CS 349: Artificial Intelligence-II

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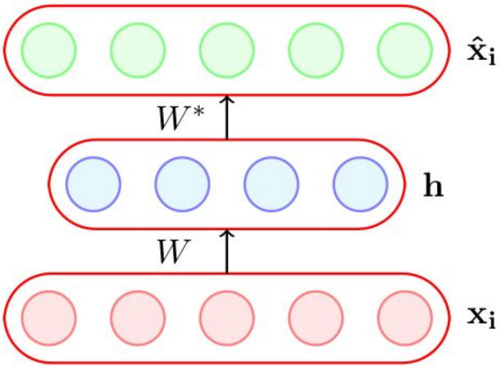
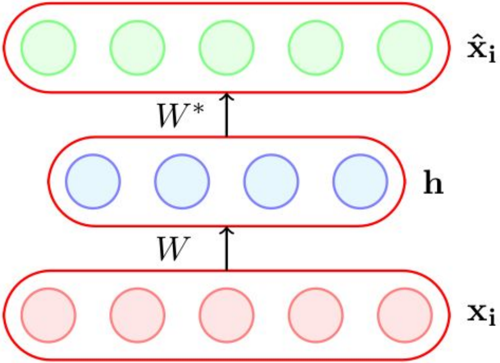
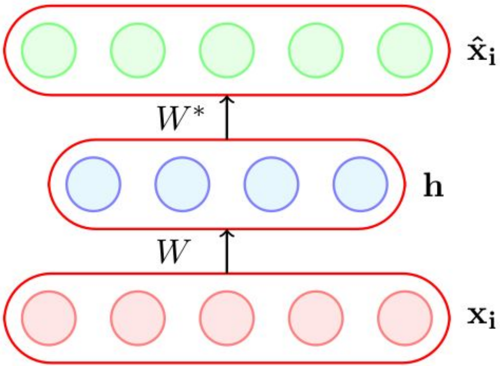
Introduction to Autoencoders



$\hat{\mathbf{x}}_\mathbf{i}$
W^*
$\mathbf{h}$
W
$\mathbf{x}_\mathbf{i}$



- An autoencoder is a special type of feed forward neural network which does the following



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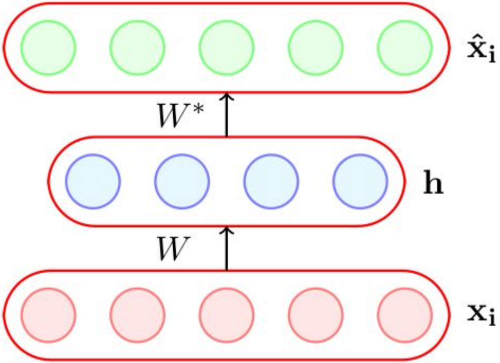
- Encodes its input $\mathbf{x_i}$ into a hidden representation $\mathbf{h}$



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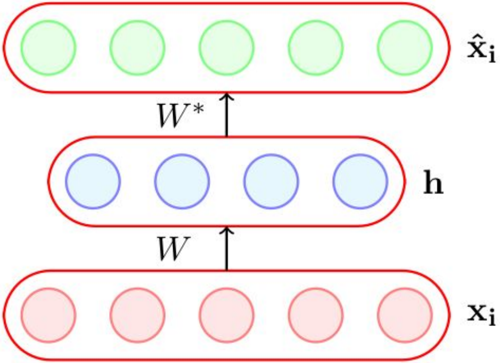

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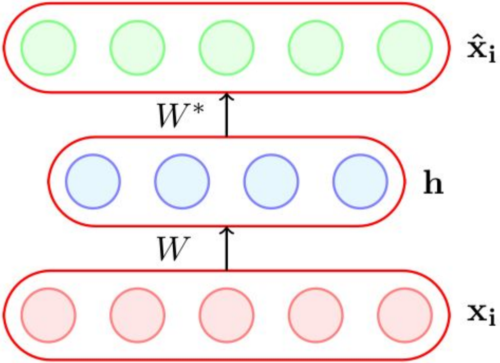
- <u>Encodes</u> its input $\mathbf{x}_\mathbf{i}$ into a hidden representation $\mathbf{h}$
- <u>Decodes</u> the input again from this hidden representation



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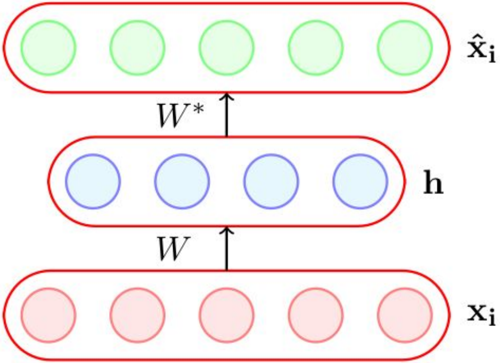

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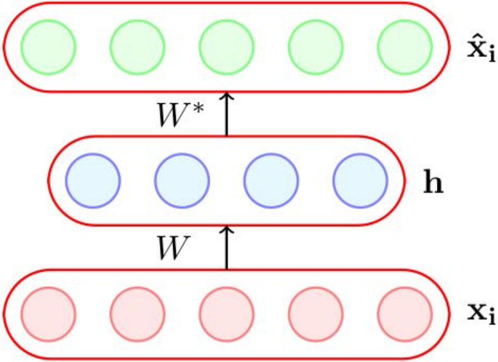
- Encodes its input $\mathbf{x}_\mathbf{i}$ into a hidden representation $\mathbf{h}$
- Decodes the input again from this hidden representation
- The model is trained to minimize a certain loss function which will ensure that $\hat{\mathbf{x}}_\mathbf{i}$ is close to $\mathbf{x}_\mathbf{i}$ (we will see some such loss functions soon)



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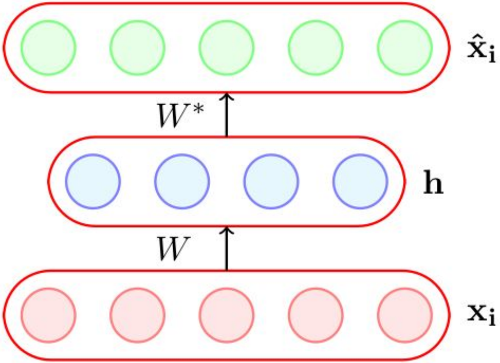

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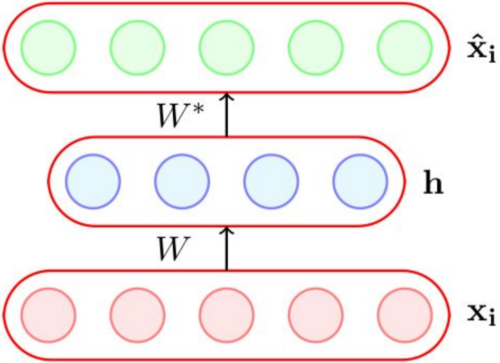
- Let us consider the case where $\dim(\mathbf{h}) < \dim(\mathbf{x_i})$



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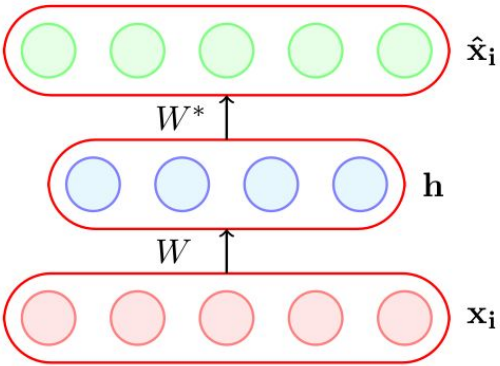

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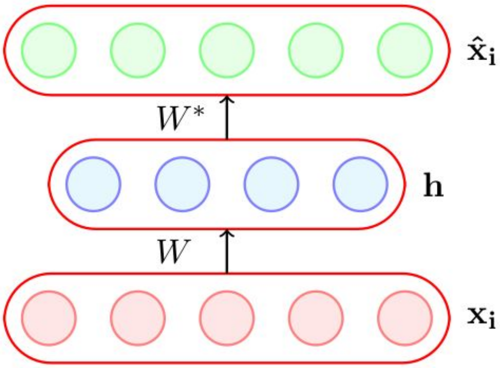

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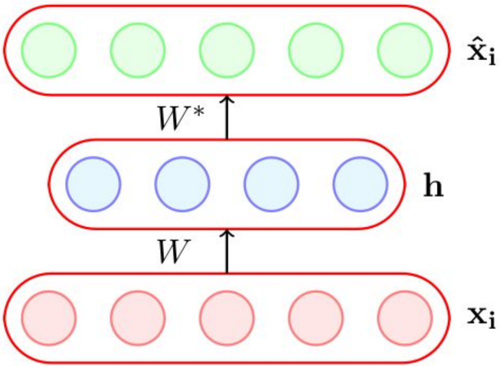
- Do you see an analogy with PCA?



