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Autoencoders and their Applications

COMP90073
Security Analytics

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Semester 2, 2021

Outline

- Introduction to Neural Networks
- Gradient Decent Learning
- Autoencoders and their architectures
- Denoising Autoencoder (DAE)
- Variational Autoencoder (VAE)

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Artificial Neural Networks

- A collection of simple, trainable mathematical units that collectively learn complex functions

- Given sufficient training data an artificial neural network can approximate very complex functions mapping raw data to output decisions

Artificial Neural Networks

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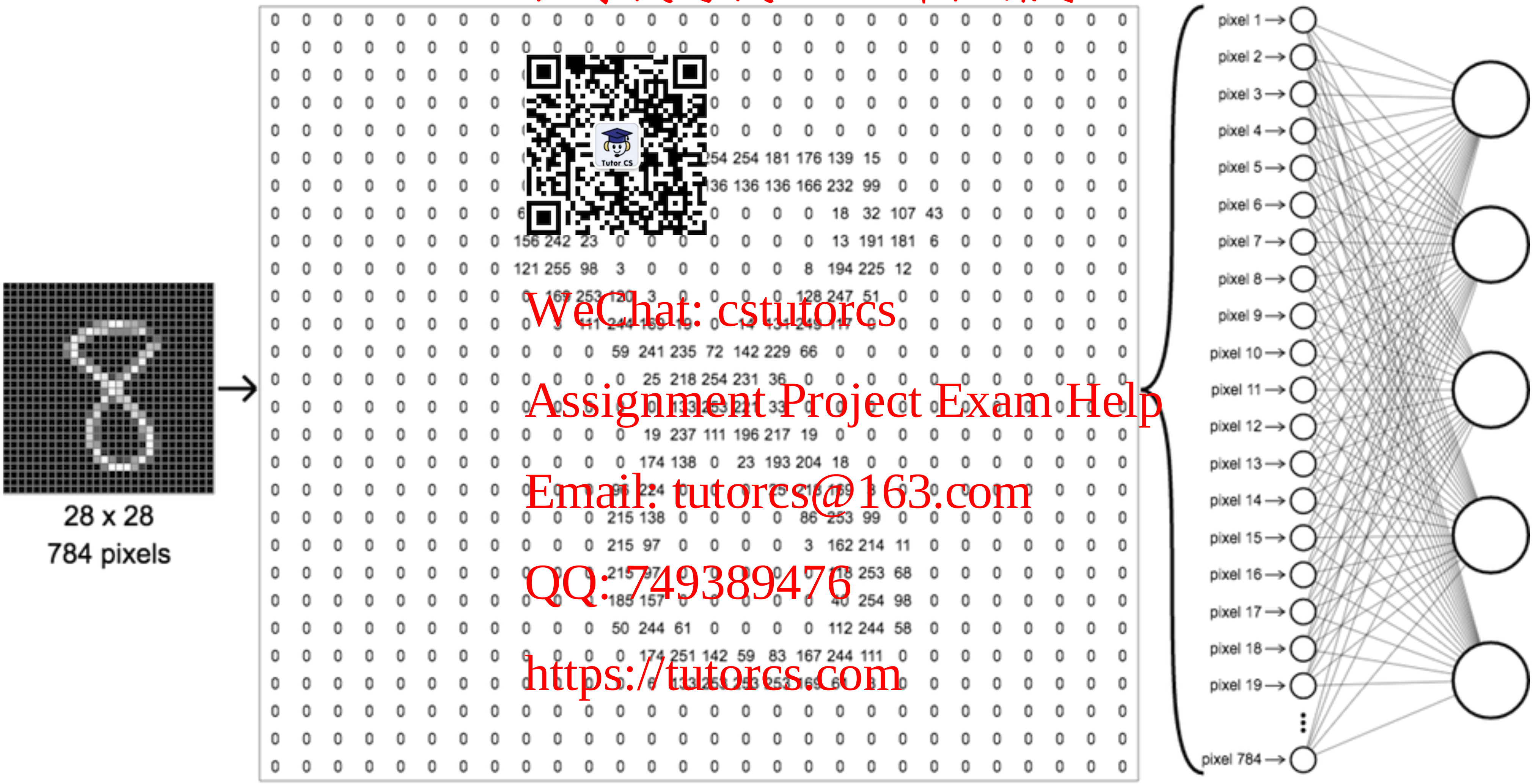
Artificial Neural Networks



Artificial Neural Networks

Types of Deep Neural Networks (DNNs)

1. DNN – all fully connected layers

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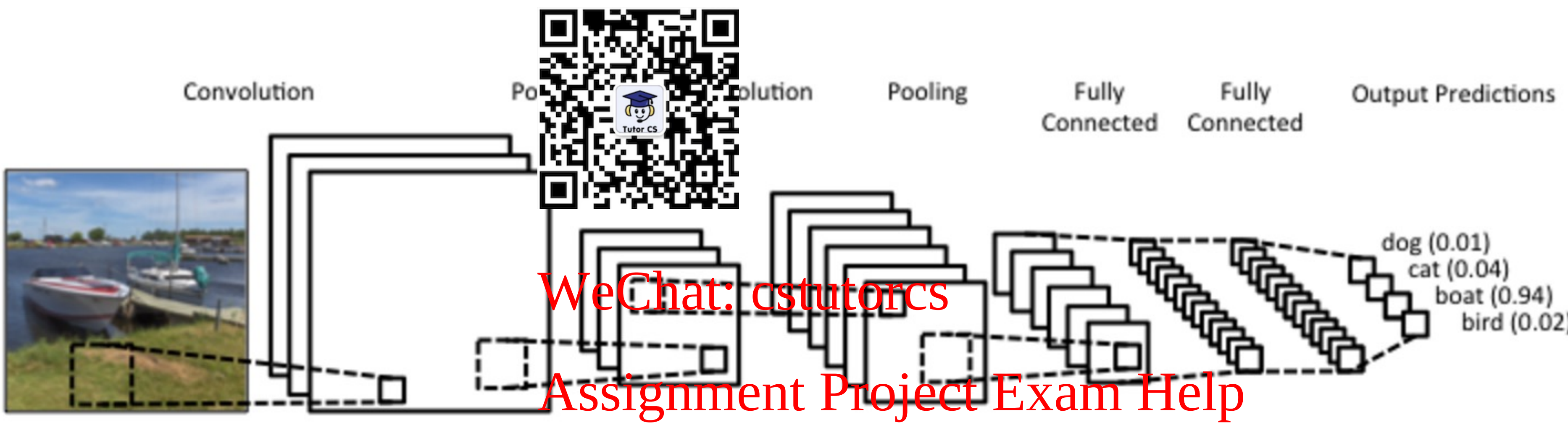
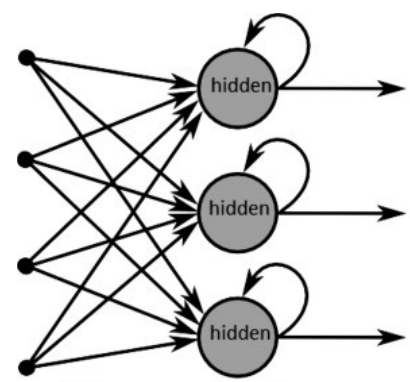
Types of Deep Neural Networks (DNNs)

2. CNNs (Convolutional Neural Networks) – some convolutional layers

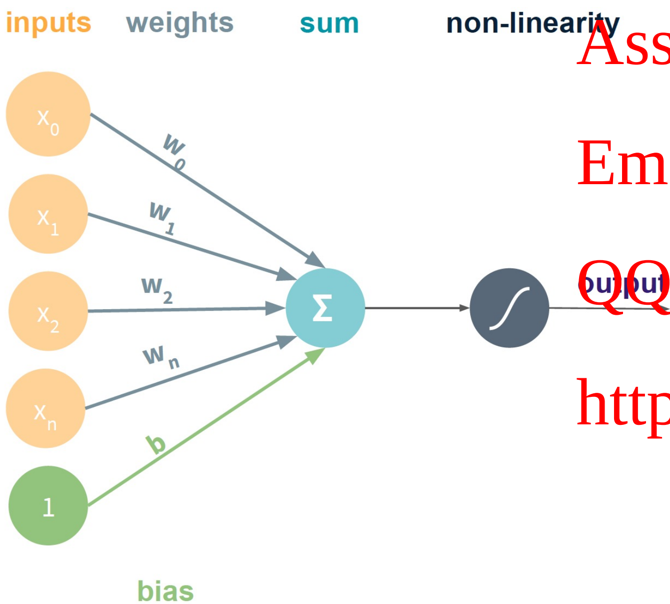


3. RNNs (Recurrent Neural Networks) – LSTM



Fundamentals of Neural Networks

- Receive signals from input neurons: $x_1, x_2, \dots, x_n$
- Weight signals according strength between neurons: $w_1x_1, w_2x_2, \dots, w_nx_n$
- Add the input signals and $_1, w_2x_2, \dots, w_nx_n + b = \sum_{i=1}^{n} w_i x_i + b$
- Emit an output signal: activation function f



Activation Function

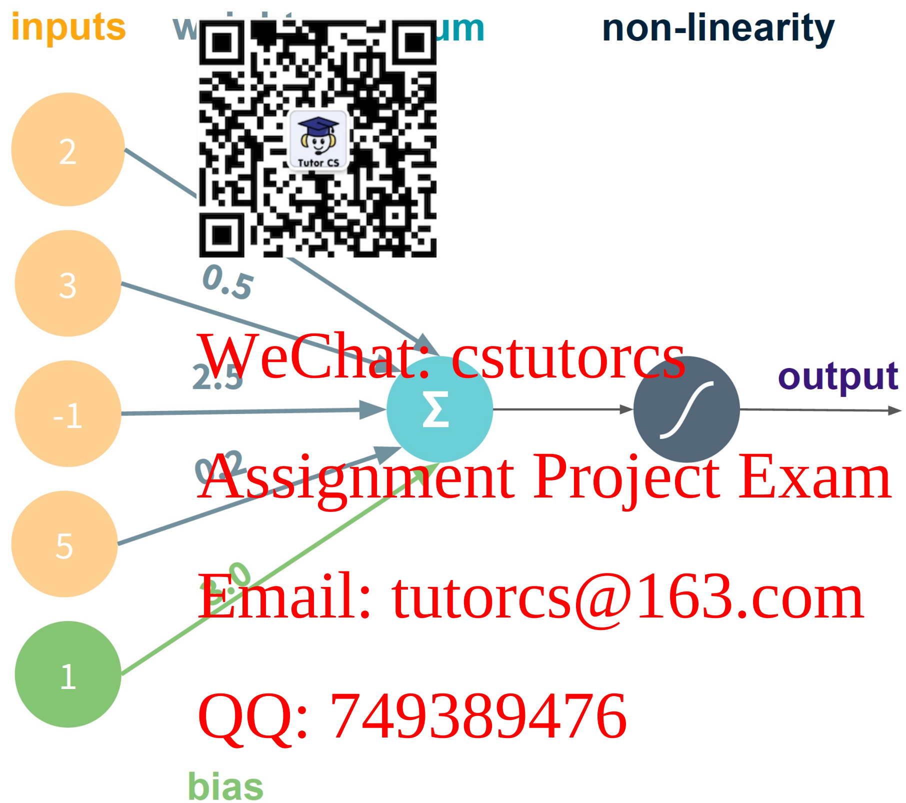
$$output = f\left(\sum_{i=1}^{n} w_i x_i + b\right)$$

Activation Functions

- Activation functions add non-linearity to our network's function
- Most real-world problems are non-linear

