

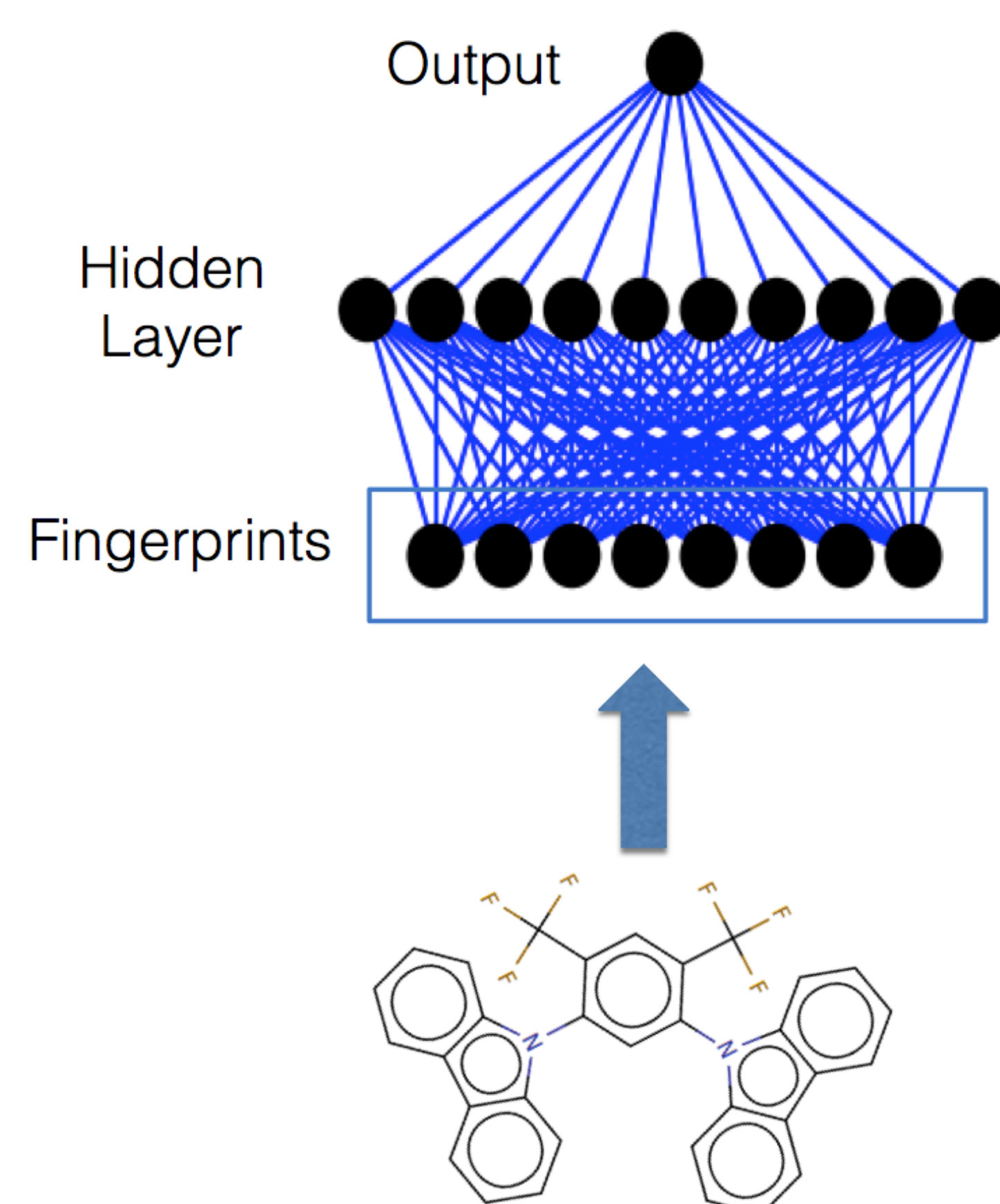
# Auto-Encoding Variational Bayes

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## How to do regression on graphs?