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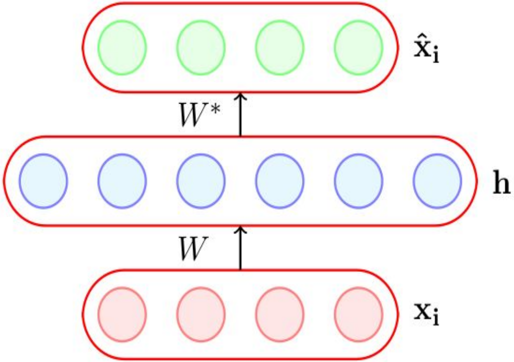
- Let us consider the case where dim(**h**) < dim($\mathbf{x}_\mathbf{i}$)
- If we are still able to reconstruct $\hat{\mathbf{x}}_\mathbf{i}$ perfectly from **h**, then what does it say about **h**?
- **h** is a loss-free encoding of $\mathbf{x}_\mathbf{i}$. It captures all the important characteristics of $\mathbf{x}_\mathbf{i}$

An autoencoder where dim(**h**) < dim($\mathbf{x}_\mathbf{i}$) is called an **under complete** autoencoder



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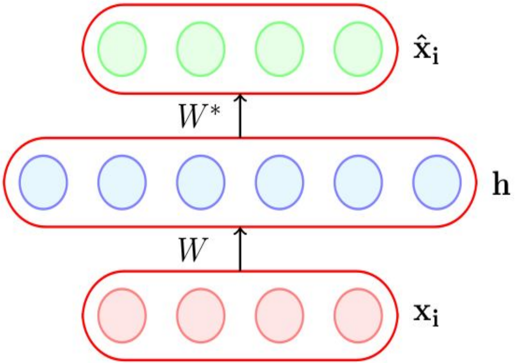

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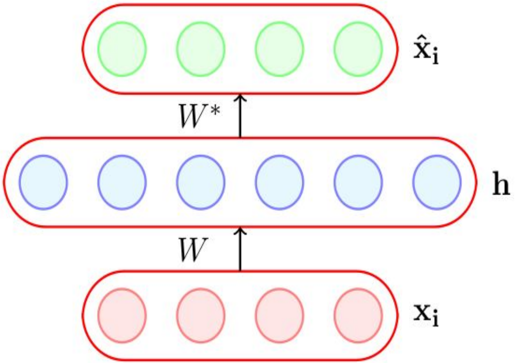

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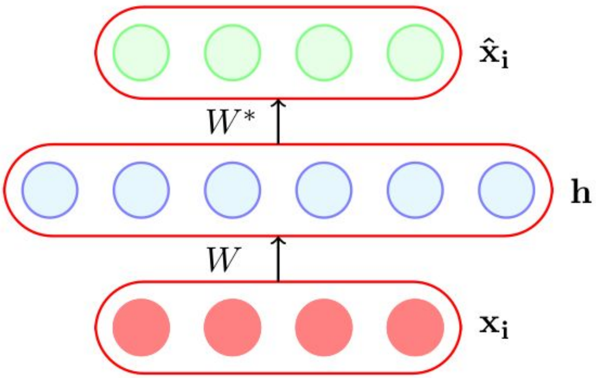

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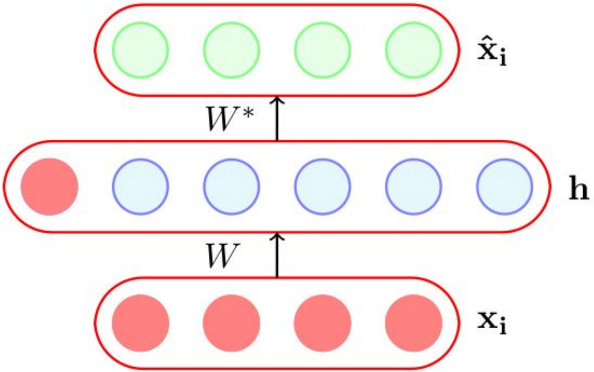

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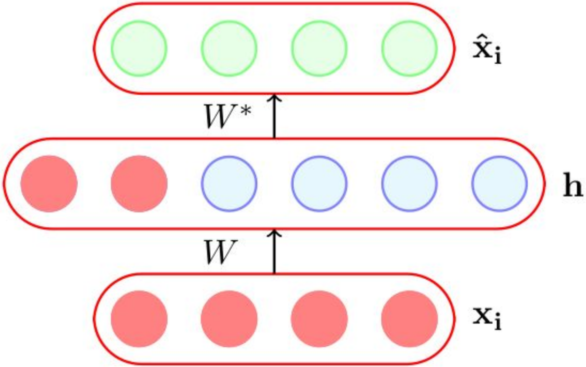

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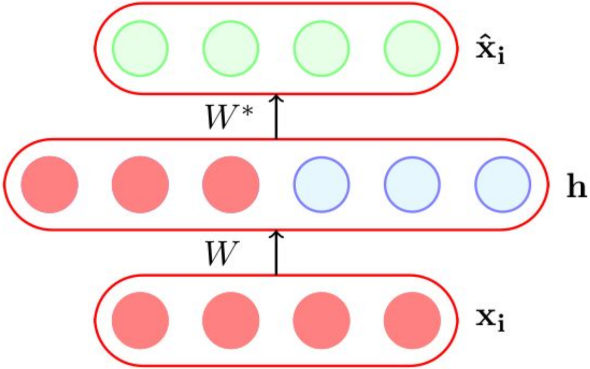

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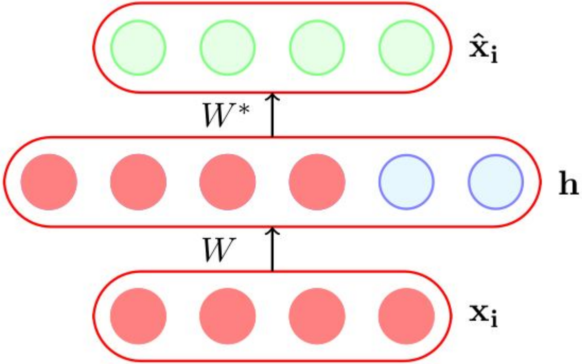

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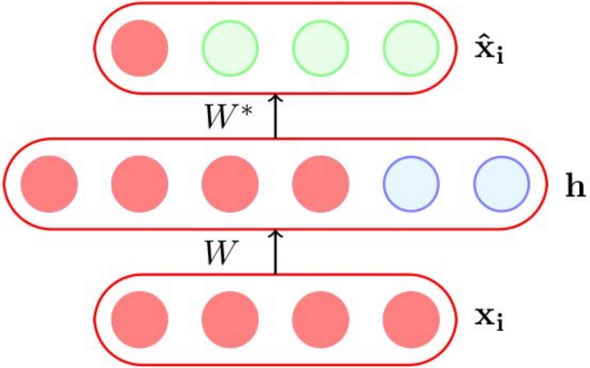

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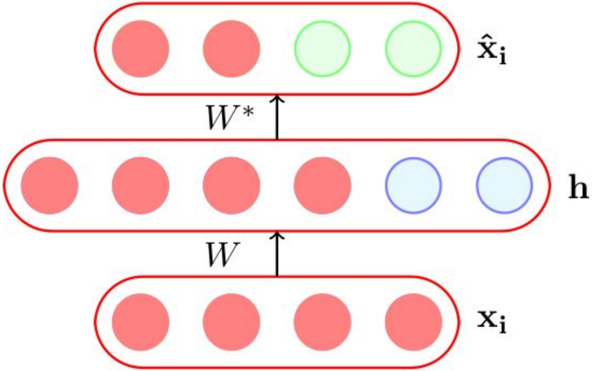

