Advanced Recurrent Neural Networks

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Manifold Hypothesis

- **Manifold:** A topological space that is locally Euclidean
- **Manifold Hypothesis:** High dimensional data lie on low dimensional manifolds embedded in high-dimensional space

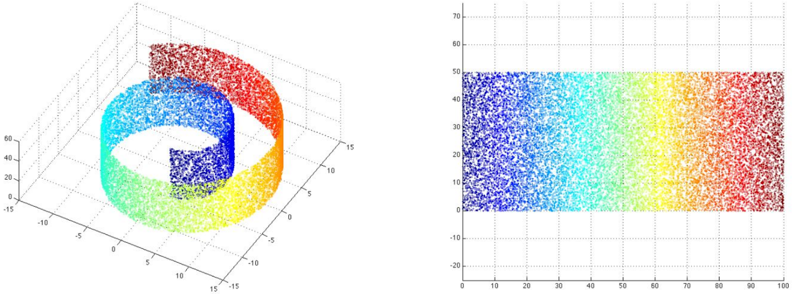

Figure: (a) A curled plane in 3-dimensional space. (b) Unrolled plane in 2-dimensional space.

Manifold Hypothesis

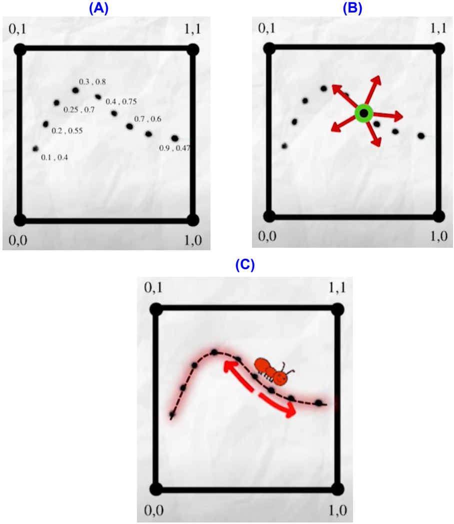

Figure: Illustration of a 1-d manifold in 2-d space.

Manifold Hypothesis

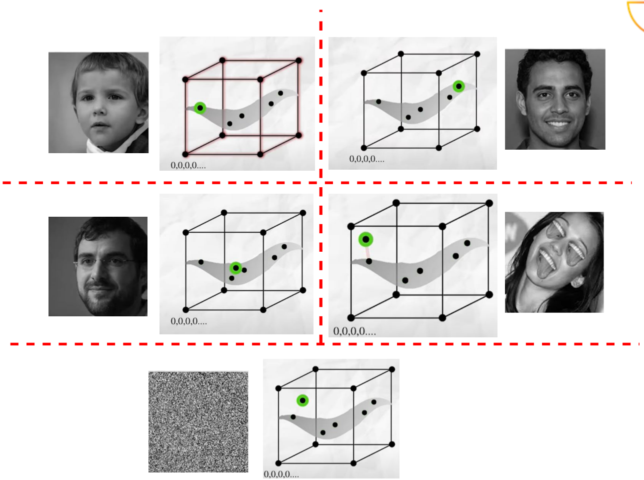

Figure: Illustration of an image manifold in image space.

Principal Component Analysis

- **Principal Components:** Orthogonal unit vectors representing variations in the data
- **Dimensionality Reduction:** Project the input N-dimensional data onto K principal components such that $K << N$

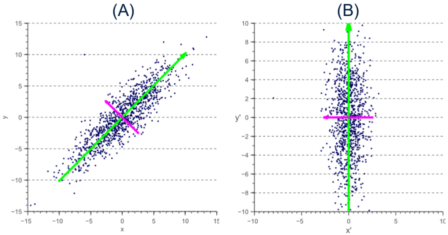

Figure: First and second principal components.

Principal Component Analysis: Algorithm

- Compute data covariance matrix:
  $$\mathbf{C} = \frac{1}{N-1}\sum_{i=1}^{N}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T$$
- Compute eigen vectors:
  $\mathbf{C} = \mathbf{U}\Sigma\mathbf{U}^T$
  - Σ is a diagonal matrix containing eigen values
  - $\mathbf{U}$ contains the corresponding eigen vectors
- Project data on M components:
  $\mathbf{x}_p = \mathbf{U}_{1:M}^T\mathbf{x}$

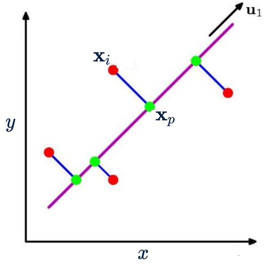

Figure: Projection on first principal component.

