Diffusion Causal Models for Counterfactual Estimation

Thomas Melistas

Sanchez, P., & Tsaftaris, S.A. (2022). Diffusion Causal Models for Counterfactual Estimation. CLEaR.

Overview

- What are counterfactuals?
- Introduction to Structural Causal Models
- Unifying Diffusion and SCMs
- Related Work

What are counterfactuals?

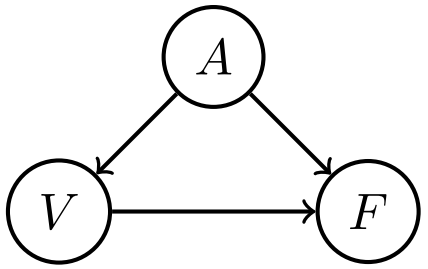
- Hypothetical scenarios
- Example: I got the vaccine and did not catch the flu, what is the probability I wouldn't catch the flu if I didn't get vaccinated?
- It cannot be computed straight away (I already got vaccinated)

Let's formalize this

Graphs as Joint Distribution Factorizations

- Represent Bayesian Networks as DAGs
- Encode conditional independence (Markovian)

$$p(a, v, f) = p(a)p(v|a)p(f|a, v)$$

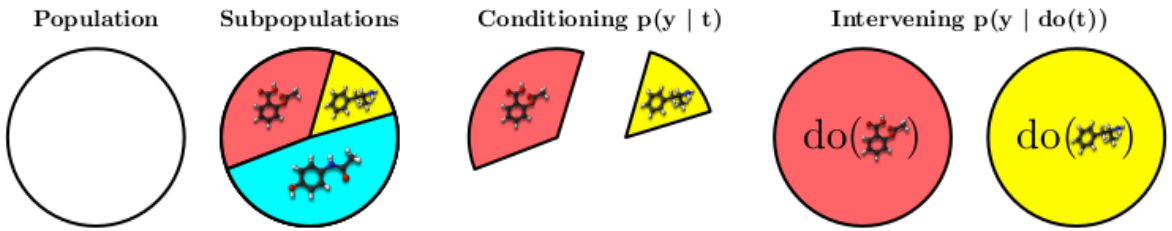


A: Age, V: Vaccination, F: Flu

Interventions

- Applying an action to a population $\rightarrow$ getting the vaccine
- We use the do-operator $do(V = v)$ or $do(v)$
- Different than conditioning: $p(f|do(v)) \neq p(f|v)$

$$p(a, f|do(v)) = p(a) \cancelto{1}{p(v|a)} p(f|a, v) \neq p(a, f|v)$$



Counterfactuals

What is the probability that I (27 years old) wouldn't get the flu if I didn't get the vaccine?

$p(f|do(v'), f, a)$?

- Conflict: first f is the hypothetical scenario and second f is the observed one
- We denote the first by $f_{v'}$:
  Counterfactual flu probability **under intervention** of no vaccination

$p(f|do(v'), a)$: How probable is flu **if** we don't vaccinate people
$p(f_{v'}|v, f, a)$: How probable the flu **would be** if I hadn't vaccinated

Pearl's Causal Hierarchy

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 $p(y \mid \mathrm{do}(x), z)$	Doing 💪	What happens to Y if I do x?	What if I take aspirin, will my headache be cured?
(3) Counterfactual $p(y_{x'} \mid x, y)$	Imagining 🤔	Was it x that caused Y?	Was it the aspirin that stopped my headache?

Pearl J. (2009). Causality

Structural Causal Models

- Extension of Bayesian Networks
- Causal relationships $\rightarrow$ Deterministic, functional equations
- Stochasticity $\rightarrow$ Some variables remain unobserved

Structural Causal Models

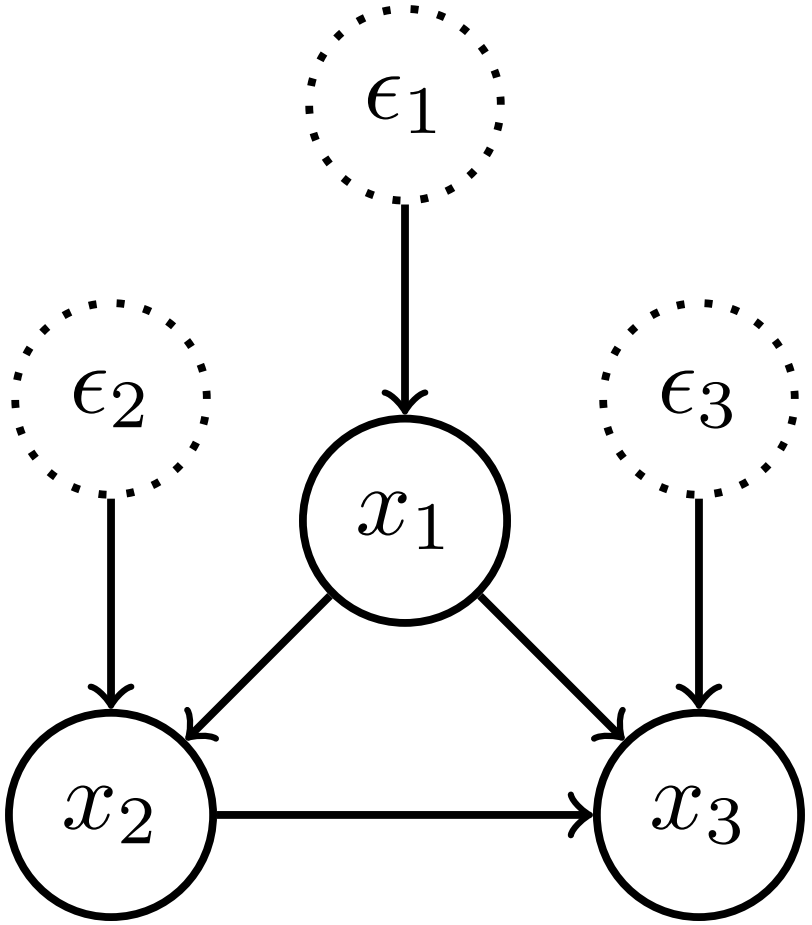
An SCM $\mathcal{M} := (\mathbf{S}, p(\boldsymbol{\epsilon}))$ consists of:

(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 $p(\boldsymbol{\epsilon}) = \prod_{i=1}^N p(\epsilon_i)$ over mutually independent noise variables

x_i: an **endogenous** variable (observed)
$\mathbf{pa}_i$: the parents of x_i (its direct *causes*, endogenous)
ϵ_i: an **exogenous** variable (unobserved)

Structural Causal Models

- In any SCM, each variable x_i is caused by parent variables and unobserved exogenous **noise** variables ϵ_i