- Input can be any size or shape
- Hard to turn into fixed-length vector
- In our case, graphs represent molecules
- Applications to photovoltaics, organic LEDs, flow batteries and pharmaceuticals



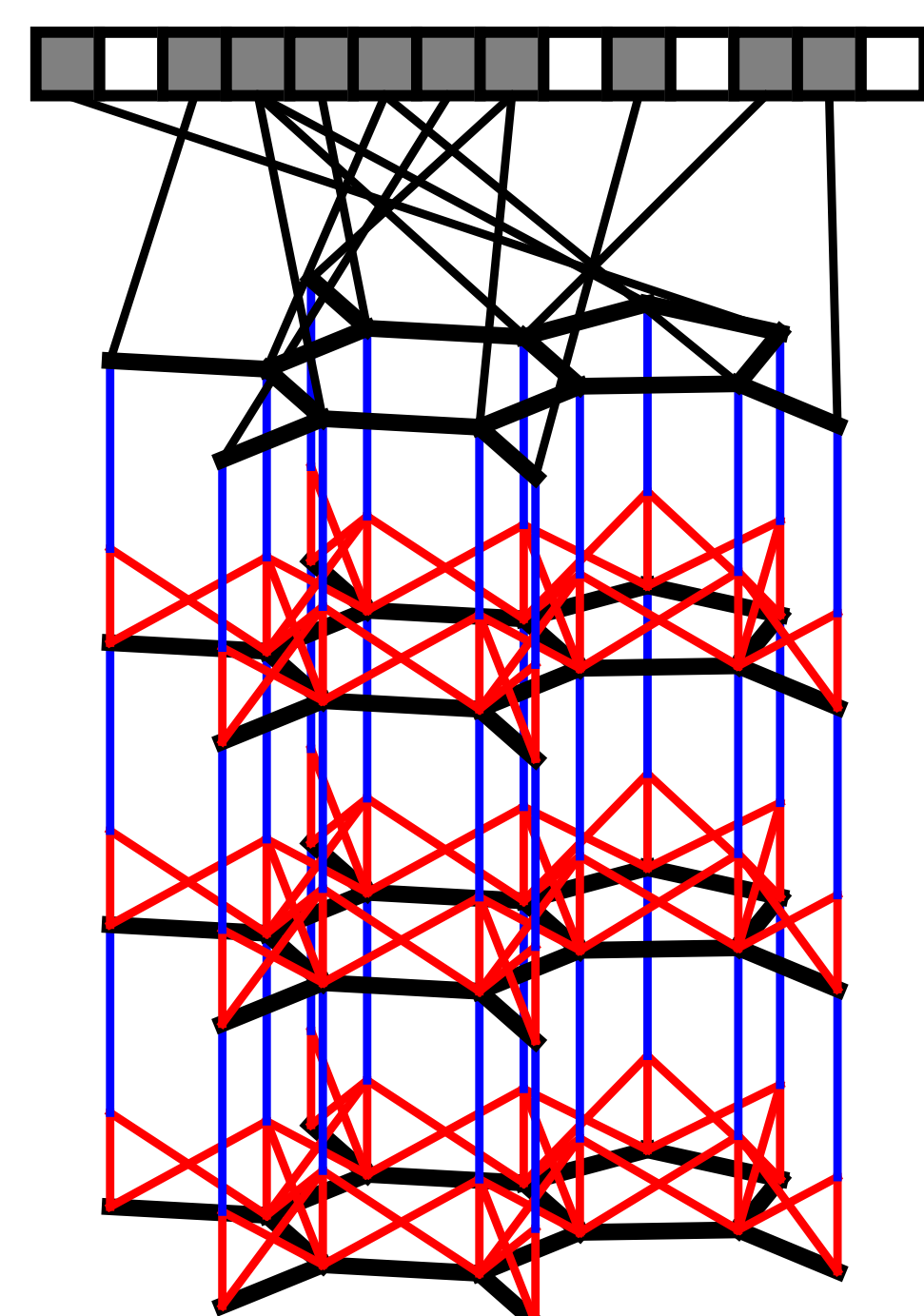
## Circular fingerprints

- Maps variable-sized molecular graph to fixed-length binary vector
- Binary features indicate presence of substructures

