Neural Cellular Automata Manifold

Abstract

Very recently, a deep Neural Cellular Automata (NCA) [1] has been proposed to simulate the complex morphogenesis process with deep networks. This model learns to grow an image starting from a fixed single pixel. In this paper, we move a step further and propose a new model that extends the expressive power of NCA from a single image to a manifold of images. In biological terms, our approach would play the role of the transcription factors, modulating the mapping of genes into specific proteins that drive cellular differentiation, which occurs right before the morphogenesis. We accomplish this by introducing dynamic convolutions inside an Auto-Encoder architecture, for the first time used to join two different sources of information, the encoding and cell’s environment information. The proposed model also extends the capabilities of the NCA to a general purpose network, which can be used in a broad range of problems. We thoroughly evaluate our approach in a dataset of synthetic emojis and also in real images of CIFAR-10.

1 Introduction

Reproduction of multi-cellular organisms entails generating entire bodies from a single cell. Complex organisms also require to create different types of somatic cells and spatially arrange them to form the different tissues while ensuring temporal stability. These three aspects, cellular differentiation, morphogenesis and cell-growth control are the pillars of developmental biology. Computational methods are a key ingredient of the developmental biology study, up to the point that the term “morphogene” itself was coined by Alan Turing decades before its empirical demonstration [2]. In this context, there exist many different simulation techniques, including systems of partial derivative equation (PDEs), particle systems, and various types of Cellular Automata (CA) [3, 4, 5, 6, 7]. In this paper we conceptually model these fundamental processes using novel dynamic neural network architectures in combination with neural cellular automata (NCA) [1]. We evaluate the proposed approach on the synthetic NotoColorEmoji [8] and real CIFAR-10 [9] datasets. In both cases our model is able to “grow” the images with a low error (see Fig. 1).

Although there is evidence of multi-cellular prokaryotes presenting differentiated cells [10], most complex organisms are eukaryotes (DNA is in a nucleus). Therefore, it seems that the existence of a protected genetic encoding is almost a requirement for the creation of complex organisms. This protection entails the use of a sophisticated transmission mechanism between the DNA and the cellular machinery, which proved to be related with the complexity of the organism [11]. Transcription Factors (TF) are the main players in transcription regulation; coded by master regulatory genes, these factors activate or deactivate the expression of other genes in a regulatory cascade. Many TF are involved in defining organism’s spatial arrangement. Most of them are Morphogenes, soluble molecules that can diffuse and carry signals via concentration gradients.

This biological model inspired our network architecture at macro-scale (see Fig. 2). We define a vector encoding where a common information for all cells is stored, as in DNA. The expression of such encoding in the “cellular machinery” is modulated by a Parameter Predictor (PP), with a
similar role to that of TF. The “cellular machinery” (NCA’s Dynamic Convolutions) receives two sources of information: one from its DNA-encoding through the Parameter Predictor and another from the gradients of Morphogenes in its surrounding environment. Both are combined to model cell differentiation, producing the “phenotype” (color) and other Morphogenes (invisible channels) that drive the expression of neighboring cells. Stochastic update of all the cells in the image for a fixed number of iterations generates the target image.

But our model goes further. It aims to learn not only a single model suitable for a single phenotype, but a single model suitable to model species with thousands of phenotypes. Using an Auto-Encoder architecture trained end to end by back-propagation, our model learns to reproduce a whole dataset of images from a common model, where different codes drive the generation of different images. For the sake of similarity with the biological model, we also included an encoding conceptually similar to that of DNA, i.e. a vector encoding on a base of four possible categorical values similar to our DNA’s cytosine, guanine, adenine and thymine bases (the well-known “CGAT” sequences).

To the best of our knowledge this is the first work to model a whole set of “species” with a neural network trainable end-to-end. Compared to the most similar approach [1], which was able to learn to generate a single image, our single model is capable of reconstructing the whole 50,000 images of the CIFAR-10 dataset. Moreover, previous restriction to work only on RGBA images has been removed boosting its applicability, first, to more abundant RGB images, but also to any kind of data in vectorial format.

We consider that the model we propose could be useful to solve problems such as those faced by Peak et al. [5], when it was not possible to completely model plant’s stomata complexity due to difficulties to obtain CA’s function from noisy real data. Its applications can spread among many other biological domains where CA-modeling has been previously used, from tumor growth processes [6] up to HIV or COVID-19 infection dynamics [7,12,13].

