

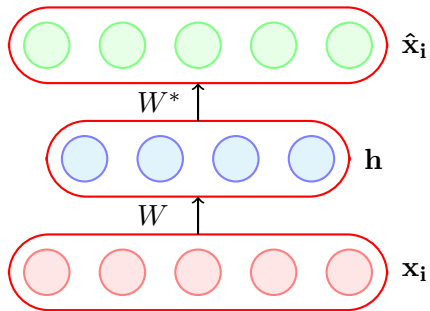
CS7015 (Deep Learning) : Lecture 7

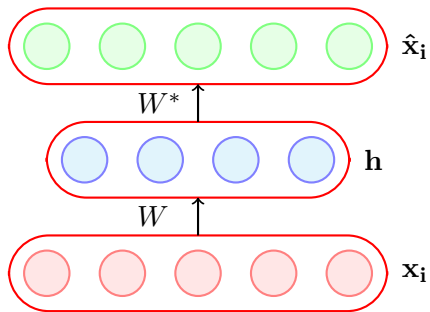
Autoencoders and relation to PCA, Regularization in autoencoders, Denoising autoencoders, Sparse autoencoders, Contractive autoencoders

Mitesh M. Khapra

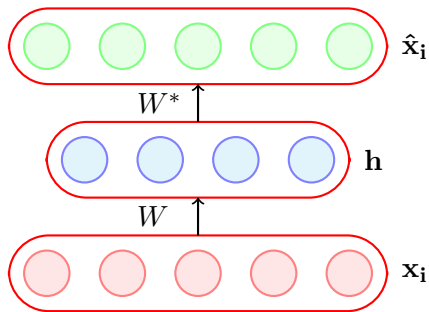
Department of Computer Science and Engineering
Indian Institute of Technology Madras

Module 7.1: Introduction to Autoencoders

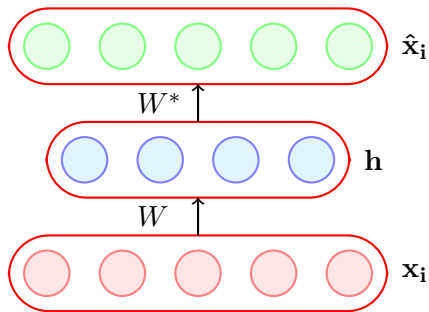




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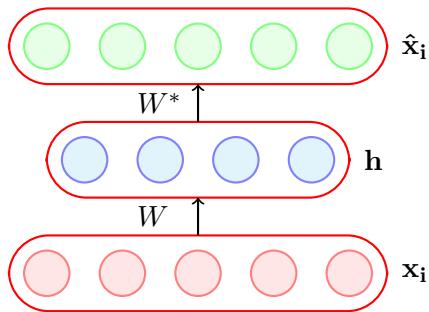


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- Encodes its input \mathbf{x}_i into a hidden representation \mathbf{h}



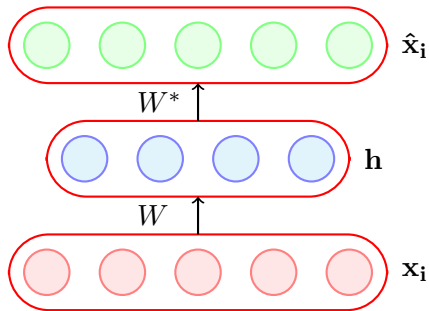
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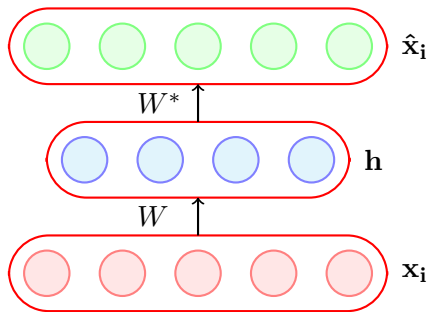


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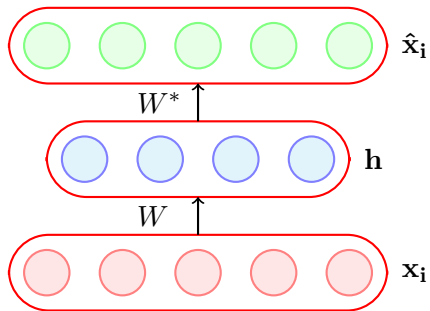
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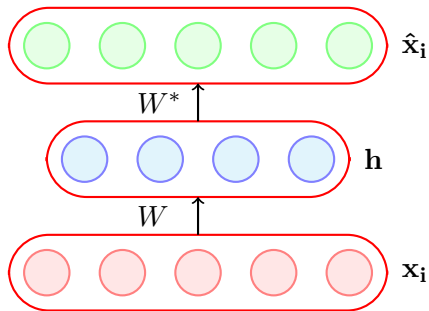


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- Encodes its input \mathbf{x}_i into a hidden representation \mathbf{h}
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- The model is trained to minimize a certain loss function which will ensure that $\hat{\mathbf{x}}_i$ is close to \mathbf{x}_i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

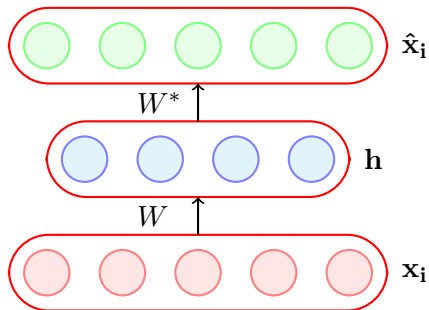


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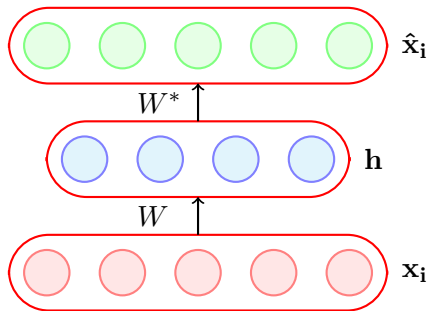
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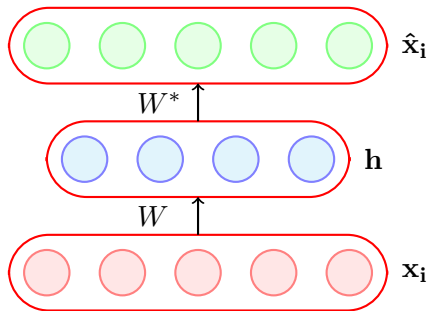
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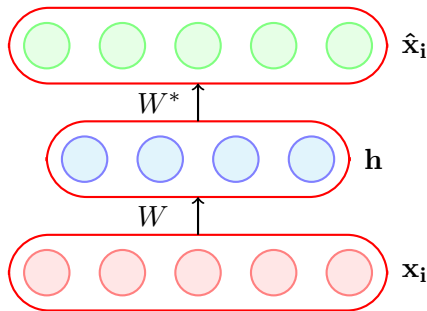
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- Do you see an analogy with PCA?

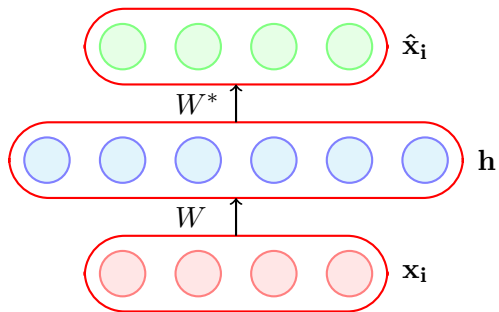


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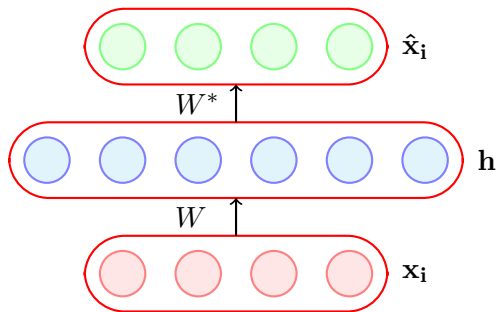
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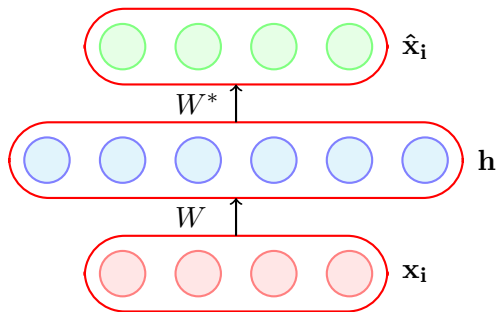
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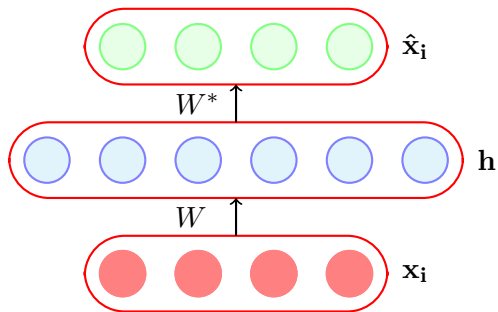
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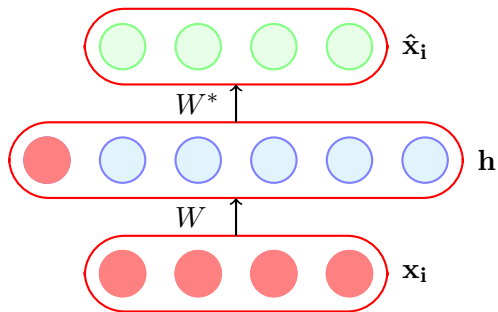
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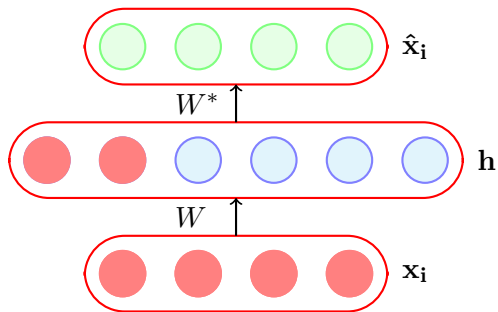
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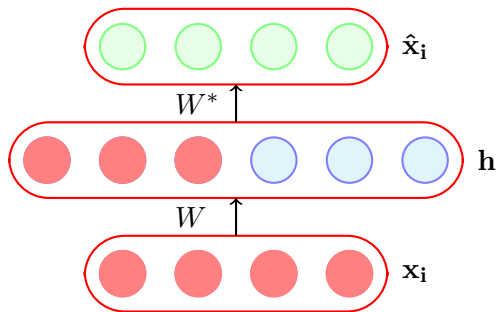
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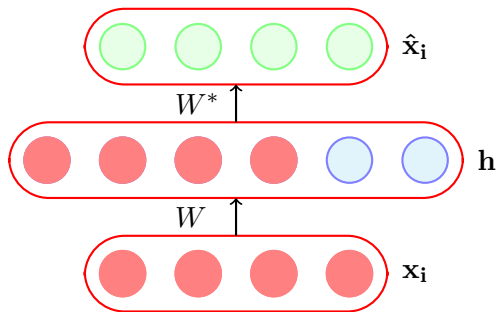
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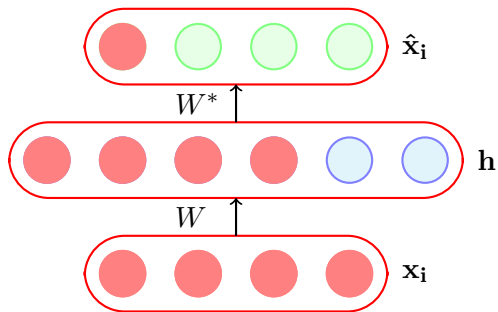
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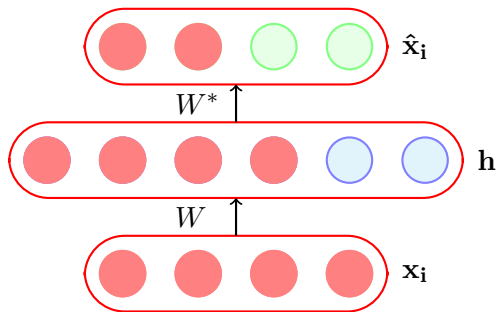
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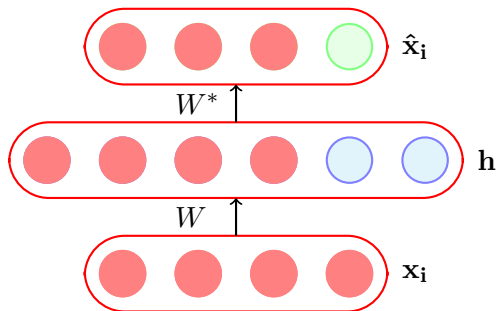
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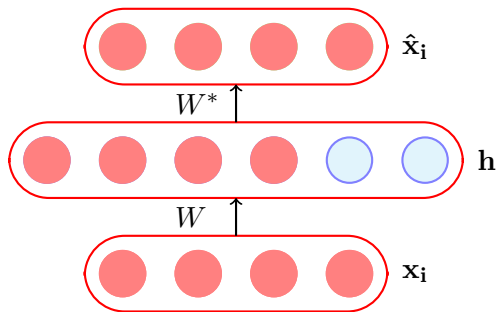
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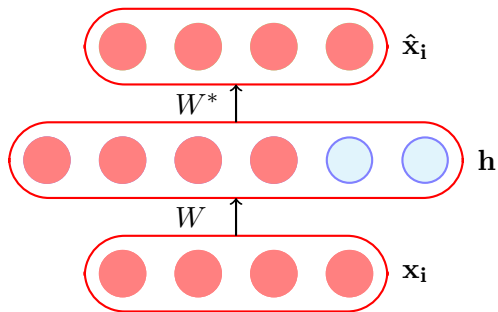
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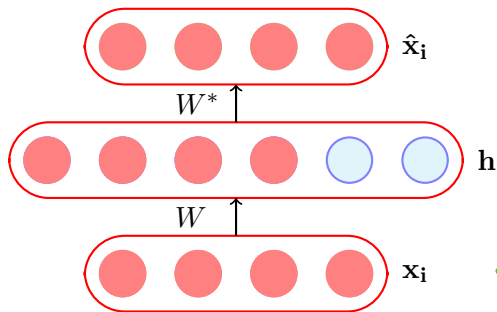
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- Such an identity encoding is useless in practice as it does not really tell us anything about the important characteristics of the data



