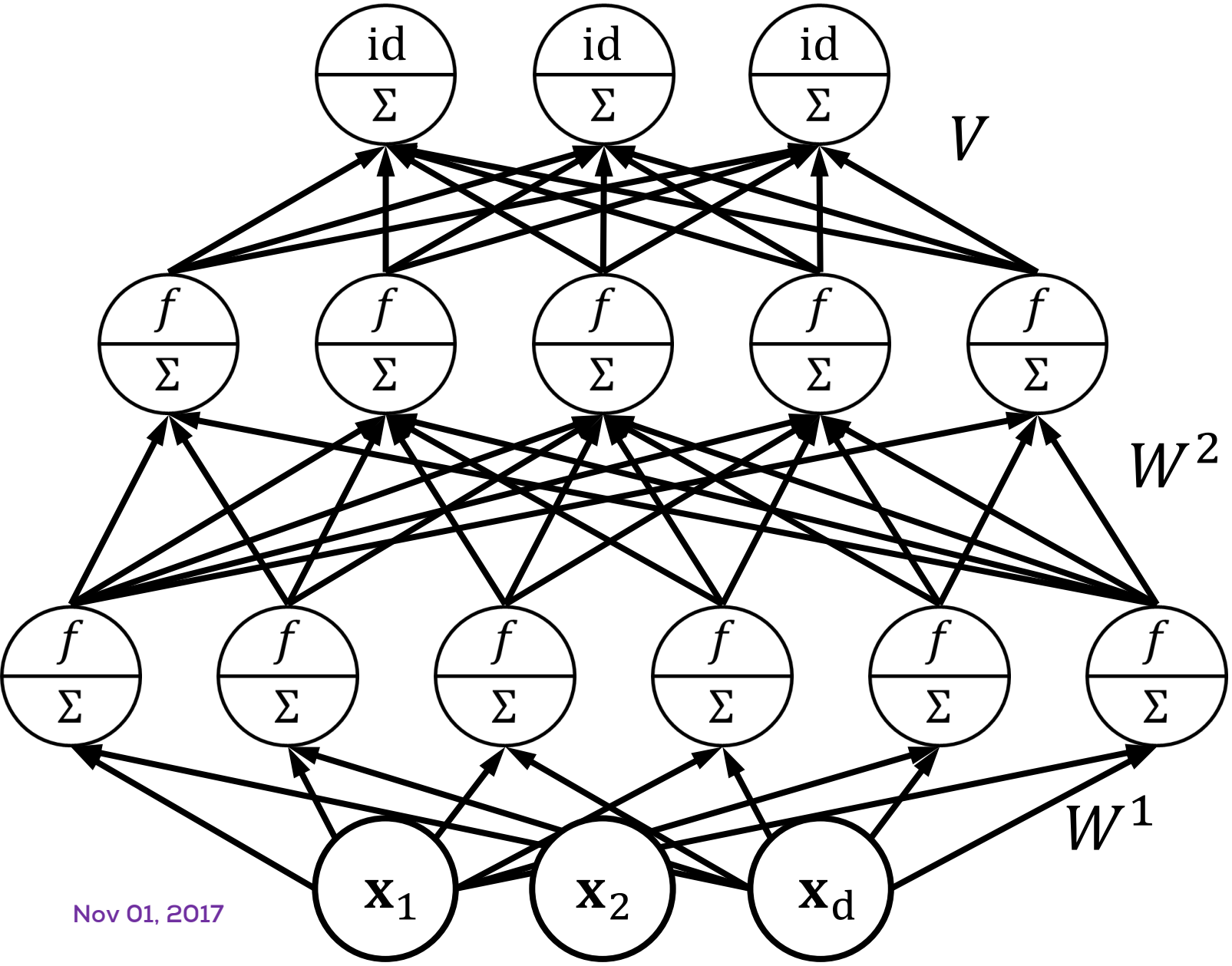
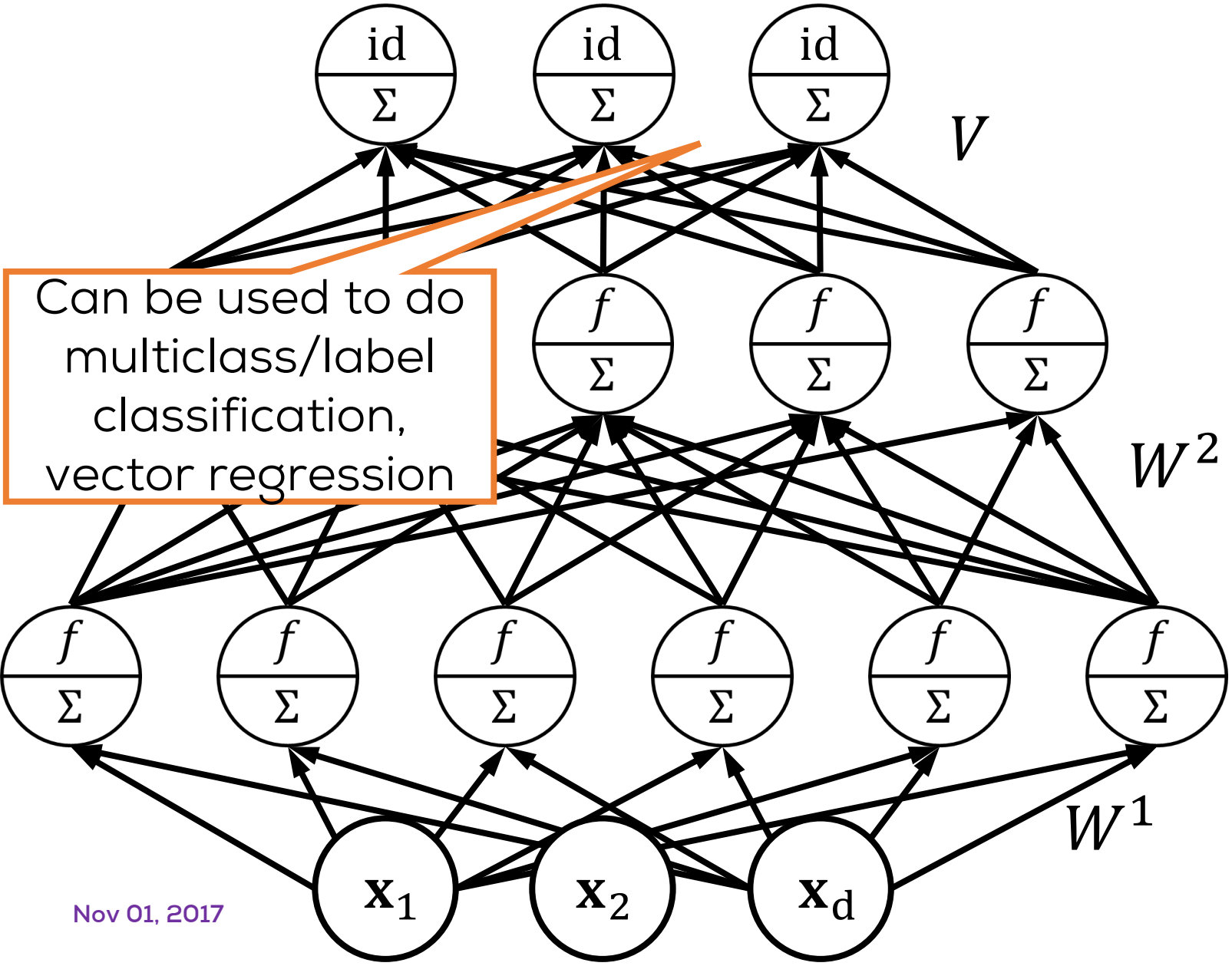


- C output nodes
- $\hat{\mathbf{y}} \in \mathbb{R}^C$ o/p of network
- $V \in \mathbb{R}^{k_L \times C}$ weights from layer L to output layer
- $\hat{\mathbf{y}} = V^\top \mathbf{h}^L$
- … or else $\hat{\mathbf{y}} = g(V^\top \mathbf{h}^L)$
- E.g. g: softmax, maxout

Feedforward Neural Network



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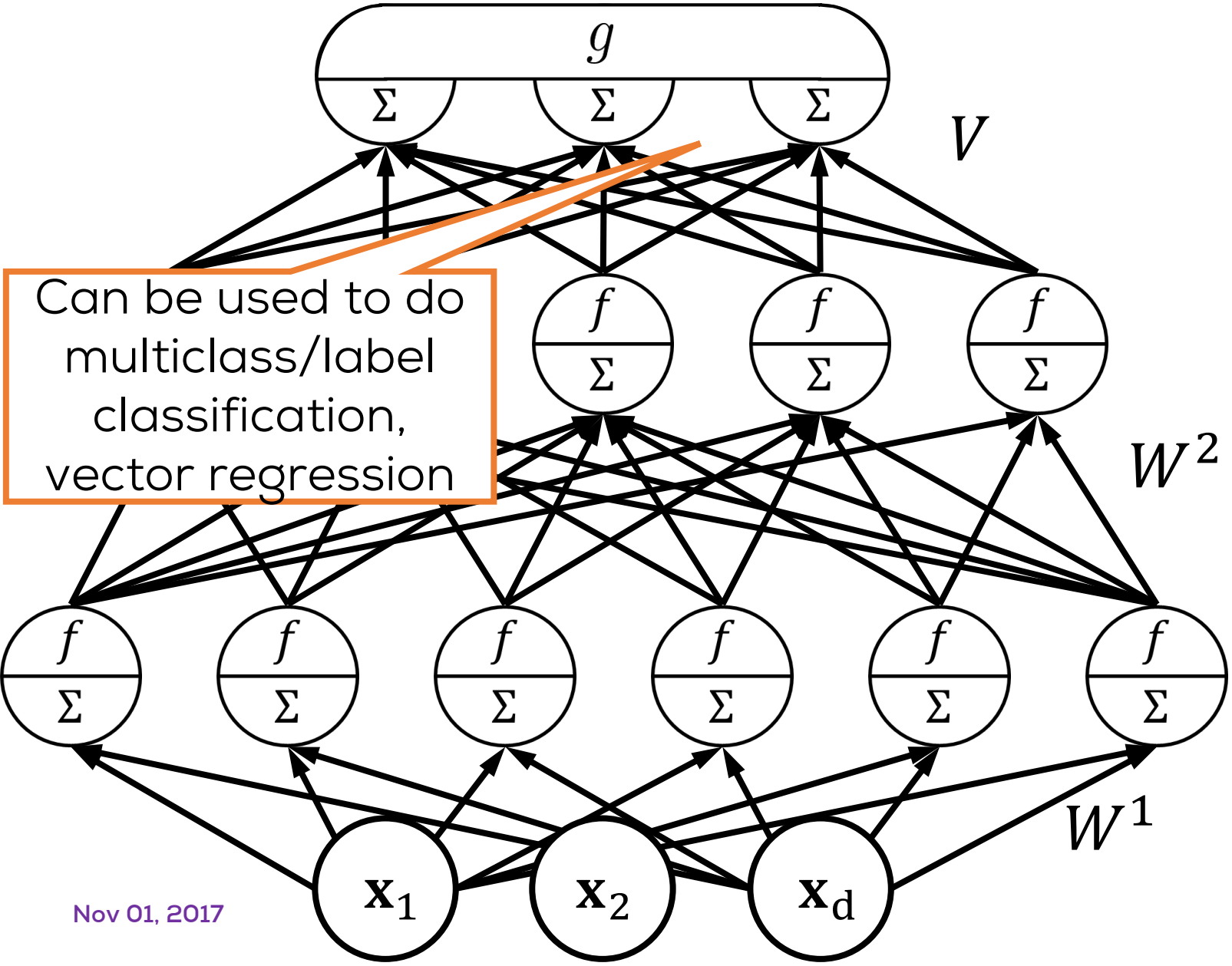

