Neural Autoregressive Flows

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January 13, 2020

Outline

- Types of Generative Models
- Normalizing Flows
- Autoregressive Models
- Inverse Autoregressive Flow
- Neural Autoregressive Flow

Types of Generative Models

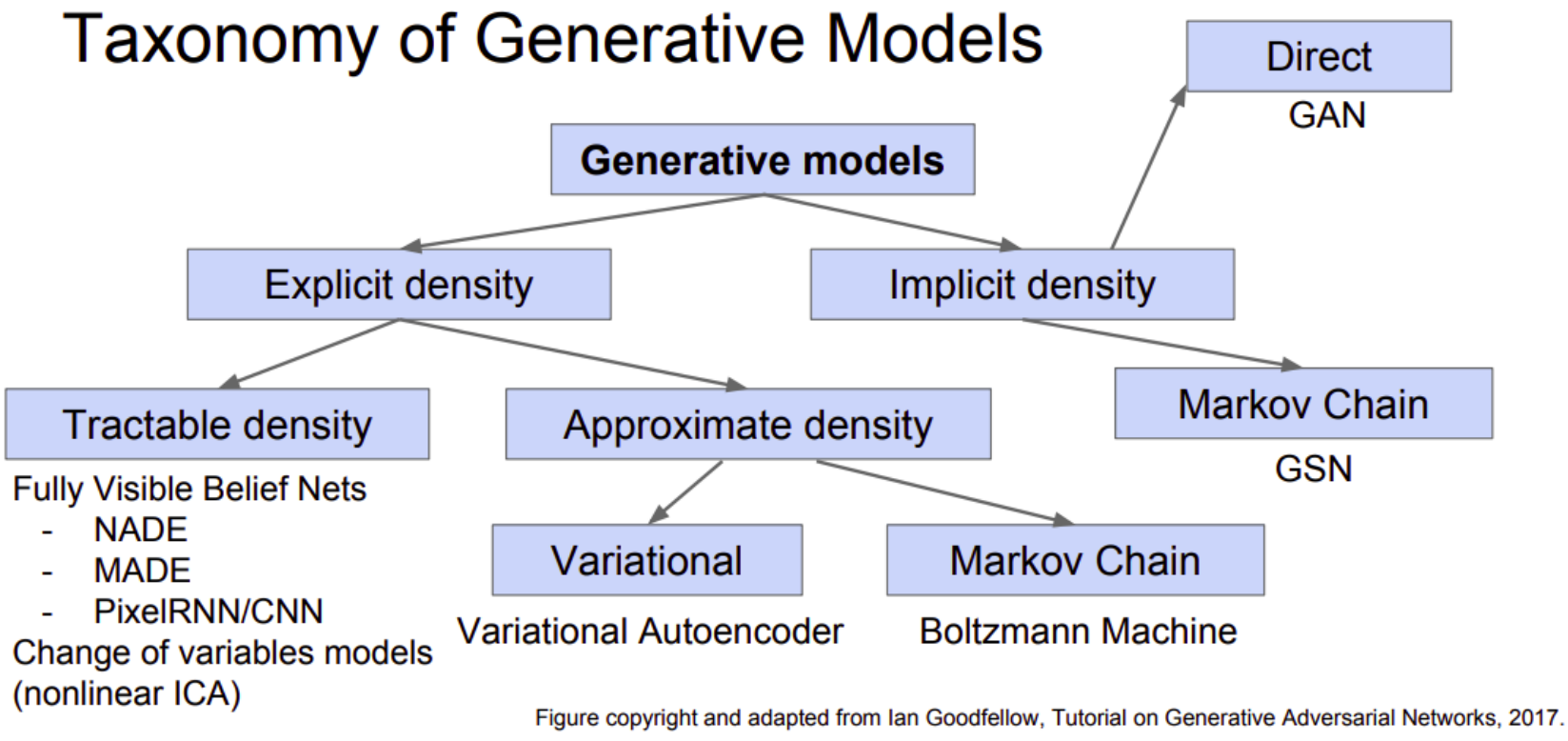

Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

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- $\mathbf{z} \in \mathbb{R}^d$ and $\mathbf{y} = f(\mathbf{z})$ where $f : \mathbb{R}^d \mapsto \mathbb{R}^d$ Let $\mathbf{z} \sim q(\mathbf{z})$. According to change of variable formula :