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The Road Ahead

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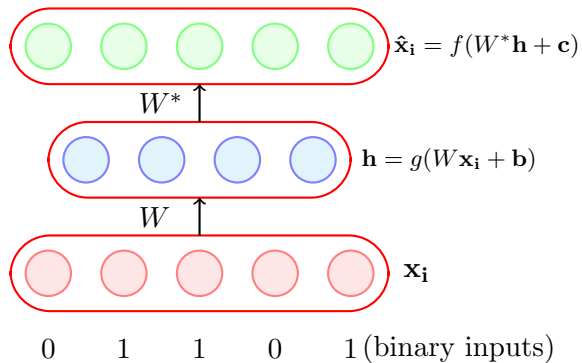
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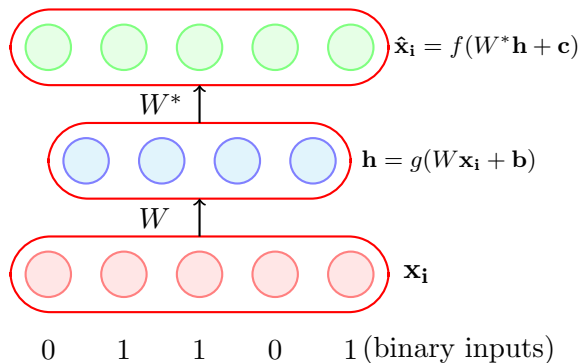
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- Choice of $f(\mathbf{x}_i)$ and $g(\mathbf{x}_i)$
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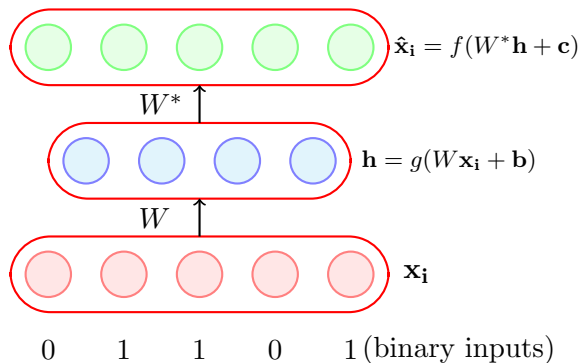
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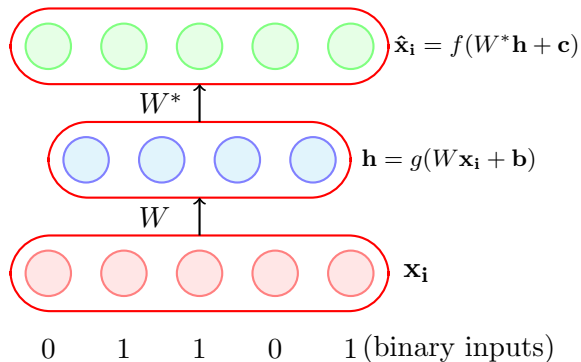




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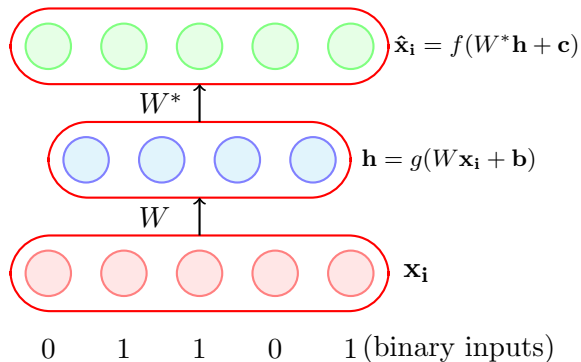


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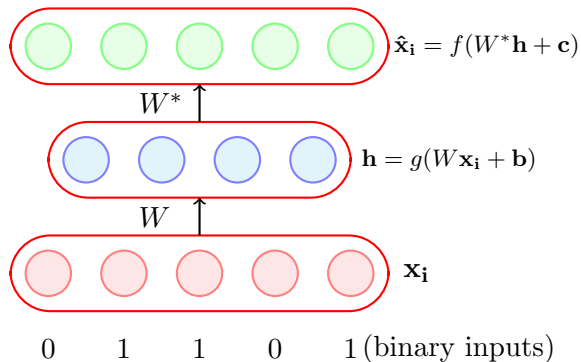
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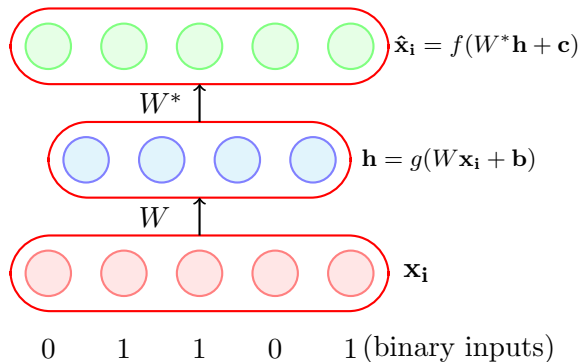


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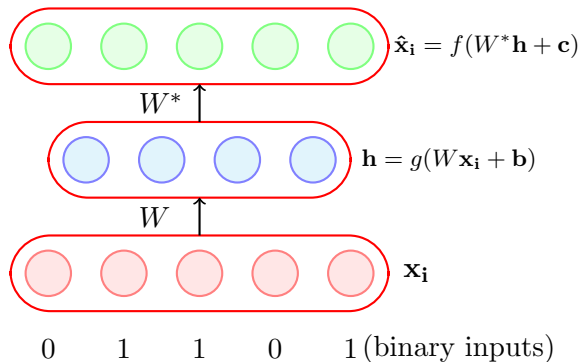
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- Logistic as it naturally restricts all outputs to be between 0 and 1



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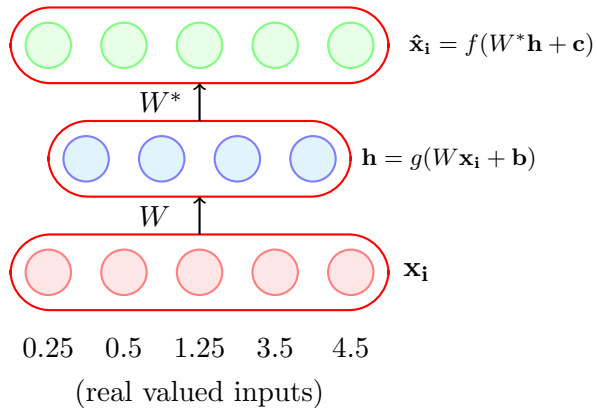
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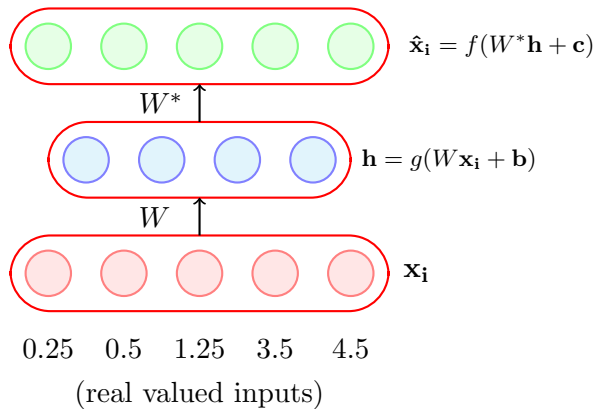
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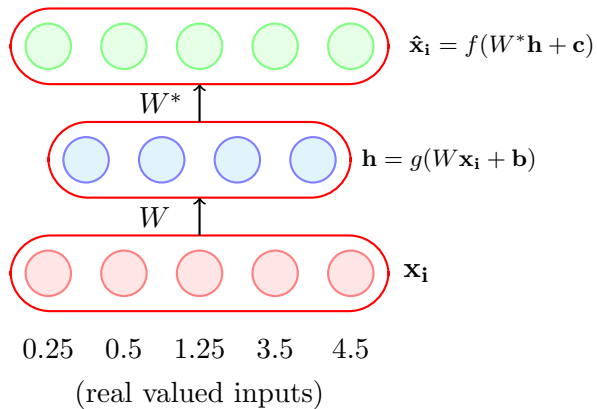
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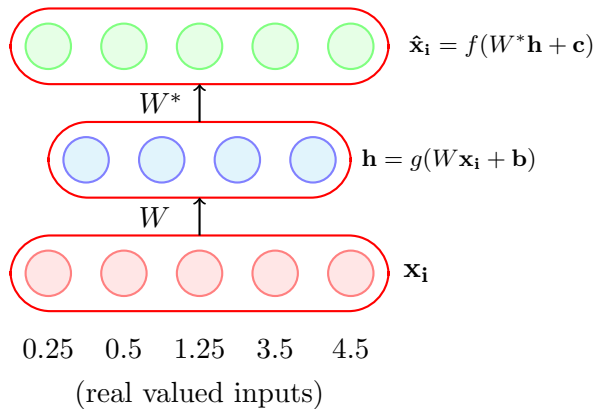




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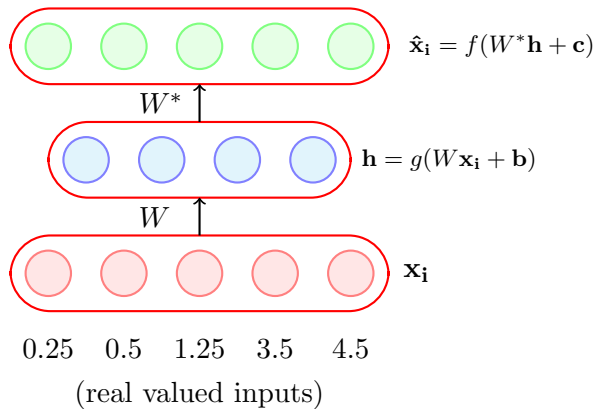


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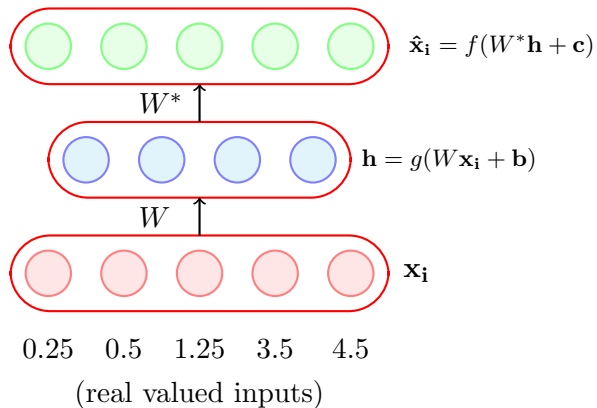
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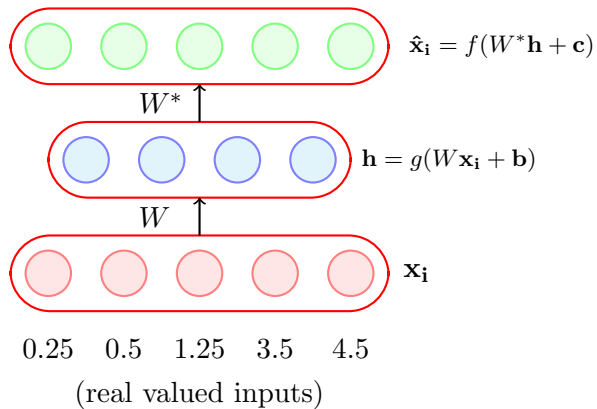


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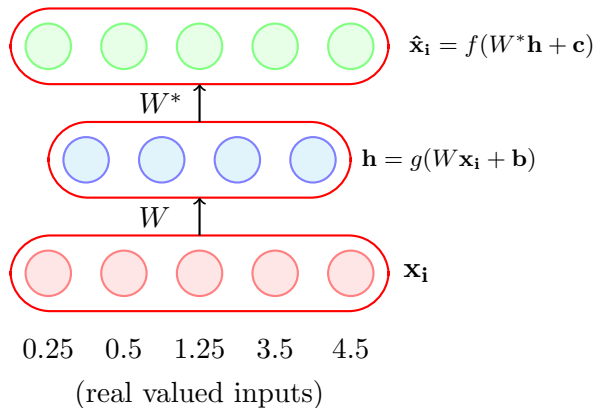
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- What will logistic and tanh do?



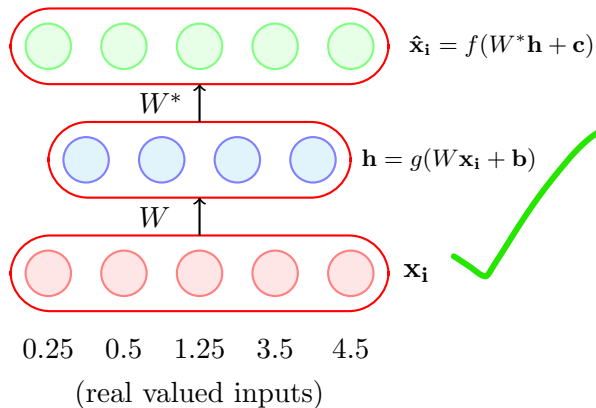
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- What will logistic and tanh do?
- They will restrict the reconstructed $\hat{\mathbf{x}}_i$ to lie between $[0,1]$ or $[-1,1]$ whereas we want $\hat{\mathbf{x}}_i \in \mathbb{R}^n$



Again, g is typically chosen as the sigmoid function

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


$$\hat{\mathbf{x}}_i = \tanh(W^* \mathbf{h} + \mathbf{c})$$

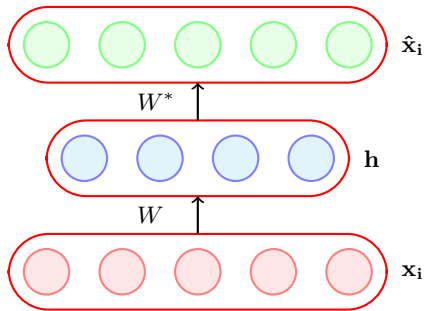
$$\hat{\mathbf{x}}_i = W^* \mathbf{h} + \mathbf{c}$$

$$\hat{\mathbf{x}}_i = \text{logistic}(W^* \mathbf{h} + \mathbf{c})$$

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

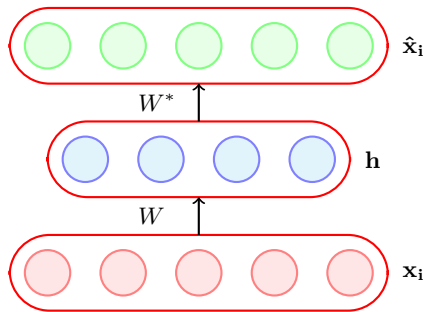
The Road Ahead

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



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

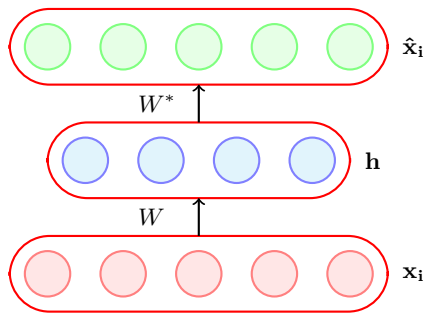
$$\hat{\mathbf{x}}_i = f(W^*\mathbf{h} + \mathbf{c})$$



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

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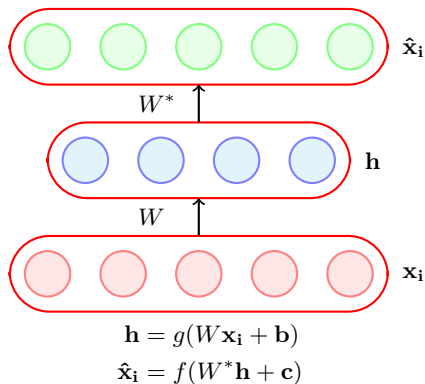
- Consider the case when the inputs are real valued



