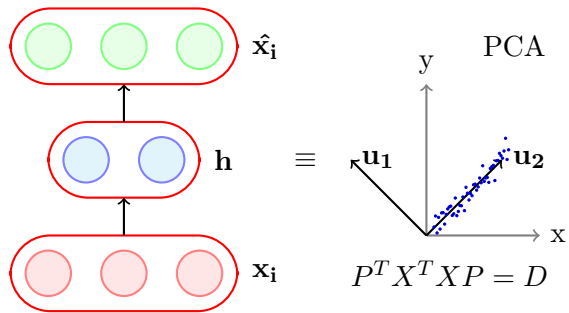
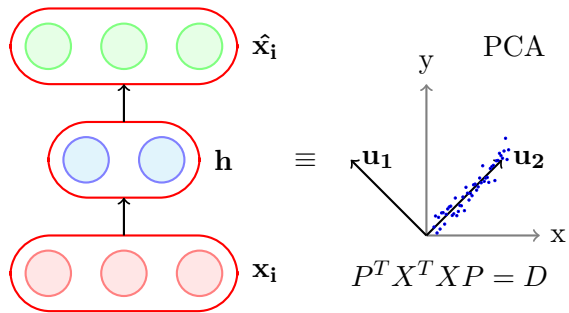


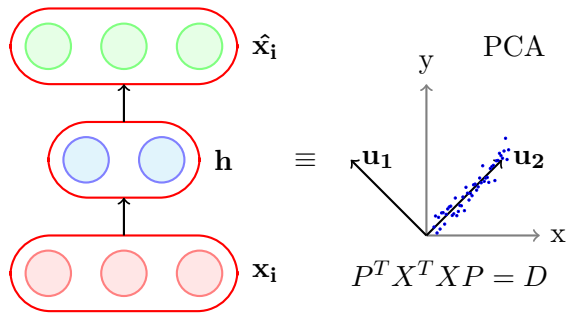
Module 7.2: Link between PCA and Autoencoders



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

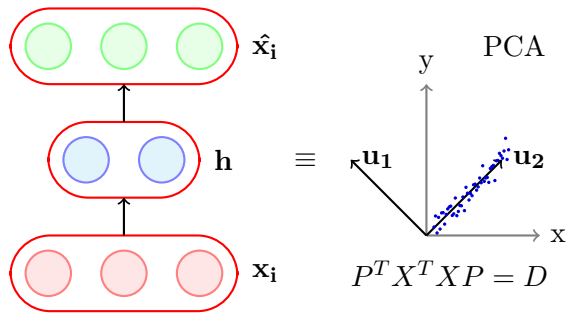


- We will now see that the encoder part of an autoencoder is equivalent to PCA if we
 - use a linear encoder



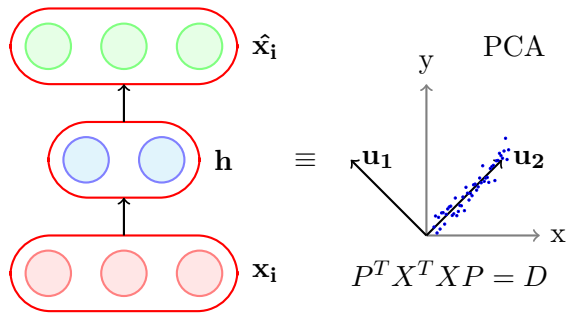
• We will now see that the encoder part of an autoencoder is equivalent to PCA if we

- use a linear encoder
- use a linear decoder



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

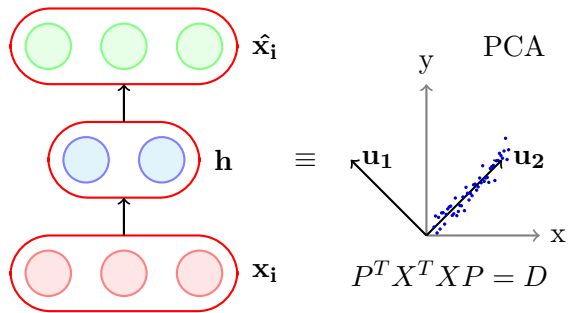
- use a linear encoder
- use a linear decoder
- use squared error loss function



