

SPATE-GAN: Improved Generative Modeling of Dynamic Spatio-Temporal Patterns with an Autoregressive Embedding Loss

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Abstract

From ecology to atmospheric sciences, many academic disciplines deal with data characterized by intricate spatio-temporal complexities, the modeling of which often requires specialized approaches. Generative models of these data are of particular interest, as they enable a range of impactful downstream applications like simulation or creating synthetic training data. Recently, COT-GAN, a new GAN algorithm inspired by the theory of causal optimal transport (COT), was proposed in an attempt to improve generation of sequential data. However, the task of learning complex patterns over time and space requires additional knowledge of the specific data structures. In this study, we propose a novel loss objective combined with COT-GAN based on an autoregressive embedding to reinforce the learning of spatio-temporal dynamics. We devise SPATE (**s**patio-**t**emporal association), a new metric measuring spatio-temporal autocorrelation. We compute SPATE for real and synthetic data samples and use it to compute an embedding loss that considers space-time interactions, nudging the GAN to learn outputs that are faithful to the observed dynamics. We test our new SPATE-GAN on a diverse set of spatio-temporal patterns: turbulent flows, log-Gaussian Cox processes and global weather data. We show that our novel embedding loss improves performance without any changes to the architecture of the GAN backbone, highlighting our model’s increased capacity for capturing autoregressive structures.

Introduction

Over the last decade, deep learning has emerged as a powerful paradigm for modeling complex data structures. It has also found successful applications in the video domain, for example for trajectory forecasting, video super-resolution or object tracking. Nevertheless, data observed over (discrete) space and time can take different shapes than just RGB videos: many of the systems and processes governing our planet, from ocean streams to the spread of viruses, exhibit complex spatio-temporal dynamics. Current deep learning approaches often struggle to account for these, as a recent survey by Reichstein et al. (2019) highlights. The authors call for more concerted research efforts aiming to improve

the capacity of deep neural networks for modeling earth systems data. Recently, the emergence of physics-informed deep learning has reinforced the integration of physical constraints as a research domain (Zhang and Zhao 2021; Rao, Sun, and Liu 2020; Wang et al. 2020b; Kim et al. 2020).

In this work, we propose a novel GAN tailored to the challenges of spatio-temporal complexities. We first devise a novel measure of spatio-temporal association—SPATE—expanding on the Moran’s I measure of spatial autocorrelation. SPATE uses the deviance of an observation from its space-time expectation, and compares it to neighboring observations to identify regions of (relative) change and regions of (relative) homogeneity over time. We propose three different approaches to calculate the space-time expectations, coming with varying assumptions and advantages for different applications. We then encode a SPATE-based embedding into COT-GAN (Xu et al. 2020) to formulate a new GAN framework, named SPATE-GAN. The motivation of choosing COT-GAN as the base model is that its principle of respecting temporal dependencies in sequential modeling is in line with our intuition for SPATE, see details in the methods section. Lastly, we test our approach on a range of different datasets. Specifically, we select data characterized by complex spatio-temporal patterns such as fluid dynamics (Wallace 2014; Wang et al. 2020b), disease spread (Brix and Diggle 2001) or global surface temperatures (Sismanidis et al. 2018). We observe that SPATE-GAN outperforms baseline models. This finding is particularly interesting as we do not change the architecture of the existing COT-GAN backbone, implying that our performance gains can be solely attributed to our novel SPATE-based embedding loss.

To summarize, the contributions of this study are as follows:

- We introduce SPATE, a new measure of spatio-temporal association, by expanding the intuition of the Moran’s I metric into the temporal dimension.
- We introduce SPATE-GAN, a novel GAN for complex spatio-temporal data utilizing SPATE to construct an embedding loss “nudging” the model to focus on the learning of autoregressive structures.
- We test SPATE-GAN against baseline GANs designed for image/video generation on datasets representing fluid dynamics, disease spread and global surface temperature.

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We show performance gains of SPATE-GAN over the baseline models.

Related Work

Autocorrelation Metrics for Spatio-temporal Phenomena

Analysing autoregressive patterns in spatial and spatio-temporal data has a long tradition in different academic domains (e.g. GIS, ecology) which over time developed diverse measures to describe these phenomena. The most commonly known of these metrics is the Moran’s I index of global and local spatial autocorrelation. Originally proposed by Anselin (1995), Moran’s I identifies both homogeneous spatial clusters and outliers. Applications of the metric range from identifying rare earth contamination (Yuan, Cave, and Zhang 2018) to analysing land cover change patterns (Das and Ghosh 2017). Throughout the years, Moran’s I has also motivated several methodological expansions, analysing for example spatial heteroskedasticity (Ord and Getis 2012) and local spatial dispersion (Westerholt et al. 2018). Moran’s I has also seen some expansions into the spatio-temporal domain. Matthews, Diawara, and Waller (2019) use the metric iteratively to model disease spread over time. Lee and Li (2017) and Gao et al. (2019) propose novel spatio-temporal expansions of the Moran’s I metric, returning static outputs at a purely spatial resolution. Siino et al. (2018) design an extended Moran’s I for spatio-temporal point processes. However, to the best of our knowledge, neither the Moran’s I nor its spatio-temporal extensions have been applied to discrete spatio-temporal video data. It is evident that metrics of spatio-temporal autocorrelation can provide meaningful embeddings of complex data, capturing underlying patterns throughout a range of different application domains.