Counterfactual Inference with SCMs

In order to compute counterfactuals we need to:

1. Estimate the noise $\boldsymbol{\epsilon}$ given the observed datum $\mathbf{x}$ (factual)
   We define $\mathcal{M}_x := (\mathbf{S}, p(\boldsymbol{\epsilon}|\mathbf{x}))$
2. To intervene on its structural assignments $\mathbf{S}$ with intervention $do(x_i = \widetilde{x}_i)$
   We define the modified, counterfactual SCM
   $\widetilde{\mathcal{M}} := \mathcal{M}_{\mathbf{x};do(\widetilde{x}_i)} = (\widetilde{\mathbf{S}}, p(\boldsymbol{\epsilon}|\mathbf{x}))$

Counterfactual Inference with SCMs

Three-step procedure:

1. **Abduction**: Infer $p(\boldsymbol{\epsilon}|\mathbf{x}))$, the state of the world (exogenous noise) that is compatible with the observations x.
2. **Action**: Replace the structural equations ($do(\widetilde{x}_i)$) corresponding to the intervention, resulting in a modified SCM $\widetilde{\mathcal{M}} := \mathcal{M}_{\mathbf{x};do(\widetilde{x}_i)} = (\widetilde{\mathbf{S}}, p(\boldsymbol{\epsilon}|\mathbf{x}))$
3. **Prediction**: Use the modified model to compute $p_{\widetilde{\mathcal{M}}}(\mathbf{x})$

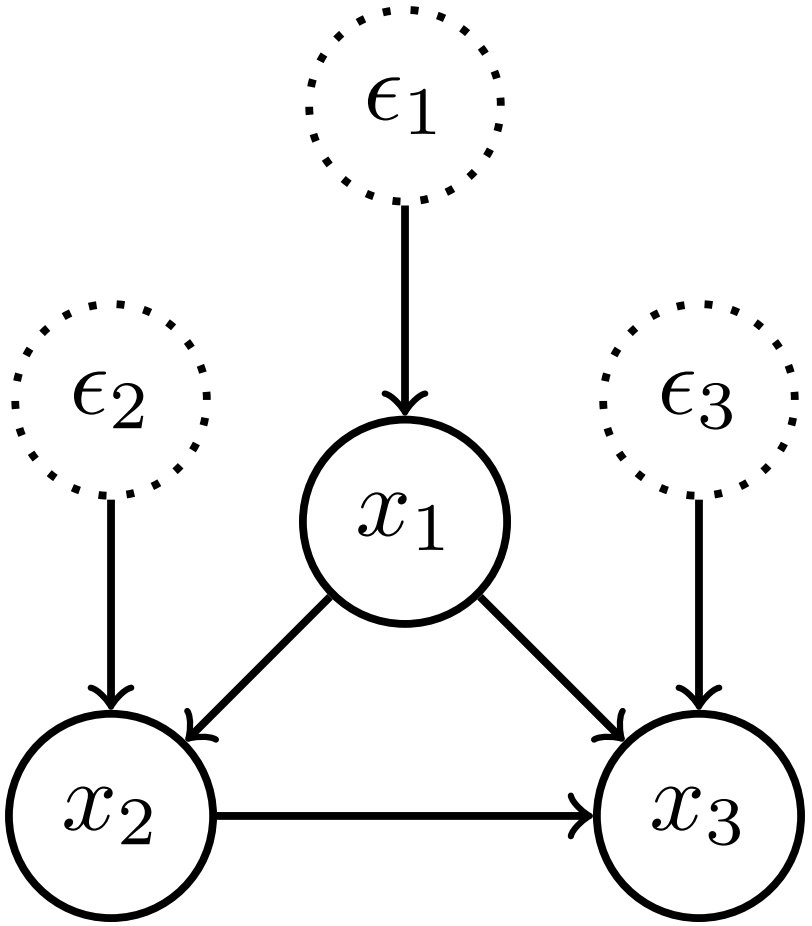
Principle of Independent Mechanisms

$p(\mathbf{x}) = \prod_{i=1}^{N} p(x_i|\mathbf{pa}_i)$

If we intervene on a subset S, then for all i:

1. If $i \notin S$, $p(x_i|\mathbf{pa}_i)$ remains unchanged
2. If $i \in S$, $p(x_i|\mathbf{pa}_i) = 1$, if x_i the value set by the intervention, otherwise 0

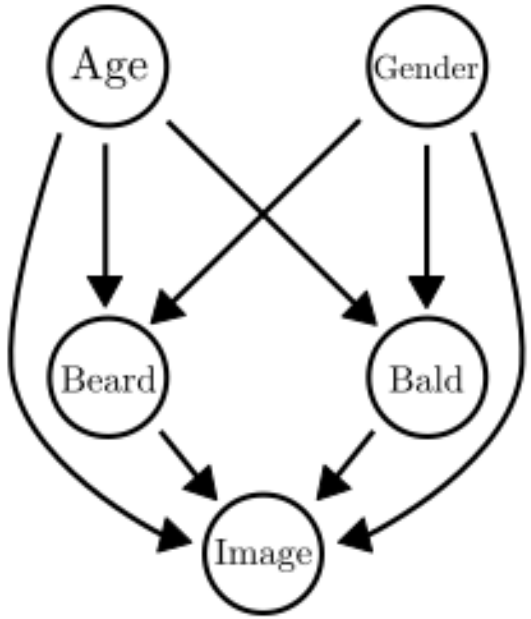
e.g. when intervening on x_2 the edges towards x_2 are removed

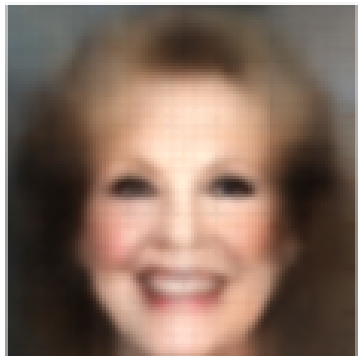


What about images?