2 Neural Cellular Automata Manifold

Let us first introduce the main concepts of CA and NCA. A Cellular Automata (CA) is a model based on a grid representation of the world. Each cell of the grid is an automaton or program which perceives the environment (i.e. its state and the state of the neighboring cells) and updates its own state according to a fixed rule, generally a mathematical function. The rule is the same for every cell and does not change over time. CA models can be universal [14], which means that they can be programmed to emulate any other system without changing its underlying construction. Despite its expressive power, the main shortcoming of CAs is that given any specific rule, it is impossible
Figure 2: Model overview. Beige elements contain trainable parameters while orange layers use only predicted parameters. See Fig.3 for details of the architecture.

To predict its behavior. This means that in order to understand its behavior, each rule has to be tried with multiple starting states, and its performance needs to be observed for many iterations. The Neural Cellular Automata (NCA), recently proposed by Mordvintsev et al. [1], is a class of Cellular Automata which uses an artificial neural network as update function, so the the NN parameters can be learned to obtain a desired behavior.

We already described in the introduction the biological inspiration of our model. Next, we move forward to its detailed formulation. Formally, our model is defined by the following equations:

$$
I^t = \{C^t_{ij}\} \quad \forall i, j \in I
$$

$$
C^t_{ij} = f(C^{t-1}_{ij}, M^{t-1}_{kl}, \kappa(e^I, \theta, \theta_{LF})) \quad \forall (k, l) \in \epsilon_{ij}
$$

$$
M^t_{ij} = g(C^{t-1}_{ij}, M^{t-1}_{kl}, \kappa(e^I, \theta, \theta_{LF})) \quad \forall (k, l) \in \epsilon_{ij}
$$

$$
\kappa(e^I, \theta) = \mathcal{P}(\mathcal{D}(e^I, \theta_D), \theta_P)
$$

$$
\theta = \{\theta_P, \theta_D\}
$$

$$
\epsilon_{ij} = \{(i-n_x, \ldots, i+n_x), (j-n_y, \ldots, j+n_y)\}
$$

where $I^t$ is the image generated at step $t$, $C^t_{ij}$ is the color vector (RGB or RGB-Alpha) of the pixel in position $(i, j)$, $M^t_{ij}$ is the corresponding vector of “Morphogenes” (i.e. invisible channels in the grid), $\epsilon_{ij}$ are indices of the neighborhood of the cell $(i, j)$ which extend $n_x, n_y$ positions to each side in $x$ and $y$ axis, and $e^I$ is the vector encoding the image. $f(\cdot)$ and $g(\cdot)$ are the functions implemented as an NCA to predict the colors and “Morphogenes”, respectively. $\kappa(e^I, \theta)$ is the function that predicts the weights of the NCA from the encoding $e^I$ and its learned parameters $\theta$, which is actually the composition of the functions learned by the DNA-decoder $\mathcal{D}(\cdot)$ and the Parameter Predictor $\mathcal{P}(\cdot)$. The learned parameters are $\theta_P, \theta_D$ and $\theta_{LF}$, the Leak Factor (see Sec. 2.1).

In order to train this model, we could simply feed it with arbitrary codes, compute the reconstruction error for corresponding target images, and back-propagate the error to learn the parameters. However, we found it more sensible to learn embedding codes that can exploit similarities between images. We, therefore, decided to use an Auto-Encoder architecture [15] at the macro level, which learns to map the set of inputs to a latent space and reconstructs them back. The Auto-Encoder consists of an Encoder and a Decoder (see Fig. 3). The Encoder is composed of two main components: a continuous encoder, that maps the input to a continuous variables encoding; and a DNA-encoder, that transforms this encoding to a categorical variables encoding. The Decoder’s structure is symmetrical, mapping first the DNA-encoding to a continuous encoding which, in turn, feeds the parameter predictor block. From an auto-encoder perspective, the NCA should be considered the third part of the decoder since it is the responsible for finally providing the reconstructed images. From a NN perspective, we can see the NCA as a stack of Residual CNN blocks sharing weights or a “Recurrent Residual CNN” [1].
2.1 Architecture Details

The architecture of the net is based on different types of residual blocks [16]. The smallest building blocks are of 3 types: Convolutional Block 3x3 (CB3), Convolutional Block 1x1 (CB1) and Fully Connected Block (FCB) (see details in Fig. 3). Unlike most of previous works [16, 17, 18], the blocks do not modify input/output representation dimensionality, neither in space resolution or number of filters. While these characteristics can be useful for classification problems, where information needs to be condensed through processing steps, our intuition is that this is not desirable in a reconstruction problem since detail information is lost.