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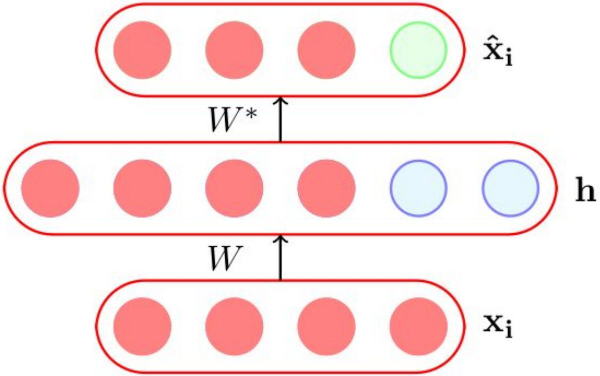

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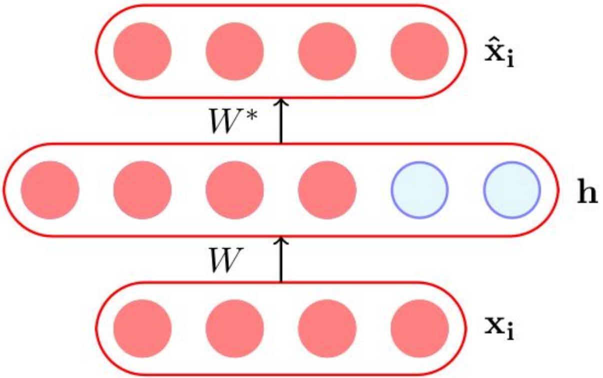

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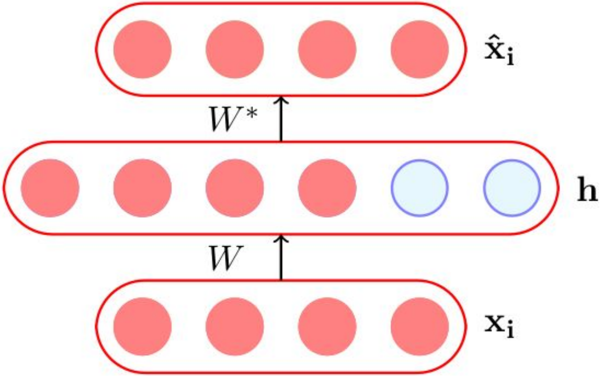

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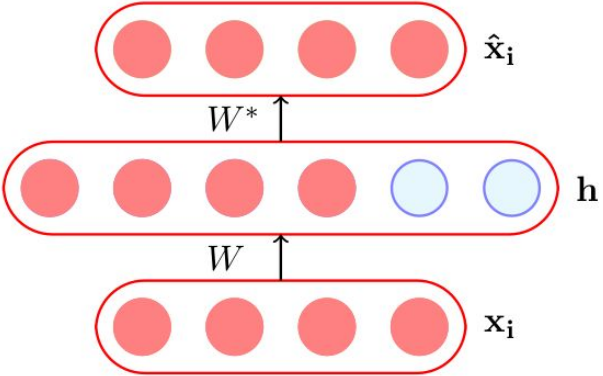
- In such a case the autoencoder could learn a trivial encoding by simply copying $\mathbf{x}_i$ into $\mathbf{h}$ and then copying $\mathbf{h}$ into $\hat{\mathbf{x}}_i$
- Such an identity encoding is useless in practice as it does not really tell us anything about the important characteristics of the data.



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An autoencoder where $\dim(\mathbf{h}) \geq \dim(\mathbf{x}_i)$ is called an **over-complete** autoencoder

The Road Ahead

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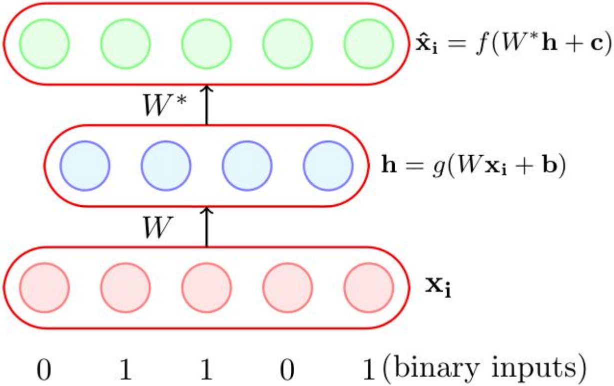
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W^*
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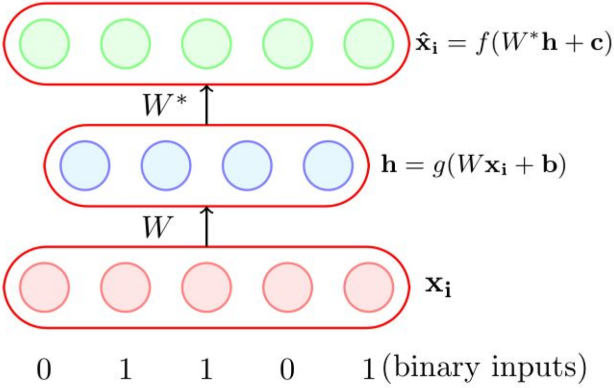
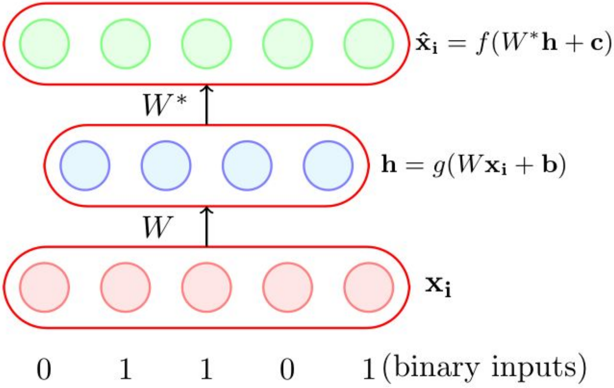
W
$\mathbf{x}_\mathbf{i}$
0 1 1 0 1 (binary inputs)



- Suppose all our inputs are binary (each $x_{ij} \in \{0, 1\}$)



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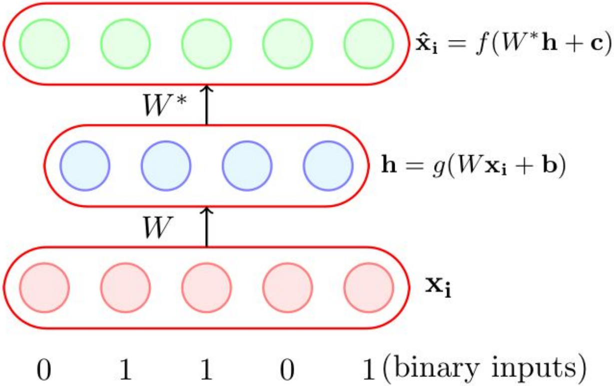
- Which of the following functions would be most apt for the decoder?