We can think of the image as a variable and its attributes as parents

Example of a possible graph and counterfactual estimation





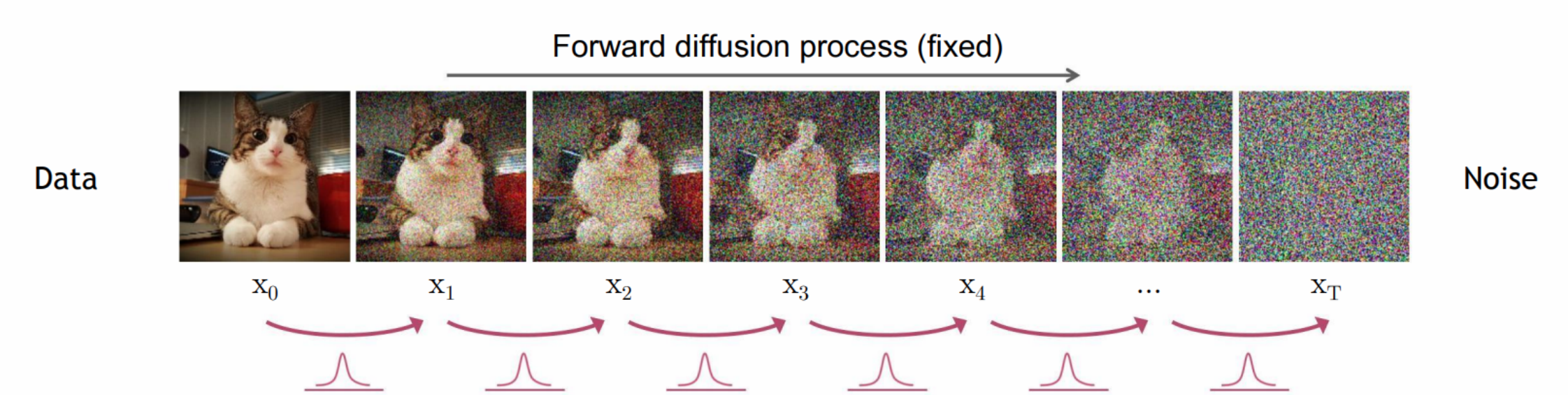
age : old
gender : female
beard : absent
bald : not

age : old
gender : male
beard* : present
bald : true

Kladny K.R., et al. (2023). Deep Backtracking Counterfactuals for Causally Compliant Explanations

Recap on DDPM

- $q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{\alpha_t}x_{t-1}, (1-\alpha_t)I)$ (noising step)
- $p_\theta(x_T) = \mathcal{N}(x_T; 0, I)$.
- $p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \sigma(x_t, t)^2 I)$ (denoising step)



$$\text{argmin}_\theta = \underbrace{\frac{(1-a_t)^2}{2\sigma_q^2(t)(1-\bar{a}_t)a_t}}_{\lambda_t} \left[||e_0 - e_\theta(x_t, t)||_2^2\right]$$

Recap on Score-based models

$$\text{argmin}_\theta = \frac{(1-a_t)^2}{2\sigma_q^2(t)a_t}\left[||s_\theta(x_t,t) - \nabla_{x_t}\log p(x_t)||_2^2\right]$$

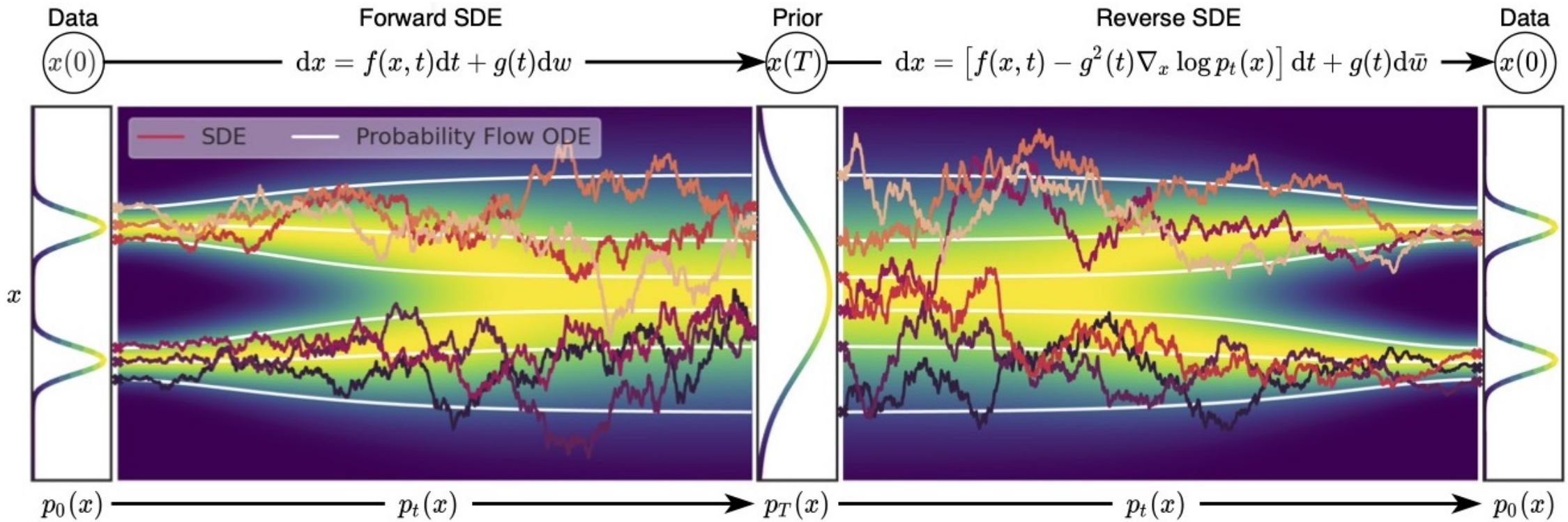
and SDEs

$$dx = f(x,t)dt + g(t)dw$$

To sample from $x(T) \sim p_T$ and get new data from p_{data}, we can reverse the SDE:
$dx = \left[f(x,t) - g^2(t)\nabla_x \log p_t(x)\right]dt + g(t)d\tilde{w}.$

With **(i)** the terminal distribution $p(T) \approx \pi(x)$ and **(ii)** the score $\nabla_x \log p_t(x)$, we train a *time dependent score model*, with objective:

$$\mathbb{E}_{t\in U(0,T)}\mathbb{E}_{p_t(x)}[\lambda(t)\|\nabla_x \log p_t(x) - s_\theta(x,t)\|_2^2]$$


Data
Forward SDE
Prior
Reverse SDE
Data
$x(0)$
$\mathrm{d}x = f(x,t)\mathrm{d}t + g(t)\mathrm{d}w$
$x(T)$
$\mathrm{d}x = \left[f(x,t) - g^2(t)\nabla_x \log p_t(x)\right]\mathrm{d}t + g(t)\mathrm{d}\bar{w}$
$x(0)$
SDE
Probability Flow ODE
x
$p_0(x)$
$p_t(x)$
$p_T(x)$
$p_t(x)$
$p_0(x)$

Teaser on DDIM and Classifier-Guidance

Algorithm 1 Classifier guided diffusion sampling, given a diffusion model $(\mu_\theta(x_t), \Sigma_\theta(x_t))$, classifier $p_\phi(y|x_t)$, and gradient scale s.