Can be efficiently computed using local operations:

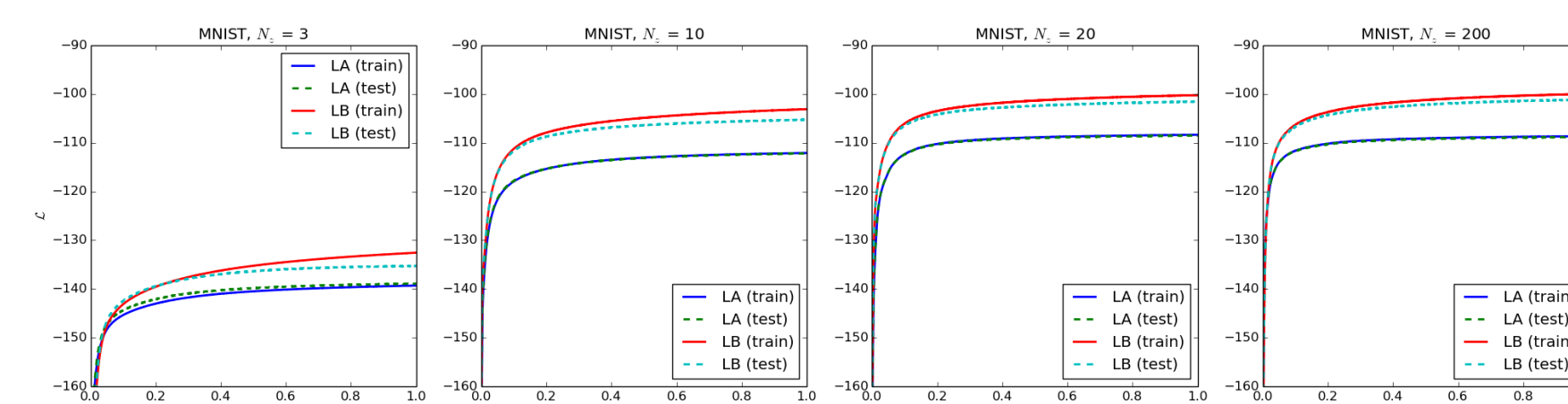
- At each layer, hash the features of each atom and its neighbors/bonds
- More layers correspond to increasing radius of substructures
- Interpret each hash as integer and set that entry to one

Was state-of-the-art for large-scale regression and classification.