Deep Learning & GANs for Spatial and Spatio-temporal Data

Deep learning describes a powerful family of methods capable of dealing with the highly complex and non-linear nature of many real world spatial and spatio-temporal patterns (Yan et al. 2017; Aodha, Cole, and Perona 2019; Chu et al. 2019; Bao et al. 2020; Geng et al. 2019). Paradigms like physics-informed deep learning aim to devise methods which integrate (geo)physical constraints explicitly into neural network models (Wang et al. 2020b). There is also an increasing number of studies tackling specific challenges associated with geographic data: Mai et al. (2020) and Yin et al. (2019) propose context-aware vector embeddings for geographic coordinates. Zammit-Mangion et al. (2019) propose to learn deep neural networks for spatial covariance patterns using injective warping functions. Intuitions for spatial autocorrelation, including the Moran’s I metric, have been integrated into machine learning frameworks tackling model selection for ensemble learners (Klemmer, Koshiyama, and Flennerhag 2019), spatial representation learning (Zhang et al. 2019), auxiliary task learning (Klemmer and Neill 2021) or residual correlation graph neural networks (Jia and Benson 2020). All these studies highlight the benefits of ex-

PLICITLY encoding spatial context into neural networks to improve performance.

Narrowing down on the GAN context specifically, we find that spatio-temporal applications have mostly focused on video data (Xu et al. 2020; Tulyakov et al. 2018; Kim, Oh, and Kim 2020). Beyond this, GANs have been used for conditional density estimation of traffic (Zhang et al. 2020), trajectory prediction (Huang et al. 2021) or extreme weather event simulation (Klemmer et al. 2021). Nevertheless, to the best of our knowledge, metrics capturing spatio-temporal autocorrelation have never been integrated into GANs. As previous studies highlight the value on encoding spatial context, this work seeks to provide a first-principle approach of integrating metrics of spatio-temporal autocorrelation into GANs for modeling of complex spatio-temporal patterns.

Embedding Loss Functions

As SPATE-GAN integrates spatio-temporal metrics into COT-GAN as embeddings, here we briefly revisit previous work and insights into embedding losses. Embedding losses describe approaches where the loss function of a model is computed on an embedding of the data. This can have desirable outcomes, such as training stability or focusing on specific patterns in the data. Embedding losses have become popular in computer vision over the last years: Ghafoorian et al. (2019) use embedding losses to improve GAN-based lane detection. Filntisis et al. (2020) use visual-semantic embedding losses to improve predictions of bodily expressed emotions. Wang et al. (2020a) introduce CLIFFNet, utilizing hierarchical embeddings of depth maps for molecular depth estimation. Bailer, Varanasi, and Stricker (2017) introduce a threshold loss to improve optical flow estimation. It is clear that embedding losses have shown great potential for particularly challenging visual problems, especially those involving complex spatio-temporal dynamics.

Method

SPATE: Spatio-temporal Association

For a static, discrete spatial pattern (e.g. a grid of pixels forming an image) consisting of continuous values $x \in \mathbb{R}^n$ where $n \in \mathbb{N}$ is the dimensionality of x , x_i for $i \in 1, \dots, n$ represents the i ’th pixel value on a regular grid. The local Moran’s I statistic I_i is computed as follows:

$$I_i = (n_i - 1) \frac{z_i}{\sum_{j=1}^{n_i} z_j^2} \sum_{j=1, j \neq i}^{n_i} w_{i,j} z_j \quad (1)$$

where $z_i = x_i - \bar{x}$ is the deviance of observation x_i from the global mean \bar{x} , n_i is the number of spatial neighbors of pixel x_i , j indexes neighbors of x_i for $j \in \{1, \dots, n_i\}$ and $j \neq i$, and $w_{i,j}$ is a binary spatial weight matrix, indicating spatial neighborhood of observations i and j . I_i can be interpreted as a measure of similarity to neighboring pixels: positive values imply homogeneous clusters, while negative values suggest outliers, change patterns or edges.

Now, let us assume that we observe a sequence of spatial patterns over time t : $x = (x_1, \dots, x_T) \in \mathbb{R}^{n \times T}$ where n is the dimensionality of x_t at each time t and T is the total time steps of the sequence. Of course, a naive adoption

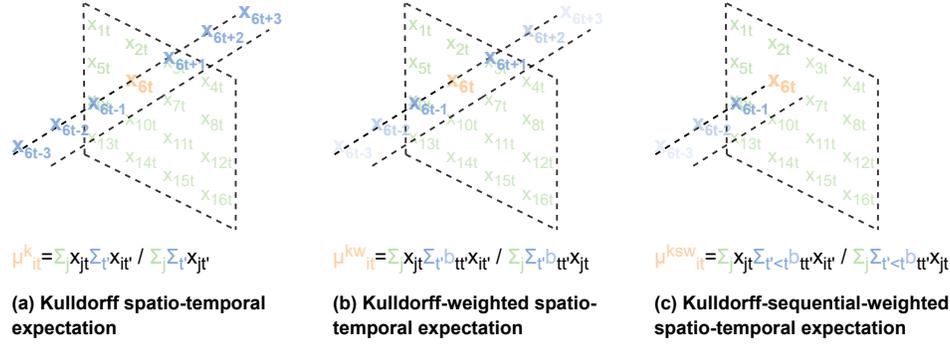


Figure 1: Illustrating the three proposed options to obtain *spatio-temporal expectations* μ_{it} used in the computation of SPATE for single-channel data. The orange value is the current observation, the green values all other spatial units at the current time step t and all values over time at the current spatial unit i are colored blue.