Input: class label y, gradient scale s
$x_T \leftarrow$ sample from $\mathcal{N}(0, \mathbf{I})$
for all t from T to 1 **do**
  $\mu, \Sigma \leftarrow \mu_\theta(x_t), \Sigma_\theta(x_t)$
  $x_{t-1} \leftarrow$ sample from $\mathcal{N}(\mu + s\Sigma \nabla_{x_t} \log p_\phi(y|x_t), \Sigma)$
end for
return x_0

Algorithm 2 Classifier guided DDIM sampling, given a diffusion model $\epsilon_\theta(x_t)$, classifier $p_\phi(y|x_t)$, and gradient scale s.

Input: class label y, gradient scale s
$x_T \leftarrow$ sample from $\mathcal{N}(0, \mathbf{I})$
for all t from T to 1 **do**
  $\hat{\epsilon} \leftarrow \epsilon_\theta(x_t) - \sqrt{1-\bar{\alpha}_t}\, \nabla_{x_t} \log p_\phi(y|x_t)$
  $x_{t-1} \leftarrow \sqrt{\bar{\alpha}_{t-1}} \left(\frac{x_t - \sqrt{1-\bar{\alpha}_t}\hat{\epsilon}}{\sqrt{\bar{\alpha}_t}} \right) + \sqrt{1-\bar{\alpha}_{t-1}}\hat{\epsilon}$
end for
return x_0

Song, J. et al. (2020). Denoising Diffusion Implicit Models
Dhariwal, P. et al. (2021). Diffusion Models Beat GANs on Image Synthesis

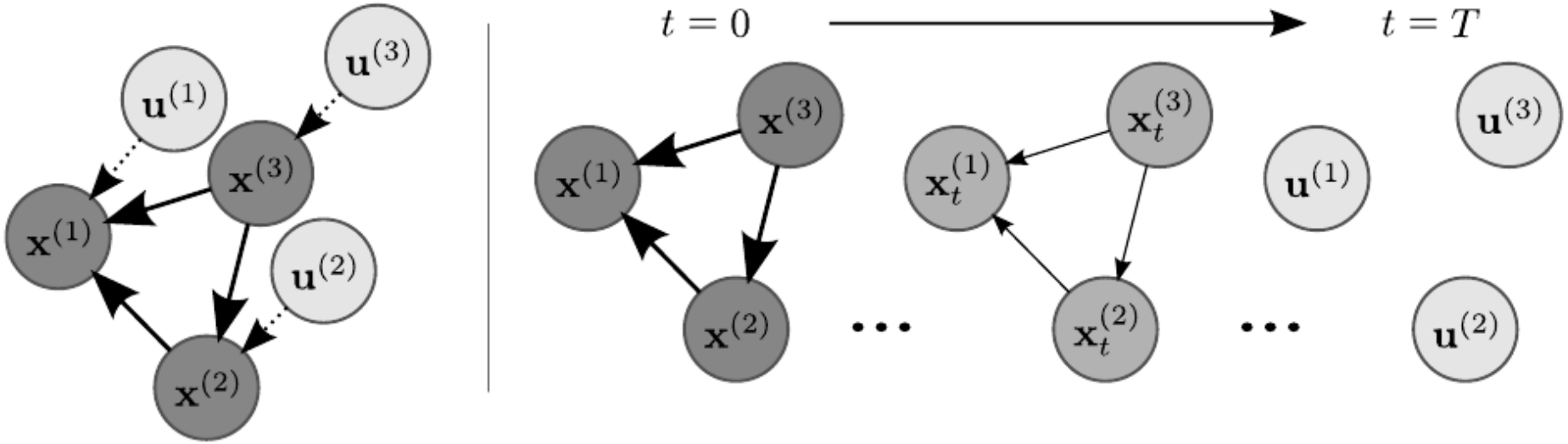
Diff-SCM: Motivation

- SCMs have been previously used to provide a causal interpretation of SDEs for modeling time-dependent problems
- SDEs have been used to formalize diffusion process in a continuous manner
- Diff-SCM models the dynamics of causal variables as an Ito process $\mathbf{x}_t^{(k)}, \forall t \in [0, T]$, going from an observed endogenous variable $\mathbf{x}_0^{(k)} = \mathbf{x}^{(k)}$ to its respective exogenous noise $\mathbf{x}_T^{(k)} = \mathbf{u}^{(k)}$ and back

Sokol, A. & Hansen N. (2014). Causal interpretation of stochastic differential equations
Bongers, S., & Mooij, J.M. (2018). From Random Differential Equations to Structural Causal Models: the stochastic case
Song, Y. et al. (2020). Score-Based Generative Modeling through Stochastic Differential Equations

Diff-SCM: Unifying Diffusion Processes and Causal Models

- Forward diffusion $\rightarrow$ gradual weakening of the causal relations between variables of a SCM



- The original joint distribution $p_{\mathcal{G}}$ diffuses to independent Gaussians $p(U)$

Diff-SCM: Unifying Diffusion Processes and Causal Models

- We can define a Deep SCM as a set of SDEs (1 for each node k):

$$d\mathbf{x}^{(k)} = -\frac{1}{2}\beta_t \mathbf{x}^{(k)} dt + \sqrt{\beta_t} d\mathbf{w}, \forall k \in [1, K],$$

where $p(\mathbf{x}_0^{(k)}) = \prod_{j=k}^{K} p(\mathbf{x}^{(j)} | \mathbf{pa}^{(j)})$ and $p(\mathbf{x}_T^{(k)}) = p(\mathbf{u}^{(k)})$

- The reverse-time SDE of the above is given by:

$$d\mathbf{x}^{(k)} = \left[-\frac{1}{2}\beta_t + \beta_t \nabla_{\mathbf{x}_t^{(k)}} \log p(\mathbf{x}_t^{(k)}) \right] + \sqrt{(\beta_t)} \bar{\mathbf{w}}$$

To solve: Iteratively update $\mathbf{x}_T^{(k)} = \mathbf{u}^{(k)}$ with the gradient w.r.t. the input variable $\nabla_{\mathbf{x}_t^{(k)}} \log p(\mathbf{x}_t^{(k)})$ until it becomes $\mathbf{x}_0^{(k)} = \mathbf{x}^{(k)}$

Apply Interventions with Anti-Causal Predictors

- We train an anti-causal classifier for each edge and a diffusion model for each node
- We use the gradients of the classifiers and diffusion models to propagate the intervention in the causal direction over the nodes

