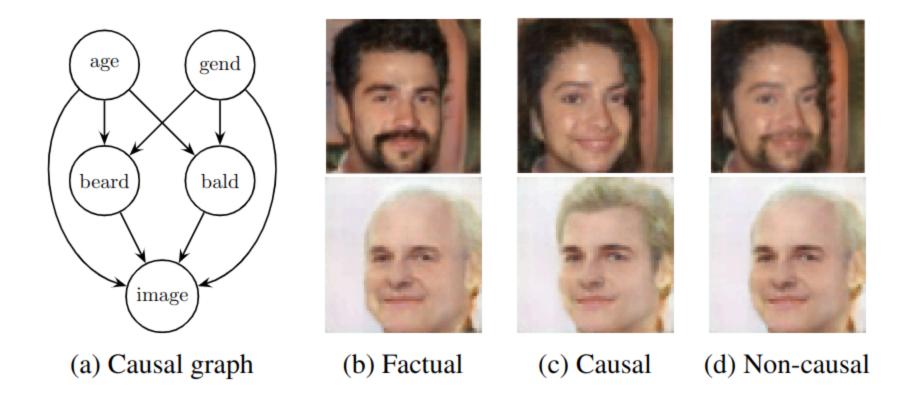
# **Benchmarking Counterfactual Image Generation**

**Thomas Melistas** 

### **Overview**

- Background
  - What is Counterfactual Image Generation?
  - Methods and Models
- Evaluation Metrics
- Benchmarking Setup
- Results

# **Counterfactual Image Generation**



### **Structural Causal Models**

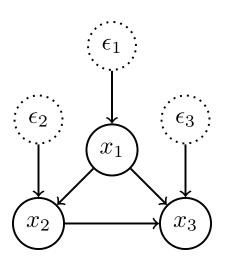
An SCM  $\mathcal{G}:=(\mathbf{S},p(oldsymbol{\epsilon}))$  consists of:

- (i) structural assignments  $\mathbf{S} = \{f_i\}_{i=1}^N$ , s.t.  $x_i := f_i(\epsilon_i, \mathbf{pa}_i)$ ,
- (ii) a joint distribution  $p(m{\epsilon}) = \prod_{i=1}^N p(\epsilon_i)$  over mutually independent noise variables

 $x_i$ : an **endogenous** variable (observed)

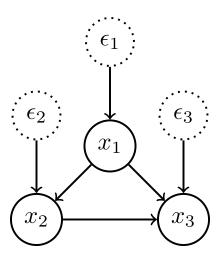
 $\mathbf{pa}_i$ : the parents of  $x_i$  (its direct *causes*, endogenous)

 $\epsilon_i$ : an **exogenous** variable (unobserved)



### **Structural Causal Models**

- Causal relations → directed acyclic graph (DAG)
- ullet Acyclic o solve recursively for  $x_i$  and obtain  $\mathbf{x} = \mathbf{f}(oldsymbol{\epsilon})$
- $\mathbf{x}$ : a collection of observable variables, where  $x_i$ : image and  $\mathbf{pa}_i$ : image attributes



### **Interventions and Counterfactuals**

- Interventional distributions  $P(x_j|do(x_i=y))$ :
  - $\circ$  interventions:  $x_i = f_i(\epsilon_i, \mathbf{pa}_i) o x_i = y$
  - $\circ$  exogenous noise is sampled from the prior  $P(oldsymbol{\epsilon})$
- Counterfactual distributions  $P(x_{j,x_i=y}|\mathbf{x})$ :
  - o interventions: as above
  - $\circ$  exogenous noise same with the observation  $P(oldsymbol{\epsilon}|\mathbf{x})$

### **Interventions and Counterfactuals**

Layer	Activity	Semantics	Example
(1) Associational $p(y \mid x)$	Seeing ••	How would seeing $x$ change my belief in $Y$ ?	What does a symptom tell us about the disease?
(2) Interventional $p(y \mid do(x), z)$	Doing 🢪	What happens to $Y$ if I do $x$ ?	What if I take aspirin, will my headache be cured?
(3) Counterfactual Imaginin $p(y_{x'} \mid x, y)$		Was it $x$ that caused $Y$ ?	Was it the aspirin that stopped my headache?