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

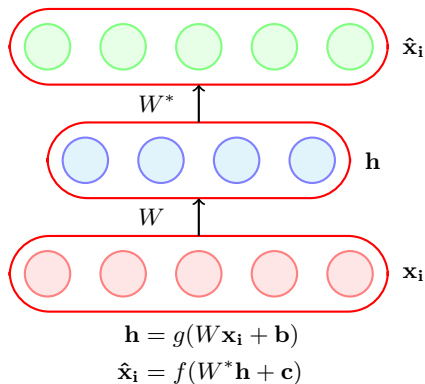
$$\hat{\mathbf{x}}_i = f(W^*\mathbf{h} + \mathbf{c})$$

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



- Consider the case when the inputs are real valued
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- This can be formalized using the following objective function:

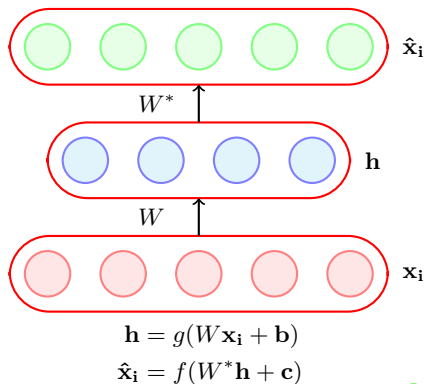
$$\min_{W, W^*, \mathbf{c}, \mathbf{b}} \frac{1}{m} \sum_{i=1}^m \sum_{j=1}^n (\hat{x}_{ij} - x_{ij})^2$$



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$$i.e., \min_{W, W^*, \mathbf{c}, \mathbf{b}} \frac{1}{m} \sum_{i=1}^m (\hat{\mathbf{x}}_i - \mathbf{x}_i)^T (\hat{\mathbf{x}}_i - \mathbf{x}_i)$$

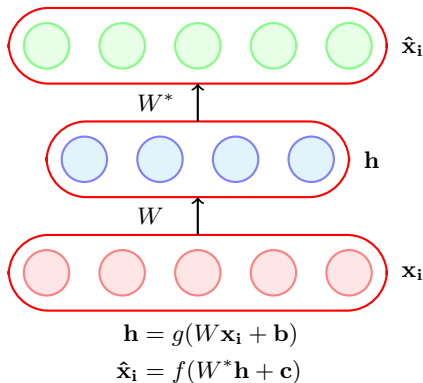


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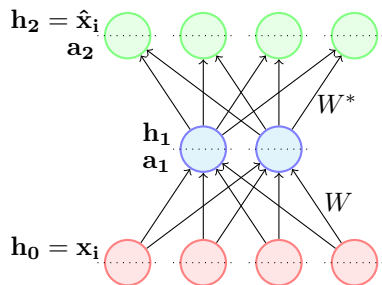
i.e., $\min_{W, W^*, \mathbf{c}, \mathbf{b}} \frac{1}{m} \sum_{i=1}^m (\hat{\mathbf{x}}_i - \mathbf{x}_i)^T (\hat{\mathbf{x}}_i - \mathbf{x}_i)$

A green arrow points from the handwritten note below to the first minimization term. A pink arrow points from the second minimization term to the handwritten note below.

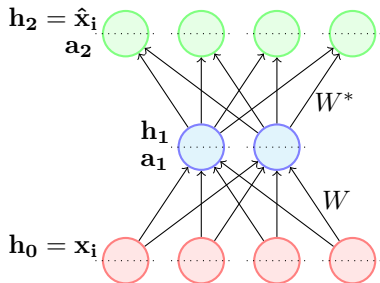
- We can then train the autoencoder just like a regular feedforward network using back-propagation
- All we need is a formula for $\frac{\partial \mathcal{L}(\theta)}{\partial W^*}$ and $\frac{\partial \mathcal{L}(\theta)}{\partial W}$ which we will see now

i/o → real valued
o/p → discrete
So → discrete
encoder

$$\mathcal{L}(\theta) = (\hat{\mathbf{x}}_i - \mathbf{x}_i)^T (\hat{\mathbf{x}}_i - \mathbf{x}_i)$$



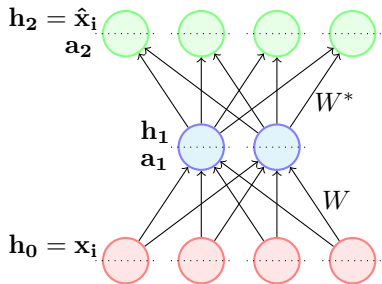
$$\mathcal{L}(\theta) = (\hat{\mathbf{x}}_i - \mathbf{x}_i)^T (\hat{\mathbf{x}}_i - \mathbf{x}_i)$$



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

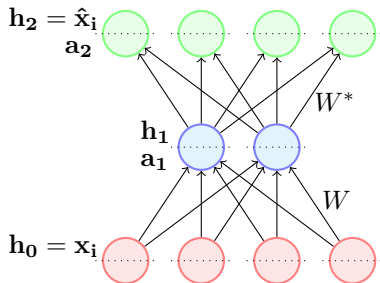
$$\mathcal{L}(\theta) = (\hat{\mathbf{x}}_i - \mathbf{x}_i)^T (\hat{\mathbf{x}}_i - \mathbf{x}_i)$$

$$\bullet \quad \frac{\partial \mathcal{L}(\theta)}{\partial W^*} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} \boxed{\frac{\partial \mathbf{h}_2}{\partial \mathbf{a}_2} \frac{\partial \mathbf{a}_2}{\partial W^*}}$$



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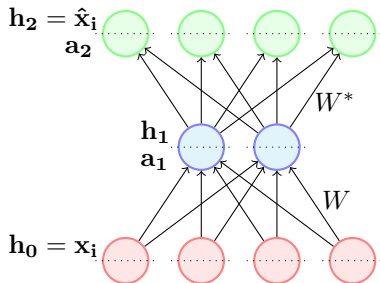
$$\mathcal{L}(\theta) = (\hat{\mathbf{x}}_i - \mathbf{x}_i)^T (\hat{\mathbf{x}}_i - \mathbf{x}_i)$$



- $\frac{\partial \mathcal{L}(\theta)}{\partial W^*} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} \boxed{\frac{\partial \mathbf{h}_2}{\partial \mathbf{a}_2} \frac{\partial \mathbf{a}_2}{\partial W^*}}$
- $\frac{\partial \mathcal{L}(\theta)}{\partial W} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} \boxed{\frac{\partial \mathbf{h}_2}{\partial \mathbf{a}_2} \frac{\partial \mathbf{a}_2}{\partial \mathbf{h}_1} \frac{\partial \mathbf{h}_1}{\partial \mathbf{a}_1} \frac{\partial \mathbf{a}_1}{\partial W}}$

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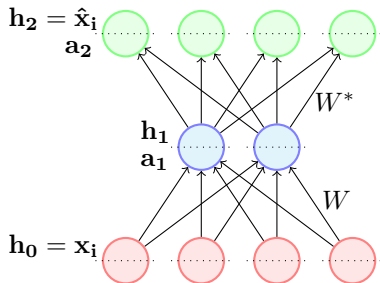
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- $\frac{\partial \mathcal{L}(\theta)}{\partial W^*} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} \boxed{\frac{\partial \mathbf{h}_2}{\partial \mathbf{a}_2} \frac{\partial \mathbf{a}_2}{\partial W^*}}$
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- We have already seen how to calculate the expression in the boxes when we learnt backpropagation

$$\mathcal{L}(\theta) = (\hat{\mathbf{x}}_i - \mathbf{x}_i)^T (\hat{\mathbf{x}}_i - \mathbf{x}_i)$$



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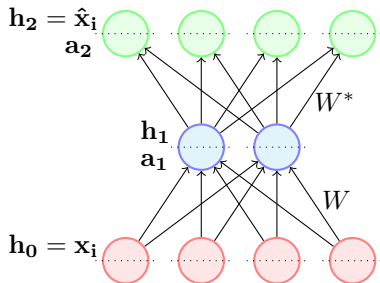
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- We have already seen how to calculate the expression in the boxes when we learnt backpropagation

$$\frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} = \frac{\partial \mathcal{L}(\theta)}{\partial \hat{\mathbf{x}}_i}$$

$$\mathcal{L}(\theta) = (\hat{\mathbf{x}}_i - \mathbf{x}_i)^T (\hat{\mathbf{x}}_i - \mathbf{x}_i)$$



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

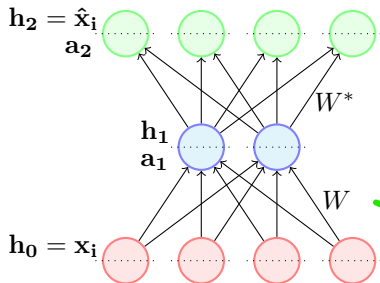
- $$\frac{\partial \mathcal{L}(\theta)}{\partial W^*} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} \boxed{\frac{\partial \mathbf{h}_2}{\partial \mathbf{a}_2} \frac{\partial \mathbf{a}_2}{\partial W^*}}$$

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

$$\begin{aligned} \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} &= \frac{\partial \mathcal{L}(\theta)}{\partial \hat{\mathbf{x}}_i} \\ &= \nabla_{\hat{\mathbf{x}}_i} \{(\hat{\mathbf{x}}_i - \mathbf{x}_i)^T (\hat{\mathbf{x}}_i - \mathbf{x}_i)\} \end{aligned}$$

$$\mathcal{L}(\theta) = (\hat{\mathbf{x}}_i - \mathbf{x}_i)^T (\hat{\mathbf{x}}_i - \mathbf{x}_i)$$



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

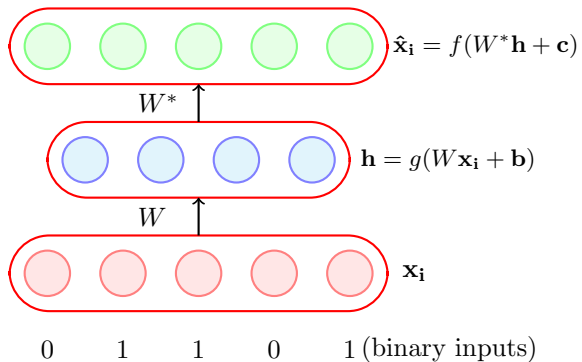
- $\frac{\partial \mathcal{L}(\theta)}{\partial W^*} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} \boxed{\frac{\partial \mathbf{h}_2}{\partial \mathbf{a}_2} \frac{\partial \mathbf{a}_2}{\partial W^*}}$

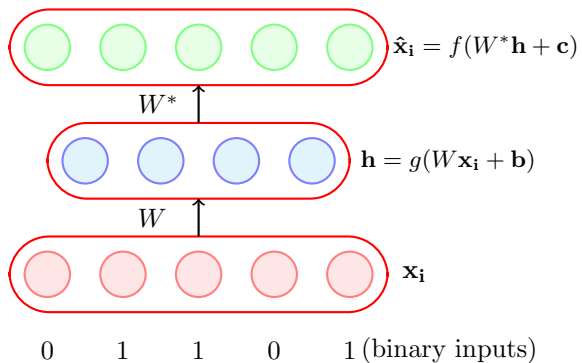
- $\frac{\partial \mathcal{L}(\theta)}{\partial W} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} \boxed{\frac{\partial \mathbf{h}_2}{\partial \mathbf{a}_2} \frac{\partial \mathbf{a}_2}{\partial \mathbf{h}_1} \frac{\partial \mathbf{h}_1}{\partial \mathbf{a}_1} \frac{\partial \mathbf{a}_1}{\partial W}}$

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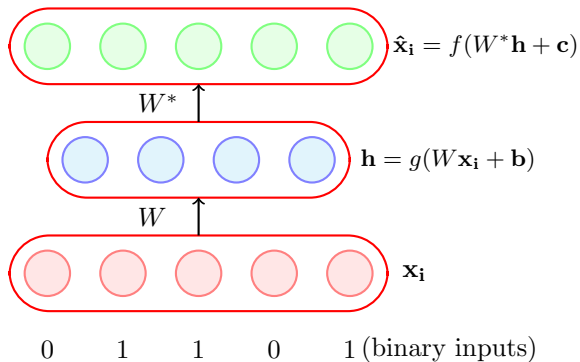
$$\begin{aligned} \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} &= \frac{\partial \mathcal{L}(\theta)}{\partial \hat{\mathbf{x}}_i} \\ &= \nabla_{\hat{\mathbf{x}}_i} \{(\hat{\mathbf{x}}_i - \mathbf{x}_i)^T (\hat{\mathbf{x}}_i - \mathbf{x}_i)\} \\ &= 2(\hat{\mathbf{x}}_i - \mathbf{x}_i) \end{aligned}$$

$\hookrightarrow \text{Loss}$





- 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.

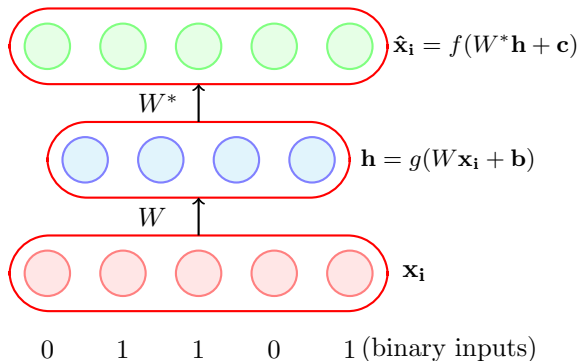
Handwritten notes in green:

Decoder

0.5, 0.5, 0.5, 0.5, 0.5

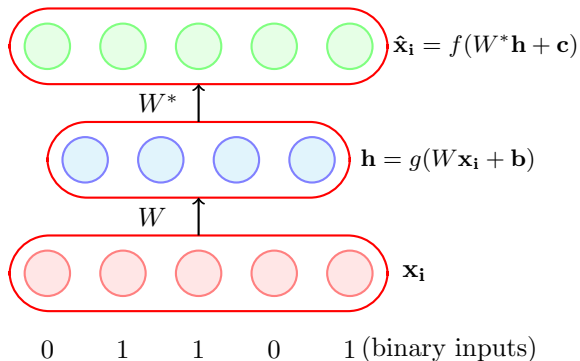
0.5, 0.5, 0.5, 0.5, 0.5

0.5, 0.5, 0.5, 0.5, 0.5



- 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

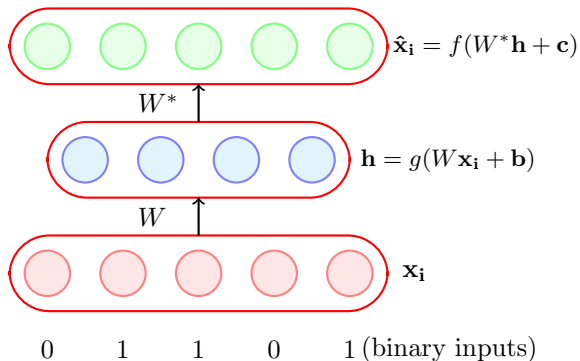
$$\min\left\{-\sum_{j=1}^n (x_{ij} \log \hat{x}_{ij} + (1 - x_{ij}) \log(1 - \hat{x}_{ij}))\right\}$$



What value of \hat{x}_{ij} will minimize this function?

