Other types of networks and some example applications

Anders Krogh

Many different types of neural networks used for different tasks

Generative models

Generative neural networks

Aim:

Model the distribution of your data, *P(x),* by mapping from a low-dimensional representation space

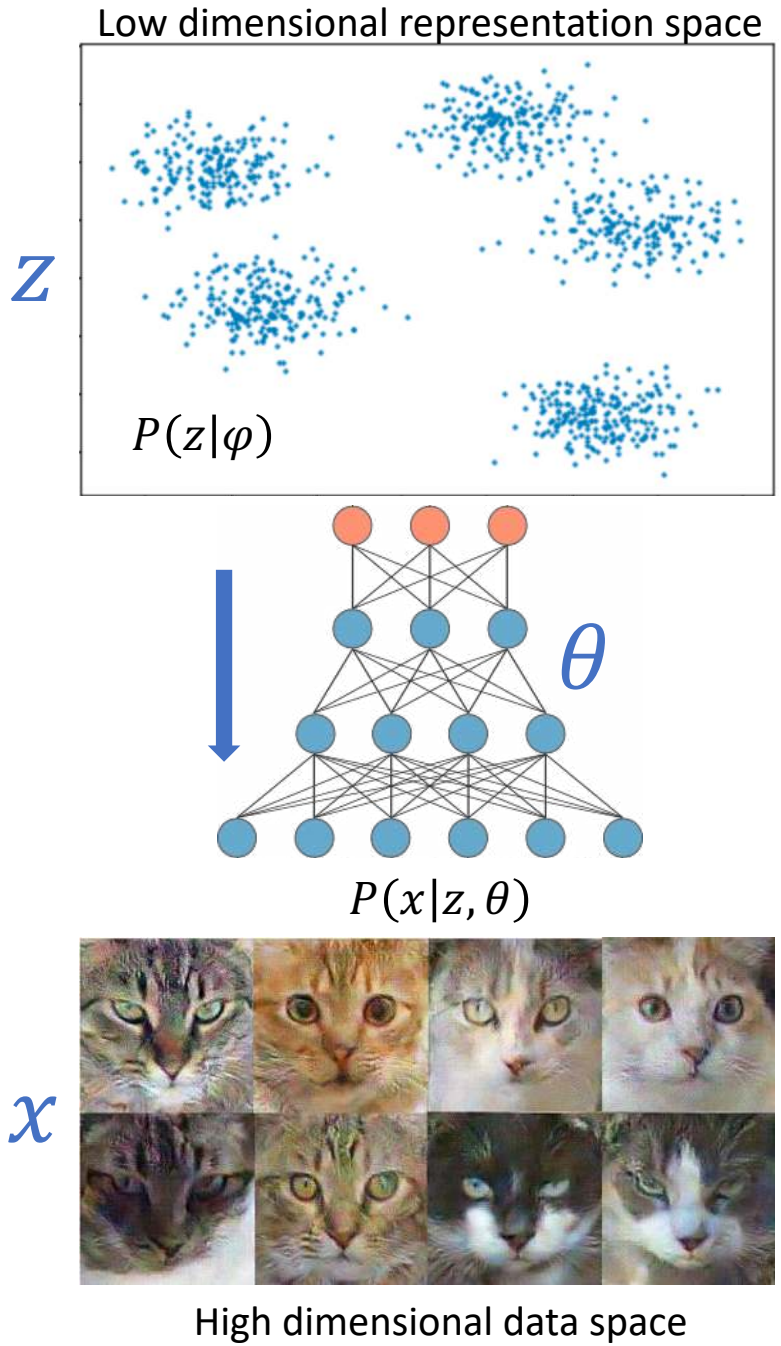
Ingredients:

- Distribution over representations: $P(z|\varphi)$
- Decoder (neural network): $P(x|z,\theta)$ *

Generative:

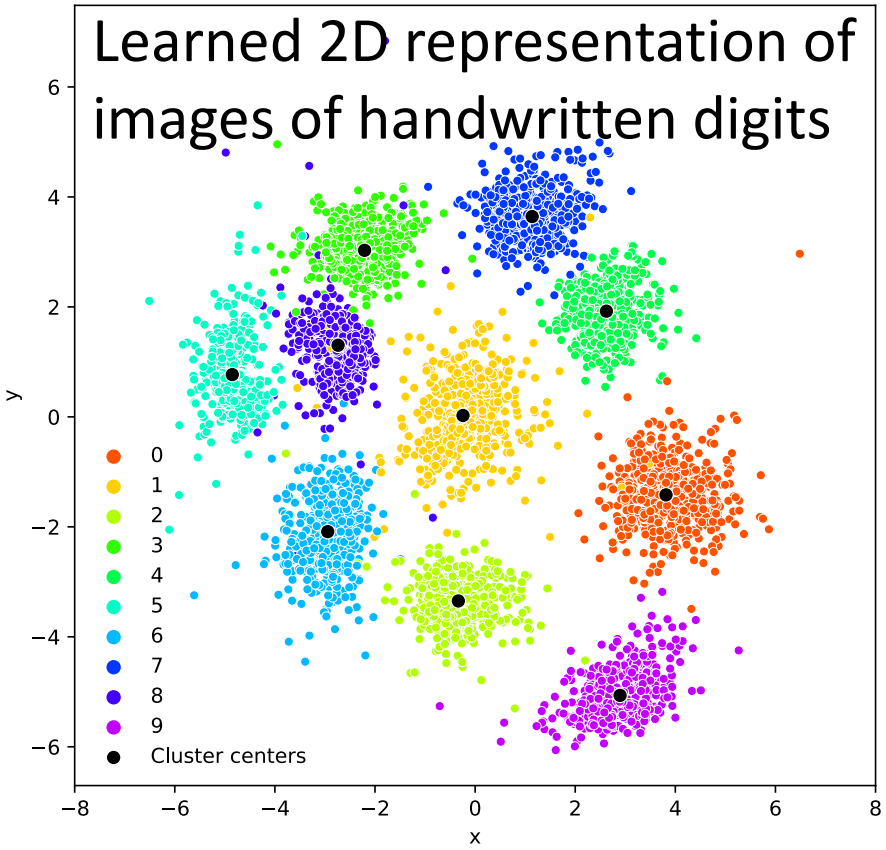
1. Sample random z from $P(z|\varphi)$
2. Sample random x from $P(x|z,\theta)$

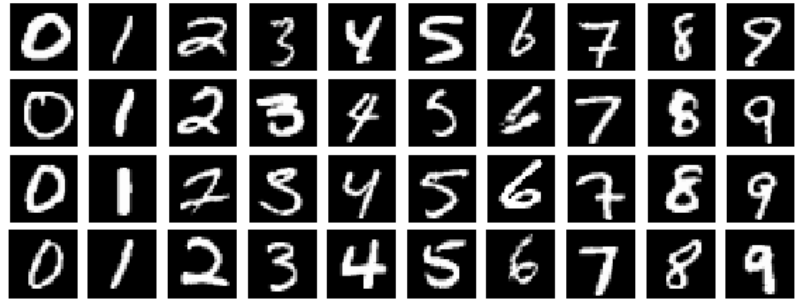
*) Neural network may for instance output a mean of a normal with fixed variance



Why generate images of fake cats?

- Model learns a low dimensional representation
- Related to manifold learning
  - UMAP
  - tSNE
- This may be useful for other puposes
  - Representations useful for other tasks
  - Grouping of tumor types, stocks, cats,…
  - Imputation
  - Interpolation





Images from MNIST

Latent space interpolation

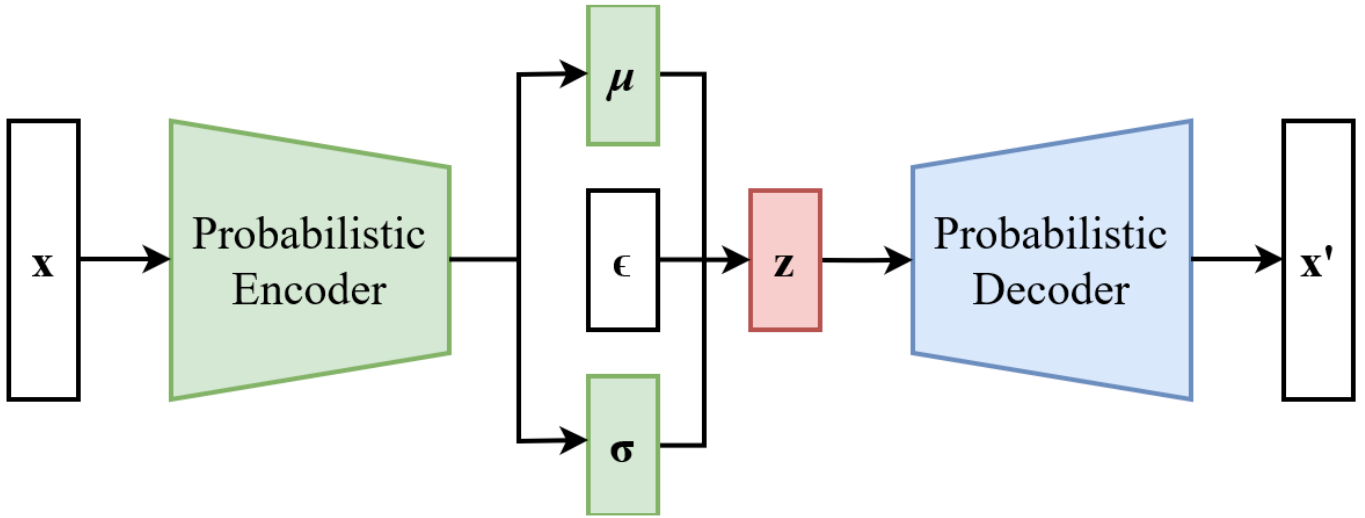
Copied from
“Generative Modeling with Variational Auto Encoder (VAE). Understanding the intuition behind Variational Autoencoder”
By Fathy Rashad