### **Abduction-Action-Prediction**

Counterfactuals using SCMs are computed in three steps:

- (i) **Abduction**: Infer  $P(\epsilon|\mathbf{x})$ , the state of the world (exogenous noise) that is compatible with the observation  $\mathbf{x}$ .
- (ii) **Action**: Replace the structural equations  $do(x_i=y)$ , resulting in a modified SCM

$$\widetilde{\mathcal{G}} := \mathcal{G}_{\mathbf{x}; do(x_i = y)} = (\widetilde{\mathbf{S}}, P(oldsymbol{\epsilon} | \mathbf{x})).$$

(iii) **Prediction**: Use the modified model to compute  $P_{\widetilde{\mathcal{G}}}(\mathbf{x})$ .

### **Using Neural Networks for Abduction**

Three categories of mechanisms:

- (i) **Invertible**, **explicit**: Conditional Normalising Flows  $\rightarrow$  attributes
- (ii) **Amortised, explicit**: Conditional VAEs or Hierarchical VAEs o image
- (iii) **Amortised, implicit**: Conditional GANs  $\rightarrow$  image

# Invertible, explicit

- Normalising flows perform mappings between probability densities
- A series of invertible transformations
- For an attribute  $x_i$  we utilise a conditional NF  $f(\epsilon_i; \mathbf{pa}_i)$  which is invertible:  $\epsilon_i = f^{-1}(x_i; \mathbf{pa}_i)$

$$P(x_i|\mathbf{pa}_i) = p(\epsilon_i) |\mathrm{det}\, 
abla_{\epsilon_i} f(\epsilon_i;\mathbf{pa}_i)|^{-1}$$

### Amortised, explicit (with VAE)

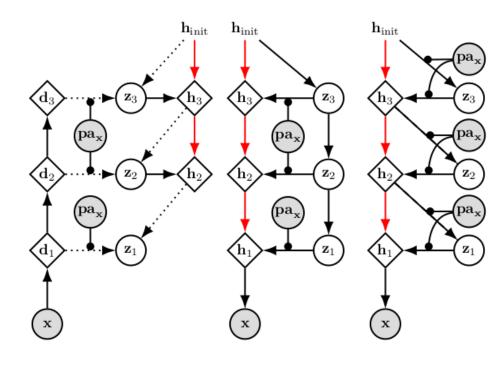
- Encoder:  $q_\phi(z|x,pa_x)$  and Decoder:  $p_\theta(x|z,pa_x)$ , trained with:  $ext{ELBO}_\beta(\phi,\theta) = \mathbb{E}_{z\sim q_\phi(z|x,pa_x)}[p_\theta(x|z,pa_x)] \beta D_{KL}[q_\phi(z|x,pa_x)||p(z)]$
- $\bullet$  The above likelihood and posterior are diagonal gaussians, whose  $\mu$  and  $\sigma$  we predict with neural networks
- ullet Prior  $p(z) \sim N(0,I)$ .

### Amortised, explicit (with VAE)

- ullet Noise  $\epsilon$  is decomposed into  $z \sim q_\phi(z|x,pa_x)$  and  $u \sim N(0,I)$
- To perform counterfactual inference:
  - $\circ$  We sample the latent  $z = \mu_\phi(x,pa_x) + \sigma_\phi(x,pa_x) * i$ ,  $i \sim N(0,I)$
  - $\circ$  We sample the counterfactual  $x^*=\mu_ heta(z,pa_x^*)+\sigma_ heta(z,pa_x^*)*u,$  where  $u=rac{x-\mu_ heta(z,pa_x)}{\sigma_ heta(z,pa_x)}$

# Amortised, explicit (HVAE)

- ullet We have L layers of hierarchical latent variables  $oldsymbol{z} = \{z_1, z_2, \dots, z_L\}$
- $egin{align} oldsymbol{\cdot} h_i &= h_{i+1} + f_\omega^i(z_i, pa_x) \ z_i &\sim p_ heta(z_i|z_{>i}), \ p_ heta(x|z_{1:L}, pa_x) &= N(x|\mu_ heta(h_1), \sigma_ heta(h1)) \ \end{matrix}$
- $egin{aligned} ullet q_{\phi}(z_{1:L}|x,pa_x) &= q_{\phi}(z_L|x,pa_x) \ q_{\phi}(z_{L-1}|z_L,x,pa_x) \ldots q_{\phi}(z_1|z_{i>1},x,pa_x) \end{aligned}$