- Consider the case when the inputs are binary
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- For a single n -dimensional i^{th} input we can use the following loss function

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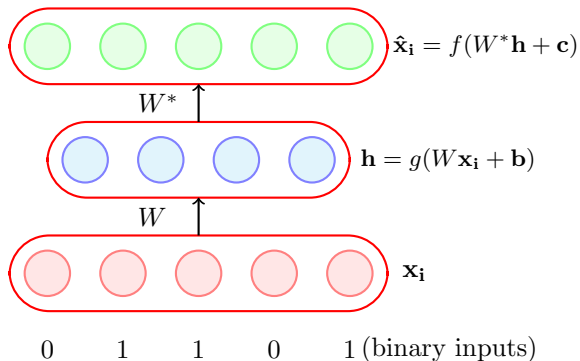
- If $x_{ij} = 1$?

- 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

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



What value of \hat{x}_{ij} will minimize this function?

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

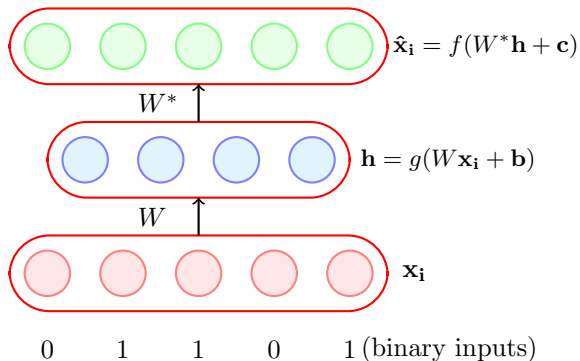
- Consider the case when the inputs are binary

- 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

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

- Again we need a formula for $\frac{\partial \mathcal{L}(\theta)}{\partial W^*}$ and $\frac{\partial \mathcal{L}(\theta)}{\partial W}$ to use backpropagation



What value of \hat{x}_{ij} will minimize this function?

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

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

- Consider the case when the inputs are binary

Logistic

- We use a sigmoid decoder which will produce outputs between 0 and 1, and can be interpreted as probabilities.

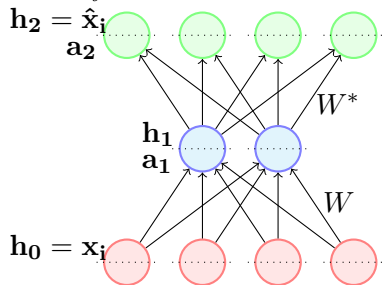
- For a single n-dimensional i^{th} input we can use the following loss function

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

- Again we need a formula for $\frac{\partial \mathcal{L}(\theta)}{\partial W^*}$ and $\frac{\partial \mathcal{L}(\theta)}{\partial W}$ to use backpropagation

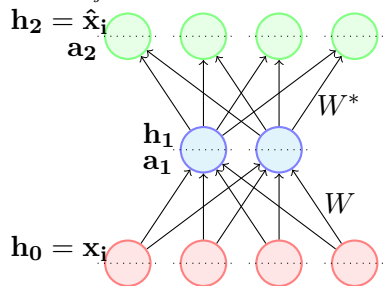
Cross Entropy Loss

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



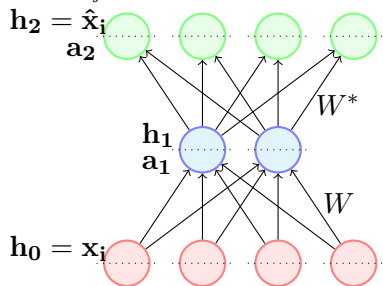
→ weights for binary i/o

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



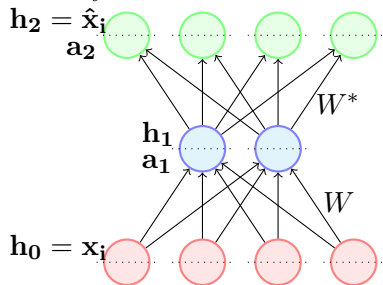
$$\bullet \quad \frac{\partial \mathcal{L}(\theta)}{\partial W^*} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} \frac{\partial \mathbf{h}_2}{\partial \mathbf{a}_2} \boxed{\frac{\partial \mathbf{a}_2}{\partial W^*}}$$

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



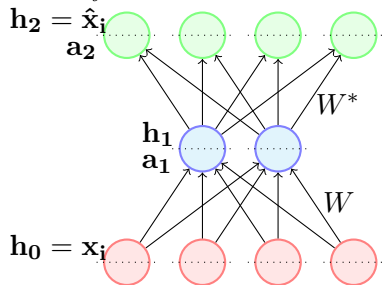
- $\frac{\partial \mathcal{L}(\theta)}{\partial W^*} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} \frac{\partial \mathbf{h}_2}{\partial \mathbf{a}_2} \boxed{\frac{\partial \mathbf{a}_2}{\partial W^*}}$
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$$\mathcal{L}(\theta) = - \sum_{j=1}^n (x_{ij} \log \hat{x}_{ij} + (1 - x_{ij}) \log(1 - \hat{x}_{ij}))$$



- $\frac{\partial \mathcal{L}(\theta)}{\partial W^*} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} \frac{\partial \mathbf{h}_2}{\partial \mathbf{a}_2} \boxed{\frac{\partial \mathbf{a}_2}{\partial W^*}}$
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- We have already seen how to calculate the expressions in the square boxes when we learnt BP

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



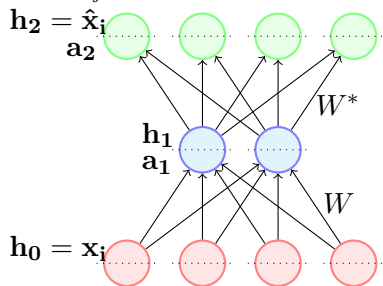
- $$\frac{\partial \mathcal{L}(\theta)}{\partial W^*} = \frac{\partial \mathcal{L}(\theta)}{\partial h_2} \frac{\partial h_2}{\partial a_2} \boxed{\frac{\partial a_2}{\partial W^*}}$$
- $$\frac{\partial \mathcal{L}(\theta)}{\partial W} = \frac{\partial \mathcal{L}(\theta)}{\partial h_2} \frac{\partial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

- 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:

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

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

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



$$\frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} = \begin{pmatrix} \frac{\partial \mathcal{L}(\theta)}{\partial h_{21}} \\ \frac{\partial \mathcal{L}(\theta)}{\partial h_{22}} \\ \vdots \\ \frac{\partial \mathcal{L}(\theta)}{\partial h_{2n}} \end{pmatrix}$$



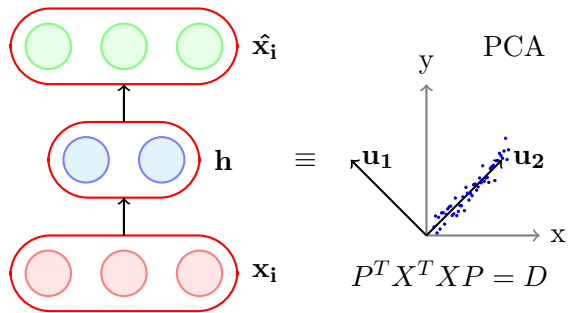
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- $\frac{\partial \mathcal{L}(\theta)}{\partial W} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_2} \frac{\partial \mathbf{h}_2}{\partial \mathbf{a}_2} \boxed{\frac{\partial \mathbf{a}_2}{\partial \mathbf{h}_1} \frac{\partial \mathbf{h}_1}{\partial \mathbf{a}_1} \frac{\partial \mathbf{a}_1}{\partial W}}$

- 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:

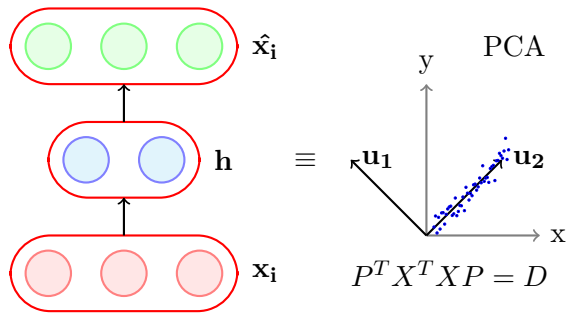
$$\frac{\partial \mathcal{L}(\theta)}{\partial h_{2j}} = -\frac{x_{ij}}{\hat{x}_{ij}} + \frac{1 - x_{ij}}{1 - \hat{x}_{ij}}$$

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

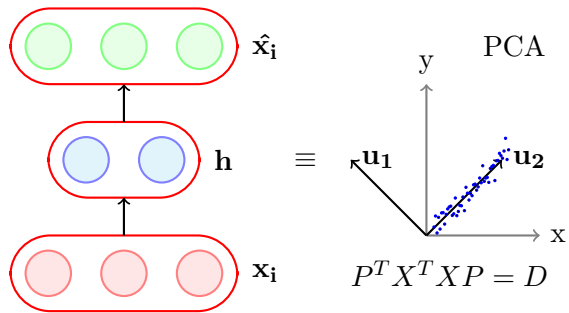
Module 7.2: Link between PCA and Autoencoders



- We will now see that the encoder part of an autoencoder is equivalent to PCA if we

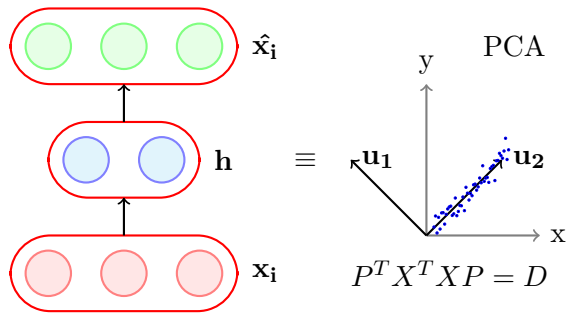


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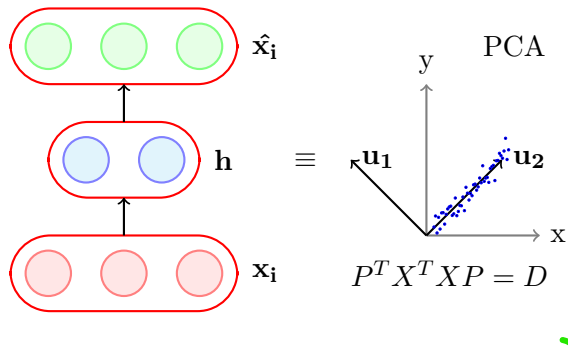
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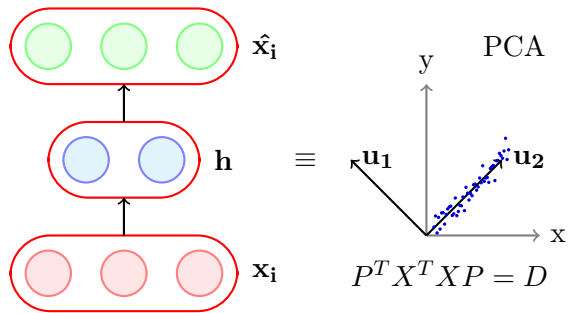
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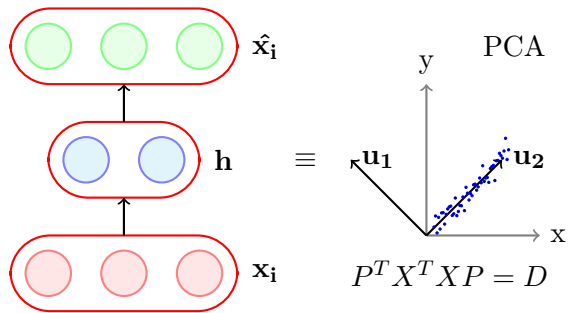
- use a linear encoder
- use a linear decoder
- use squared error loss function
- normalize the inputs to

$$\hat{x}_{ij} = \frac{1}{\sqrt{m}} \left(x_{ij} - \frac{1}{m} \sum_{k=1}^m x_{kj} \right)$$



- First let us consider the implication of normalizing the inputs to

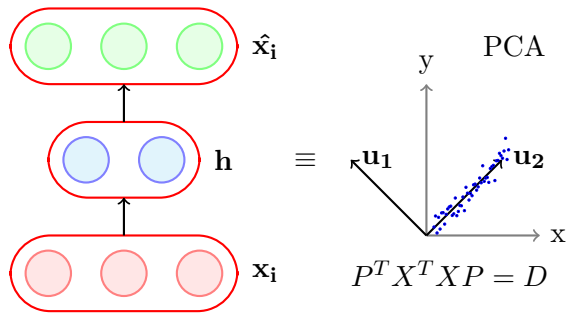
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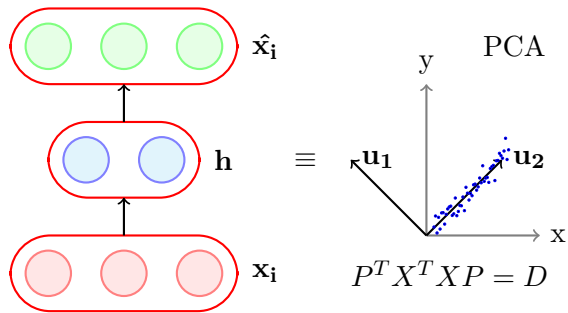
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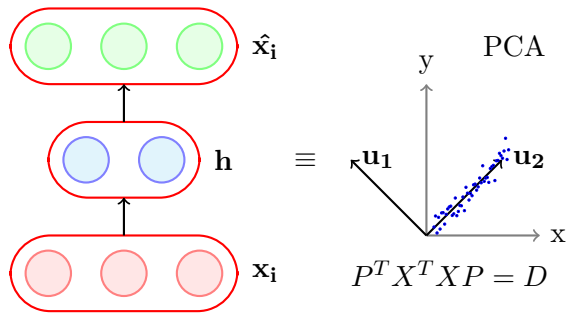
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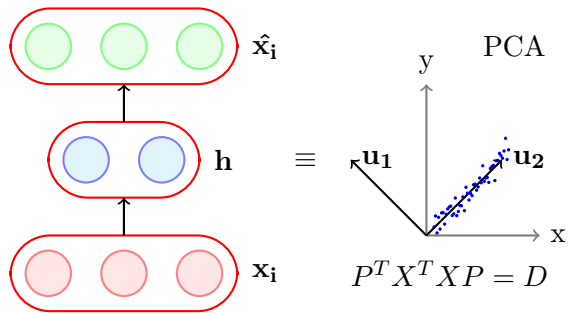


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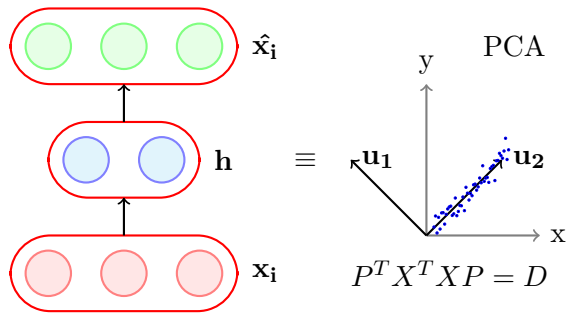
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- Let X' be this zero mean data matrix then what the above normalization gives us is $X = \frac{1}{\sqrt{m}} X'$
- Now $(X)^T X = \frac{1}{m} (X')^T X'$ is the covariance matrix (recall that covariance matrix plays an important role in PCA)

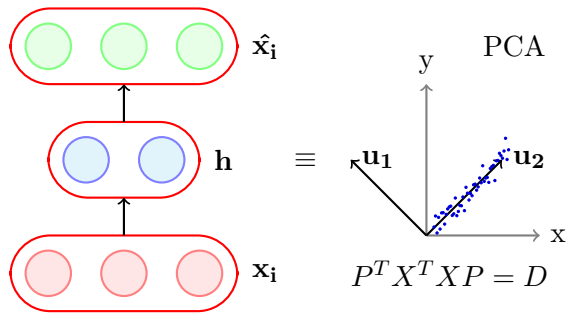




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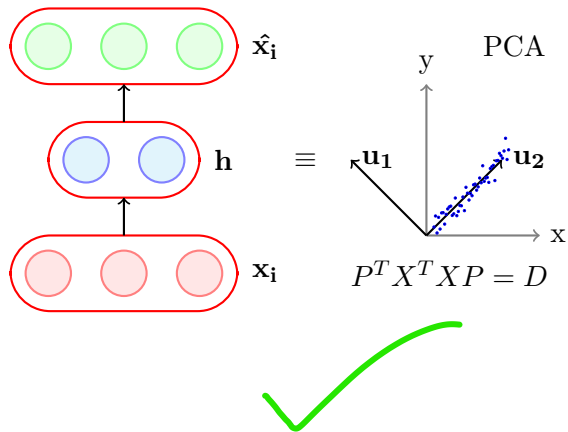


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is obtained when we use a linear encoder.