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$$q_y(\mathbf{y}) = q(\mathbf{z}) \left| \det \frac{\partial f^{-1}}{\partial \mathbf{y}} \right| = q(\mathbf{z}) \left| \det \frac{\partial f}{\partial \mathbf{z}} \right|^{-1} \tag{1}$$

by applying the inverse function theorem, $J_{f^{-1}}(q) = [J_f(p)]^{-1}$

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$$\log q(\mathbf{z}_K) = \log q(\mathbf{z}_0) - \sum_{k=1}^{K} \log \left| \det \frac{\partial f_k}{\partial \mathbf{z}_{k-1}} \right| \tag{4}$$

Normalizing Flows

Loss Function :[1]

$$\begin{aligned}
\mathcal{F}(x) &= E_{\mathbf{z}\sim q}[\log q(\mathbf{z}) - \log P(x, \mathbf{z})] && (5)\\
&= E_{z\sim q}[\log q(\mathbf{z_K}) - \log P(x, \mathbf{z_K})] && (6)\\
&= E_{z\sim q}[\log q(\mathbf{z_0}) - \sum_{k=1}^{K} \log \left| \det \frac{\partial f_k}{\partial \mathbf{z_{k-1}}} \right| - \log P(x, \mathbf{z_K})] && (7)
\end{aligned}$$

[1] For the derivation of the Variational Free Energy, see Slide 26: Appendix

Planar Flows

- Transformation function f_k should satisfy two properties:
  - It is easily invertible.
  - Its Jacobian determinant is easy to compute.
- Planar Flows : $f(\mathbf{z}) = \mathbf{z} + \mathbf{u}h(\mathbf{w}^T\mathbf{z} + b)$

$$\psi(z) = h'(w^T z + b)w \tag{8}$$

$$\left|\det \frac{\partial f}{\partial z}\right| = \left|\det(I + u\psi(z)^T)\right| = \left|1 + u^T\psi(z)\right| \tag{9}$$