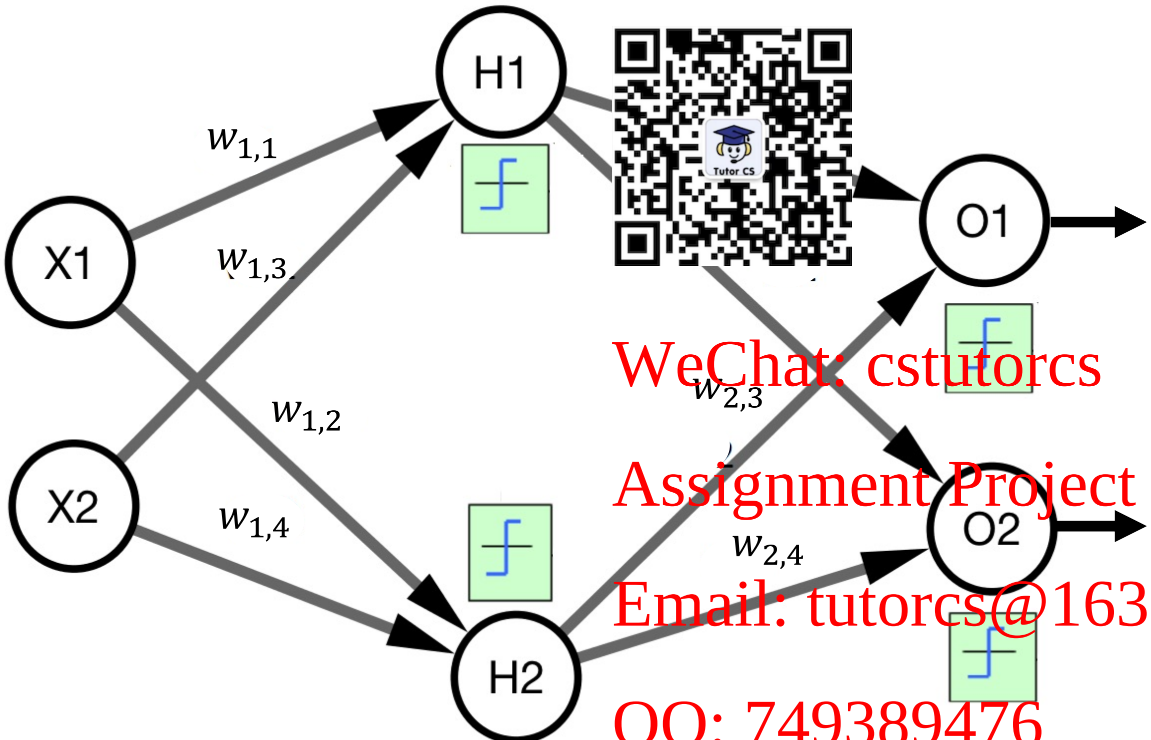
Common Activation Functions:

Fundamentals of Neural Networks



$$output = sigmoid(2\times0.1 + 3\times0.5\ + (-1)\times2.5 + 5\times0.2 + 1\times3) = 0.96$$

Functional Form of Neural Networks



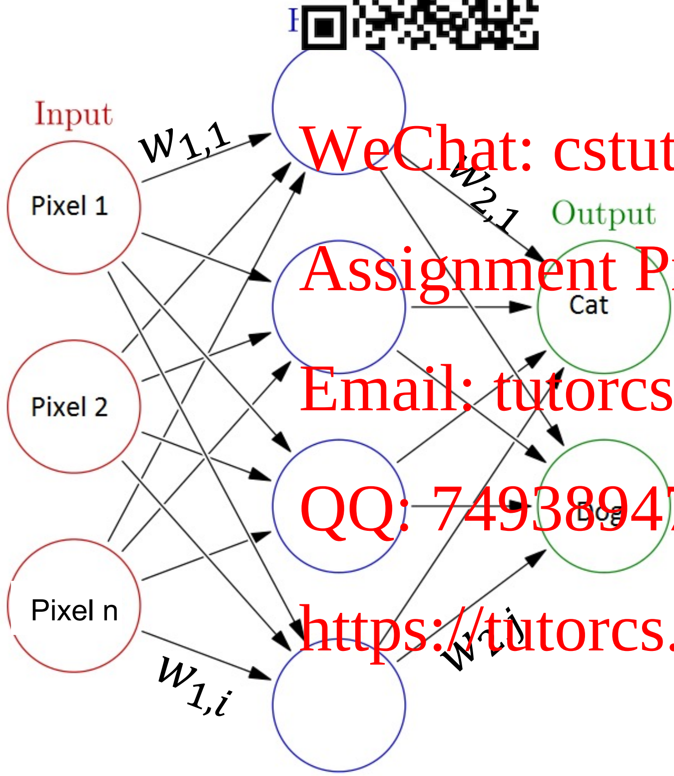
Feed-Forward pass:

$$H_1 = f_1(X_1 w_{1,1} + X_2 w_{1,3})$$
$$H_2 = f_1(X_1 w_{1,2} + X_2 w_{1,4})$$
$$O_1 = f_2(H_1 w_{2,1} + H_2 w_{2,3})$$
$$O_2 = f_2(H_1 w_{2,2} + H_2 w_{2,4})$$

Training a Neural Network

- Find a set of weights so that the network exhibits the desired behaviour
- Example: cat vs. dog



Output	Label	
0.8,0.7	1,1	(Cat & dog)
0.08,0.6	0,1	(Dog)
0.92,0.01	1,0	(Cat)
0.02, 0.0	0,0	(No cat or dog)

Error Function

- Measure the difference between actual output and expected output
- One popular measure: sum-squared error

$$E(input, weights, label) = \sum (output - label)^2$$

- Note: Neural network is a composite/nested function that map the input to the output.

$$output = f_{NN}(input, weights)$$

Gradient Decent Learning

- A training example is a vector of inputs and the desirable output(s), i.e., $(\{x_1, x_2, \dots, x_n\}, \{t_1, t_2, \dots, t_m\})$, $t_i = 1$ iff the data point $\{x_1, x_2, \dots, x_n\}$, belongs to the ith class.
- **Objective:** finding the weights that minimise the difference between t and o (predicted output) for each of our training inputs.
- Define an error function E to be the sum of squared errors.

$$E = \frac{1}{2} \sum_{k=1} (o_k - t_k)^2$$

- If we think of E as height, it defines an error landscape on the weight space. *The aim is to find a set of weights for which E is very low.*

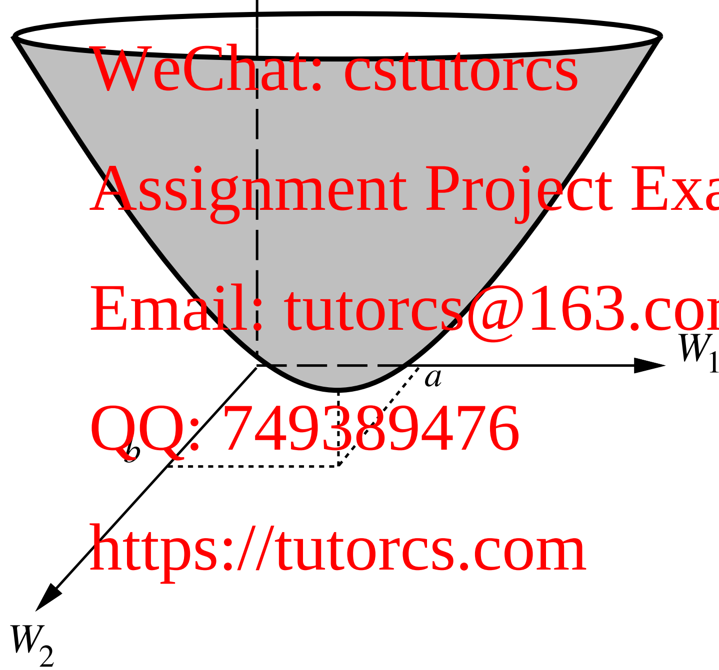
- This is done by moving in the steepest downhill direction (Gradient descent), i.e., $-\frac{\partial E}{\partial w_i}$

$$w_i \leftarrow w_i - \eta \frac{\partial E}{\partial w_i}$$

Weight update rule
η : Learning rate

Example Error Landscape

- An example error landscape for gradient descent search in weight space



Intuition of Gradient Descent Learning

$$w_1 = w_0 - \eta \frac{\partial E}{\partial w}(w_0)$$

$$w_2 = w_1 - \eta \frac{\partial E}{\partial w}(w_1)$$

$$\vdots$$

$$w_{\text{optimal}}$$

Negative gradient points towards a local minimum.

Weight update rule

To derive the weight update rule, we need to remember the chain rule from differential calculus:

if $y = y(u)$ and $u = u$

then $\partial y/\partial x = (\partial y/\partial u)($

So, if $\mathrm{E} = \frac{1}{2}\sum(o-t)^2$, $o = \sum w_i x_i + b$, and $\mathrm{t} = $ true output

$$\frac{\partial E}{\partial w_i} = \frac{\partial\left[\frac{1}{2}(o-t)^2\right]}{\partial o}\frac{\partial o}{\partial w_i}$$

$$= (o-t)\ \frac{\partial o}{\partial w_i}$$

$$= (o-t)x$$

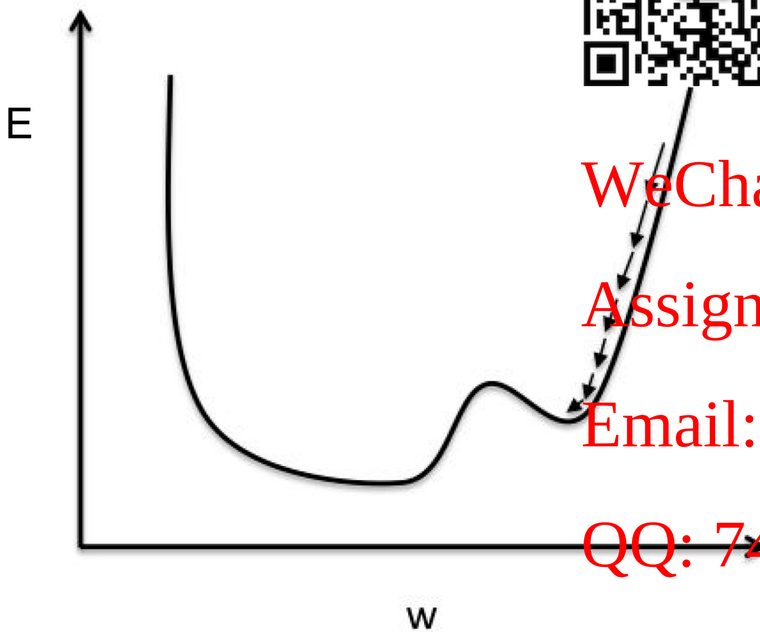
Normally we include a learning rate parameter η to control the update of weights in a stable manner

$$w_i \leftarrow w_i - \eta(o-t)x$$

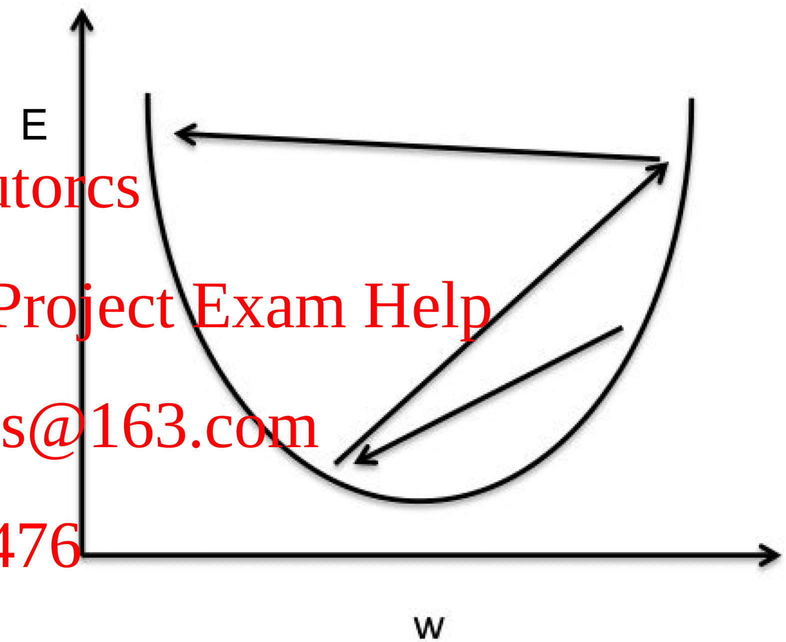
We repeatedly update the weights based on each example until the weights converge

Adjusting Learning Rate

- Learning rate parameter η is a small value (usually $0.0001 - 0.1$) to control the update of weights in a sta[illegible]er.