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The Backpropagation Algorithm

- We have seen how to use Gradient Descent to train perceptron
- Backprop is used to perform GD on multilayer networks
- Basically chain-rule + intelligent bookkeeping
- Recall, we used bookkeeping to do coordinate descent in $\mathcal{O}(n)$ time
- Backprop is still the defacto training technique for most NN
- Indications that this may (have to) change [Hinton 2017]

The Rules that Chain

- Let $x = f(y), y = g(z), z = h(w)$ where $x, y, z, w \in \mathbb{R}$ and f, g, h: $\mathbb{R} \rightarrow \mathbb{R}$
- Chain rule of calculus

$$\frac{dx}{dw} = \frac{dx}{dy} \cdot \frac{dy}{dz} \cdot \frac{dz}{dw} = f'(y) \cdot g'(z) \cdot h'(w)$$

- What about multivariate versions?
- Let $x = f(\mathbf{y})$ where $x \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^q$ and f: $\mathbb{R}^q \rightarrow \mathbb{R}$ - notion of gradient

$$\frac{dx}{d\mathbf{y}} = \nabla f(\mathbf{y}) \in \mathbb{R}^{1 \times q}$$

- If $\mathbf{x} = f(\mathbf{y})$ where $\mathbf{x} \in \mathbb{R}^p, \mathbf{y} \in \mathbb{R}^q$ and f: $\mathbb{R}^q \rightarrow \mathbb{R}^p$ - notion of Jacobian
- Think of $f(\mathbf{y}) = \left[f_1(\mathbf{y}), \ldots, f_p(\mathbf{y})\right]^\top$ as a vector of functions

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\mathbf{y}} = J^f \text{ where }, J^f_{ij} = \frac{d\mathbf{x}_i}{d\mathbf{y}_j} \text{ i. e. } J^f = \begin{bmatrix} \nabla f_1(\mathbf{y}) \\ \vdots \\ \nabla f_p(\mathbf{y}) \end{bmatrix} \in \mathbb{R}^{p \times q}$$

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Notice slightly different notation where $\nabla f(\mathbf{y})$ is a row vector

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The Rules that Chain

- Let $x = f(\mathbf{y}), \mathbf{y} = g(\mathbf{z})$ where $x \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^q, \mathbf{z} \in \mathbb{R}^r$ and $f\colon \mathbb{R}^q \rightarrow \mathbb{R}, g\colon \mathbb{R}^r \rightarrow \mathbb{R}^q$
- The chain rule becomes a bit more involved here (proof nontrivial)

$$\frac{dx}{d\mathbf{z}_j} = \sum_{i=1}^{q} \frac{dx}{d\mathbf{y}_i} \cdot \frac{d\mathbf{y}_i}{d\mathbf{z}_j}$$

- Thus we have

$$\frac{dx}{d\mathbf{z}} = \nabla f(\mathbf{y}) \cdot J^g \in \mathbb{R}^{1 \times r}$$

Remember our slightly different notation where $\nabla f(\mathbf{y})$ is a row vector

- Similarly, if we have $\mathbf{x} = f(\mathbf{y}), \mathbf{y} = g(\mathbf{z})$ where $x \in \mathbb{R}^p, \mathbf{y} \in \mathbb{R}^q, \mathbf{z} \in \mathbb{R}^r$

$$\frac{d\mathbf{x}}{d\mathbf{z}} = J^f \cdot J^g$$

The Rules that Chain

- This actually extends very cleanly to more complex instances
- If $\mathbf{x} = f(\mathbf{y}), \mathbf{y} = g(\mathbf{z}), \mathbf{z} = h(\mathbf{w})$ where $x \in \mathbb{R}^p, \mathbf{y} \in \mathbb{R}^q, \mathbf{z} \in \mathbb{R}^r, \mathbf{w} \in \mathbb{R}^s$

$$\frac{d\mathbf{x}}{d\mathbf{w}} = J^f \cdot J^g \cdot J^h$$

- It also unifies the previous cases beautifully
- Consider a function $\mathbf{x} = f(\mathbf{y})$ where $x \in \mathbb{R}^p, \mathbf{y} \in \mathbb{R}^q$
  - If $p = q = 1$ (basic case), Jacobian is simply a 1×1 matrix (a real number)
  - If $p = 1$ and $q > 1$ (real valued function on vector space), Jacobian becomes a row vector
  - If $p > 1$ and $q = 1$ and no $\mathbf{w}$ (vector valued function on the real line), Jacobian becomes a column vector
- However, $\frac{d\mathbf{x}}{d\mathbf{w}} = J^f \cdot J^g \cdot J^h$ always applies if careful with dimensions

The Rules that Chain

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- If $\mathbf{x} = f(\mathbf{y}), \mathbf{y} = g(\mathbf{z}), \mathbf{z} = h(\mathbf{w})$ where $x \in \mathbb{R}$, $\mathbf{y} \in$

$$\frac{d\mathbf{x}}{d\mathbf{w}} = J^f \cdot J^g \cdot J^h$$

Mimics earlier result

$$\frac{dx}{dw} = f'(y) \cdot g'(z) \cdot h'(w)$$

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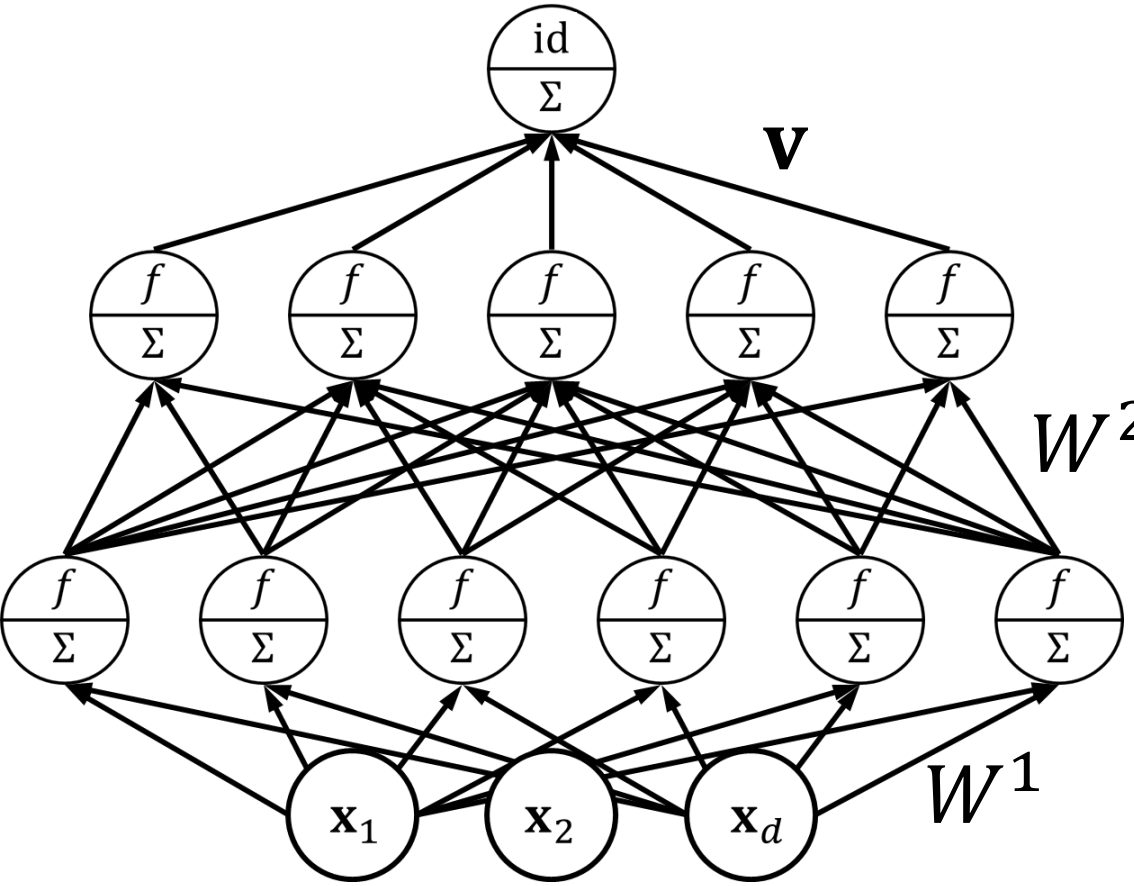
Back to Backpropagation



- $\hat{y} = \langle \mathbf{v}, \mathbf{h}^2 \rangle$ is the output of the NN
- We wish to train using GD on

$$F(\mathbf{v}, W^2, W^1) = \sum_{i=1}^{n} \ell(\hat{y}^i, y^i) = \sum_{i=1}^{n} \ell^i$$