- Matrix-determinant lemma : $\det(I + uv^T) = (1 + v^T u)$

Normalizing Flows

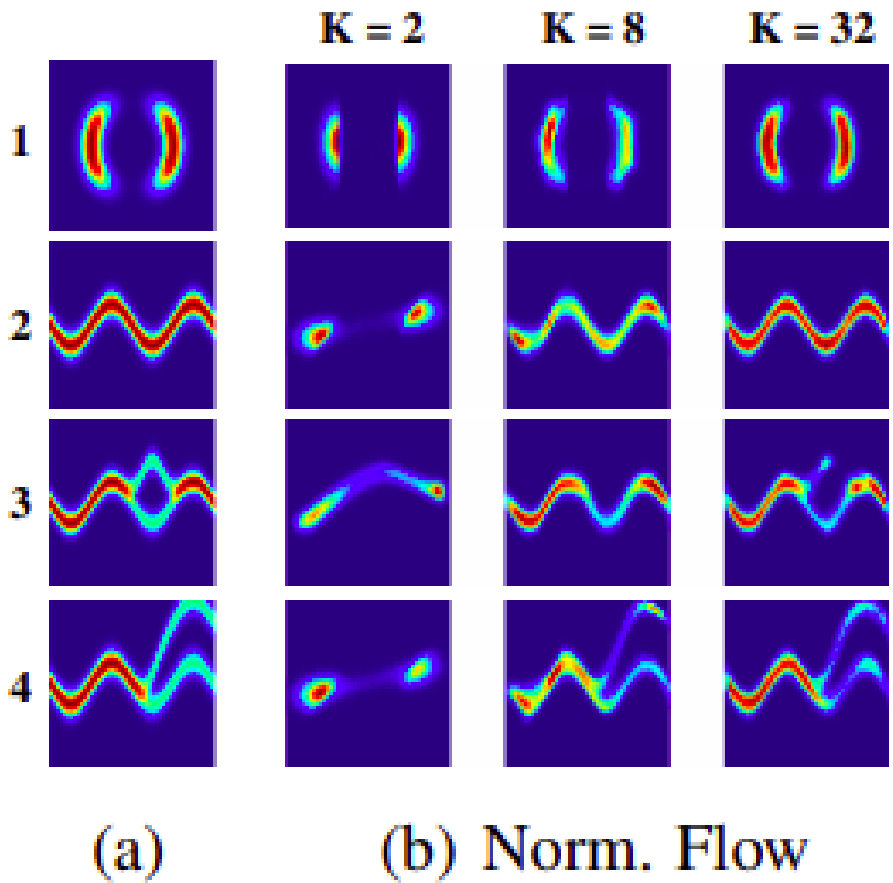

Figure: (a) Target Distribution. (b)) Approx posterior using NF[2]

[2] Image Source : Rezende and Mohamed (2015)

Autoregressive Models

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$$p(\mathbf{x}) = \prod_{i=1}^{D} p(x_i|x_1, \ldots, x_{i-1}) = \prod_{i=1}^{D} p(x_i|x_{1:i-1}) \tag{10}$$

