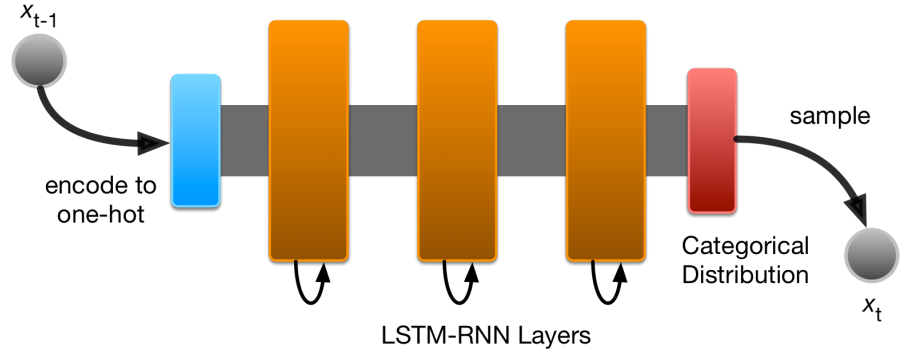
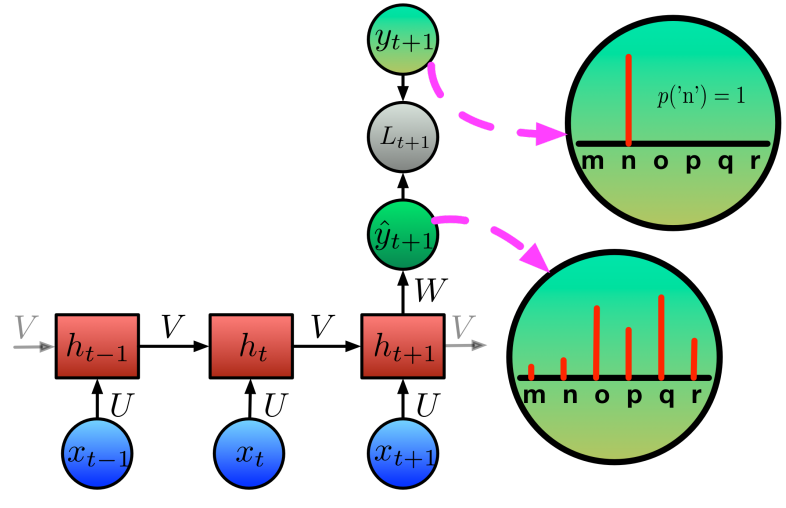
MIXTURE DENSITY NETWORKS

Charles Martin

SO FAR; RNNS THAT MODEL CATEGORICAL DATA





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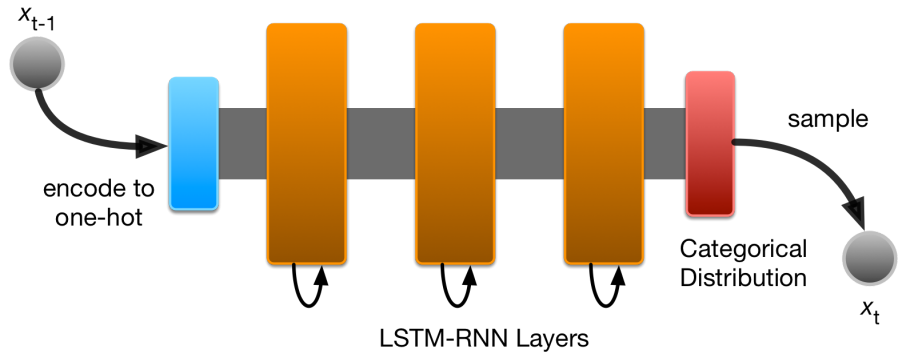

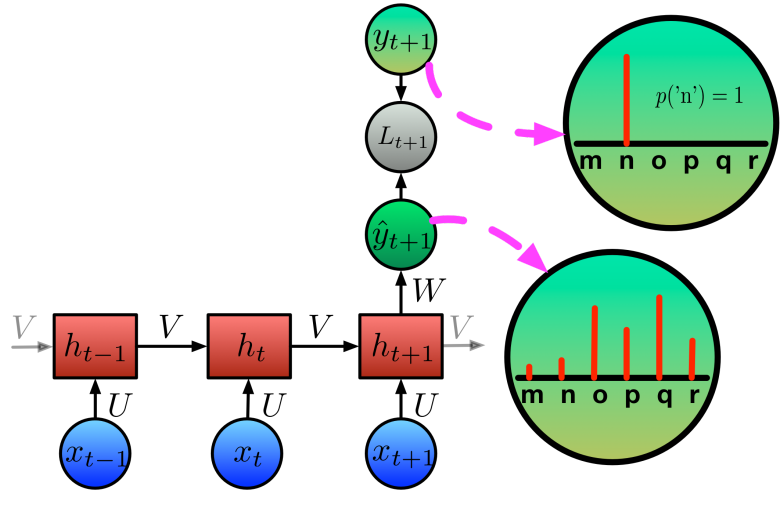

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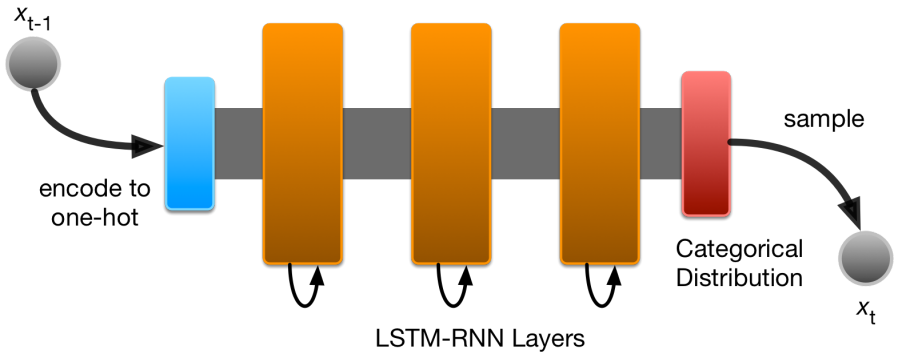

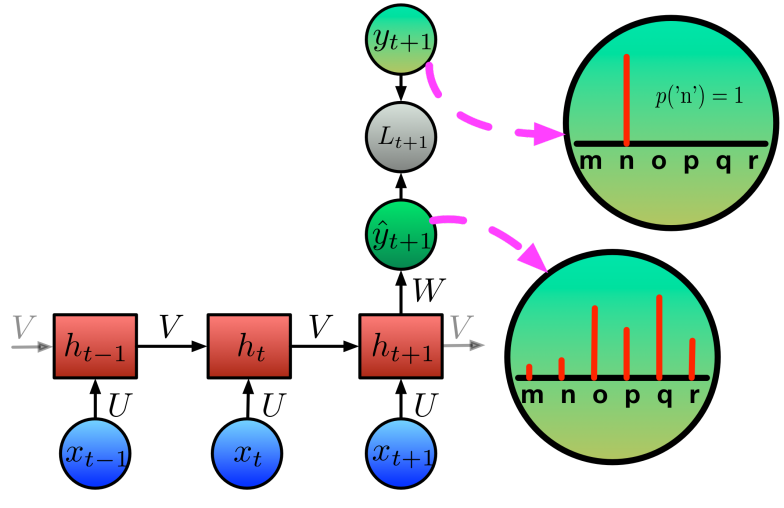

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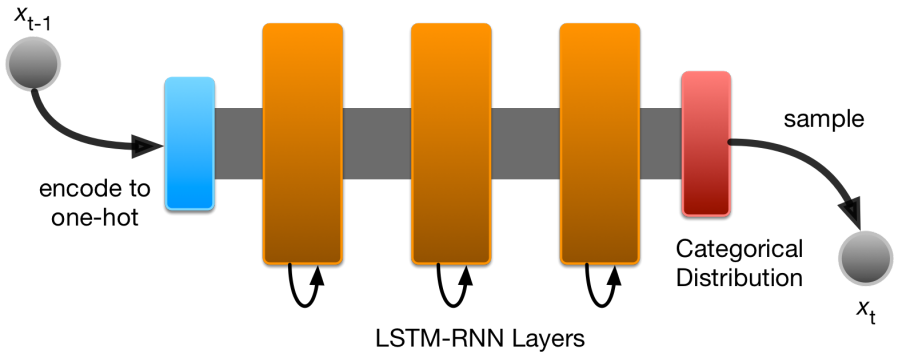

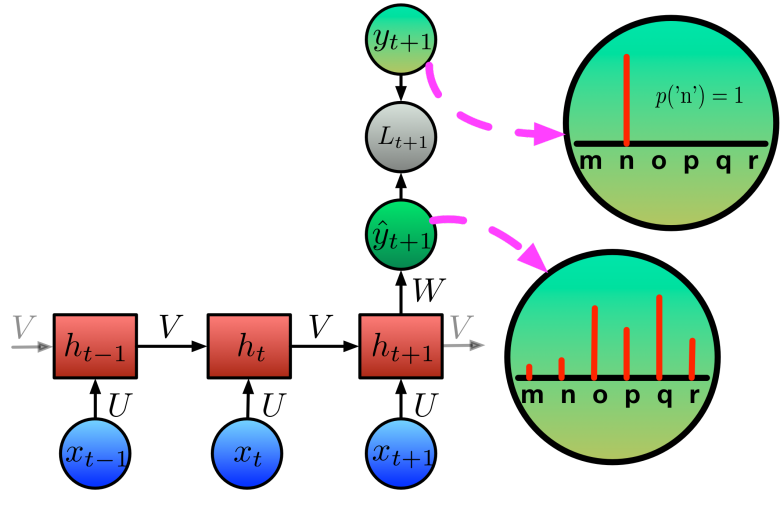

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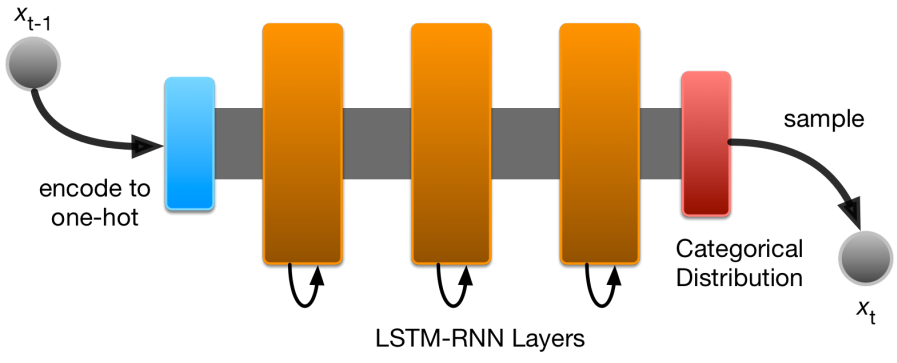

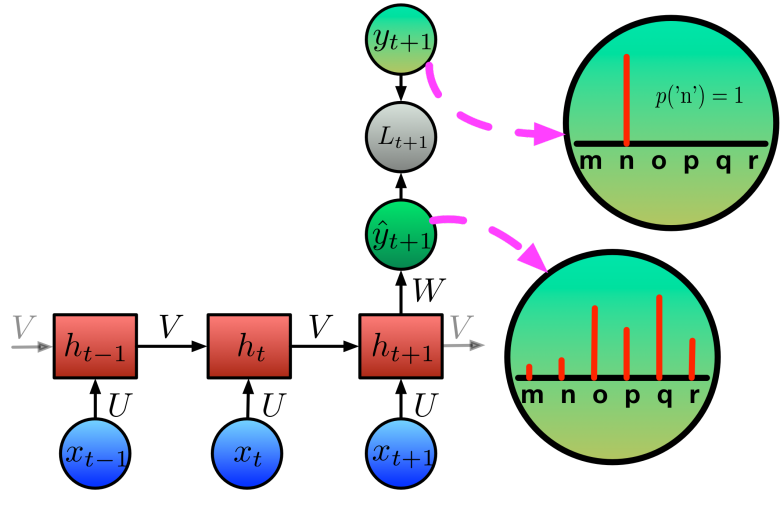

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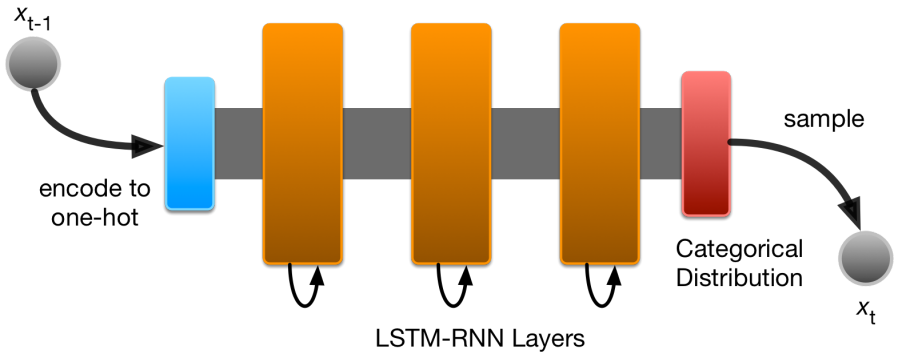

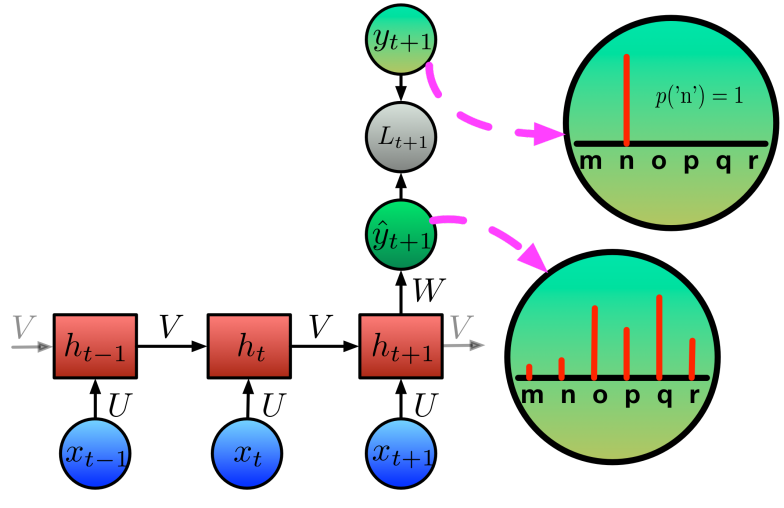

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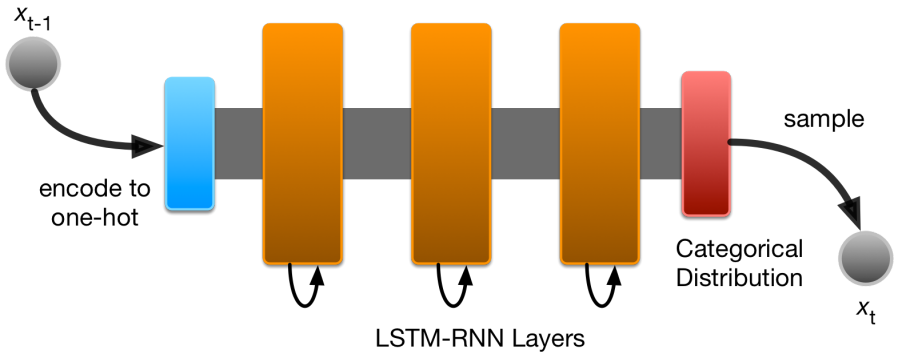

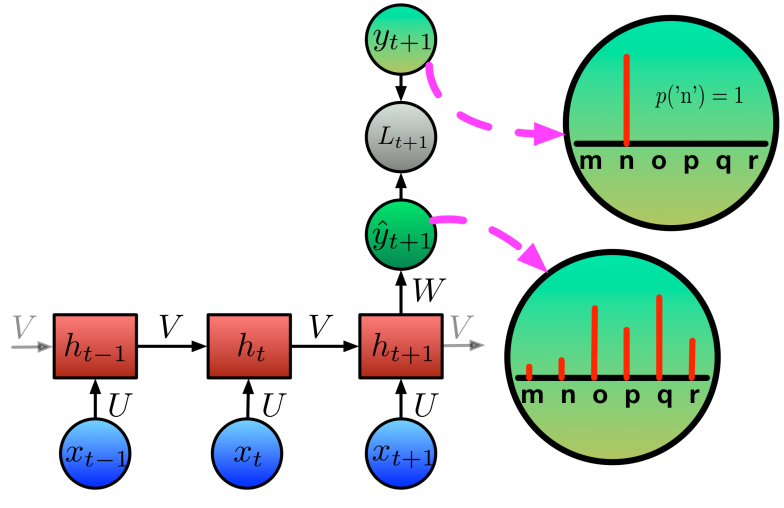

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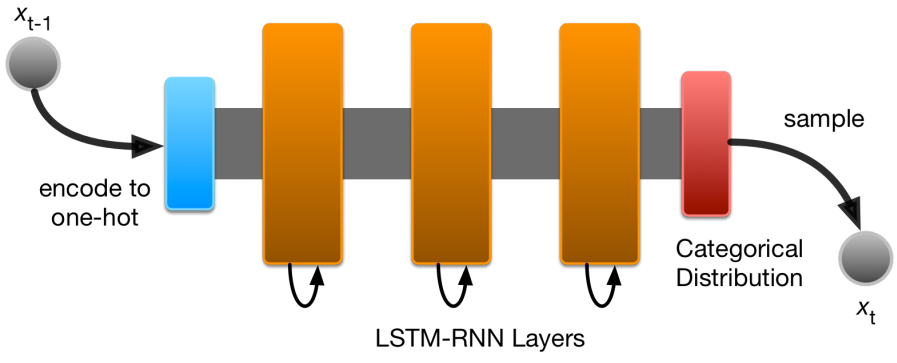