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- By matching variables one possible solution is

$$H = U_{\cdot, \leq k} \Sigma_{k,k}$$

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 &= X V I_{.,\leq k} && (\Sigma^{-1} I_{.,\leq k} = \Sigma_{k,k}^{-1}) \\
 H &= X V_{.,\leq k}
 \end{aligned}$$

Thus H is a linear transformation of X and $W = V_{.,\leq k}$

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- Thus, the encoder matrix for linear autoencoder(W) and the projection matrix(P) for PCA could indeed be the same. Hence proved

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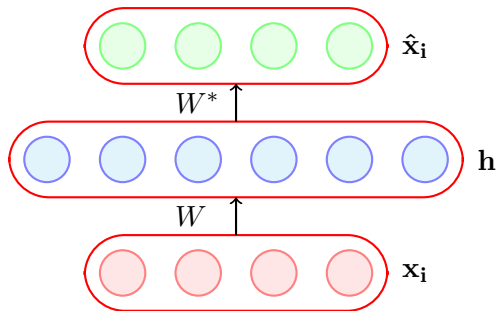
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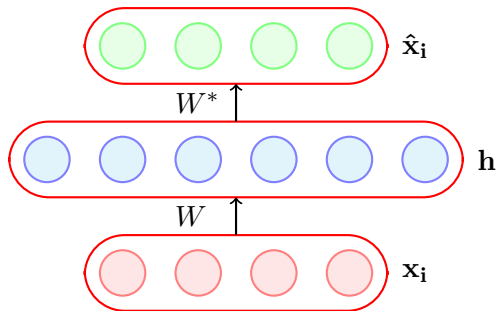
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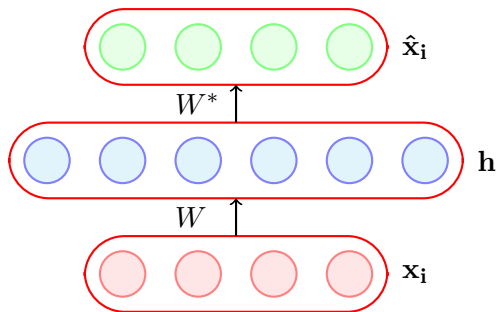
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Module 7.3: Regularization in autoencoders (Motivation)

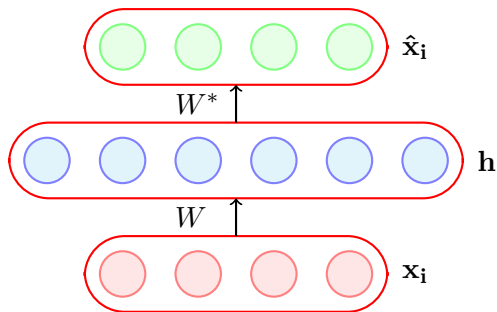


- While poor generalization could happen even in undercomplete autoencoders it is an even more serious problem for overcomplete auto encoders

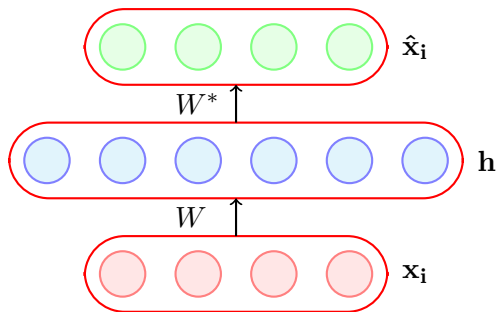




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- Here, (as stated earlier) the model can simply learn to copy \mathbf{x}_i to \mathbf{h} and then \mathbf{h} to $\hat{\mathbf{x}}_i$

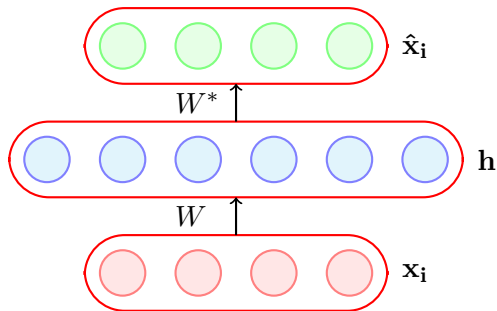


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- Here, (as stated earlier) the model can simply learn to copy \mathbf{x}_i to \mathbf{h} and then \mathbf{h} to $\hat{\mathbf{x}}_i$
- To avoid poor generalization, we need to introduce regularization



- The simplest solution is to add a L_2 -regularization term to the objective function

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

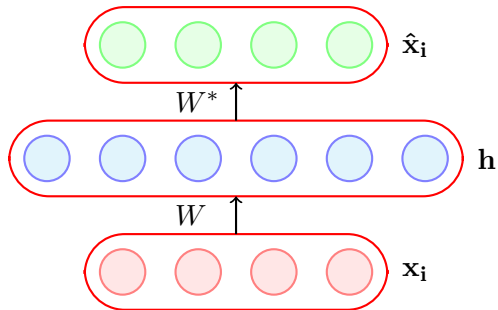


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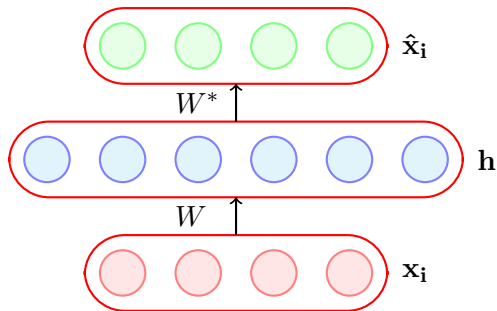
$$\min_{\theta, w, w^*, \mathbf{b}, \mathbf{c}} \frac{1}{m} \sum_{i=1}^m \sum_{j=1}^n (\hat{x}_{ij} - x_{ij})^2 + \lambda \|\theta\|^2$$

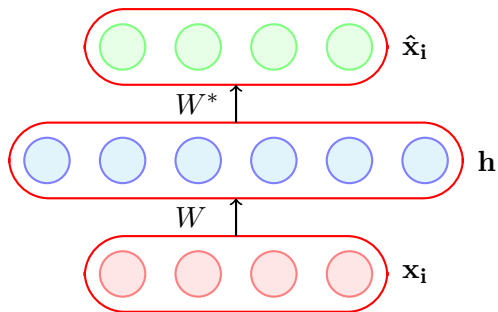
- This is very easy to implement and just adds a term λW to the gradient $\frac{\partial \mathcal{L}(\theta)}{\partial W}$ (and similarly for other parameters)

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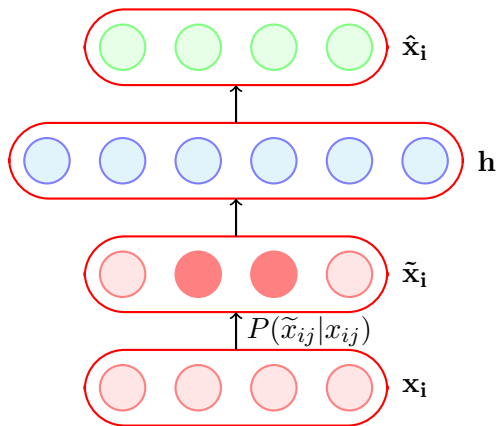


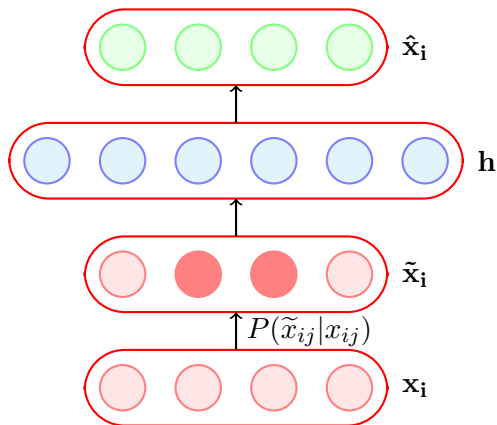


- Another trick is to tie the weights of the encoder and decoder i.e., $W^* = W^T$
- This effectively reduces the capacity of Autoencoder and acts as a regularizer

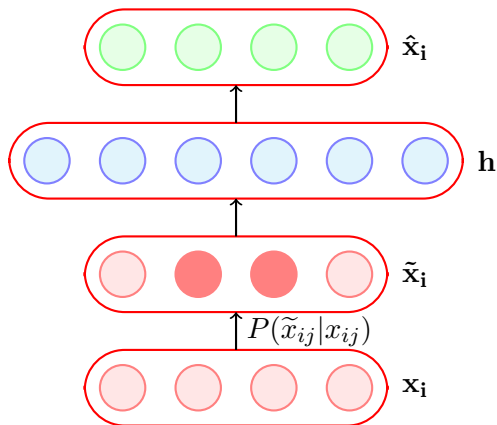
Module 7.4: Denoising Autoencoders

- A denoising encoder simply corrupts the input data using a probabilistic process ($P(\tilde{x}_{ij}|x_{ij})$) before feeding it to the network



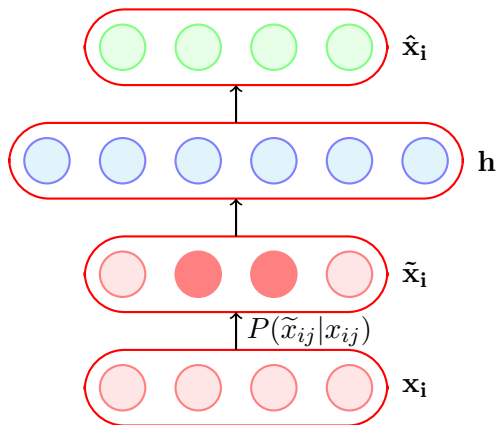


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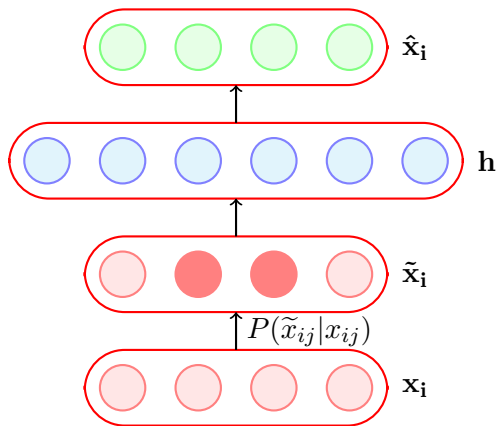
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$$P(\tilde{x}_{ij} = x_{ij}|x_{ij}) = 1 - q$$



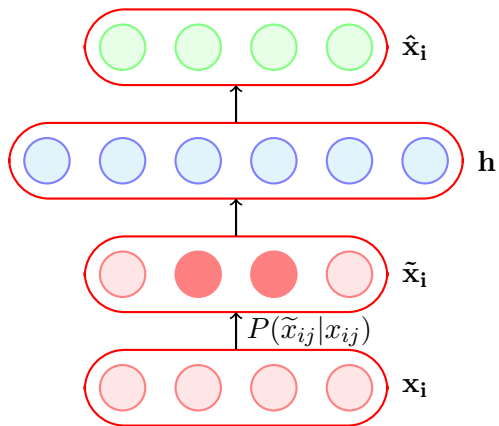
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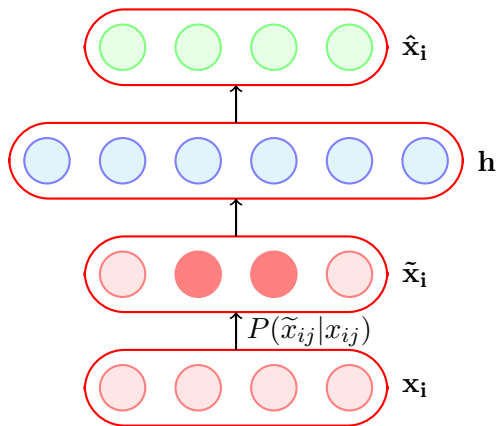
$$P(\tilde{x}_{ij} = 0|x_{ij}) = q$$

$$P(\tilde{x}_{ij} = x_{ij}|x_{ij}) = 1 - q$$

- In other words, with probability q the input is flipped to 0 and with probability $(1 - q)$ it is retained as it is

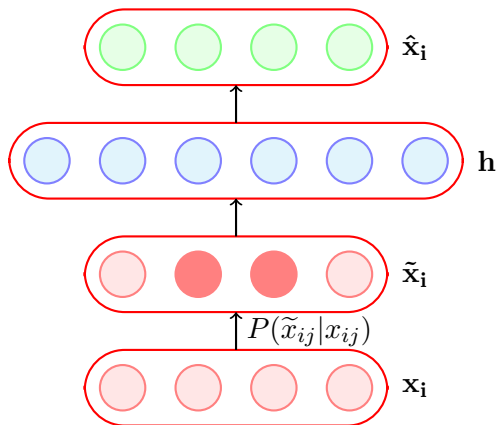
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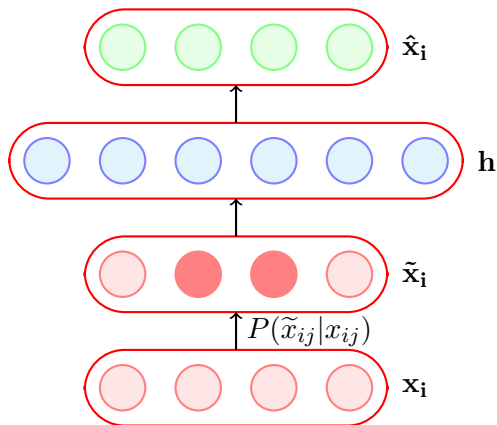
$$\arg \min_{\theta} \frac{1}{m} \sum_{i=1}^m \sum_{j=1}^n (\hat{x}_{ij} - x_{ij})^2$$



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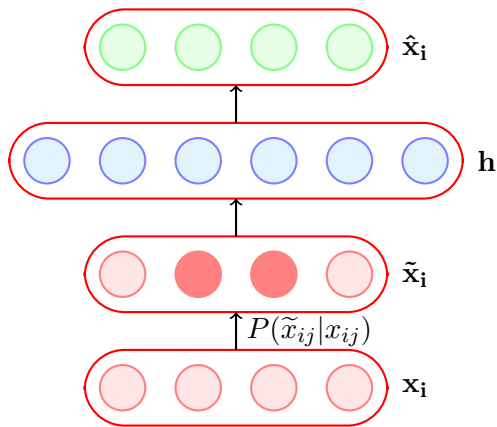
- It no longer makes sense for the model to copy the corrupted $\tilde{\mathbf{x}}_i$ into $h(\tilde{\mathbf{x}}_i)$ and then into $\hat{\mathbf{x}}_i$ (the objective function will not be minimized by doing so)



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- Instead the model will now have to capture the characteristics of the data correctly.