Principal Component Analysis: Algorithm

- **Reconstruction:** Obtaining data from the projected space to the original space:

$$\hat{\mathbf{x}} = \mathbf{X}_p \mathbf{U}_{1:M} + (\mathbf{U}_{M:D}^T \bar{\mathbf{x}}) \mathbf{U}_{M:D} \tag{1}$$

- **Objective:** Minimise $\sum_{i=1}^{N} ||\mathbf{x}_i - \hat{\mathbf{x}}_i||_2^2$
- Optimal solution if $\mathbf{U}_{M:D}$ represents least information
- $\mathbf{U}_{M:D}$ should correspond to lesser eigenvalues

Principal Component Analysis: Eigenfaces

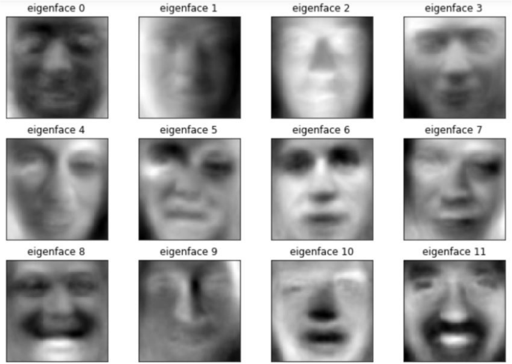

Figure: An application of PCA: Eigenfaces.

Credit: *towardsdatascience.com/eigenfaces-recovering-humans-from-ghosts-17606c328184*

Principal Component Analysis is Linear!

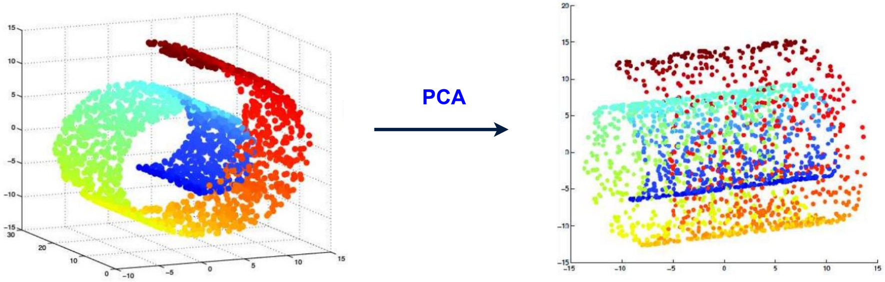

Figure: PCA on Swiss roll dataset.

Credit: *Barnabas Pozcos*

Autoencoder

- A neural network trained to reconstruct its input
- Autoencoder consists of two components:
  - **Encoder:** A function $f()$ that maps an input example $(\mathbf{x})$ to a latent representation or code or bottleneck embedding $(\mathbf{h})$
  - **Decoder:** A function $g()$ that reconstructs the input $(\mathbf{x})$ back from the code $(\mathbf{h})$

$$\mathbf{h} = f(\mathbf{x}), \qquad \hat{\mathbf{x}} = g(\mathbf{h}) \tag{2}$$

- **Loss function:** Minimise the deviation between $\mathbf{x}$ and $\hat{\mathbf{x}}$
- Not helpful if autoencoder is an identity function: $\mathbf{x} = g(f(\mathbf{x})), \forall \mathbf{x}$

Autoencoder: Illustration

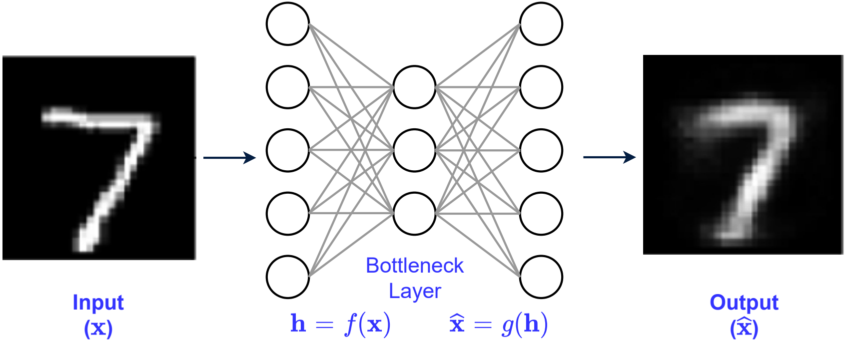

Figure: A feed-forward autoencoder.