A significant peculiarity of CB1 and CB3 is the expansion of the number features in the internal layer by a factor of 4 and 2, respectively. We consider that this increase of dimensionality of the representation space allows for a better disentanglement of the data manifold. Notice that CB1 needs to be used in combination with CB3 to introduce neighbourhood information. This detail is opposed to previous residual architectures [16, 17, 18] that reduce the number of filters in the inner layer of the block, while using higher dimensionality in the short-cut path.

A specific detail of the architecture is the use of a Leak Factor (LF) as an aid for training stability. LF is a single learnable parameter that regulates how much each successive step contributes to the output. A low value of LF encourages the network to retain most of the knowledge from previous steps, avoiding to distort the image too abruptly at any given step. After the network has learnt the basics of the problem this scenario is less likely, thus the network can learn to let more and more information to leak through each step. LF is constrained between $10^{-3}$ and $10^3$, initialized at $10^{-1}$.

Unlike many architectures that only take the spatial mean of the convolutional output tensor to feed FC layers [16, 17, 18], we use 3 additional slices. Being $(c \times h \times w)$ the dimensions of the output tensor, a spatial mean over $h, w$ provides a $(c)$ dimensional encoding of the image. A mean over $h$ yields a $(c \times w)$ dimensional vector, and doing similarly over the other 2 dimensions $(c \text{ and } w)$, we obtain the input to our FCB of dimension $= c + (c \times h) + (c \times w) + (h \times w)$.

2.2 DNA-encoding

The latent vector representation can be interpreted as the source code that dictates the behavior on the cells of each of the NCAs. This definition inspired us to think of a possible alternative representation of such source code: each value in the latent vector can be encoded into a categorical base, making our encoding compatible to that of the DNA. Notice that a simple quantization on the continuous variable would provide an ordinal discrete variable instead of a DNA-like categorical one.
Figure 4: Growth images/results. First row is a random set of images from the full NotoColorEmoji dataset. Following rows are images generated by different variants of NCAM for the corresponding target images codified as: CE: Continuous encoding, DNA: DNA-encoding; STO: Stochastic update, SYN: Synchronous update; 16-512: number of channels in NCA (16,32) - Dimensionality of the continuous embedding (256, 512, 1024) (DNA dimensionality is 16 times that of continuous).

This encoding is dimensioned to handle the same 32 bits of information of the corresponding float variable, thus no additional bottleneck or expansion is introduced here.

As we can see in Fig.[8] the DNA-encoder is composed of 4 successive CB1 feeding a softmax layer to obtain the 4-categories DNA-embedding. The DNA-decoder follows a symmetrical structure, mapping back each “gene” to a continuous feature. These CB1 are all 1D convolutions, independently expanding each feature of the continuous encoding to a 16-features “gene”. This independent processing of different variables makes no assumption about the “meaning” of each category for one variable in relation to its “meaning” in other variables, so the actual “meaning” depends only on latter interaction between corresponding continuous variables.

In order to train our encoding, we add a biologically plausible noise replacing half of the letters by randomly drawn letters. Our intent is not to precisely mimic the mutation rate of DNA \((2.5 \times 10^{-8}/\text{generation})\) but to enforce a high level of redundancy in the encoding.

2.3 Dynamic Convolutions

Several architectures have been proposed to augment CNNs capabilities, all performing some kind of scaling over intermediate representations between convolutional layers. Attention models [20,21] scale the input according to a spatial probability distribution, being essentially a mask that tells the CNN which parts of the input are the most relevant. Conditioning models use information either from the same network [22], from another network [23] or from a completely independent source [24], to scale the internal representation channel-wise.