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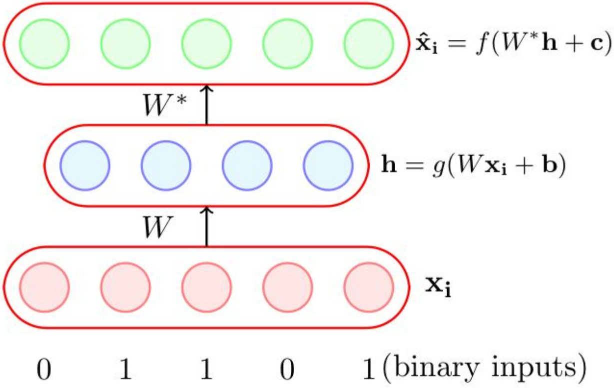

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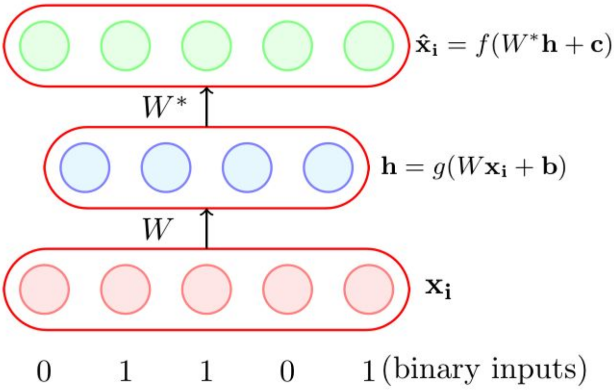

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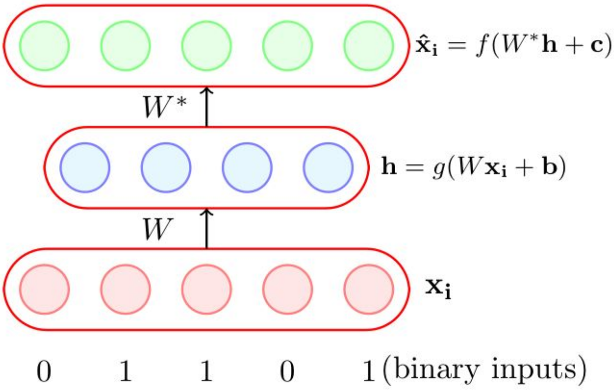

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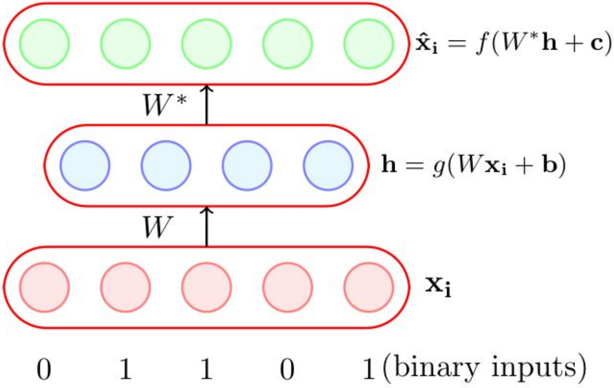
- Logistic as it naturally restricts all outputs to be between 0 and 1



g is typically chosen as the sigmoid function

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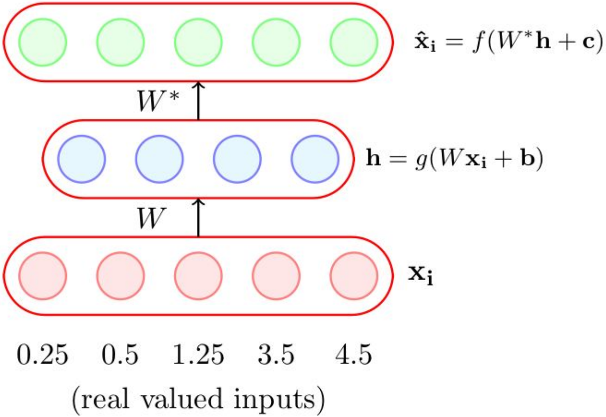
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W^*
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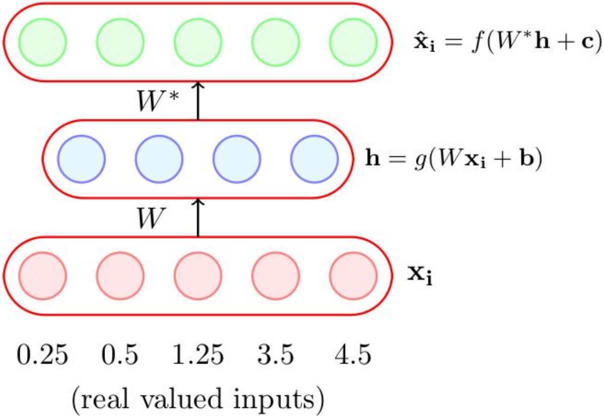
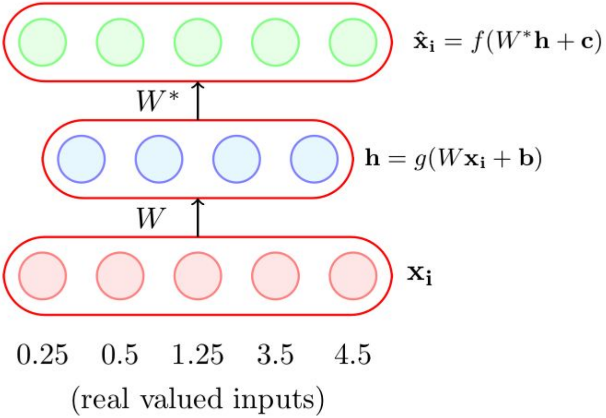
W
$\mathbf{x}_{\mathbf{i}}$
0.25 0.5 1.25 3.5 4.5
(real valued inputs)



- Suppose all our inputs are real (each $x_{ij} \in \mathbb{R}$)



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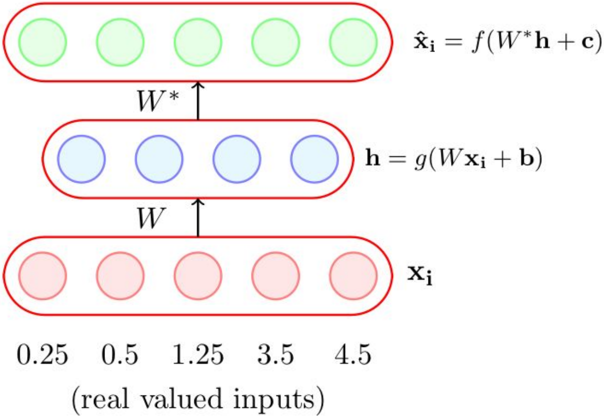

- Suppose all our inputs are real (each $x_{ij} \in \mathbb{R}$)
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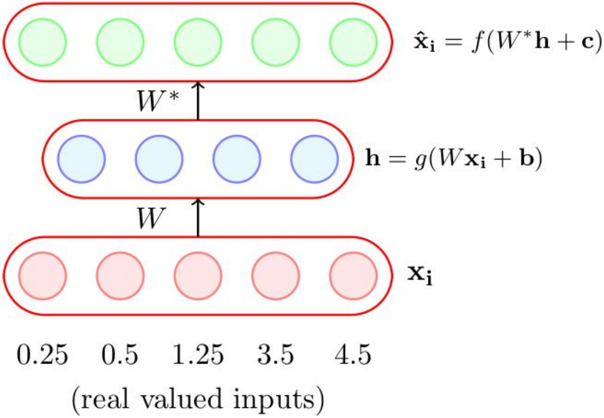

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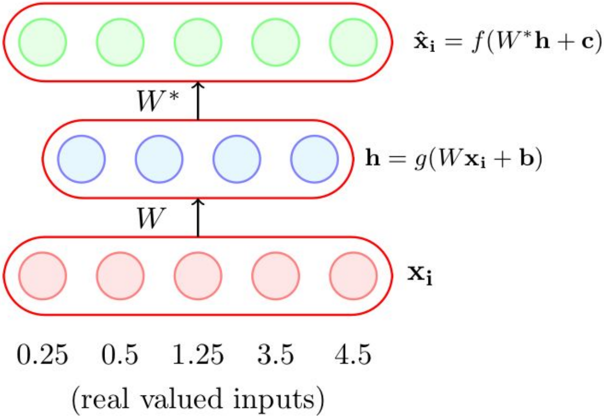

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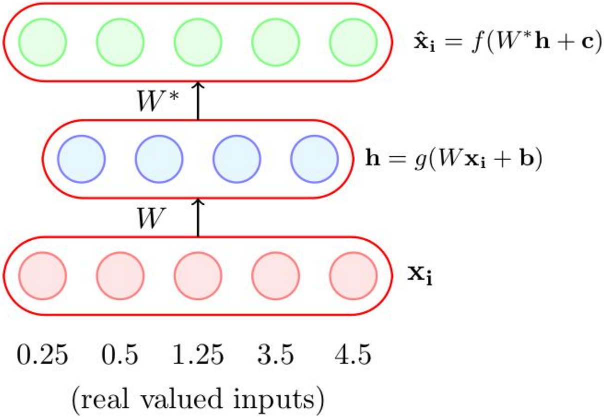

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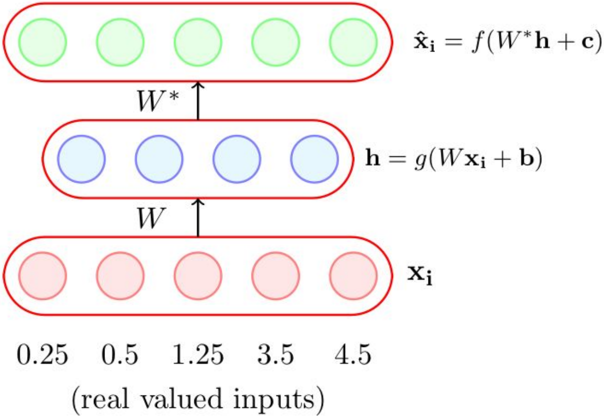
- What will logistic and tanh do?