https://medium.com/vitrox-publication/generative-modeling-with-variational-auto-encoder-vae-fc449be9890e

Similar: App that can predict how you will look when you get old

VAE: Variational Autoencoder

- Training of generative models require additional “tricks”
- One method is to train an encoder together with the decoder to give a distribution P(z|x) to sample from
- This is called a variational autoencoder



- Generative adversarial network (GAN) is another type

Image credits: https://en.wikipedia.org/wiki/Variational_autoencoder, EugenioTL, https://commons.wikimedia.org/wiki/User:EugenioTL

Generative models for gene expression

Bioinformatics, 36(16), 2020, 4415–4422
doi: 10.1093/bioinformatics/btaa293
Advance Access Publication Date: 16 May 2020
Original Paper

Gene expression

scVAE: variational auto-encoders for single-cell gene expression data

Christopher Heje Grønbech[1,2,3,*], Maximillian Fornitz Vording[3], Pascal N. Timshel[4], Casper Kaae Sønderby[1], Tune H. Pers[4] and Ole Winther[1,2,3]

nature methods
ARTICLES
https://doi.org/10.1038/s41592-019-0494-8

scGen predicts single-cell perturbation responses

Mohammad Lotfollahi[1,2], F. Alexander Wolf[1*] and Fabian J. Theis[1,2,3*]

nature COMMUNICATIONS

ARTICLE
https://doi.org/10.1038/s41467-019-14018-z OPEN

Realistic in silico generation and augmentation of single-cell RNA-seq data using generative adversarial networks

Mohamed Marouf[1,5], Pierre Machart[1,5], Vikas Bansal[1], Christoph Kilian[1,2], Daniel S. Magruder[1,3], Christian F. Krebs[2] & Stefan Bonn[1,4*]

Bioinformatics, 36(11), 2020, 3418–3421
doi: 10.1093/bioinformatics/btaa169
Advance Access Publication Date: 16 March 2020
Original Paper

Gene expression

Interpretable factor models of single-cell RNA-seq via variational autoencoders

Valentine Svensson[1,*], Adam Gayoso[2], Nir Yosef[2,3,4] and Lior Pachter[1,5]