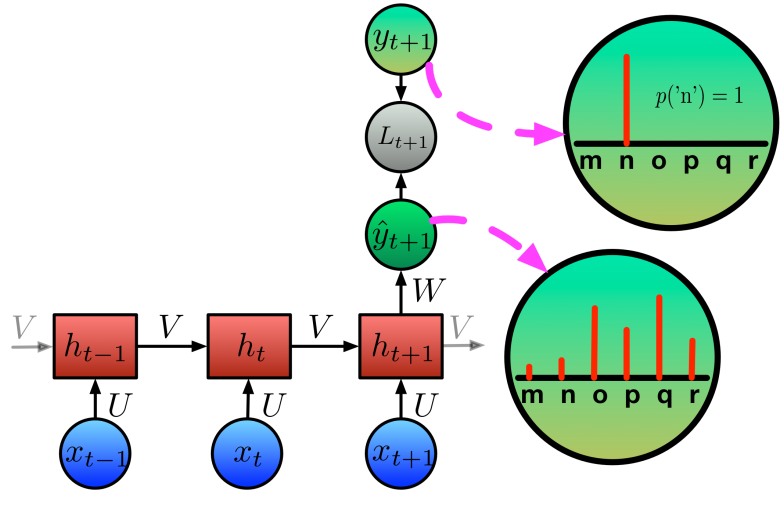

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  - image labels,
  - letters, words,
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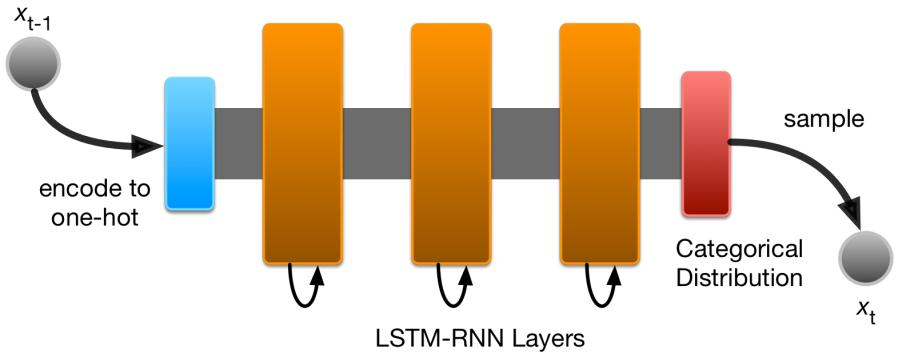
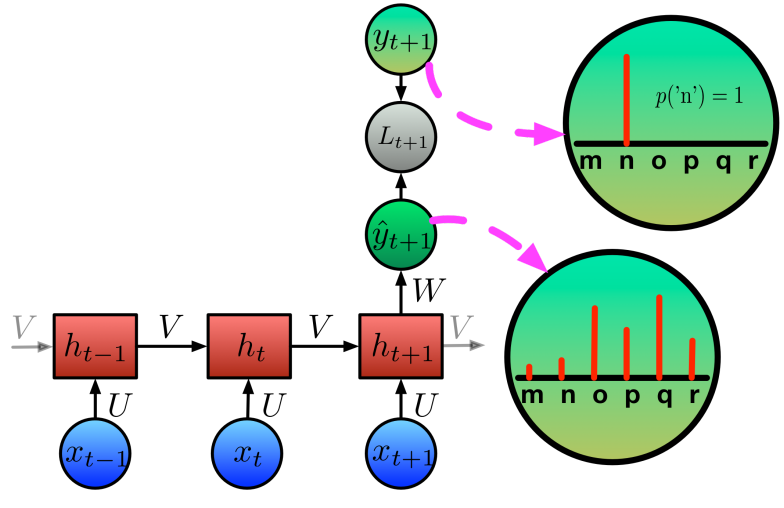
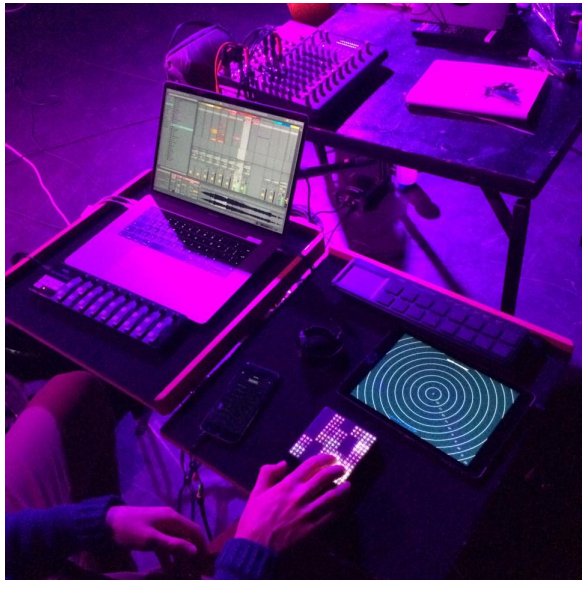
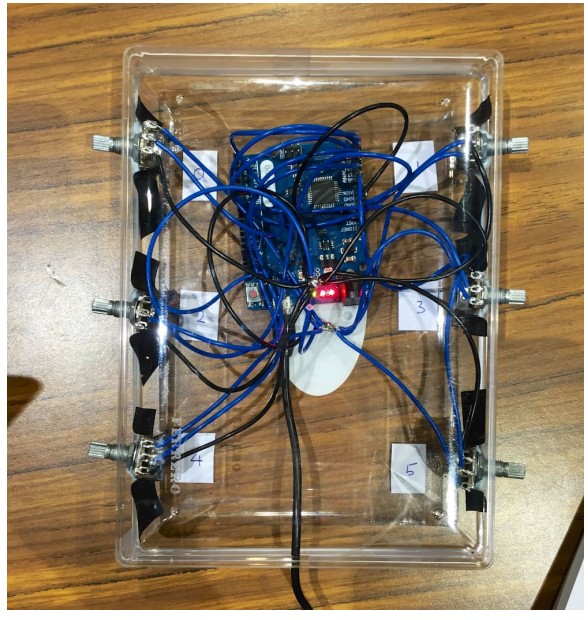
  - robot commands,
  - moves in chess.





EXPRESSIVE DATA IS OFTEN CONTINUOUS

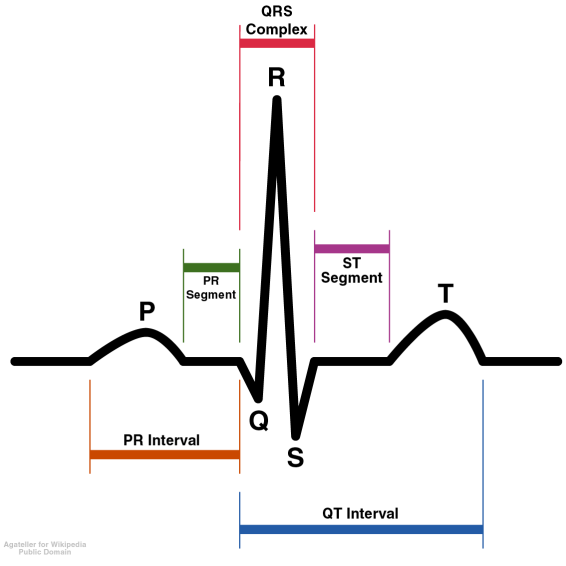




The Snyderphonics Birl Electronic Wind Instrument (Sneak Preview)

Jeff Snyder of **Snyderphonics**, developer of the **Manta** controller, shared this video preview of the upcoming **Birl** electronic wind instrument.

SO ARE BIO-SIGNALS



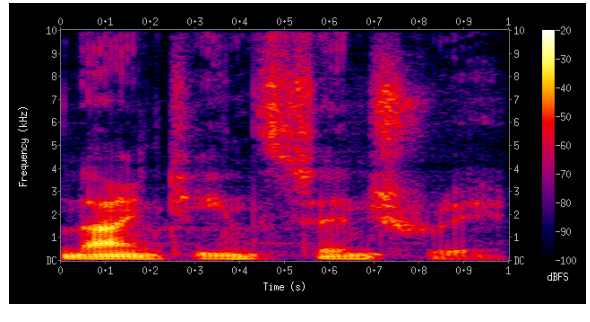
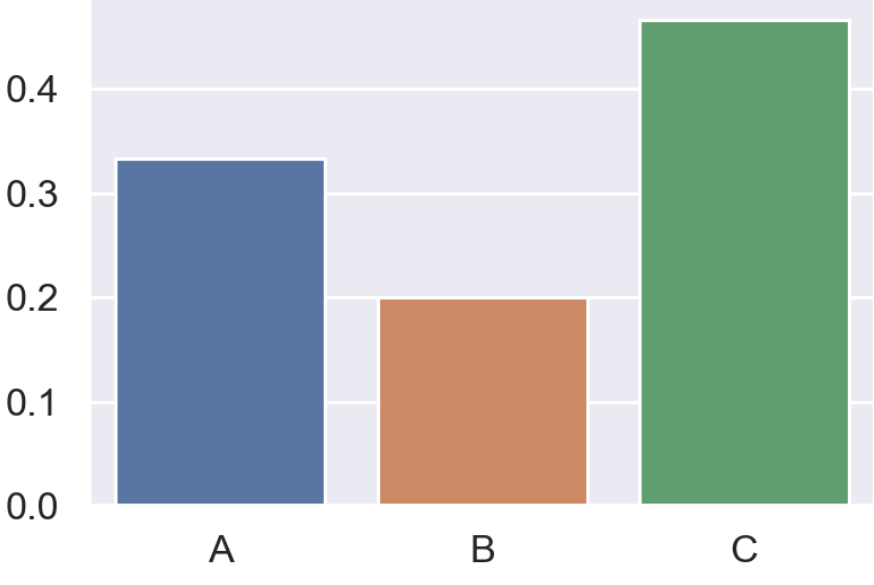
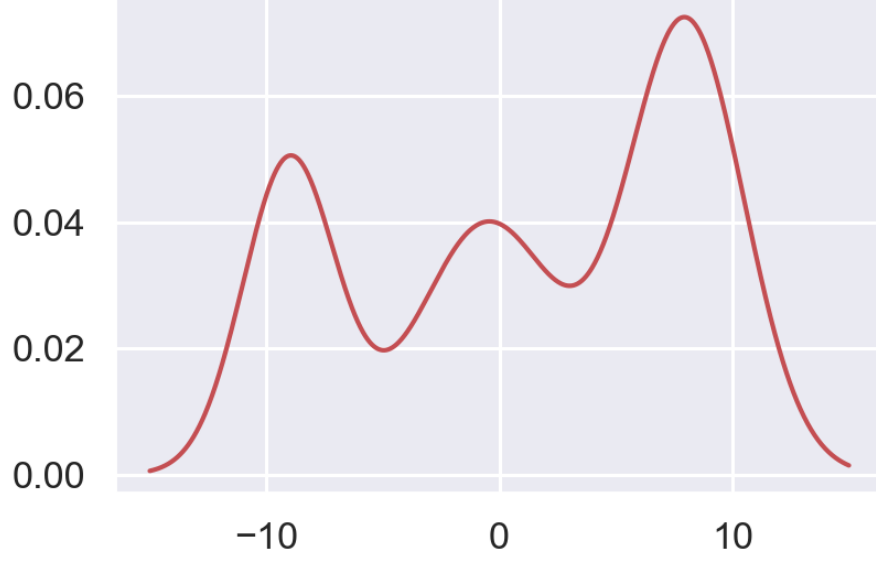


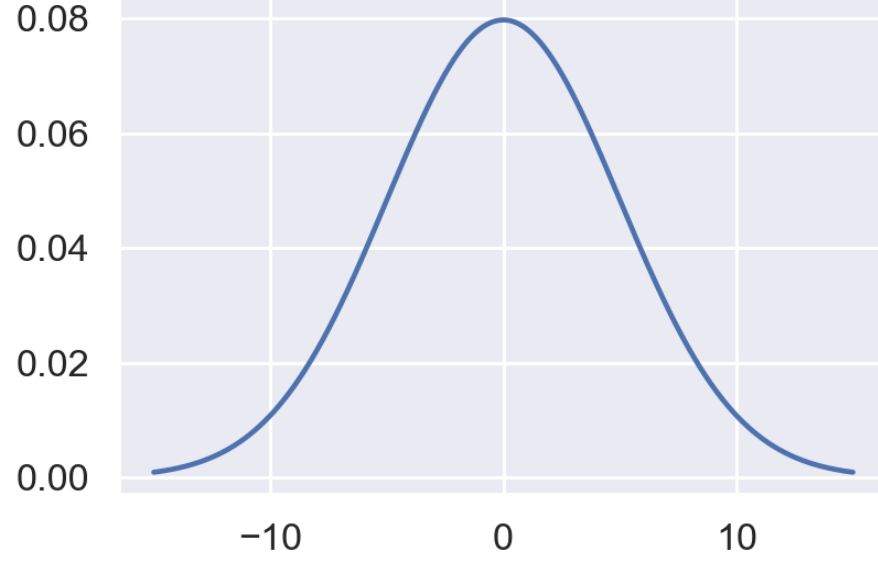
Image Credit: Wikimedia

CATEGORICAL VS. CONTINUOUS MODELS



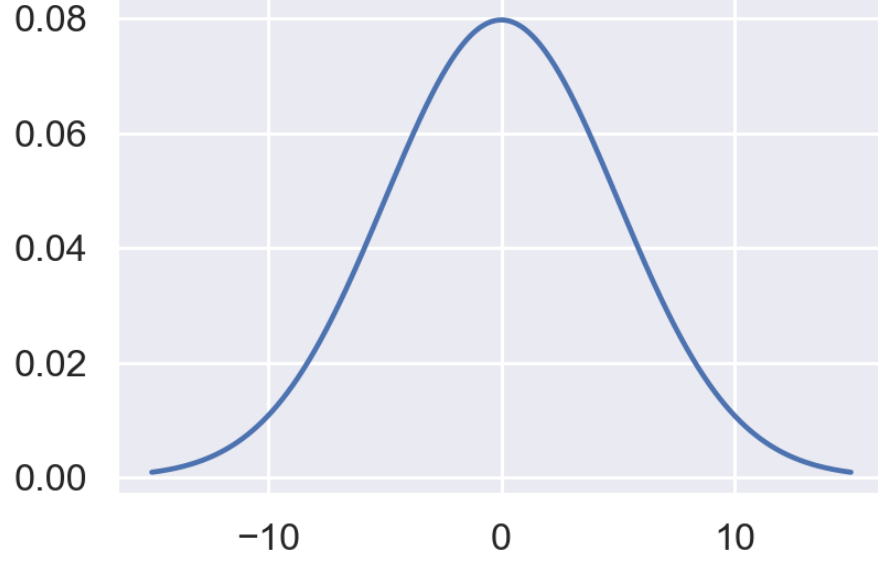


NORMAL (GAUSSIAN) DISTRIBUTION



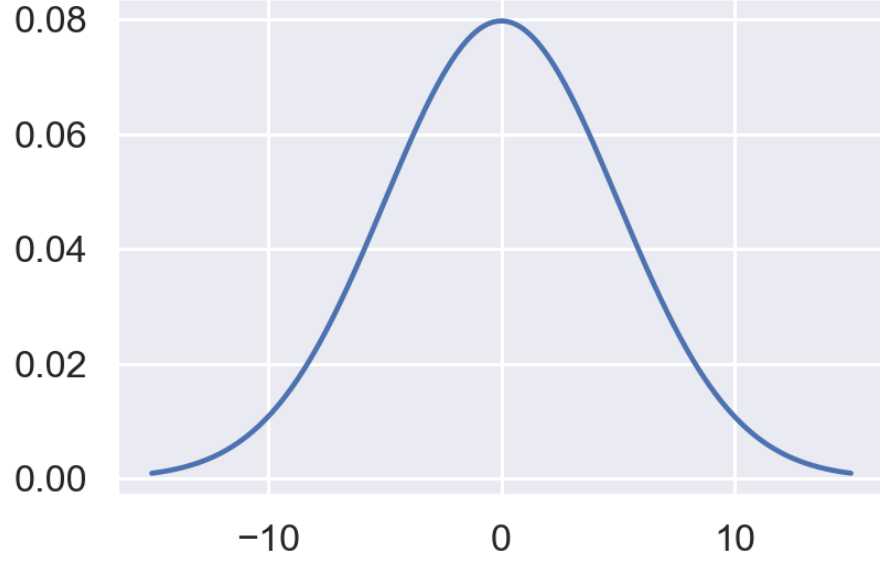
NORMAL (GAUSSIAN) DISTRIBUTION

- “Standard” probability distribution



NORMAL (GAUSSIAN) DISTRIBUTION

- “Standard” probability distribution
- Has two parameters:



NORMAL (GAUSSIAN) DISTRIBUTION

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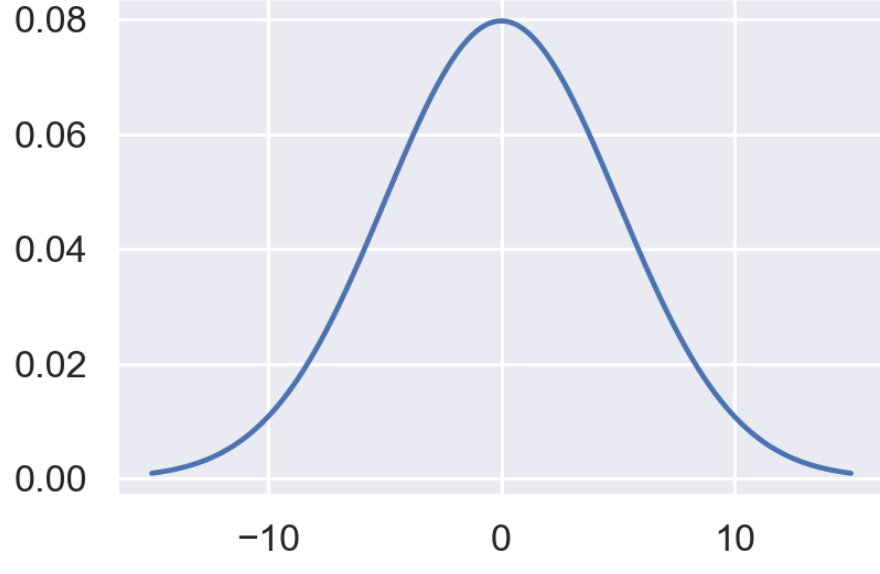