of the approach above is simply to ignore the time component of a sequence and compute the local Moran’s I values I_{it} around pixel i using mean values \bar{x}_t at each time t . Unfortunately, this approach would strictly separate spatial and temporal effects. In fact, the much more realistic assumption is that space and time are not separable, but do in fact interact and form joint patterns. For this reason, we expand the concept of Moran’s I for spatio-temporal expectations. First, we follow the intuition outlined in Kulldorff et al. (2005) and define expected values of $\mu_{it}(x)$. We refer to this approach as Kulldorff spatio-temporal expectation (“k”):

$$\mu_{it}^{(k)} = \frac{\sum_j x_{jt} \sum_{t'} x_{it'}}{\sum_j \sum_{t'} x_{jt'}}. \quad (2)$$

$\mu_{it}^{(k)}$ in (2) involves utilizing all spatial units (pixels) available at time step t and across all time steps at a single spatial unit (pixel position) i . This computation of the *spatio-temporal expectations* assumes independence of space and time, and thus the residual $z_{it} = x_{it} - \mu_{it}^{(k)}$ can be thought of as a local measure of space-time interaction at pixel i and time t . Moreover, this formulation of μ_{it} makes two critical assumptions: (1) Different time steps are equally important, irrespective of how distant they are from the current time step. (2) At each time step, we assume availability of the whole time series (i.e. looking into the future is possible). We can modify the computation of μ_{it} by imposing alternative assumptions.

First, assuming that distant time steps have less significant impact on the current time step, we can integrate temporal weights into the computation, and apply decreasingly lower weights to more distant time steps. For example, one can consider an exponential kernel:

$$\mu_{it}^{(kw)} = \frac{\sum_j x_{jt} \sum_{t'} b_{tt'} x_{it'}}{\sum_j \sum_{t'} b_{tt'} x_{jt'}}, \quad (3)$$

where $b_{tt'} = \exp(-|t - t'|/l)$ and l is the lengthscale of the exponential kernel. We refer to this approach as Kulldorff-weighted spatio-temporal expectation (“kw”).

Second, we can restrict the computation of μ_{it} at time step t to only account for time steps $< t$, so that the expectation at

each time step is independent of future observations. Thus, the computation respects the generating logic of sequential data. We refer to this last approach as Kulldorff-sequential-weighted spatio-temporal expectation (“ksw”):

$$\mu_{it}^{(ksw)} = \frac{\sum_j x_{jt} \sum_{t' < t} b_{tt'} x_{it'}}{\sum_j \sum_{t' < t} b_{tt'} x_{jt'}}. \quad (4)$$

Note that for the first time step $t = 0$, we cannot access past time steps to calculate spatio-temporal expectations $\mu_{i0}^{(ksw)}$.

We can now simply plug in our new spatio-temporal expectations into the Moran’s I metric at time t by replacing spatial only expectations with a spatio-temporal expectation of our choice. As such, we define our novel measure of **spatio-temporal association** (SPATE),

$$S_{it}(x, w) = (n_i - 1) \frac{z_{it}}{\sum_{j=1}^{n_x} z_{jt}^2} \sum_{j=1, j \neq i}^{n_x} w_{i,j} z_{jt} \quad (5)$$

where $z_{it} = x_{it} - \mu_{it}$ and μ_{it} can be any option from $\mu_{it}^{(k)}$, $\mu_{it}^{(kw)}$ and $\mu_{it}^{(ksw)}$. When using $\mu_{it}^{(ksw)}$, SPATE does not return values for $t = 0$, as no previous time steps are available to calculate spatio-temporal expectations. See Fig 1 for an illustration of the three proposed options.

SPATE measures spatio-temporal autocorrelation at the input resolution. Its behavior can be closely related to that of the Moran’s I metric. While Moran’s I evaluates the deviance z_i between each pixel and the spatial expectation, SPATE does so by using the spatio-temporal expectation z_{it} . Like Moran’s I, SPATE acts as a detector of spatio-temporal clusters and change patterns. Like Moran’s I, SPATE identifies positive and negative space-time autocorrelation, i.e. homogeneous areas of similar behavior and outliers that behave differently from their immediate neighborhood. The difference between Moran’s I and SPATE is that the later explicitly captures space-time interactions. For example, if pixel x_i and all other data points (not just its neighbors) are increased at a given time step t , Moran’s I at time t (for all points) will be high, but SPATE will not be. SPATE of x_{it} will be high if (a) pixel x_{it} is high compared to its expectation at the same

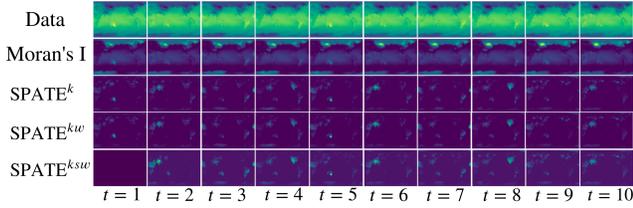


Figure 2: The SPATE metric in its different forms computed for an example from the LGCP datasets. While SPATE^k and SPATE^{kw} are visually undistinguishable, SPATE^{ksw} changes as increasingly more past time steps become available, converging to SPATE^{kw} at time T . We can also observe how the Moran’s I metric remains static in time, while all versions of SPATE behave dynamically in space and time.

time t , (b) its neighbors are high compared to their expectations, while (c) its non-neighbors are not particularly high compared to their expectations.

