Flow-based models

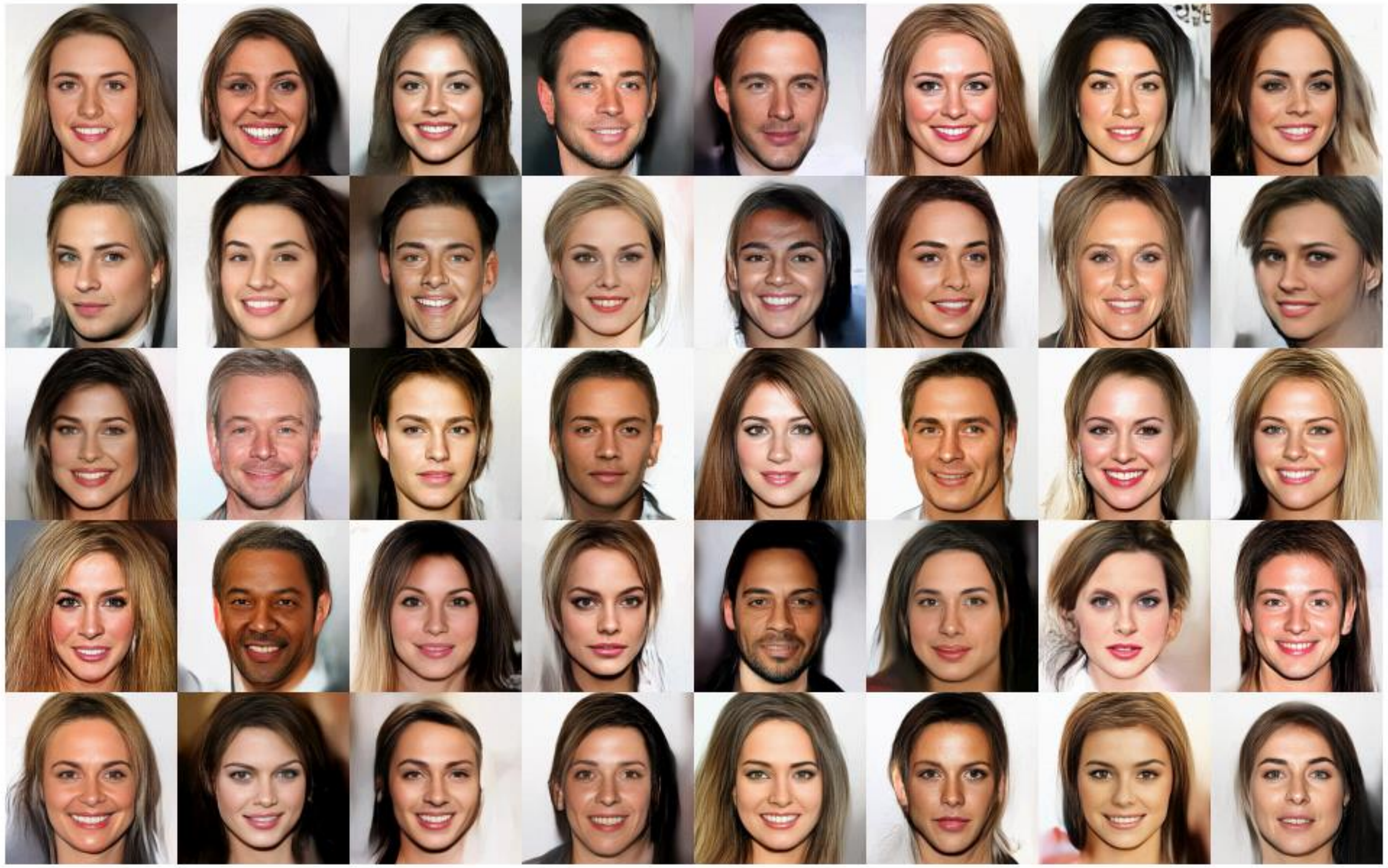


Figure 4: Random samples from the model, with temperature 0.7

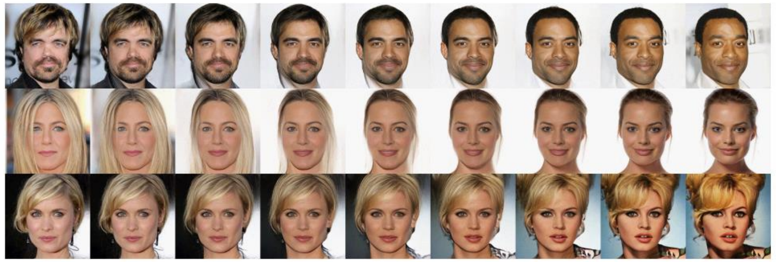
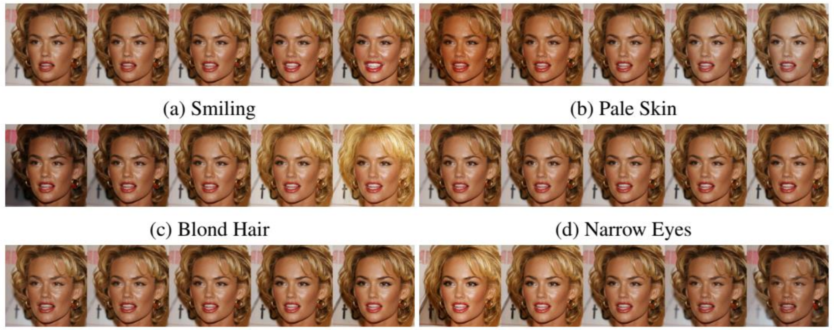


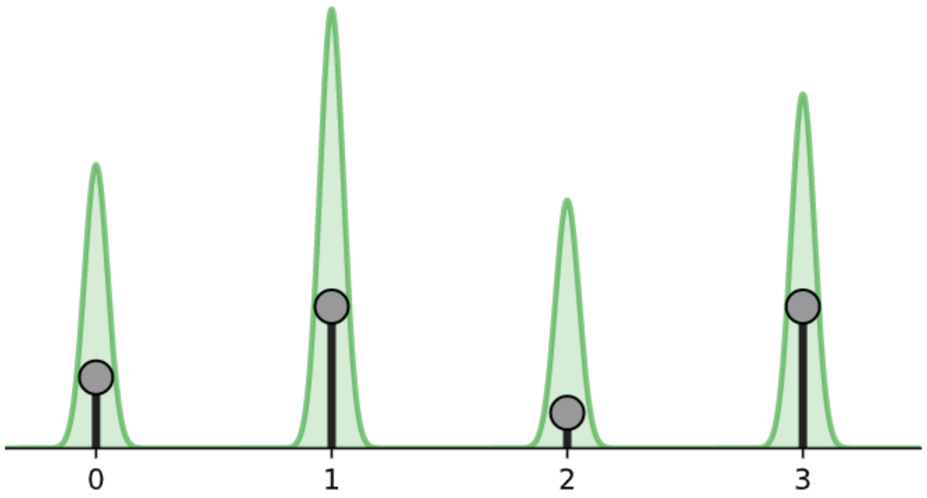
Figure 5: Linear interpolation in latent space between real images



(a) Smiling (b) Pale Skin (c) Blond Hair (d) Narrow Eyes (e) Young (f) Male

Normalizing flows on images

- Normalizing flows are continuous transformations
- Images contain discrete values
  → The model will assign δ-peak probabilities on integer (pixel) values only
  - These probabilities will be nonsensical, there is no smoothness



UVADLC tutorial

(Variational) dequantization

- Add (continuous) noise $u \sim q(u|x)$ to input variables $v = x + u$
- The data log-likelihood then is

$$\log p(x) = \log \int p(x+u)\, du = \log \mathbb{E}_{u\sim q(u|x)} \left[\frac{p(x+u)}{q(u|x)} \right] \geq \mathbb{E}_{u\sim q(u|x)} \log \left[\frac{p(x+u)}{q(u|x)} \right]$$