NORMAL (GAUSSIAN) DISTRIBUTION

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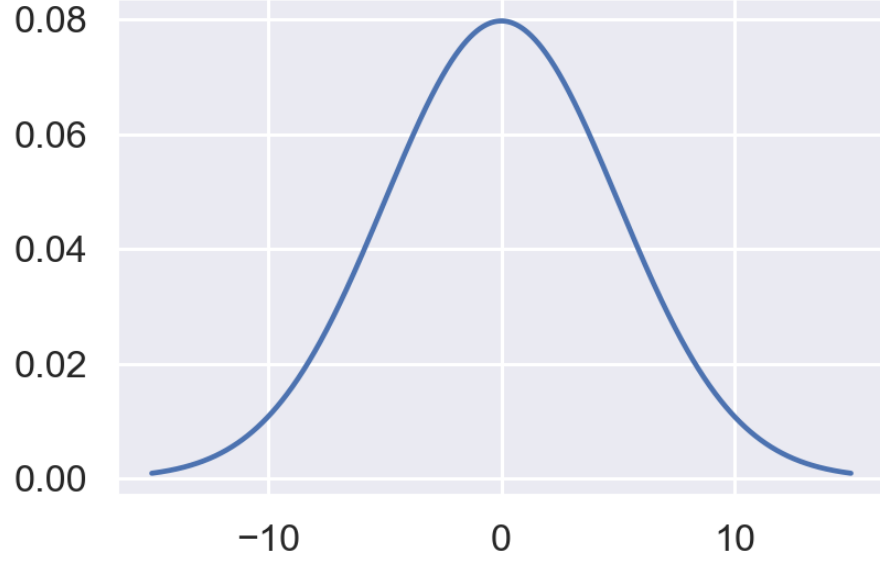

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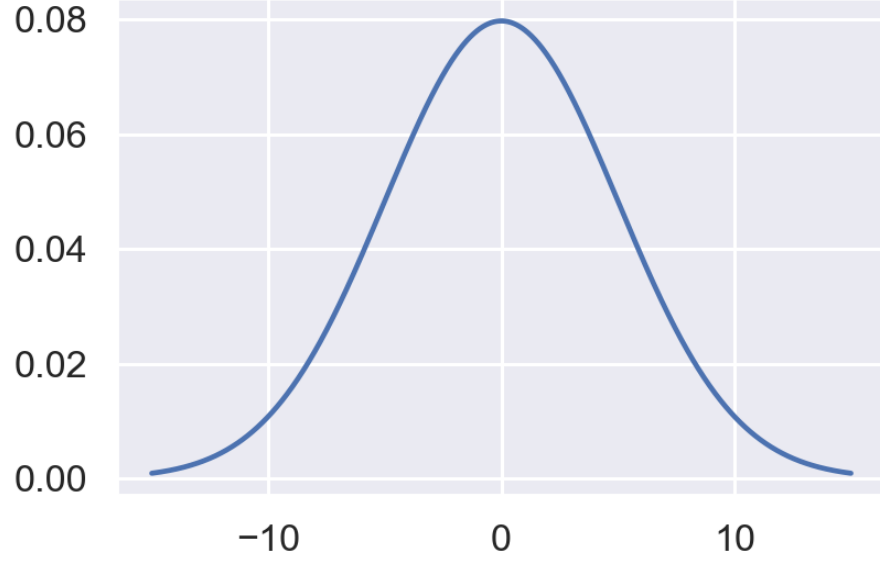

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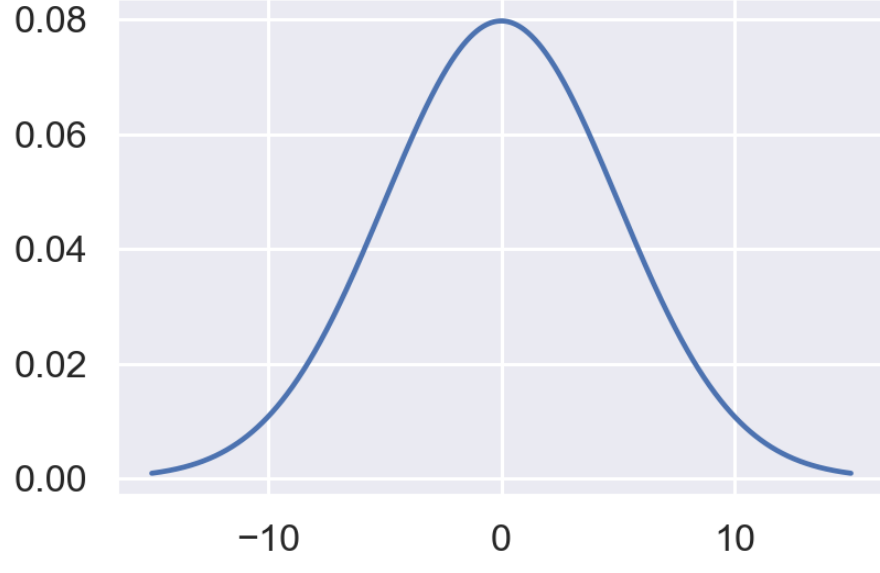
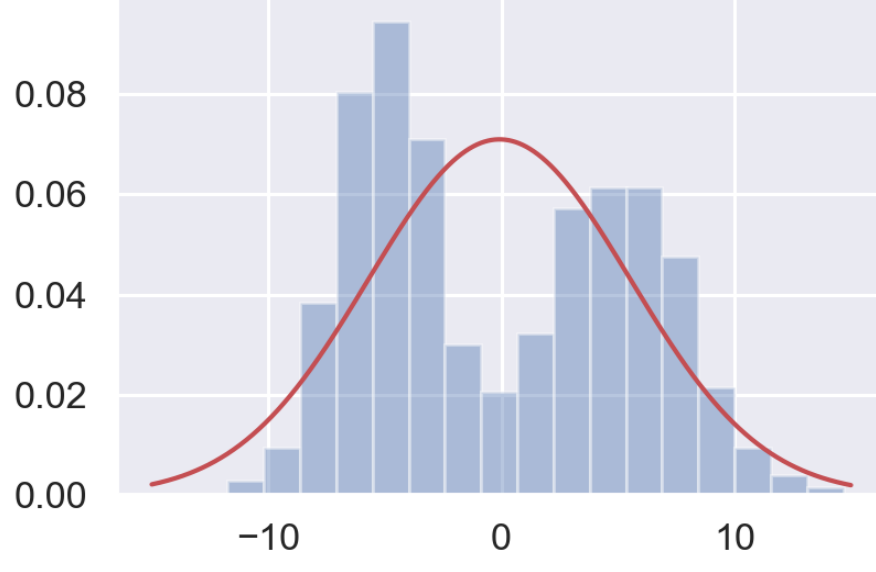
  - $$N(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$



PROBLEM: NORMAL DISTRIBUTION MIGHT NOT FIT DATA

What if the data is complicated?



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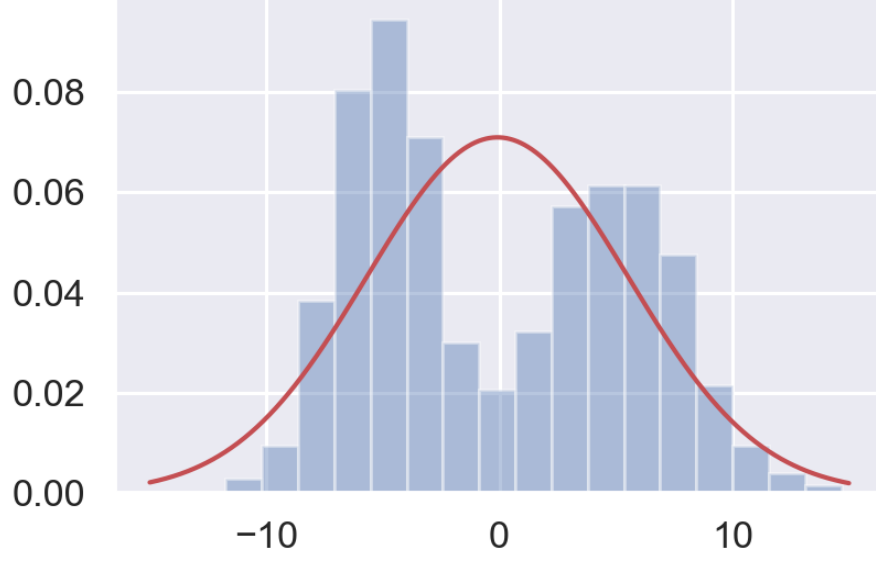

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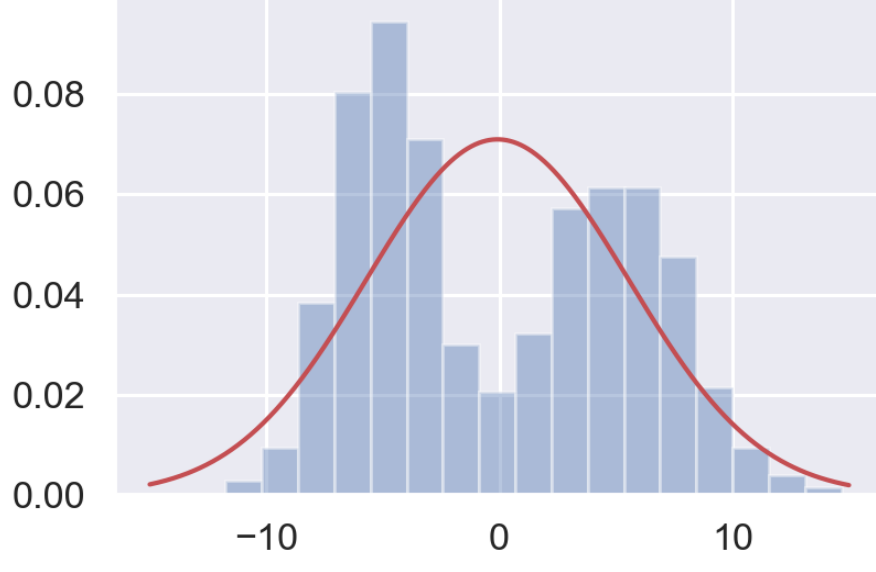
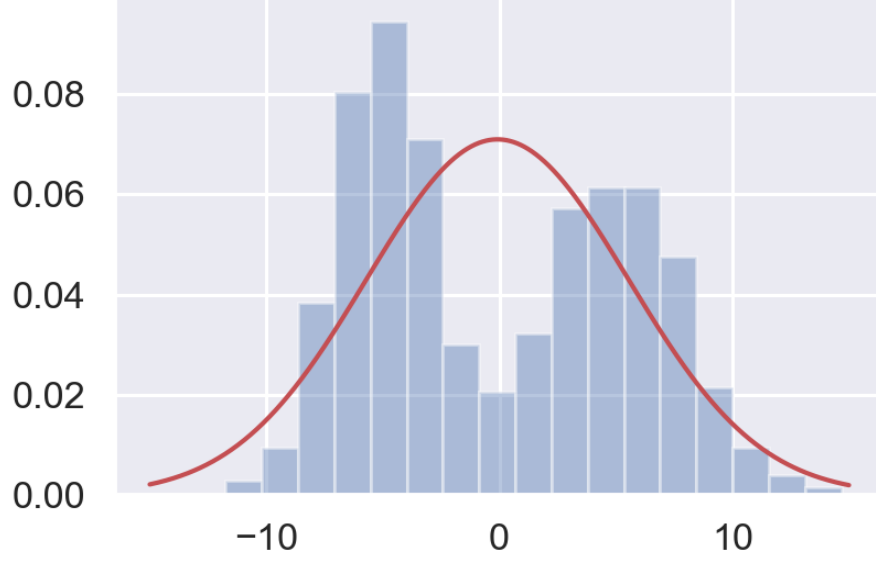


PROBLEM: NORMAL DISTRIBUTION MIGHT NOT FIT DATA

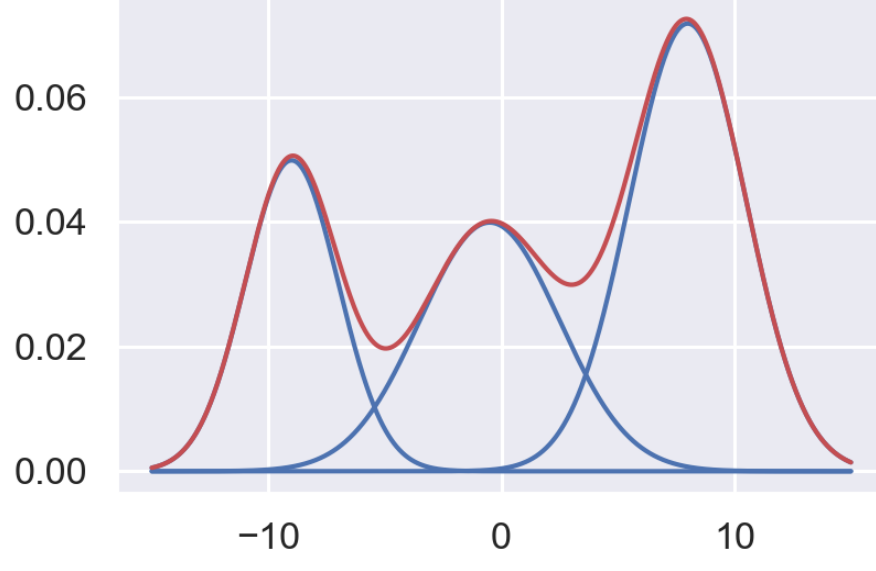
What if the data is complicated?

- It's easy to "fit" a normal model to any data.
  - Just calculate μ and σ
- But this might not fit the data well.



MIXTURE OF NORMALS

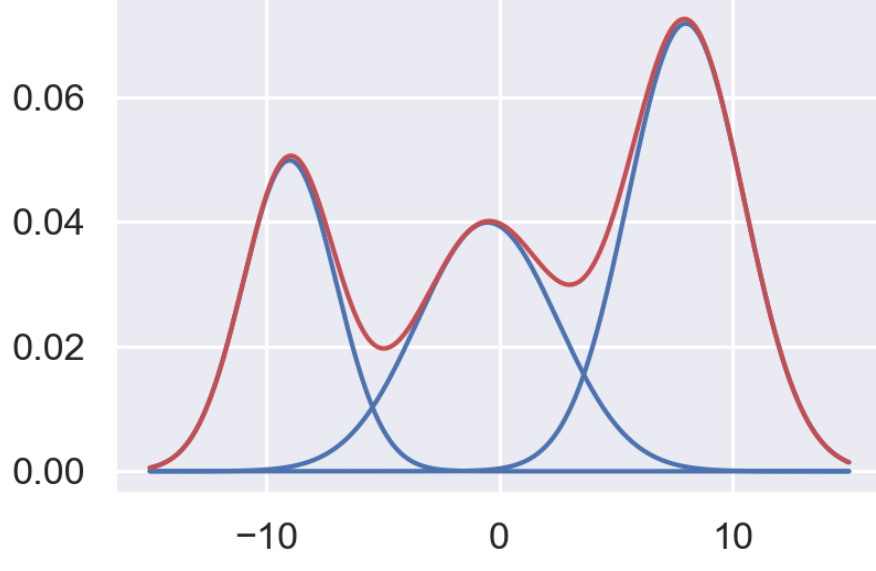
Three groups of parameters:



MIXTURE OF NORMALS

Three groups of parameters:

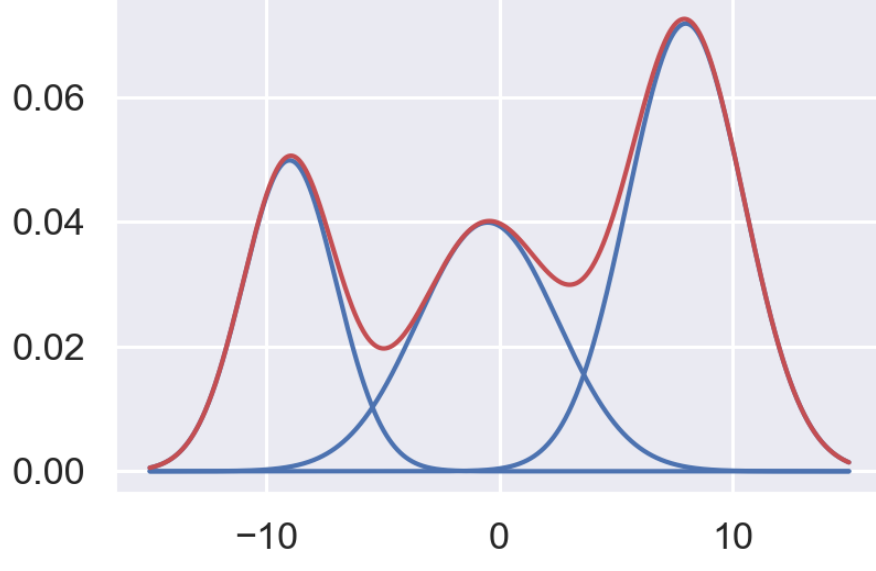
- means (μ): location of each component



MIXTURE OF NORMALS

Three groups of parameters:

- means (μ): location of each component
- standard deviations (σ): width of each component



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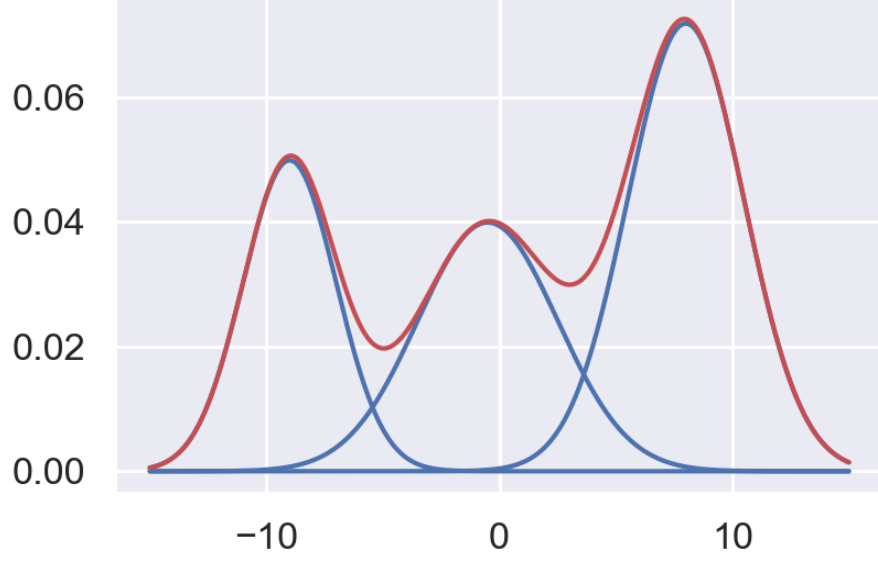