In the kw and ksw settings, the lengthscale parameter l governs whether the metric captures longer or shorter term temporal patterns. For example, if pixel x_{it} and its neighbors increase slowly over time, that change will only cause SPATE to be high for larger lengthscales l , while smaller l values imply that current values are compared to those that are close in time. As such, the lengthscale determines what changes are considered ”slow” (incorporated into the mean, not detected as space-time interaction) and ”fast” (current values are different from the mean, detected as space-time interaction). The ksw setting further allows for scenarios where we might wish to compute the metric based on previous time-steps alone, i.e. to preserve sequential logic.

COT-GAN

COT-GAN was introduced by Xu et al. (2020) as an adversarial algorithm to train implicit generative models for sequential learning, which enforces a temporal causality constraint on the classical optimal transport (OT) by restricting the transporting of mass on the arrival sequence at any time t to depend on the starting sequence only up to time t . We provide a detailed introduction of COT-GAN because, not only did it motivate us to design the spatio-temporal expectation μ_{it}^{ksw} in a similar autoregressive manner in order to respect the nature of sequential data, this consistency between the embedding metrics and the backbone model also leads to the best performance as shown in the experiments.

In sequential generation, we are interested in learning a model that produces $y = (y_1, \dots, y_T) \in \mathbb{R}^{n \times T}$ to mimic $x = (x_1, \dots, x_T) \in \mathbb{R}^{n \times T}$. Given two probability measures μ, ν defined on $\mathbb{R}^{n \times T}$, and a cost function $c : \mathbb{R}^{n \times T} \times \mathbb{R}^{n \times T} \rightarrow \mathbb{R}$, the causal optimal transport of μ into ν is formulated as

$$\mathcal{W}_c^{\mathcal{K}}(\mu, \nu) := \inf_{\pi \in \Pi^{\mathcal{K}}(\mu, \nu)} \mathbb{E}^{\pi}[c(x, y)], \quad (6)$$

where $\Pi^{\mathcal{K}}(\mu, \nu)$ is the set of probability measures π on $\mathbb{R}^{n \times T} \times \mathbb{R}^{n \times T}$ with marginals μ, ν , which also satisfy the constraint $\pi(dy_t | dx_{1:T}) = \pi(dy_t | dx_{1:t})$ for all $t =$

$\{1, \dots, T - 1\}$. Such plans in $\Pi^{\mathcal{K}}(\mu, \nu)$ are called *causal transport plans*. Here $c(x, y)$ is a cost function that measures the loss incurred by transporting a unit of mass from x to y . $\mathcal{W}_c^{\mathcal{K}}(\mu, \nu)$ is thus the minimal total cost for moving the mass μ to ν in a causal way.

In comparison, the (classic) OT is defined on \mathbb{R}^n and differs from COT by searching an optimal plan that leads to the least cost in a less restricted space $\Pi(\mu, \nu)$ which contains all transport plans,

$$\mathcal{W}_c(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \mathbb{E}^{\pi}[c(x, y)]. \quad (7)$$

COT-GAN constructed an adversarial objective by reformulating the COT (6) as below,

$$\mathcal{W}_c^{\mathcal{K}}(\mu, \nu) = \sup_{c^{\mathcal{K}} \in \mathcal{C}^{\mathcal{K}}(\mu, c)} \inf_{\pi \in \Pi(\mu, \nu)} \{\mathbb{E}^{\pi}[c^{\mathcal{K}}(x, y)]\}, \quad (8)$$

where $\mathcal{C}^{\mathcal{K}}(\mu, c)$ is a special family of costs that encode the causality constraint, see Appendix A for details. Note that the inner optimization problem is equivalent to OT in (7) with a specific class of cost function, i.e., $\mathcal{W}_{c^{\mathcal{K}}}(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \{\mathbb{E}^{\pi}[c^{\mathcal{K}}(x, y)]\}$.

In the implementation of COT-GAN, learning is done via stochastic gradient descent (SGD) on mini-batches. Given a distribution ζ on some latent space \mathcal{Z} , the generator g_{θ} is a function that maps a latent variable $z \sim \zeta$ to the generated sequence y in the path space. Given a mini-batch of size m from training data $\{x_{1:T}^d\}_{d=1}^m$ and that from generated samples $\{y_{1:T}^d\}_{d=1}^m$, we define the empirical measures for the mini-batches as

$$\hat{\mu} := \frac{1}{m} \sum_{d=1}^m \delta_{x_{1:T}^d}, \quad \hat{\nu}_{\theta} := \frac{1}{m} \sum_{d=1}^m \delta_{y_{1:T}^d},$$

where $\hat{\nu}_{\theta}$ incorporates the parameterization of g_{θ} . Thus, the duality of COT given by (8) between the empirical measures of two mini-batches can be written as

$$\mathcal{W}_c^{\mathcal{K}}(\hat{\mu}, \hat{\nu}_{\theta}) = \sup_{c^{\mathcal{K}} \in \mathcal{C}^{\mathcal{K}}(\hat{\mu}, c)} \mathcal{W}_{c^{\mathcal{K}}}(\hat{\mu}, \hat{\nu}_{\theta}). \quad (9)$$

