MAF:
Masked Autoregressive Flow for Density Estimation

Lorne Whiteway
lorne.whiteway@star.ucl.ac.uk

Astrophysics Group
Department of Physics and Astronomy
University College London

27 April 2020

Find the presentation at https://tinyurl.com/???

Context

- *Supervised machine learning* i.e. selecting from a highly-parameterised family of non-linear functions to fit some training data.
- Fitting is done to optimise a utility function that rewards a close match to the training data and penalises complexity i.e. enforces *regularization*.
- Regularisation is also provided by any lack-of-flexibility in the fitting functions.
- Bayesian framework: adherence to training data = likelihood; regularisation = prior.

Density Estimation

- We want to do ML to do density estimation:
- Find the probability density p, given a set of training data $\{x_i\}$ that we suppose to be a fair random sample from p.

MAF

- We will discuss the MAF algorithm: Papamakarios et al. 2018; Masked Autoregressive Flow for Density Estimation; `https://arxiv.org/abs/1705.07057`.
- Based on earlier algorithms of which the most relevant is MADE: Germain et al. 2015; MADE: Masked Autoencoder for Distribution Estimation; `https://arxiv.org/abs/1502.03509`.
- I will focus first on MADE as all the key ideas are present there.

Analogy

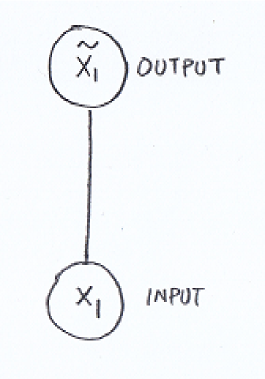
- An *autoencoder* is like a parrot - it learns to mimic.
- An *autoregressive autoencoder* is like a deaf parrot - it learns to play the probabilities (and hence becomes a density estimator).

Parrot training

- Simple example: single binary outcome. We want the parrot to mimic us when we say 'Yes' or 'No'.
- So give lots of 'Yes', 'No' training data; give the parrot treats but reduce the treats by the non-positive number log(% correctness of the parrot's response). This is called *cross-entropy loss*.

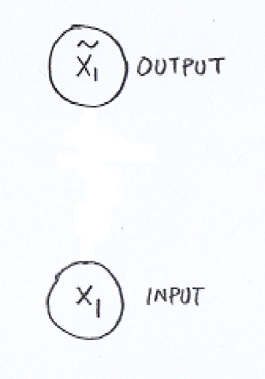
Parrot training

- The neural network is incentivised to model the identity function $\tilde{x_1} = x_1$.
- Depending on the flexibility of the neural network the parrot will get this exactly or approximately correct.



Deaf parrot

- Deaf parrot = no link between input and output.
- Parrot still squawks and gets feedback (more treats if the squawk accidentally matched the unheard training input).
- If say 75% of the training data was 'Yes' then the parrot will learn to say 'Yes' more often. Optimal strategy will be a word that is 75% 'Yes' and 25% 'No'.



Deaf parrot

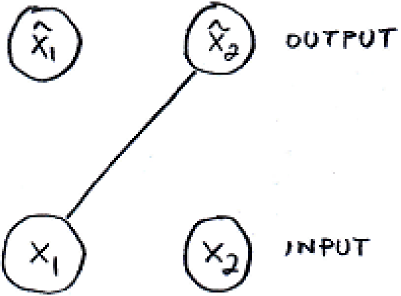
- So by removing links from the neural network but still rewarding the network for mimicry we create a density estimator.

Two word phrase

- Now consider two word phrases ("Yes, No").
- If there is no correlation between the two words then we just need two deaf parrots.
- But generally $p(x_1 \& x_2) = p(x_1)p(x_2|x_1)$.
- To model this: one deaf parrot for $p(x_1)$ as before. But for the second parrot: unmask its ears, let it hear the training word told to the first parrot, the re-mask its ears for the second word.
- Give treats as before (still encouraging mimicry).
- Easy to show that the second parrot learns $p(x_2|x_1)$.