# Amortised, implicit

- ullet Encoder E:  $z_x=E(x,pa_x)$
- ullet Generator G:  $x'=G(z',pa_x)$ , where  $z'\sim N(0,I)$  or  $z'=z_x$
- Discriminator  $D(x', z', pa_x)$ : generated  $\rightarrow$  fake, data  $\rightarrow$  real

$$\min_{E,G}\max_{D}V(D,G,E)=\mathbb{E}_{q(x)p(pa_x)}[log(D(x,E(x,pa_x),pa_x))]+\mathbb{E}_{p(z)p(pa_x)}[log(1-D(G(z,pa_x),z,pa_x))]$$

#### Finetuning the encoder:

$$egin{align} L_x &= \mathbb{E}_{x\sim q(x)} \|x - G(E(x,pa_x),pa_x)\|_2 \ L_z &= \mathbb{E}_{z\sim p(z)} \|z - E(G(z,pa_x),pa_x)\| \ \end{aligned}$$

#### To produce counterfactuals:

$$x^st = G(E(x,pa_x),pa_x^st))$$

Dumoulin et al, Adversarially learned inference. 2017

### **Metrics**

We use 4 metrics to evaluate the generated counterfactuals

- Composition
- Effectiveness
- Realism (FID)
- Minimality (CLD)

# Composition

- Conceptually: the image and its attributes do not change without intervention
- ullet If we force a variable X to a value x it would have without the intervention, it should have no effect on the other variables
- ullet Therefore, a *null-intervention* applied m times:  $f_\emptyset^m$  should change no variable
- composition  $^m(x,pa_x)=d(x,f_\emptyset^m(x,pa_x))$ , where d(.,.) is a suitable distance metric

### **Effectiveness**

- Conceptually: how successful was the performed intervention
- ullet If we force a variable X to have the value x, then X will take on the value x
- ullet We train an anti-causal predictor  $g_{ heta}^i$  on observations, for each  $pa_x^i$
- effectiveness  $_i(x^*,pa^*{}_x^i)=d(g^i_\theta(x^*),pa^*{}_x^i)$ , where  $d(.\,,.\,)$ : classification metric for categorical variables, regression for continuous

# **Fréchet Inception Distance (FID)**

- Conceptually: Counterfactual image quality
- Measures the similarity of counterfactual images to observational data
- We use Inception-v3 trained on ImageNet to extract features
- Defined as:

$$d^2((m_q,C_q),(m_p,C_p)) = ||m_q-m_p||_2^2 + \mathrm{Tr}(C_q+C_p-2(C_qC_p)^{rac{1}{2}})|_2^2$$

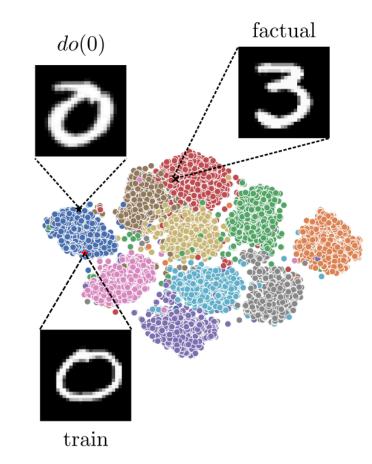
where q: counterfactual features distribution, p: factual features distribution Fréchet distance d is defined as the distance between the Gaussian with mean  $(m_q, C_q)$  obtained from q and the Gaussian with mean  $(m_p, C_p)$  obtained from p.

# **Counterfactual Latent Divergence (CLD)**

- Conceptually: Counterfactual only differs in the intervened parent attribute
- Formally:

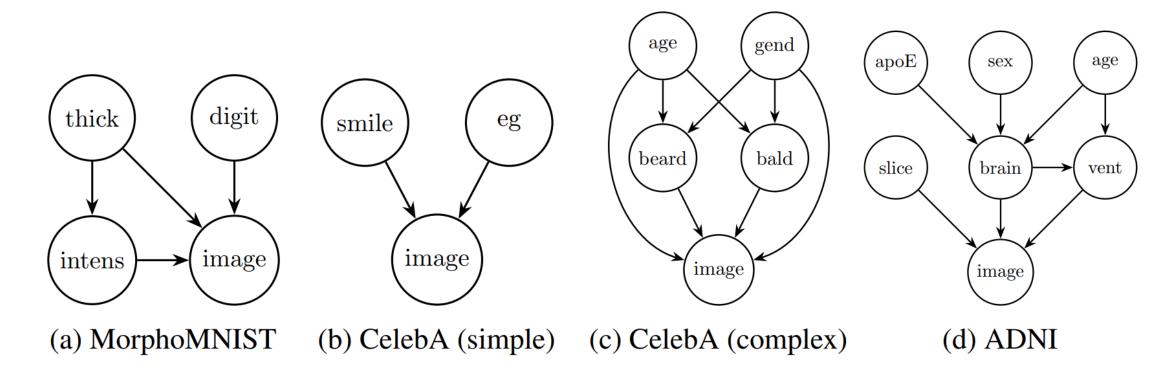
$$ext{CLD} = \log(w_1 \exp P(S_{x^*} \leq div) + w_2 \exp P(S_x \geq div))$$
 ,where:  $div = d(x,x*)$  ,  $S_x = \{d(x,x')|pa_{x'} = pa_x\}$  ,  $S_{x^*} = \{d(x,x')|pa_{x'} = pa_{x^*}\}$ 

•  $d(.\,,.\,)$ : KL-divergence between the latents given by an unconditional VAE

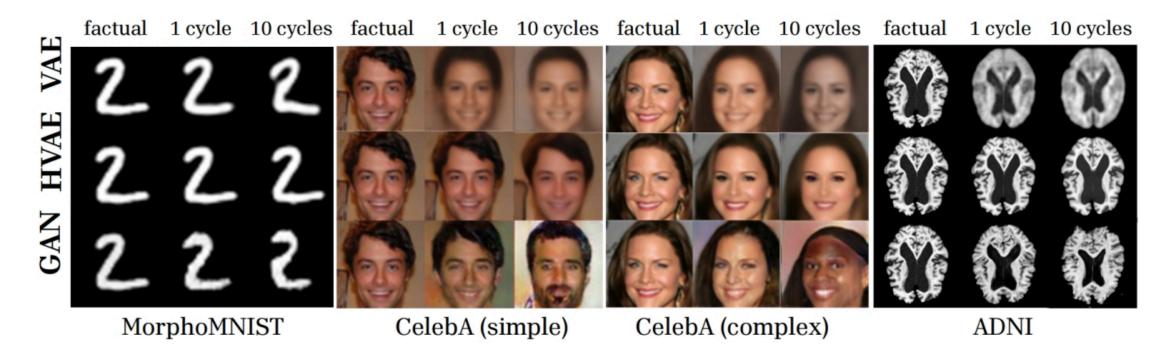


### **Datasets used for benchmarking**

- MorphoMNIST: Synthetic dataset of digits (32  $\times$  32)
- CelebA: Human faces (64  $\times$  64)  $\rightarrow$  simple & complex causal graph
- **ADNI**: 2D slices of brain MRIs (192  $\times$  192)