Small learning rate: Many iterations until convergence and trapping in local minima.



Large learning rate: Overshooting.

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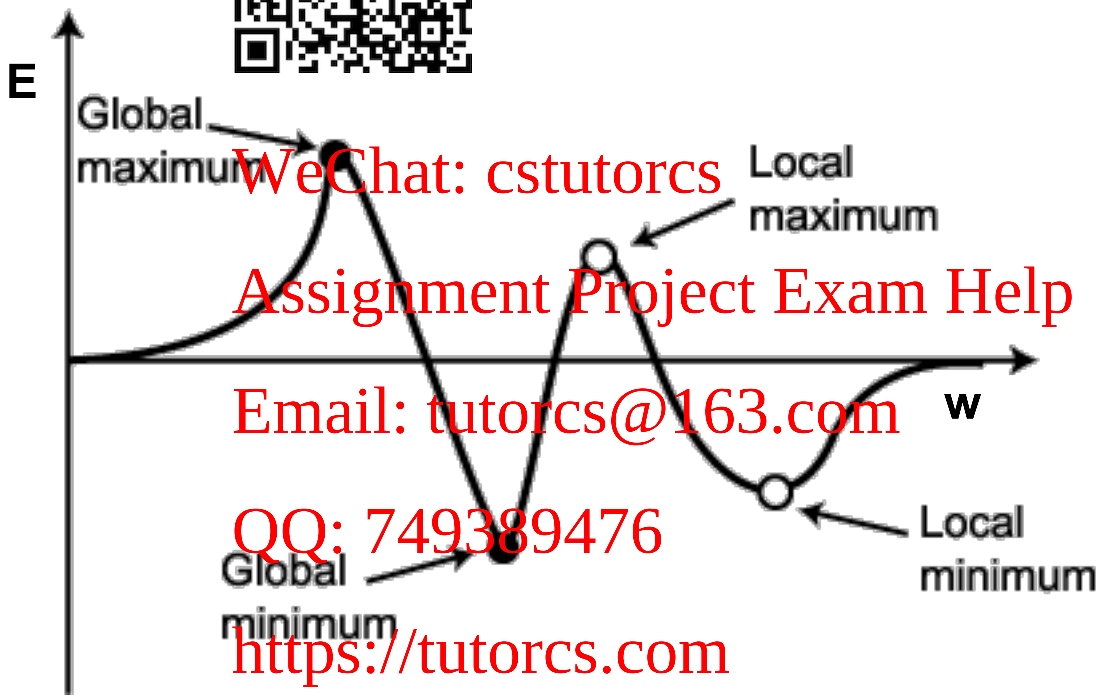
Minimizing Error by Gradient Descent

- The iterative algorithm might converge to one of the many local minima



Backpropagation Algorithm

Backpropagation(network, training data D, label T)

Initialise the weights ***w*** to small random values

Repeat

For each $d \in D, d =< x_1, \ldots, x_n, t_c >$

Forward pass: calculate hidden h_i and output O_j values

Backward pass:

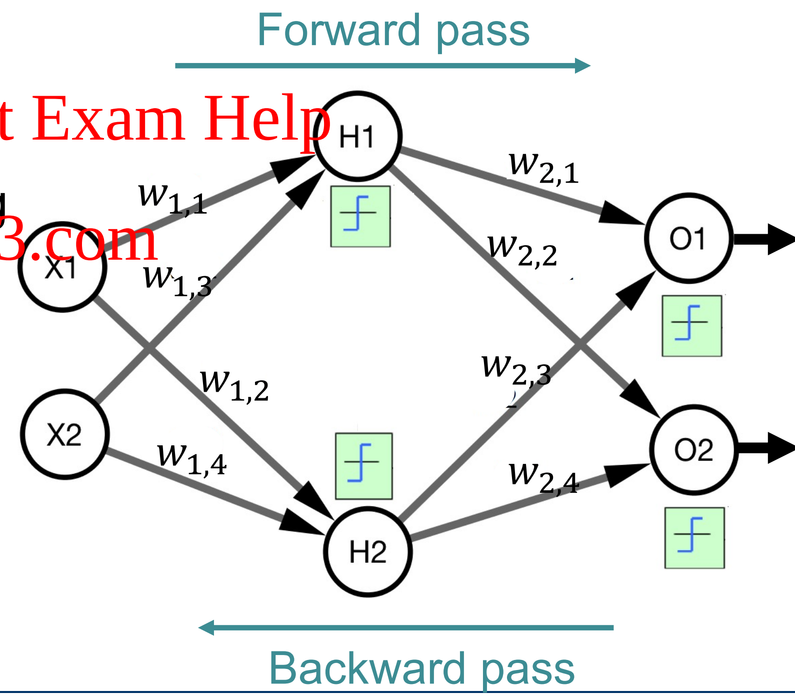
Calculate error between o_k and t_k at output

Update the weights in each layer $w_{i,j}$

(in proportion to their effect on the error using

gradient descent $w_i \leftarrow w_i - \eta(o - t)x$)

Until network has converged



Network Architectures/Parameters

- Number of input nodes = number of features
- Number of output nodes = [illegible] of classes
  - *Neural networks can [illegible] rally with multi-class classification problems (compare [illegible])*
- Number of hidden layers
- Number of nodes in each hidden layers
- Learning rate
- Regularization parameters (similar to C in SVM): control the complexity of the model, preventing overfitting.

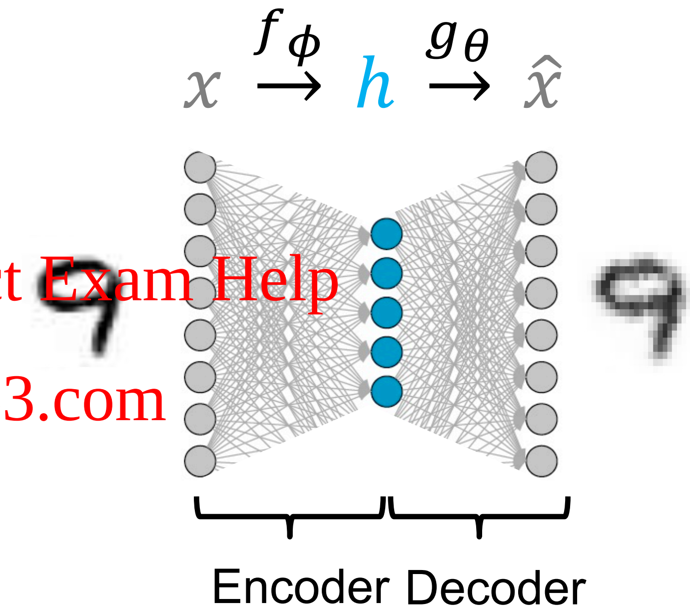
Live Demo:
http://playground.tensorflow.org/#activation=tanh&batchSize=10&dataset=circle&regDataset=reg-plane&learningRate=0.03&regularizationRate=0&noise=0&networkShape=4,2&seed=0.13820&showTestData=false&discretize=false&percTrainData=50&x=true&y=true&xTim

Autoencoder [1]

- A a neural net which aim is to take an input $x \in \mathbb{R}^d$ and reproduce it $\hat{x} \in \mathbb{R}^d$.
- To make this non-trivial, we [illegible]d a *bottleneck* layer $h \in \mathbb{R}^k$ whose dimension is much smaller t[illegible]ut, $k \ll d$.
- Architecture:
  - Encoder: $h = f_\phi(x) = sigmoid(Wx + b)$
  - Decoder: $\hat{x} = g_\theta(h) = sigmoid(\widehat{W}h + \hat{b})$
  - Often use tied weights, $\widehat{W} = W^T$
- Minimize a loss function

$$\mathcal{L}(\theta, \phi) = \frac{1}{2}\sum_{i=1}^{n}\left(x_i - \overbrace{g_\theta\left(f_\phi(x_i)\right)}^{\hat{x}_i}\right)^2$$

- Parameters are obtained using backpropagation
- Demo: https://cs.stanford.edu/people/karpathy/convnetjs/demo/autoencoder.html



Using AEs Unsupervised Problems

Only input vectors $\{x_1, x_2, \dots, x_n\}$ are available, not corresponding labels.

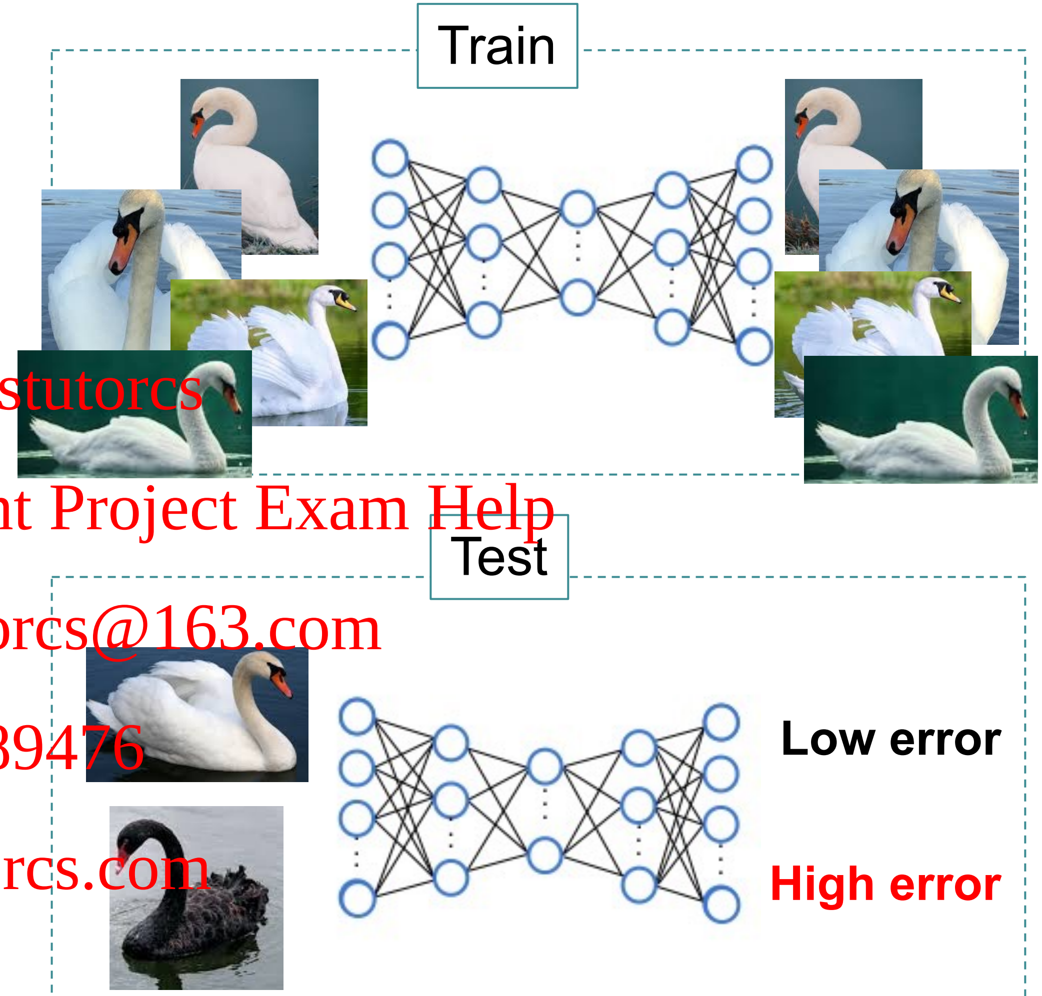
- Anomaly detection
- Extracting interesting infor[illegible]m data
  - Data compression (dimension reduction)
  - Clustering
  - Visualisation
- Representations learning

Using Autoencoder for Anomaly Detection

- Train an autoencoder on normal data
- Learn the distribution of normal data
- μ: mean of error in training data
- σ: standard deviation of error in training data
- **Identifying anomalies with 3σ rule:**

$$\left\| x_{anomaly} - \hat{x}_{anomaly} \right\|^2 \geq \mu + 3\sigma$$

  – Generate high error for anomalies.