Computing (9) involves solving the optimization problem of classic OT. COT-GAN opted for the Sinkhorn algorithm, see (Cuturi 2013; Genevay, Peyre, and Cuturi 2018), and a modified version of Sinkhorn divergence for an approximation. Here we have the entropic-regularized OT defined as

$$\mathcal{W}_{c, \varepsilon}(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \{\mathbb{E}^{\pi}[c(x, y)] - \varepsilon H(\pi)\}, \quad \varepsilon > 0,$$

where $H(\pi)$ is the Shannon entropy of π . Whilst the Sinkhorn divergence was also computed between two mini-batches, the authors of COT-GAN noticed the bias was better reduced by the mixed Sinkhorn divergence,

$$\begin{aligned} \widehat{\mathcal{W}}_{c, \varepsilon}^{\text{mix}}(\hat{\mu}, \hat{\nu}, \hat{\mu}', \hat{\nu}') &:= \mathcal{W}_{c, \varepsilon}(\hat{\mu}, \hat{\nu}) + \mathcal{W}_{c, \varepsilon}(\hat{\mu}', \hat{\nu}') \\ &\quad - \mathcal{W}_{c, \varepsilon}(\hat{\mu}, \hat{\mu}') - \mathcal{W}_{c, \varepsilon}(\hat{\nu}, \hat{\nu}'), \end{aligned}$$

where $\hat{\mu}$ and $\hat{\mu}'$ represent the empirical measures corresponding to two different mini-batches of the training data, and $\hat{\nu}$ and $\hat{\nu}'$ are the ones to the generated samples.

Finally, we have the following objective function for COT-GAN:

$$\inf_{\theta} \sup_{\varphi} \left\{ \widehat{\mathcal{W}}_{c_{\varphi}^{\mathcal{K}}, \varepsilon}^{\text{mix}}(\hat{\mu}, \hat{\nu}_{\theta}, \hat{\mu}', \hat{\nu}'_{\theta}) - \lambda [p_{\mathcal{M}_{\varphi_2}}(\hat{\mu}) + p_{\mathcal{M}_{\varphi_2}}(\hat{\mu}')] \right\},$$

where the role of discriminator is played by the cost function $c^{\mathcal{K}}$ parameterized by φ , and $p_{\mathcal{M}_{\varphi_2}}$ is the martingale penalization required for the formulation of the new class of costs $\mathcal{C}_{\varphi}^{\mathcal{K}}$, and φ_2 is a subset of the discriminator parameters φ , see details in Appendix A. The discriminator learns the worst-case cost $c_{\varphi}^{\mathcal{K}}$ by maximizing the objective over φ , and the generator is updated by minimizing it over θ .

SPATE-GAN

In SPATE-GAN, we integrate our newly devised spatio-temporal metric into the COT-GAN objective function. We compute the embedding for each x_{it}^d and y_{it}^d in minibatches $\{x_{1:T}^d\}_{d=1}^m$ and $\{y_{1:T}^d\}_{d=1}^m$ by

$$\hat{x}_{it}^d = S_{it}(x_{1:T}^d, w) \quad \text{and} \quad \hat{y}_{it}^d = S_{it}(y_{1:T}^d, w),$$

where the binary spatial weight matrix w is pre-defined.

The corresponding embeddings are then concatenated with the training data and generated samples on the channel dimension. We define the empirical measures for the concatenated sequences as

$$\begin{aligned} \hat{\mu}^e &:= \frac{1}{m} \sum_{d=1}^m \delta_{\text{concat}(x_{1:T}^d, \hat{x}_{1:T}^d)}, \\ \hat{\nu}_{\theta}^e &:= \frac{1}{m} \sum_{d=1}^m \delta_{\text{concat}(y_{1:T}^d, \hat{y}_{1:T}^d)}, \end{aligned}$$

where $\text{concat}(\cdot, \cdot)$ is an operator that concatenates inputs along the channel dimension.

We thus arrive at the objective function for SPATE-GAN:

$$\inf_{\theta} \sup_{\varphi} \left\{ \widehat{\mathcal{W}}_{c_{\varphi}^{\mathcal{K}}, \varepsilon}^{\text{mix}}(\hat{\mu}^e, \hat{\nu}_{\theta}^e, \hat{\mu}^{e'}, \hat{\nu}_{\theta}^{e'}) - \lambda [p_{\mathcal{M}_{\varphi_2}}(\hat{\mu}^e) + p_{\mathcal{M}_{\varphi_2}}(\hat{\mu}^{e'})] \right\}.$$

We maximize the objective function over φ to search for a worst-case distance between the two empirical measures, and minimize it over θ to learn a distribution that is as close as possible to the real distribution. The algorithm is summarized in Algorithm 1. Its time complexity scales as $\mathcal{O}((J + 2n)LTm^2)$ in each iteration where J is the output dimension of the discriminator (see Appendix A for details), and L is the number of Sinkhorn iterations (see Genevay, Peyre, and Cuturi (2018); Cuturi (2013) for details).

In the experiment section, we will compare SPATE-GAN with three different expectations $\mu_{it}^{(k)}$, $\mu_{it}^{(kw)}$ and $\mu_{it}^{(ksw)}$ in the computation of SPATE. Hence, we denote the corresponding models as SPATE-GAN^{*k*}, SPATE-GAN^{*kw*}, and SPATE-GAN^{*ksw*}, respectively.