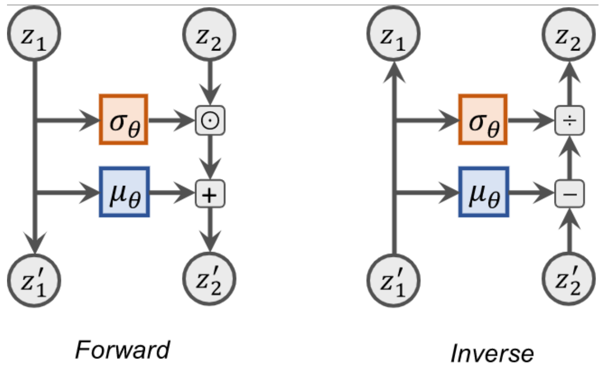
- If $q(u|x)$ is the uniform distribution the standard dequantization
  - Probability between two consecutive values is fixed
    → resemble boxy boundaries between values
- Better learn $q(u|x)$ in a variational manner
  → Variational dequantization

Coupling layers

- Given input $\boldsymbol{z}$ the output of the transformation is

$$\boldsymbol{z}' = \begin{bmatrix} \boldsymbol{z}'_{1:j} \\ \boldsymbol{z}'_{j+1:d} \end{bmatrix} = \begin{bmatrix} \boldsymbol{z}_{1:j} \\ \mu_\theta(\boldsymbol{z}_{1:j}) + \sigma_\theta(\boldsymbol{z}_{1:j}) \odot \boldsymbol{z}_{j+1:d} \end{bmatrix}$$

  - $\mu_\theta, \sigma_\theta$ are neural networks with shared parameters

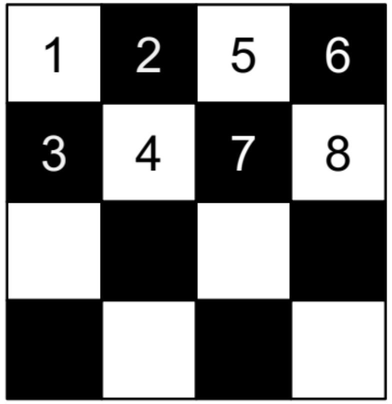


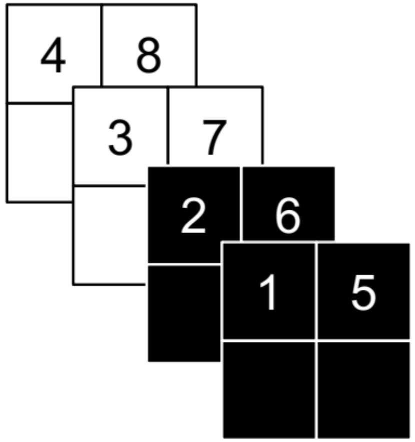
- Easy inverse: $\boldsymbol{z} = \begin{bmatrix} \boldsymbol{z}_{1:j} \\ \frac{\left(\boldsymbol{z}'_{j+1:d} - \mu_\theta(\boldsymbol{z}_{1:j})\right)}{\sigma_\theta(\boldsymbol{z}_{1:j})} \end{bmatrix}$

- Easy triangular Jacobian $\frac{\partial \boldsymbol{z}'}{\partial \boldsymbol{z}} = \begin{bmatrix} \mathbb{I}_d & 0 \\ \frac{\partial \boldsymbol{z}'_{j+1:d}}{\partial \boldsymbol{z}_{1:j}} & \mathrm{diag}\left(\sigma_\theta(\boldsymbol{z}_{1:j})\right) \end{bmatrix}$
  - The log determinant is $\sum_j \log \sigma_\theta(\boldsymbol{z}_j)$

Splitting dimensions in images

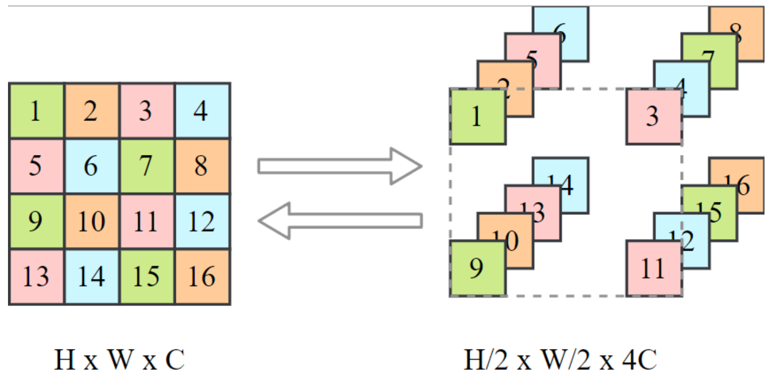
- Use masking
  - Checkers pattern
  - Splitting across channels
- Alternate dimensions between consecutive layers
  $\rightarrow$ not always the same $1:d$ dimensions remain untouched