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

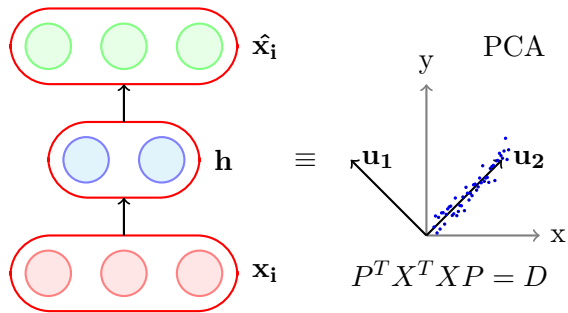
- use a linear encoder
- use a linear decoder
- use squared error loss function
- normalize the inputs to

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



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

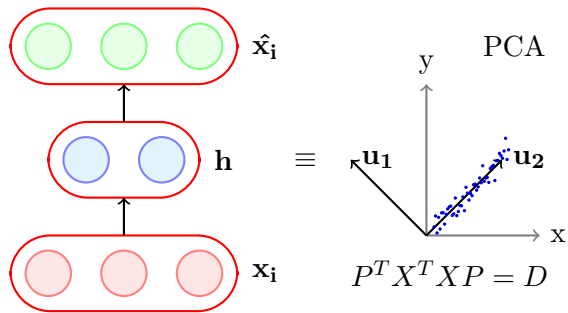
$$\hat{x}_{ij} = \frac{1}{\sqrt{m}} \left(x_{ij} - \frac{1}{m} \sum_{k=1}^m x_{kj} \right)$$



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

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

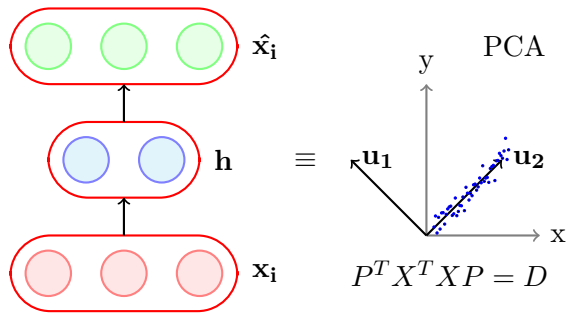
- The operation in the bracket ensures that the data now has 0 mean along each dimension j (we are subtracting the mean)



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

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

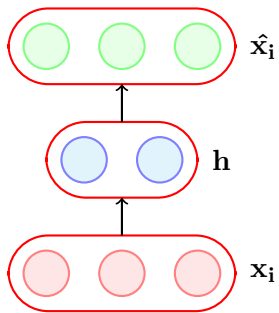
- The operation in the bracket ensures that the data now has 0 mean along each dimension j (we are subtracting the mean)
- Let X' be this zero mean data matrix then what the above normalization gives us is $X = \frac{1}{\sqrt{m}} X'$



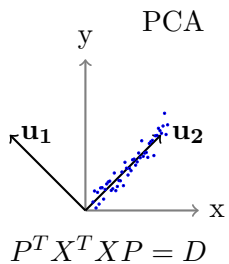
- First let us consider the implication of normalizing the inputs to

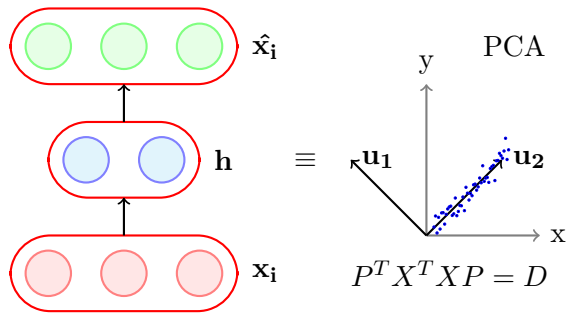
$$\hat{x}_{ij} = \frac{1}{\sqrt{m}} \left(x_{ij} - \frac{1}{m} \sum_{k=1}^m x_{kj} \right)$$