Autoencoders: Undercomplete and Overcomplete

- **Undercomplete AE:** Dimensions of code (**h**) is less than dimensions of the input (**x**)
- Encourages the model to learn only relevant features

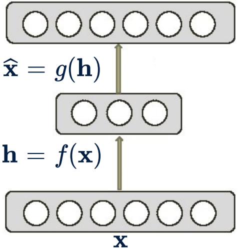

Figure: An undercomplete autoencoder.

Autoencoders: Undercomplete and Overcomplete

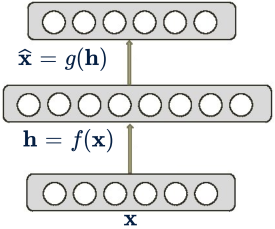

Figure: An overcomplete autoencoder.

- **Overcomplete AE:** Dimensions of code (**h**) is larger than dimensions of the input (**x**)
- No guarantee that relevant features will be extracted
- May result in AE just copying the input

Overcomplete Autoencoders

- **Sparse AE:** Requires regularisation to encourage sparsity over **h**:

$$\ell_{AE} = ||\mathbf{x} - \hat{\mathbf{x}}||_2^2 + \lambda ||\mathbf{h}||_1 \tag{3}$$

Minimise ℓ_1 norm of **h** along with improving reconstruction

- **Contractive AE:** Regularise AE by penalising derivatives:

$$\ell_{AE} = ||\mathbf{x} - \hat{\mathbf{x}}||_2^2 + \lambda \nabla_{\mathbf{x}} \mathbf{h} \tag{4}$$

Penalise larger changes in **h** due to small changes in **x**

Denoising Autoencoders

- Training AE to reconstruct a noise-free version ($\mathbf{x}'$) from the noisy input example ($\mathbf{x}$)
- $\hat{\mathbf{x}} = g(f(\mathbf{x}))$. Then, the loss function becomes:

$$\ell_{AE} = ||\mathbf{x}' - \hat{\mathbf{x}}||_2^2 \tag{5}$$

- No issue of identity AE as inputs and outputs are different
- Overcompleteness may help in better estimation of the noisy features

Denoising Autoencoders

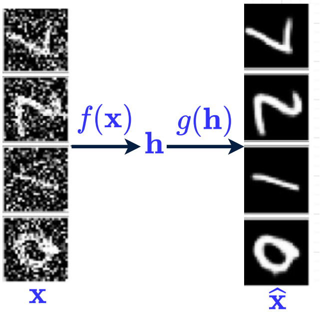

Figure: An illustration of denoising capabilities of AEs.

Denoising Autoencoders

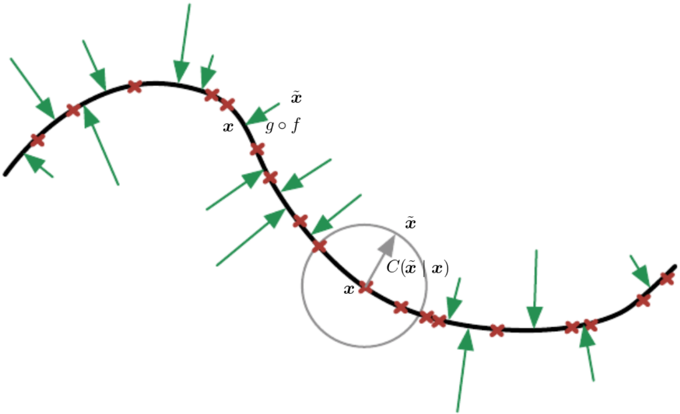

Figure: An illustration of denoising capabilities of AEs.