Using Autoencoder for Anomaly Detection – Example

- Train samples

Sample	x	[illegible]
1	30, 12, 85	[illegible], 78
2	22, 18, 83	25, 13, 89
3	32, 21, 68	28, 18, 74

- Test samples

Sample	x_t	$\hat{x}_t$
1	32, 16, 81	29, 12, 79
2	19, 28, 63	27, 16, 88

Using Autoencoder for Anomaly Detection – Example

- Train samples

Sample	x	[illegible]	Error
1	30, 12, 85	[illegible], 78	8.3
2	22, 18, 83	25, 13, 89	8.4
3	32, 21, 68	28, 18, 74	7.8

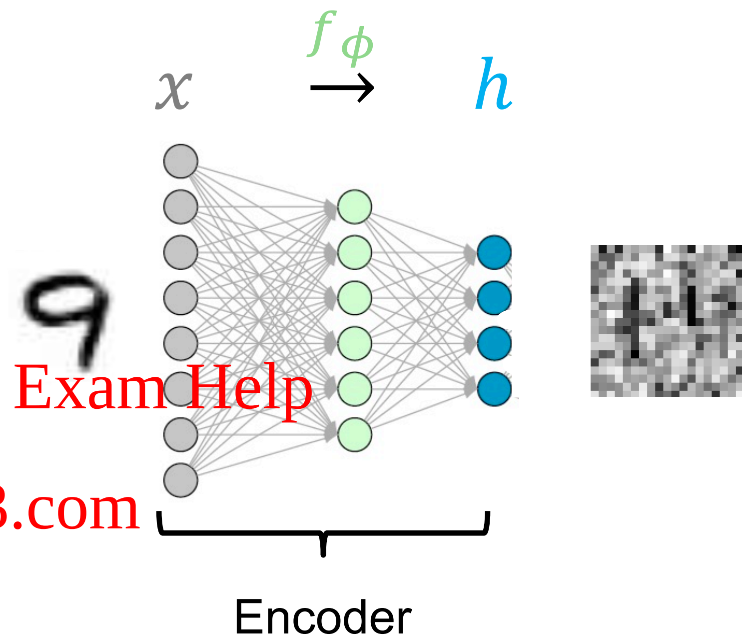
$$8.2 + 3\times 0.26 = 8.98$$

- Test samples

Sample	x	$\hat{x}$	Error
1	32, 16, 81	29, 12, 79	5.3
2	19, 28, 63	27, 16, 88	28.5

Data Compression

- **Objective:** Find a way to appropriately compress our input into a … “…ttleneck” vector of smaller dimensi… …coder).
  - Learns a Lossy Com… …f the input data.



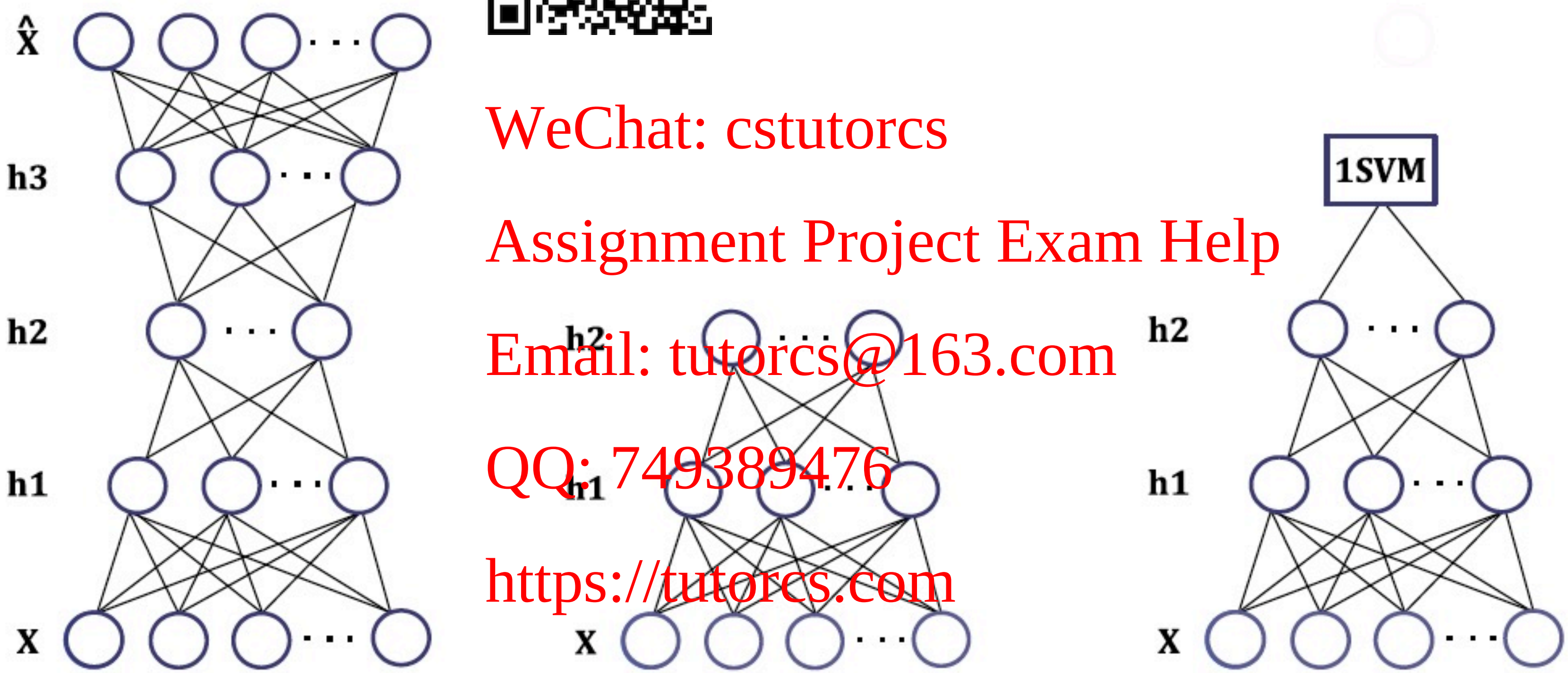
- **Special case:** f, g linear, $\mathcal{L}$ mean square error: reduces to Principal Component Analysis (PCA)
  - PCA: Data compression methods that reduces the dimensionality of the data while maintaining its essence.

Unsupervised Representation Learning

- Force the representations to better model input distribution
  - Not just extracting fe classification
  - Asking the model to representing the data and not overfitting to a particular task
  - Potentially allowing for better generalization

Application: Hybrid Anomaly Detection Model [3]

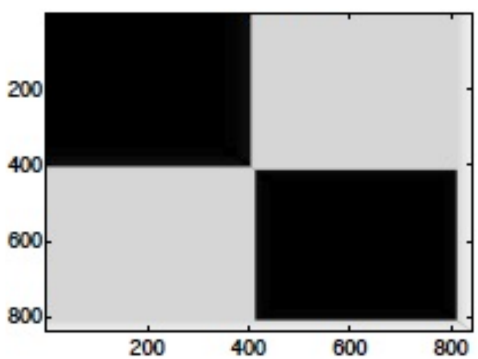
- Feed the output of the bottleneck into a simple model (e.g. k-NN, 1SVM, logistic regression. . .).



Application: Hybrid Anomaly Detection Model

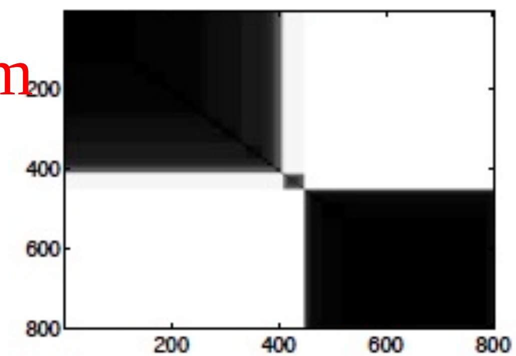
- Example of 2 dimensional Banana (two moon) dataset:

- iVAT images of 100 dimensional Banana dataset (with 5% random anomaly)



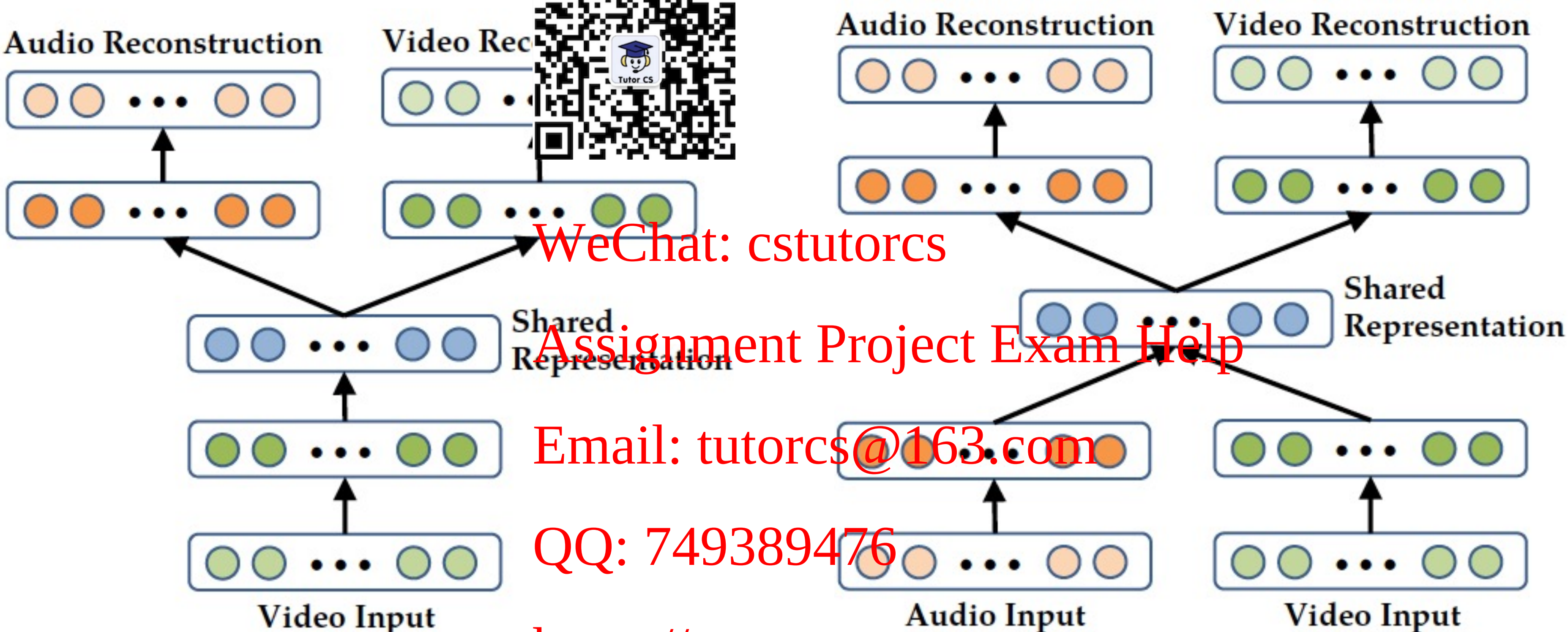
Input data

Output of 1st hidden layer



Output of 2nd hidden layer

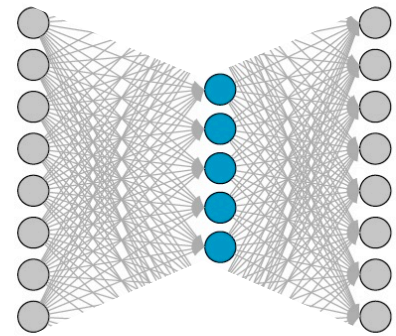
Application: Multimodal Learning [4]