Autoregressive Models

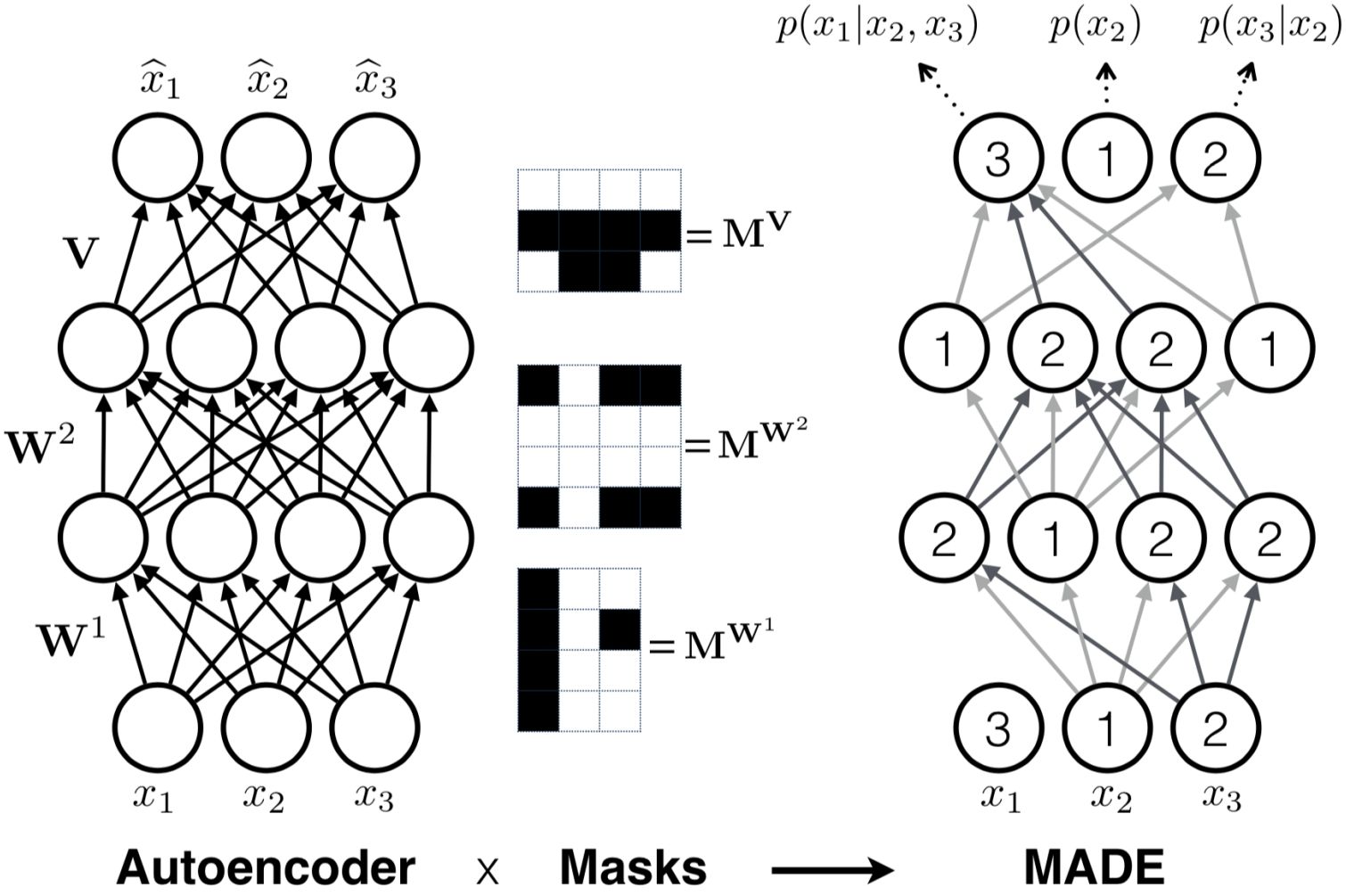

Figure: Demonstration MADE in a 3-layer NN. Germain et al. (2015)[3]

[3] Image Source : Germain et al. (2015)

Autoregressive Flows

- flow transformation framed as an autoregressive model — **autoregressive flow**.

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- The Jacobian $J = \frac{\partial z'}{\partial z}$ becomes lower triangular.

$$\det J = \prod_{i=1}^{D} J_{ii} \tag{12}$$

Autoregressive Transformation

- Let $z' = f(z)$, and the first dimension of the transformed variable be defined by:

$$z \sim \mathcal{N}(0, I) \quad \text{[base distribution: } q(\mathbf{z})\text{]} \tag{13}$$

$$z'_0 = \mu_0 + \sigma_0 \odot z_0 \quad \text{[Randomly Sampled]} \tag{14}$$

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- The other dimensions $i > 0$ are computed by :

$$z'_i = \mu_i(z'_{1:i-1}) + \sigma_i(z'_{1:i-1}) \cdot z_i \tag{15}$$

Inverse Autoregressive Transformation

- Inverse of Equation (14) and (15) are :

$$z_0 = \frac{z'_0 - \mu_0}{\sigma_0} \tag{16}$$

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$$\det \left| \frac{d\mathbf{z}}{d\mathbf{z}'} \right| = \prod_{i=1}^{D} \frac{1}{\sigma_i(z_{1:i-1})} \tag{18}$$

$$\log \det \left| \frac{d\mathbf{z}}{d\mathbf{z}'} \right| = \sum_{i=1}^{D} -\log \sigma_i(z_{1:i-1}) \tag{19}$$

Inverse Autoregressive Flow (IAF)

- Kingma et al. (2016) has defined two functions $\mathbf{s}_t = \frac{1}{\sigma_t(\cdot)}$ and $\mathbf{m}_t = \frac{-\mu_t(\cdot)}{\sigma_t(\cdot)}$.
- $\mathbf{s}_t$ and $\mathbf{m}_t$ can be modeled by **autoregressive neural networks**.

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z_t &= \frac{z_{t-1} - \mu_t(z_{t-1})}{\sigma_t(z_{t-1})} && (20)\\
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&= z_{t-1} \odot \mathbf{s}_t(z_{t-1}) + \mathbf{m}_t(z_{t-1}) && (22)
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\end{aligned}
$$

- And finally for numerical stability they modify Equation (22)

$$
\begin{aligned}
g_t &= \text{sigmoid}(\mathbf{s}_t(z_{t-1})) && (23)\\
z_t &= z_{t-1} \odot g_t + (1 - g_t) \odot \mathbf{m}_t(z_{t-1}) && (24)
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$$

Neural Autoregressive Flow

- Re-write Equation (24) as a combination of an autoregressive **conditioner**, c and an invertible **transformer**, τ

$$y \doteq f(x_{1:t}) = \tau(c(x_{1:t-1}), x_t) \tag{25}$$

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Notice the similarity between Eq (24) and (26).