Credit: *Chapter 14, Deep Learning Book.*

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Dimensionality Reduction using AEs

- **Visualisation:** Maps high dimensional data to two or three dimensions
- **Dimensionality Reduction:** Maps high dimensional data to any lower dimensional space

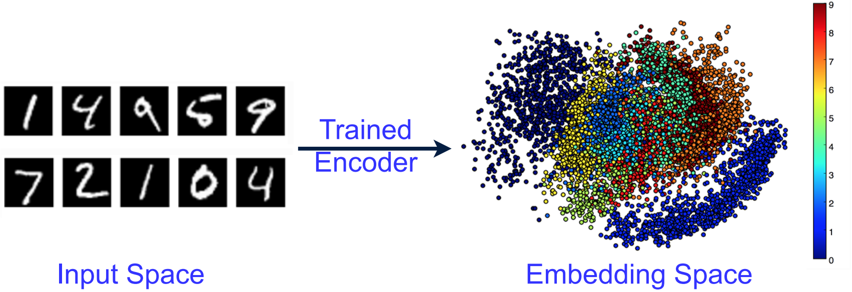

Figure: Data visualisation using trained AEs.

Segmentation using AEs

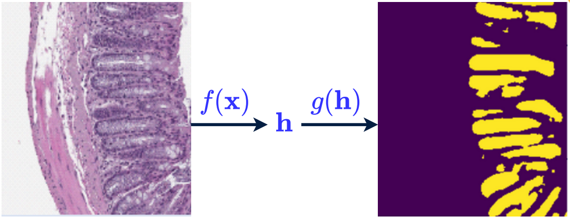

Figure: An illustration of image segmentation using AEs.

- AEs are trained to reconstruct a version of input image that only highlights the regions of interest
- Suppose $\mathbf{x}$ and $\mathbf{m}_x$ be input and mask pair. Then, the loss function for training AE is of the following form:

$$\ell_{AE} = ||g(f(\mathbf{x})) - \mathbf{m}_x||_2^2 \tag{6}$$

Unsupervised Learning

- Latent embedding or bottleneck features are semantically rich
- Latent embedding can be used for semantic clustering
- The principle of autoencoding can be used for pre-training neural networks
  - Usually helpful in case of labelled data scarcity
- Latent embedding can be used as predictive features

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Autoencoders for Time-series

- **Sequence-to-sequence AE:**
  - Encoder transforms a time-series to the latent vector
  - Decoder converts the latent representation to the input time-series
- **Conditioned seq2seq AEs:**
  - Generation/Decoding at next time-step is explicitly conditioned on the previous step
  - Previous time-step prediction is given as input to the current step
- **Unconditioned seq2seq AEs:** No explicit conditioning

Sequence-to-sequence AE: No Teaching

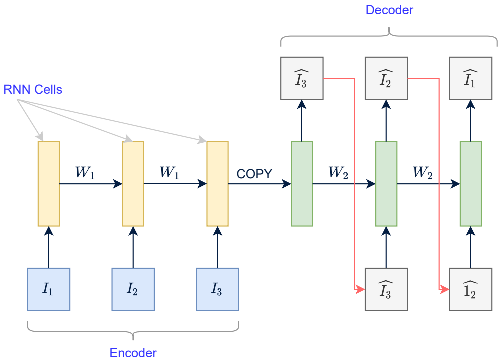


Figure: Recurrent Autoencoder Model. $\{\mathbf{I}_1, \mathbf{I}_2, \mathbf{I}_3\}$ are the vectors at three steps of the time-series.

Credit: *Unsupervised Learning with LSTMs, Srivastava et. al*

Sequence-to-sequence AE: Teaching

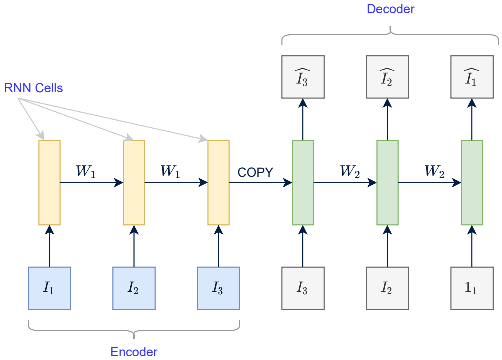


Figure: Seq2Seq Model. $\{\mathbf{I}_1, \mathbf{I}_2, \mathbf{I}_3\}$ are the vectors at three steps of the input time-series $\mathbf{I}$.