Undercomplete vs. Overcomplete Hidden Layer

Undercomplete Representation:

- Hidden layer is undercom[illegible]aller than the input layer
- Hidden layer compresses [illegible]
- Compresses well only for the training distribution
- Hidden units will be good features for the training distribution, but bad for other inputs



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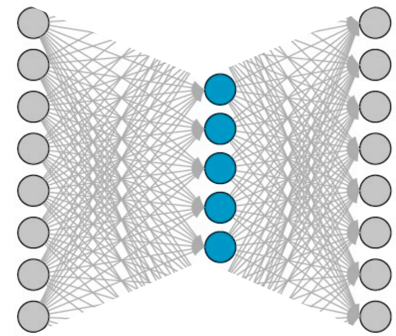
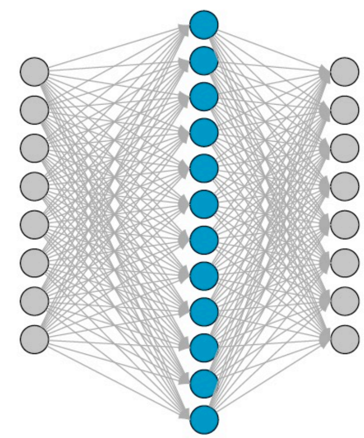


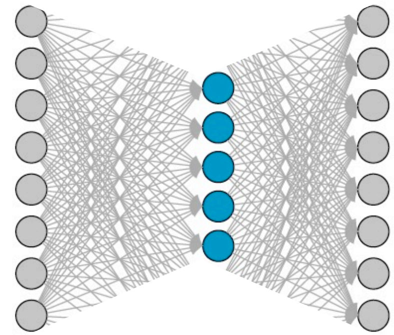
Overcomplete Representation:

- Hidden layer is overcomplete if greater than the input layer
- No compression in the hidden layer
- Each hidden unit could copy a different component
- No guarantee that the hidden unit will extract meaningful structure



Undercomplete vs. Overcomplete Hidden Layer

Undercomplete Representation:



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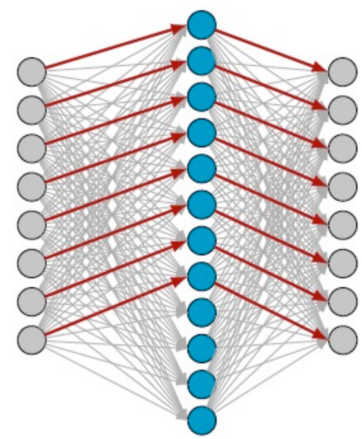
Overcomplete Representation:

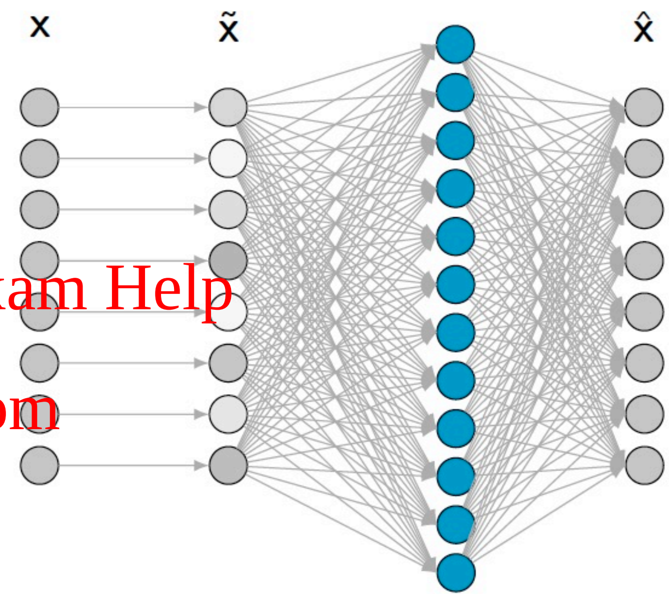


- Hidden layer is overcomplete if greater than the input layer
- No compression in the hidden layer
- Each hidden unit could copy a different component $x = \hat{x}$
- No guarantee that the hidden unit will extract meaningful structure

Denoising Autoencoder (DAE)

- **Idea:** Add noise to input but learn to reconstruct the original
  - Randomly assign a s [illegible] ata to 0, with probability ρ
  - Add Gaussian noise
- Reconstruct $\hat{x}$ from corrupted $\tilde{x}$
- Loss function minimises error between $\hat{x}$ and original sample x

$$\mathcal{L}(\theta,\phi) = \frac{1}{2}\sum_{i=1}^{n}\left(x_i - \overbrace{g_\theta\left(f_\phi(\tilde{x}_i)\right)}^{\hat{x}_i}\right)^2$$

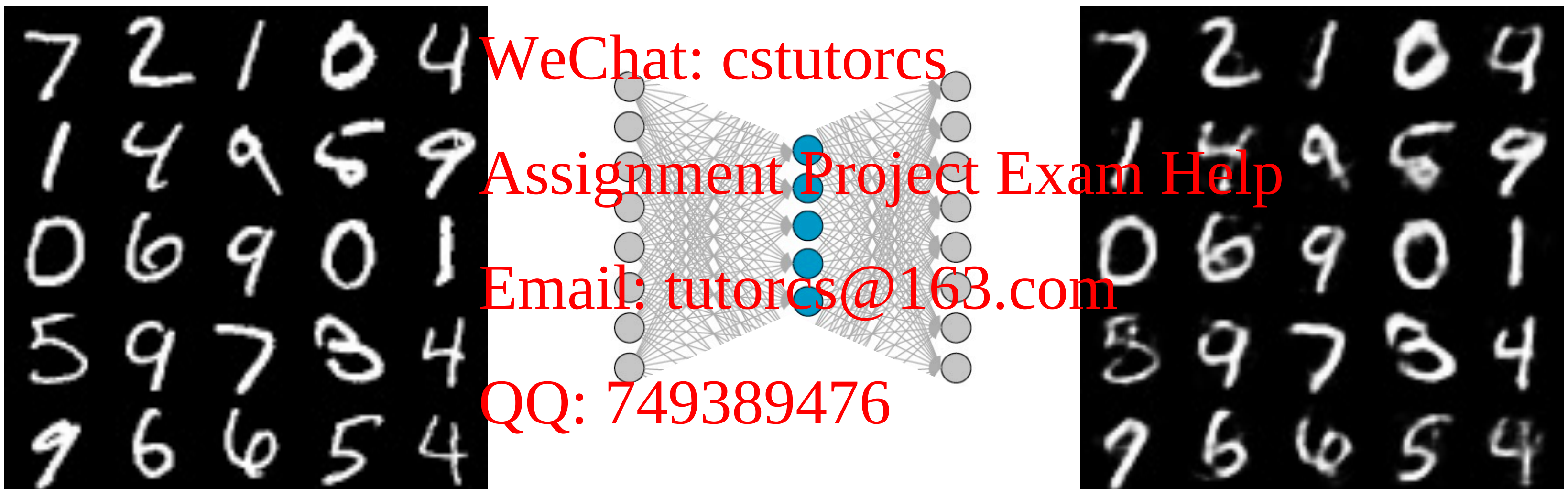


- Prevents copying
- Improves the representations and robustness
- **Note:** different noise is added during each epoch

Example of Autoencoder

Input x

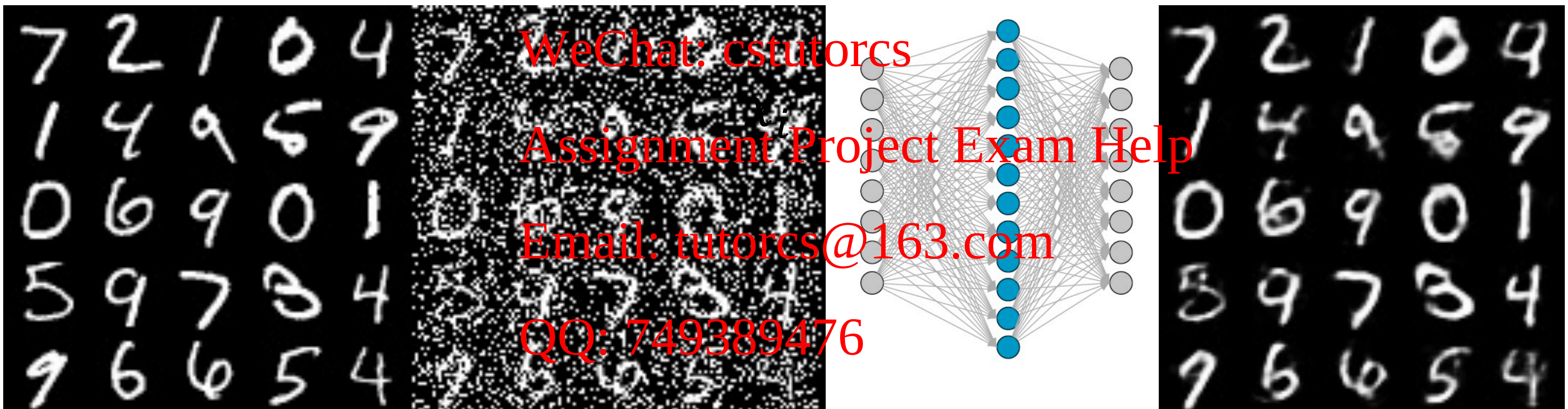
Output $\hat{x}$



$$\mathcal{L}(\theta, \phi) = \frac{1}{2}\sum_{i=1}^{n}(x_i - \hat{x}_i)^2$$

Example of Denoising Autoencoder

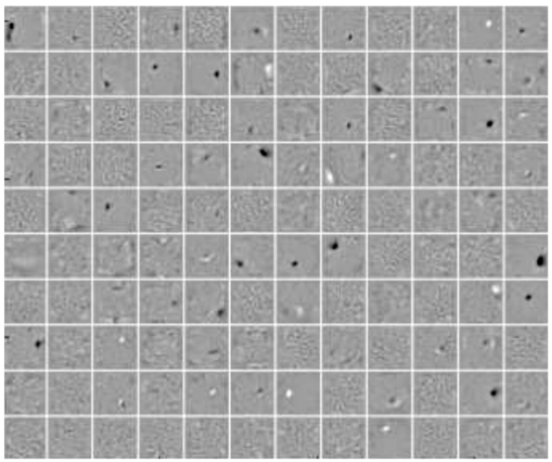
Original Data x Noisy Input $\tilde{x}$ Output $\hat{x}$