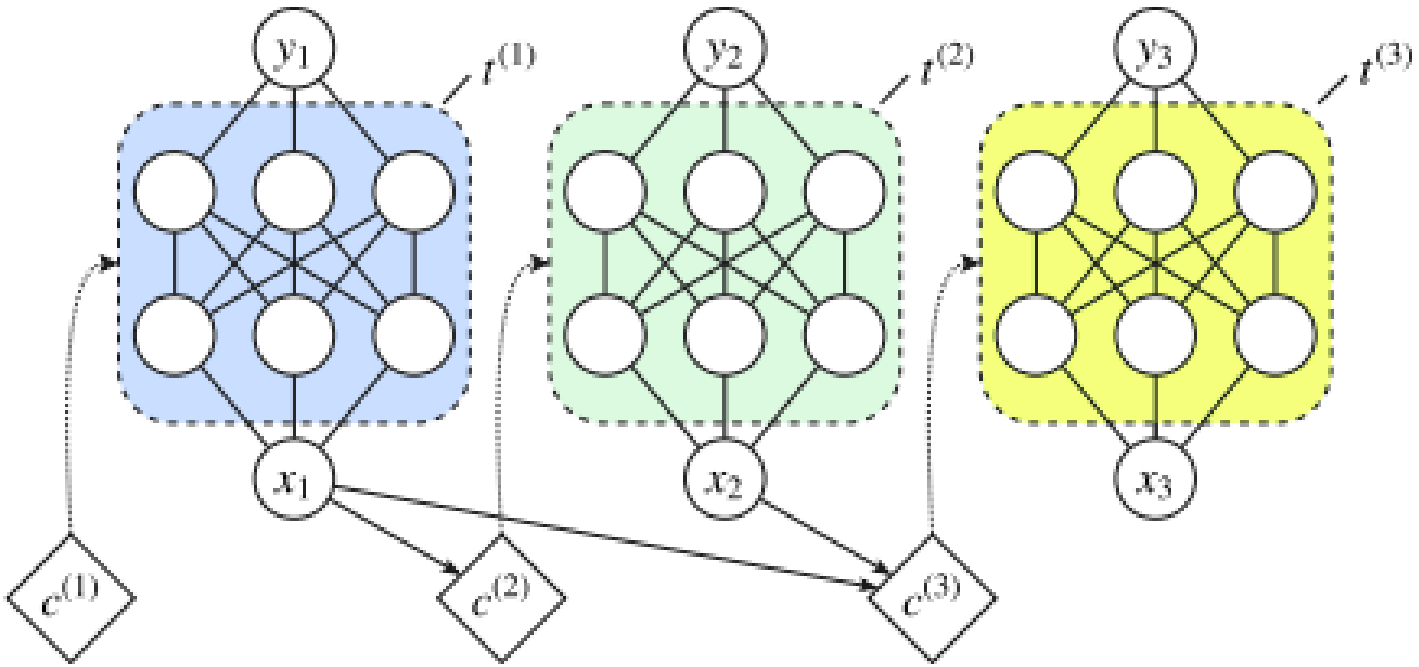
Neural Autoregressive Flow

- Two requirements for transformer τ
  - must be invertible as a function of x_t
  - $\frac{dy_t}{dx_t}$ must be cheap to compute.
- In IAF, τ is affine, trivially invertible. In NAF, τ is a neural network.

$$\tau(c(x_{1:t-1}), x_t) = DNN(x_t; \phi = c(x_{1:t-1})) \tag{27}$$

- where ϕ are the **pseudo-parameters**

Architecture of NAF



(a) NAF: each $c^{(i)}$ is a neural network that predicts pseudo-parameters for $t^{(i)}$, which in turns processes x_i.