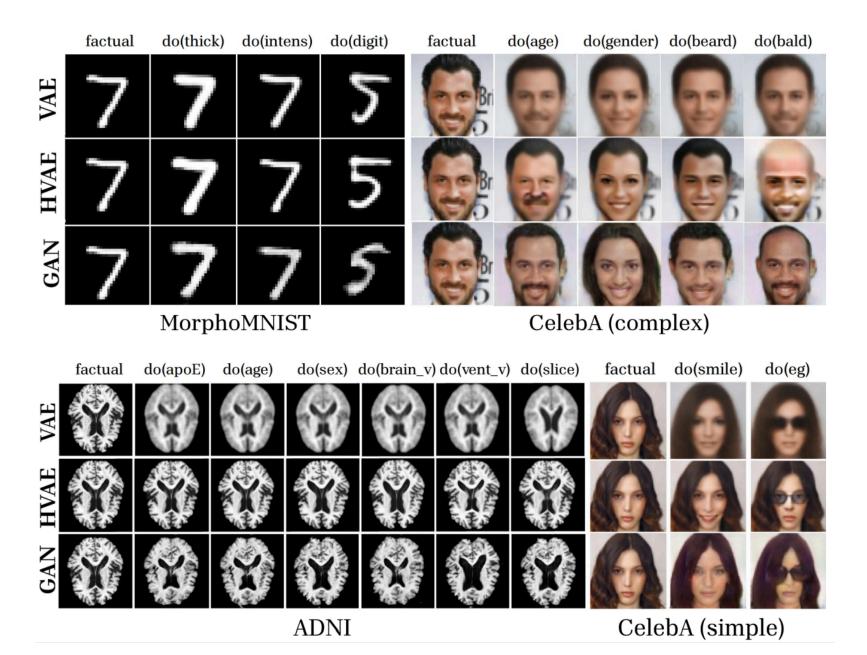
# Composition



# Composition

	$\overline{l_1}$ image	space \	LPI	PS↓						
Model	1 cycle 10 cycles		1 cycle	10 cycles						
	MorphoMNIST									
VAE	$2.600_{1.454}$	$7.698_{4.199}$	$0.026_{0.003}$	$0.075_{0.003}$						
HVAE	$0.438_{0.178}$	$1.550_{0.541}$	$0.006_{0.001}$	$0.024_{0.003}$						
GAN	$3.807_{1.822}$	$11.697_{5.750}$	$0.049_{0.004}$	$0.184_{0.008}$						
	CelebA (simple/complex)									
VAE	$127.8_{18.1}/\mathbf{121.2_{13.2}}$	$123.4_{22.1}/127.9_{21.1}$	$0.295_{0.004}/0.282_{0.061}$	$0.424_{0.005}/0.412_{0.091}$						
HVAE	$129.4_{11.6}/122.7_{10.4}$	$138.8_{23.4}/\mathbf{124.6_{16.4}}$	$0.063_{0.003}/0.122_{0.033}$	$0.200_{0.008}/0.240_{0.053}$						
GAN	$115.3_{22.0}/127.6_{17.3}$	$128.4_{21.4}/131.8_{23.3}$	$0.290_{0.003}/0.276_{0.074}$	$0.462_{0.005}/0.490_{0.121}$						
	ADNI									
VAE	$18.882_{1.786}$	$30.250_{3.389}$	$0.306_{0.008}$	$0.384_{0.006}$						
HVAE	$3.384_{0.367}$	$\bf 7.456_{0.622}$	$\mathbf{0.101_{0.012}}$	$0.156_{0.014}$						
GAN	$24.261_{1.821}$	$32.794_{3.578}$	$0.268_{0.009}$	$0.323_{0.007}$						

# **Qualitative Results**



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# **Effectiveness**

	Thickness (t) MAE ↓			Intensity (i) MAE ↓			Digit (y) Acc. ↑		
Model	do(t)	do(i)	do(y)	do(t)	do(i)	do(y)	do(t)	do(i)	do(y)
VAE	$0.109_{0.01}$	$0.333_{0.02}$	$0.139_{0.01}$	$3.15_{0.26}$	$5.33_{0.29}$	$4.64_{0.35}$	$0.989_{0.01}$	$0.988_{0.01}$	$0.775_{0.02}$
HVAE	$0.086_{0.09}$	$0.224_{0.03}$	$\mid 0.117_{0.01} \mid$	$1.99_{0.18}$	$3.52_{0.26}$	$2.10_{0.17}$	$0.985_{0.01}$	$0.935_{0.02}$	$0.972_{0.02}$
GAN	$0.228_{0.01}$	$0.680_{0.02}$	$0.393_{0.02}$	$9.43_{0.59}$	$15.14_{0.99}$	$12.39_{0.57}$	$0.961_{0.02}$	$0.966_{0.01}$	$0.451_{0.024}$