For example, it will have to learn to reconstruct a corrupted x_{ij} correctly by relying on its interactions with other elements of \mathbf{x}_i

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We will now see a practical application in which AEs are used and then compare Denoising Autoencoders with regular autoencoders

Task: Hand-written digit recognition

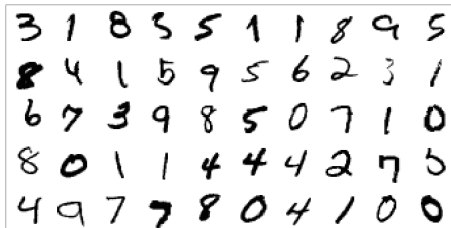
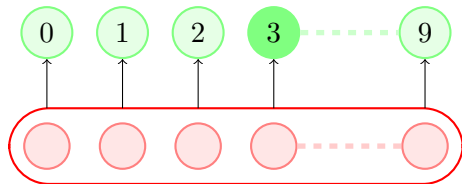


Figure: MNIST Data



$$|\mathbf{x}_i| = 784 = 28 \times 28$$



28*28

Figure: Basic approach (we use raw data as input features)

Task: Hand-written digit recognition

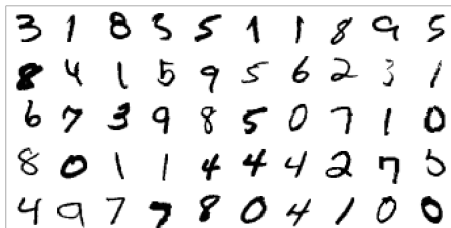


Figure: MNIST Data

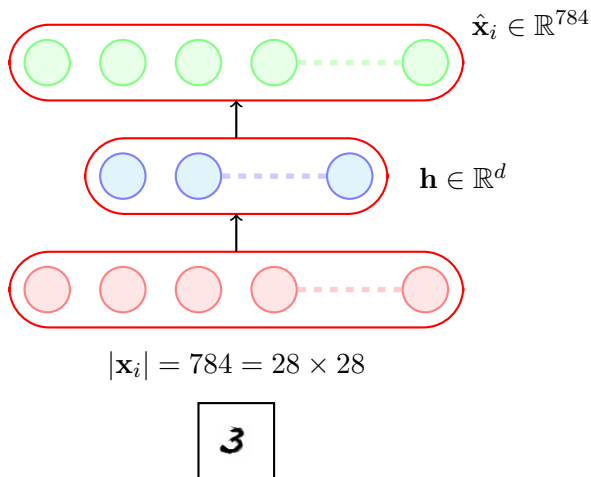


Figure: AE approach (first learn important characteristics of data)

Task: Hand-written digit recognition

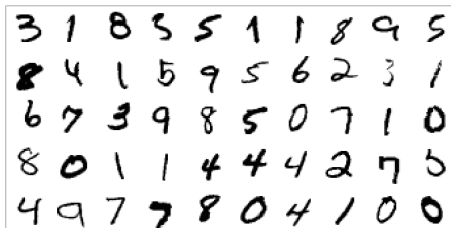


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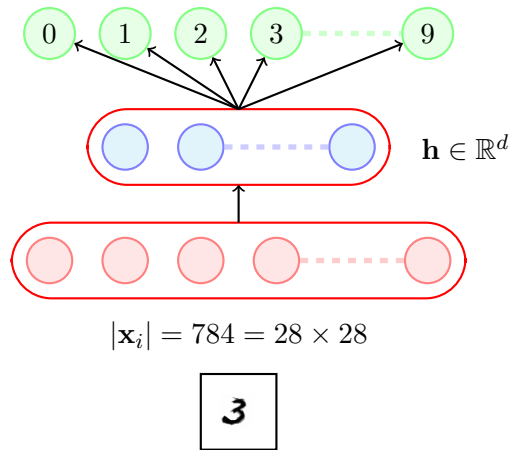
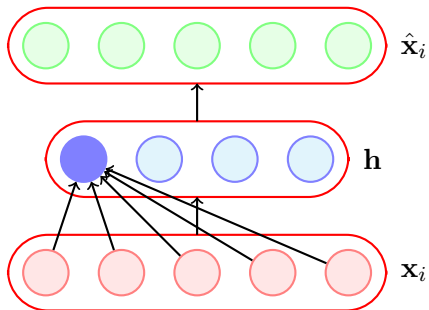
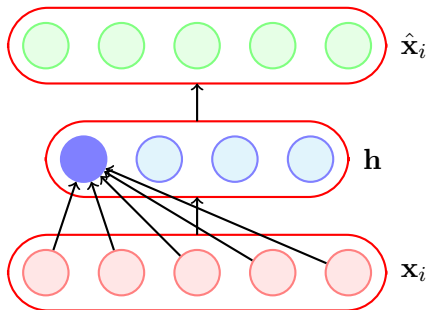


Figure: AE approach (and then train a classifier on top of this hidden representation)

We will now see a way of visualizing AEs and use this visualization to compare different AEs



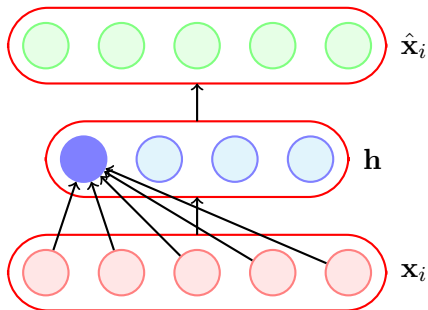
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- For example,

$$\mathbf{h}_1 = \sigma(W_1^T \mathbf{x}_i) \text{ [ignoring bias } b]$$

Where W_1 is the trained vector of weights connecting the input to the first hidden neuron

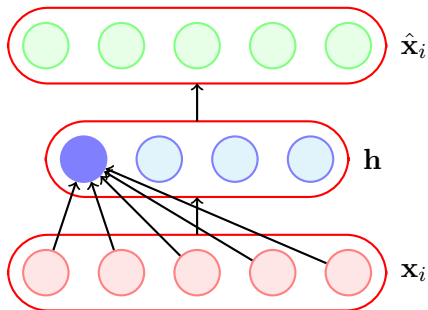


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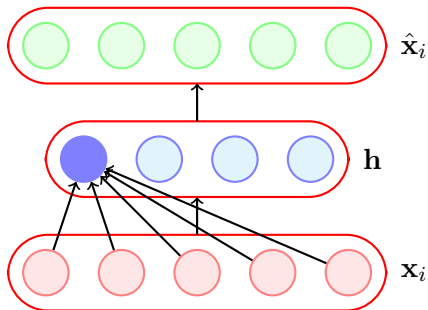


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- Suppose we assume that our inputs are normalized so that $\|\mathbf{x}_i\| = 1$



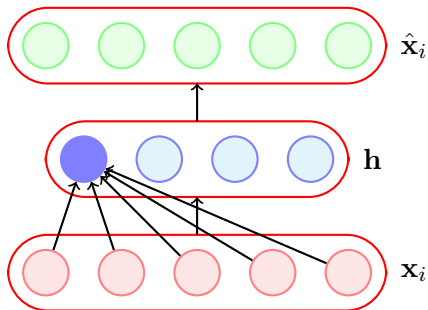
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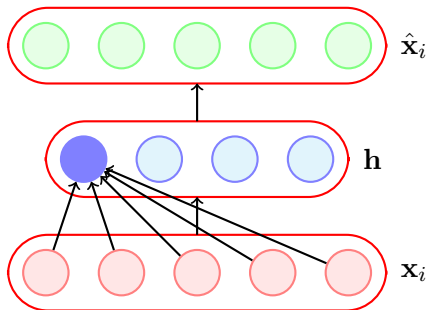
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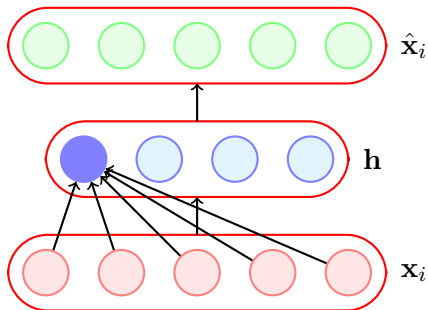


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will respectively cause hidden neurons 1 to n to maximally fire

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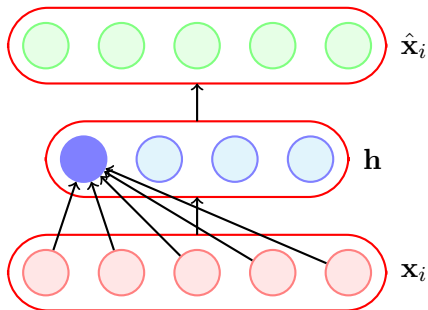
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- These \mathbf{x}_i 's are computed by the above formula using the weights ($W_1, W_2 \dots W_k$) learned by the respective autoencoders

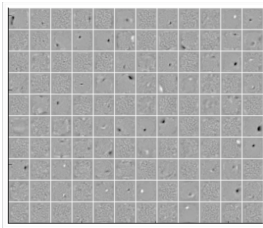


Figure: Vanilla AE
(No noise)

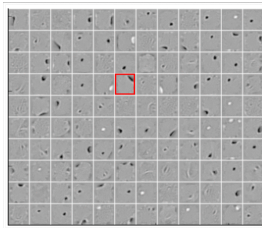


Figure: 25% Denoising
AE ($q=0.25$)

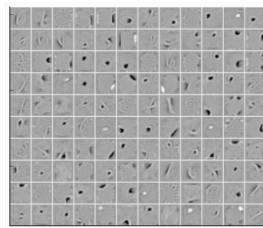


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AE ($q=0.5$)

- The vanilla AE does not learn many meaningful patterns

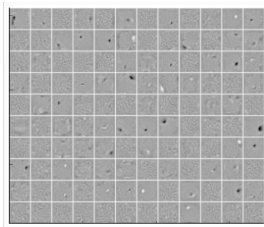


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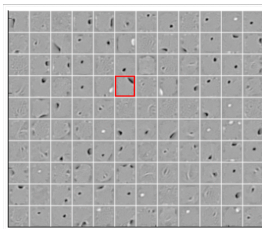


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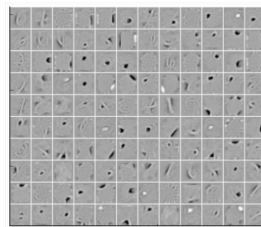


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- The vanilla AE does not learn many meaningful patterns
- The hidden neurons of the denoising AEs seem to act like pen-stroke detectors (for example, in the highlighted neuron the black region is a stroke that you would expect in a '0' or a '2' or a '3' or a '8' or a '9')

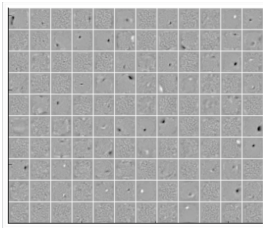


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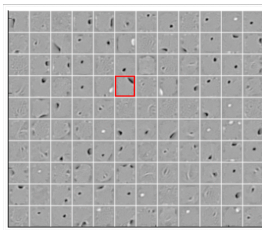


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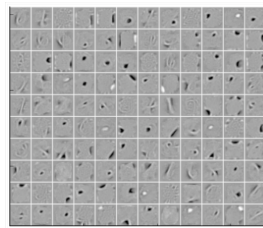
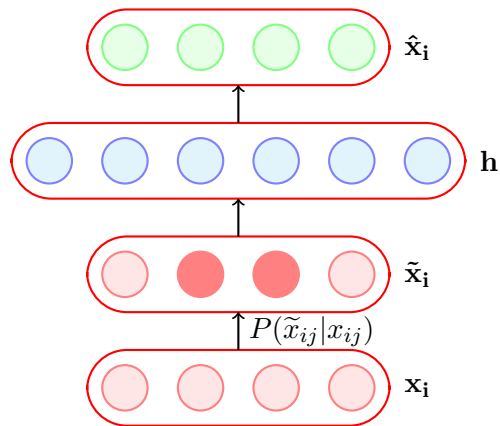
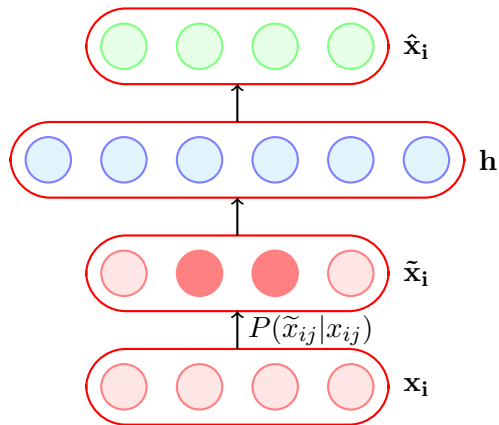


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- The hidden neurons of the denoising AEs seem to act like pen-stroke detectors (for example, in the highlighted neuron the black region is a stroke that you would expect in a '0' or a '2' or a '3' or a '8' or a '9')
- As the noise increases the filters become more wide because the neuron has to rely on more adjacent pixels to feel confident about a stroke

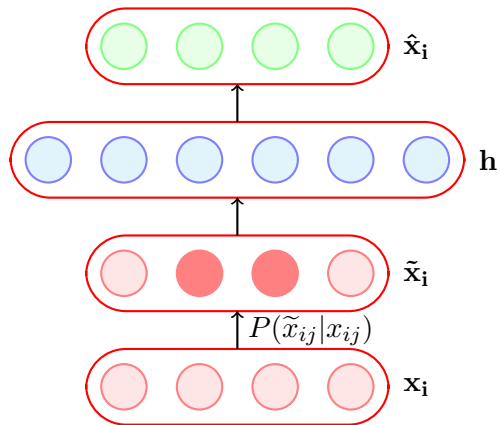


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$$\tilde{x}_{ij} = x_{ij} + \mathcal{N}(0, 1)$$



- We saw one form of $P(\tilde{x}_{ij}|x_{ij})$ which flips a fraction q of the inputs to zero
- Another way of corrupting the inputs is to add a Gaussian noise to the input

$$\tilde{x}_{ij} = x_{ij} + \mathcal{N}(0, 1)$$

- We will now use such a denoising AE on a different dataset and see their performance