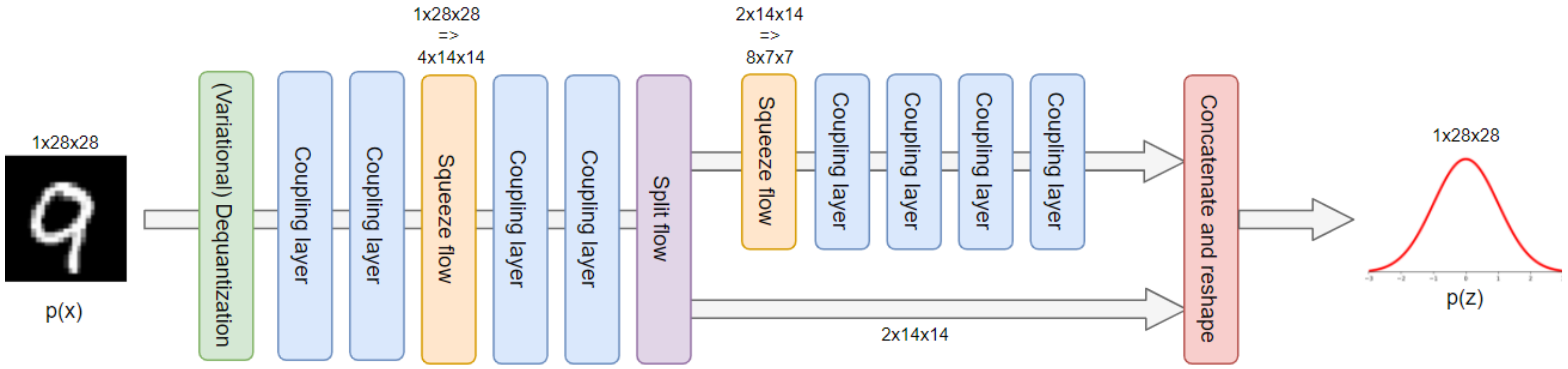




Multi-scale architecture

- Invertibility → number of dimensions before and after f is the same
  - High computational complexity for large images
- Apply new transformations to half the input only
  - For the other half use the prior (previous) trasnfromations
- Use squeeze to turn spatial to channel dimensions
  - And split for halving the input