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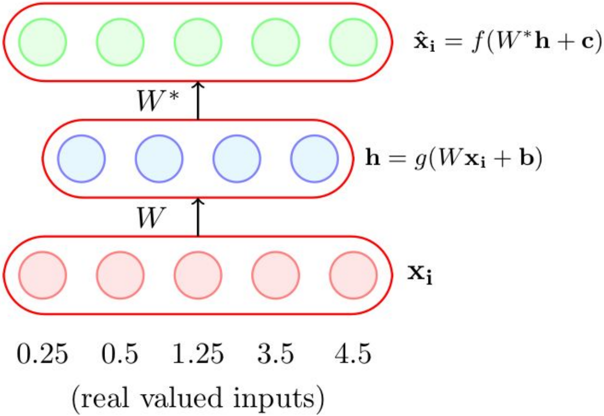
- What will logistic and tanh do?
- They will restrict the reconstructed $\hat{\mathbf{x}}_\mathbf{i}$ to lie between [0,1] or [-1,1] whereas we want $\hat{\mathbf{x}}_\mathbf{i} \in \mathbb{R}^n$



Again, g is typically chosen as the sigmoid function

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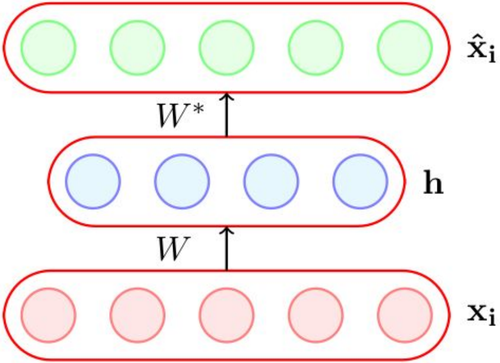
The Road Ahead

- Choice of $f(\mathbf{x_i})$ and $g(\mathbf{x_i})$
- Choice of loss function



$$\mathbf{h} = g(W\mathbf{x}_\mathbf{i} + \mathbf{b})$$

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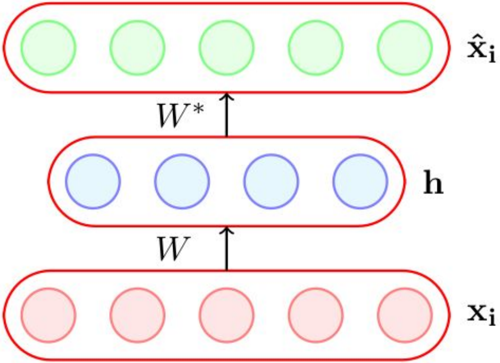

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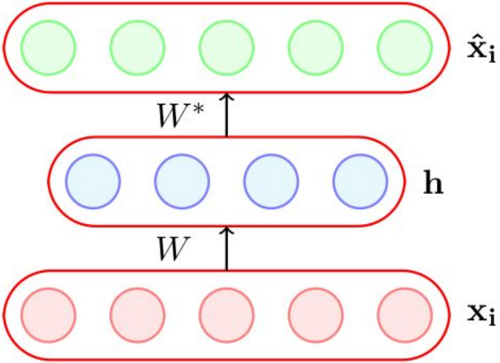
- Consider the case when the inputs are real valued



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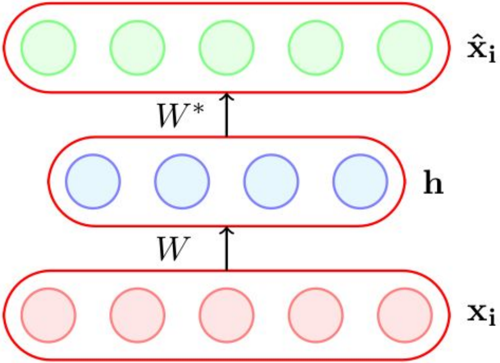
- Consider the case when the inputs are real valued
- The objective of the autoencoder is to reconstruct $\hat{\mathbf{x}}_\mathbf{i}$ to be as close to $\mathbf{x}_\mathbf{i}$ as possible



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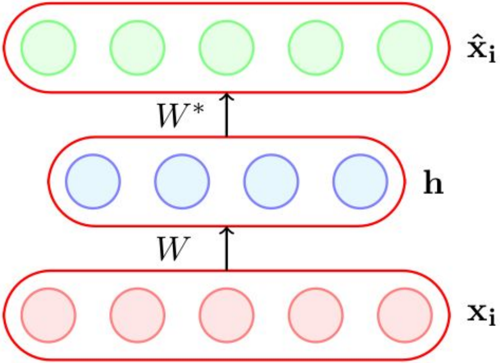
- The objective of the autoencoder is to reconstruct $\hat{\mathbf{x}}_\mathbf{i}$ to be as close to $\mathbf{x}_\mathbf{i}$ as possible
- This can be formalized using the following objective function:

$$\min_{W, W^*, \mathbf{c}, \mathbf{b}} \frac{1}{m} \sum_{i=1}^{m} \sum_{j=1}^{n} (\hat{x}_{ij} - x_{ij})^2$$



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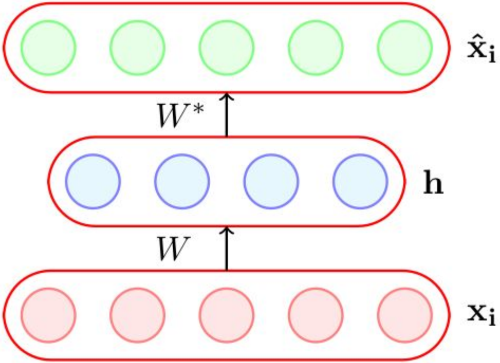

$$\mathbf{h} = g(W\mathbf{x_i} + \mathbf{b})$$
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- *there are m instances*
- *each $\boldsymbol{x}_{\boldsymbol{i}}$ is n-dimensional*

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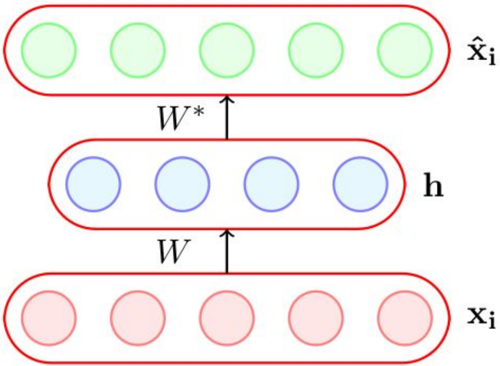
- We can then train the autoencoder just like a regular feedforward network using backpropagation



$$\mathbf{h} = g(W\mathbf{x_i} + \mathbf{b})$$
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- All we need is a formula for $\frac{\partial \mathscr{L}(\theta)}{\partial W^*}$ and $\frac{\partial \mathscr{L}(\theta)}{\partial W}$

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- The objective of the autoencoder is to reconstruct $\hat{\mathbf{x}}_\mathbf{i}$ to be as close to $\mathbf{x_i}$ as possible
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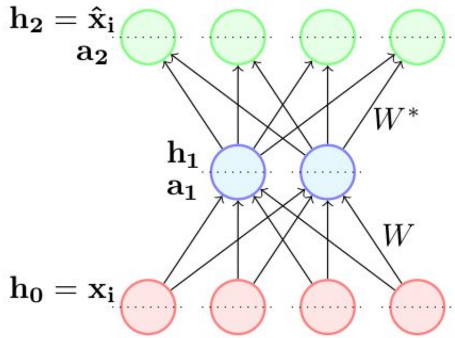
$$\mathscr{L}(\theta) = (\mathbf{\hat{x}_i} - \mathbf{x_i})^T(\mathbf{\hat{x}_i} - \mathbf{x_i})$$



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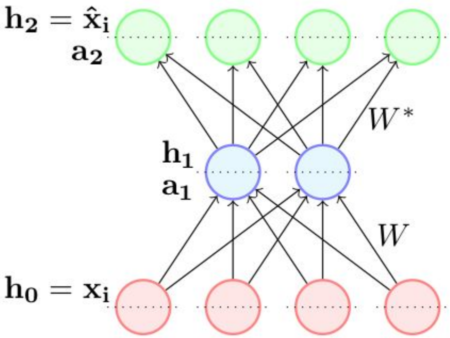

- Note that the loss function is shown for only one training example.