- Need only describe how to calculate

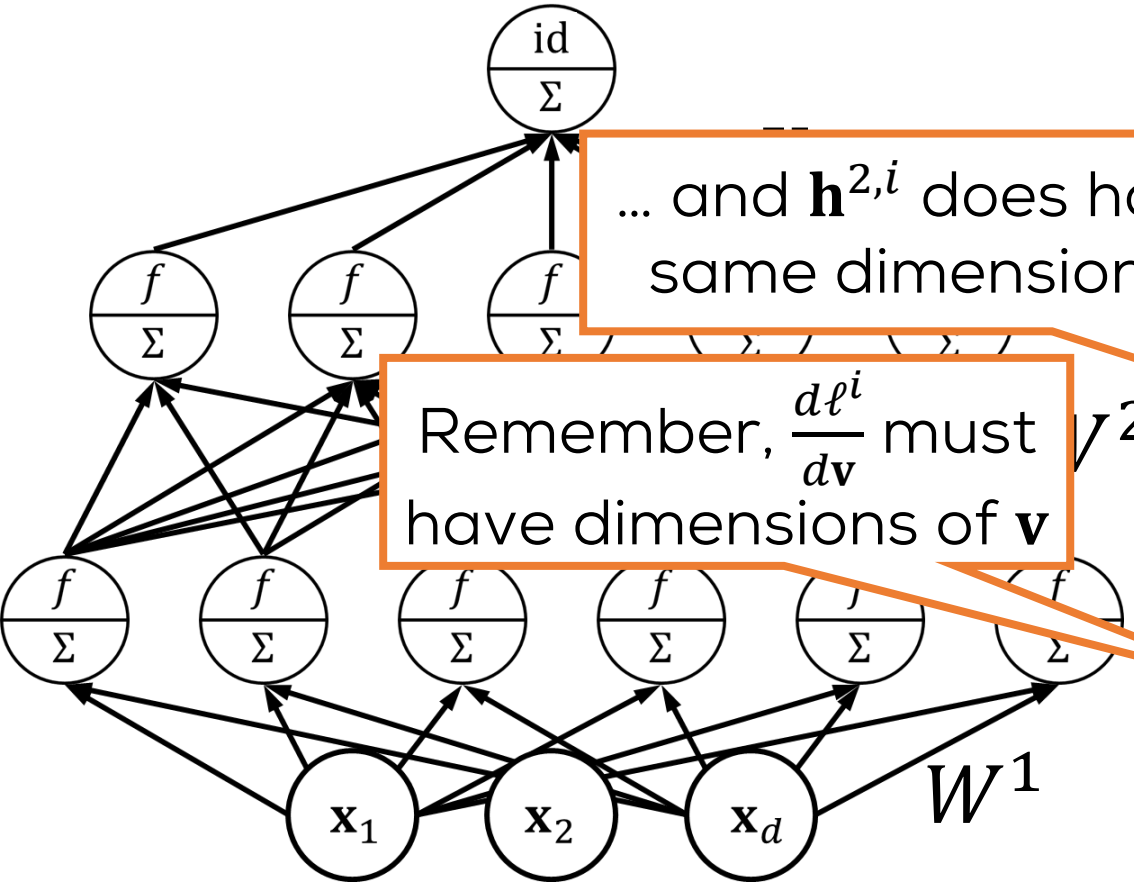
$$\frac{d\ell^i}{d\mathbf{v}}, \frac{d\ell^i}{dW^2}, \frac{d\ell^i}{dW^1}$$

- First is easy

$$\frac{d\ell^i}{d\mathbf{v}} = \frac{d\ell^i}{d\hat{y}^i} \cdot \frac{d\hat{y}^i}{d\mathbf{v}} = \ell'(\hat{y}^i, y^i) \cdot \mathbf{h}^{2,i}$$

- $\mathbf{h}^{2,i}$ is the o/p of the 2nd hidden layer on the i-th data point

Back to Backpropagation



… and $\mathbf{h}^{2,i}$ does have the same dimensions as $\mathbf{v}$

Remember, $\frac{d\ell^i}{d\mathbf{v}}$ must have dimensions of $\mathbf{v}$

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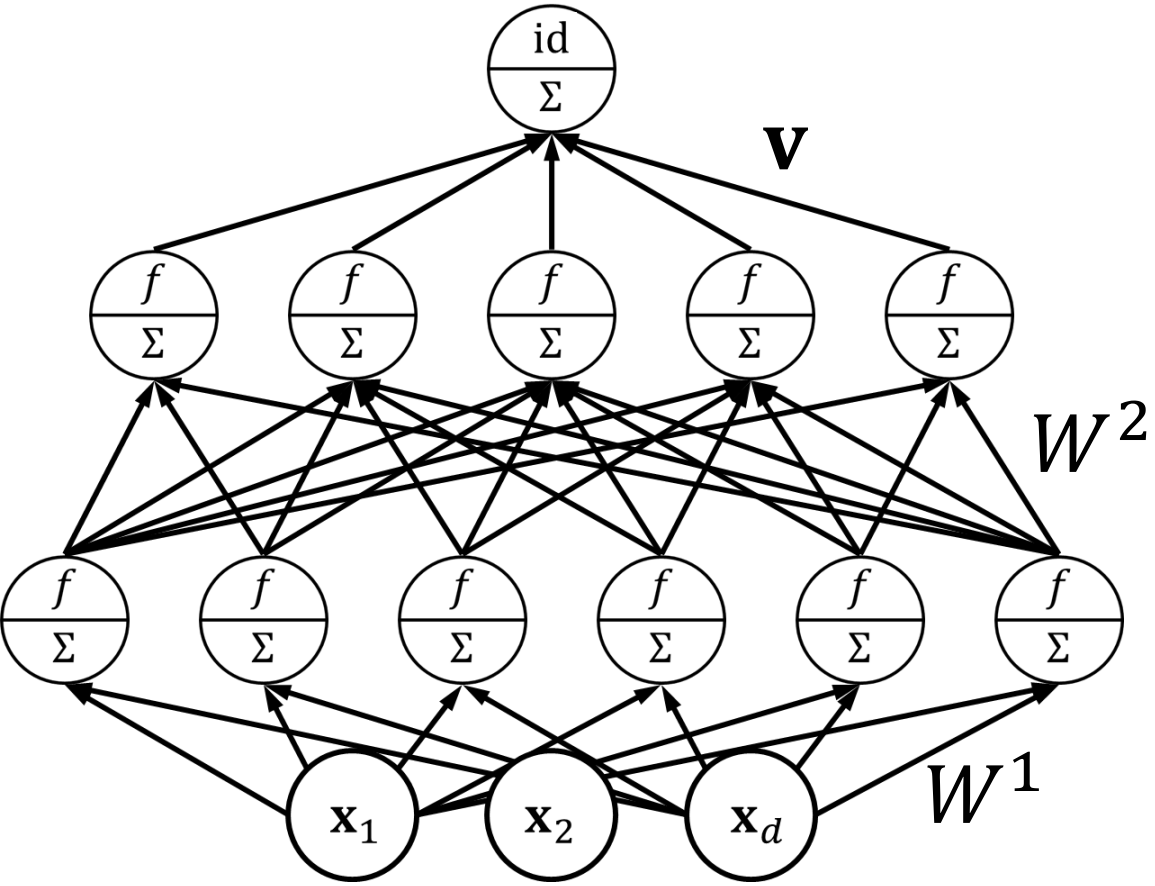


- Second is more challenging

$$\frac{d\ell^i}{dW^2} = \frac{d\ell^i}{d\hat{y}^i} \cdot \frac{d\hat{y}^i}{dW^2} = \ell'(\hat{y}^i, y^i) \cdot \frac{d\hat{y}^i}{dW^2}$$

$$= \ell'(\hat{y}^i, y^i) \cdot \frac{d\hat{y}^i}{d\mathbf{h}^{2,i}} \cdot \frac{d\mathbf{h}^{2,i}}{dW^2} = \ell'(\hat{y}^i, y^i) \cdot \mathbf{v} \cdot \frac{d\mathbf{h}^{2,i}}{dW^2}$$

- Use the fact that $\mathbf{h}^{2,i} = f\left((W^2)^\top \mathbf{h}^{1,i}\right)$
- Why did we not consider $\frac{d\hat{y}^i}{d\mathbf{v}}$ above?

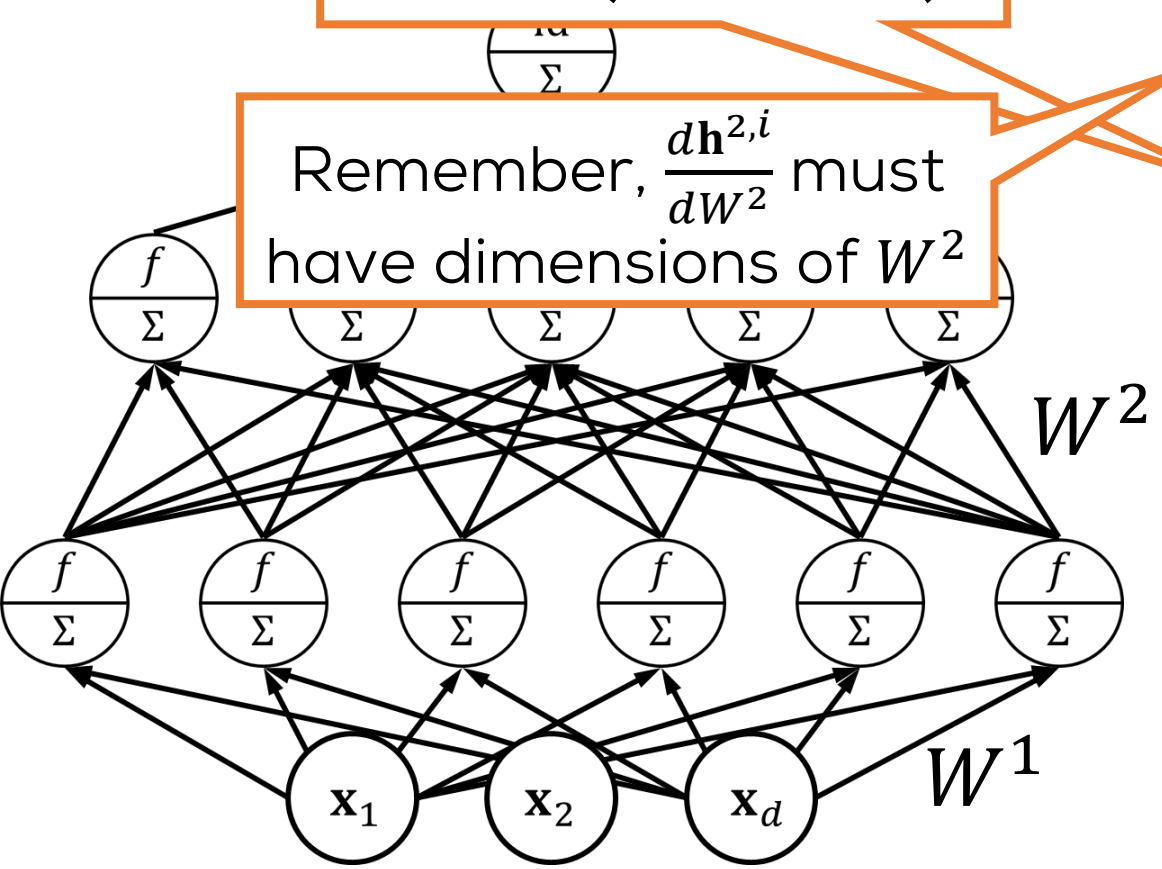
$$\frac{d\hat{y}^i}{dW^2} = \frac{d\hat{y}^i}{d\mathbf{h}^{2,i}} \cdot \frac{d\mathbf{h}^{2,i}}{dW^2} + \frac{d\hat{y}^i}{d\mathbf{v}} \cdot \frac{d\mathbf{v}}{dW^2}$$