Last, we would like to emphasize that, although all three embeddings consider the space-time interactions in a certain way, the non-anticipative assumption of $\mu_{it}^{(ksw)}$ is consistent with the generating process of the type of data we

Algorithm 1: training SPATE-GAN by SGD

Data: $\{x_{1:T}^d\}_{d=1}^n$ (input data), ζ (latent distribution)
Parameters: θ_0, φ_0 (parameter initializations), m (batch size), ε (regularization parameter), α (learning rate), λ (martingale penalty coefficient)

Initialize: $\theta \leftarrow \theta_0, \varphi \leftarrow \varphi_0$

for $b = 1, 2, \dots$ **do**

Sample $\{x_{1:T}^d\}_{d=1}^m$ from real data;

Sample $\{z_{1:T}^d\}_{d=1}^m$ from ζ ;

Generate sequences from latent:

$(y_{1:T}^d) \leftarrow g_{\theta}(z_{1:T}^d)$;

Compute the embeddings:

$\hat{x}_{it}^d = S_{it}(x_{1:T}^d, w), \hat{y}_{it}^d = S_{it}(y_{1:T}^d, w)$;

Concatenated the data with embeddings:

$\text{concat}(x_{1:T}^d, \hat{x}_{1:T}^d), \text{concat}(y_{1:T}^d, \hat{y}_{1:T}^d)$;

Update discriminator parameter:

$\varphi \leftarrow \varphi + \alpha \nabla_{\varphi} \left(\widehat{\mathcal{W}}_{c_{\varphi}^{\mathcal{K}}, \varepsilon}^{\text{mix}}(\hat{\mu}^e, \hat{\nu}_{\theta}^e, \hat{\mu}^{e'}, \hat{\nu}_{\theta}^{e'}) - \lambda [p_{\mathcal{M}_{\varphi_2}}(\hat{\mu}^e) + p_{\mathcal{M}_{\varphi_2}}(\hat{\mu}^{e'})] \right)$;

Sample $\{z_{1:T}^d\}_{d=1}^m$ from ζ ;

Generate sequences from latent:

$(y_{1:T}^d) \leftarrow g_{\theta}(z_{1:T}^d)$;

Compute the embeddings:

$\hat{x}_{it}^d = S_{it}(x_{1:T}^d, w), \hat{y}_{it}^d = S_{it}(y_{1:T}^d, w)$;

Concatenated the data with embeddings:

$\text{concat}(x_{1:T}^d, \hat{x}_{1:T}^d), \text{concat}(y_{1:T}^d, \hat{y}_{1:T}^d)$;

Update generator parameter:

$\theta \leftarrow \theta - \alpha \nabla_{\theta} \left(\widehat{\mathcal{W}}_{c_{\varphi}^{\mathcal{K}}, \varepsilon}^{\text{mix}}(\hat{\mu}^e, \hat{\nu}_{\theta}^e, \hat{\mu}^{e'}, \hat{\nu}_{\theta}^{e'}) \right)$;

end

are investigating. As the causality constraint in COT-GAN also restricts the search of transport plans to those that satisfy non-anticipative transporting of mass, SPATE-GAN^{*ksw*} is a model that fully respects temporal causality in learning, whilst SPATE-GAN^{*k*} and SPATE-GAN^{*kw*} also combine information from the future.

Experiments

To empirically evaluate SPATE-GAN, we use three datasets characterized by different spatio-temporal complexities.

Extreme Weather (EW) This dataset, introduced by Racah et al. (2017), was originally proposed for detecting extreme weather events from a range of climate variables (e.g. zonal winds, radiation). Each of these climate variables is observed four times a day for a 128×192 pixel representation of the whole earth. We chose to model surface temperature, as it comes with several interesting spatio-temporal characteristics: It exhibits both static (e.g. continent outlines) and dynamic patterns as well as abnormal patterns (e.g. in the presence of tropical cyclones or atmospheric rivers). Furthermore, simulating climate data is an

important potential downstream application of deep generative models.

LGCP This dataset represents the intensities (number of events in a grid cell) of a log-Gaussian Cox process (LGCP), a continuous spatio-temporal point process. LGCPs are a popular class of models for simulating contagious spatio-temporal patterns and have various applications, for example in epidemiology. We simulate 300 different LGCP intensities on a 64×64 grid over 10 time steps using the *R* package *LGCP* (Taylor et al. 2015).

Turbulent Flows (TF) This dataset, proposed by Wang et al. (2020b), simulates velocity fields according to the Navier-Stokes equation. This is a class of partial differential equations describing the motion of fluids. Fluid dynamics and simulation is another potential application of deep generative models. Following the approach of Wang et al. (2020b), we divide the data into 7 steps of 64×64 pixel frames. Please note that we only utilize the first velocity field, so that all our utilized datasets are single-channel.

Baselines and Evaluation Metrics

We are limited in our choice of benchmark methods, as most video GANs are developed for RGB (multi-channel) videos and often make use of pre-trained models. For example, to the best of our knowledge, no GAN has ever been applied to LGCP data. Here, we use COT-GAN (Xu et al. 2020) and the GAN proposed by Genevay, Peyre, and Cuturi (2018), which we name as SinkGAN, as baseline models. We augment both models with our new embedding loss, using SPATE with k , kw and ksw configurations. We refer to all models using a COT-GAN backbone with our new embedding loss as SPATE-GAN. We further denote the SinkGAN models corresponding to three SPATE settings as SinkGAN ^{k} , SinkGAN ^{kw} and SinkGAN ^{ksw} . To compare our approach to a non-time-sensitive embedding, we also deploy models using the Moran’s I metric using the same embedding loss procedure, denoted as COT-GAN ^{M} and SinkGAN ^{M} .