$$\mathcal{L}(\theta, \phi) = \frac{1}{2}\sum_{i=1}^{n}(x_i - \hat{x_i})^2$$

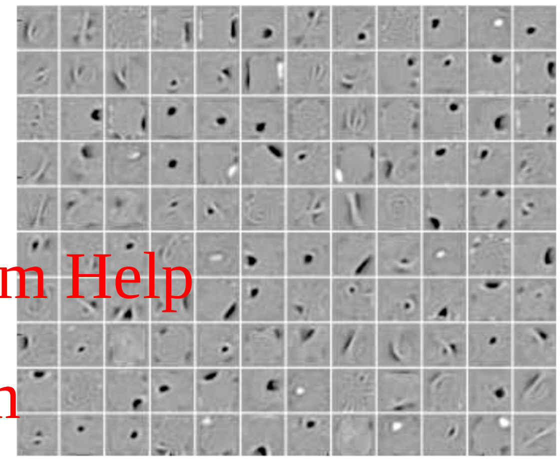
Example of Denoising Autoencoder

0% Noise

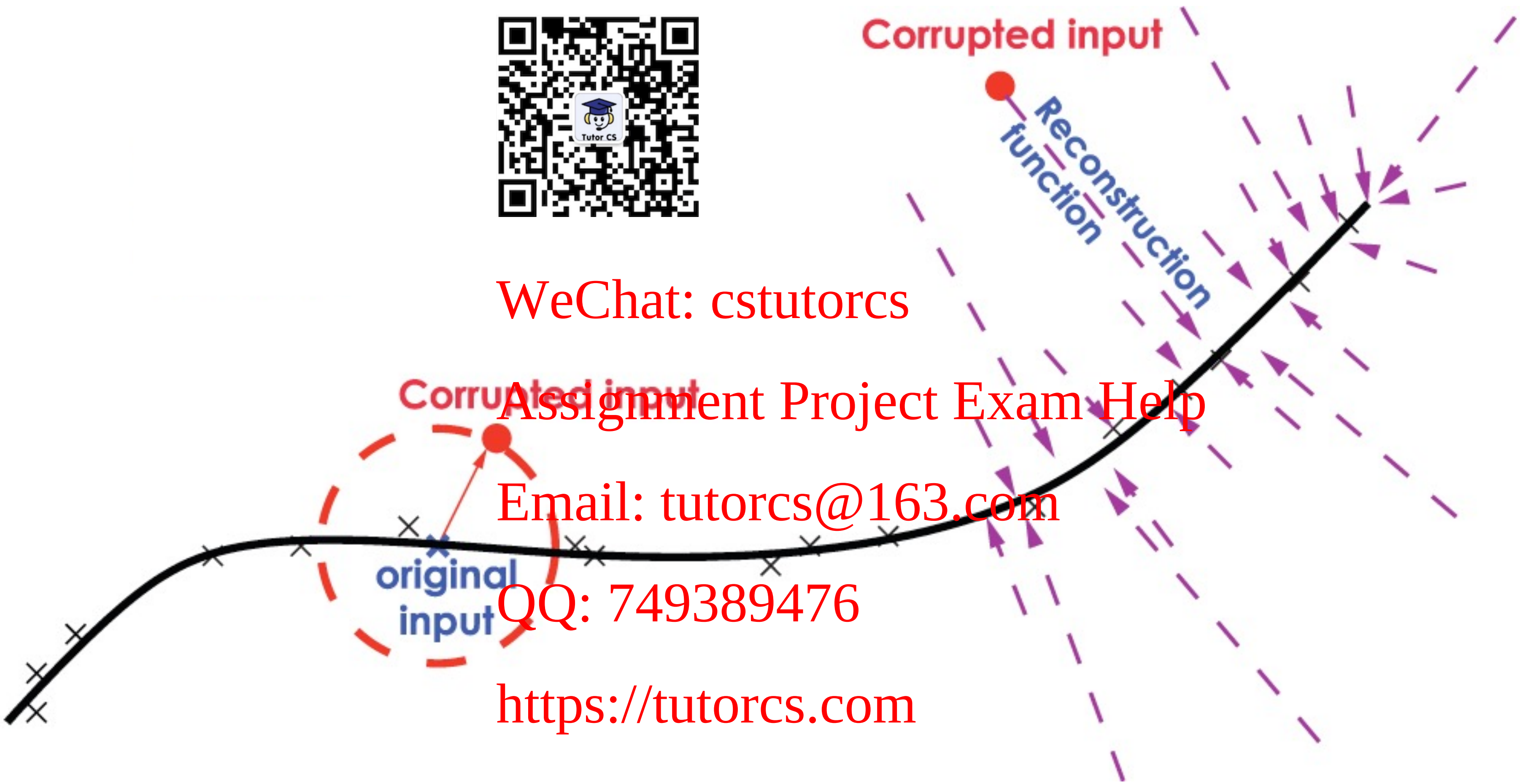


% Noise

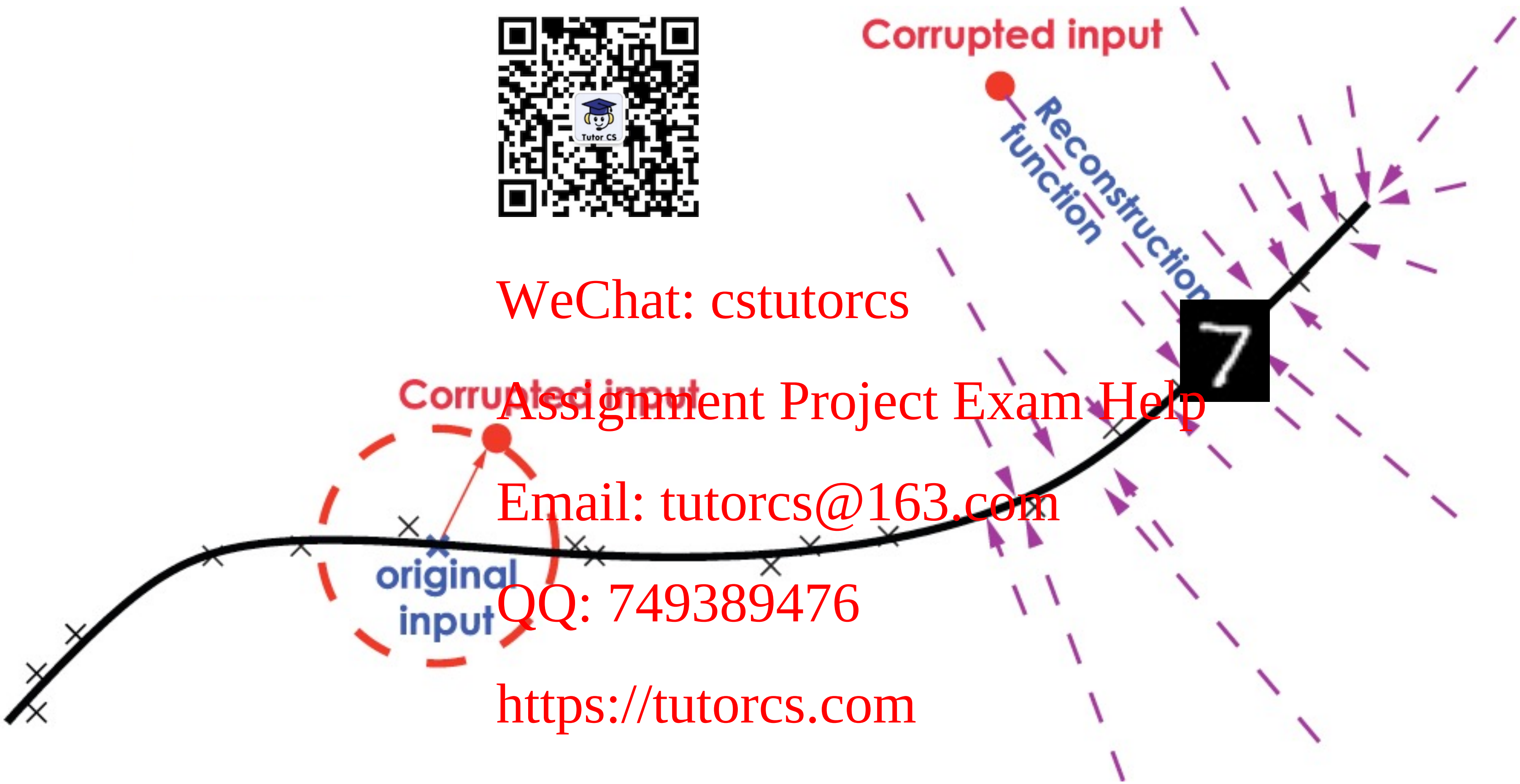
50% Noise



Intuition of Denoising Autoencoder



Intuition of Denoising Autoencoder



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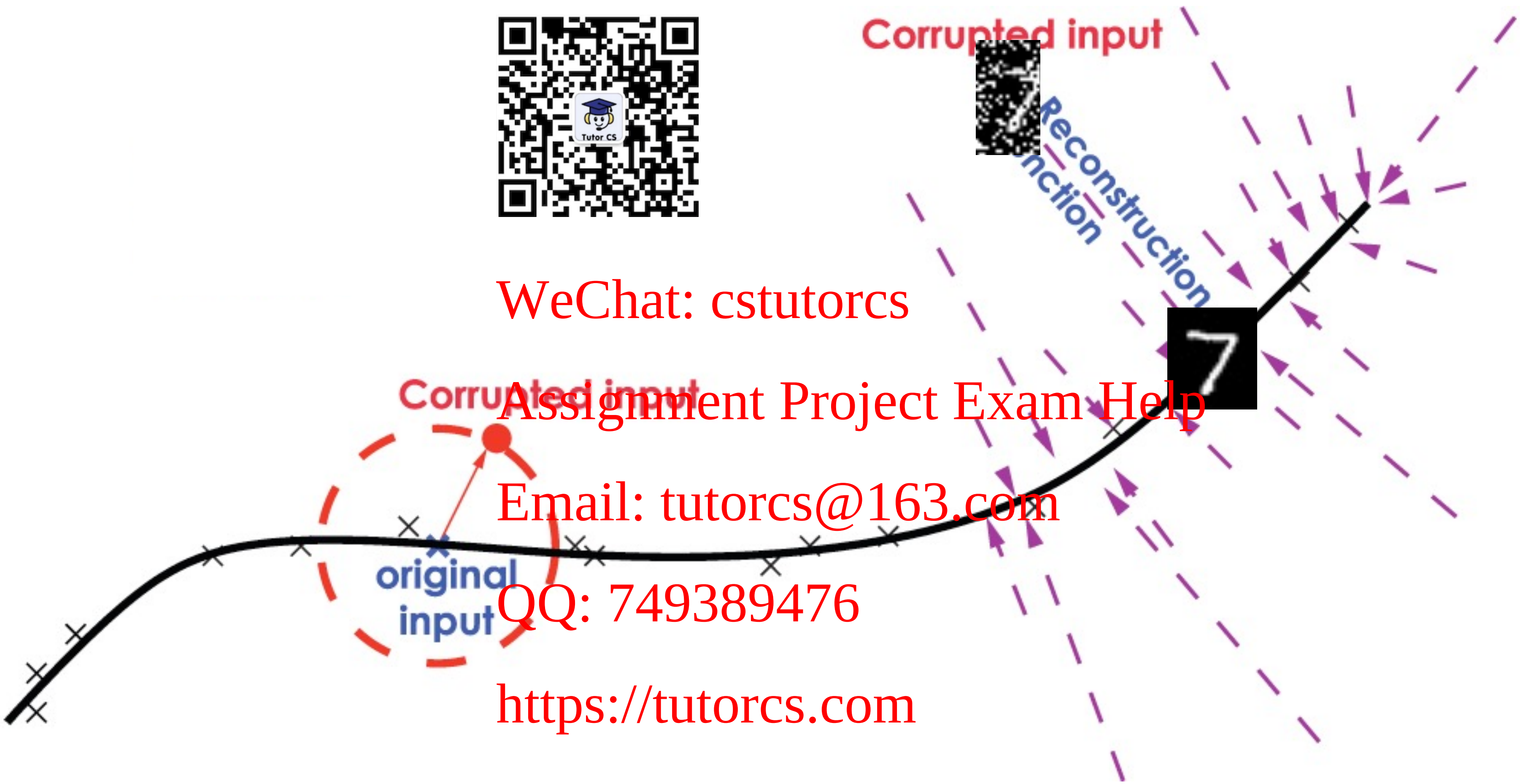