UVADLC tutorial

GLOW, FLOW, FLOW++

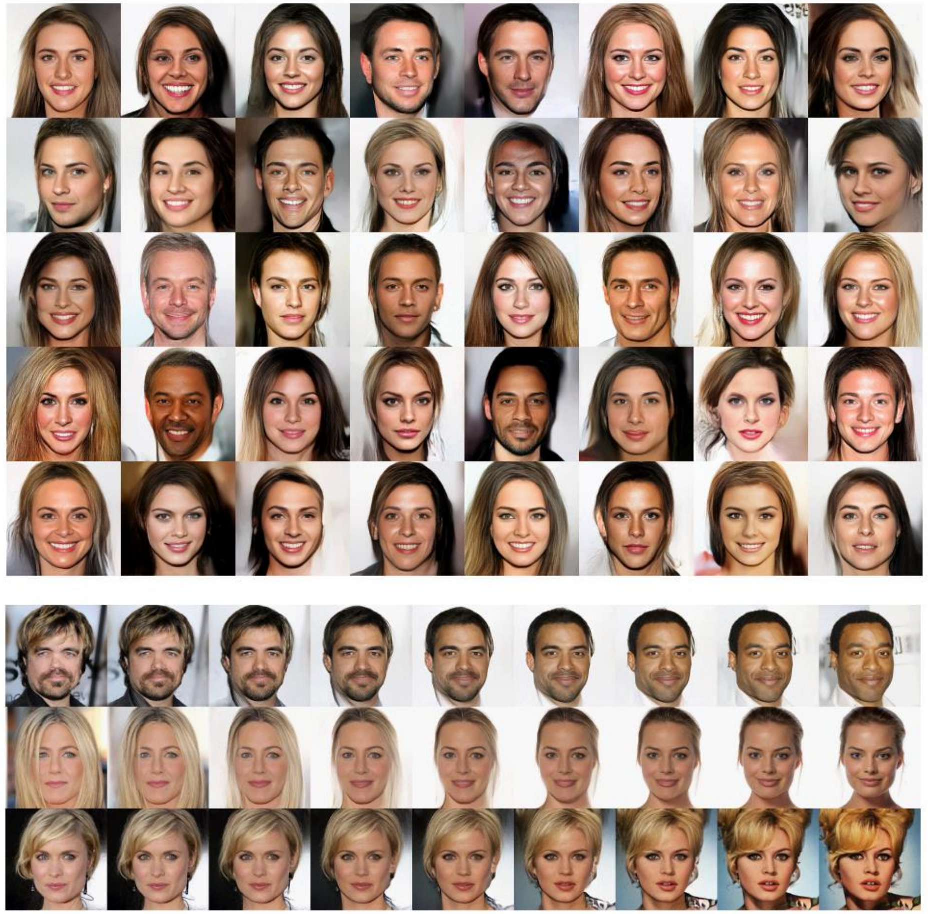


Figure 5: Linear interpolation in latent space between real images

Kingma, Dhariwal, Glow: Generative Flow with Invertible 1x1 Convolutions

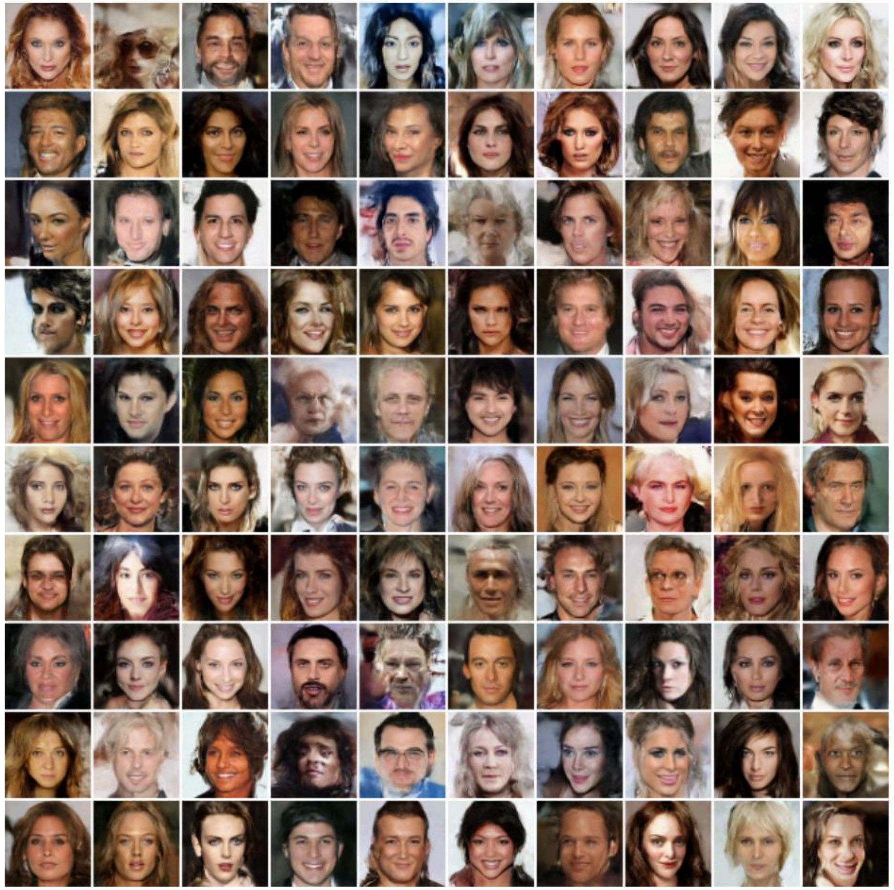


Figure 4. Samples from Flow++ trained on 5-bit 64x64 CelebA, without low-temperature sampling.

