


University
of Glasgow



ML
in
Science

What can Generative Models do for Science?

April 22nd 1pm-2pm
Online Zoom Seminar
Meeting ID: 995 9590 5918

- 1 **Adalberto Claudio Quiros (Comp. Sci.):**
Intro to Generative Adversarial Networks (GANs)
- 2 **Valentin Kapitany (Physics):**
GANs for super-resolution microscopy
- 3 **Dr. Catherine Higham (Comp. Sci.):**
Applications of GANs in Science

All disciplines welcome!

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Applications of GANs in science

Catherine Higham

Wednesday 22nd April

Talk Outline

- Long Short Term Memory (LSTM)
 - Generative model used with sequence data
 - Alice in Wonderland example
 - Complexity and Learnability of language
- Conditional GANs
 - Generating images conditioned on a 'label'
 - Comparison to GAN MNIST example
 - Hybrid LiDAR – RGB and single pixel LiDAR

Long Short Term Memory LSTM

Sequence data

Embedding

Input/output remember/forget

Distribution over classes

Applications Natural Language

Considerations

Training data

- Preparing and storing for efficiency
- labels/ground truth
- simulations

Architecture

- Type of layers: Size/number of filters/weights
- Connections between layers/networks

Training options

- Learning rates, dropout, gradient descent, regularizers

Prediction

- Classification, segmentation, end user
- Uncertainty quantification

Training Data: Natural Language

HTML code from Alice's Adventures in Wonderland by Lewis Carroll from Project Gutenberg.

Parse HTML code into short paragraphs using Text Analysis Tools

- *"In another moment down went Alice after it, never once considering how in the world she was to get out again. "*

Create a datastore that contains the data for training.

- For the predictors, this datastore converts the documents into sequences of word indices using a word encoding.
- For the responses, the datastore returns categorical sequences of the words shifted by one.

Architecture

Layers	Learnable Weights	Activations
Sequence Input		1
Word Embedding	100 x 2920	100
LSTM	4 x 100 x 100 input 4 x 100 x 100 recurrent + 4 x 100 bias	100
Dropout		100
Fully Connected	2920 x 100 + 2920 bias	2920
SoftMax		2920
Classification		

- Training Options:
 - 'adam',
 - 'MaxEpochs',300,
 - 'InitialLearnRate',0.01,
 - 'MiniBatchSize',32,
 - 'Shuffle','never',
 - 'Plots','training-progress',
 - 'Verbose',false.

Prediction

```
generatedText = "";
```

Predict the "next word" score

Network
Sequence Input (wordIndex)
Word Embedding
LSTM
Dropout
Fully Connected
SoftMax
Classification

Sample the "next word"

```
generatedText = generatedText + "next word"
```



Prediction

```
generatedText = "";
```

Predict the "next word" score

Network
Sequence Input (wordIndex)
Word Embedding
LSTM
Dropout
Fully Connected
SoftMax
Classification

Sample the "next word"

```
generatedText = generatedText + "next word"
```

```
generatedText = " 'Sure, it's a good Turtle!' said the Queen in a low, weak voice."
```