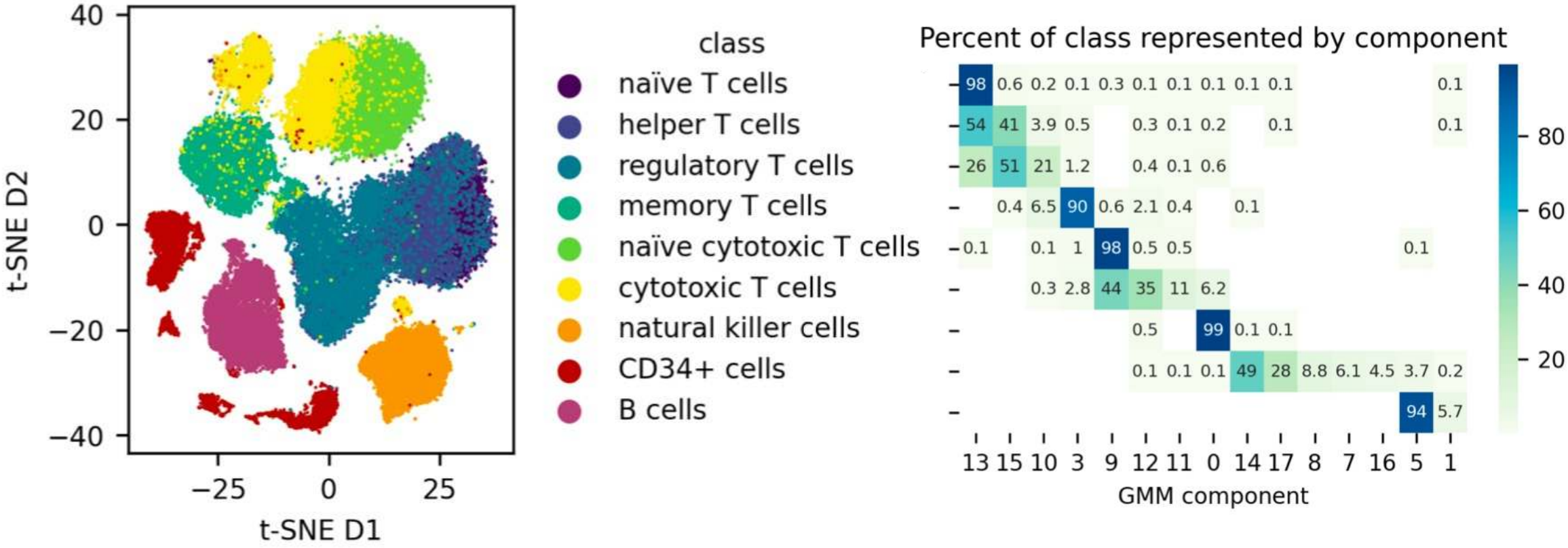
nature COMMUNICATIONS

ARTICLE
https://doi.org/10.1038/s41467-021-26017-0 OPEN

VEGA is an interpretable generative model for inferring biological network activity in single-cell transcriptomics

Lucas Seninge[1], Ioannis Anastopoulos[1], Hongxu Ding[1✉] & Joshua Stuart[1✉]

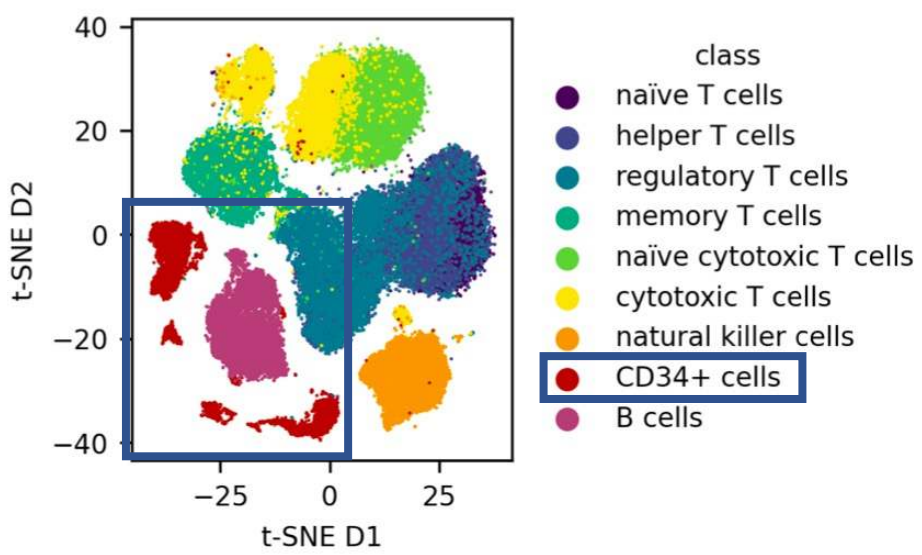
A Deep Generative model applied to a single-cell dataset from peripheral blood mononuclear cells*