Credit: *Unsupervised Learning with LSTMs, Srivastava et. al*

Neural Machine Translation

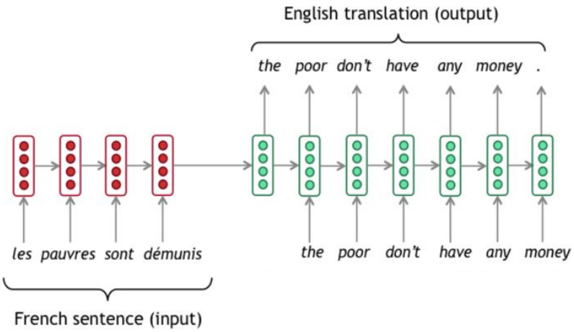


Figure: Neural machine translation using Seq2Seq encoder-decoder model.

Sequence-to-sequence AE

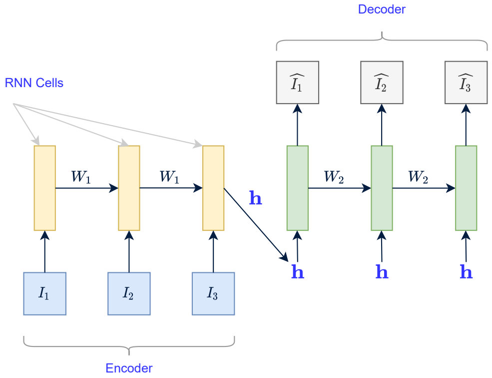


Figure: Recurrent Autoencoder Model. $\{\mathbf{I}_1, \mathbf{I}_2, \mathbf{I}_3\}$ are the vectors at three steps of the time-series.

Encoder Setup: AEs for Time-Series

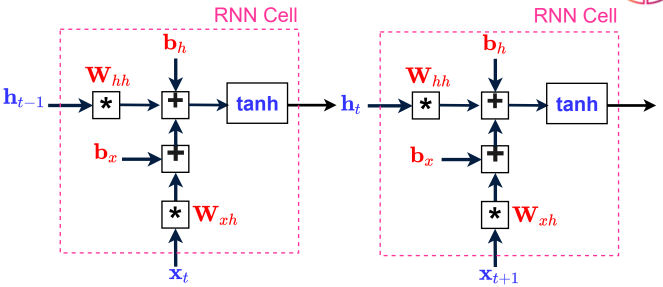


Figure: RNN cell. Biases are optional.

- $\mathbf{h}_t = \text{RNNCell}(\mathbf{x}_t, \mathbf{h}_{t-1}) = \tanh(\mathbf{W}_{hh}\mathbf{h}_{t-1} + \mathbf{b}_h + \mathbf{W}_{xh}\mathbf{x}_t + \mathbf{b}_x)$
- $\mathbf{h}_0 = \mathbf{0}$

Decoder Setup: AEs for Time-Series

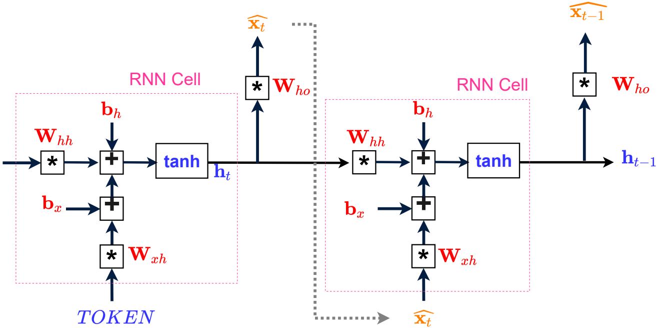


Figure: RNN based decoder setup in sequence-to-sequence AE.