- We could have but $\frac{d\mathbf{v}}{dW^2} = \mathbf{0}$ since $\mathbf{v}$ is not a function of W^2

Back to Backpropagation

Careful, $\frac{d\mathbf{h}^{2,i}}{dW^2}$ is a 3-D matrix (3D tensor)

Remember, $\frac{d\mathbf{h}^{2,i}}{dW^2}$ must have dimensions of W^2



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$$\frac{d\hat{y}^i}{dW^2} = \frac{d\hat{y}^i}{d\mathbf{h}^{2,i}} \cdot \frac{d\mathbf{h}^{2,i}}{dW^2} + \frac{d\hat{y}^i}{d\mathbf{v}} \cdot \frac{d\mathbf{v}}{dW^2}$$

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Bookkeeping in Backprop

- Lower derivatives get more and more costly

$$\frac{d\ell^i}{dW^1} = \frac{d\ell^i}{d\hat{y}^i} \cdot \frac{d\hat{y}^i}{d\mathbf{h}^{2,i}} \cdot \frac{d\mathbf{h}^{2,i}}{d\mathbf{h}^{1,i}} \cdot \frac{d\mathbf{h}^{1,i}}{dW^1}$$

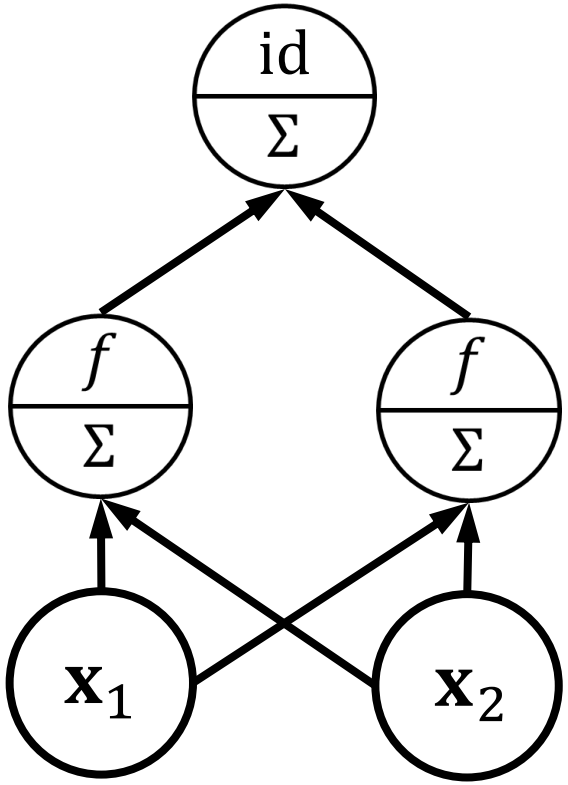
- We have ignored the terms $\frac{\mathrm{d}\ell^i}{dy^i}, \frac{d\hat{y}^i}{d\mathbf{v}}, \frac{d\mathbf{h}^{2,i}}{dW^2}, \frac{d\mathbf{h}^{1,i}}{d\mathbf{x}^i}$ ($\mathbf{x}^i$ is the input layer) since $\frac{dy^i}{dW^1} = \frac{d\mathbf{v}}{dW^1} = \frac{dW^2}{dW^1} = \frac{d\mathbf{x}^i}{dW^1} = \mathbf{0}$ ($\mathbf{x}^i, y^i$ are constants)
- Note that quantities like $\frac{d\ell^i}{d\hat{y}^i}, \frac{d\hat{y}^i}{d\mathbf{h}^{2,i}}$ get used again and again
- Better to compute them once and store them – bookkeeping
- Basically what frameworks like Theano, TensorFlow, Torch do
- Which is why they take up so much memory as well!

Dropout

Dropout

- An effort to make networks more resilient to noise, node failure
- Side effect is slightly faster training and regularization
- Basic idea is to train sparse networks (lots of edges missing)
- The lead author of the Dropout paper is an IITK alumni ☺
- During training, before applying mini-batch gradient descent
  - Randomly sample a subset of input nodes (choose each with prob 20%)
  - Randomly sample a subset of hidden nodes (choose each w/p 50%)
  - Remove those nodes, and corresponding edges from the network
  - Apply mini-batch gradient descent-backprop to the remaining network
  - Keep using NAG, AdaGrad etc as usual
- Forces nodes to learn to work in absence of other nodes – robust!

Dropout at Work



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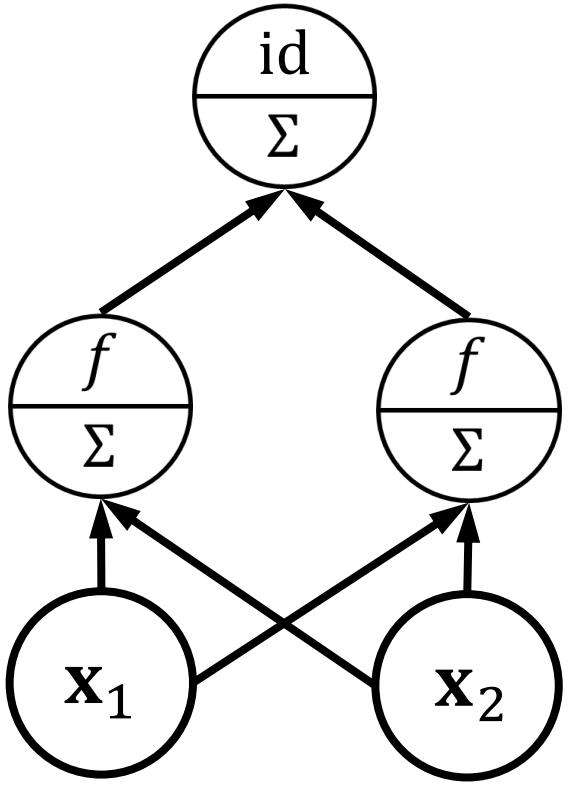

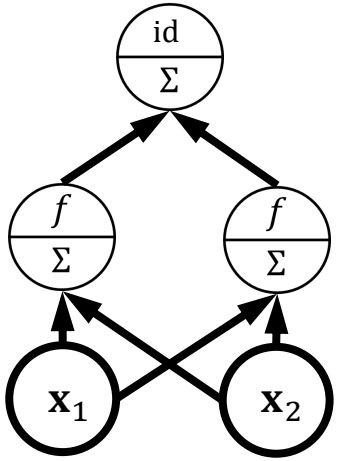

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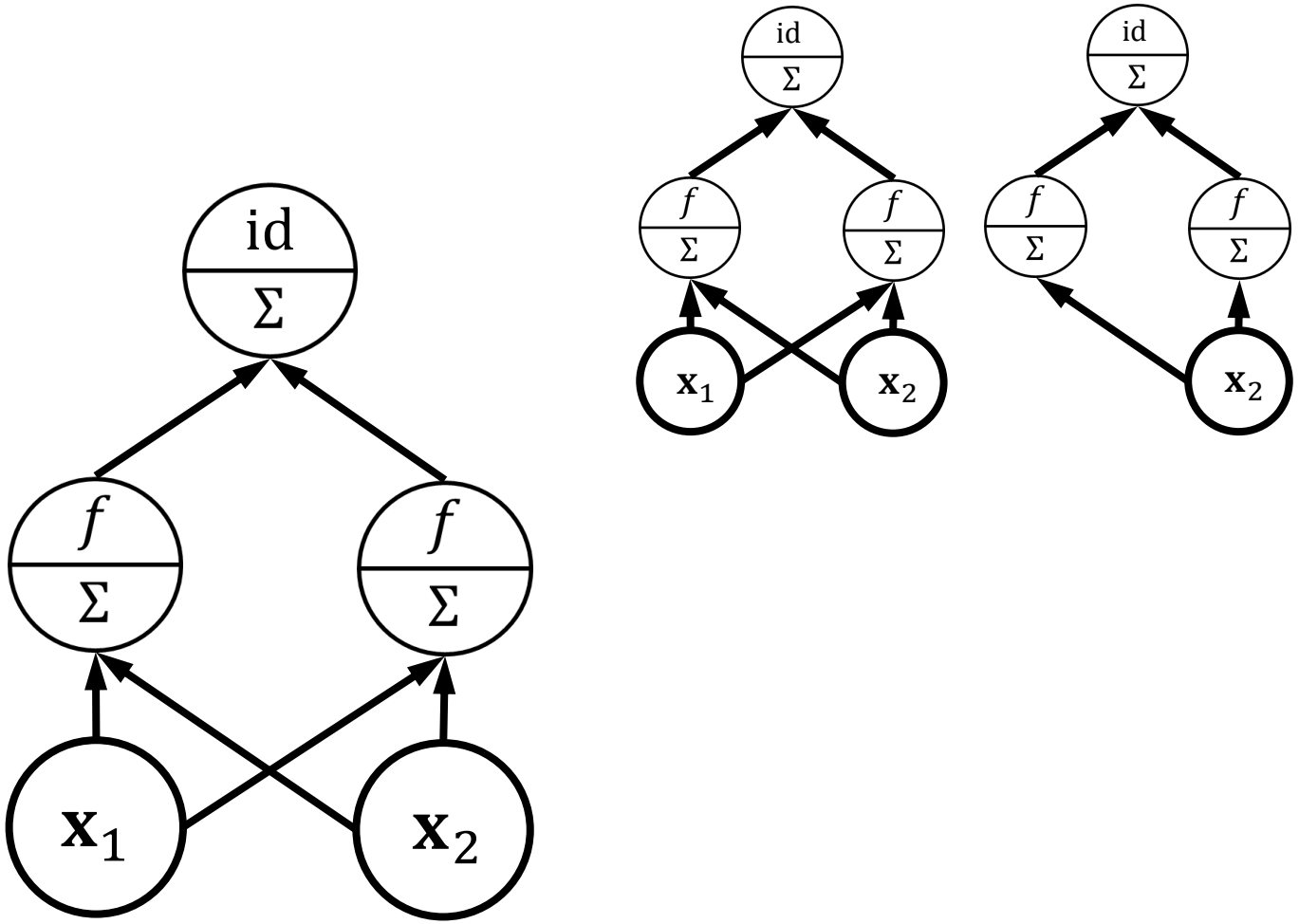

