

UNIVERSITY OF LIÈGE  
Faculty of Applied Sciences  
Department of Electrical Engineering & Computer Science

PhD dissertation

---

# CONTRIBUTIONS TO DEEP GENERATIVE MODELING

FROM BLACK-BOX TO HYBRID APPROACHES

---

by ANTOINE WEHENKEL



Advisor: Prof. GILLES LOUPPE  
August 2022



## JURY MEMBERS

---

???, Professor at the Université de Liège (President);

GILLES LOUPPE, Professor at the Université de Liège (Advisor);

???, Professor at the Université de Liège;

???, ???;

???, ???;

???, ???;



## ABSTRACT

---

To be completed.



## ACKNOWLEDGMENTS

---

To be completed.





## CONTENTS

---

1	INTRODUCTION	1
1.1	Outline and contributions . . . . .	1
1.2	Publications . . . . .	1
2	BACKGROUND	3
2.1	Unsupervised learning . . . . .	3
i	BLACK-BOX GENERATIVE MODELING	5
3	DEEP LATENT VARIABLES GENERATIVE MODELS	7
3.1	Variational Auto Encoders . . . . .	7
3.2	Diffusion Models . . . . .	7
3.3	Contribution: <i>Diffusion Priors in Variational Autoencoders</i>	7
4	UNSTRUCTURED DENSITY ESTIMATION WITH NORMAL- IZING FLOWS	9
4.1	Normalizing Flows . . . . .	9
4.2	Contribution: <i>You say Normalizing Flows I see Bayesian Networks</i> . . . . .	9
4.3	Contribution: <i>Unconstrained Monotonic Neural Networks</i>	9
5	DIGRESSION ON MONOTONIC FUNCTIONS IN MACHINE LEARNING	11
ii	HYBRID GENERATIVE MODELING	13
6	STRUCTURED DENSITY ESTIMATION WITH NORMALIZ- ING FLOWS	15
6.1	Contribution: <i>Graphical normalizing flows</i> . . . . .	15
7	HYBRID GENERATIVE MODELS	17
7.1	Contribution: <i>Robust Hybrid Learning With Expert Aug- mentation</i> . . . . .	17
iii	APPENDIX	19
A	NOTATIONS	21
B	REFERENCES	25



# INTRODUCTION

---

If you erase this you are almost there! :D

## 1.1 OUTLINE AND CONTRIBUTIONS

If you erase this you are almost there! :D

## 1.2 PUBLICATIONS

To be completed.



## BACKGROUND

---

### OUTLINE

This chapter concerns the definition of unsupervised learning with a brief review of classical methods. Graphical models (in particular B-net are introduced here.) It continues with a review of deep generative modeling, with a discussion between explicit and implicit generative modeling. We introduce the concepts of GANs, VAEs, Normalizing Flows and diffusion models. With a note that VAEs and diffusions models are discussed in more details in further chapters.

### 2.1 UNSUPERVISED LEARNING



## Part I

### BLACK-BOX GENERATIVE MODELING





## DEEP LATENT VARIABLES GENERATIVE MODELS

---

### OUTLINE ???

3.1 VARIATIONAL AUTO ENCODERS

3.2 DIFFUSION MODELS

3.3 CONTRIBUTION: *diffusion priors in variational autoencoders*



## UNSTRUCTURED DENSITY ESTIMATION WITH NORMALIZING FLOWS

---

### OUTLINE

???

4.1 NORMALIZING FLOWS

4.2 CONTRIBUTION: *you say normalizing flows i see bayesian networks*

4.3 CONTRIBUTION: *unconstrained monotonic neural networks*



# 5

## DIGRESSION ON MONOTONIC FUNCTIONS IN MACHINE LEARNING

---

OUTLINE

???



## Part II

### HYBRID GENERATIVE MODELING





## STRUCTURED DENSITY ESTIMATION WITH NORMALIZING FLOWS

---

### OUTLINE

???