- The operation in the bracket ensures that the data now has 0 mean along each dimension j (we are subtracting the mean)
- 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)

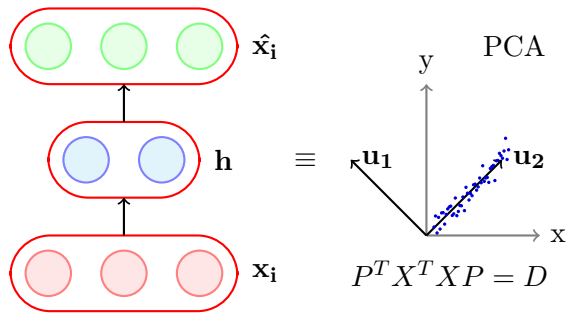


\equiv

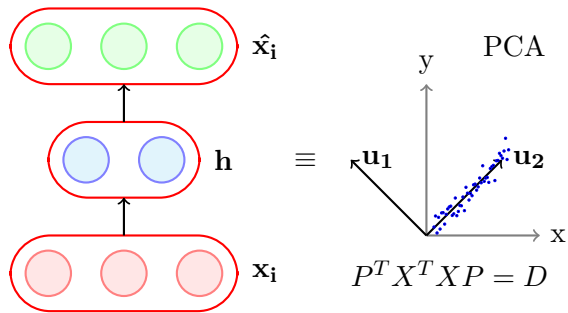




- First we will show that if we use linear decoder and a squared error loss function then

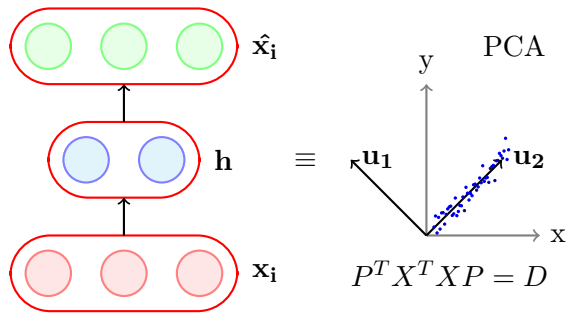


- First we will show that if we use linear decoder and a squared error loss function then
- The optimal solution to the following objective function



- First we will show that if we use linear decoder and a squared error loss function then
- The optimal solution to the following objective function

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



- First we will show that if we use linear decoder and a squared error loss function then
- The optimal solution to the following objective function

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

is obtained when we use a linear encoder.

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

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

- This is equivalent to

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

- This is equivalent to

$$\min_{W^*H} (\|X - HW^*\|_F)^2$$

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

- This is equivalent to

$$\min_{W^*H} (\|X - HW^*\|_F)^2 \qquad \|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n a_{ij}^2}$$

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

- This is equivalent to

$$\min_{W^*H} (\|X - HW^*\|_F)^2 \qquad \|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n a_{ij}^2}$$

(just writing the expression (1) in matrix form and using the definition of $\|A\|_F$) (we are ignoring the biases)

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

- This is equivalent to

$$\min_{W^*H} (\|X - HW^*\|_F)^2 \qquad \|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n a_{ij}^2}$$

(just writing the expression (1) in matrix form and using the definition of $\|A\|_F$) (we are ignoring the biases)

- From SVD we know that optimal solution to the above problem is given by

$$HW^* = U_{\cdot, \leq k} \Sigma_{k,k} V_{\cdot, \leq k}^T$$

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

- This is equivalent to

$$\min_{W^*H} (\|X - HW^*\|_F)^2 \qquad \|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n a_{ij}^2}$$

(just writing the expression (1) in matrix form and using the definition of $\|A\|_F$) (we are ignoring the biases)

- From SVD we know that optimal solution to the above problem is given by

$$HW^* = U_{\cdot, \leq k} \Sigma_{k,k} V_{\cdot, \leq k}^T$$

- By matching variables one possible solution is

$$\begin{aligned} H &= U_{\cdot, \leq k} \Sigma_{k,k} \\ W^* &= V_{\cdot, \leq k}^T \end{aligned}$$