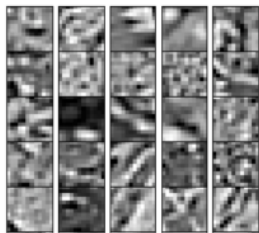


Figure: Data

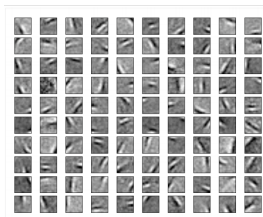


Figure: AE filters

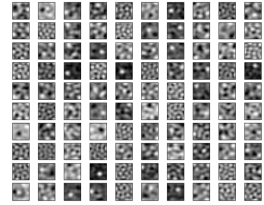


Figure: Weight decay filters

- The hidden neurons essentially behave like edge detectors

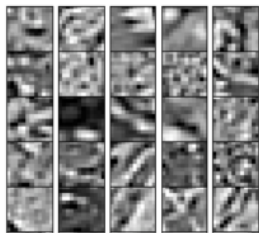


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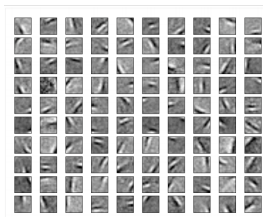


Figure: AE filters

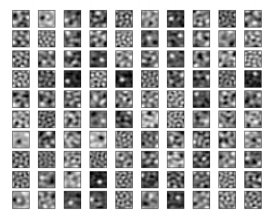
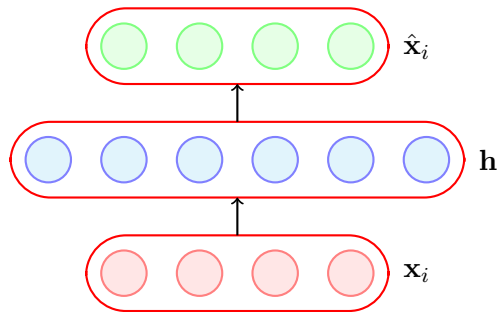
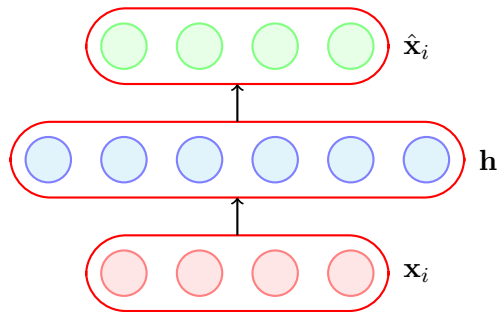


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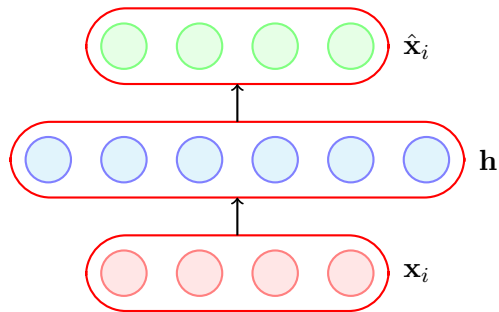
- The hidden neurons essentially behave like edge detectors
- PCA does not give such edge detectors

Module 7.5: Sparse Autoencoders

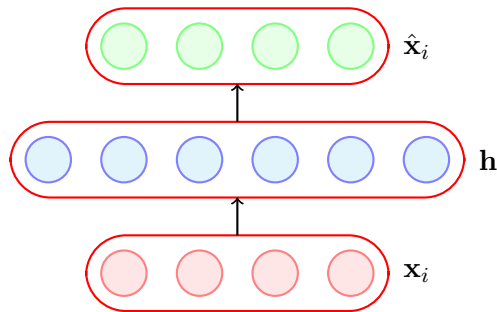




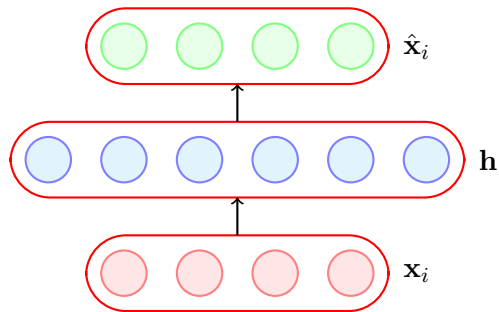
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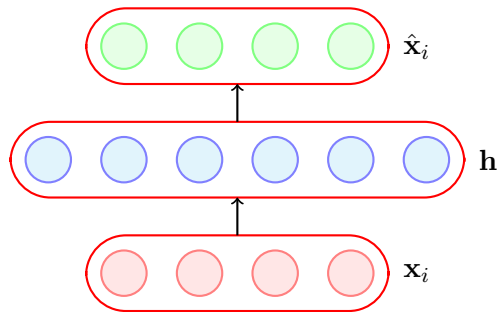
- A hidden neuron with sigmoid activation will have values between 0 and 1
- We say that the neuron is activated when its output is close to 1 and not activated when its output is close to 0.
- A sparse autoencoder tries to ensure the neuron is inactive most of the times.



- If the neuron l is sparse (i.e. mostly inactive) then $\hat{\rho}_l \rightarrow 0$

The average value of the activation of a neuron l is given by

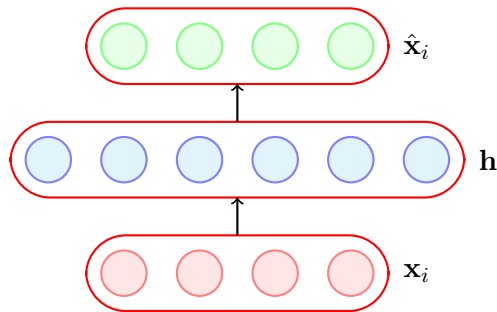
$$\hat{\rho}_l = \frac{1}{m} \sum_{i=1}^m h(\mathbf{x}_i)_l$$



- If the neuron l is sparse (i.e. mostly inactive) then $\hat{\rho}_l \rightarrow 0$
- A sparse autoencoder uses a sparsity parameter ρ (typically very close to 0, say, 0.005) and tries to enforce the constraint $\hat{\rho}_l = \rho$

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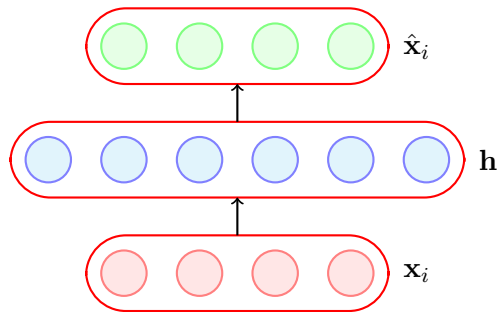


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- A sparse autoencoder uses a sparsity parameter ρ (typically very close to 0, say, 0.005) and tries to enforce the constraint $\hat{\rho}_l = \rho$
- One way of ensuring this is to add the following term to the objective function

The average value of the activation of a neuron l is given by

$$\hat{\rho}_l = \frac{1}{m} \sum_{i=1}^m h(\mathbf{x}_i)_l$$

$$\Omega(\theta) = \sum_{l=1}^k \rho \log \frac{\rho}{\hat{\rho}_l} + (1 - \rho) \log \frac{1 - \rho}{1 - \hat{\rho}_l}$$



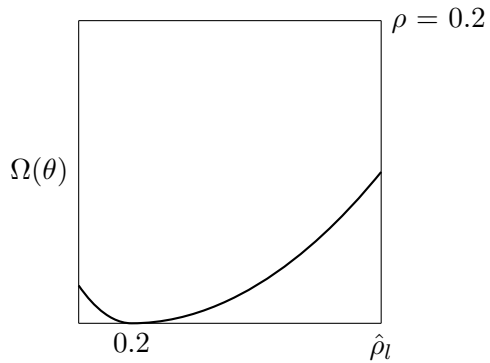
- If the neuron l is sparse (i.e. mostly inactive) then $\hat{\rho}_l \rightarrow 0$
- A sparse autoencoder uses a sparsity parameter ρ (typically very close to 0, say, 0.005) and tries to enforce the constraint $\hat{\rho}_l = \rho$
- One way of ensuring this is to add the following term to the objective function

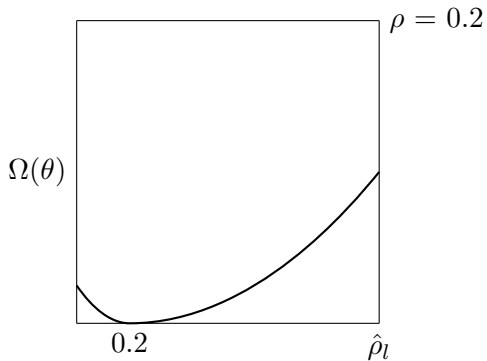
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- When will this term reach its minimum value and what is the minimum value? Let us plot it and check.





- The function will reach its minimum value(s) when $\hat{\rho}_l = \rho$.

- Now,

$$\hat{\mathcal{L}}(\theta) = \mathcal{L}(\theta) + \Omega(\theta)$$

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By Chain rule:

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and $\frac{\partial \hat{\rho}_l}{\partial W} = \mathbf{x}_i (g'(W^T \mathbf{x}_i + \mathbf{b}))^T$ (see next slide)

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- We already know how to calculate $\frac{\partial \mathcal{L}(\theta)}{\partial W}$
- Let us see how to calculate $\frac{\partial \Omega(\theta)}{\partial W}$.
- Finally,

$$\frac{\partial \hat{\mathcal{L}}(\theta)}{\partial W} = \frac{\partial \mathcal{L}(\theta)}{\partial W} + \frac{\partial \Omega(\theta)}{\partial W}$$

(and we know how to calculate both terms on R.H.S)

Derivation

$$\frac{\partial \hat{\rho}}{\partial W} = \left[\frac{\partial \hat{\rho}_1}{\partial W} \quad \frac{\partial \hat{\rho}_2}{\partial W} \quad \dots \quad \frac{\partial \hat{\rho}_k}{\partial W} \right]$$

For each element in the above equation we can calculate $\frac{\partial \hat{\rho}_l}{\partial W}$ (which is the partial derivative of a scalar w.r.t. a matrix = matrix). For a single element of a matrix W_{jl} :-

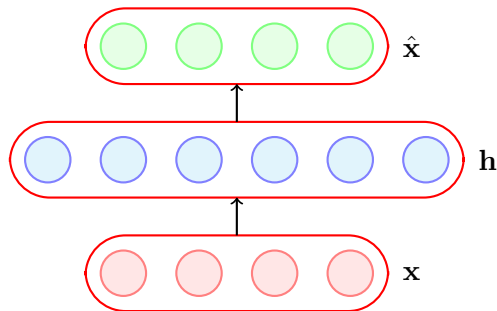
$$\begin{aligned} \frac{\partial \hat{\rho}_l}{\partial W_{jl}} &= \frac{\partial \left[\frac{1}{m} \sum_{i=1}^m g(W_{:,l}^T \mathbf{x}_i + b_l) \right]}{\partial W_{jl}} \\ &= \frac{1}{m} \sum_{i=1}^m \frac{\partial \left[g(W_{:,l}^T \mathbf{x}_i + b_l) \right]}{\partial W_{jl}} \\ &= \frac{1}{m} \sum_{i=1}^m g'(W_{:,l}^T \mathbf{x}_i + b_l) x_{ij} \end{aligned}$$

So in matrix notation we can write it as :

$$\frac{\partial \hat{\rho}_l}{\partial W} = \mathbf{x}_i (g'(W^T \mathbf{x}_i + \mathbf{b}))^T$$

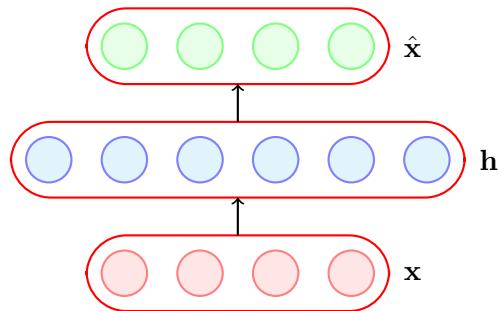
Module 7.6: Contractive Autoencoders

- A contractive autoencoder also tries to prevent an overcomplete autoencoder from learning the identity function.



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- It does so by adding the following regularization term to the loss function

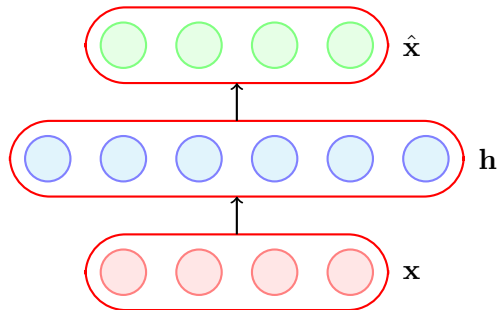
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where $J_{\mathbf{x}}(\mathbf{h})$ is the Jacobian of the encoder.

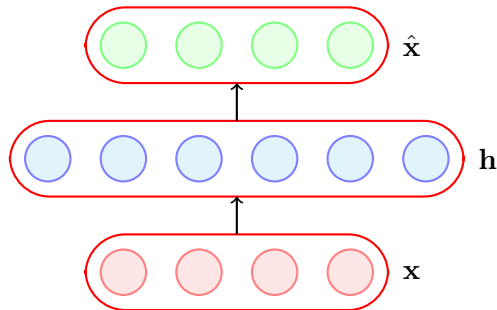


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- Let us see what it looks like.



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$$J_{\mathbf{x}}(\mathbf{h}) = \begin{bmatrix} \frac{\partial h_1}{\partial x_1} & \cdots & \cdots & \cdots & \frac{\partial h_1}{\partial x_n} \\ \frac{\partial h_2}{\partial x_1} & \cdots & \cdots & \cdots & \frac{\partial h_2}{\partial x_n} \\ \vdots & & \ddots & & \vdots \\ \frac{\partial h_k}{\partial x_1} & \cdots & \cdots & \cdots & \frac{\partial h_k}{\partial x_n} \end{bmatrix}$$

- If the input has n dimensions and the hidden layer has k dimensions then
- In other words, the (l, j) entry of the Jacobian captures the variation in the output of the l^{th} neuron with a small variation in the j^{th} input.

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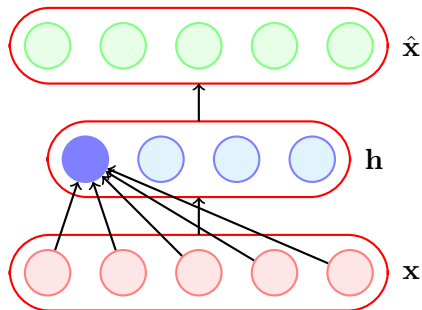
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$$\|J_{\mathbf{x}}(\mathbf{h})\|_F^2 = \sum_{j=1}^n \sum_{l=1}^k \left(\frac{\partial h_l}{\partial x_j} \right)^2$$

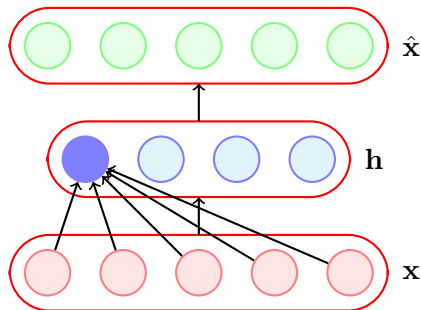
- What is the intuition behind this ?