Proposition 1 (Interventions as anti-causal gradient updates) *We consider the SCM* $\mathfrak{G}$ *and a variable* $\mathbf{x}^{(j)} \in \mathbf{an}^{(k)}$. *The effect observed on* $\mathbf{x}^{(k)}$ *caused by an intervention on* $\mathbf{x}^{(j)}$, $p_{\mathfrak{G}}(\mathbf{x}^{(k)} \mid do(\mathbf{x}^{(j)} = x^{(j)}))$, *is equivalent to solving a reverse-diffusion process for* $\mathbf{x}_t^{(k)}$. *Since the sampling process involves taking into account the distribution entailed by* $\mathfrak{G}$, *it is guided by the gradient of an* ***anti-causal*** *predictor w.r.t. the effect when the cause is assigned a specific value:*

$$\nabla_{x_t^{(k)}} p_{\mathfrak{G}^-}(\mathbf{x}^{(j)} = x^{(j)} \mid x_t^{(k)})$$

Schölkopf, B. et al. (2012). On Causal and Anticausal Learning

Counterfactual Estimation with Diff-SCM

Three step procedure:

1. **Abduction**: Infer $p(\boldsymbol{u}|\mathbf{x})) \rightarrow$ **Forward diffusion***
2. **Action**: Modify SCM $\widetilde{\mathcal{M}} := \mathcal{M}_{\mathbf{x};do(\widetilde{x}_i)} = (\widetilde{\mathbf{S}}, p(\boldsymbol{u}|\mathbf{x})) \rightarrow$ **Remove the edges between the intervened variable and its parents**
3. **Prediction**: Compute $p_{\widetilde{\mathcal{M}}}(\mathbf{x}) \rightarrow$ **Reverse diffusion* controlled by the gradients of an anti-causal classifier**

*It actually follows the DDIM algorithm:

Song, J. et al. (2020). Denoising Diffusion Implicit Models

Counterfactual Estimation with Diff-SCM

Formally: Estimate counterfactual $x_{CF}^{(k)}$ based on factual (observed) $x_{F}^{(k)}$ after $do(\mathbf{x}^{(j)} = x_{CF}^{(j)}), \mathbf{x}^{(j)} \in \mathbf{an}^{(k)}$

They do experiments for the simple case, two variables: $\mathbf{x}^{(j)} \rightarrow \mathbf{x}^{(k)}$

Counterfactual Estimation with Diff-SCM

Abduction of Exogenous Noise By performing forward diffusion with an invertible process (e.g. DDIM, Neural ODEs) we get a latent $u^{(k)}$ that is invertible

Prediction under Intervention Counterfactual estimation: apply an intervention in the reverse diffusion process with the gradients of an anti-causal predictor
(*see classifier guidance of DDIM*)

Algorithm 1 Inference of **counterfactual** for a variable $\mathbf{x}^{(k)}$ from an intervention on $\mathbf{x}^{(j)} \in \mathbf{an}^{(k)}$

Models: trained diffusion model ϵ_θ and anti-causal predictor $p_\phi(x^{(j)} \mid x_t^{(k)})$

Input : factual variable $x_{0,\mathrm{F}}^{(k)}$, target intervention $x_{0,\mathrm{CF}}^{(j)}$, scale s

Output: counterfactual $x_{0,\mathrm{CF}}^{(k)}$

Abduction of Exogenous Noise – Recovering $u^{(k)}$ from $x_{0,\mathbf{F}}^{(k)}$

for $t \leftarrow 0$ **to** T **do**

$$x_{t+1,\mathrm{F}}^{(k)} \leftarrow \sqrt{\alpha_{t+1}} \left(\frac{x_{t,\mathrm{F}}^{(k)} - \sqrt{1-\alpha_t}\ \epsilon_\theta(x_{t,\mathrm{F}}^{(k)}, t)}{\sqrt{\alpha_t}} \right) + \sqrt{\alpha_{t+1}}\ \epsilon_\theta(x_{t,\mathrm{F}}^{(k)}, t)$$

end

$$u^{(k)} = x_{T,\mathrm{F}}^{(k)} = x_T^{(k)}$$

Generation under Intervention

for $t \leftarrow T$ **to** 0 **do**

$$\epsilon \leftarrow \epsilon_\theta(x_t^{(k)}, t) - s\sqrt{1-\alpha_t}\ \nabla_{x_t^{(k)}} \log p_\phi(x_{0,\mathrm{CF}}^{(j)} \mid x_t^{(k)})$$

$$x_{t-1}^{(k)} \leftarrow \sqrt{\alpha_{t-1}} \left(\frac{x_t^{(k)} - \sqrt{1-\alpha_t}\ \epsilon}{\sqrt{\alpha_t}} \right) + \sqrt{\alpha_{t-1}}\ \epsilon$$

end

$$x_{0,\mathrm{CF}}^{(k)} = x_0^{(k)}$$

Controlling the Intervention

Three factors enable counterfactual estimation:

(i) The inferred $u^{(k)}$ keeps information of the factual observation

(ii) $\nabla_{\mathbf{x}_t^{(k)}} \log p_\phi(x_{CF}^{(j)} | x_t^{(k)})$ guides the intervention towards the desired counterfactual class

(iii) $\epsilon_\theta(x_t^{(k)}, t)$ forces the estimation to belong to the data distribution

A hyperparameter s controls the scale of $\nabla_{\mathbf{x}_t^{(k)}} \log p_\phi(x_{CF}^{(j)} | x_t^{(k)})$