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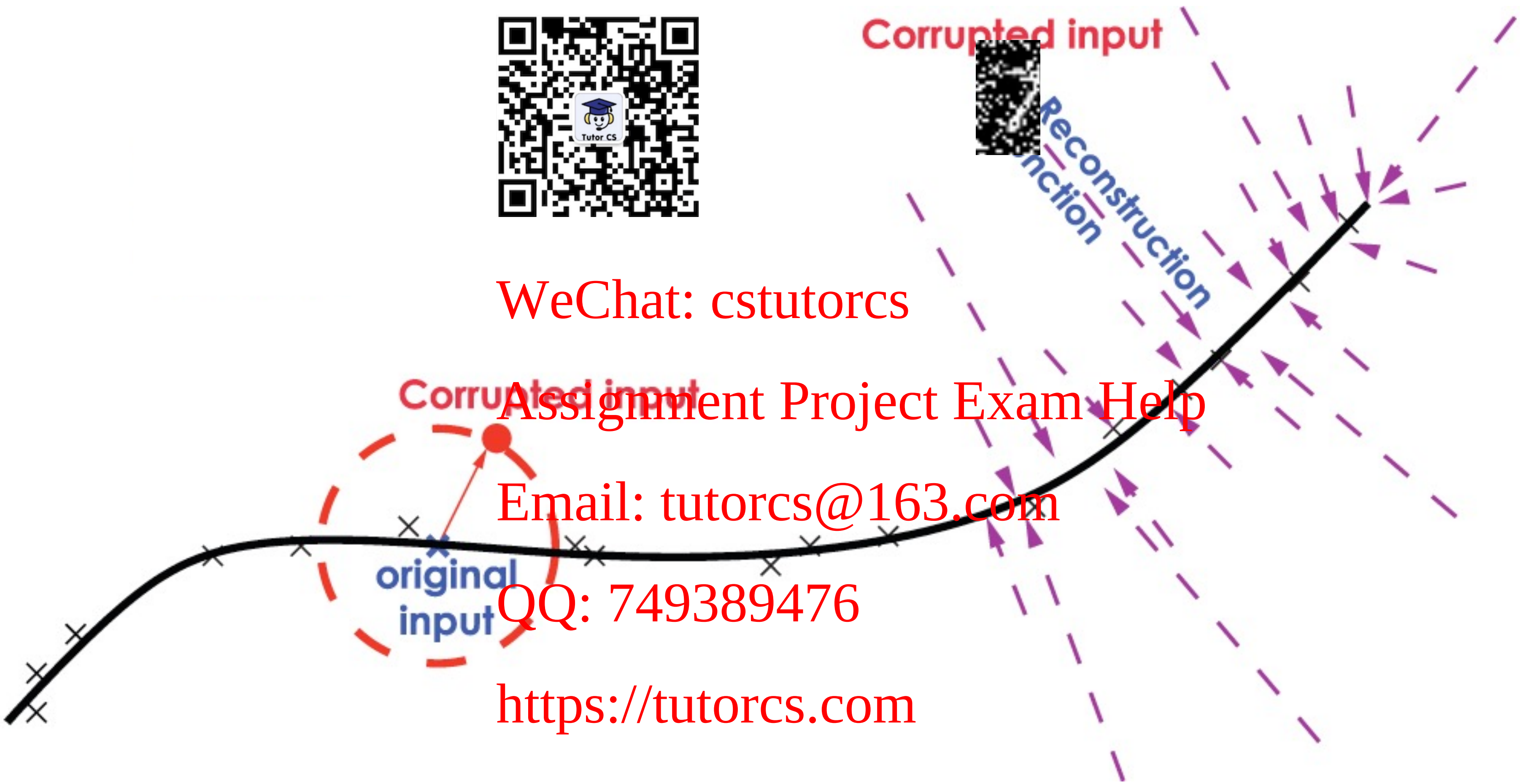
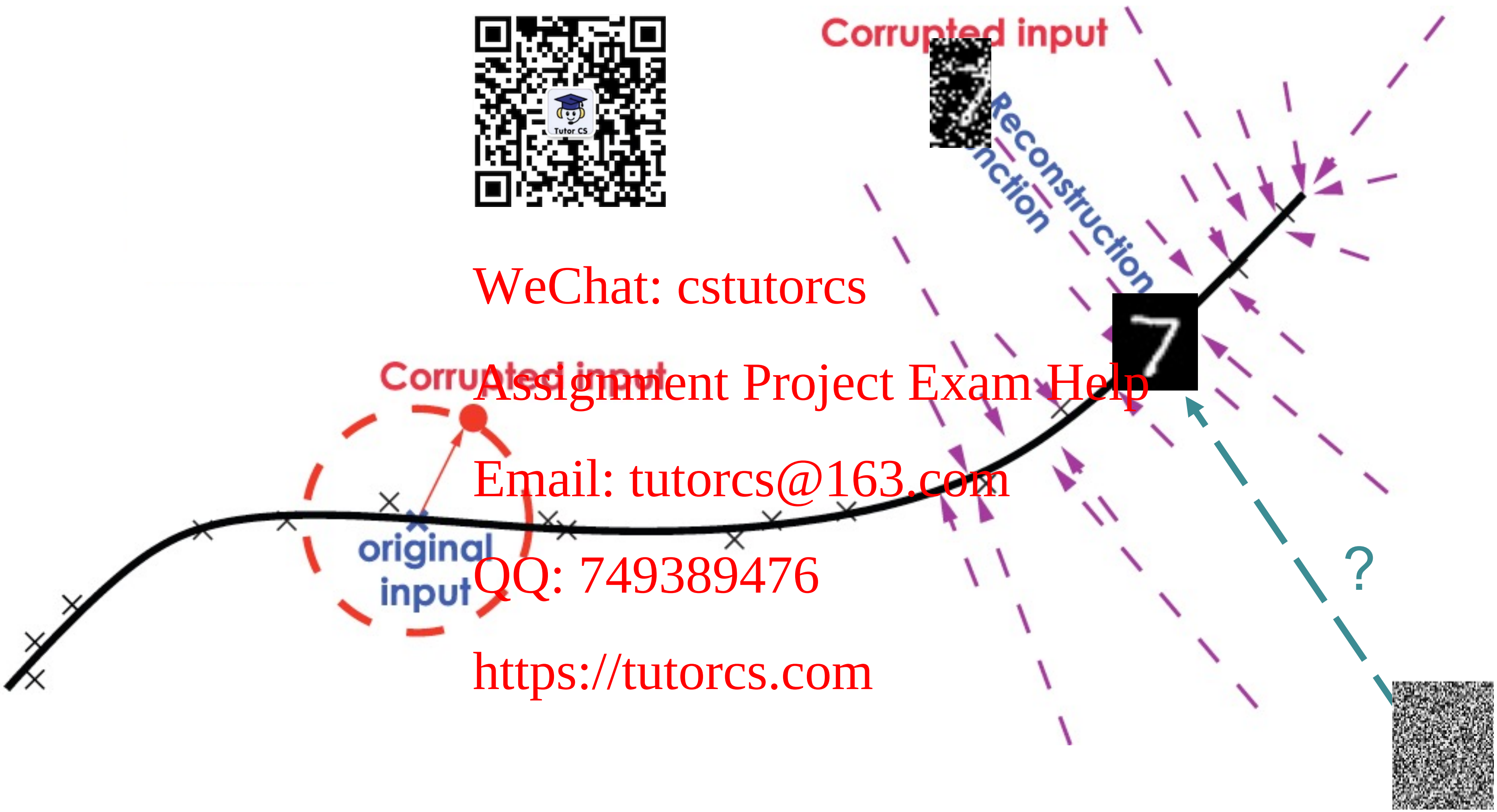
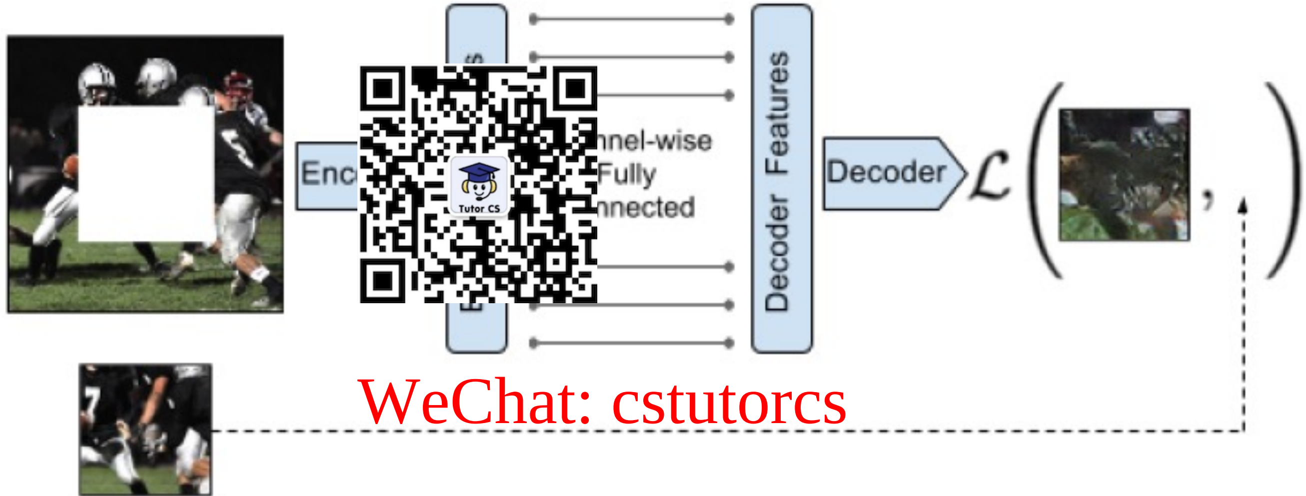


Intuition of Denoising Autoencoder



Application: Image Patching (Neural Inpainting) [9]



Problem with AEs

- Their latent space and their encoded vectors, may not be continuous.

Variational Autoencoder (VAE) [6]

- VAEs are in a class of models called generative models, they can be used to generate examples of in[illegible]y learning their statistics (e.g., mean and variance).

- Instead of learning $f_\phi(x)$ [illegible]), VAEs learn distributions of the features given the input, and the input given the activations, i.e., probabilistic versions of f_ϕ and g_θ. The VAE will learn:

  – $q_\phi(h|x)$: the distribution of the features given the input.

  – $p_\theta(x|h)$: the distribution of the input given the features.

- **Objective:** Find a distribution $q_\phi(h|x)$ of some latent variables h, which we can sample from $h \sim q_\phi(h|x)$, to generate new samples $\hat{x} \sim p_\theta(x|h)$.

Encoding of AE vs. VAE

Standard Autoencoder
(direct encoding coordinates)

Variational Autoencoder
(μ and σ initialize a probability distribution)

Why VAE Learns Data Distribution?

- Often times the data is noisy, and a model of the distribution of the data is more useful for a given applicat[illegible]

- The relationship between [illegible]ved variables and the latent variables can be nonlinear, in which cas[illegible] provides a way to do inference.

- The VAE is a generative model; by learning $p_\theta(x|h)$, it is possible to sample h and then sample x. This enables the generation of data that has similar statistics to the input.

VAE Architecture

VAE's Loss Function

$$\mathcal{L}(\theta, \phi) = \underbrace{\mathbb{E}_{q_\phi(h|x)}[\log p_\theta(x|h)]}_{\text{Reconstruction Loss}} - \underbrace{D_{KL}(q_\phi(h|x) \| p_\theta(h))}_{\text{Regulariser (KL divergence)}}$$

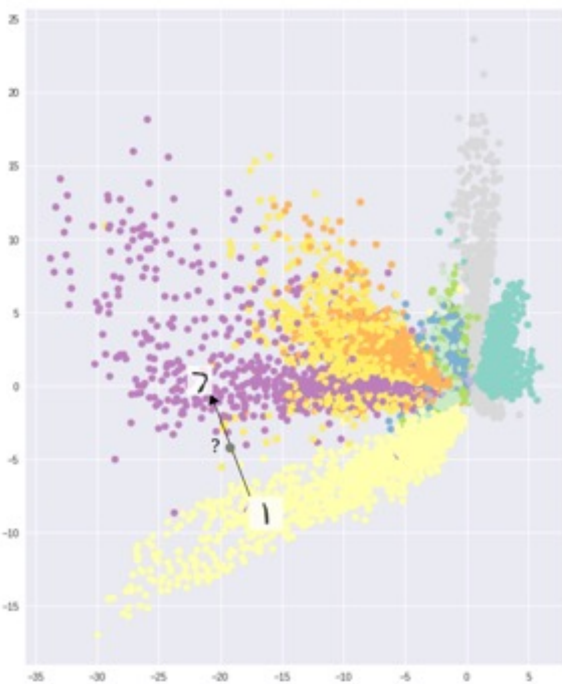
- **Reconstruction Loss:** The expected log-likelihood measures how well samples from $q_\phi(h|x)$ are able to explain the data x.