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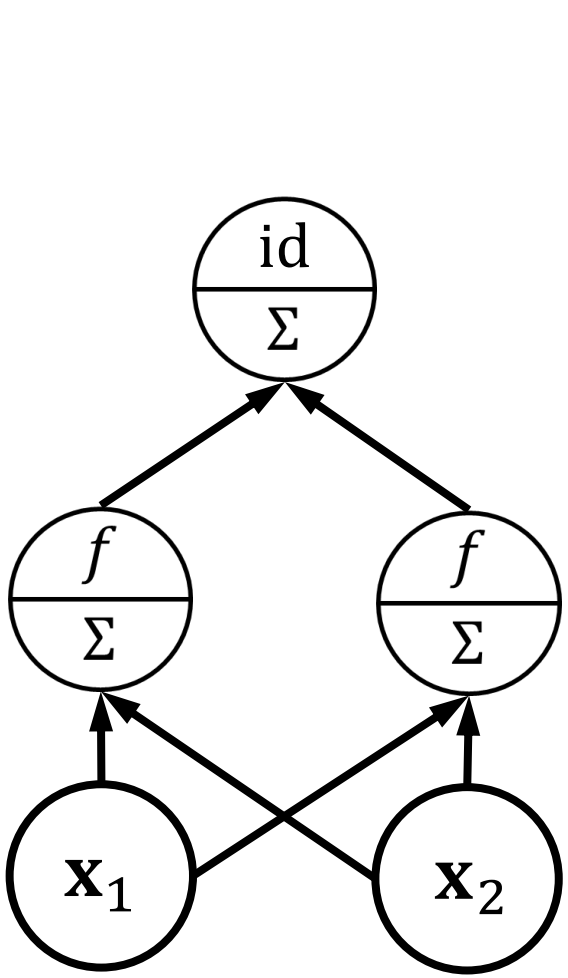

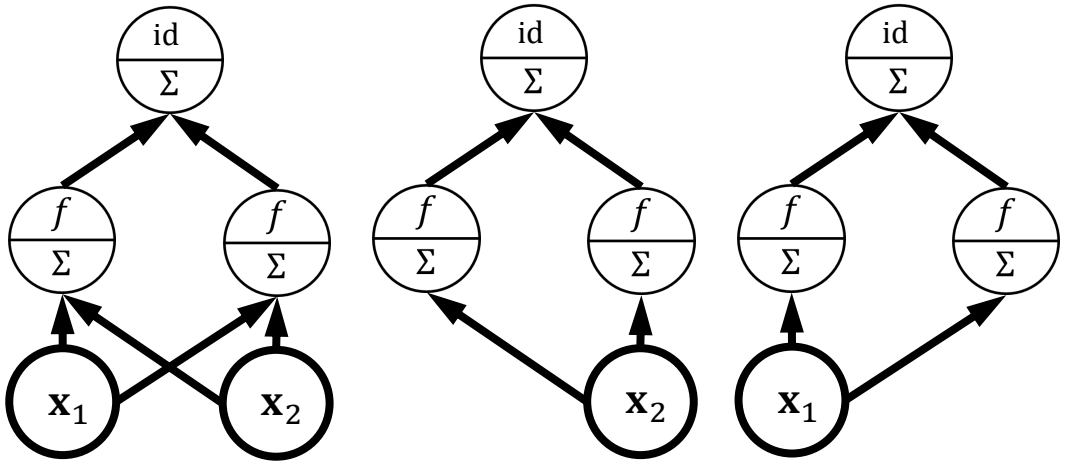

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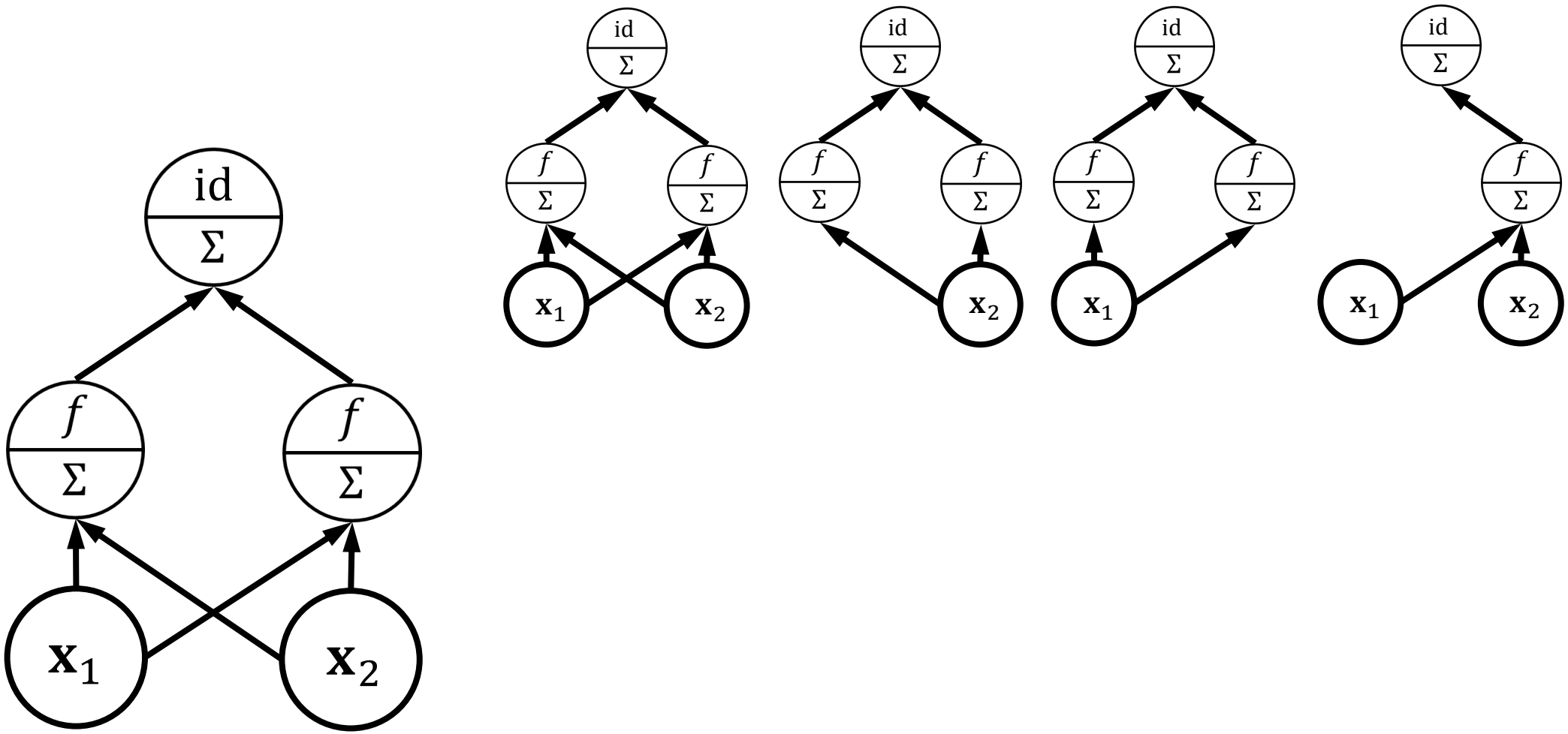

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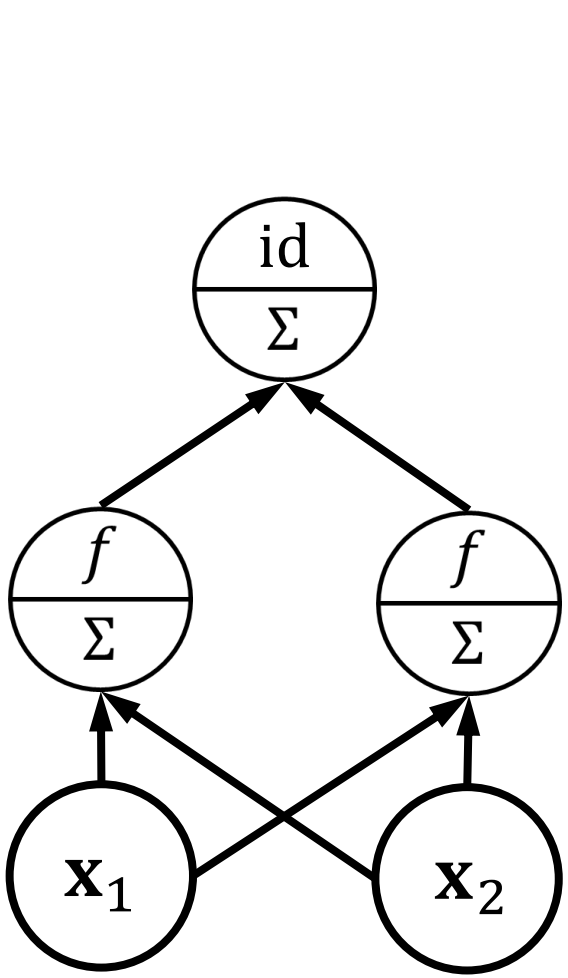