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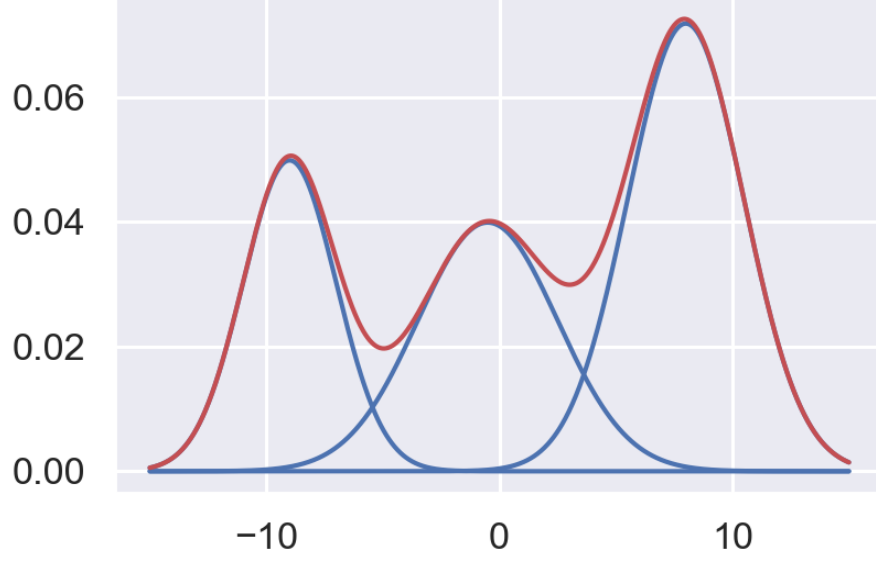

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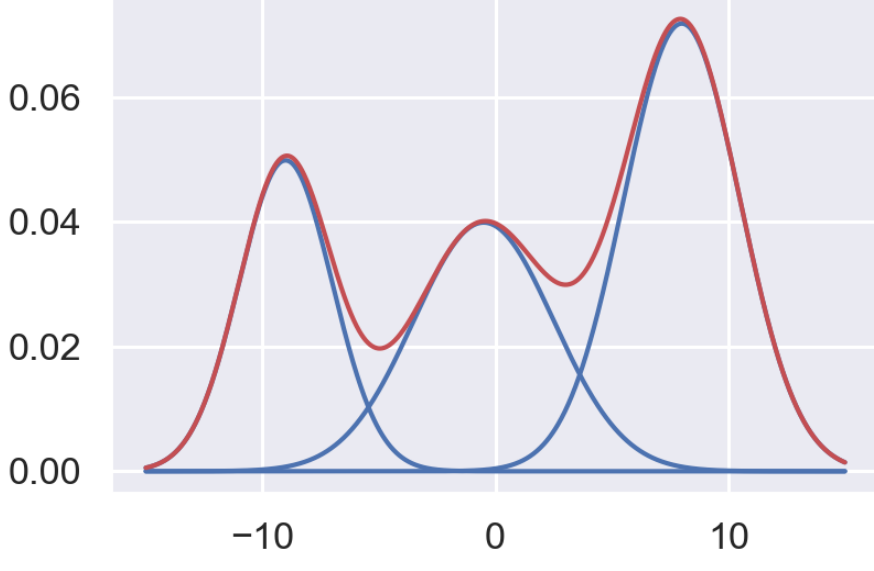

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Returning to our modelling problem, let's plot the PDF of a evenly-weighted mixture of the two sample normal models.

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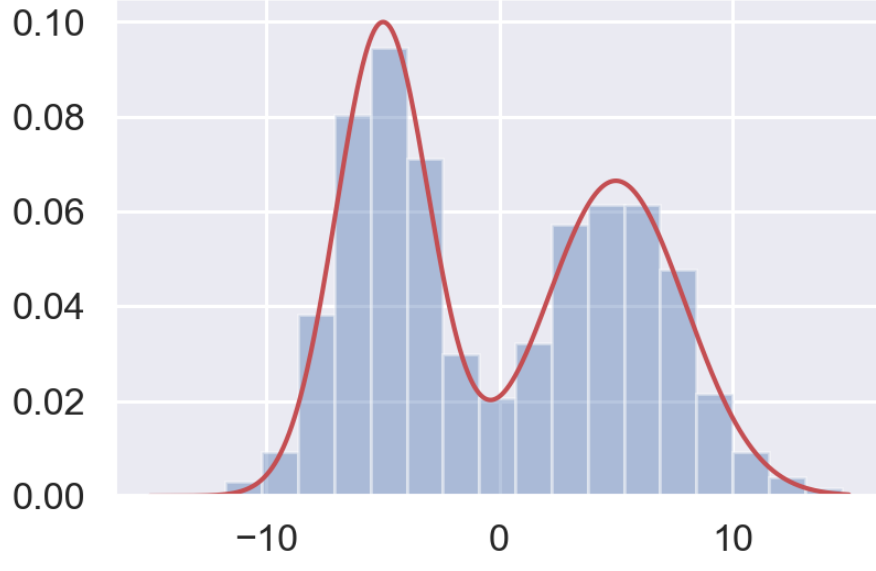

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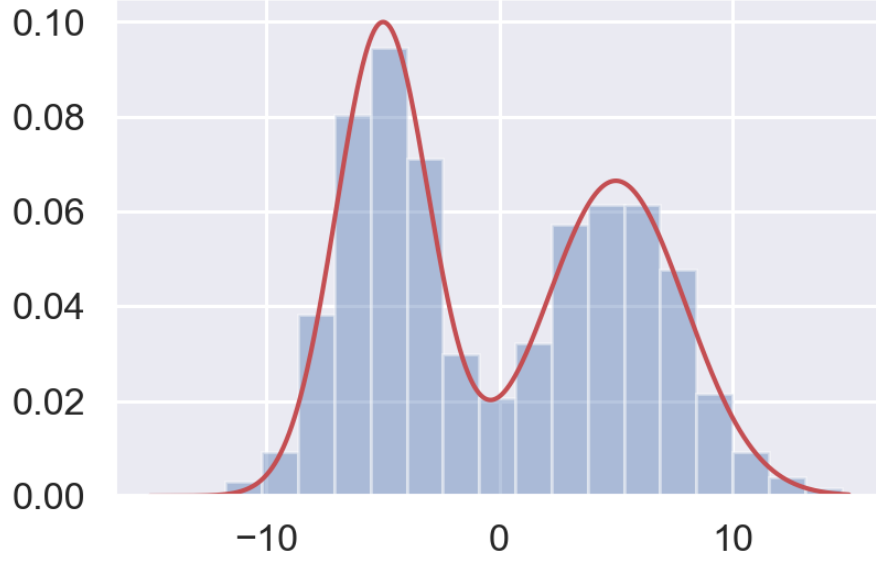

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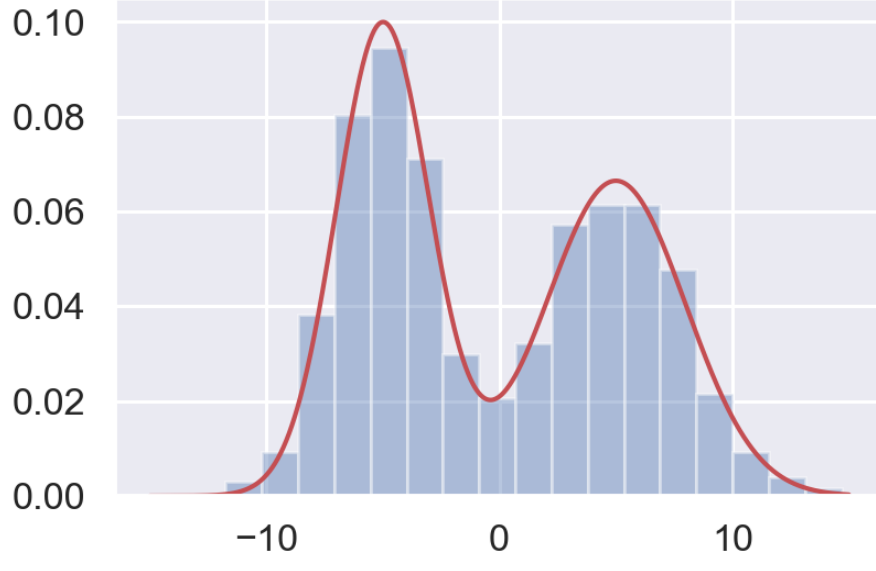

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Returning to our modelling problem, let's plot the PDF of a evenly-weighted mixture of the two sample normal models.

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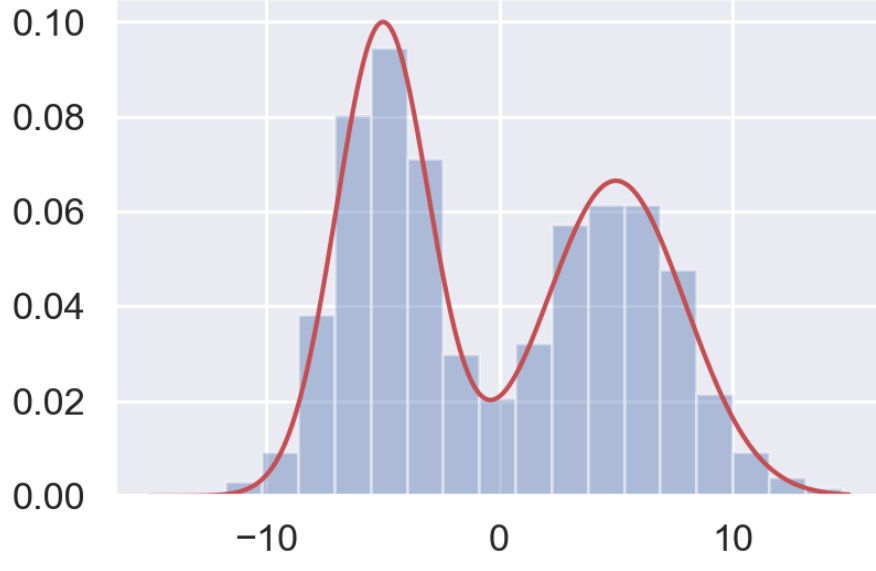

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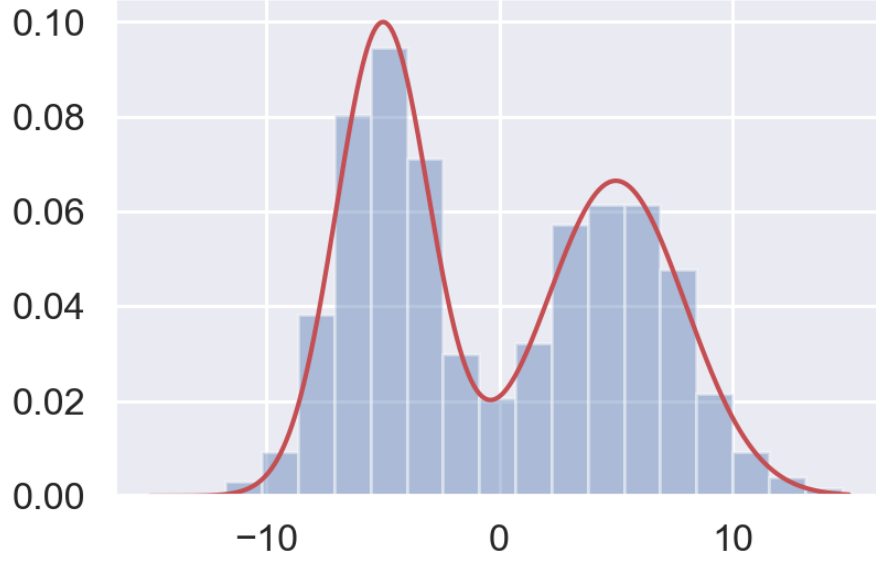

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- (bold used to indicate the vector of parameters for each component)

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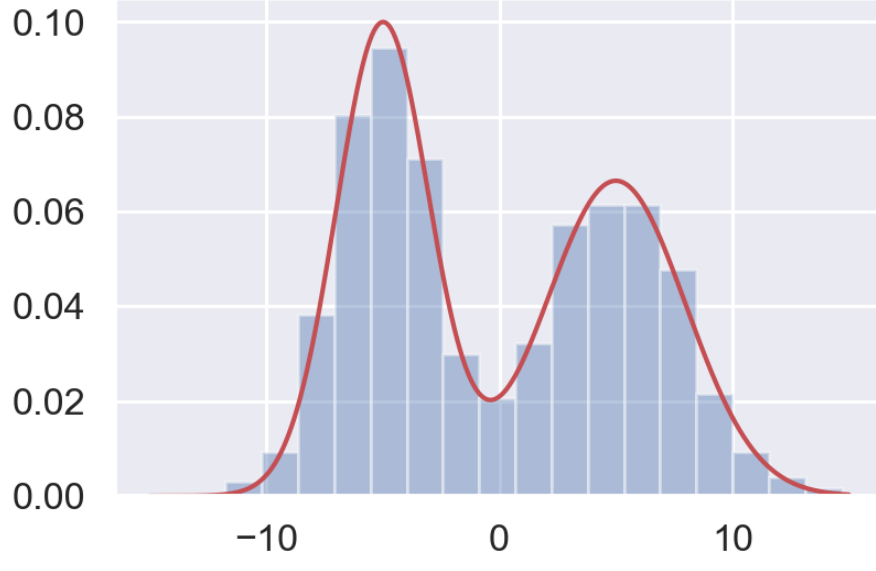
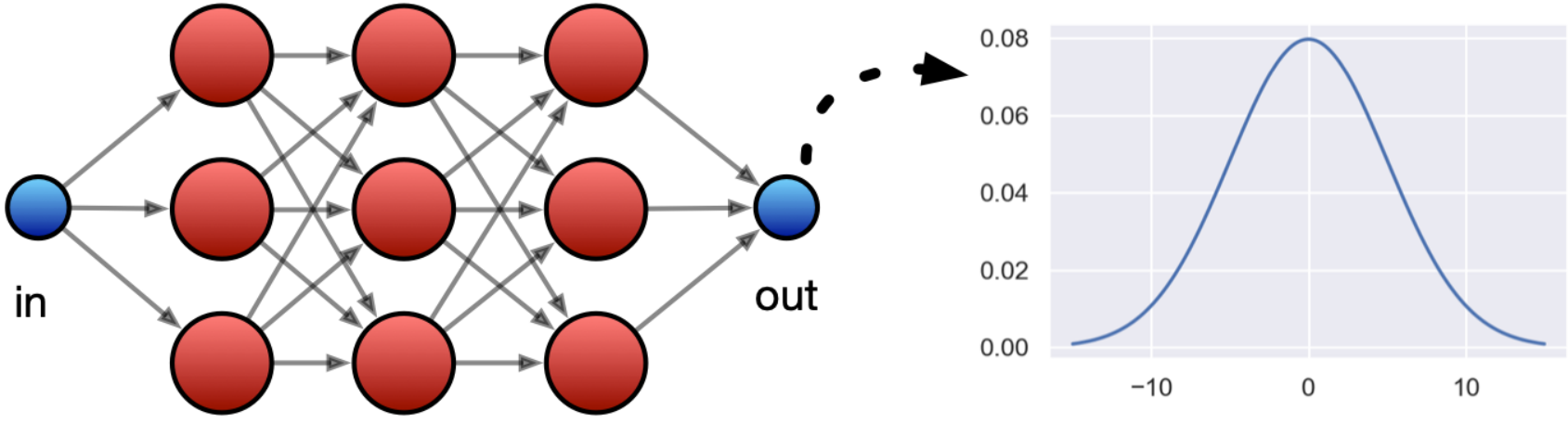


MIXTURE DENSITY NETWORKS



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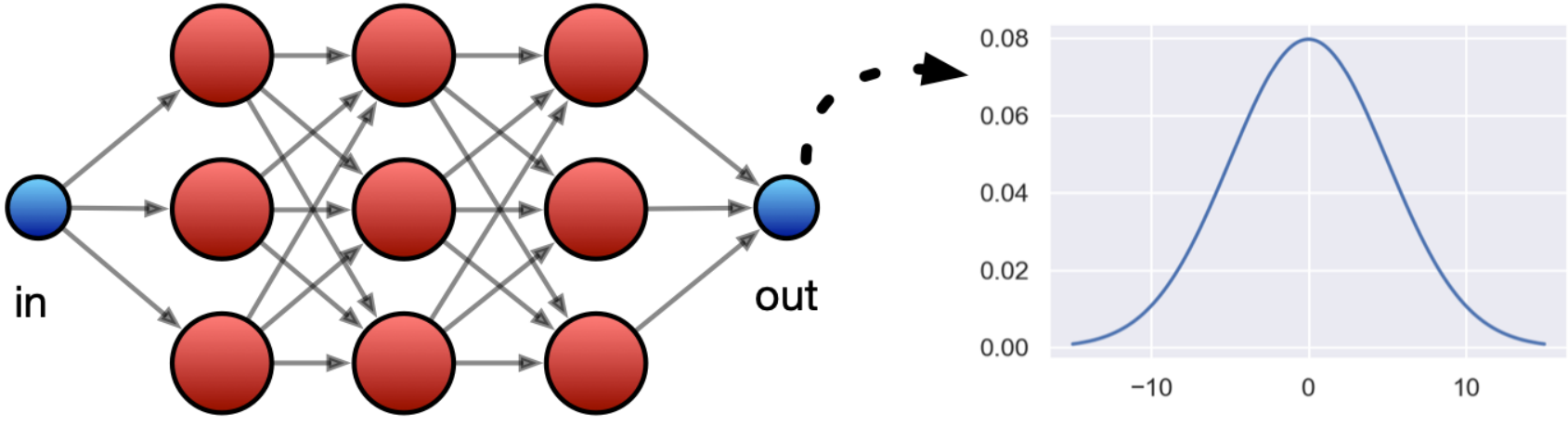

- Neural networks used to model complicated real-valued data.