- **Regulariser:** Ensures that the explanation of the data $q_\phi(h|x)$ doesn't deviate too far from the prior distribution $p_\theta(h)$.

- **Kullback–Leibler (KL)-divergence:** Measure of difference between two distributions (the approximate posterior and the prior for h)

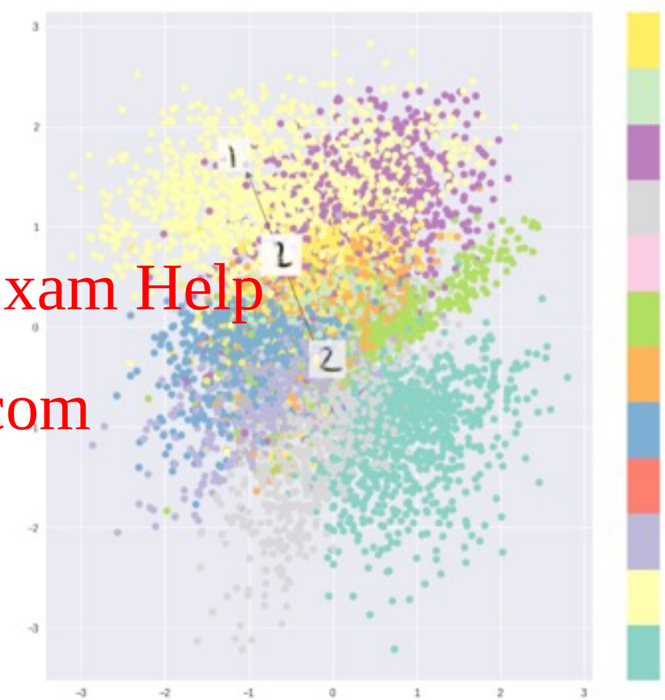
Intuition of VAE’s Loss Function [10]

Only reconstruction loss



divergence

Combination



Example: Two-dimensional Latent Space for MNIST

Demo: https://www.siarez.com/projects/variational-autoencoder

Application: Generating celebrity-lookalike photos

Application: Forecasting [7]

Disentangled VAE (β-VAE)

- Disentangle Representation: Each variable in the inferred latent representation h is only se[illegible] one single generative factor and relatively invariant to other factors.

- Extract very useful feature[illegible]y high dimensional space and use them to a task it wants to learn.

- Those features *generalise* to domains outside the training data, and enhance *interpretability*.

Non examinable

Disentangled VAE (β-VAE)

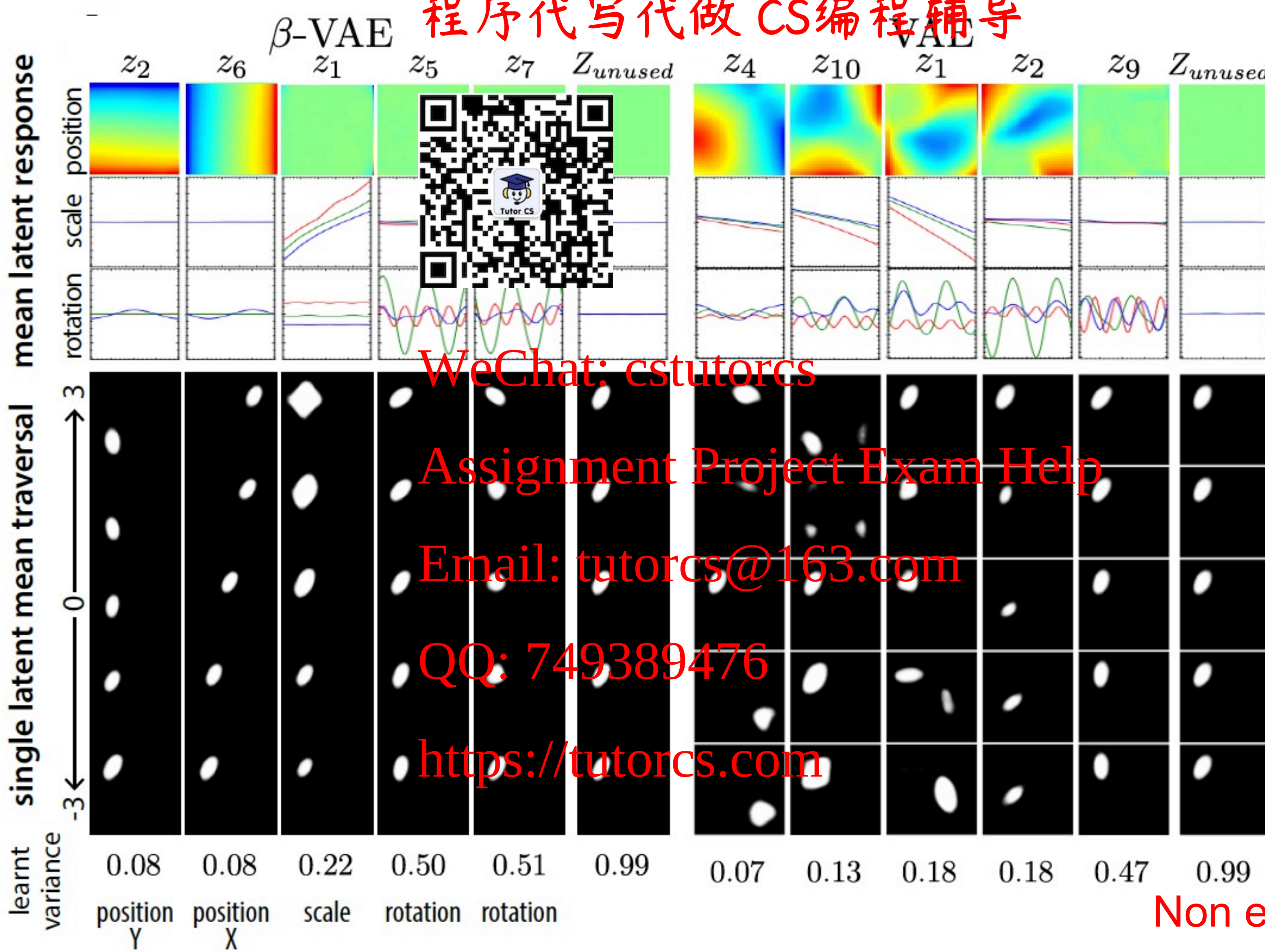
$$\mathcal{L}(\theta, \phi) = \mathbb{E}_{q_\phi(h|x)}[\log p_\theta(x|h)] - \boxed{\beta} D_{KL}(q_\phi(h|x) \| p_\theta(h))$$

- For $\beta > 1$, it applies a stronger constraint on the latent bottleneck and limits the representation capacity of h.

- **Advantages:** Extremely flexible, even if each conditional is simple (e.g. conditional Gaussian), the marginal likelihood can be arbitrarily complex

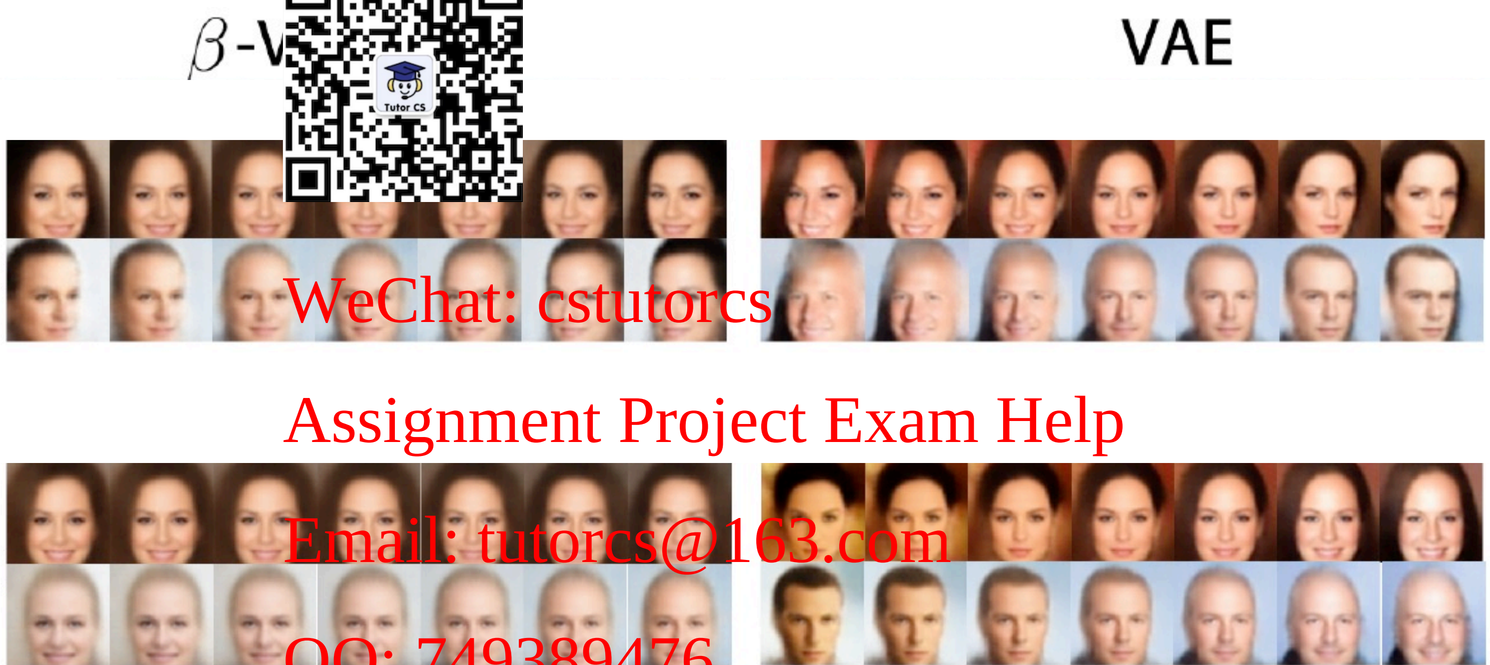
Non examinable

Representation Learning by β-VAE and VAE



Non examinable

Manipulating Latent Variables



Azimuth (Rotation)

Emotion (Smile)

Non examinable

Using VAE for Anomaly Detection [11]

- Training VAE: using only data of normal instances to learn $q_\phi(h|x)$ and $p_\theta(x|h)$
- For a test instance z
  - Evaluate the mean and standard deviation vectors with the probabilistic encoder $(\mu_z, \sigma_z) = q_\phi(h|z)$
  - Draw L samples from $h \sim N(\mu_z, \sigma_z)$
  - Compute the reconstruction probability

$$P_{recons}(z) = \frac{1}{L}\sum_{l=1}^{L} p_\theta(z|\mu_{\hat{z}_l}, \sigma_{\hat{z}_l})$$

$$(\mu_{\hat{z}_l}, \sigma_{\hat{z}_l}) = q_{\phi(x|h_l)}$$

  - z is anomaly if $P_{recons}(z) > \alpha$

Advantages of VAE for Anomaly Detection

- Latent variables are stochastic variables
  - The probabilistic enc[illegible]AE models the distribution of the latent variables (rather than [illegible] variable itself).
  - It can capture normal [illegible]alies which share the same mean, but different variance.

- Reconstructions are stochastic variables

  - Reconstruction probability considers the reconstruction error, as well as the variability of the reconstruction (by considering the variance parameter of the distribution function).

  - This property enables selective sensitivity to reconstruction according to variable variance.

Summary

- How to train a neural network?
- What is an autoencoder and what are its applications?
- How we can apply autoencoders to noisy data?
- What is a generative autoencoder and how we can use it for anomaly detection?

Next: Graph anomaly detection

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