We will now show that H is a linear encoding and find an expression for the encoder weights W

We will now show that H is a linear encoding and find an expression for the encoder weights W

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

We will now show that H is a linear encoding and find an expression for the encoder weights W

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

$$= (XX^T)(XX^T)^{-1}U_{., \leq K} \Sigma_{k,k}$$

$$(\text{pre-multiplying } (XX^T)(XX^T)^{-1} = I)$$

We will now show that H is a linear encoding and find an expression for the encoder weights W

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

$$= (XX^T)(XX^T)^{-1}U_{., \leq K} \Sigma_{k,k}$$

$$(pre-multiplying (XX^T)(XX^T)^{-1} = I)$$

$$= (XV\Sigma^T U^T)(U\Sigma V^T V\Sigma^T U^T)^{-1}U_{., \leq k} \Sigma_{k,k}$$

$$(using X = U\Sigma V^T)$$

We will now show that H is a linear encoding and find an expression for the encoder weights W

$$\begin{aligned} H &= U_{.,\leq k} \Sigma_{k,k} \\ &= (XX^T)(XX^T)^{-1} U_{.,\leq K} \Sigma_{k,k} && \text{(pre-multiplying } (XX^T)(XX^T)^{-1} = I) \\ &= (XV\Sigma^T U^T)(U\Sigma V^T V\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && \text{(using } X = U\Sigma V^T) \\ &= XV\Sigma^T U^T (U\Sigma\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && (V^T V = I) \end{aligned}$$

We will now show that H is a linear encoding and find an expression for the encoder weights W

$$\begin{aligned}
 H &= U_{.,\leq k} \Sigma_{k,k} \\
 &= (XX^T)(XX^T)^{-1} U_{.,\leq K} \Sigma_{k,k} && \text{(pre-multiplying } (XX^T)(XX^T)^{-1} = I) \\
 &= (XV\Sigma^T U^T)(U\Sigma V^T V\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && \text{(using } X = U\Sigma V^T) \\
 &= XV\Sigma^T U^T (U\Sigma\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && (V^T V = I) \\
 &= XV\Sigma^T U^T U (\Sigma\Sigma^T)^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && ((ABC)^{-1} = C^{-1}B^{-1}A^{-1})
 \end{aligned}$$

We will now show that H is a linear encoding and find an expression for the encoder weights W

$$\begin{aligned}
 H &= U_{.,\leq k} \Sigma_{k,k} \\
 &= (XX^T)(XX^T)^{-1}U_{.,\leq K} \Sigma_{k,k} && \text{(pre-multiplying } (XX^T)(XX^T)^{-1} = I) \\
 &= (XV\Sigma^T U^T)(U\Sigma V^T V\Sigma^T U^T)^{-1}U_{.,\leq k} \Sigma_{k,k} && \text{(using } X = U\Sigma V^T) \\
 &= XV\Sigma^T U^T (U\Sigma\Sigma^T U^T)^{-1}U_{.,\leq k} \Sigma_{k,k} && (V^T V = I) \\
 &= XV\Sigma^T U^T U (\Sigma\Sigma^T)^{-1}U^T U_{.,\leq k} \Sigma_{k,k} && ((ABC)^{-1} = C^{-1}B^{-1}A^{-1}) \\
 &= XV\Sigma^T (\Sigma\Sigma^T)^{-1}U^T U_{.,\leq k} \Sigma_{k,k} && (U^T U = I)
 \end{aligned}$$

We will now show that H is a linear encoding and find an expression for the encoder weights W

$$\begin{aligned}
 H &= U_{.,\leq k} \Sigma_{k,k} \\
 &= (XX^T)(XX^T)^{-1} U_{.,\leq K} \Sigma_{k,k} && \text{(pre-multiplying } (XX^T)(XX^T)^{-1} = I) \\
 &= (XV\Sigma^T U^T)(U\Sigma V^T V\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && \text{(using } X = U\Sigma V^T) \\
 &= XV\Sigma^T U^T (U\Sigma\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && (V^T V = I) \\
 &= XV\Sigma^T U^T U (\Sigma\Sigma^T)^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && ((ABC)^{-1} = C^{-1}B^{-1}A^{-1}) \\
 &= XV\Sigma^T (\Sigma\Sigma^T)^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && (U^T U = I) \\
 &= XV\Sigma^T \Sigma^{T^{-1}} \Sigma^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && ((AB)^{-1} = B^{-1}A^{-1})
 \end{aligned}$$