Dhariwal, P. et al. (2021). Diffusion Models Beat GANs on Image Synthesis

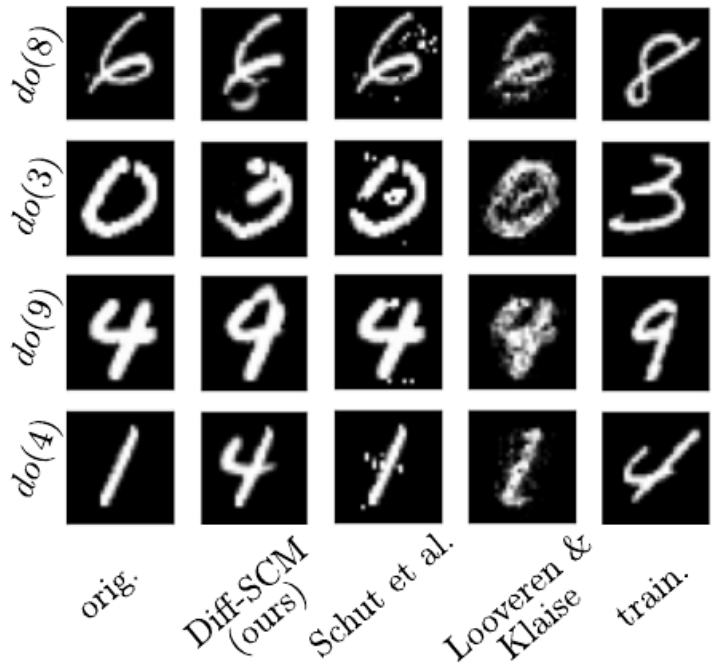
Experimental Setup

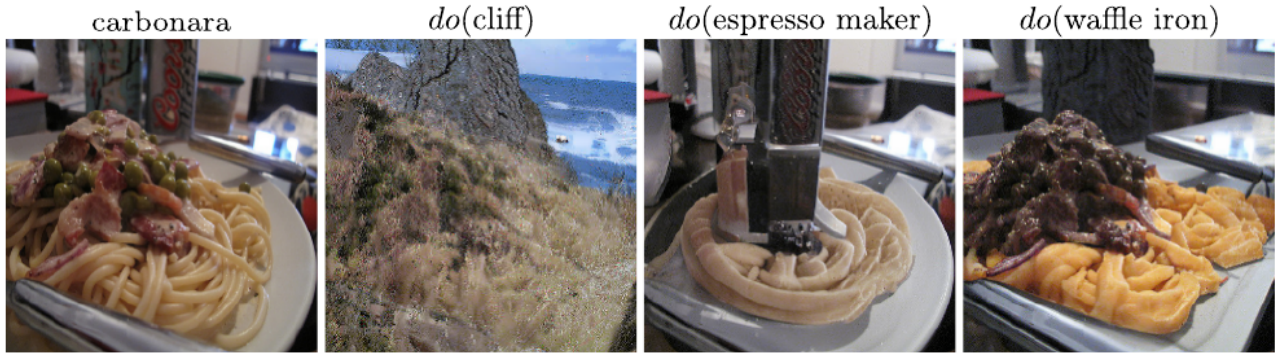
Given an SCM $\mathcal{G}_{image}$ with two variables $\mathbf{x}^{(1)} \leftarrow \mathbf{x}^{(2)}$, $\mathbf{x}^{(1)}$: image, $\mathbf{x}^{(2)}$: class

- A diffusion model ϵ_θ (U-Net) learns the score of the marginal distribution of $\mathbf{x}^{(1)}$
- An anticausal classifier $p_\phi(\mathbf{x}^{(2)}|\mathbf{x}^{(1)})$ (encoder of ϵ_θ + pooling + linear layer)

Both conditioned on t and trained separately

Trained and tested on MNIST and ImageNet





Schut, L. et al. (2021) Generating Interpretable Counterfactual Explanations By Implicit Minimisation of Epistemic and Aleatoric Uncertainties

Van Looveren, A et al. (2021). Interpretable Counterfactual Explanations Guided by Prototypes

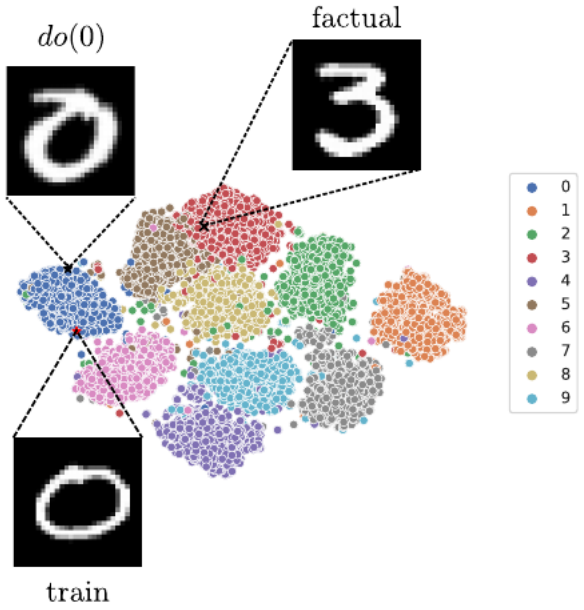
Counterfactual Latent Divergence (CLD)

- Used to evaluate minimality of intervention in latent space
- They train a VAE and measure KL divergence

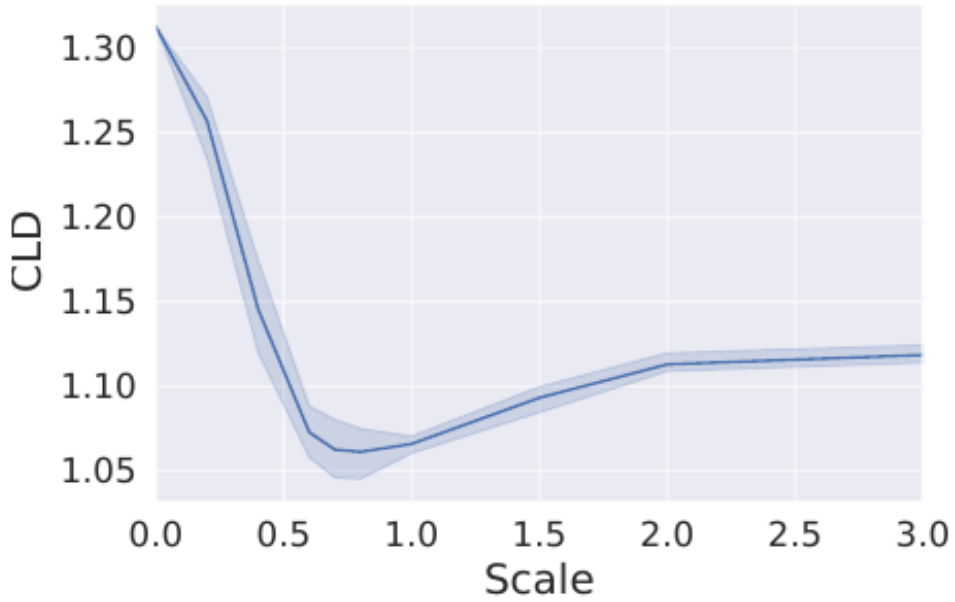
$$div = D(x_{\text{CF}}^{(1)}, x_{\text{F}}^{(1)}), \qquad \text{with } D(x_i^{(1)}, x_j^{(1)}) = D_{\text{KL}}(\mathcal{N}(\mu_i, \sigma_i), \mathcal{N}(\mu_j, \sigma_j))$$

$$\mathcal{S}_{\text{class}} = \{D(x^{(1)}, x_{\text{F}}^{(1)}) \mid (x^{(1)}, x^{(2)}) \in \mathcal{D} \wedge x^{(2)} = x_{\text{class}}^{(2)}\}$$

$$\text{CLD} = \log\left(\exp\left(P\left(\mathcal{S}_{\text{CF}} \leq div\right)\right) + \exp\left(P\left(\mathcal{S}_{\text{F}} \geq div\right)\right)\right)$$