Figure: Block Diagram of NAF Architecture.Here $t^{(i)}$ means $\tau^{(i)}$[4]

[4]Image Source : De Cao et al. (2019)

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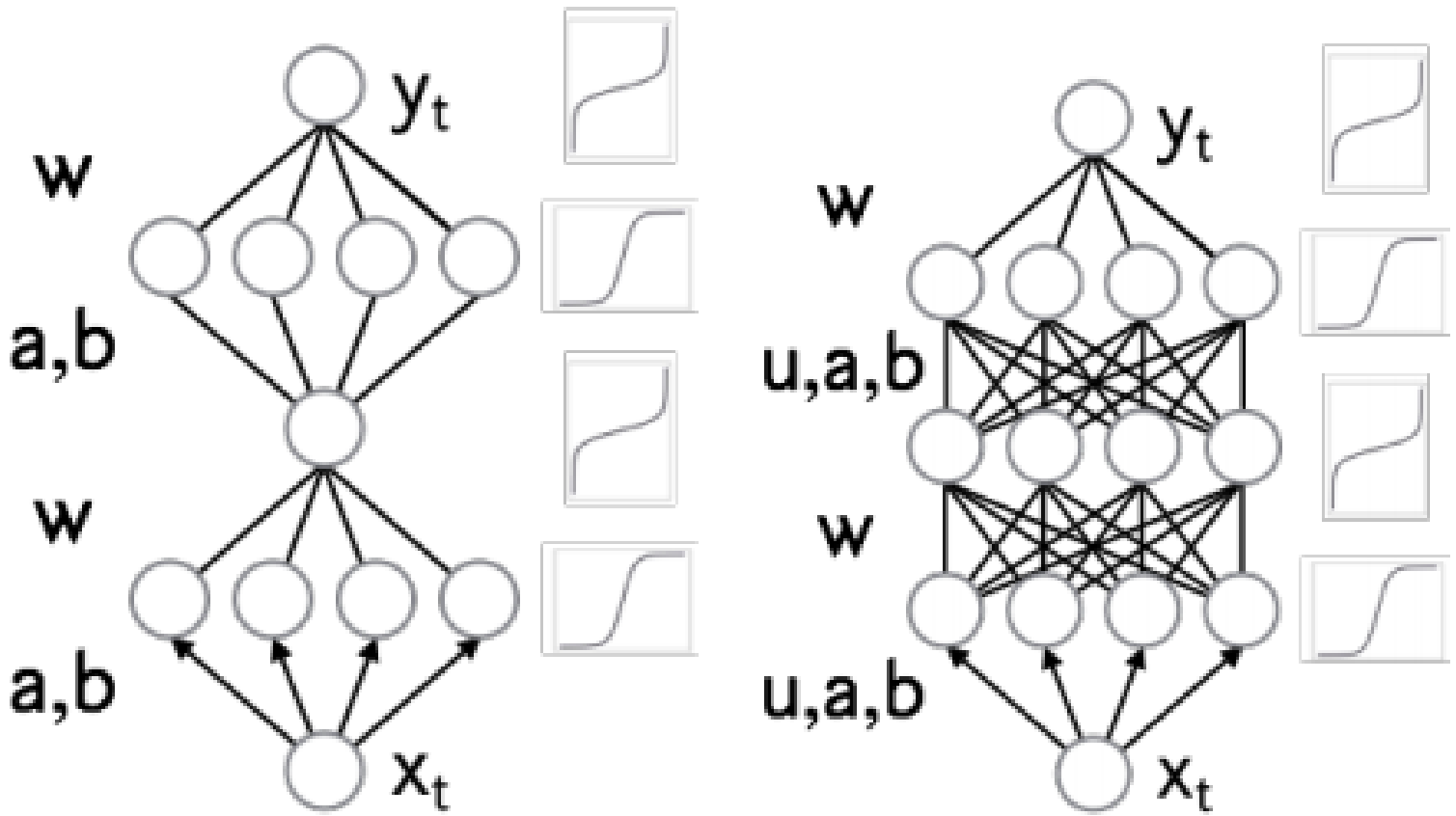

