Analyzing Inverse Problems with Invertible Neural Networks

Ardizzone et al., ICLR 2019
Example

Forward process:

\[(x_1, x_2) \rightarrow \text{Red}\]

Inverse process:

\[\text{Red} \rightarrow (x_1, x_2)\]
Generative Modelling: Why?

• **Bayesian:**
  Model represents a distribution, not just a point estimate

• **Data augmentation** to train other models:
  Can generate data in a guided way

• Understand the relations between $x$ and $y$ better
Architecture: Invertible Blocks

\[ v_1 = u_1 \odot \exp(s_2(u_2)) + t_2(u_2) \]
\[ v_2 = u_2 \odot \exp(s_1(v_1)) + t_1(v_1) \]

**u**: Input to the layer

**v**: Output of the layer

Neural Network Layers!
Data flow diagram

https://hci.iwr.uni-heidelberg.de/vislearn/wp-content/uploads/2018/07/INN-coupling-layer.png
\[ \mathcal{L}_y : \quad f_y(x) \approx y_{\text{true}} \]

\[ \mathcal{L}_z : \quad \text{Sample } z \text{ independently of } y \]

\[ p(z|y) \overset{!}{=} p_{\text{true}}(z) = \mathcal{N}(0, 1) \]

\[ \mathcal{L}_x : \quad \text{Sample } x \text{ correctly} \]

\[ p_{x,\text{sampling}} \overset{!}{=} p_{x,\text{true}} \]
$L_{reconstruction}:$

$$f^{-1}(f(x) + \text{noise}) \approx x$$
Comparing distributions: MMD

**Goal:** Compare distributions $p$, $q$ when only given samples

$x, x' \sim p$ $\quad$ $x, x'$ indep.

$y, y' \sim q$ $\quad$ $y, y'$ indep.

$$\text{MMD}^2 [\mathcal{F}, p, q] = \mathbb{E}_{x,x'} [k(x, x')] - 2\mathbb{E}_{x,y} [k(x, y)] + \mathbb{E}_{y,y'} [k(y, y')]$$

Inverse Multiquadratic $k(x, x') = 1/(1 + \| (x - x')/h \|^2_2)$
Losses: Summary

- Punish wrong distributions of $x$ and $z$ with MMD
- Punish wrong $x \rightarrow y$ map with MSE
Results

Ground truth  INN, all losses  INN, only $L_y + L_z$  INN, only $L_x$
https://hci.iwr.uni-heidelberg.de/vislearn/inverse-problems-invertible-neural-networks/
Questions?
Appendix:
Recent results in generative Modelling
Advances and challenges in deep generative models for de novo molecule generation

- Goal:
  Find new molecules with desired properties
- Still ongoing research
Glow: Better Reversible Generative Models
Analyzing and Improving the Image Quality of StyleGAN

https://www.thispersondoesnotexist.com/