An even more precise adjustment is provided by the Dynamic convolutions, where the weights of the convolutional kernel are specifically computed for each sample. In previous works [25,26], the architecture branches in two paths from the input image: one to compute the kernels, and the other to process the input through the dynamic kernels. In contrast, in our approach, the kernel weights are generated from an encoding which is completely independent (and different) from the image to be processed by them. Indeed, the image to be processed in the first step is the pixel seed, which is the same for all targets. Similarly to [25], for an image sample \(I\), being \(X^I\) the input tensor of the convolution and \(Y^I\) the output tensor, we define the dynamic convolution as

\[
Y^I_n = \sum_m \kappa(e^I)_mn \ast X^I_m,
\]

where \(\kappa(e^I)_mn\) is the convolution kernel dynamically computed from the encoding for \(I\), and \((m,n)\) are the input and output channels of the convolution.
2.4 Neural Cellular Automata Architecture

The last component of the decoder is an NCA. To reconstruct an image, the NCA starts from a pixel seed image (typically a blank image with a different pixel). Then, each cell in the grid recurrently perceives the environment and computes an update. After a fixed number of steps, the output is evaluated and the reconstruction error back-propagated. In [1], NCA’s kernel weights are directly updated, but in our case the error is back-propagated further, through the NCA and to the parameter predictor, updating its weights instead of the NCA’s. We can divide the NCA architecture in two main blocks, perception and update.

The **Perception Layer** was designed to propagate the gradients across the grid in the 16 channels composing it (the first four corresponding to the visible RGBA). This is achieved with manually defined Sobel filters (see Fig. 2), similarly to [1]. Since our network’s architecture has only ReLU activation functions, the activations have an unbounded positive value. Given the recurrent architecture of the NCA, during the training process, an exponential reinforcement can occur, leading activations and weights to $\infty$ and degenerate states. To avoid this problem, we apply instance normalization [27] on top of the Sobel filters.

To compute the **Update**, we use the same network architecture as in [1], consisting on 2 pixel-wise dense layers (implemented as 1x1 convolutions). The update is modulated by the Leak Factor (the only trainable parameter of the NCA), which is analogous to the LF used in the Continuous Encoder. Finally, the update is stochastically applied on the current state with an independent probability of $p = 0.5$ for each cell.

3 Experiments

We next present several experiments to highlight different aspects of our Neural Cellular Automata Manifold (NCAM). We also provide qualitative and quantitative evaluation (MSE error).

**Datasets.** NotoColorEmoji dataset [8]: 2924 images of synthetic emojis. This kind of images are very simple and with sharp edges, therefore it is relatively easy to visually assess the quality of the produced images. The original images are 128x128 pixels but in our experiments we downsampled them to 64x64 to reduce the computational requirements. CIFAR-10 dataset [9]: 50,000 real 32x32 images from 10 categories: plane, car, bird, cat, deer, dog, frog, horse, ship, truck. The number of images and its variability make it a challenging dataset to reconstruct.
Continuos vs. DNA encoding. Generation images/results for these two sets of experiments are very similar, both visually (see Fig. 4, rows 1-2) and numerically in MSE (CE: 0.01591, DNA: 0.01633). images/results show no clear reduction or increase on performance with the extra processing involved in the DNA encoding and decoding process. We consider that the proposed DNA-encoding methodology achieves the desired objective of obtaining an equivalent encoding. It is remarkable the absence of artifacts in the background of the emojis given that we removed the alive masking feature used in [1], proving that our design is able to learn by itself the limits of the figure.

Stochastic vs. synchronous update. We consider that the stochastic update feature of the NCA, while being relevant in the biological analogy, may suppose an extra difficulty in the learning process. In these experiments we remove the stochastic update ($p = 0.5$) making it synchronous at every time step ($p = 1.0$). Notice that this change implies, on average, doubling the number of steps on the NCA processing. It also makes more reliable the expected state of neighboring cells. This modification reduced the error significantly in both scenarios, continuous and DNA encoding. Note that images generated with this approach succeed in reconstructing even the finest details (see Fig. 4, rows 3-4). Numeric error is almost one order of magnitude below stochastic approaches (MSE: CE: 0.00199, DNA: 0.00262).

Effect of encoding dimensionality. In our preliminary experiments we set what we found to be good dimensionalities for different elements of the network. We next evaluate our method under significant changes in the encoding dimensionality setting it to half (256) and double (1024) size. Notice that these dimensionalities refer to the continuous encoding, the actual DNA-encoding dimensions are 16 times larger. The experiments show (see Fig. 4, rows 5-6) that there is a significant quality degradation when the dimensionality is reduced to half while there is no appreciable improvement when it is doubled (MSE: 256: 0.02302, 1024: 0.01584). Therefore, we consider that the embedding size is not a bottleneck for the problem at hand.