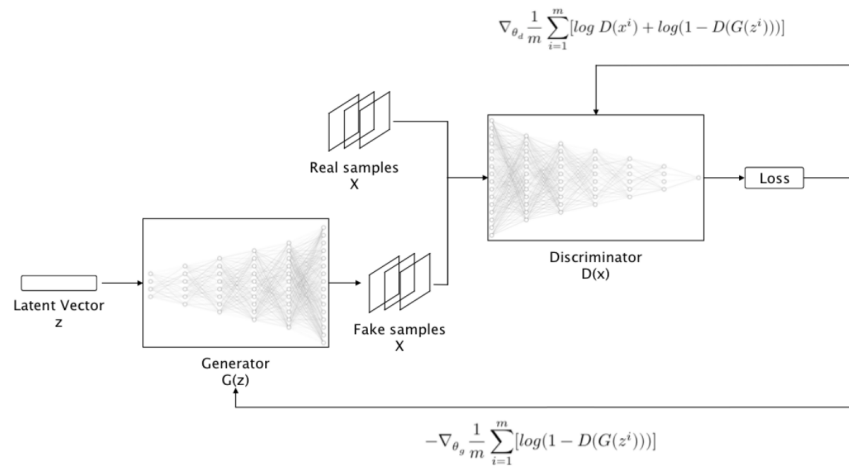
Conditional GAN

Generator and Discriminator

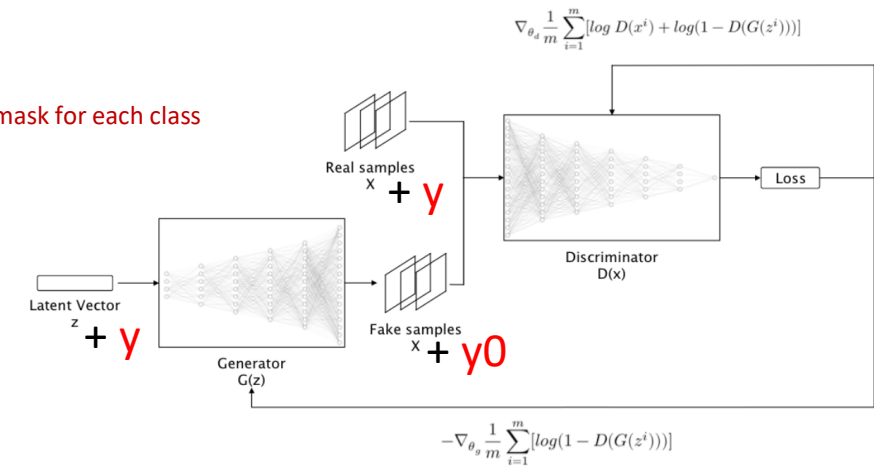
Embedding the label

Pitfalls, mode collapse, drift

Applications Images, Data Fusion



Embed z, x with learned mask for each class



GAN CODE $x|z$

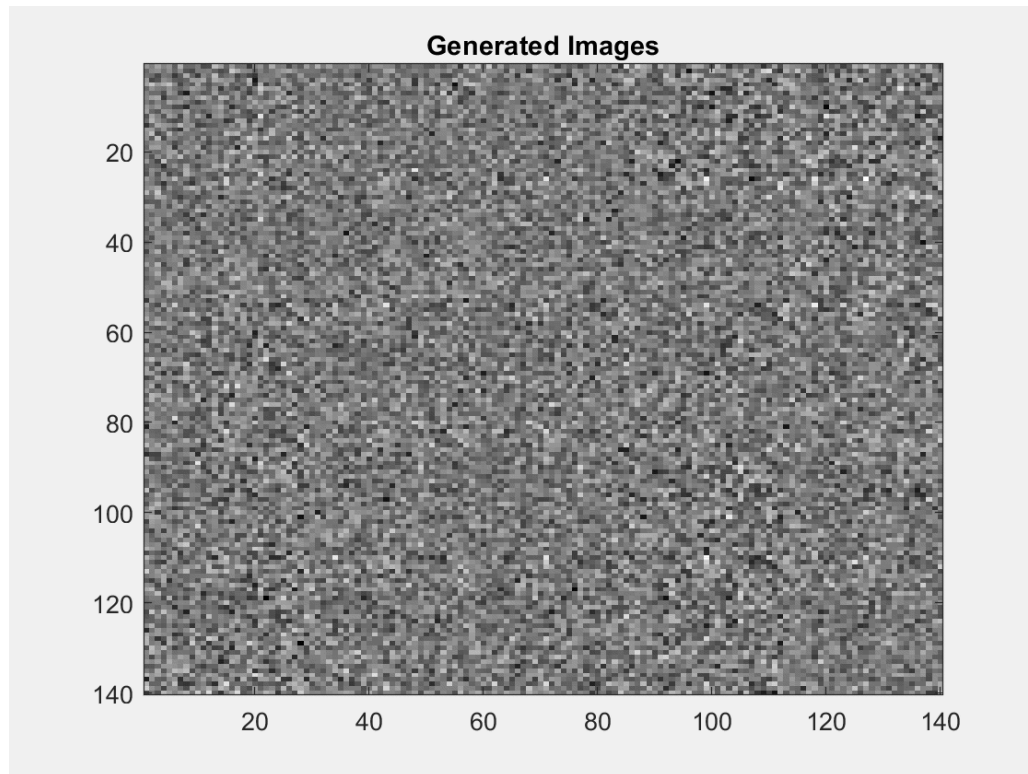
```
fake_images = Generator(z);
d_output_real = Discriminator(x);
d_output_fake = Discriminator(fake_images);
% Loss due to true or not
d_loss = -mean(log(d_output_real)+log(1-d_output_fake));
g_loss = -mean(log(d_output_fake));
% For each network, calculate the gradients with respect to the loss
GradGen = dlgradient(g_loss);
GradDis = dlgradient(d_loss);
```