- $\hat{\mathbf{x}}_{t-1} = \mathbf{W}_{ho}.\text{RNNCELL}(\hat{\mathbf{x}}_t, \mathbf{h}_t)$

Loss Function: AEs for Time-Series

- **Mean squared error:** $\mathcal{L}(\mathbf{I}, \hat{\mathbf{I}}) = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{I}_i - \hat{\mathbf{I}}_i)^2$
- **Mean absolute error:** $\mathcal{L}(\mathbf{I}, \hat{\mathbf{I}}) = \frac{1}{N}\sum_{i=1}^{N}|\mathbf{I}_i - \hat{\mathbf{I}}_i|$

Future Predictor: Sequence-to-sequence AE

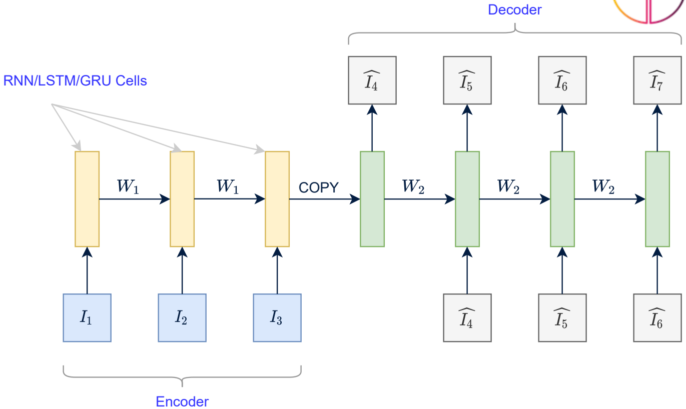
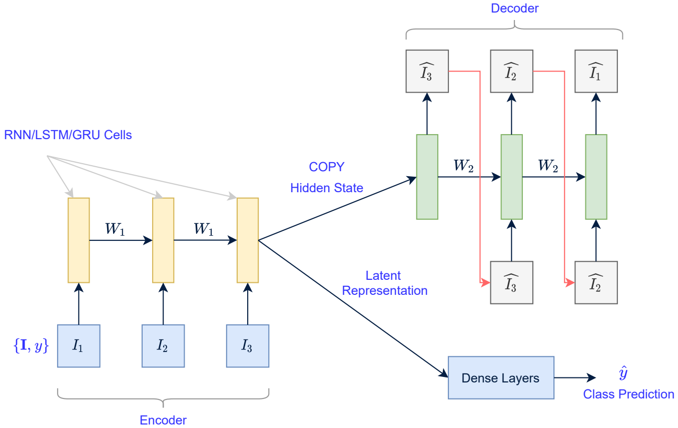


Figure: Predicting values at future time-steps.

Credit: *Unsupervised Learning with LSTMs, Srivastava et. al*

Auxiliary tasks: Sequence-to-sequence AE

- **Auxiliary tasks** can help in learning the **main tasks**
- For example: Classification and Reconstruction of time-series



$$\mathscr{L}_{AE} = \alpha.\, L(\hat{y}, y) + \beta.\, L(\mathbf{I}, \hat{\mathbf{I}})$$

Figure: A time-series classification setup with an auxiliary reconstruction task.

Skip Connections and Sparsely Connected RNNs

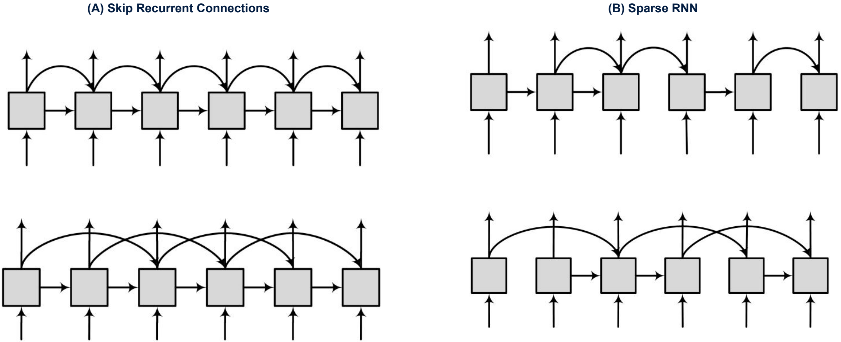


Figure: Skip connections and sparse recurrent connections between recurrent units.