Figure: Proposed Transformer Networks (τ). **Left**: Deep Sigmoidal Flows(DSF). **Right**: Deep Dense Sigmoidal Flows(DDSF).[5]

[5] Image Source: Huang et al. (2018)

More on DSF and DDSF

- DSF:

$$y_t = \sigma^{-1}(\underbrace{w^T}_{1\times d} \cdot \sigma(\underbrace{a}_{d\times 1} \cdot \underbrace{x_t}_{1\times 1} + \underbrace{b}_{d\times 1})) \tag{28}$$

where $0 < w_{i,h} < 1, \sum_i w_{i,j} = 1$ and d denotes the number of hidden units.

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- DDSF :

$$h^{(l+1)} = \sigma^{-1}(\underbrace{w^{(l+1)}}_{d_{l+1}\times d_{l+1}} \cdot \sigma(\underbrace{a^{(l+1)}}_{d_{l+1}} \odot \underbrace{u^{(l+1)}}_{d_{l+1}\times d_l} \cdot \underbrace{h^{(l)}}_{d_l} + \underbrace{b^{(l+1)}}_{d_{l+1}})) \tag{29}$$

for $1 < l < L$, $h_0 = x$ and $y = h_L; d_0 = d_L = 1$; $\mathbf{w}$ and $\mathbf{u}$ are softmax-weighted.

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for $1 < l < L$, $h_0 = x$ and $y = h_L$;$d_0 = d_L = 1$; **w** and **u** are softmax-weighted.

- Log-determinant of the Jacobian:

$$\nabla_x y = \left[\nabla_{h^{(L-1)}} h^{(L)}\right] \left[\nabla_{h^{(L-2)}} h^{(L-1)}\right], \cdots, \left[\nabla_{h^{(0)}} h^{(1)}\right] \tag{30}$$

Result

Figure: **Left**: Target Distribution, **Right**: Modeled by NAF.[6]
Resemblance of the distribution with any animal, living or extinct, is purely co-incidental.

[6] Image Source: https://medium.com/element-ai-research-lab/neural-autoregressive-flows-f164d6b8e462

Comparison with AAF(IAF)

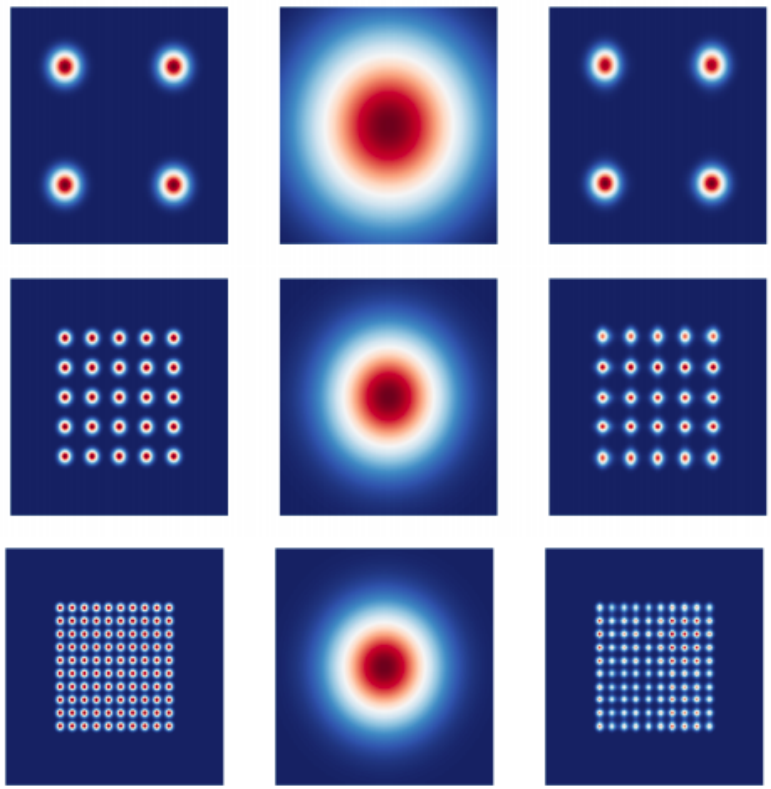

Figure: Fitting grid of Gaussian distributions using maximum likelihood. Left: true distribution. Center: AAF. Right: NAF[7]