Conditional GAN CODE $x|z, y$

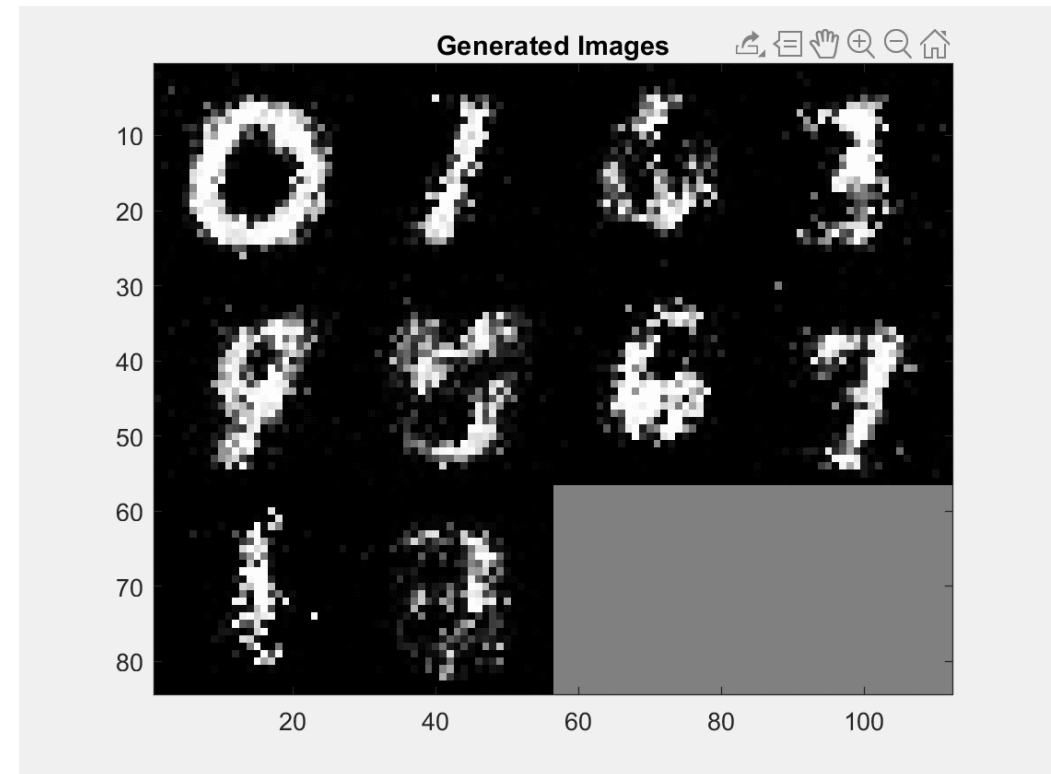
```
fake_images = Generator(z,y);
d_output_real = Discriminator(x,y);
d_output_fake = Discriminator(fake_images,y);
fake_images0 = Generator(z,y0);
y0 = randomly sampled from label classes;
d_out_fake0 = Discriminator(fake_images0,y0);
% Loss due to true or not
d_loss = -mean(log(d_output_real)+log(1-d_output_fake));
g_loss = -mean(log(d_out_fake0));
% For each network, calculate the gradients with respect to the loss
GradGen = dlgradient(g_loss);
GradDis = dlgradient(d_loss);
```