Credit: *Outlier Detection for Time Series with Recurrent Autoencoder Ensembles, Kieu et. al (2019)*

Case study: Denoising using Recurrent AEs

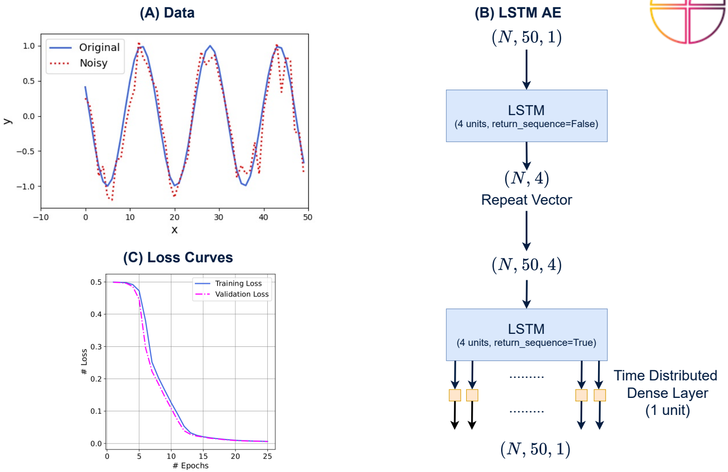


Figure: Training Recurrent AE to denoise sine waves. Means square error is used as the loss function.

Case study: Denoising using Recurrent AEs

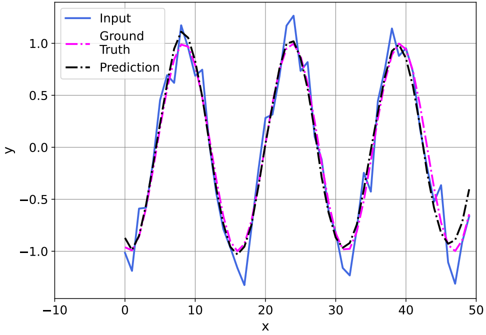


Figure: Denoising using trained Recurrent AE.

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Generative vs Discriminative Models

- **Discriminative models:** Capture conditional probability $p(y|\mathbf{x})$
  - Tells us how likely a label is to apply to an instance
- **Generative models:** Capture $p(\mathbf{x}, y)$ or $p(\mathbf{x})$ if no labels
  - Tells us how likely a given instance is

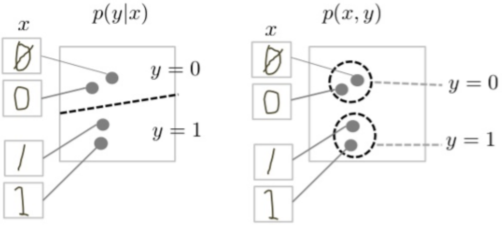

Figure: Discriminative vs generative modelling of hand-written digits.

Credit: `developers.google.com/machine-learning/gan/generative`

Autoencoder as generative model?

- **Autoencoder:** Encoder maps an input example $(\mathbf{x})$ to the latent embedding $(\mathbf{h})$ and a decoder maps this embedding back to the input space
- How will the reconstructed example look like if we use $\mathbf{h} + \delta$ to reconstruct $\mathbf{x}$?
- If $\mathbf{h} + \delta$ is on manifold, we will be fine
- Any idea about distribution of $\mathbf{h}$ can allow us to generate meaning examples in input space

Variational Autoencoder

- Learns a distribution over latent space
- Samples a hidden embedding from this distribution
- Use decoder to map the sampled embedding to input space

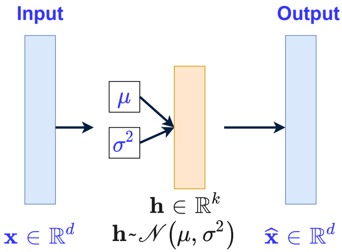

Figure: An illustration of basic VAE framework.

Variational Autoencoder

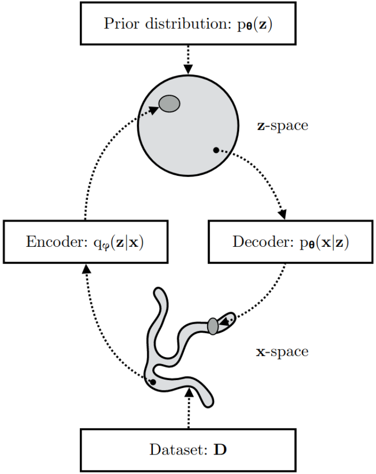

Figure: An illustration of basic VAE framework.