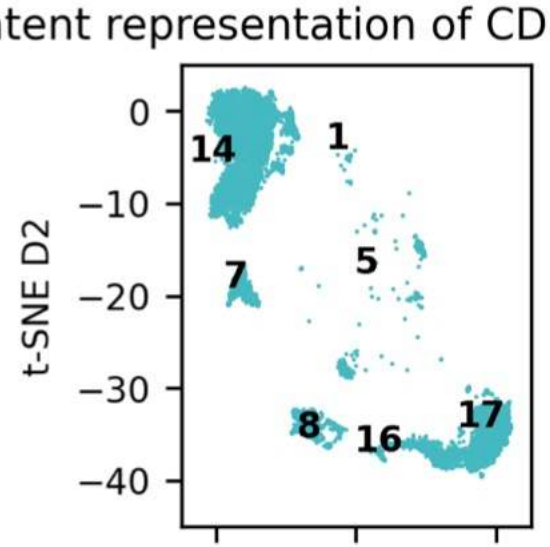


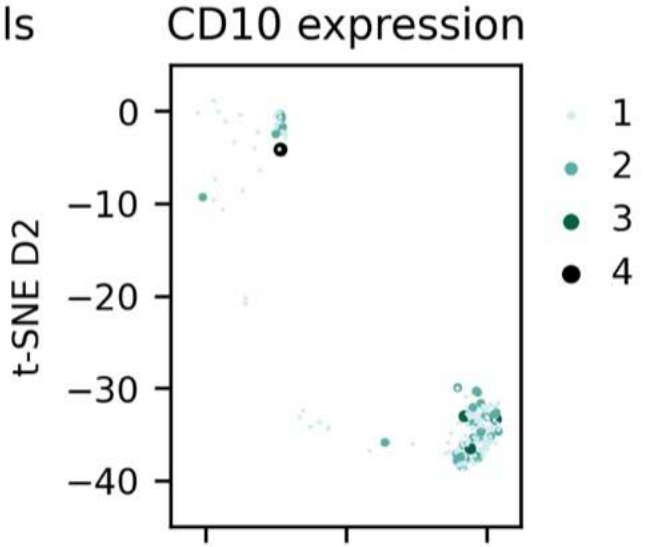
Schuster & Krogh: https://arxiv.org/abs/2110.06672

*) Data from Zheng, et al. Nat Commun. 2017 Apr;8(1):14049. https://doi.org/10.1038/ncomms14049.