MNIST digit generation

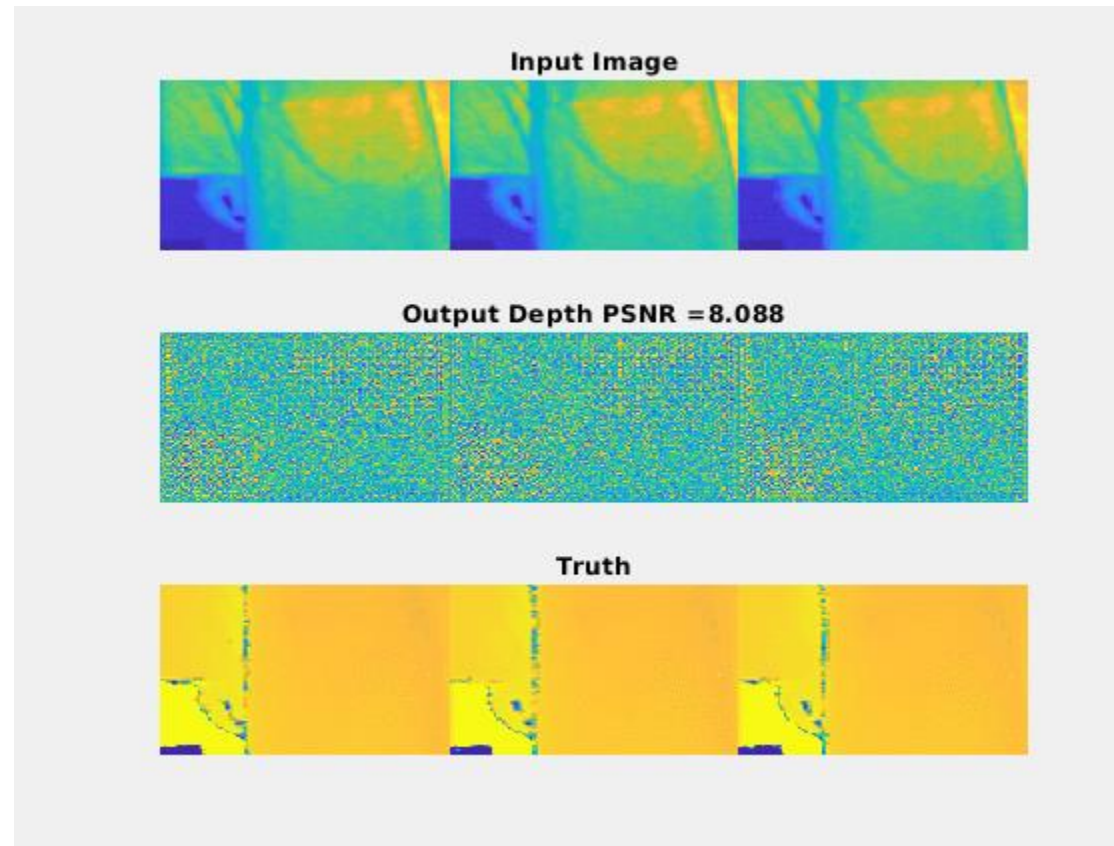
GAN



CGAN



Hybrid LiDAR generate Depth | G (RGB)+single LiDAR signal



Joint work with Steven Johnson, Neal Radwell, Rod Murray-Smith and Miles Padgett