Smaller datasets. In order to assess the challenge that the size of the dataset and its visual complexity poses on the proposed method, we experiment on 4 different subsets of the NotoColorEmoji dataset, classified by the authors according to their visual appearance. Chars (96 images): emojis containing characters of the Latin set and a few symbols. They are simple shapes, usually with straight lines and few colors. Emos (103 images): round yellow faces showing emotions. Heads (858 images): images of person heads, typically showing different professions. All these images include the full set of versions according to skin tone. Variety (684 images): images not present in previous sets that are also visually different among them. It mainly includes animals, objects and food.

images/results show that, as expected, problems have a growing level of difficulty in terms of MSE: Chars: 0.00976 < Emos: 0.01799 < Heads: 0.02439 < Variety: 0.05035 which can also be visually assessed on Fig. 5. The primary factor is the visual complexity or variety, not the size of the dataset. Linear simple shapes seem easier to generate than more rounded or intricate ones.

"Genetic engineering". We next play a little of "genetic engineering", injecting part of the DNA-encoding from some images to others. To do so, we first generate a mean encoding of a group of
source images that share a visual trait. We compute the mean of the 4 discrete features over the
samples (i.e. DNA categories) and take the ones with values over a defined threshold. Notice that
since they are produced by a softmax we can not have two values over 0.5. If none of the values is
over the threshold we would have new category “none” which the DNA-decoder will ignore. With
this encoding we generate the mean image. The parts of the mean encoding that are not “none” will
substitute corresponding parts of target image encoding.

images/results in Fig. 6 show some interesting properties of the embedding. The lack of several
features in the mean encoding causes no perturbation in the common traits and usually also provides
a reasonable solution for the uncommon. The transfer process does not disrupt other common traits in
target images. If the traits transferred collide with existing traits, they produce mixed shapes. We can
observe that some traits that are not common in the source images are also transferred, suggesting
some kind of trait dominance.

CIFAR-10 images/results. Finally, we report images/results on CIFAR-10 dataset [9]. Note that in
this case, our NCAM model is capable to generate up to 50K different images. In Fig. 1 we show an
example of image formation for this case. On this dataset we only experimented with the synchronous
update (best solution) since it is difficult to appreciate the level of detail required to visually evaluate
the quality of the images/results (see Fig. 7). However, MSE values obtained are CE: 0.00717 DNA:
0.00720, perfectly comparable with those of NotoColorEmoji.

4 Conclusions

Machine learning techniques are already considered critical for the study of epigenetic processes,
meddling between genetic information and their expression, which hold immense promise for
medical applications [28]. The model proposed here successfully simulates the main components of
developmental biology, from ADN encoding to morphogenesis, at a high conceptual level. In our
experiments, it is capable of reproducing almost 3,000 different emoji images, with a great level of
detail, and up to 50,000 real images of the CIFAR-10 dataset. Given its unique structure, capable of
combining DNA-encoded and environment information, demonstrated scalability and robustness to
noise, we consider it has an enormous potential in modeling genetic expression problems.

It is important to notice that the properties of the manifold learnt by the proposed Auto-Encoder will
depend on the loss function used for training. In our work, we use MSE loss to learn to reproduce
original images with high fidelity. If we were to use an adversarial loss [29], we likely would obtain
visually plausible images of the same class but not an exact replica. We consider that the application
of a reinforcement learning loss [30] could allow to produce a model driven by a fitness metric, such
model would then be similar to genetic evolution. These simple adaptations open unfathomable use
possibilities for the NCAM.

As stated in the introduction, CA models are widespread in biology and we consider that the
generalization capabilities shown by the proposed method can be of interest in many different fields,
specially where the model needs to be universal and able to fit noisy data. Cellular automata models
have been proposed to obtain predictions on disease spreading [31, 7, 32] and, more recently, on the
COVID 19 pandemic evolution [12, 13]. We consider our model could also be of special interest for
these tasks due to the capabilities shown and the ease to adapt it to different problems.
Acknowledgments

Broader Impact

As stated before, CA models are widespread in biology and many other fields. We consider that the generalization capabilities shown by the proposed method can be of interest in many different fields, specially where the model needs to be universal and able to fit noisy data. Considering the myriad of possible adaptations, we cannot anticipate its use cases. It is of special relevance nowadays CA's modeling to obtain predictions on disease spreading, more precisely on current COVID 19 pandemic evolution. We consider our model could be of special interest for these task due to the capabilities shown and the ease to adapt it to different problems. On the other side, we must recognize our lack of imagination to foresee possible negative outcomes.

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