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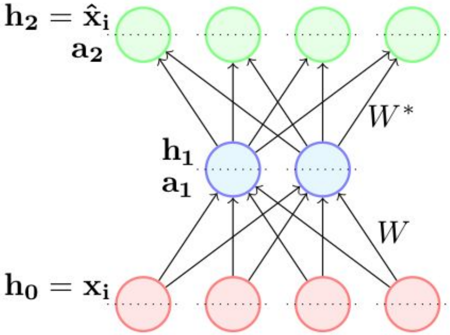

- $$\frac{\partial \mathscr{L}(\theta)}{\partial W^*} = \frac{\partial \mathscr{L}(\theta)}{\partial \mathbf{h_2}} \boxed{\frac{\partial \mathbf{h_2}}{\partial \mathbf{a_2}} \frac{\partial \mathbf{a_2}}{\partial W^*}}$$

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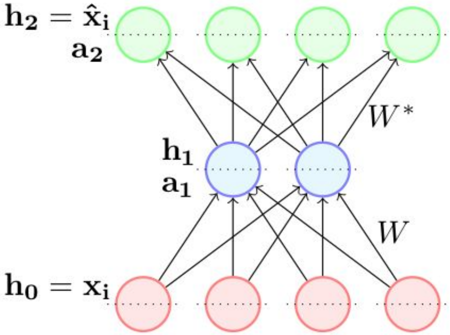

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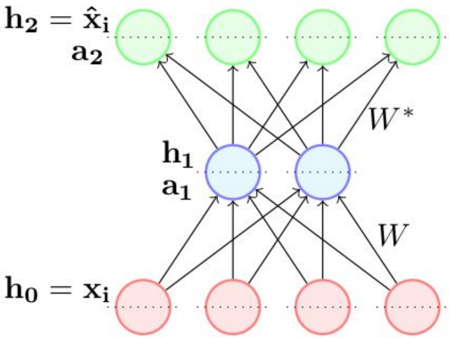

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- expression in the boxes can be calculated using backpropagation

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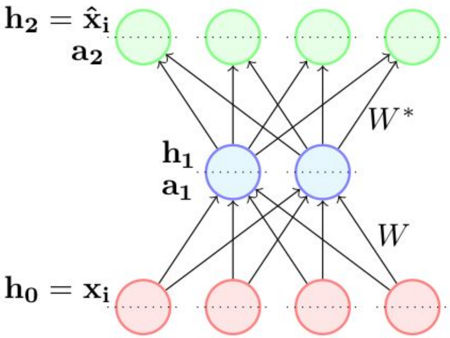
$$\mathscr{L}(\theta) = (\hat{\mathbf{x}}_\mathbf{i} - \mathbf{x}_\mathbf{i})^T(\hat{\mathbf{x}}_\mathbf{i} - \mathbf{x}_\mathbf{i})$$



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- Expression in the boxes are calculated through backpropagation

$$\frac{\partial \mathscr{L}(\theta)}{\partial \mathbf{h_2}} = \frac{\partial \mathscr{L}(\theta)}{\partial \hat{\mathbf{x}}_\mathbf{i}}$$

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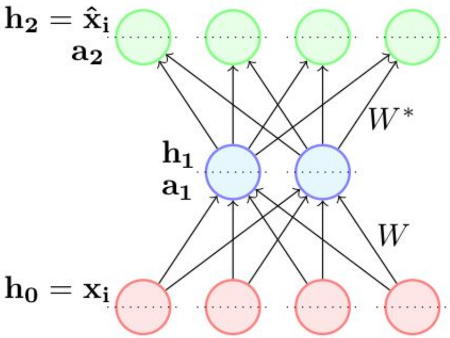

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- We have already seen how to calculate the expression in the boxes when we learnt backpropagation

$$\frac{\partial \mathscr{L}(\theta)}{\partial \mathbf{h_2}} = \frac{\partial \mathscr{L}(\theta)}{\partial \hat{\mathbf{x}}_\mathbf{i}}$$
$$= \nabla_{\hat{\mathbf{x}}_\mathbf{i}} \{(\hat{\mathbf{x}}_\mathbf{i} - \mathbf{x}_\mathbf{i})^T(\hat{\mathbf{x}}_\mathbf{i} - \mathbf{x}_\mathbf{i})\}$$

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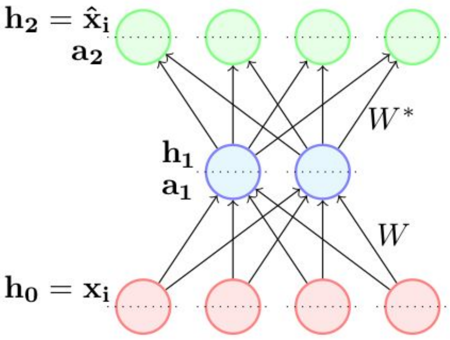
$$\mathscr{L}(\theta) = (\hat{\mathbf{x}}_\mathbf{i} - \mathbf{x}_\mathbf{i})^T(\hat{\mathbf{x}}_\mathbf{i} - \mathbf{x}_\mathbf{i})$$



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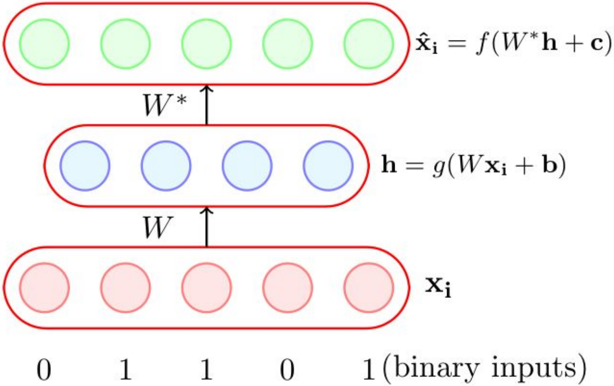
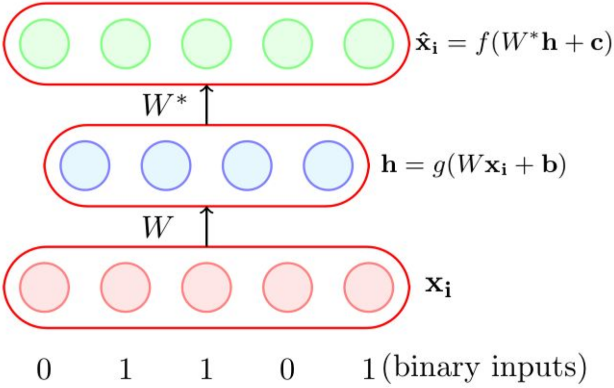
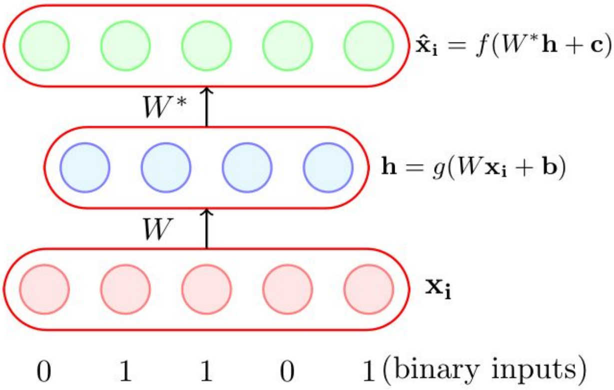
$$\begin{aligned}\frac{\partial \mathscr{L}(\theta)}{\partial \mathbf{h_2}} &= \frac{\partial \mathscr{L}(\theta)}{\partial \hat{\mathbf{x}}_\mathbf{i}} \\ &= \nabla_{\hat{\mathbf{x}}_\mathbf{i}} \{(\hat{\mathbf{x}}_\mathbf{i} - \mathbf{x}_\mathbf{i})^T(\hat{\mathbf{x}}_\mathbf{i} - \mathbf{x}_\mathbf{i})\} \\ &= 2(\hat{\mathbf{x}}_\mathbf{i} - \mathbf{x}_\mathbf{i})\end{aligned}$$