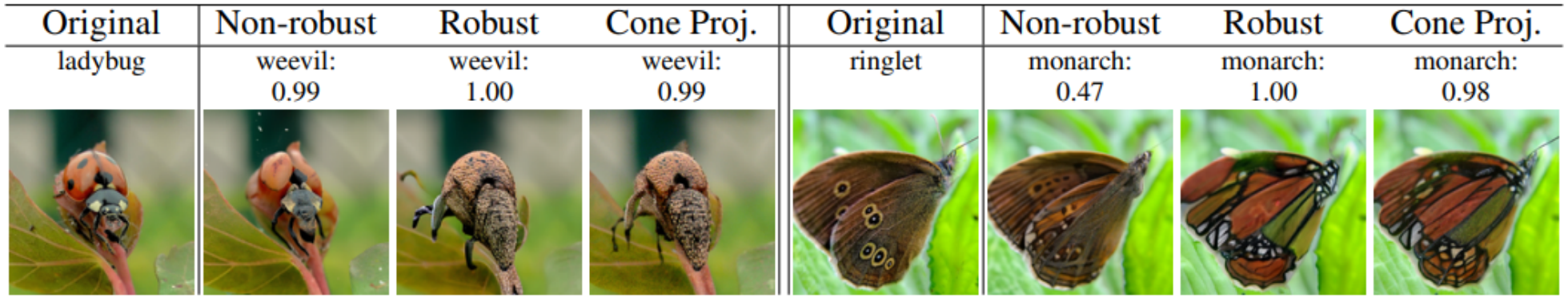


Use CLD to tune s



Related work

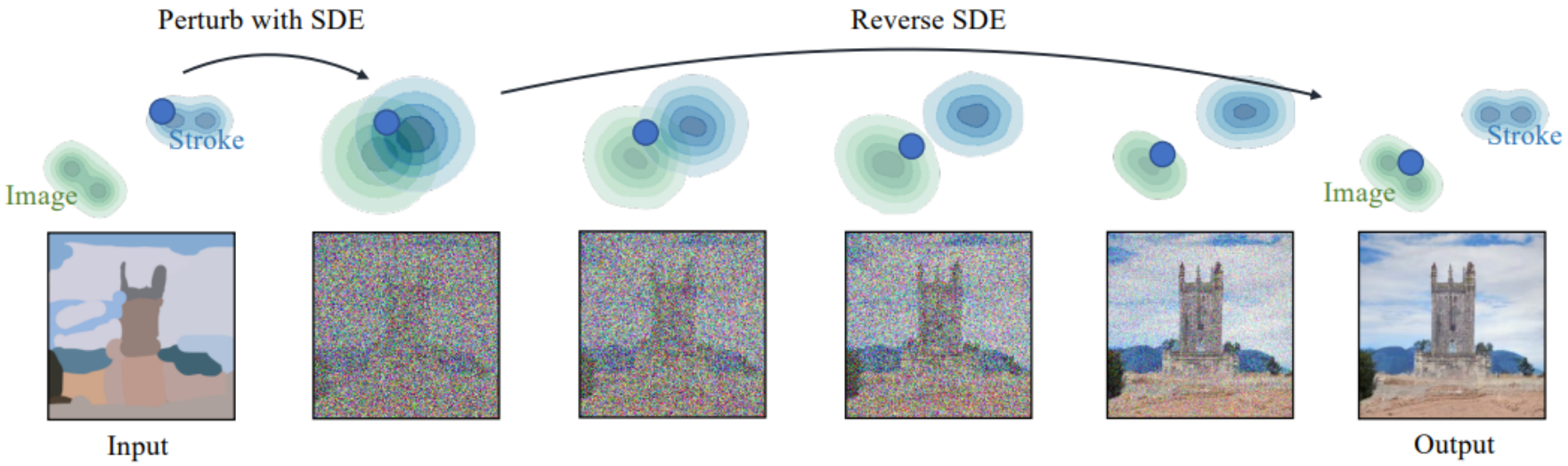
- Counterfactual Explanations is a technique to test the robustness and bias of models by making minimal changes in order to change a classifier's prediction



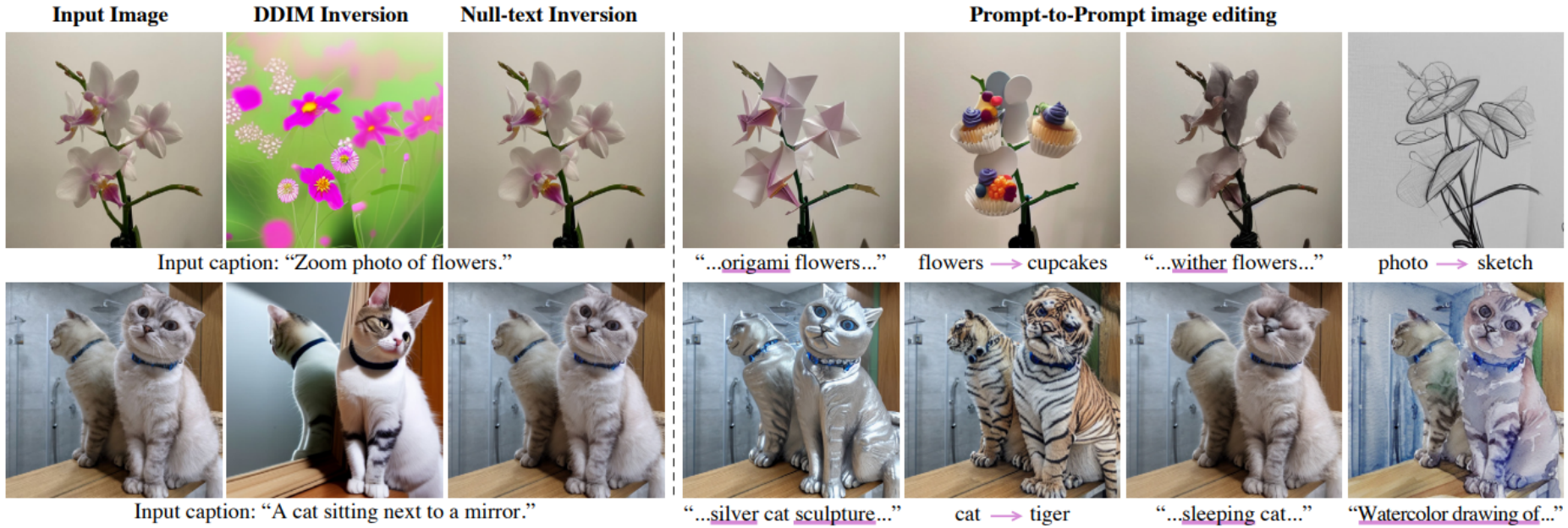
Augustin, M. (2022). Diffusion Visual Counterfactual Explanations