To compare our GAN output to real data samples, we use three different metrics: Earth Mover Distance (EMD), Maximum Mean Discrepancy (MMD) (Borgwardt et al. 2006) and a classifier two-sample test based on a k -nearest-neighbor (KNN) classifier with $k = 1$ (Lopez-Paz and Oquab 2019). All these measures are general purpose GAN metrics. While GAN metrics specialized on video data exist, they rely on extracting features from models pre-trained on three-channel RGB video data. As we are working with single-channel, non-image data, these methods are not applicable in our case.

Experimental Setting

We compare SPATE-GAN to a range of baseline configurations. We use the same GAN architecture for all these settings to ensure comparability. Our GAN generators feed the noise input through two LSTM layers to obtain time-dependent features. These are then mapped into the desired shape for deconvolutional operations using a fully-connected layer with a leaky ReLU activation. Lastly, 4 deconvolutional layers map the output into video frames, all

also with leaky ReLU activations. Our discriminators initially feed video input through three convolutional layers with leaky ReLU activations. The outputs from the convolutional operations are then reshaped and fed through two LSTM layers to create the final discriminator outputs.

All our models are implemented in PyTorch (Paszke et al. 2019) and optimized using the Adam algorithm (Kingma and Ba 2015). Our experiments are conducted on a single Geforce 1080Ti or RTX 3090 GPU. Further training details can be found in Appendix B.

Results

Results from our experiments are shown in Table 1. Visual comparisons between real and generated data from the different models are shown in Figures 2, ??, and ??. For larger figures including results from all tested model configurations, please see the Appendix D. For all three datasets, all SinkGAN results are visually worse than those of COT-GAN. When combined with Moran’s I, samples generated from SinkGAN ^{M} can be seen with obvious defects while those from COT-GAN ^{M} for the Turbulent Flows dataset are also worse than other models for failing to capture the brightness of the highlights in the real data. The differences in samples produced by the remaining models are difficult to distinguish visually. We therefore rely primarily on numerical evaluations in Table 1 for comparison of methods. Through all experiments we can observe that SPATE-GAN ^{ksw} consistently outperforms the competing approaches, achieving the best scores across all datasets and evaluation metrics.

This finding is interesting as the ksw setting theoretically loses information over the k and kw approaches, which both have access to future time steps when calculating the SPATE metric. Nevertheless, this result underlines the strong synergies between SPATE ^{ksw} and the COT-GAN backbone: The metric is calculated in sequential fashion and thus respects the same causality constraints that restrict COT-GAN. As such, the outcome, while noteworthy, is not surprising.

This result is strengthened by a comparison with the SinkGAN-based approaches: SinkGAN does not follow the same restrictions and, as we observe, is not improved as consistently by the SPATE-based embedding losses. In fact, in some cases the naive SinkGAN performs better than its derivatives using SPATE or Moran’s I based embedding losses.

We also observe that throughout all settings, models using Moran’s I perform similarly to their naive counterparts. This confirms that in fact, simply using measures of spatial autocorrelation computed over a sequence is not sufficient for capturing complex spatio-temporal effects. On the contrary, the other two SPATE settings, k and kw , both appear to have beneficial effects and improve performance.

In summary, our results highlight how COT-GAN combined with a non-anticipative measure of space-time association can improve the modeling of complex spatio-temporal patterns. This finding represents another step on the way towards deep learning methods specialized on the dynamics driving many systems on our planet.

LGCP	EMD	MMD	KNN
SinkGAN	12.46 (0.02)	0.38 (0.001)	0.14 (0.001)
SinkGAN ^M	12.46 (0.02)	0.38 (0.001)	0.14 (0.001)
SinkGAN ^k	12.65 (0.03)	0.38 (0.001)	0.15 (0.001)
SinkGAN ^{kw}	10.60 (0.01)	0.63 (0.008)	0.30 (0.002)
SinkGAN ^{ksw}	13.33 (0.01)	0.36 (0.001)	0.38 (0.003)
COT-GAN	12.38 (0.02)	0.30 (0.001)	0.20 (0.004)
COT-GAN ^M	12.38 (0.02)	0.30 (0.001)	0.20 (0.004)
SPATE-GAN ^k	11.56 (0.02)	0.32 (0.01)	0.31 (0.01)
SPATE-GAN ^{kw}	10.92 (0.03)	0.64 (0.035)	0.15 (0.006)
SPATE-GAN ^{ksw}	10.47 (0.02)	0.30 (0.001)	0.39 (0.01)
Extreme Weather			
SinkGAN	29.40 (0.05)	0.49 (0.001)	0.41 (0.004)
SinkGAN ^M	29.27 (0.05)	0.72 (0.002)	0.22 (0.01)
SinkGAN ^k	32.57 (0.03)	0.81 (0.001)	0.16 (0.004)
SinkGAN ^{kw}	32.78 (0.05)	0.81 (0.001)	0.18 (0.004)
SinkGAN ^{ksw}	30.00 (0.04)	0.50 (0.001)	0.41 (0.004)
COT-GAN	26.66 (0.09)	0.43 (0.002)	0.42 (0.002)
COT-GAN ^M	36.42 (0.14)	0.65 (0.002)	0.09 (0.01)
SPATE-GAN ^k	33.58 (0.07)	0.73 (0.002)	0.15 (0.01)
SPATE-GAN ^{kw}	33.36 (0.09)	0.72 (0.002)	0.13 (0.003)
SPATE-GAN ^{ksw}	26.24 (0.07)	0.42 (0.002)	0.42 (0.002)
Turbulent Flows			
SinkGAN	26.52 (0.007)	1.23 (0.001)	0.15 (0.001)
SinkGAN ^M	28.02 (0.005)	1.22 (0.0002)	0.01 (0.002)
SinkGAN ^k	28.14 (0.002)	1.32 (0.002)	0.08 (0.001)
SinkGAN ^{kw}	30.98 (0.001)	1.50 (0.001)	0.03 (0.001)
SinkGAN ^{ksw}	25.47 (0.008)	1.24 (0.0002)	0.13 (0.002)
COT-GAN	27.03 (0.01)	1.22 (0.001)	0.16 (0.002)
COT-GAN ^M	24.93 (0.01)	1.19 (0.001)	0.09 (0.002)
SPATE-GAN ^k	25.70 (0.02)	1.21 (0.001)	0.12 (0.003)
SPATE-GAN ^{kw}	24.30 (0.002)	1.42 (0.001)	0.13 (0.004)
SPATE-GAN ^{ksw}	22.98 (0.01)	1.16 (0.001)	0.16 (0.002)