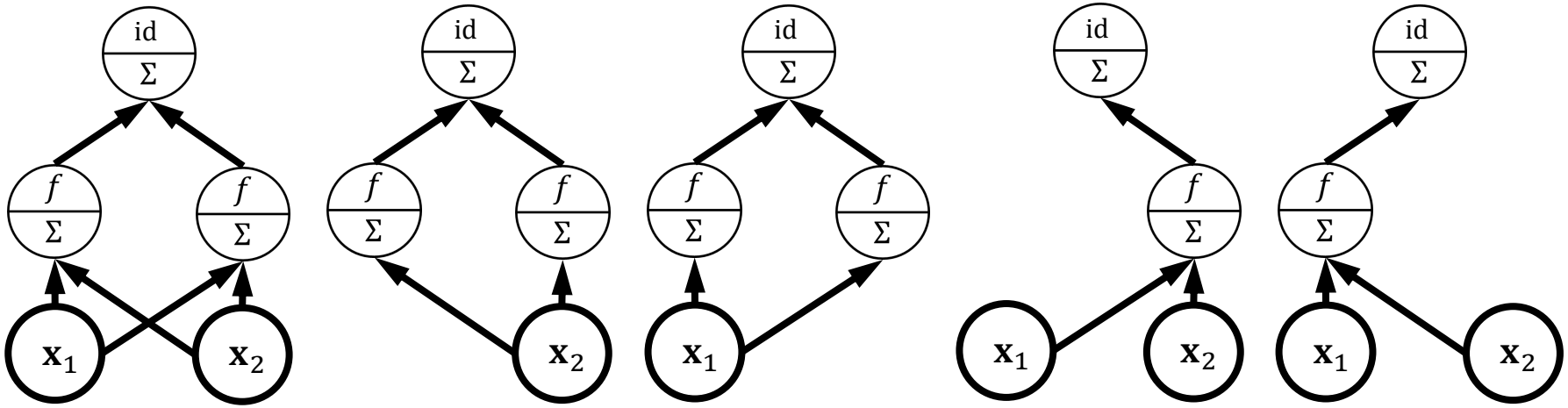

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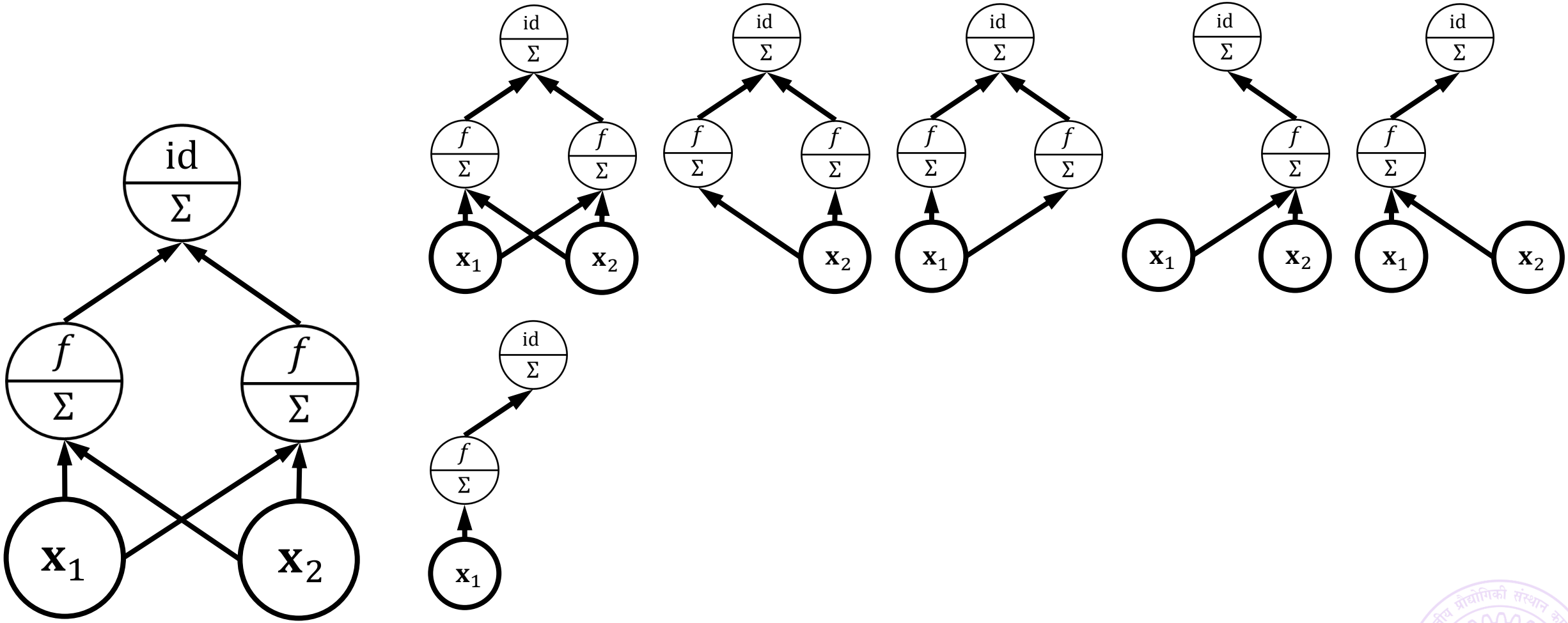

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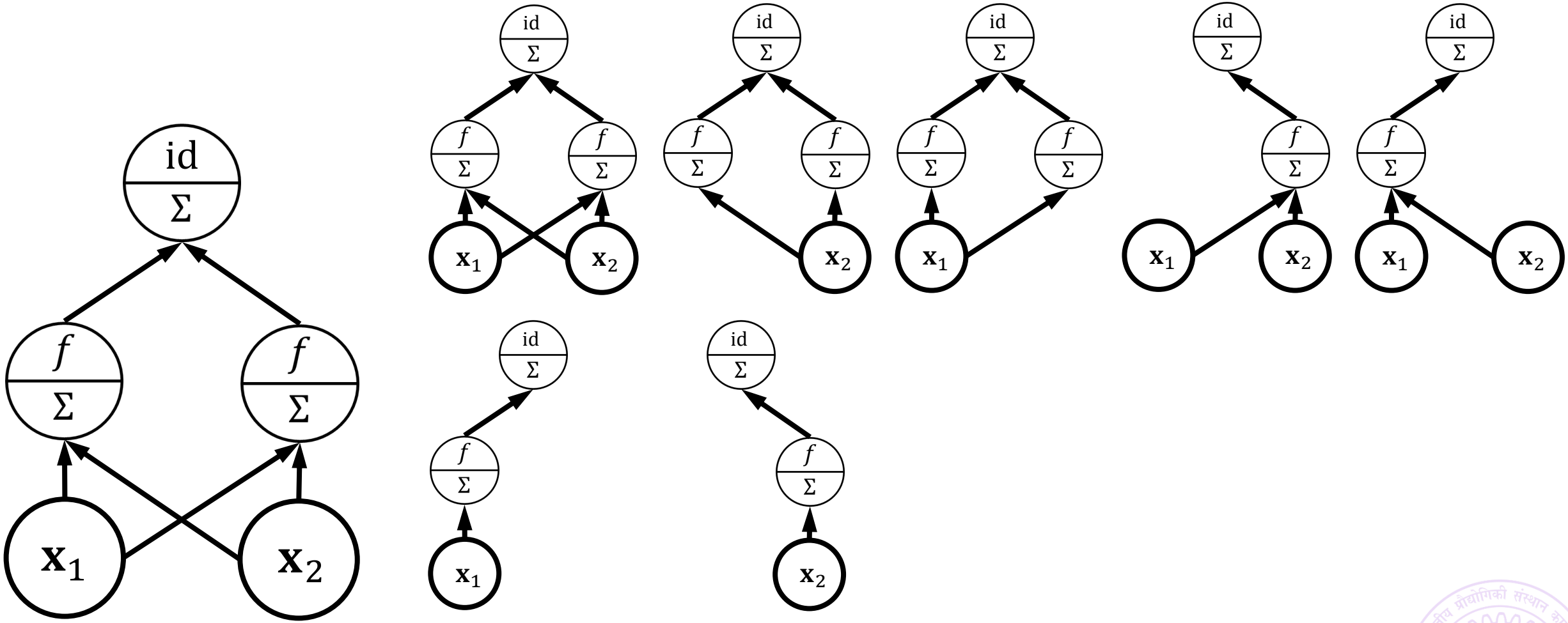

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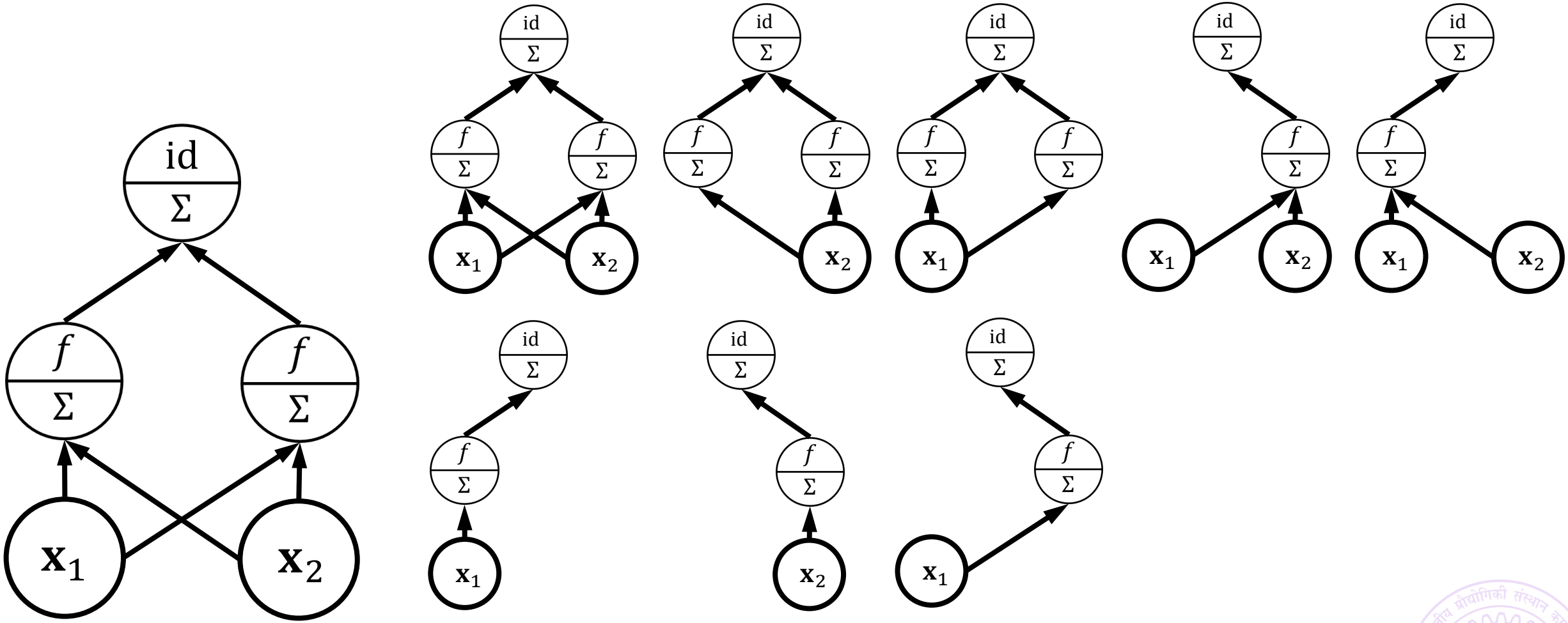