[7] Image Source : Huang et al. (2018)

Detailed Comparison

Model	POWER	GAS	HEPMASS	MINIBOONE	BSDS300
MADE MoG	0.40 ± 0.01	8.47 ± 0.02	-15.15 ± 0.02	-12.27 ± 0.47	153.71 ± 0.28
MAF-affine (5)	0.14 ± 0.01	9.07 ± 0.02	-17.70 ± 0.02	-11.75 ± 0.44	155.69 ± 0.28
MAF-affine (10)	0.24 ± 0.01	10.08 ± 0.02	-17.73 ± 0.02	-12.24 ± 0.45	154.93 ± 0.28
MAF-affine MoG (5)	0.30 ± 0.01	9.59 ± 0.02	-17.39 ± 0.02	-11.68 ± 0.44	156.36 ± 0.28
TAN (various architectures)	0.48 ± 0.01	11.19 ± 0.02	-15.12 ± 0.02	-11.01 ± 0.48	157.03 ± 0.07
MAF-DDSF (5)	$\mathbf{0.62 \pm 0.01}$	11.91 ± 0.13	$\mathbf{-15.09 \pm 0.40}$	$\mathbf{-8.86 \pm 0.15}$	$\mathbf{157.73 \pm 0.04}$
MAF-DDSF (10)	0.60 ± 0.02	$\mathbf{11.96 \pm 0.33}$	-15.32 ± 0.23	-9.01 ± 0.01	157.43 ± 0.30
MAF-DDSF (5) valid	0.63 ± 0.01	11.91 ± 0.13	15.10 ± 0.42	-8.38 ± 0.13	172.89 ± 0.04
MAF-DDSF (10) valid	0.60 ± 0.02	11.95 ± 0.33	15.34 ± 0.24	-8.50 ± 0.03	172.58 ± 0.32

Figure: Test log-likelihood and error bars of 2 standard deviations on the 5 datasets.[8]

[8] Table taken from : https://medium.com/element-ai-research-lab/neural-autoregressive-flows-f164d6b8e462

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Rezende, D. J. and Mohamed, S. (2015). Variational inference with normalizing flows. *arXiv preprint arXiv:1505.05770*.

Acknowledgements

Slides made with help from the following blogs :

- https://lilianweng.github.io/lil-log/2018/10/13/flow-based-deep-generative-models.html
- http://akosiorek.github.io/ml/2018/04/03/norm_flows.html
- https://medium.com/element-ai-research-lab/neural-autoregressive-flows-f164d6b8e462
- https://www.ritchievink.com/

Thank you

Appendix

- Derivation of the variational free enery :

$$
\begin{aligned}
F(x) &= D_{KL}(Q(z)||P(z)) - E_{z\sim Q}[\log P(x|z)] && (31)\\
&= \int_z Q(z) \log \frac{Q(z)}{P(z)} dz - E_{z\sim Q}[\log P(x|z)] && (32)\\
&= E_{z\sim Q}[\log \frac{Q(z)}{P(z)}] - E_{z\sim Q}[\log P(x|z)] && (33)\\
&= E_{z\sim Q}[\log \frac{Q(z)}{P(z)} - \log P(x|z)] && (34)\\
&= E_{z\sim Q}[\log Q(z) - \log P(z) - \log P(x|z)] && (35)\\
&= E_{z\sim Q}[\log Q(z) - (\log P(z) + \log P(x|z))] && (36)\\
&= E_{z\sim Q}[\log Q(z) - \log P(x,z))] && (37)
\end{aligned}
$$