#### 6.1 CONTRIBUTION: *graphical normalizing flows*



## HYBRID GENERATIVE MODELS

---

### OUTLINE ???

#### 7.1 CONTRIBUTION: *robust hybrid learning with expert augmentation*



### Part III

## APPENDIX



## NOTATIONS

---

$\mathcal{A}$	A supervised learning algorithm .....??
$\mathcal{A}(\theta, \mathcal{L})$	The model $\varphi_{\mathcal{L}}$ produced by algorithm $\mathcal{A}$ over $\mathcal{L}$ and hyper-parameters $\theta$ .....??
$\alpha_s$	The proportion of samples in a random patch ....??
$\alpha_f$	The proportion of features in a random patch ....??
$b_l$	The $l$ -th value of a categorical variable .....??
$B$	A subset $B \subseteq V$ of variables .....??
$c_k$	The $k$ -th class .....??
$C_p^k$	The number of $k$ -combinations from a set of $p$ elements .....??
$C(N)$	The time complexity for splitting $N$ samples .....??
$\mathbb{E}$	Expectation .....??
$\bar{E}(\varphi_{\mathcal{L}}, \mathcal{L}')$	The average prediction error of $\varphi_{\mathcal{L}}$ over $\mathcal{L}'$ .....??
$\text{Err}(\varphi_{\mathcal{L}})$	The generalization error of $\varphi_{\mathcal{L}}$ .....??, ??
$H(X)$	The Shannon entropy of $X$ .....??
$H(X Y)$	The Shannon entropy of $X$ conditional to $Y$ .....??
$\mathcal{H}$	The space of candidate models .....??
$i(t)$	The impurity of node $t$ .....??, ??
$i_R(t)$	The impurity of node $t$ based on the local resubstitution estimate .....??, ??
$i_H(t)$	The entropy impurity of node $t$ .....??
$i_G(t)$	The Gini impurity of node $t$ .....??
$\Delta i(s, t)$	The impurity decrease of the split $s$ at node $t$ .....??
$I(X; Y)$	The mutual information between $X$ and $Y$ .....??
$\text{Imp}(X_j)$	The variable importance of $X_j$ .....??, ??
$J$	The number of classes .....??
$K$	The number of folds in cross-validation .....?? The number of input variables drawn at each node for finding a split .....??
$K(\mathbf{x}_i, \mathbf{x}_j)$	The kernel of $\mathbf{x}_i$ and $\mathbf{x}_j$ .....??, ??
$L$	A loss function .....?? The number of values of a categorical variable ....??
$\mathcal{L}$	A learning set $(\mathbf{X}, \mathbf{y})$ .....??
$\mathcal{L}^m$	The $m$ -th bootstrap replicate of $\mathcal{L}$ .....??