Evidence Lower Bound (ELBO)

- Given $q_\phi(\mathbf{z}|\mathbf{x})$, the log likelihood can be represented as:

$$
\begin{aligned}
\log p_{\boldsymbol{\theta}}(\mathbf{x}) &= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log p_{\boldsymbol{\theta}}(\mathbf{x})\right] \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log\left[\frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})}\right]\right] \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log\left[\frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})}\right]\right] \\
&= \underbrace{\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log\left[\frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right]\right]}_{\substack{=\mathcal{L}_{\boldsymbol{\theta},\phi}(\mathbf{x}) \\ \text{(ELBO)}}} + \underbrace{\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log\left[\frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})}\right]\right]}_{=D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}))}
\end{aligned}
$$

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

Variational Autoencoder

- Let $q_\phi()$ be the encoder and p_θ be the decoder
- **Loss function:** $\mathcal{L}(\phi, \theta) = \sum_{i=1}^{N} l_i(\phi, \theta)$
- $l_i = -\mathbb{E}_{\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x}_i)} \left[\log p_\theta(\mathbf{x}_i|\mathbf{z})\right] + \mathrm{KL}\left(q_\phi(\mathbf{z}|\mathbf{x}_i)||p(\mathbf{z})\right)$
- First term encourages better reconstruction
- Second term acts as regulariser: Produces $\mathbf{z}$ that follow normal distribution

Reparameterisation Trick

- Stochastic sampling is non-differentiable
- $\mathbf{z} \sim q_\phi(\mathbf{z}|x) = \mathcal{N}(\mu, \sigma^2)$
- $\mathbf{z} = \mu + \sigma \odot \epsilon$

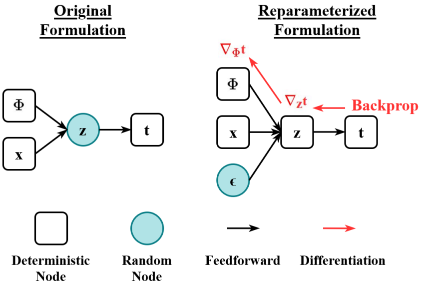

Figure: The schematic representation of reparameterisation trick.

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RNN-VAE for Time-series Modelling

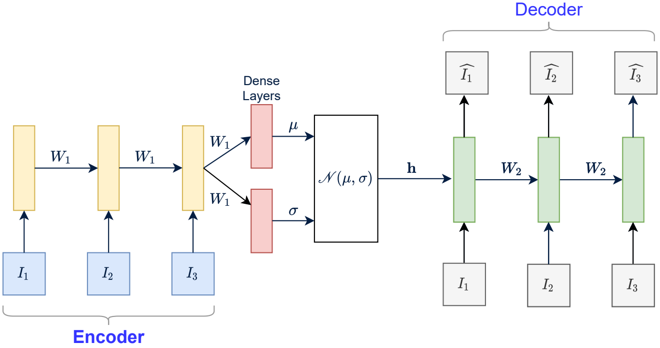

Figure: A schematic illustration of RNN-VAE.

Credit: *Latent ODEs for Irregularly-Sampled Time Series, Rubanova et. al* (2019)

What RNN-VAE can do?

- can generate EHR time-series data
- can compose music! (MusicVAE)
- can be used to generate sentences

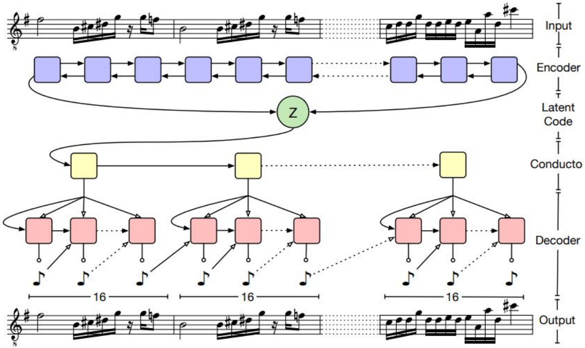

Figure: Schematic of hierarchical recurrent Variational Autoencoder model, MusicVAE.

Credit: *A Hierarchical Latent Vector Model for Learning Long-Term Structure in Music, Roberts et. al (2019)*

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Further Reading

- Transformers
- Conv1d architectures for seq2seq modelling: WavNet
- Generative adversarial networks for time-series generation
- Neural ODE for continuous modelling of RNN hidden dynamics