Table 1: Evaluations for LGCP, EW and TF datasets. Lower values in EMD and MMD indicate better sample quality, while values close to 0.5 are more desirable for KNN.

Furthermore, we provide an investigation on the impact of the lengthscale parameter l in the spatio-temporal expectations for $l \in \{1, 10, 20, 30, 50\}$. As shown in Figure 4, $l = 20$ leads to better EMD and KNN results whilst all MMD scores remain unchanged. For the results presented in this paper, we set $l = 20$ in all our experiments.

Conclusion

Recent studies have called for more research into improving deep learning models for spatio-temporal earth systems data (Reichstein et al. 2019). Other academic domains have dealt with these data for many decades and have developed methods for capturing specific spatial and spatio-temporal effects. Inspired by their approaches, we devise SPATE, a measure of spatio-temporal association capable of detecting emerging space-time clusters and homogeneous areas in the data. We then develop a novel embedding loss for video GANs utilizing SPATE as a means of reinforcing the learning of these patterns-of-interest. Our new generative modeling approach, SPATE-GAN, shows performance increases on a

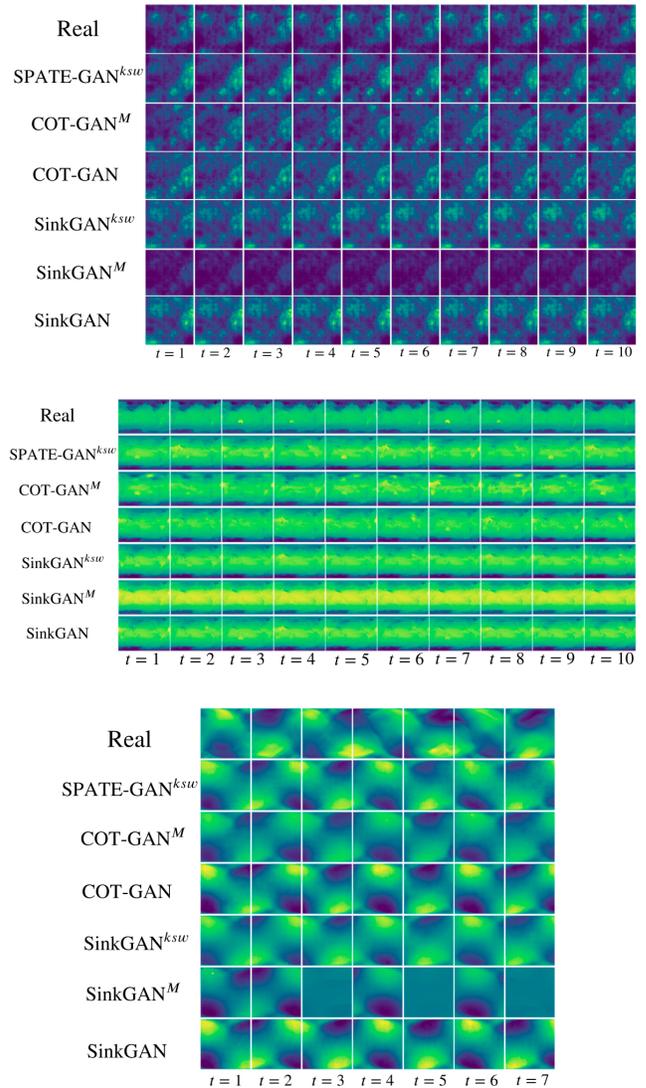


Figure 3: Selected samples from the LGCP, Extreme Weather and Turbulent Flows datasets (top to bottom).

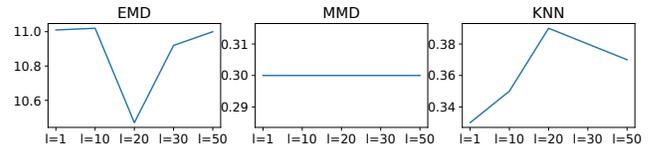


Figure 4: Evaluations of SPATE-GAN^{ksw} (left: EMD, middle: MMD, and right: KNN) on LGCP dataset given length-scale $l \in \{1, 10, 20, 30, 50\}$.

range of different datasets emulating the real-world complexities of spatio-temporal dynamics. As such, this study highlights how domain expertise from applied academic areas can help to motivate methodological advances in machine learning.

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