	CelebA (simple)											
Model		Smiling	(s) F1 ↑		Eyeglasses (e) F1 ↑							
	do(s)		do(e)		do(s)		do(e)					
VAE		$7_{0.02}$	$0.987_{0.01}$		$0.938_{0.05}$		$0.810_{0.02}$					
HVAE		$8_{0.01}$	$0.997_{0.01}$		$0.883_{0.06}$		$0.981_{0.02}$					
GAN	0.81	$9_{0.02}$	$0.873_{0.01}$		$0.957_{0.03}$		0.89	$1_{0.01}$				
	CelebA (complex)											
		Age (a	a) F1 ↑		Gender (g) F1 ↑							
	do(a)	do(g)	do(br)	do(bl)	do(a)	do(g)	do(br)	do(bl)				
VAE	$0.35_{0.04}$	$0.782_{0.02}$	$0.816_{0.02}$	$0.819_{0.02}$	$0.977_{0.01}$	$0.909_{0.02}$	$0.959_{0.02}$	$0.973_{0.01}$				
HVAE	$\boldsymbol{0.654_{0.1}}$	$0.893_{0.04}$	$0.908_{0.03}$	$0.899_{0.03}$	$0.988_{0.02}$	$0.949_{0.03}$	$0.994_{0.01}$	$0.95_{0.03}$				
GAN	$0.413_{0.04}$	$0.71_{0.02}$	$0.818_{0.02}$	$0.799_{0.01}$	$0.952_{0.01}$	$0.982_{0.01}$	$0.92_{0.01}$	$0.961_{0.01}$				
		Beard (	br) F1 ↑		Bald (bl) F1 ↑							
	do(a)	do(g)	do(br)	do(bl)	do(a)	do(g)	do(br)	do(bl)				
VAE	$0.944_{0.01}$	$0.828_{0.03}$	$0.296_{0.05}$	$0.945_{0.02}$	$0.023_{0.03}$	$0.496_{0.05}$	$0.045_{0.04}$	$0.412_{0.03}$				
HVAE	$0.952_{0.03}$	$0.951_{0.03}$	$0.441_{0.11}$	$0.916_{0.04}$	$0.02_{0.05}$	$0.86_{0.05}$	$0.045_{0.07}$	$0.611_{0.04}$				
GAN	$0.908_{0.01}$	$0.838_{0.02}$	$0.233_{0.03}$	$0.907_{0.01}$	$0.021_{0.02}$	$0.82_{0.02}$	$0.055_{0.02}$	$0.492_{0.02}$				

	Brain volume (b) MAE ↓		Ventricular volume (v) MAE ↓			Slice (s) F1 ↑			
Model	do(b)	do(v)	do(s)	do(b)	do(v)	do(s)	do(b)	do(v)	do(s)
VAE	$0.17_{0.03}$	$0.15_{0.06}$	$0.15_{0.06}$	$0.08_{0.05}$	$0.20_{0.04}$	$0.08_{0.05}$	$0.52_{0.15}$	$0.48_{0.15}$	$0.46_{0.10}$
HVAE	$0.09_{0.03}$	$0.12_{0.06}$	$0.13_{0.06}$	$0.06_{0.04}$	$0.04_{0.01}$	$0.06_{0.04}$	$0.38_{0.15}$	$0.41_{0.16}$	$0.41_{0.11}$
GAN	$0.17_{0.02}$	$0.16_{0.07}$	$0.16_{0.06}$	$0.12_{0.02}$	$0.22_{0.03}$	$0.12_{0.03}$	$0.14_{0.03}$	$0.16_{0.03}$	$0.05_{0.02}$

# Realism (FID) & Minimality (CLD)

	MorphoMNIST		CelebA (simp	ADNI		
Model	FID↓	CLD↓	FID↓	CLD↓	FID ↓	CLD↓
VAE	10.124	0.268	66.412/59.393	0.301/ <b>0.299</b>	278.245	0.352
HVAE	5.362	0.272	<b>22.047</b> /35.712	<b>0.295</b> /0.305	74.696	0.347
GAN	35.568	0.286	31.560/ <b>27.861</b>	0.38/0.304	113.749	0.353

### **Conclusions**

- HVAE outperforms other models across metrics and datasets
- GAN counterfactuals more realistic than VAE but far from factuals for complex datasets
- Amortised implicit mechanisms → better abduction,
   but hierarchical latents are important

#### **Future Work**

- Extend to other
  - Generative models for the image mechanism (i.e. Diffusion Models)
  - Counterfactual paradigms (i.e. Deep Twin Networks, Backtracking Counterfactuals)
- Metrics
  - Limit bias of used model-dependent metrics (i.e. effectiveness, CLD)
  - Come up with new metrics

 $Thank \quad you \quad for \quad your \quad attention!!!$