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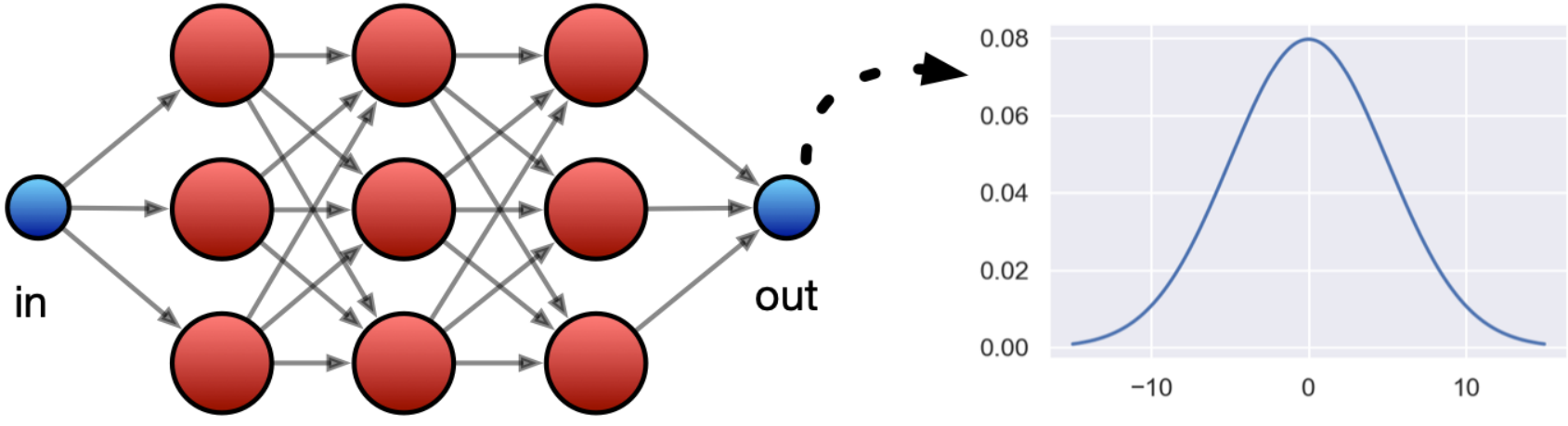

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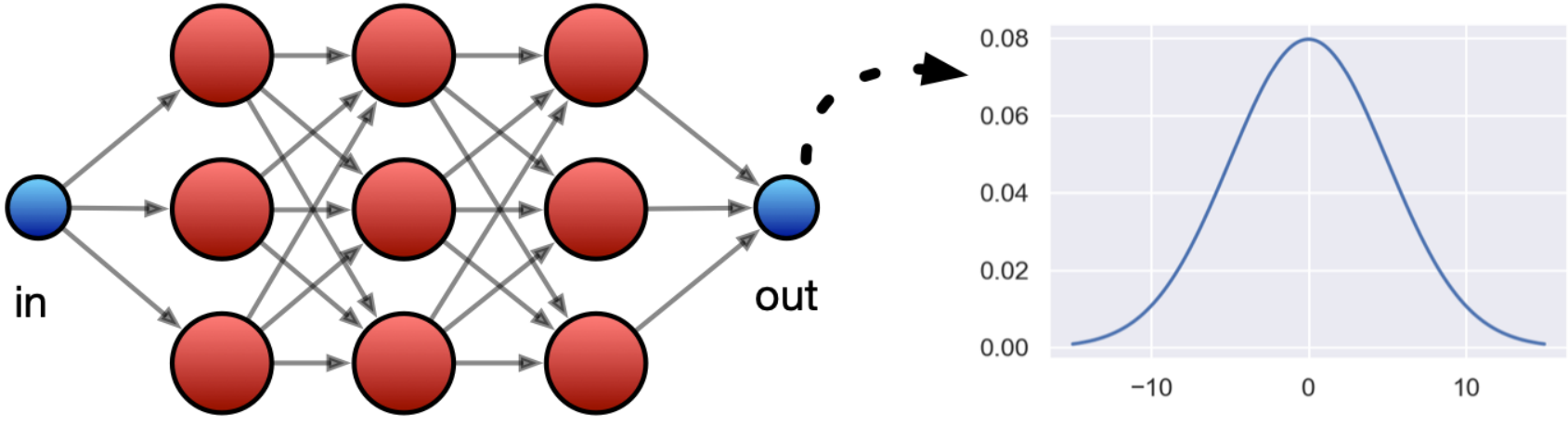

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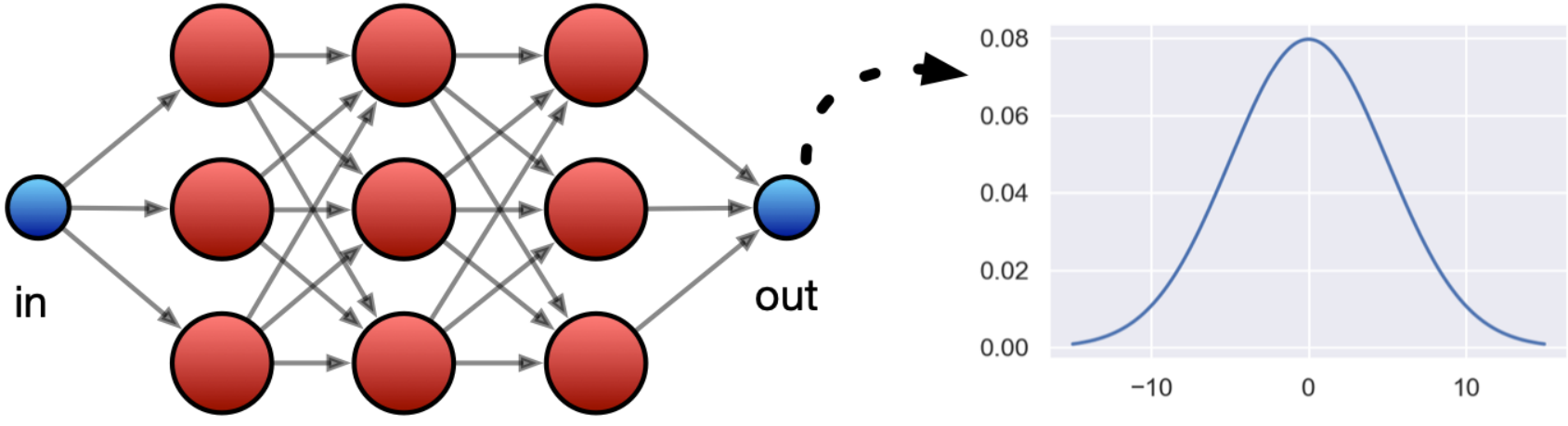

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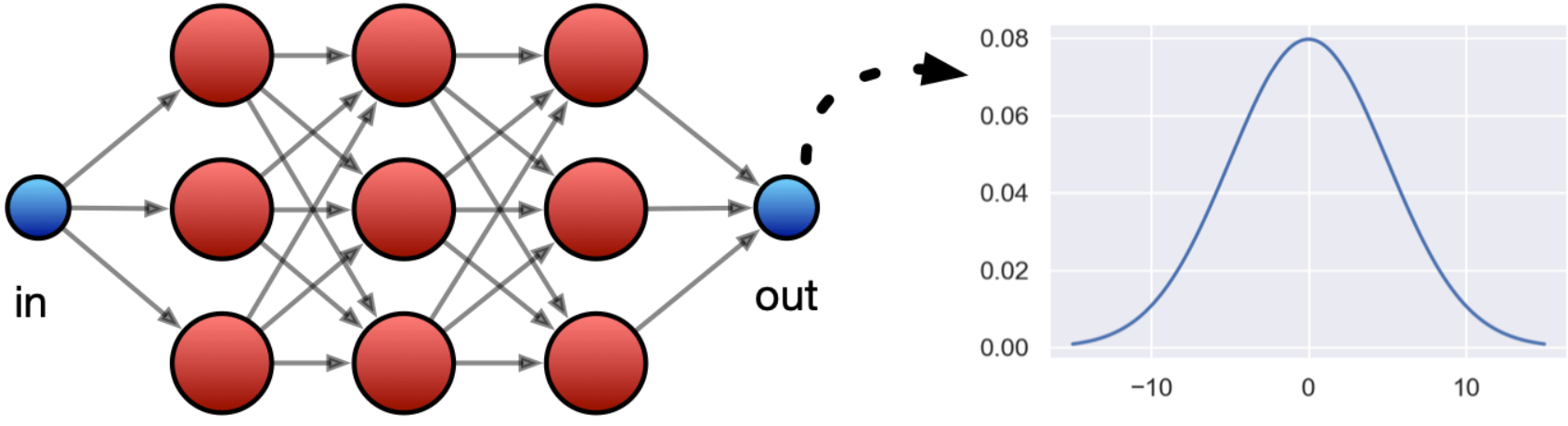

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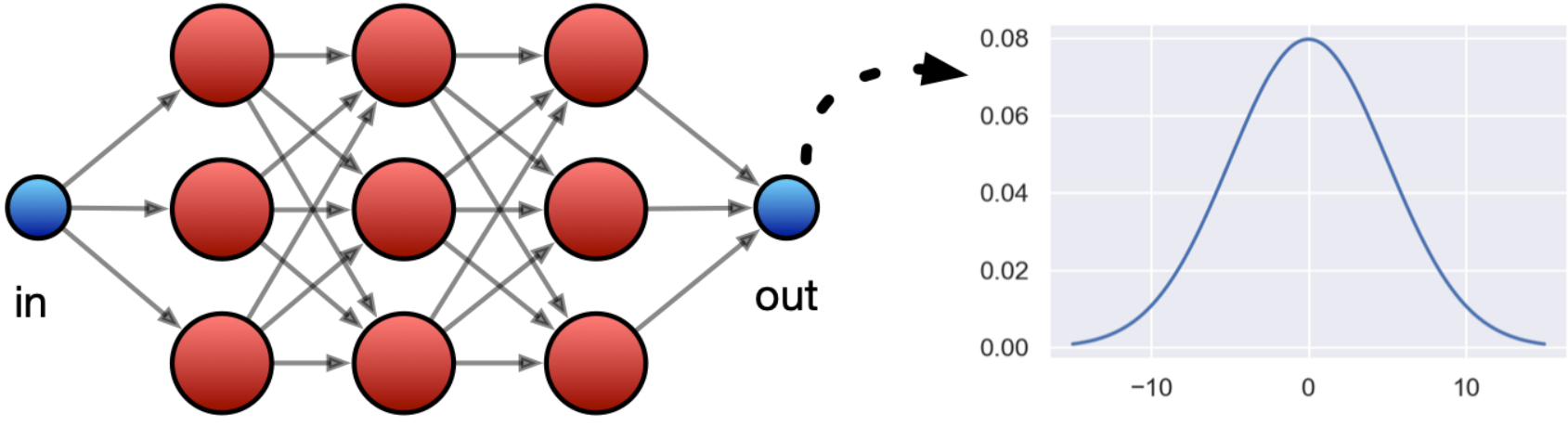

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- (See Bishop, C (1994) for proof and more details)

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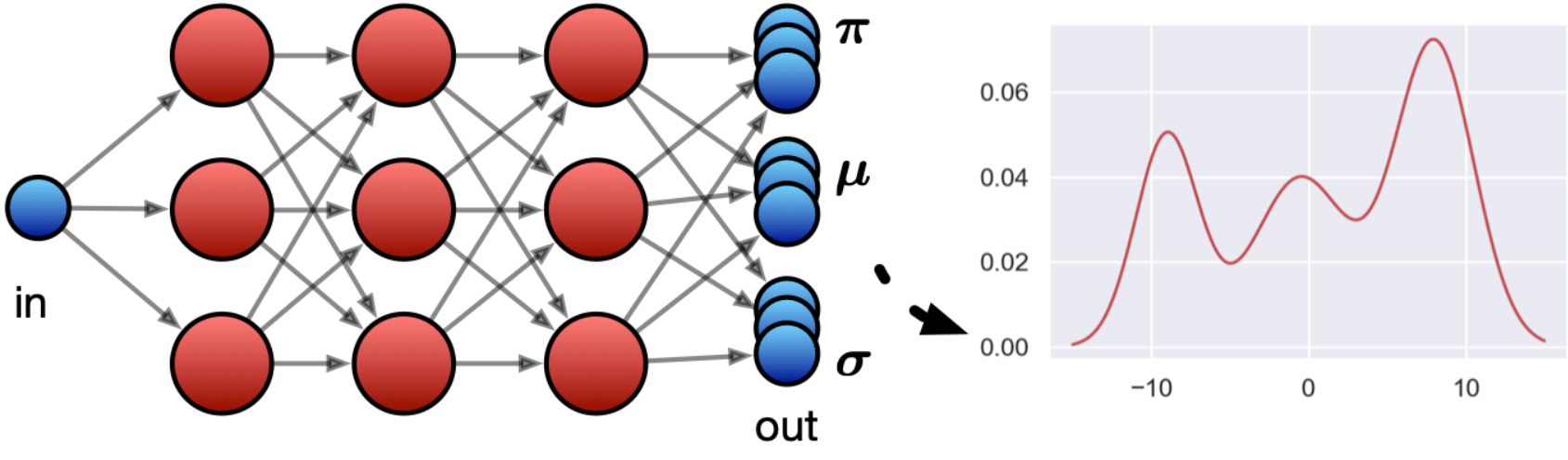

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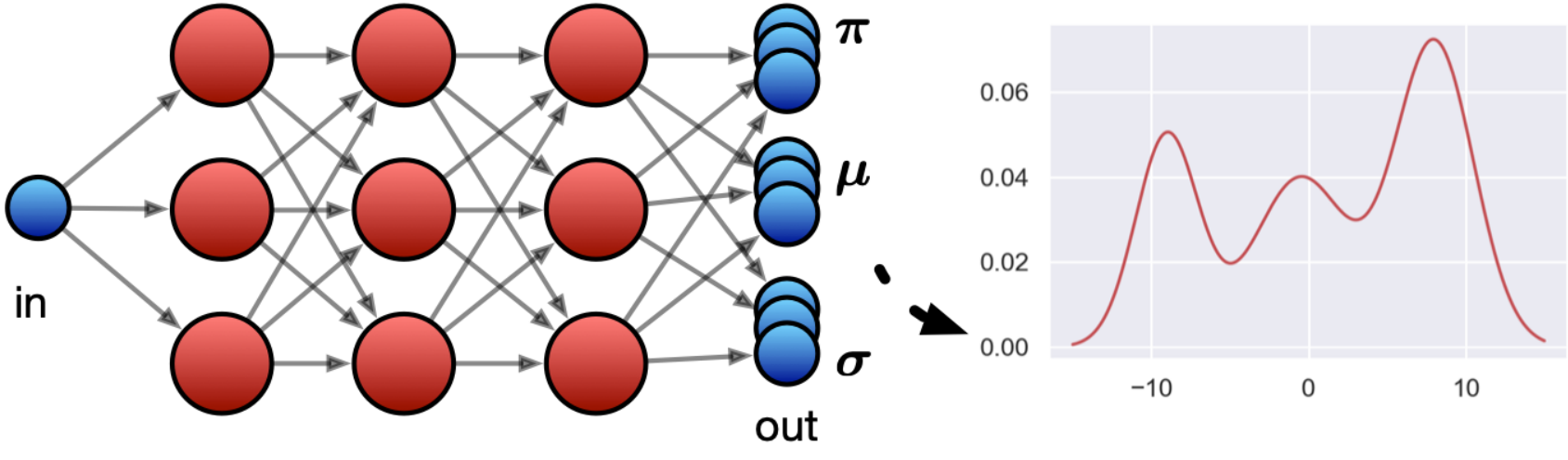

- Idea: output parameters of a mixture model instead!

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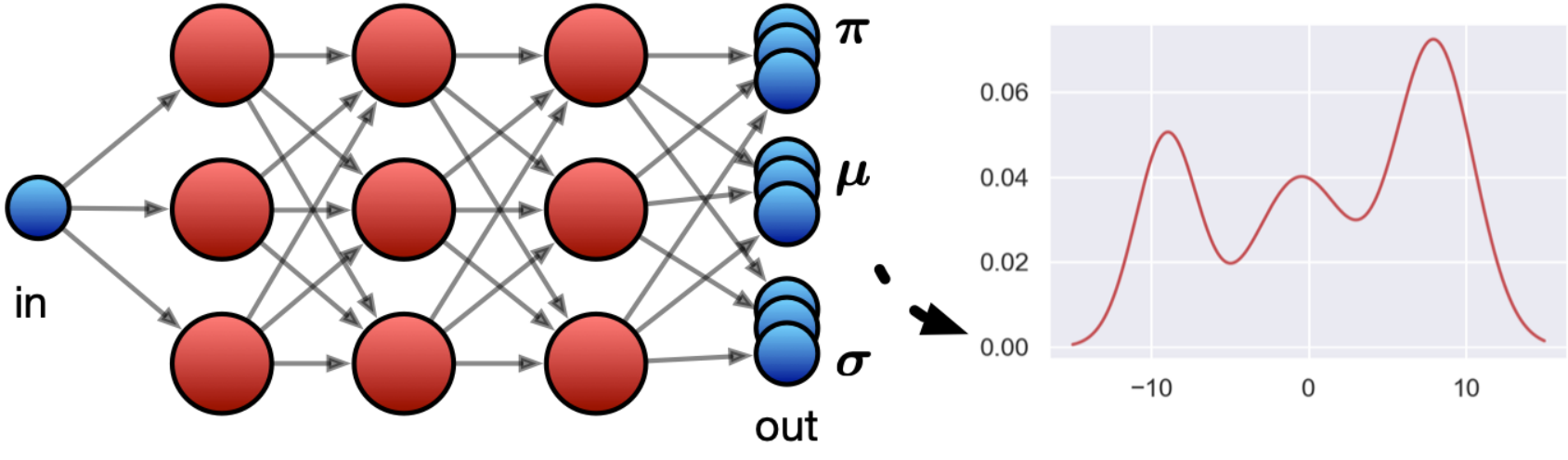

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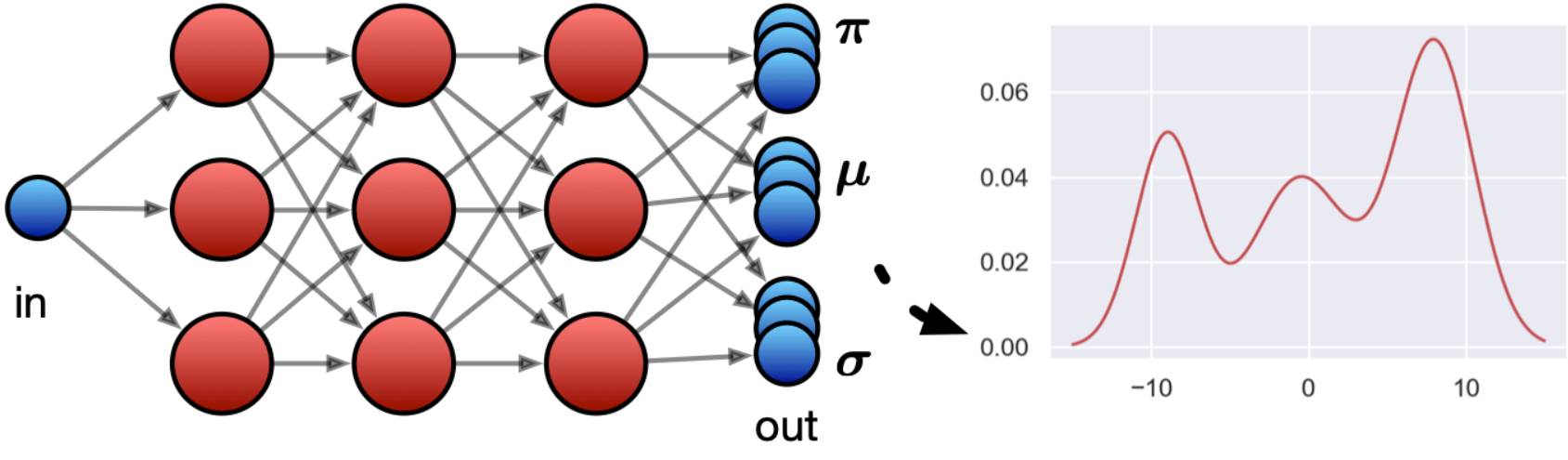