Two word phrase

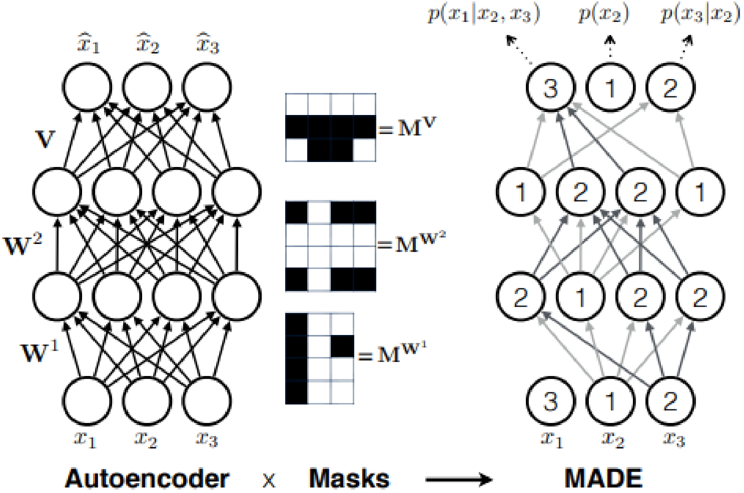
- More generally if $\tilde{x}_i$ is linked only to $x_1, \ldots x_{i-1}$ then we learn $p(x_1), \ldots, p(x_i|x1 \ldots x_{i-1})$ whose product is $p(x)$.



Autoencoder; Autoregressive autoencoder

- The 'hearing' parrot (that mimics) is an *autoencoder*.
- The network of partially-deaf parrots (that learns the conditional probabilities) is called an *autoregressive autoencoder*.
- Autoregression appears in other contexts e.g. predicting the next element in a causal sequence.

Figure 1 from MADE paper



Sampling from the inferred probability density

- Use $(0,0)$ as input to get $(\tilde{x}_1, \tilde{x}_2)$ as output;
- Randomly choose s_1 in $\{0,1\}$ with probability $\tilde{x}_1$ of being 1;
- Use $(s_1, 0)$ as input to get new $(\tilde{\tilde{x}}_1, \tilde{\tilde{x}}_2)$ as output;
- Randomly choose s_2 in $\{0,1\}$ with probability $\tilde{\tilde{x}}_2$ of being 1;
- Then (s_1, s_2) is a new sample from the inferred density.
- Takes D evaluations of the net to get one new sample.

More complicated distributions

- So far we have looked at binary distributions.
- Here the probability density could be described by a single number ($= p(x_i = 1)$). So output $\tilde{x}_i$ has dual meaning as 'best guess at x_i' and as '$p(x_i = 1 | x1, \ldots, x_{i-1})$'.

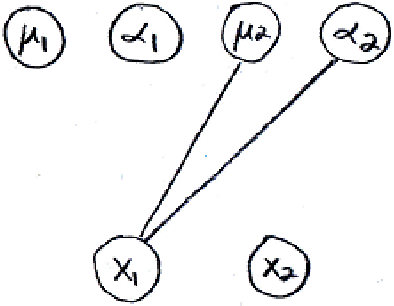
More complicated distributions

- To handle continuous distributions:
- Assume each univariate conditional distribution $p(x_i|x_1, \ldots, x_{i-1})$ is Gaussian;
- Two output cells for each input: one for mean and one for (log of) standard deviation - from this we easily calculate the conditional probabilities and hence the overall probability of any given input;
- Loss function is now sum of negative logs of probabilities of training data.

More complicated distributions

$$p(x_1) = N(\mu_1, \exp(\alpha_1))$$

$$p(x_2|x_1) = N(\mu_2, \exp(\alpha_2))$$



Sampling from the inferred probability density $\tilde{p}$

- As before we can create new samples with D calls to the neural net.
- At each step we randomly choose u_i from $N(0,1)$ and scale and shift it to get $\tilde{x_i} = \exp(\alpha) * u_i + \mu$.
- At each step the α and μ come from a call to the net with $\tilde{x_1}, \ldots, \tilde{x_{i-1}}$ as inputs.

Sampling from the inferred probability density 1

- Thus we get a mapping f from $u \sim N(0, I)$ to $\tilde{x} \sim \tilde{p}$.
- The mapping is easily invertible!
- $u_i = (\tilde{x}_i - \mu) \exp(-\alpha)$
- All the μ and α that we need are available in **one** call to the net (as here we have all the net input values that we need).
- This gives f^{-1} mapping $\tilde{p}$ to $N(0, I)$.