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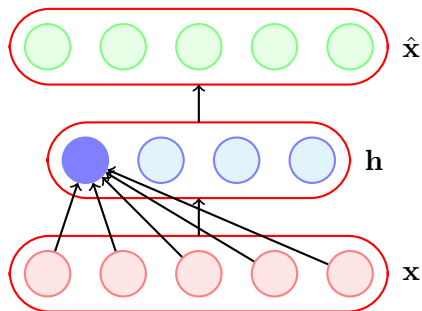
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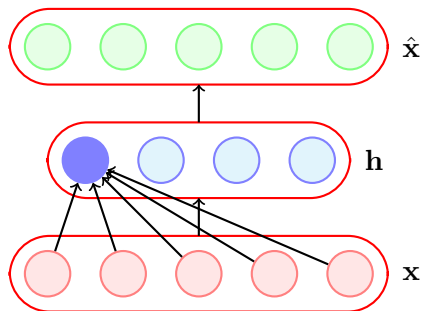
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- It means that this neuron is not very sensitive to variations in the input x_1 .

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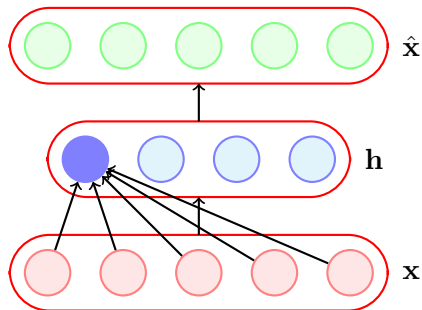
- What is the intuition behind this ?
- Consider $\frac{\partial h_1}{\partial x_1}$, what does it mean if $\frac{\partial h_1}{\partial x_1} = 0$
- It means that this neuron is not very sensitive to variations in the input x_1 .
- But doesn't this contradict our other goal of minimizing $\mathcal{L}(\theta)$ which requires \mathbf{h} to capture variations in the input.

$$\|J_{\mathbf{x}}(\mathbf{h})\|_F^2 = \sum_{j=1}^n \sum_{l=1}^k \left(\frac{\partial h_l}{\partial x_j} \right)^2$$



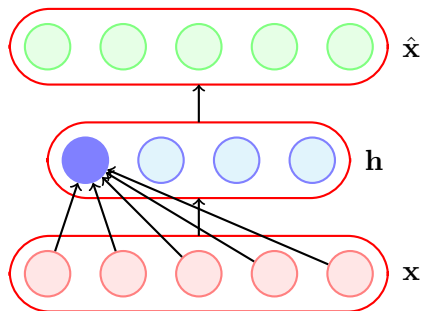
- Indeed it does and that's the idea

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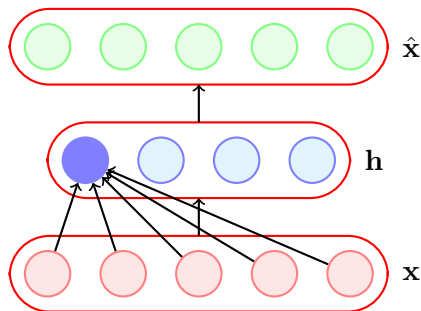
- Indeed it does and that's the idea
- By putting these two contradicting objectives against each other we ensure that \mathbf{h} is sensitive to only very important variations as observed in the training data.

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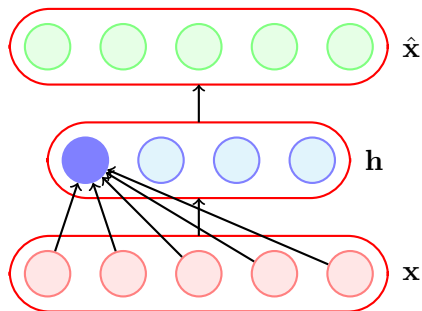
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- $\mathcal{L}(\theta)$ - capture important variations in data

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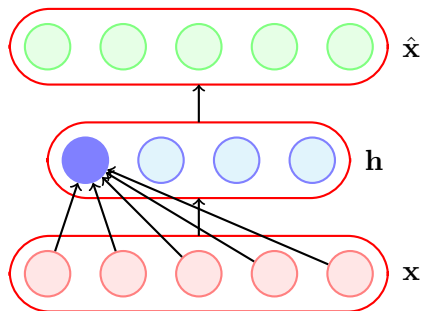
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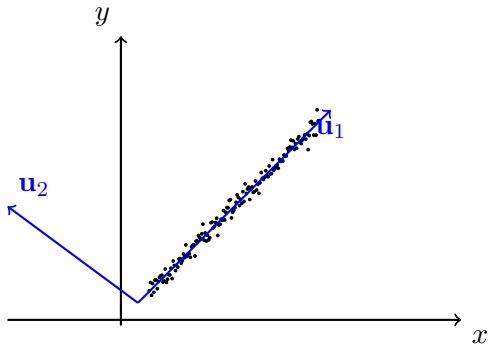


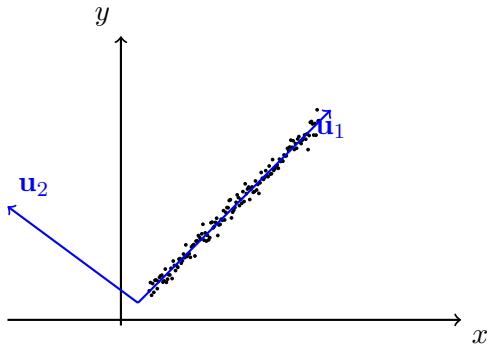
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- $\Omega(\theta)$ - do not capture variations in data
- Tradeoff - capture only very important variations in the data

$$\|J_{\mathbf{x}}(\mathbf{h})\|_F^2 = \sum_{j=1}^n \sum_{l=1}^k \left(\frac{\partial h_l}{\partial x_j} \right)^2$$

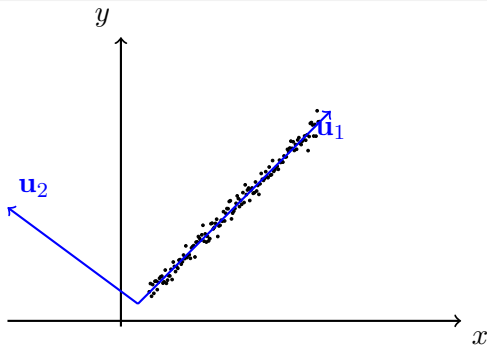


Let us try to understand this with the help of an illustration.

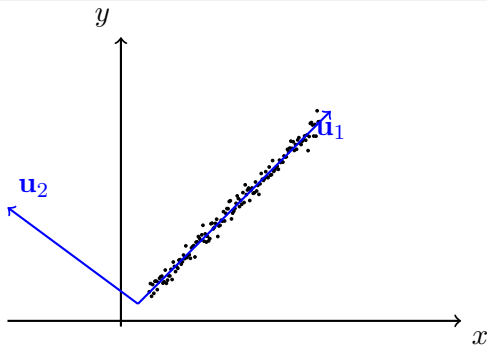




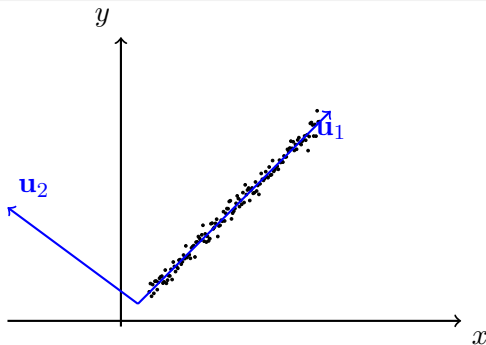
- Consider the variations in the data along directions \mathbf{u}_1 and \mathbf{u}_2



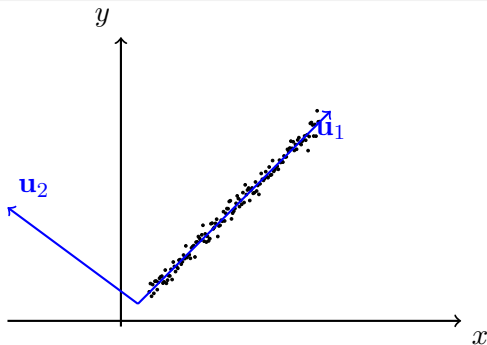
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- Consider the variations in the data along directions \mathbf{u}_1 and \mathbf{u}_2
- It makes sense to maximize a neuron to be sensitive to variations along \mathbf{u}_1
- At the same time it makes sense to inhibit a neuron from being sensitive to variations along \mathbf{u}_2 (as there seems to be small noise and unimportant for reconstruction)

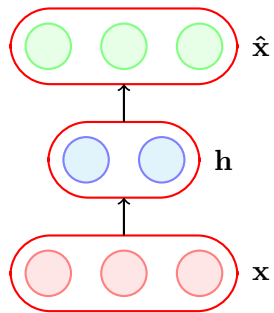


- Consider the variations in the data along directions \mathbf{u}_1 and \mathbf{u}_2
- It makes sense to maximize a neuron to be sensitive to variations along \mathbf{u}_1
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- By doing so we can balance between the contradicting goals of good reconstruction and low sensitivity.

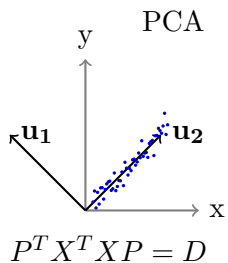


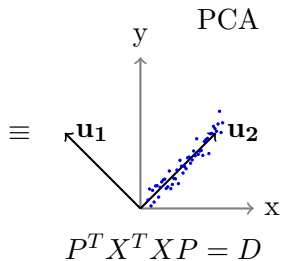
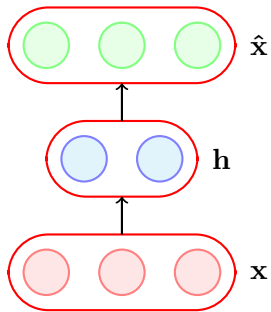
- Consider the variations in the data along directions \mathbf{u}_1 and \mathbf{u}_2
- It makes sense to maximize a neuron to be sensitive to variations along \mathbf{u}_1
- At the same time it makes sense to inhibit a neuron from being sensitive to variations along \mathbf{u}_2 (as there seems to be small noise and unimportant for reconstruction)
- By doing so we can balance between the contradicting goals of good reconstruction and low sensitivity.
- What does this remind you of ?

Module 7.7 : Summary

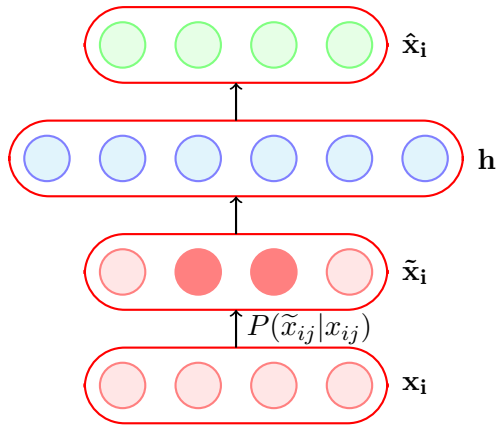


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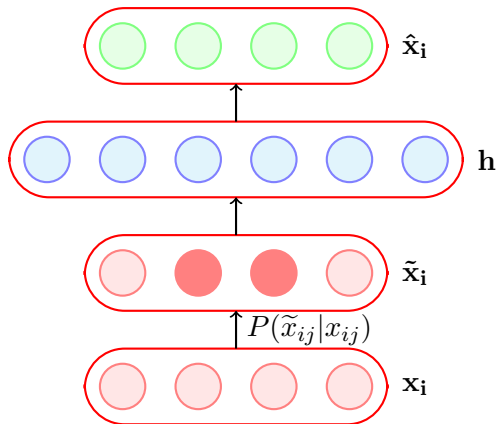


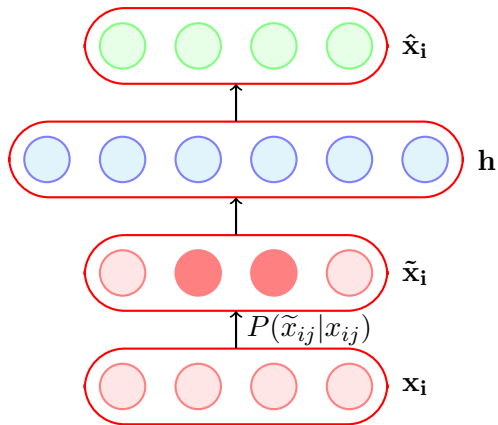


$$\min_{\theta} \|X - \underbrace{HW^*}_{\substack{U\Sigma V^T \\ \text{(SVD)}}}\|_F^2$$



Regularization

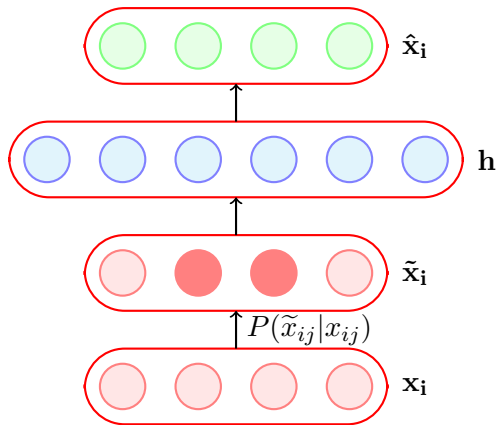




Regularization

$$\Omega(\theta) = \lambda \|\theta\|^2$$

Weight decaying



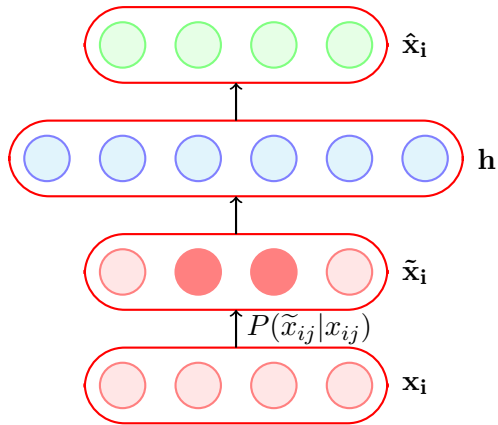
Regularization

$$\Omega(\theta) = \lambda \|\theta\|^2$$

Weight decaying

$$\Omega(\theta) = \sum_{l=1}^k \rho \log \frac{\rho}{\hat{\rho}_l} + (1 - \rho) \log \frac{1 - \rho}{1 - \hat{\rho}_l}$$

Sparse



Regularization

$$\Omega(\theta) = \lambda \|\theta\|^2 \quad \boxed{\text{Weight decaying}}$$

$$\Omega(\theta) = \sum_{l=1}^k \rho \log \frac{\rho}{\hat{\rho}_l} + (1 - \rho) \log \frac{1 - \rho}{1 - \hat{\rho}_l} \quad \boxed{\text{Sparse}}$$

$$\Omega(\theta) = \sum_{j=1}^n \sum_{l=1}^k \left(\frac{\partial h_l}{\partial x_j} \right)^2 \quad \boxed{\text{Contractive}}$$