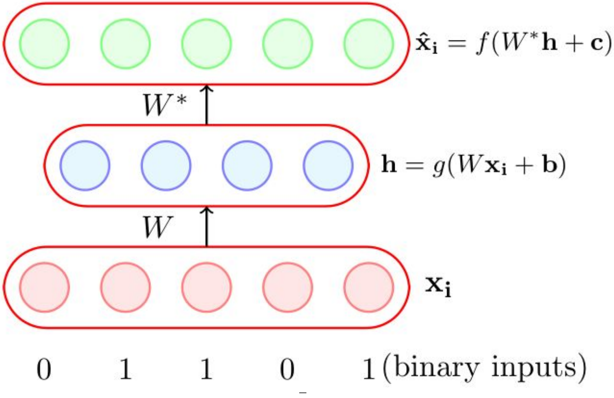

$\hat{\mathbf{x}}_{\mathbf{i}} = f(W^*\mathbf{h} + \mathbf{c})$
W^*
$\mathbf{h} = g(W\mathbf{x}_{\mathbf{i}} + \mathbf{b})$
W
$\mathbf{x}_{\mathbf{i}}$
0 1 1 0 1 (binary inputs)



- Consider the case when the inputs are binary

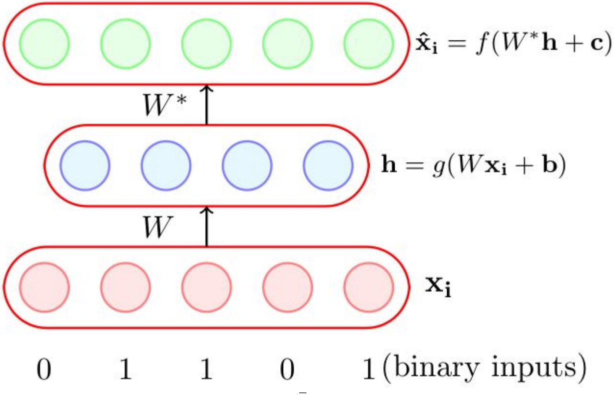


- Consider the case when the inputs are binary
- We use a sigmoid decoder which will produce outputs between 0 and 1, and can be interpreted as probabilities.



- Consider the case when the inputs are binary
- We use a sigmoid decoder which will produce outputs between 0 and 1, and can be interpreted as probabilities.
- For a single n-dimensional i^th input we can use the following loss function

$$\min\{-\sum_{j=1}^{n}(x_{ij}\log\hat{x}_{ij} + (1 - x_{ij})\log(1 - \hat{x}_{ij}))\}$$



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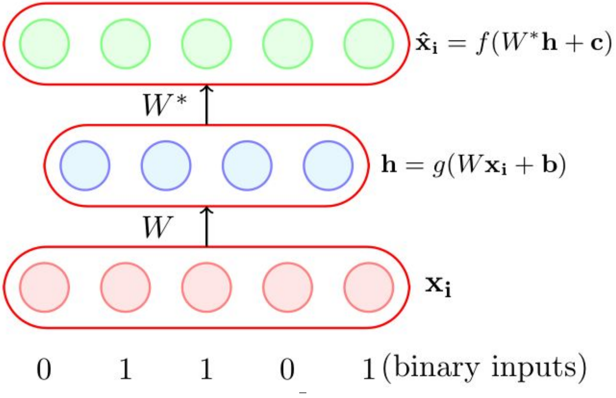
What value of $\hat{\mathbf{x}}_{\mathbf{i}}$ will minimize this function?



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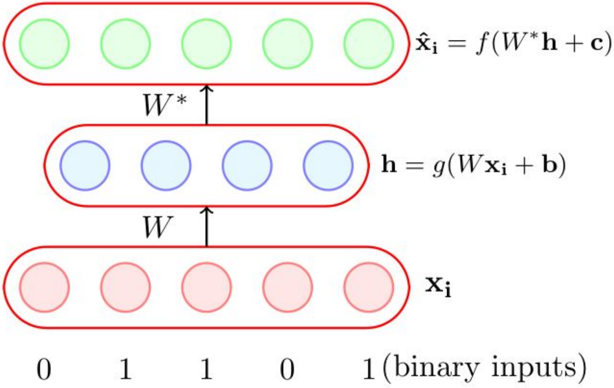
What value of $\hat{\mathbf{x}}_\mathbf{i}$ will minimize this function?

- If $x_{ij} = 1$?



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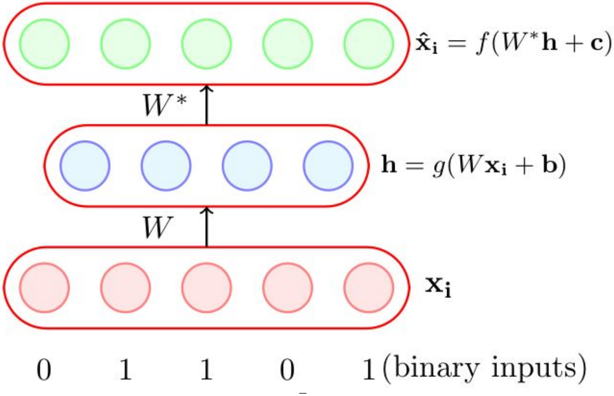
What value of $\hat{\mathbf{x}}_\mathbf{i}$ will minimize this function?

- If $x_{ij} = 1$?
- If $x_{ij} = 0$?



What value of $\hat{\mathbf{x}}_\mathbf{i}$ will minimize this function?

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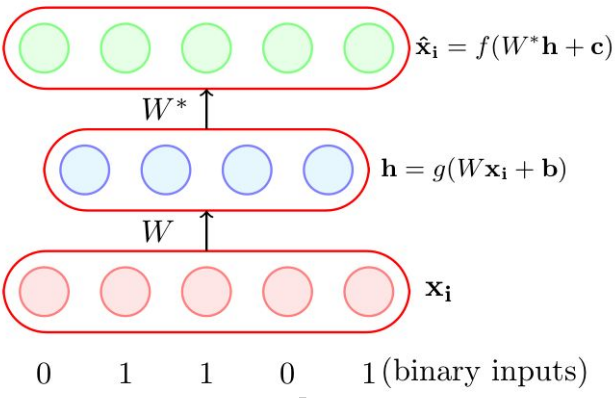
- Again we need formula for $\frac{\partial \mathscr{L}(\theta)}{\partial W^*}$ and $\frac{\partial \mathscr{L}(\theta)}{\partial W}$ to use back propagation



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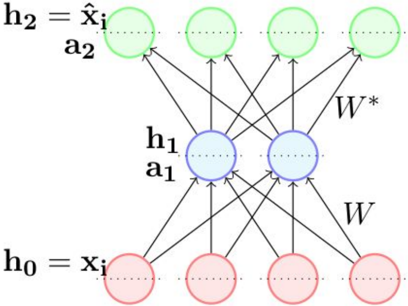
- Again we need formula for $\frac{\partial\mathscr{L}(\theta)}{\partial W^*}$ and $\frac{\partial\mathscr{L}(\theta)}{\partial W}$ to use back propagation

What value of $\hat{\mathbf{x}}_\mathbf{i}$ will minimize this function?