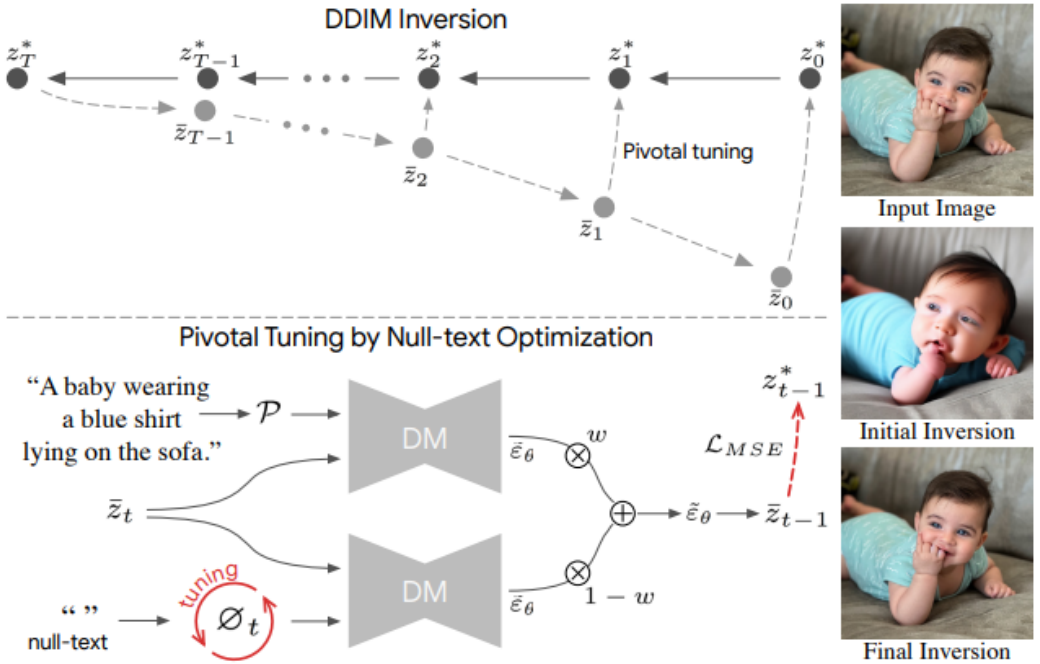
Related work

- Image-to-Image translation can be thought of as a case of counterfactual estimation
- Existing methods such as SDEdit or Null-text-Inversion deploy a very similar technique



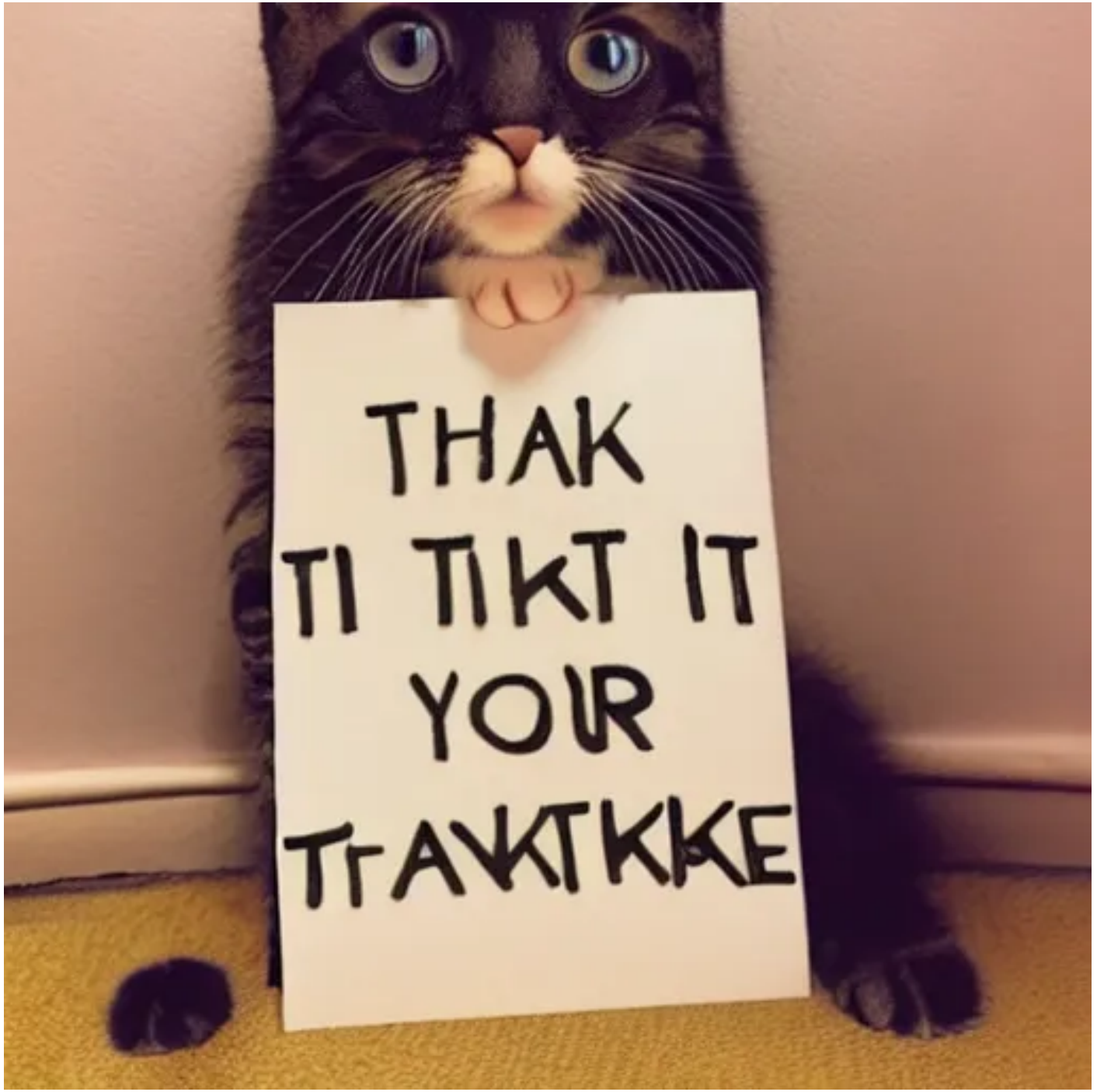
Meng, Ch. et al. (2022). SDEdit: Guided Image Synthesis and Editing with Stochastic Differential Equations





Mokady, R et al. (2022). Null-text Inversion for Editing Real Images using Guided Diffusion Models

Thank you
for your time!



Questions

- What are the difficulties in extending Diff-SCM to the general case?
- How can counterfactual properties such as minimality be evaluated?
- What can this framework offer, more than the classic image editing framework?