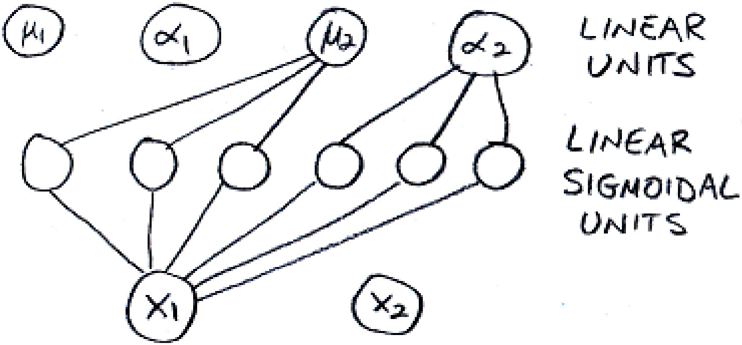
Sampling from the inferred probability density 2

- Furthermore the autoregressive property means that the Jacobian of $f^{-}1$ is triangular.
- Its diagonal elements are just the $exp(-\alpha_i)$ factors.
- So the determinant of $Jac(f^{-}1)$ is easy to calculate.

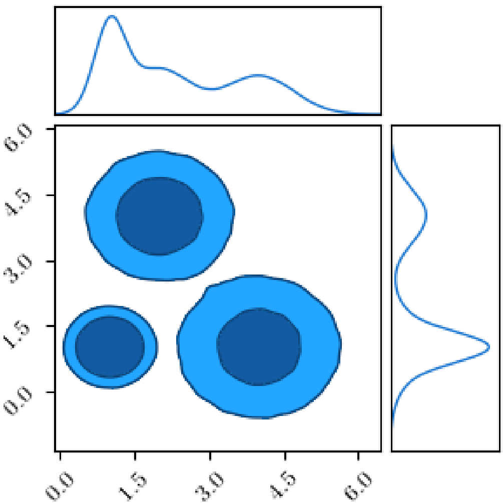
Normalising flow

- So f maps $N(0, I)$ to $\tilde{p}$.
- Such f is called a normalising flow.
- Recall how probability densities transform: $\tilde{p}(x) = \mathcal{N}_{(0,I)}(f^{-1}(x))|det(Jac(f^{-1}))|$
- All of these components are easy to calculate, and let us evaluate and sample from $\tilde{p}$.

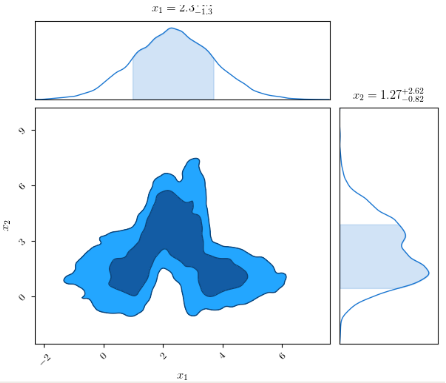
Example - Neural net



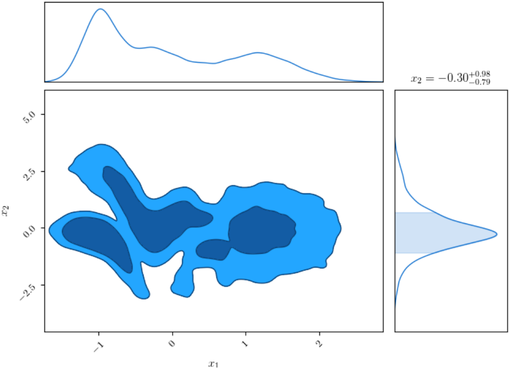
Example - Target distribution



Example - inferred distribution



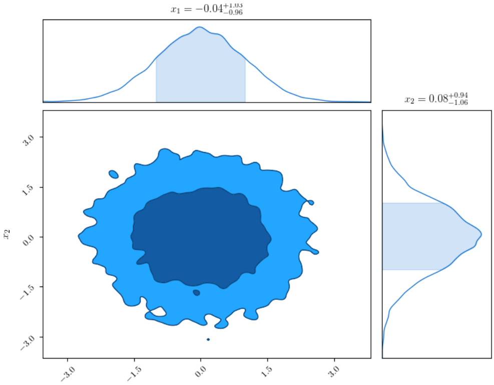
Inverse image of inferred distribution - should be $N(0, I)$



MAF idea

- Map the original training data back through f^{-1} to get $\{u_i\}$ that should be $N(0, I)$ but aren't;
- Repeat the whole process! Treat the u as training data for a new neural net that is trying to model the u as a distorted $N(0, I)$
- Be prepared to do this five or ten iterations.

MAF - after two iterations


$x_1 = -0.04^{+1.03}_{-0.96}$
$x_2 = 0.08^{+0.94}_{-1.06}$
x_2
3.0
1.5
0.0
−1.5
−3.0
−3.0
−1.5
0.0
1.5
3.0