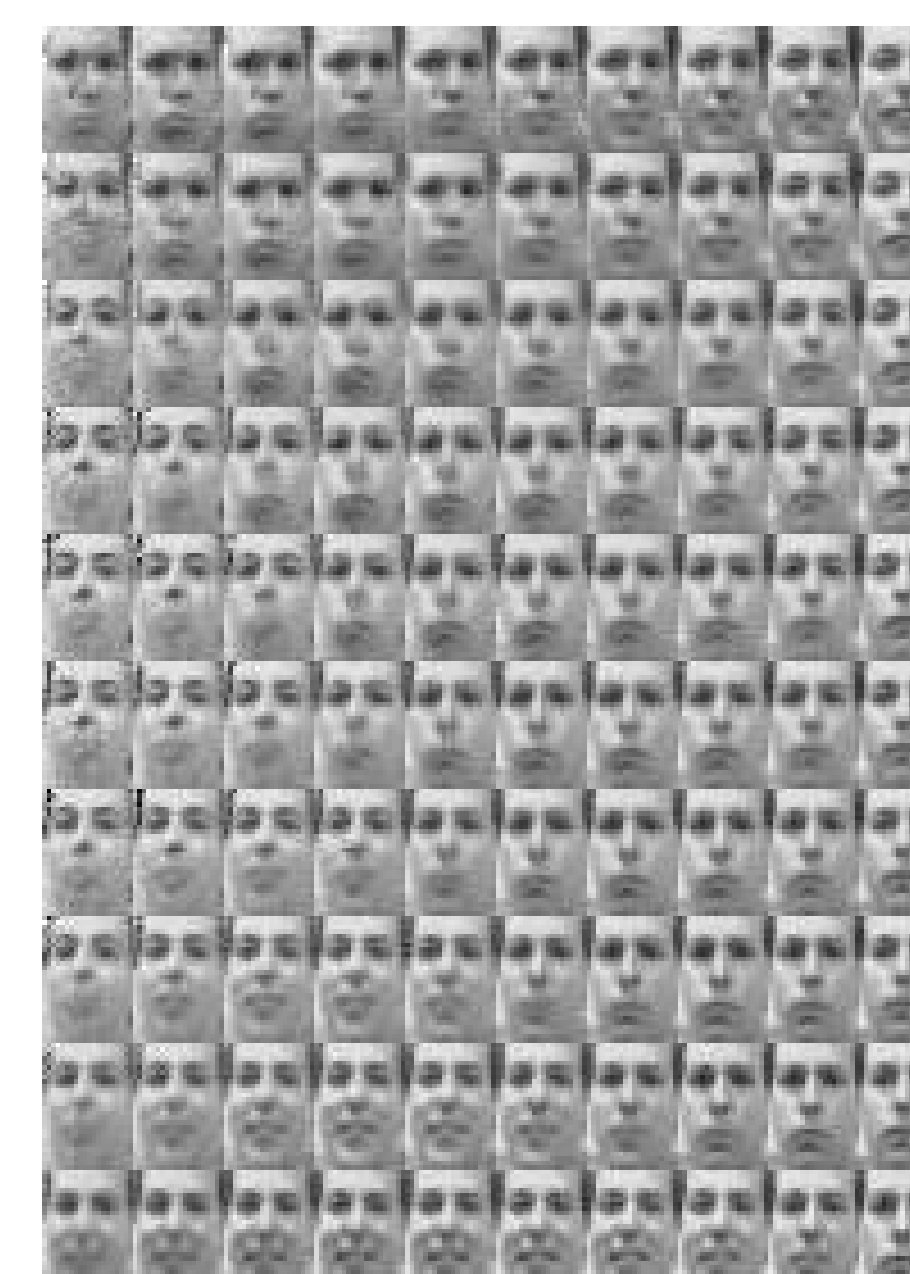
## Learning Curves - la vs lb

Comparison of learning



## Visualisation of learned manifolds

It is possible to observe what the encoder learnt during training if we choose a low-dimensional latent space e.g.  $2D$ . The linearly spaced grid of coordinates over the unit square is mapped through the inverse CDF of the Gaussian (our prior for the latent space is Gaussian) to obtain the value of  $z$ . Then, we plotted the output of our decoder  $p_{\theta}(x|z)$  with the estimated parameters  $\theta$ .