Kingma, Dhariwal, Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design

Categorical normalizing flows [not in exams]

- Normalizing flows with variational inference to learn representations of categorical data on continuous space
  - Learnable, smooth, support for higher dimensions
- Learning must ensure no loss of information
  → the volumes that represent categorical data must not-overlap
  - Otherwise, to which category does the representation correspond to?

$$p(\boldsymbol{x}) \geq \mathbb{E}_{\boldsymbol{z}\sim q(\cdot|\boldsymbol{x})}\left[\frac{\prod_i p(x_i|\boldsymbol{z}_i)}{q(\boldsymbol{z}|\boldsymbol{x})} p(\boldsymbol{z})\right]$$

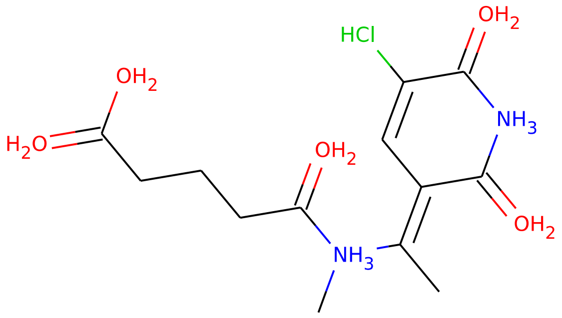
  - Factorized posterior $\prod_i p(x_i|\boldsymbol{z}_i)$ to encourage learning non-overlapping $\boldsymbol{z}_i$

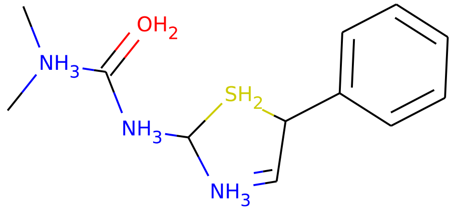
Lippe and Gavves, Categorical Normalizing Flows via Continuous Transformations, in submission to ICLR 2021

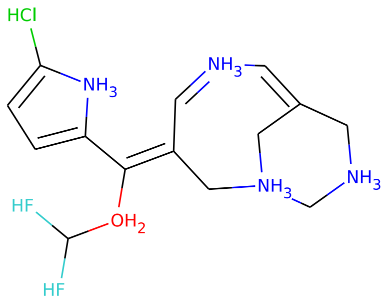
Graph generation with categorical normalizing flows

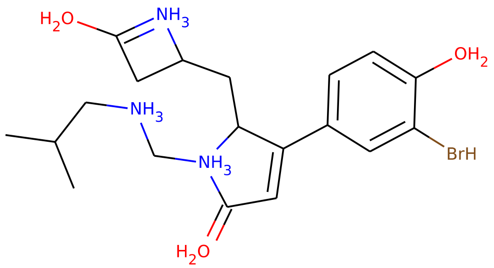
Results on the Zinc250k dataset (224k examples)

Method	Validity	Uniqueness	Novelty	Reconstruction	Parallel	General
JT-VAE	100%	100%	100%	71%	✗	✗
GraphAF	68%	99.10%	100%	100%	✗	✓
R-VAE	34.9%	100%	–	54.7%	✓	✓
GraphNVP	42.60%	94.80%	100%	100%	✓	✓
GraphCNF	83.41% (±2.88)	99.99% (±0.01)	100% (±0.00)	100% (±0.00)	✓	✓
+ Sub-graphs	96.35% (±2.21)	99.98% (±0.01)	99.98% (±0.02)	100% (±0.00)	✓	✓









Normalizing flows: pros and cons

- Starting from a simple density like a unit Gaussian we can obtain any complex density that match our data without even knowing its analytic form
- Tractable density estimation
- Efficient parallel sampling and learning
- Often very many transformations required → Very large networks needed
- Constrained to invertible transformations with tractable determinant
- Tied encoder and decoder weights
- Transformations cannot easily introduce bottlenecks

UVADLC tutorial

A summary of properties

	Training	Likelihood	Sampling	Compression
Autoregressive models (e.g., PixelCNN)	Stable	Yes	Slow	No
Flow-based models (e.g., RealNVP)	Stable	Yes	Fast/Slow	No
Implicit models (e.g., GANs)	Unstable	No	Fast	No
Prescribed models (e.g., VAEs)	Stable	Approximate	Fast	Yes

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J. Tomczak's lecture from April, 2019

Summary

- Early autoregressive models
- Modern autoregressive models
- Normalizing flows
- Flow-based models

All mentioned papers as reading material