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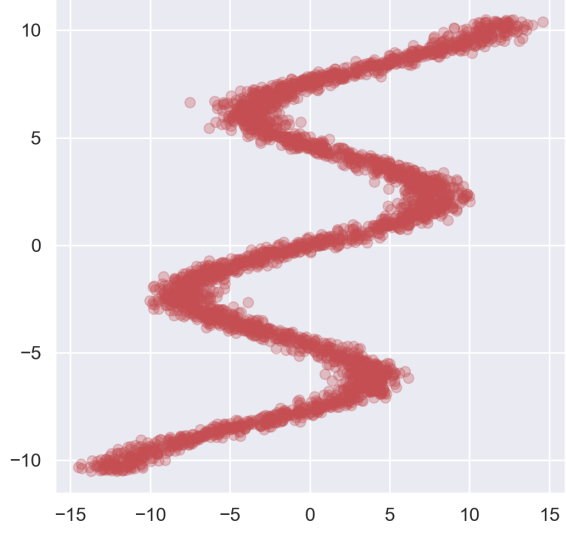
- Rather than MSE for training, use the PDF of the mixture model.
- Now network can model complicated distributions! 😌

SIMPLE EXAMPLE IN KERAS



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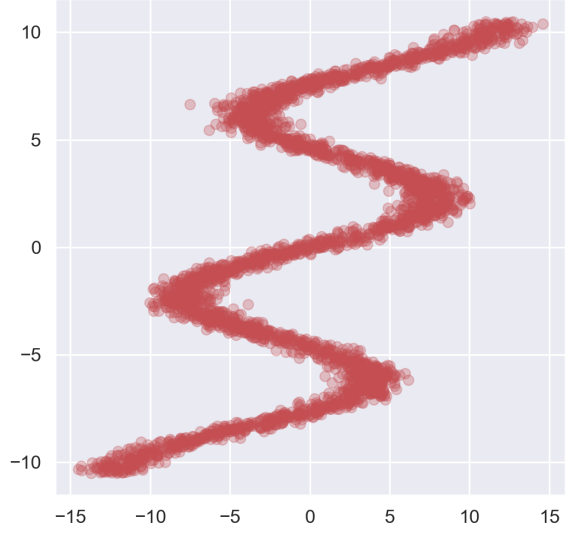

- Difficult data is not hard to find! Think about modelling an inverse sine (arcsine) function.

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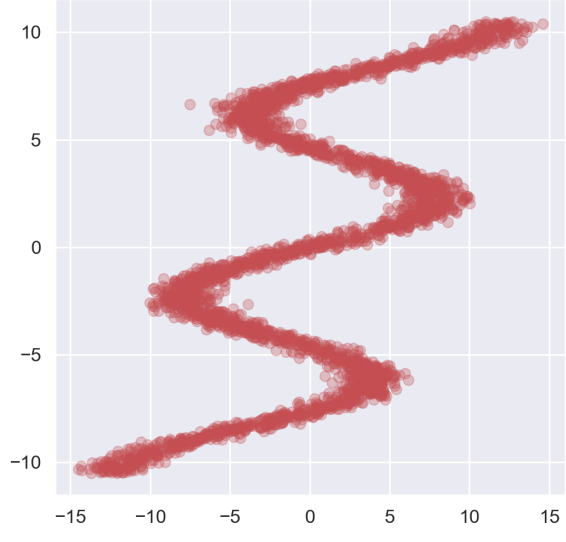

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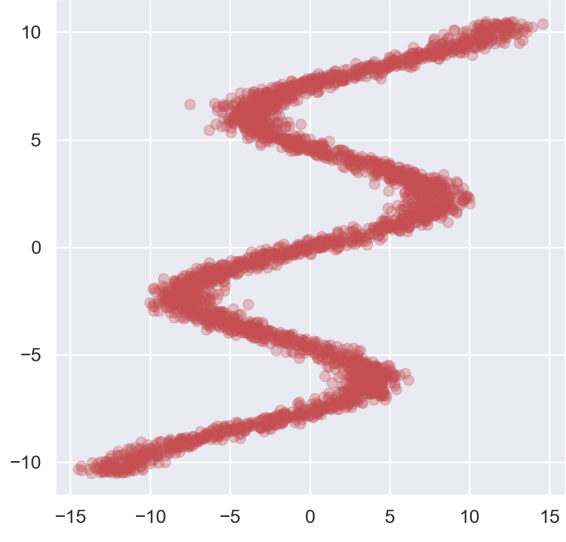
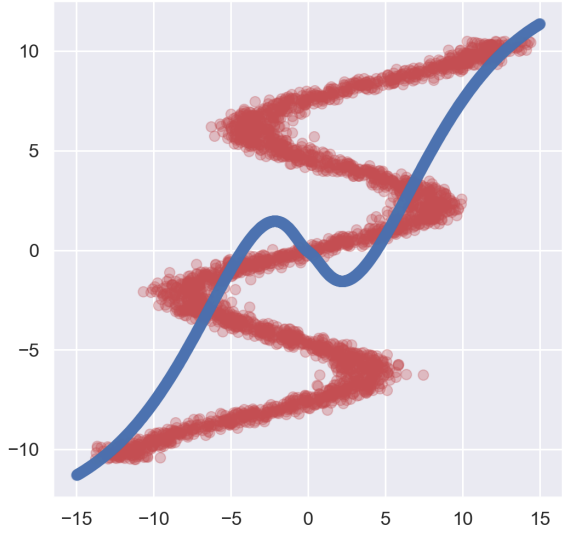
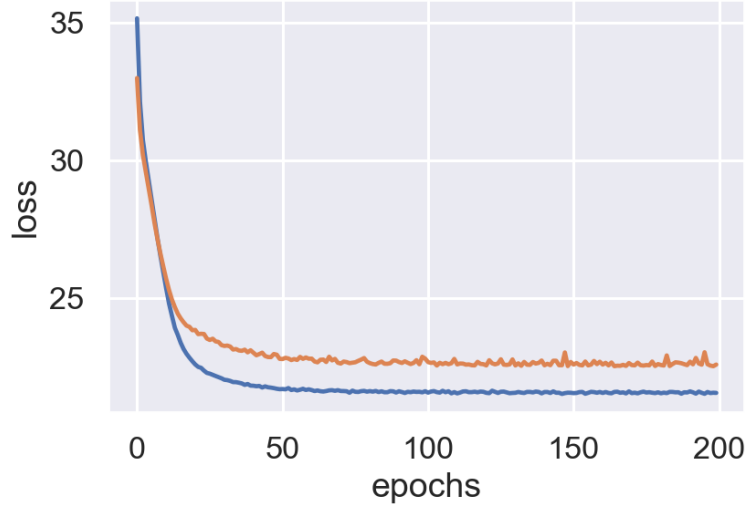


- Difficult data is not hard to find! Think about modelling an inverse sine (arcsine) function.
  - Each input value takes multiple outputs…
  - This is not going to go well for a single normal model.

FEEDFORWARD MSE NETWORK

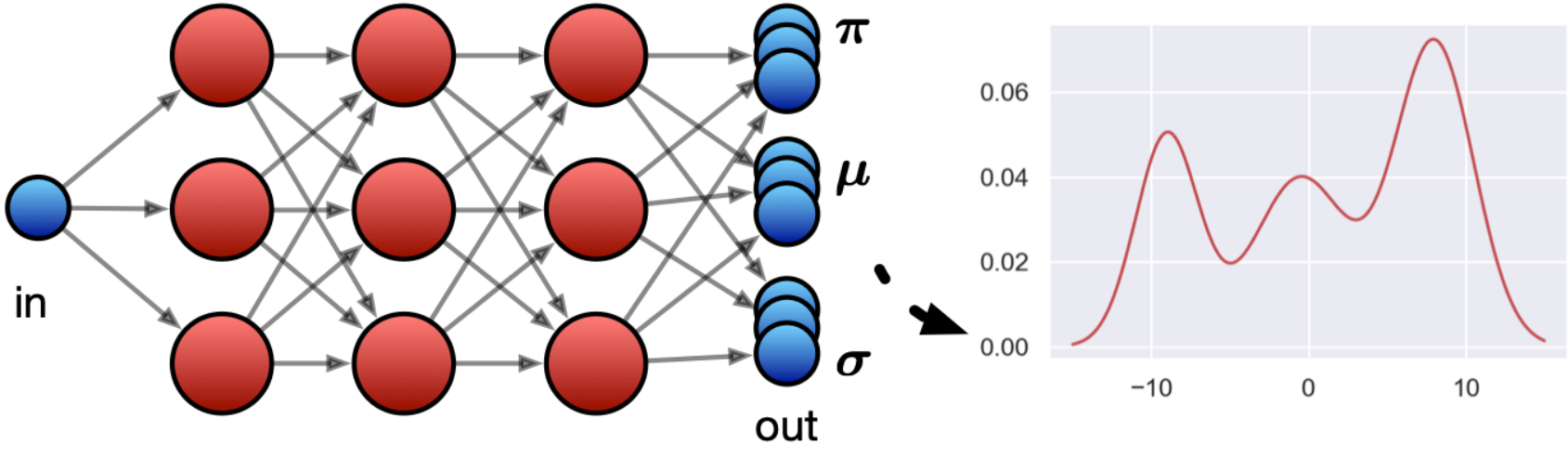




Here's a simple two-hidden-layer network (286 parameters), trained to produce the above result.

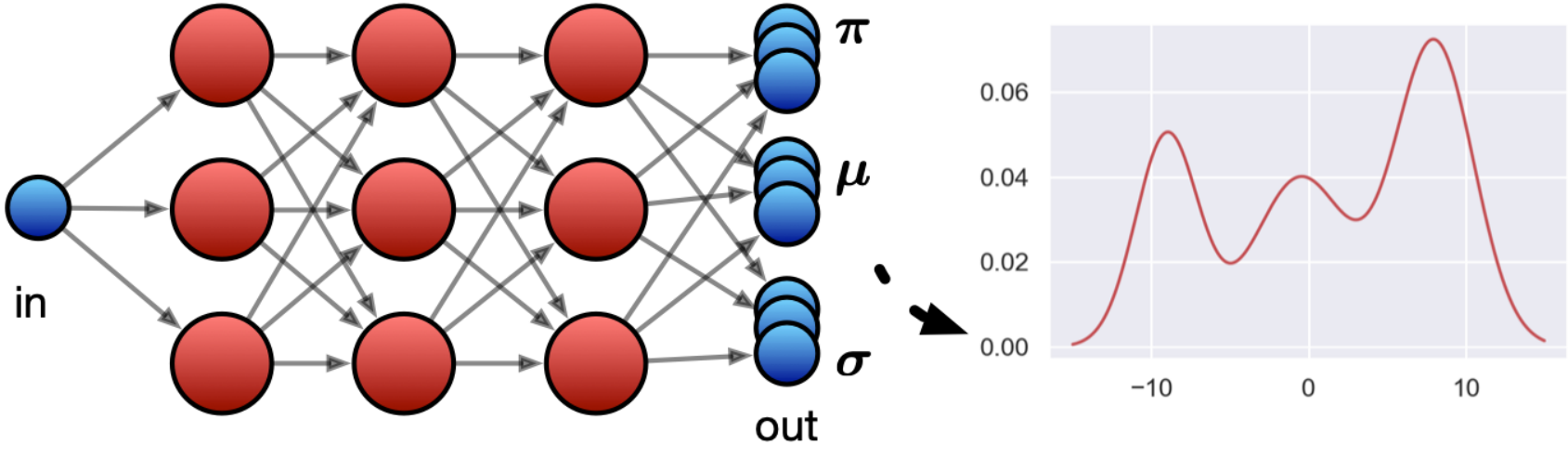
```
model = Sequential()
model.add(Dense(15, batch_input_shape=(None, 1), activation='tanh'))
model.add(Dense(15, activation='tanh'))
model.add(Dense(1, activation='linear'))
model.compile(loss='mse', optimizer='rmsprop')
model.fit(x=x_data, y=y_data, batch_size=128, epochs=200, validation_split=0.15)
```

MDN ARCHITECTURE:



$$\mathcal{L} = \sum_{i=1}^{K} \pi_i(\mathbf{x}) \mathcal{N}\left(\mu_i(\mathbf{x}), \sigma_i^2(\mathbf{x}); \mathbf{t}\right)$$

MDN ARCHITECTURE:



- Loss function for MDN is negative log of likelihood function L.

$$L = \sum_{i=1}^{K} \pi_i(x) N\left(\mu_i(x), \sigma_i^2(x); t\right)$$

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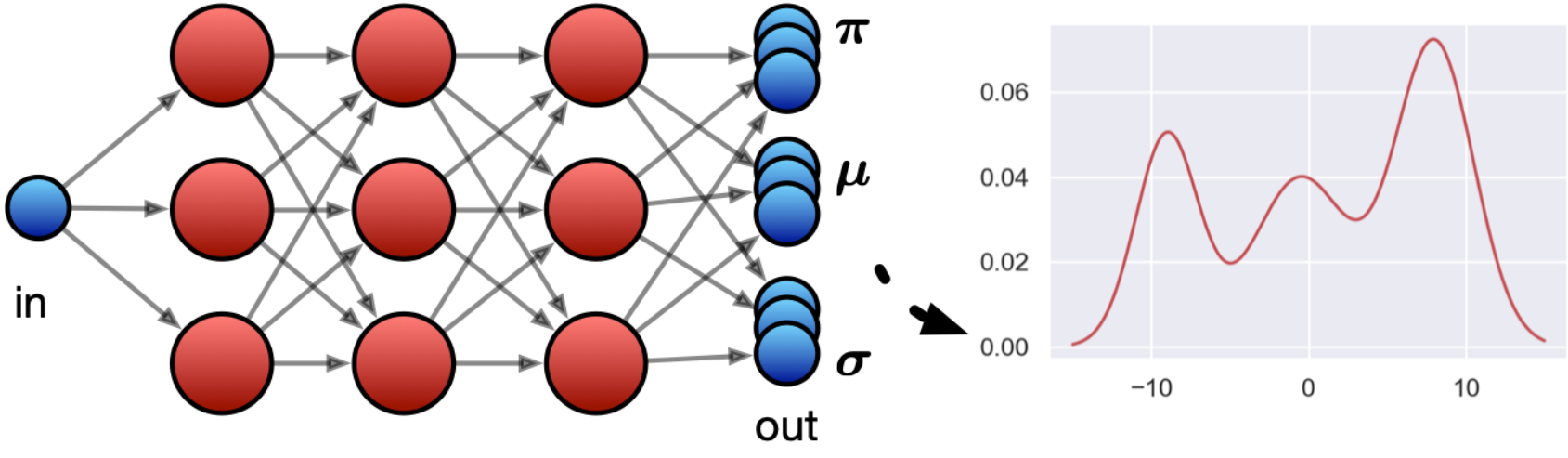
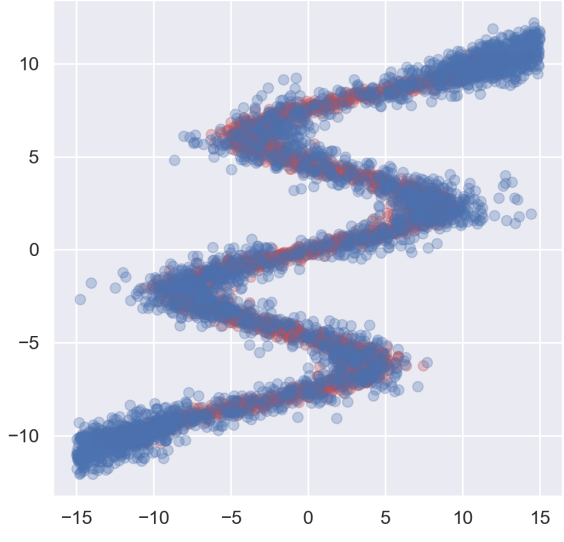
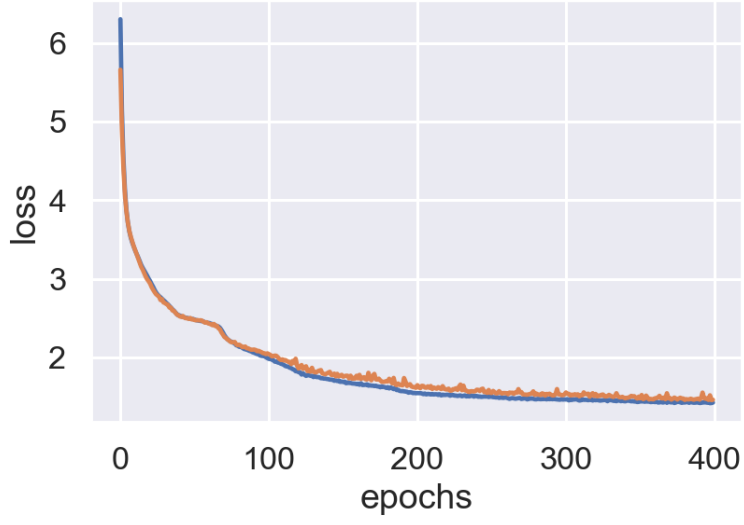


- Loss function for MDN is negative log of likelihood function L.
- L measures likelihood of t being drawn from a mixture parametrised by μ, σ, and π which are generated by the network inputs x:

$$L = \sum_{i=1}^{K} \pi_i(x) N\left(\mu_i(x), \sigma_i^2(x); t\right)$$

FEEDFORWARD MDN SOLUTION





And, here's a simple two-hidden-layer MDN (510 parameters), that achieves the above result! Much better!

```
N_MIXES = 5

model = Sequential()
model.add(Dense(15, batch_input_shape=(None, 1), activation='relu'))
model.add(Dense(15, activation='relu'))
model.add(mdn.MDN(1, N_MIXES)) # here's the MDN layer!
model.compile(loss=mdn.get_mixture_loss_func(1,N_MIXES), optimizer='rmsprop')
model.summary()
```

GETTING INSIDE THE MDN LAYER

Here's the same network wihtout using the MDN layer abstraction (this is with Keras' functional API):

```
def elu_plus_one_plus_epsilon(x):
    """ELU activation with a very small addition to help prevent NaN in loss."""
    return (K.elu(x) + 1 + 1e-8)

N_HIDDEN = 15
N_MIXES = 5

inputs = Input(shape=(1,), name='inputs')
hidden1 = Dense(N_HIDDEN, activation='relu', name='hidden1')(inputs)
hidden2 = Dense(N_HIDDEN, activation='relu', name='hidden2')(hidden1)

mdn_mus = Dense(N_MIXES, name='mdn_mus')(hidden2)
mdn_sigmas = Dense(N_MIXES, activation=elu_plus_one_plus_epsilon, name='mdn_sigmas')
  (hidden2)
mdn_pi = Dense(N_MIXES, name='mdn_pi')(hidden2)

mdn_out = Concatenate(name='mdn_outputs')([mdn_mus, mdn_sigmas, mdn_pi])

model = Model(inputs=inputs, outputs=mdn_out)
model.summary()
```

LOSS FUNCTION: THE TRICKY BIT.