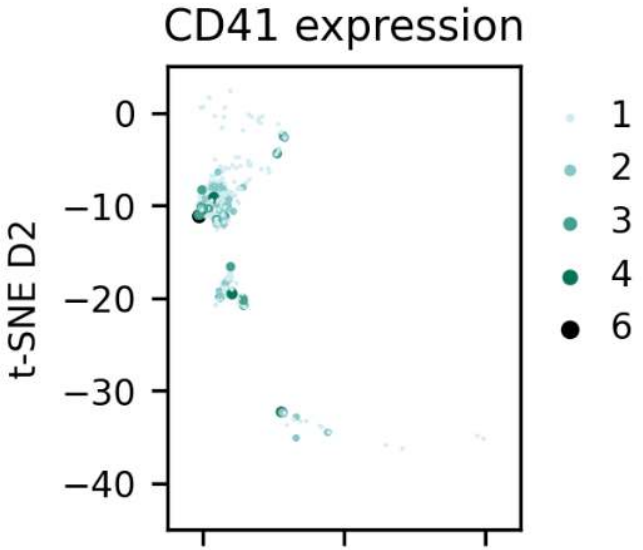
Sub-clustering for marker genes

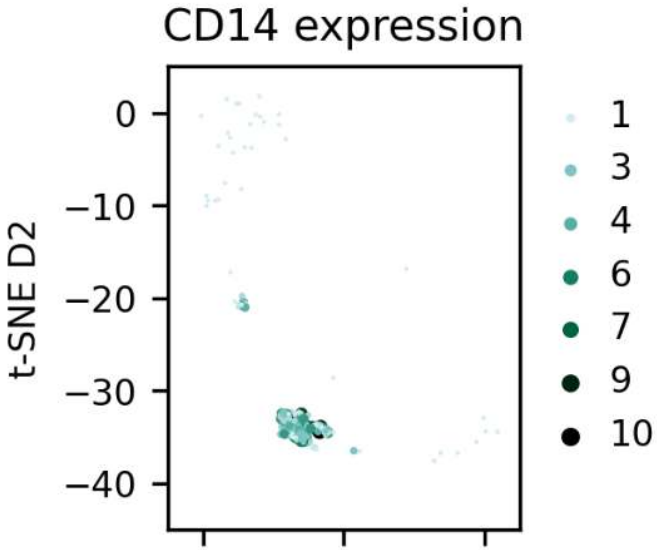


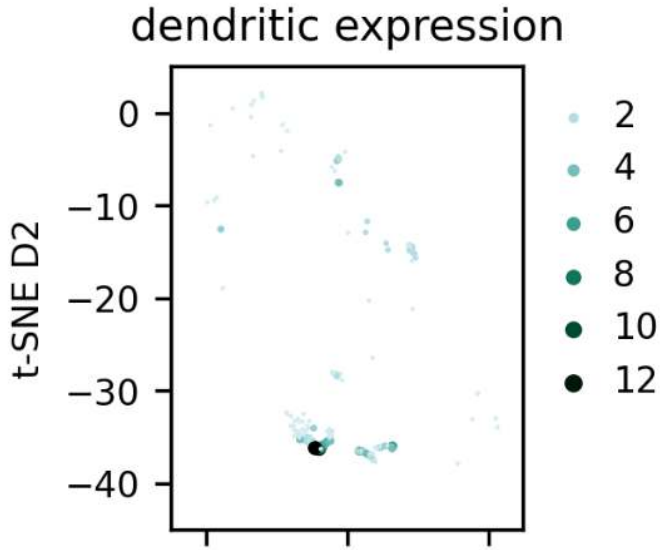




Heatmaps shows expression count







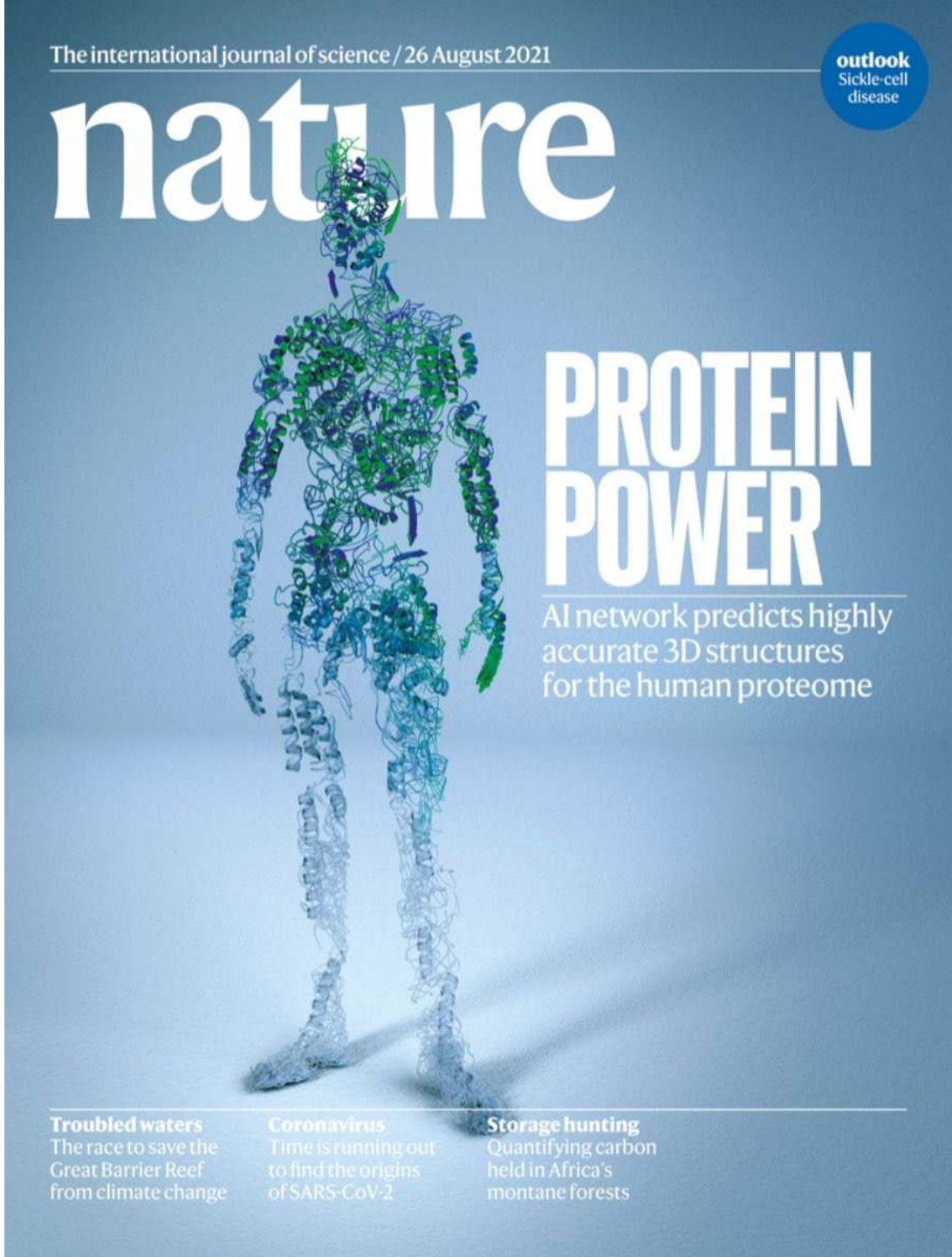
Transformers