We will now show that H is a linear encoding and find an expression for the encoder weights W

$$\begin{aligned}
 H &= U_{.,\leq k} \Sigma_{k,k} \\
 &= (XX^T)(XX^T)^{-1} U_{.,\leq K} \Sigma_{k,k} && \text{(pre-multiplying } (XX^T)(XX^T)^{-1} = I) \\
 &= (XV\Sigma^T U^T)(U\Sigma V^T V\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && \text{(using } X = U\Sigma V^T) \\
 &= XV\Sigma^T U^T (U\Sigma\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && (V^T V = I) \\
 &= XV\Sigma^T U^T U (\Sigma\Sigma^T)^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && ((ABC)^{-1} = C^{-1}B^{-1}A^{-1}) \\
 &= XV\Sigma^T (\Sigma\Sigma^T)^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && (U^T U = I) \\
 &= XV\Sigma^T \Sigma^{T^{-1}} \Sigma^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && ((AB)^{-1} = B^{-1}A^{-1}) \\
 &= XV\Sigma^{-1} I_{.,\leq k} \Sigma_{k,k} && (U^T U_{.,\leq k} = I_{.,\leq k})
 \end{aligned}$$

We will now show that H is a linear encoding and find an expression for the encoder weights W

$$\begin{aligned}
 H &= U_{.,\leq k} \Sigma_{k,k} \\
 &= (XX^T)(XX^T)^{-1} U_{.,\leq K} \Sigma_{k,k} && \text{(pre-multiplying } (XX^T)(XX^T)^{-1} = I) \\
 &= (XV\Sigma^T U^T)(U\Sigma V^T V\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && \text{(using } X = U\Sigma V^T) \\
 &= XV\Sigma^T U^T (U\Sigma\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && (V^T V = I) \\
 &= XV\Sigma^T U^T U (\Sigma\Sigma^T)^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && ((ABC)^{-1} = C^{-1}B^{-1}A^{-1}) \\
 &= XV\Sigma^T (\Sigma\Sigma^T)^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && (U^T U = I) \\
 &= XV\Sigma^T \Sigma^{T^{-1}} \Sigma^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && ((AB)^{-1} = B^{-1}A^{-1}) \\
 &= XV\Sigma^{-1} I_{.,\leq k} \Sigma_{k,k} && (U^T U_{.,\leq k} = I_{.,\leq k}) \\
 &= XVI_{.,\leq k} && (\Sigma^{-1} I_{.,\leq k} = \Sigma_{k,k}^{-1})
 \end{aligned}$$

We will now show that H is a linear encoding and find an expression for the encoder weights W

$$\begin{aligned}
 H &= U_{.,\leq k} \Sigma_{k,k} \\
 &= (XX^T)(XX^T)^{-1} U_{.,\leq K} \Sigma_{k,k} && \text{(pre-multiplying } (XX^T)(XX^T)^{-1} = I) \\
 &= (XV\Sigma^T U^T)(U\Sigma V^T V\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && \text{(using } X = U\Sigma V^T) \\
 &= XV\Sigma^T U^T (U\Sigma\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && (V^T V = I) \\
 &= XV\Sigma^T U^T U (\Sigma\Sigma^T)^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && ((ABC)^{-1} = C^{-1}B^{-1}A^{-1}) \\
 &= XV\Sigma^T (\Sigma\Sigma^T)^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && (U^T U = I) \\
 &= XV\Sigma^T \Sigma^{T^{-1}} \Sigma^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && ((AB)^{-1} = B^{-1}A^{-1}) \\
 &= XV\Sigma^{-1} I_{.,\leq k} \Sigma_{k,k} && (U^T U_{.,\leq k} = I_{.,\leq k}) \\
 &= X V I_{.,\leq k} && (\Sigma^{-1} I_{.,\leq k} = \Sigma_{k,k}^{-1}) \\
 H &= X V_{.,\leq k}
 \end{aligned}$$