Loss function for the MDN should be the negative log likelihood:

```
def mdn_loss(y_true, y_pred):
    # Split the inputs into paramaters
    out_mu, out_sigma, out_pi = tf.split(y_pred, num_or_size_splits=[N_MIXES, N_MIXES,
  N_MIXES],
                                         axis=-1, name='mdn_coef_split')
    mus = tf.split(out_mu, num_or_size_splits=N_MIXES, axis=1)
    sigs = tf.split(out_sigma, num_or_size_splits=N_MIXES, axis=1)
    # Construct the mixture models
    cat = tfd.Categorical(logits=out_pi)
    coll = [tfd.MultivariateNormalDiag(loc=loc, scale_diag=scale) for loc, scale
            in zip(mus, sigs)]
    mixture = tfd.Mixture(cat=cat, components=coll)
    # Calculate the loss function
    loss = mixture.log_prob(y_true)
    loss = tf.negative(loss)
    loss = tf.reduce_mean(loss)
    return loss

model.compile(loss=mdn_loss, optimizer='rmsprop')
```

Let’s go through bit by bit…

LOSS FUNCTION: PART 1:

First we have to extract the mixture paramaters.

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# Split the inputs into paramaters
out_mu, out_sigma, out_pi = tf.split(y_pred, num_or_size_splits=[N_MIXES, N_MIXES, N_MIXES],
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- Split up the parameters μ, σ, and π, remember that there are N_MIXES = K of each of these.

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- Split up the parameters μ, σ, and π, remember that there are N_MIXES = K of each of these.
- μ and σ have to be split *again* so that we can iterate over them (you can't iterate over an axis of a tensor…)

LOSS FUNCTION: PART 2:

Now we have to construct the mixture model's PDF.

```
# Construct the mixture models
cat = tfd.Categorical(logits=out_pi)
coll = [tfd.Normal(loc=loc, scale=scale) for loc, scale
        in zip(mus, sigs)]
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- Each normal PDF is contructed using `tfd.Normal`.
- Can do this from first principles as well, but good to use abstractions that are available (?)

LOSS FUNCTION: PART 3:

Finally, we calculate the loss:

```
loss = mixture.log_prob(y_true)
loss = tf.negative(loss)
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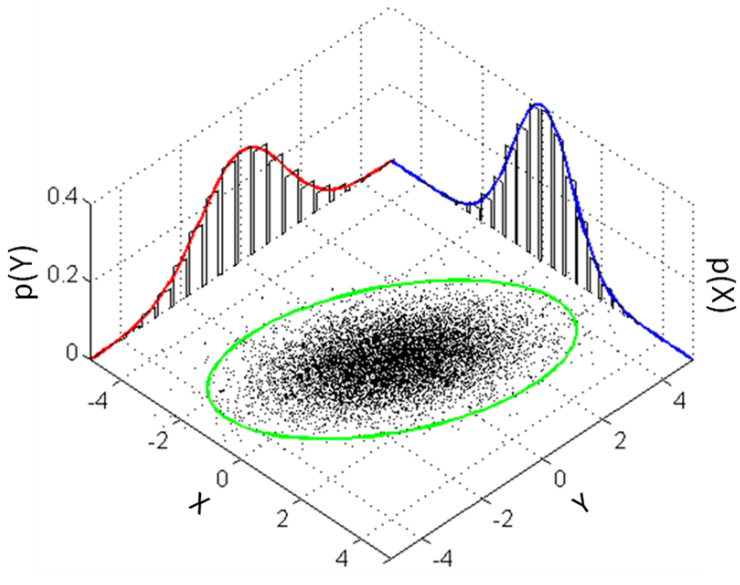
- `mixture.log_prob(y_true)` means “the log-likelihood of sampling `y_true` from the distribution called `mixture`.”

SOME MORE DETAILS….



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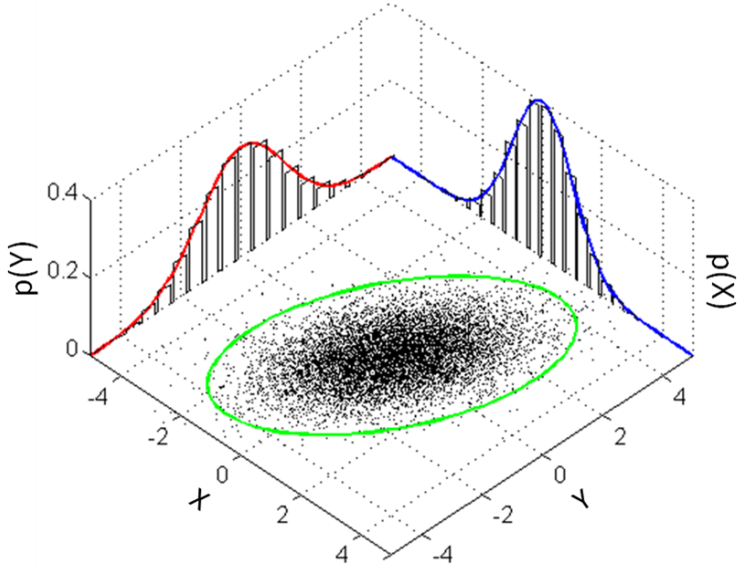
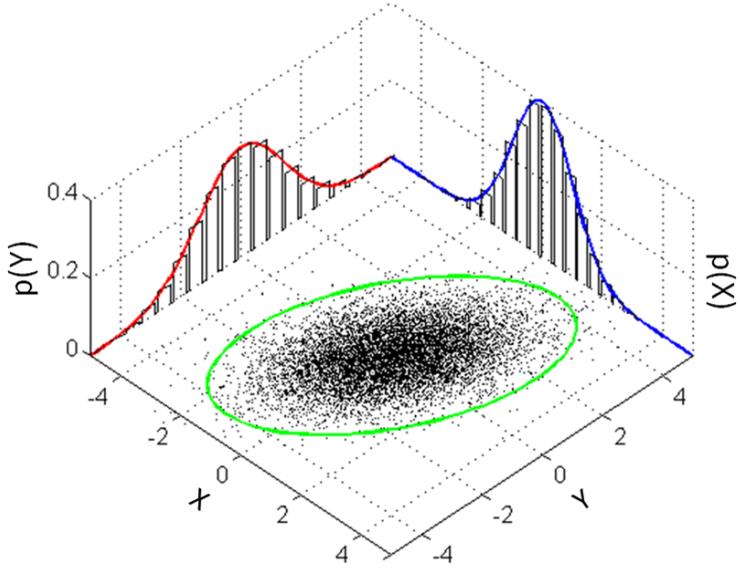


- This “version” of a mixture model works for a mixture of 1D normal distributions.

SOME MORE DETAILS….



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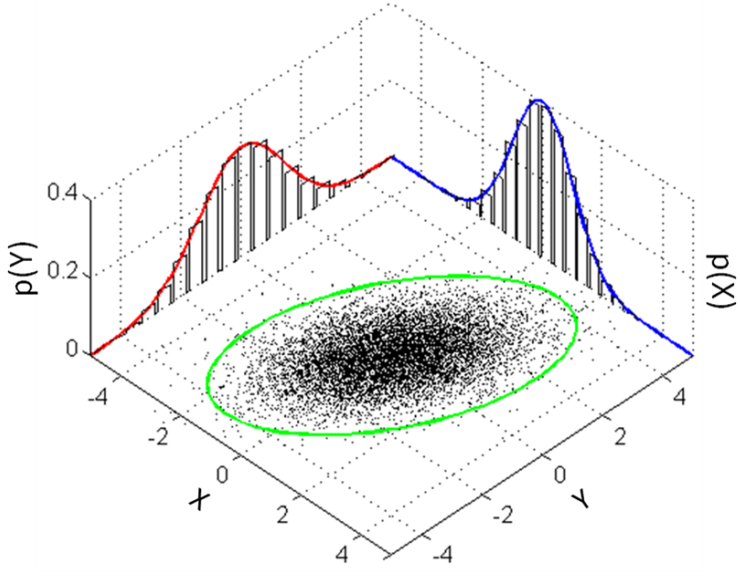
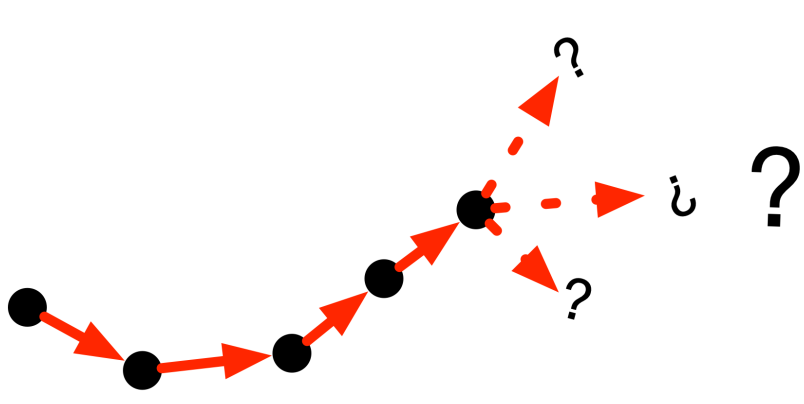
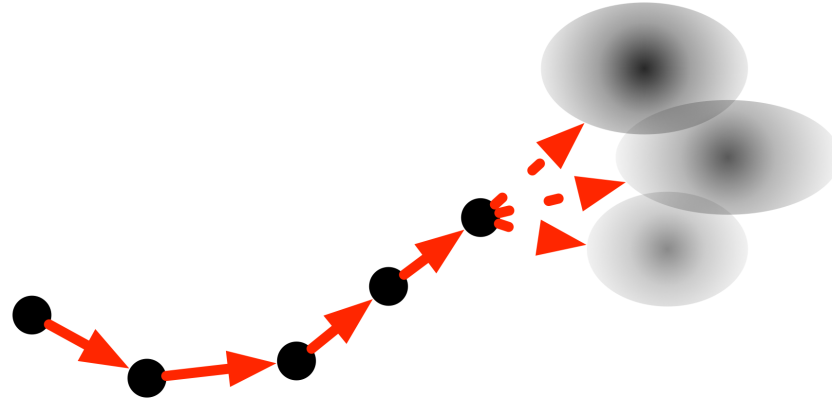


- This “version” of a mixture model works for a mixture of 1D normal distributions.
- Not too hard to extend to multivariate normal distributions, which are useful for lots of problems.
- This is how it actually works in my Keras MDN layer, have a look at the code for more details…

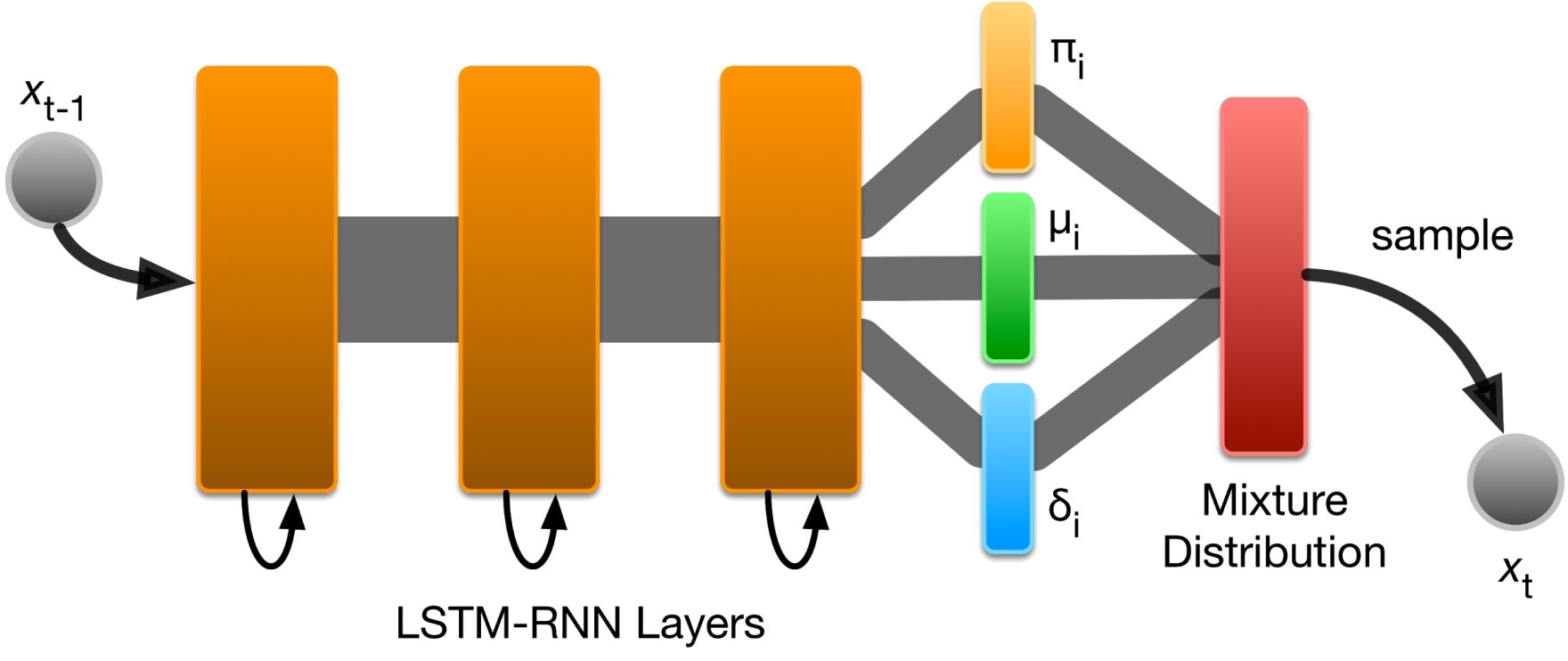
MDN-RNNS





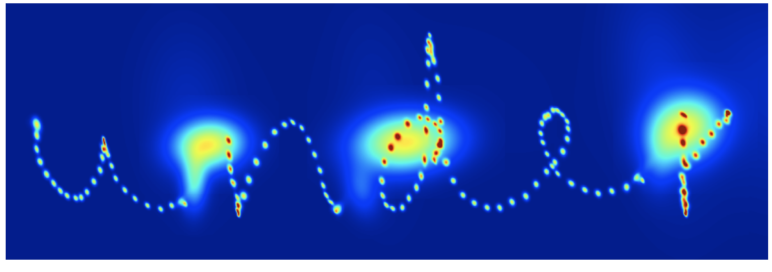
MDNs can be handy at the end of an RNN! Imagine a robot calculating moves forward through space, it might have to choose from a number of valid positions, each of which could be modelled by a 2D Normal model.

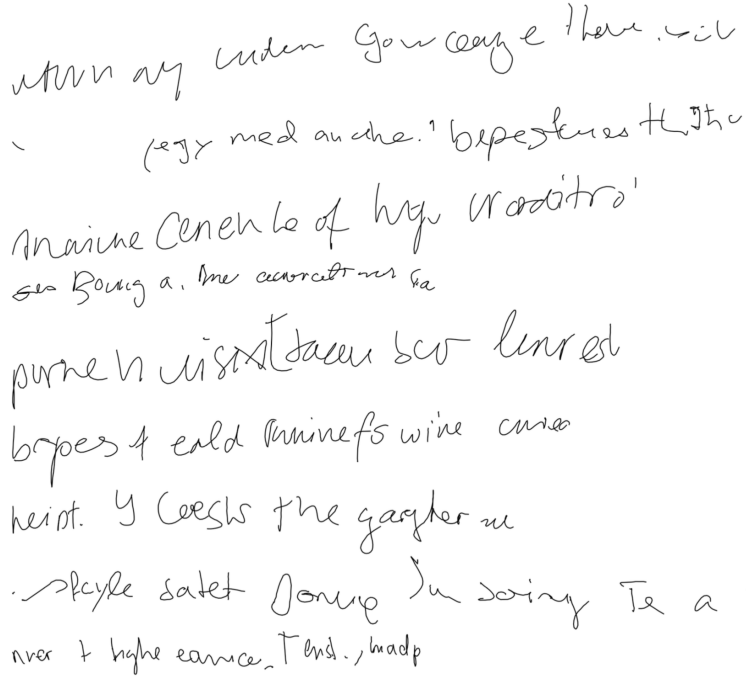
MDN-RNN ARCHITECTURE



Can be as simple as putting an MDN layer after recurrent layers!