- If $x_{ij} = 1$?
- If $x_{ij} = 0$?

Indeed the above function will be minimized when $\hat{\mathbf{x}}_\mathbf{i} = x_{ij}$!

$$\mathscr{L}(\theta) = -\sum_{j=1}^{n} (x_{ij} \log \hat{x}_{ij} + (1 - x_{ij}) \log(1 - \hat{x}_{ij}))$$



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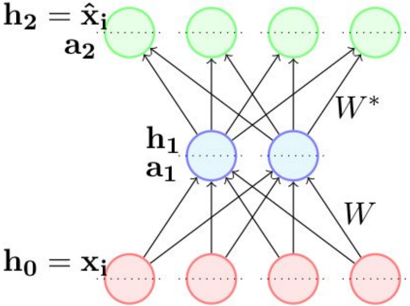
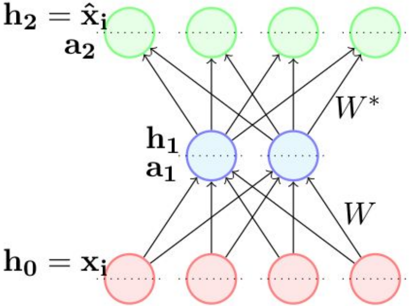


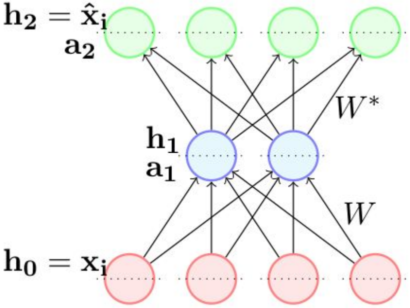
- $$\frac{\partial \mathscr{L}(\theta)}{\partial W^*} = \frac{\partial \mathscr{L}(\theta)}{\partial \mathbf{h_2}} \frac{\partial \mathbf{h_2}}{\partial \mathbf{a_2}} \boxed{\frac{\partial \mathbf{a_2}}{\partial W^*}}$$

$$\mathscr{L}(\theta) = -\sum_{j=1}^{n}(x_{ij}\log\hat{x}_{ij} + (1-x_{ij})\log(1-\hat{x}_{ij}))$$



- $$\frac{\partial \mathscr{L}(\theta)}{\partial W^*} = \frac{\partial \mathscr{L}(\theta)}{\partial \mathbf{h_2}}\frac{\partial \mathbf{h_2}}{\partial \mathbf{a_2}}\boxed{\frac{\partial \mathbf{a_2}}{\partial W^*}}$$
- $$\frac{\partial \mathscr{L}(\theta)}{\partial W} = \frac{\partial \mathscr{L}(\theta)}{\partial \mathbf{h_2}}\frac{\partial \mathbf{h_2}}{\partial \mathbf{a_2}}\boxed{\frac{\partial \mathbf{a_2}}{\partial \mathbf{h_1}}\frac{\partial \mathbf{h_1}}{\partial \mathbf{a_1}}\frac{\partial \mathbf{a_1}}{\partial W}}$$

$$\mathscr{L}(\theta) = -\sum_{j=1}^{n} \left(x_{ij} \log \hat{x}_{ij} + (1 - x_{ij}) \log(1 - \hat{x}_{ij})\right)$$

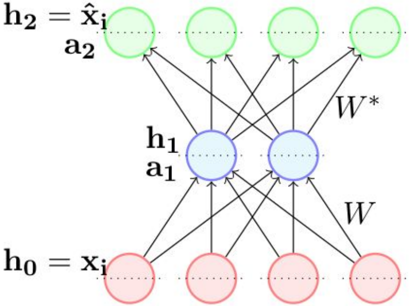


- $$\frac{\partial \mathscr{L}(\theta)}{\partial W^*} = \frac{\partial \mathscr{L}(\theta)}{\partial \mathbf{h_2}} \frac{\partial \mathbf{h_2}}{\partial \mathbf{a_2}} \boxed{\frac{\partial \mathbf{a_2}}{\partial W^*}}$$

- $$\frac{\partial \mathscr{L}(\theta)}{\partial W} = \frac{\partial \mathscr{L}(\theta)}{\partial \mathbf{h_2}} \frac{\partial \mathbf{h_2}}{\partial \mathbf{a_2}} \boxed{\frac{\partial \mathbf{a_2}}{\partial \mathbf{h_1}} \frac{\partial \mathbf{h_1}}{\partial \mathbf{a_1}} \frac{\partial \mathbf{a_1}}{\partial W}}$$

- We have already seen how to calculate the expressions in the square boxes when we learnt BP

$$\mathscr{L}(\theta) = -\sum_{j=1}^{n} (x_{ij} \log \hat{x}_{ij} + (1 - x_{ij}) \log(1 - \hat{x}_{ij}))$$

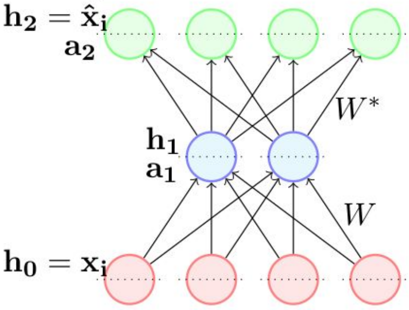


- $$\frac{\partial \mathscr{L}(\theta)}{\partial W^*} = \frac{\partial \mathscr{L}(\theta)}{\partial \mathbf{h_2}} \frac{\partial \mathbf{h_2}}{\partial \mathbf{a_2}} \boxed{\frac{\partial \mathbf{a_2}}{\partial W^*}}$$
- $$\frac{\partial \mathscr{L}(\theta)}{\partial W} = \frac{\partial \mathscr{L}(\theta)}{\partial \mathbf{h_2}} \frac{\partial \mathbf{h_2}}{\partial \mathbf{a_2}} \boxed{\frac{\partial \mathbf{a_2}}{\partial \mathbf{h_1}} \frac{\partial \mathbf{h_1}}{\partial \mathbf{a_1}} \frac{\partial \mathbf{a_1}}{\partial W}}$$
- We have already seen how to calculate the expressions in the square boxes when we learnt BP
- The first two terms on RHS can be computed as:

$$\frac{\partial \mathscr{L}(\theta)}{\partial h_{2j}} = -\frac{x_{ij}}{\hat{x}_{ij}} + \frac{1 - x_{ij}}{1 - \hat{x}_{ij}}$$

$$\frac{\partial h_{2j}}{\partial a_{2j}} = \sigma(a_{2j})(1 - \sigma(a_{2j}))$$

$$\mathscr{L}(\theta) = -\sum_{j=1}^{n}(x_{ij}\log\hat{x}_{ij} + (1-x_{ij})\log(1-\hat{x}_{ij}))$$



$$\frac{\partial\mathscr{L}(\theta)}{\partial\mathbf{h_2}} = \begin{pmatrix} \frac{\partial\mathscr{L}(\theta)}{\partial h_{21}} \\ \frac{\partial\mathscr{L}(\theta)}{\partial h_{22}} \\ \vdots \\ \frac{\partial\mathscr{L}(\theta)}{\partial h_{2n}} \end{pmatrix}$$

- $$\frac{\partial\mathscr{L}(\theta)}{\partial W^*} = \frac{\partial\mathscr{L}(\theta)}{\partial\mathbf{h_2}}\frac{\partial\mathbf{h_2}}{\partial\mathbf{a_2}}\boxed{\frac{\partial\mathbf{a_2}}{\partial W^*}}$$
- $$\frac{\partial\mathscr{L}(\theta)}{\partial W} = \frac{\partial\mathscr{L}(\theta)}{\partial\mathbf{h_2}}\frac{\partial\mathbf{h_2}}{\partial\mathbf{a_2}}\boxed{\frac{\partial\mathbf{a_2}}{\partial\mathbf{h_1}}\frac{\partial\mathbf{h_1}}{\partial\mathbf{a_1}}\frac{\partial\mathbf{a_1}}{\partial W}}$$
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Deep Learning Course, IITM
Deep Learning for NLP, Stanford University

Thank you for Your Attention