We will now show that H is a linear encoding and find an expression for the encoder weights W

$$\begin{aligned}
 H &= U_{.,\leq k} \Sigma_{k,k} \\
 &= (XX^T)(XX^T)^{-1} U_{.,\leq K} \Sigma_{k,k} && \text{(pre-multiplying } (XX^T)(XX^T)^{-1} = I) \\
 &= (XV\Sigma^T U^T)(U\Sigma V^T V\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && \text{(using } X = U\Sigma V^T) \\
 &= XV\Sigma^T U^T (U\Sigma\Sigma^T U^T)^{-1} U_{.,\leq k} \Sigma_{k,k} && (V^T V = I) \\
 &= XV\Sigma^T U^T U (\Sigma\Sigma^T)^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && ((ABC)^{-1} = C^{-1}B^{-1}A^{-1}) \\
 &= XV\Sigma^T (\Sigma\Sigma^T)^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && (U^T U = I) \\
 &= XV\Sigma^T \Sigma^{T^{-1}} \Sigma^{-1} U^T U_{.,\leq k} \Sigma_{k,k} && ((AB)^{-1} = B^{-1}A^{-1}) \\
 &= XV\Sigma^{-1} I_{.,\leq k} \Sigma_{k,k} && (U^T U_{.,\leq k} = I_{.,\leq k}) \\
 &= X V I_{.,\leq k} && (\Sigma^{-1} I_{.,\leq k} = \Sigma_{k,k}^{-1}) \\
 H &= X V_{.,\leq k}
 \end{aligned}$$

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

- We have encoder $W = V_{\cdot, \leq k}$

- We have encoder $W = V_{\cdot, \leq k}$
- From SVD, we know that V is the matrix of eigen vectors of $X^T X$

- We have encoder $W = V_{\cdot, \leq k}$
- From SVD, we know that V is the matrix of eigen vectors of $X^T X$
- From PCA, we know that P is the matrix of the eigen vectors of the covariance matrix

- We have encoder $W = V_{\cdot, \leq k}$
- From SVD, we know that V is the matrix of eigen vectors of $X^T X$
- From PCA, we know that P is the matrix of the eigen vectors of the covariance matrix
- We saw earlier that, if entries of X are normalized by

- We have encoder $W = V_{\cdot, \leq k}$
- From SVD, we know that V is the matrix of eigen vectors of $X^T X$
- From PCA, we know that P is the matrix of the eigen vectors of the covariance matrix
- We saw earlier that, if entries of X are normalized by

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

- We have encoder $W = V_{\cdot, \leq k}$
- From SVD, we know that V is the matrix of eigen vectors of $X^T X$
- From PCA, we know that P is the matrix of the eigen vectors of the covariance matrix
- We saw earlier that, if entries of X are normalized by

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

then $X^T X$ is indeed the covariance matrix

- We have encoder $W = V_{.,\leq k}$
- From SVD, we know that V is the matrix of eigen vectors of $X^T X$
- From PCA, we know that P is the matrix of the eigen vectors of the covariance matrix
- We saw earlier that, if entries of X are normalized by

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

then $X^T X$ is indeed the covariance matrix

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

Remember

The encoder of a linear autoencoder is equivalent to PCA if we

Remember

The encoder of a linear autoencoder is equivalent to PCA if we

- use a linear encoder

Remember

The encoder of a linear autoencoder is equivalent to PCA if we

- use a linear encoder
- use a linear decoder

Remember

The encoder of a linear autoencoder is equivalent to PCA if we

- use a linear encoder
- use a linear decoder
- use a squared error loss function

Remember

The encoder of a linear autoencoder is equivalent to PCA if we

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

Remember

The encoder of a linear autoencoder is equivalent to PCA if we

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

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