$\mathcal{L}_t$	The subset of node samples falling into node $t$ ... ??
$M$	The number of base models in an ensemble ..... ??
$\mu_{\mathcal{L}, \theta_m}(\mathbf{x})$	The mean prediction at $X = \mathbf{x}$ of $\varphi_{\mathcal{L}, \theta_m}$ ..... ??
$N$	The number of input samples ..... ??
$N_t$	The number of node samples in node $t$ ..... ??
$N_{ct}$	The number of node samples of class $c$ in node $t$ .. ??
$\Omega$	The universe, or population, from which cases are sampled ..... ??
$p$	The number of input variables ..... ??
$p_L$	The proportion of node samples going to $t_L$ ..... ??
$p_R$	The proportion of node samples going to $t_R$ ..... ??
$p(t)$	The estimated probability $p(X \in \mathcal{X}_t) = \frac{N_t}{N}$ ..... ??
$p(c t)$	The empirical probability estimate $p(Y = c X \in \mathcal{X}_t) = \frac{N_{ct}}{N_t}$ of class $c$ at node $t$ ..... ??
$\hat{p}_{\mathcal{L}}$	An empirical probability estimate computed from the learning set $\mathcal{L}$ ..... ??
$P(X, Y)$	The joint probability distribution of the input variables $X = (X_1, \dots, X_p)$ and the output variable $Y$ .. ??
$\mathcal{P}_k(V)$	The set of subsets of $V$ of size $k$ ..... ??
$\varphi$	A model or function $\mathcal{X} \mapsto \mathcal{Y}$ ..... ?? A single decision tree ..... ??
$\tilde{\varphi}$	The set of terminal nodes in $\varphi$ ..... ??
$\varphi(\mathbf{x})$	The prediction of $\varphi$ for the sample $\mathbf{x}$ ..... ??
$\varphi_{\mathcal{L}}$	A model built from $\mathcal{L}$ ..... ??
$\varphi_{\mathcal{L}, \theta}$	A model built from $\mathcal{L}$ with random seed $\theta$ ..... ??
$\varphi_B$	A Bayes model ..... ??
$\psi_{\mathcal{L}, \theta_1, \dots, \theta_M}$	An ensemble of $M$ models built from $\mathcal{L}$ and random seeds $\theta_1, \dots, \theta_M$ ..... ??
$\mathcal{Q}$	A set $\mathcal{Q} \subseteq \mathcal{S}$ of splits of restricted structure .... ??, ??
$\mathcal{Q}(X_j)$	The set $\mathcal{Q}(X_j) \subseteq \mathcal{Q}$ of univariate binary splits that can be defined on variable $X_j$ ..... ??, ??
$\rho(\mathbf{x})$	The correlation coefficient between the predictions at $X = \mathbf{x}$ of two randomized models ..... ??
$s$	A split ..... ??, ??
$s^*$	The best split ..... ??, ??
$s_j^*$	The best binary split defined on variable $X_j$ .... ??, ??
$s_j^v$	The binary split $(\{\mathbf{x}   x_j \leq v\}, \{\mathbf{x} > v\})$ defined on variable $X_j$ with discretization threshold $v$ ..... ??
$s_t$	The split labeling node $t$ ..... ??
$\tilde{s}_t^j$	The best surrogate split for $s_t$ defined from $X_j$ ... ??



$\mathcal{S}$	The set of all possible splits $s$ .....??
$\sigma_{\mathcal{L}, \theta_m}^2(\mathbf{x})$	The prediction variance at $X = \mathbf{x}$ of $\varphi_{\mathcal{L}, \theta_m}$ .....??
$t$	A node in a decision tree .....??
$t_L$	The left child of node $t$ .....??, ??
$t_R$	The right child of node $t$ .....??, ??
$\theta$	A vector of hyper-parameter values .....?? A random seed .....??
$\theta^*$	The optimal hyper-parameters .....??
$\hat{\theta}^*$	The approximately optimal hyper-parameters ....??
$\theta_m$	The seed of the $m$ -th model in an ensemble .....??
$v$	A discretization threshold in a binary split .....??
$v_k$	The $k$ -th value of an ordered variable, when node samples are in sorted order .....??
$v'_k$	The mid-cut point between $v_k$ and $v_{k+1}$ .....??
$V$	The set $\{X_1, \dots, X_p\}$ of input variables .....??
$V^{-j}$	$V \setminus \{X_j\}$ .....??
$\mathbb{V}$	Variance .....??
$\mathbf{x}$	A case, sample or input vector $(x_1, \dots, x_p)$ .....??
$\mathbf{x}_i$	The $i$ -th input sample in $\mathcal{L}$ .....??
$x_j$	The value of variable $X_j$ for the sample $\mathbf{x}$ .....??
$\mathbf{X}$	The $N \times p$ matrix representing the values of all $N$ samples for all $p$ input variables .....??
$X_j$	The $j$ -th input variable or feature .....??, ??
$X$	The random vector $(X_1, \dots, X_p)$ .....??
$\mathcal{X}_j$	The domain or space of variable $X_j$ .....??
$\mathcal{X}$	The input space $\mathcal{X}_1 \times \dots \times \mathcal{X}_p$ .....??
$\mathcal{X}_t$	The subspace $\mathcal{X}_t \subseteq \mathcal{X}$ represented by node $t$ .....??
$y$	A value of the output variable $Y$ .....??
$\hat{y}_t$	The value labelling node $t$ .....??
$\hat{y}_t^*$	The optimal value labelling node $t$ .....??
$\mathbf{y}$	The output values $(y_1, \dots, y_N)$ .....??
$Y$	The output or response variable $Y$ .....??
$\mathcal{Y}$	The domain or space of variable $Y$ .....??



REFERENCES

---