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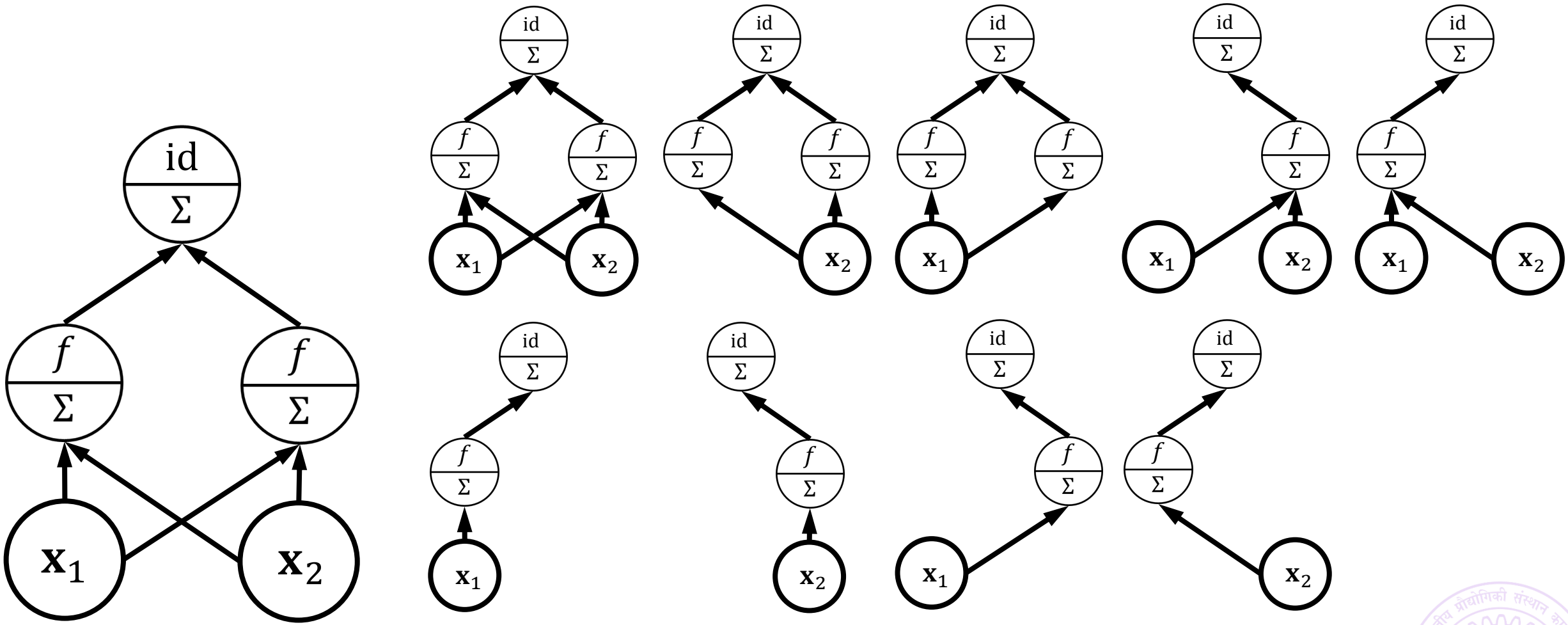

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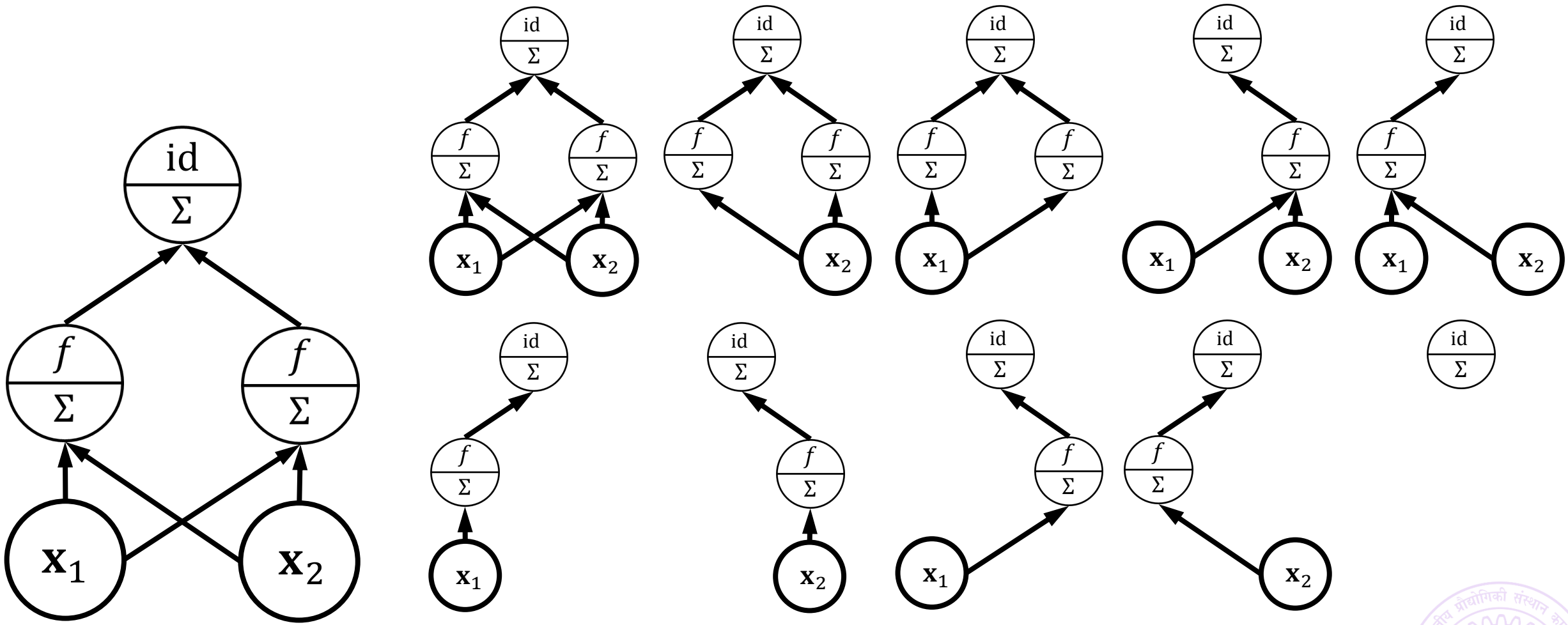

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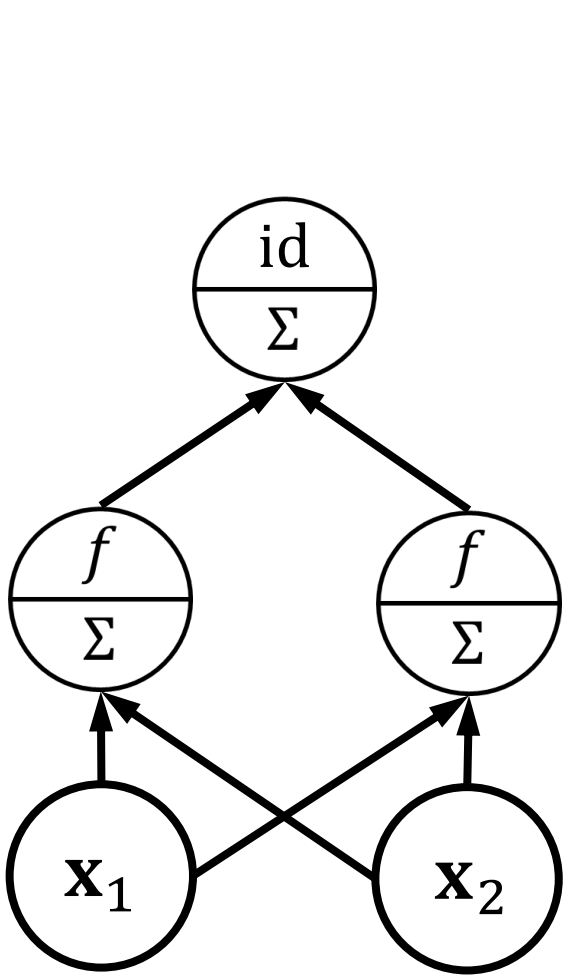

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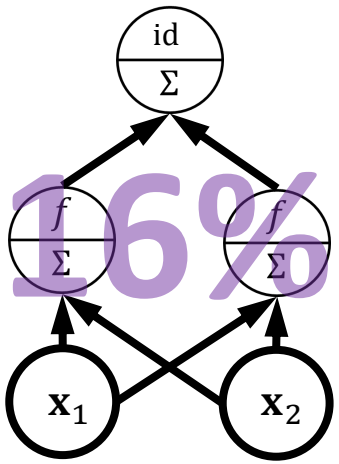

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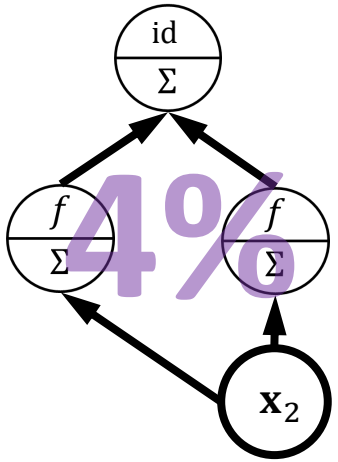

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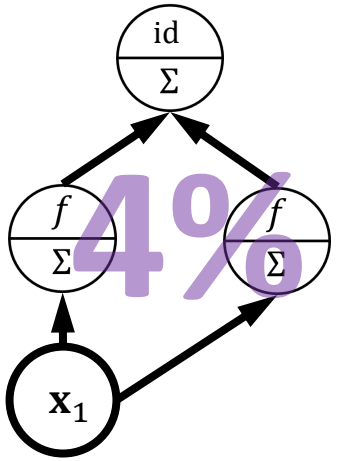

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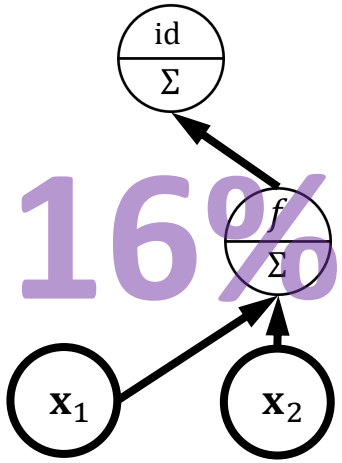

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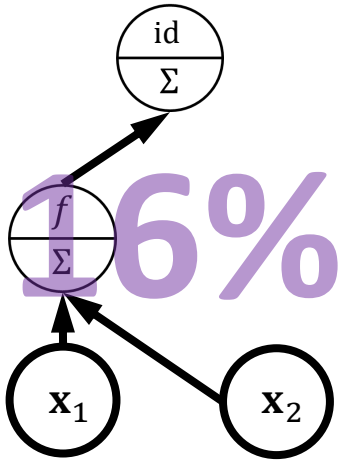

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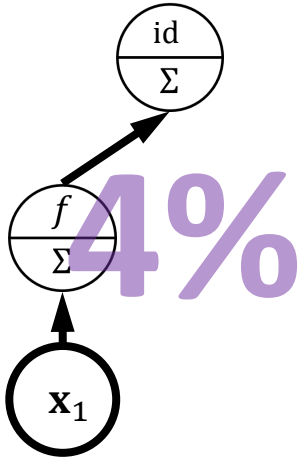

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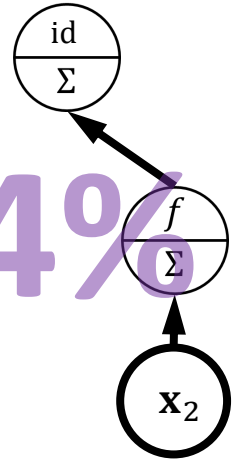