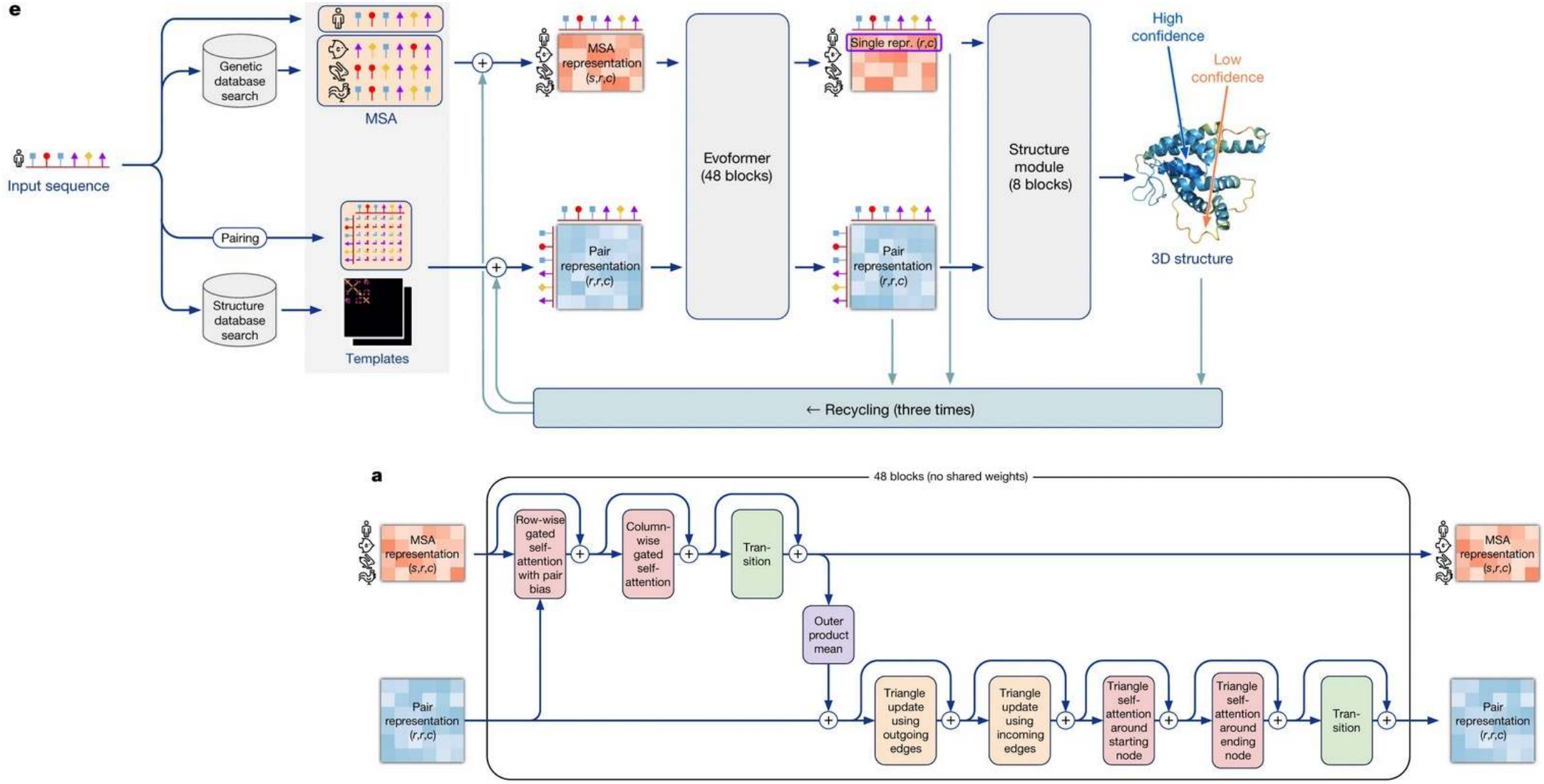
AlphaFold 2

The New York Times

A.I. Predicts the Shapes of Molecules to Come

DeepMind has given 3-D structure to 350,000 proteins, including every one made by humans, promising a boon for medicine and drug design.