USE CASES: HANDWRITING GENERATION





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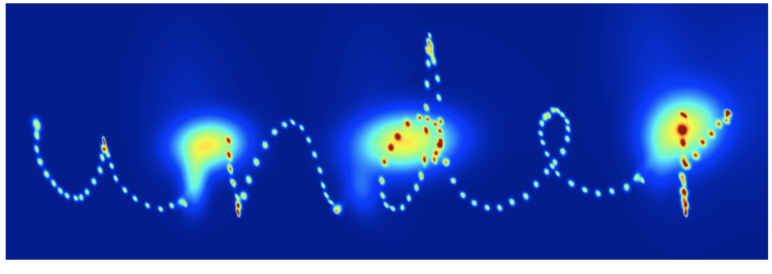

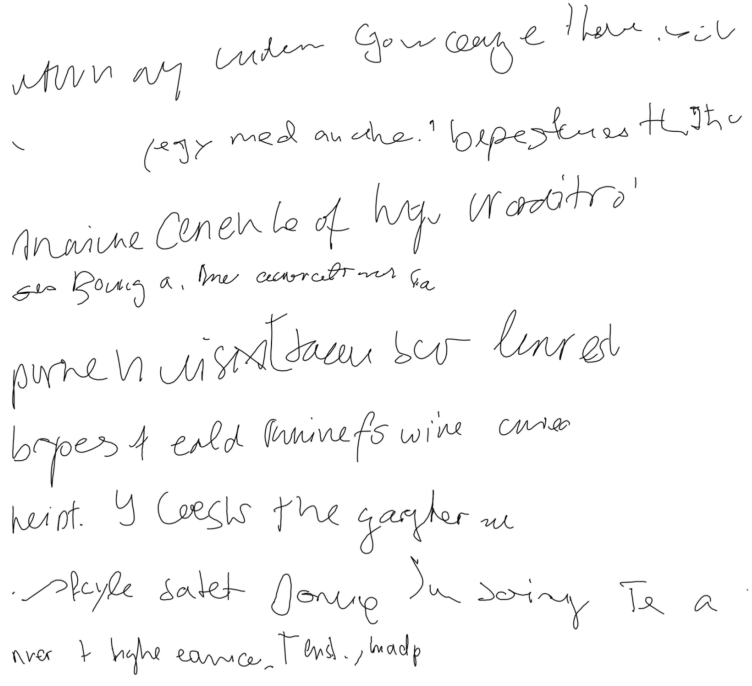

- Handwriting Generation RNN (Graves, 2013).

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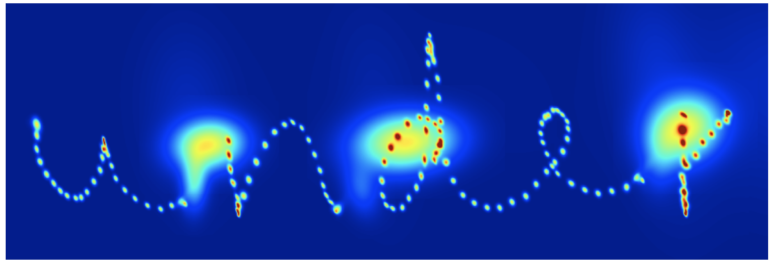

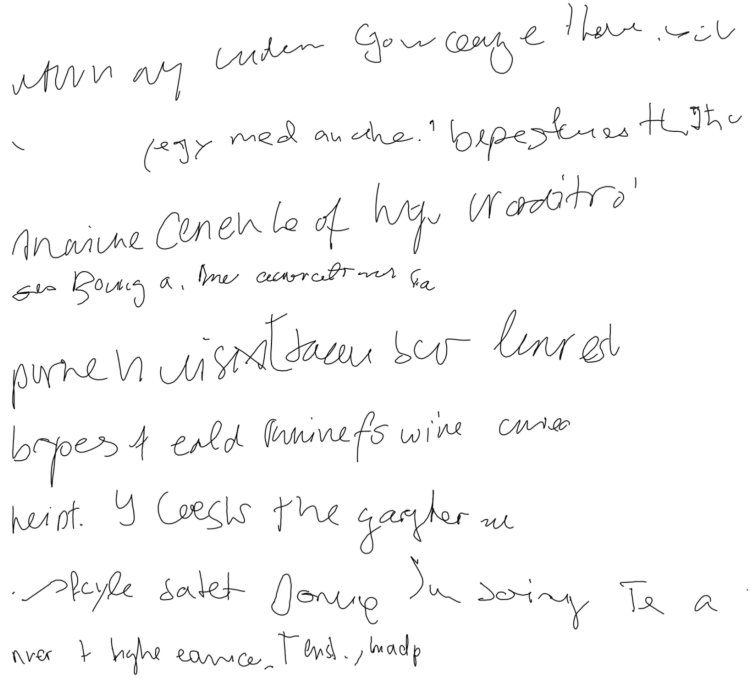

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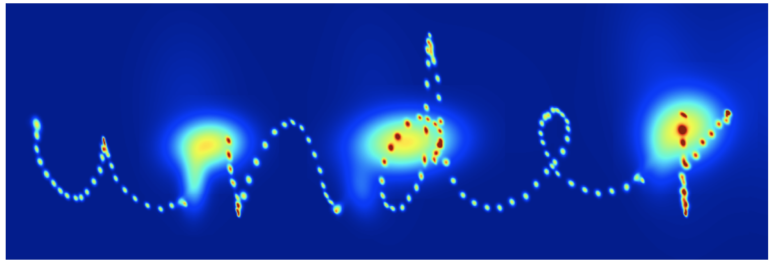

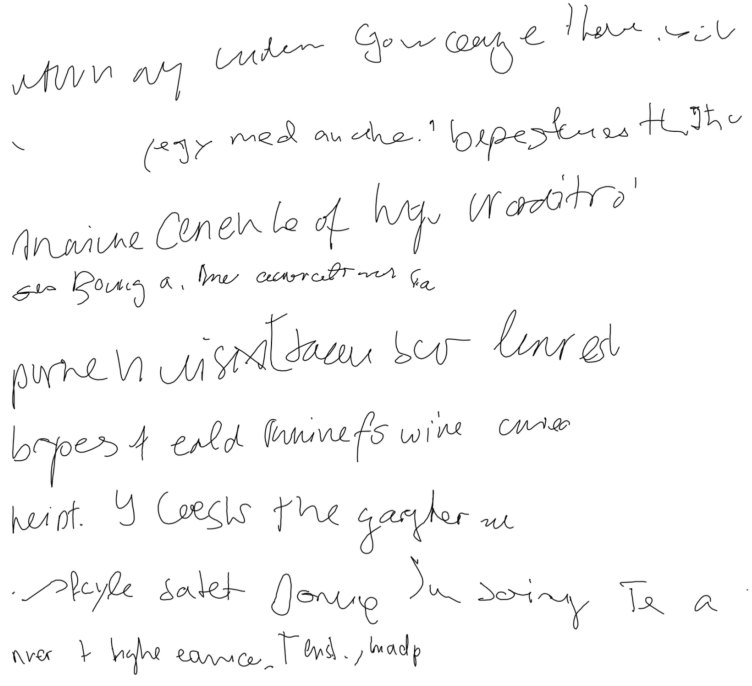

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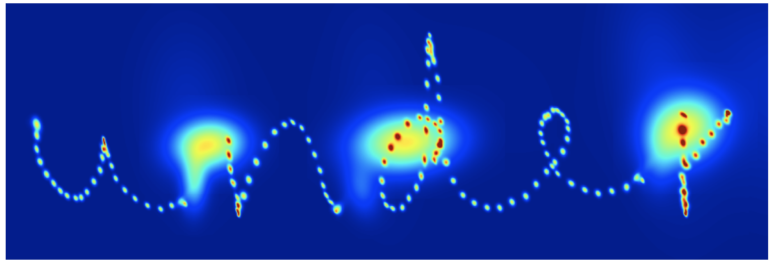
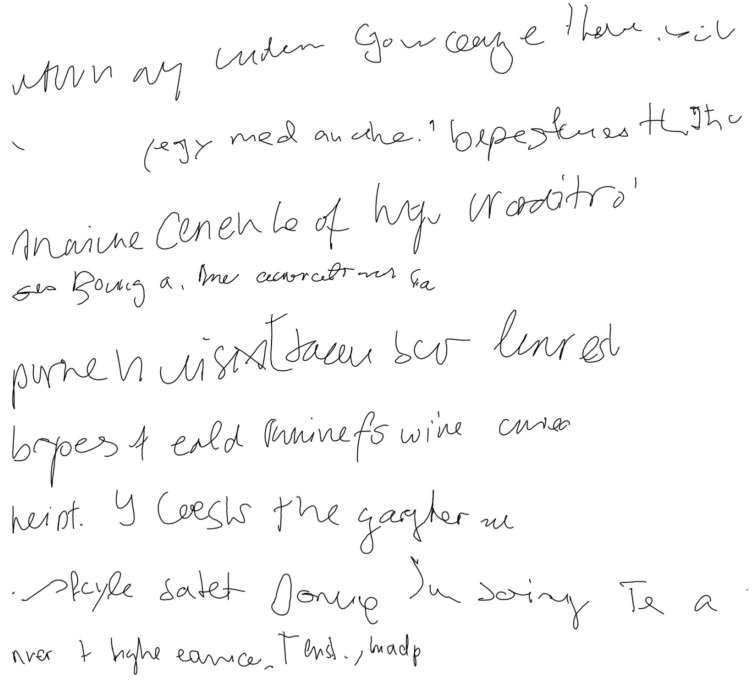
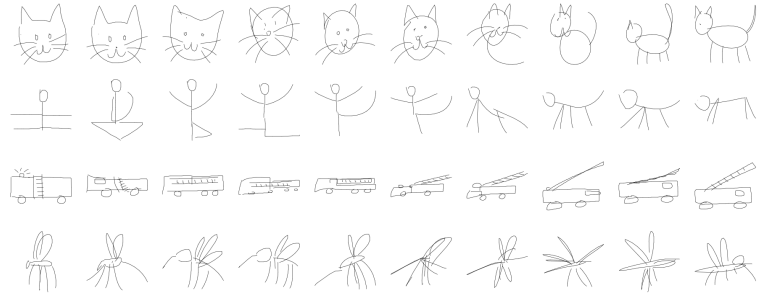




- Handwriting Generation RNN (Graves, 2013).
- Trained on handwriting data.
- Predicts the next location of the pen (dx, dy, and up/down)
- Network takes text to write as an extra input, RNN learns to decide what character to write next.

USE CASES: SKETCHRNN



USE CASES: SKETCHRNN

- SketchRNN Kanji (Ha, 2015); similar to handwriting generation, trained on kanji and then generates new “fake” characters

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- SketchRNN Kanji (Ha, 2015); similar to handwriting generation, trained on kanji and then generates new “fake” characters
- SketchRNN VAE (Ha et al., 2017); similar again, but trained on human-sourced sketches. VAE architecture with bidirectional RNN encoder and MDN in the decoder part.

USE CASES: ROBOJAM

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- RoboJam (Martin et al., 2018); similar to the kanji RNN, but trained on touchscreen musical performances

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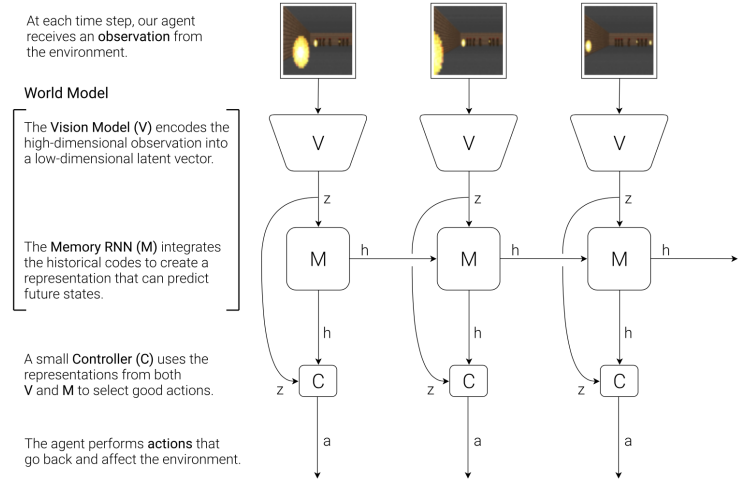
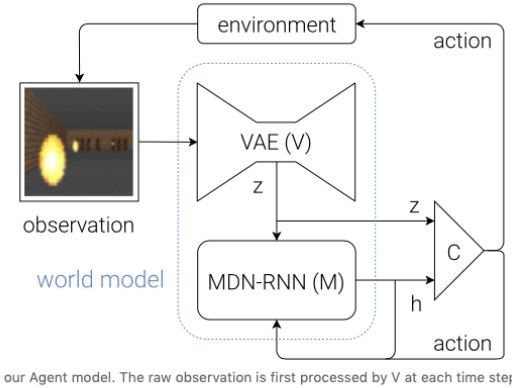
- Extra complexity: have to model touch position (x, y) and time (dt).
- Implemented in my MicroJam app (have a go: microjam.info)

USE CASES: WORLD MODELS

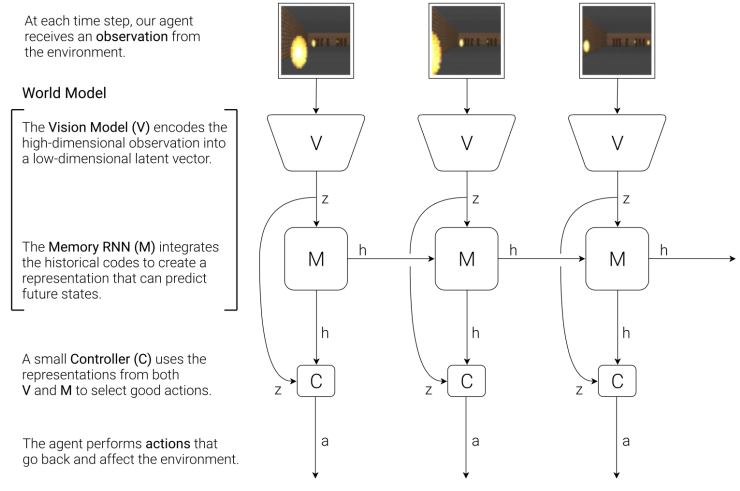


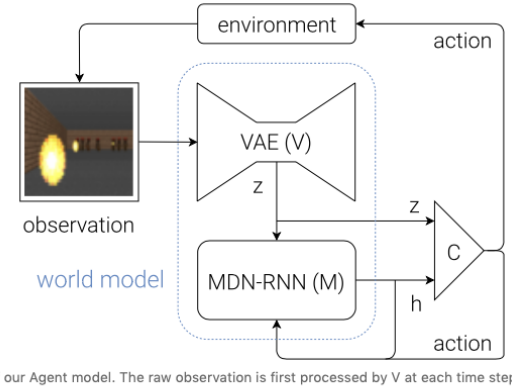


Flow diagram of our Agent model. The raw observation is first processed by V at each time step t to produce z_t. The input into C is this latent vector z_t concatenated with M's hidden state h_t at each time step. C will then output an action vector a_t for motor control. M will then take the current z_t and action a_t as an input to update its own hidden state to produce h_{t+1} to be used at time $t+1$.

USE CASES: WORLD MODELS

- World Models (Ha & Schmidhuber, 2018)





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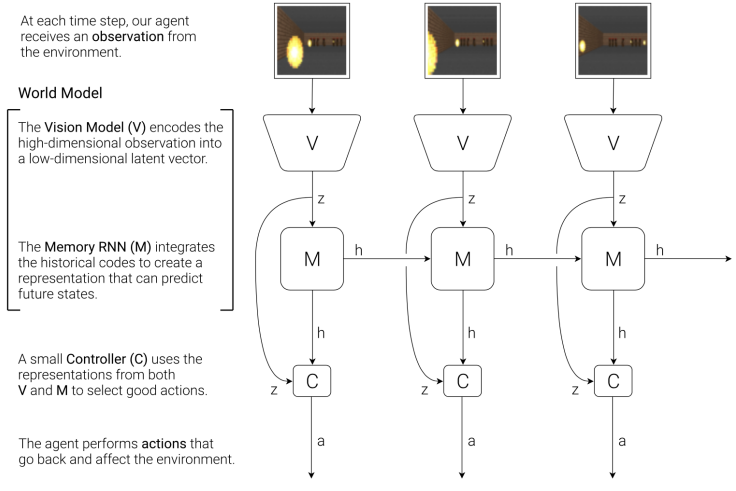
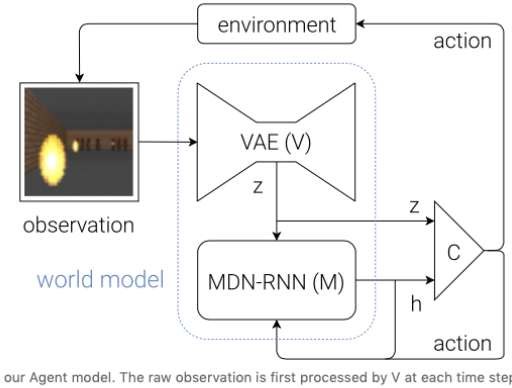
- Train a VAE for visual perception an environment (e.g., VizDoom), now each frame from the environment can be represented by a vector z





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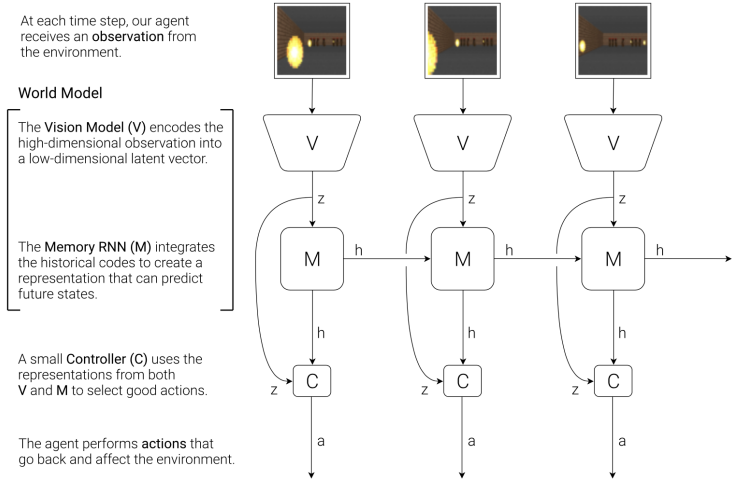
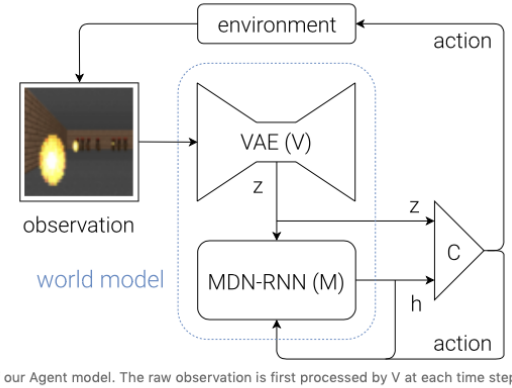
- Train MDN to predict next z, use this to help train an agent to operate in the environment.





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6. D. Ha and J. Schmidhuber. 2018. Recurrent World Models Facilitate Policy Evolution. ArXiv e-prints (Sept. 2018). ArXiv:1809.01999