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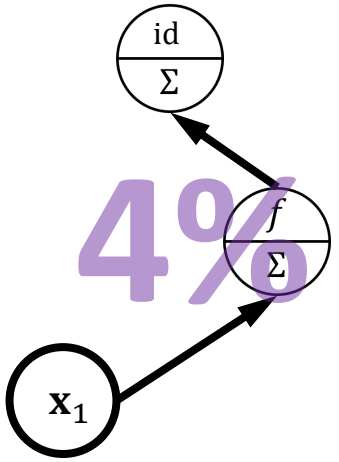

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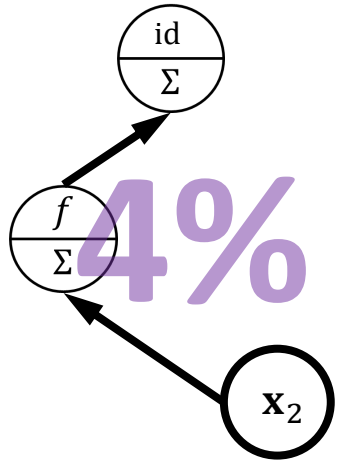

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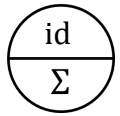

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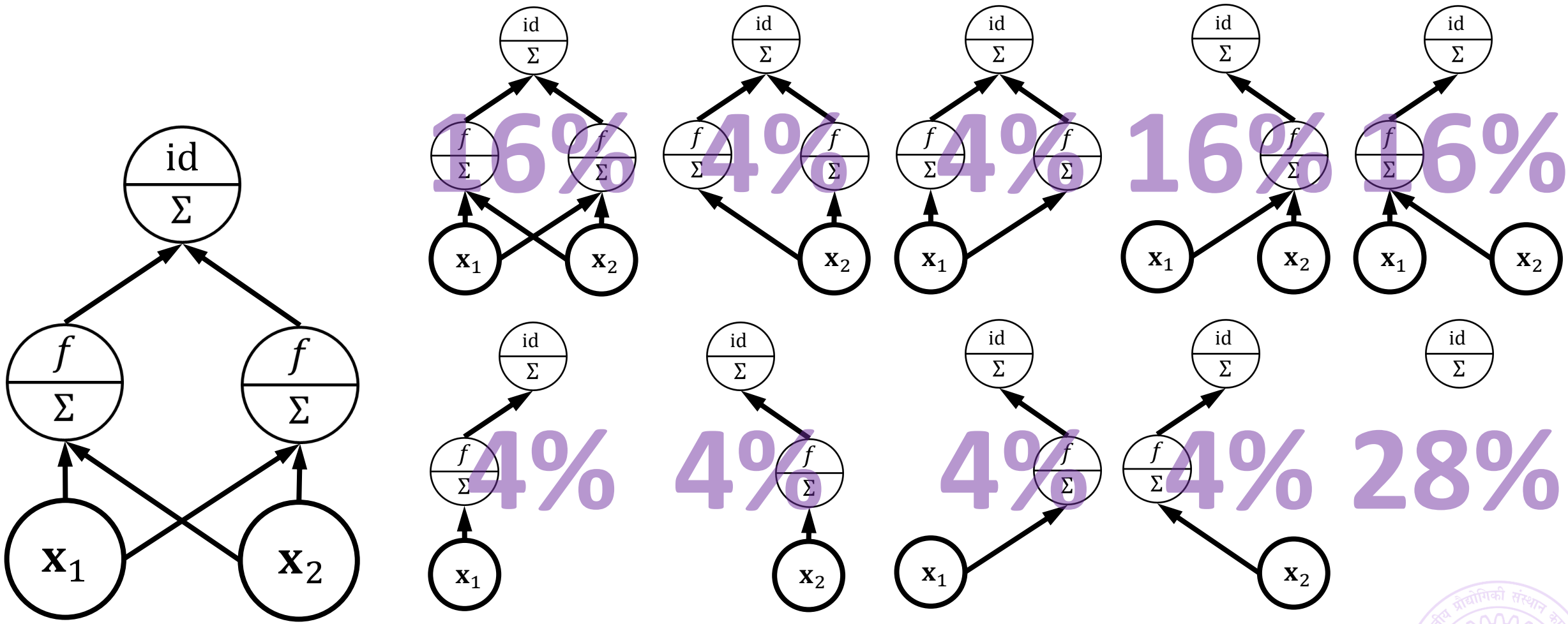


28% networks have no input nodes or no path connecting at least one input node to the output node (cannot apply GD to them)

Dropout at Test time

- Can do dropout at test time too
- What is desirable is to achieve the average effect of all the sparse subnetworks in the previous slide
- The above becomes intractable (kind of like Bayesian inference)
- Approximations used
  - Sample several networks using same sampling techniques, predict using each and take the average prediction
  - Simply scale the output of each node in the NN with the probability it would have been missing
  - See Deep Learning book [**GBC**] for a more detailed discussion

Data Modelling with NNs

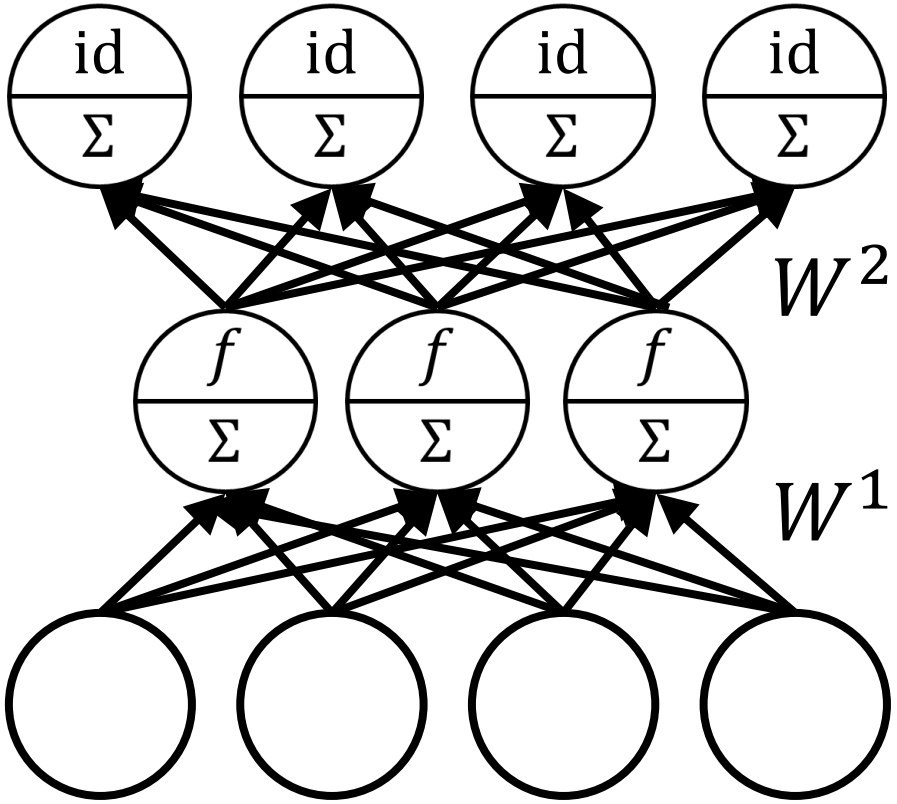
Networks that model/generate data

- Note: feedforward networks are discriminative
- Generative networks exist too!
- Too vast an area to do justice in one-and-a-half lectures
- Several flavours exist
  - Autoencoders (akin to PCA/PPCA)
  - Boltzmann machines (restricted/convolutional/fully-connected)
  - Deep belief networks
- Will just look at autoencoders briefly since they mimic PCA
- [**GBC**] contains a detailed description of other architectures

Autoencoders

- Recall that in PCA, a latent variable $\mathbf{z}$ generated the data as
$$\mathbf{x} = W\mathbf{z} + \boldsymbol{\epsilon}$$
- Also recall that if we could find W, then we had $\mathbf{z} = W^{\top}\mathbf{x}$
- Thus, we cast the problem as that of regenerating the data
$$\|\mathbf{x} - WW^{\top}\mathbf{x}\|_2^2$$
- However, since W is low-rank, we are forced to regenerate the data using a low-rank representation
- Autoencoders do pretty much the same
- An encoder converts data to a hidden representation $\mathbf{h} = e(\mathbf{x})$
- A decoder produces a reconstruction $\mathbf{r} = d(\mathbf{h})$
- Want to minimize loss $\ell(d(\mathbf{h}), \mathbf{x}) = \ell\big(d\big(e(\mathbf{x})\big), \mathbf{x}\big)$

Deep Autoencoders



- Encoder is $e(\mathbf{x}) = f\left((W^1)^\top \mathbf{x}\right)$
- Decoder is $d(\mathbf{h}) = (W^2)^\top \mathbf{h}$
- Reconstruction is $(W^2)^\top f\left((W^1)^\top \mathbf{x}\right)$
- Training done using

$$\ell\left((W^2)^\top f\left((W^1)^\top \mathbf{x}\right), \mathbf{x}\right)$$

- For example

$$\left\|(W^2)^\top f\left((W^1)^\top \mathbf{x}\right) - \mathbf{x}\right\|_2^2$$

- Undercomplete AE: # hidden nodes less than # input nodes
- Prevents encoded and decoder from being trivial indentity function

Autoencoder Variants

- Often some noise is added to input $\mathbf{x}$ to avoid overfitting,

$$\ell\big(d\big(e(\mathbf{x}+\boldsymbol{\epsilon})\big),\mathbf{x}\big)$$

  Denoising autoencoder!
- Note: PCA is an autoencoder too … just a linear one
- Also, it fixes $W^2 = W^1 = W$
- Interestingly, this was done in the past for autoencoders too
- Pretraining phase – train with constraint $W^2 = W^1$
- Fine-tuning phase – train allowing the two to differ
- However, these days it is common to learn W^1, W^2 separately from scratch. No pretraining and fine-tuning phases

Autoencoder Variants

- Can have overcomplete autoencoders as well – need to be careful
- Sparse autoencoders – force lots of edge weights to be zero
- Can have several hidden layers – learn compressed representations in several stages
- Possible to take 780-dimensional MNIST dataset and reduce to 7-dimensional representation without loss of too much information
- SVMs applied to 7-dimensional version do almost as well as SVMs applied to 780-dimensional version [LeCun]
- Such a drastic reduction not possible in practice in one shot
- AE needs several layers to gradually reduce dimensionality e.g.

$$780 \rightarrow 500 \rightarrow 100 \rightarrow 50 \rightarrow 7 \rightarrow 50 \rightarrow 100 \rightarrow 500 \rightarrow 780$$

Please give your Feedback

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