From: Jumper, J., Evans, R., Pritzel, A. *et al.* Highly accurate protein structure prediction with AlphaFold. *Nature* **596**, 583–589 (2021). https://doi.org/10.1038/s41586-021-03819-2

Transformer Neural Networks

- Introduced for natural language processing
- Used for sequential data like words in a sentence or amino acids in a sequence
- Replaces recurrent neural networks
- Use several layers of representations and an attention mechanism to focus on important parts (words)

Learn more e.g. in this blog post (where the figure is from):

https://towardsdatascience.com/transformer-neural-network-step-by-step-breakdown-of-the-beast-b3e096dc857f

or read the paper

Attention Is All You Need

Ashish Vaswani* Google Brain avaswani@google.com

Noam Shazeer* Google Brain noam@google.com

Niki Parmar* Google Research nikip@google.com

Jakob Uszkoreit* Google Research usz@google.com

Llion Jones* Google Research llion@google.com

Aidan N. Gomez* † University of Toronto aidan@cs.toronto.edu

Łukasz Kaiser* Google Brain lukaszkaiser@google.com

Illia Polosukhin* ‡ illia.polosukhin@gmail.com

31st Conference on Neural Information Processing Systems (NIPS 2017), Long Beach, CA, USA.

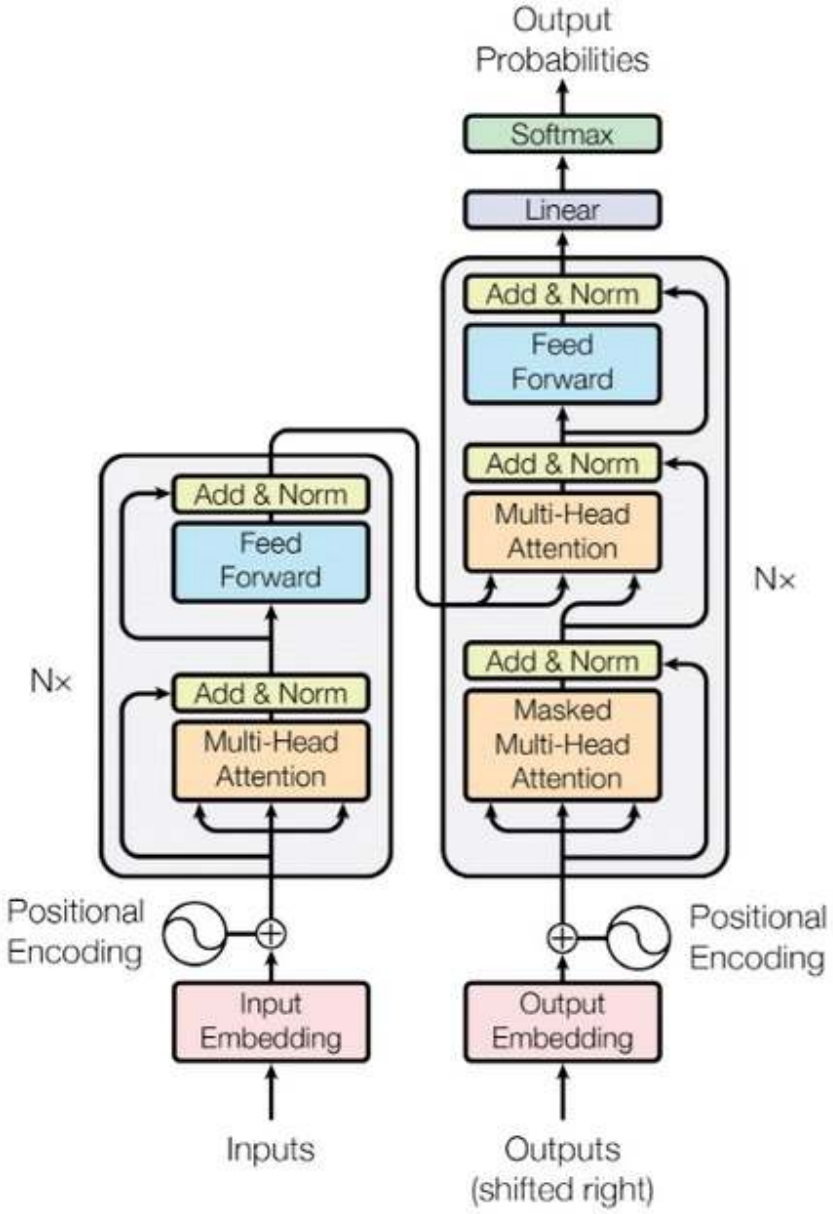


Figure 1: The Transformer - model architecture.

And so on

- DELL-E https://openai.com/dall-e-2/
- ChatGBT