## Full VB

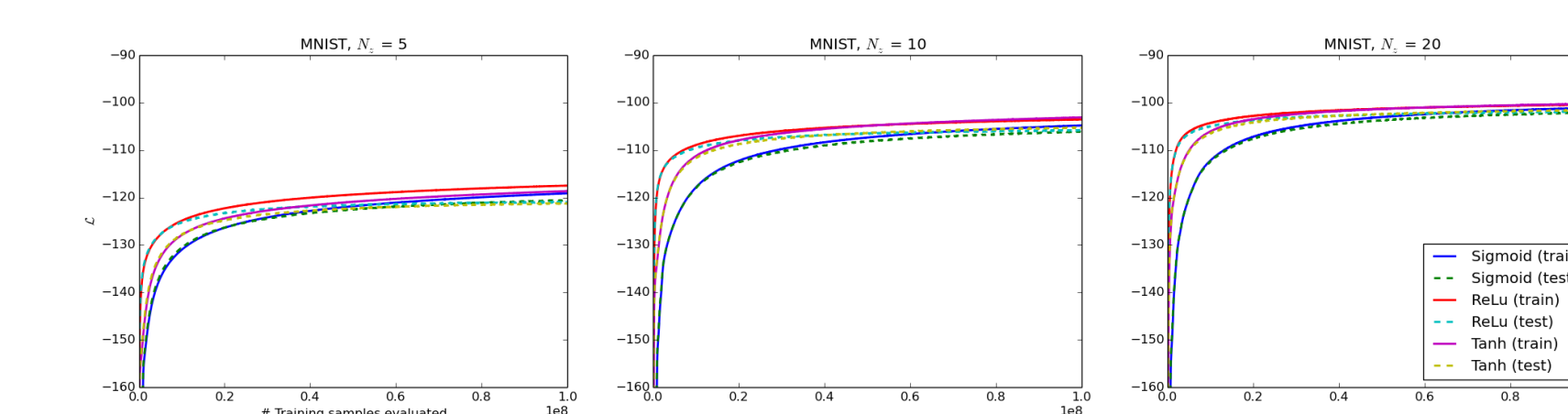
Large random weights give similar behavior to circular fingerprints:

Small random weights already much better than circular fingerprints! Can do even better by optimizing for given task.

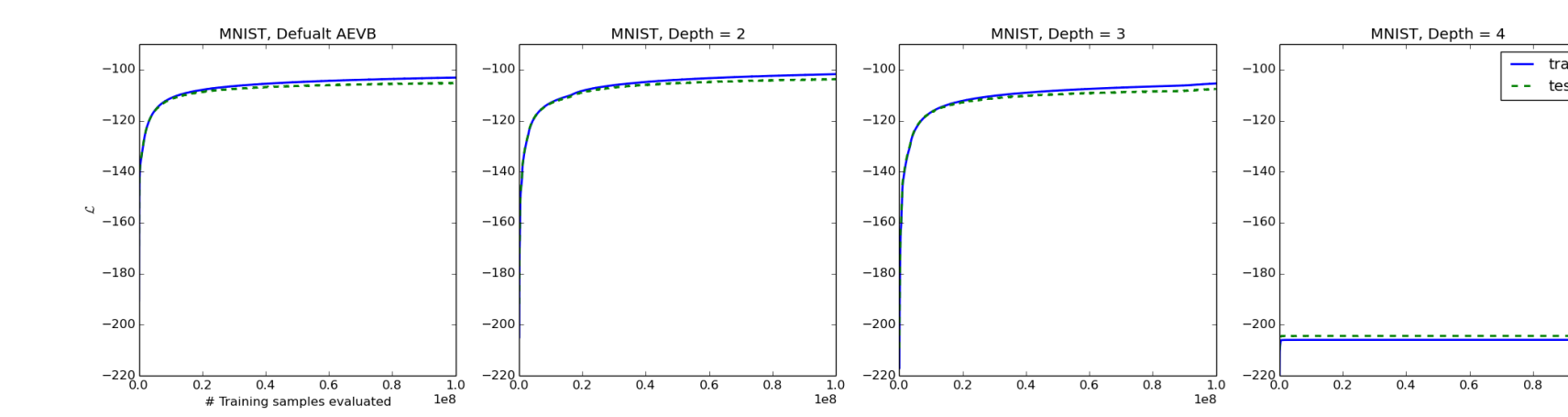
## Architecture experiments

We examined various changes to the original architecture of the auto-encoder to test the robustness and flexibility of the model which lead to improvement in terms of optimising the lower bound and computational efficiency.

- Different activation functions.



- Increasing the depth of the encoder.



## Future works

- Scheduled training of VAEB [2].

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## References

1. Kingma, D. P., and Welling M., "Auto-encoding variational bayes." arXiv preprint arXiv:1312.6114 (2013).
2. Geras, K. J., and Sutton C., "Scheduled denoising autoencoders." arXiv preprint arXiv:1406.3269 (2014).