

Recurrent Generative Stochastic Networks for Sequence Prediction

Abstract

We present a new generative model for unsupervised learning of sequence representations, the recurrent Generative Stochastic Network (RNN-GSN). This approach builds on recent deep recurrent neural network architectures for modeling high-dimensional, multimodal input distributions, and is able to predict complex sequences of these distributions. The RNN-GSN is non-probabilistic and easier to perform inference over compared to other representation models, such as the RNN-RBM or NADE variants. We provide experimental validation for this new model on sequences of MNIST images and standard MIDI music datasets.

1. Introduction

Unsupervised sequence learning is an important problem in machine learning given that most information (ranging from speech to video to music to even consumer behavior) is often unlabeled and has a sequential structure. Most of these sequences consist of high-dimensional, complex objects such as words in text, images in video, or chords in music. Recently, recurrent neural networks (RNN) (Rumelhart et al., 1986) have become state-of-the-art for sequence representation because they have an internal memory that can learn long-term, temporal dependencies. Further advances with Hessian-free optimization and Long Short-term Memory for RNNs (Martens & Sutskever, 2011; Hochreiter & Schmidhuber, 1996) have enabled learning highly complex temporal dependencies.

While traditional RNNs can learn complex sequences through maintaining an internal memory, they don't deal well when modeling complex input distributions, where the conditional distribution at each time step is highly multimodal. In real-world data, we often care more about this conditional distribution rather than the expected value. In music, for example, the existence of a particular note can greatly change the probabilities with which other notes occur at the same time in a chord. In consumer behavior, the

existence of a particular action taken can greatly change the probabilities of other actions made within the same time window. We would prefer to reason and perform inference over these distributions at each time step to form a better representation of the sequences.

Deep RNN architectures have been proposed to alleviate the traditional RNN architecture shortcomings with complex input distributions (Pascanu et al., 2013). One proposed framework involves using deep input-to-hidden or hidden-to-output functions to reduce input complexity, making the RNN's temporal modeling task easier. These functions exploit the ability of deep networks to disentangle the underlying factors of variation of the original input and flatten high-density data manifolds (Goodfellow et al., 2009; Glorot et al., 2011; Bengio et al., 2012).

One such model, the RNN-RBM, replaces the output layer of an RNN with a restricted Boltzmann machine (RBM) to provide a conditional generative model over the input distribution (Boulanger-Lewandowski et al., 2012; Boulanger-Lewandowski, 2014). The RNN-RBM is a generalization of previous recurrent temporal RBM work (Sutskever et al., 2009) that has shown promise for modeling complex sequences such as MIDI representations of polyphonic music. Another possible model is to replace the RNN output layer with a neural autoregressive distribution estimator (NADE), which has been shown to provide a tractable distribution estimator that performs similarly to large, intractable RBMs (Larochelle & Murray, 2011).

Motivated by the promise of deep RNN models for learning sequence representations, we propose a model using a Generative Stochastic Network (GSN) as the hidden-to-output function of an RNN, called the RNN-GSN. GSNs are a recent generalization of denoising autoencoders (Bengio et al., 2013a) that are easier to perform inference over compared to RBMs and sample from compared to NADEs. GSNs are non-probabilistic, generative models that have also been shown to learn the same model as a deep orderless NADE, which alleviates the factorization ordering drawback of a traditional NADE model (Yao et al., 2014).

The rest of this paper explains the RNN-GSN model and provides experimental evidence for its use in modeling complex sequences. In Sections 2, 3, and 4, we introduce the GSN, RNN, and RNN-GSN architectures in more detail. We then provide experimental validation of the RNN-

GSN on sequences of MNIST images and standard MIDI datasets in Section 5.

2. Generative Stochastic Networks

Generative stochastic networks (GSN) are a generalization of the denoising auto-encoder and help solve the problem of mixing between many major modes of the input data distribution.

2.1. Denoising auto-encoder

Denoising auto-encoders use a Markov chain to learn a reconstruction distribution $P(X|\tilde{X})$ given a corruption process $C(\tilde{X}|X)$ for some data X . Denoising auto-encoders have been shown as generative models (Bengio et al., 2013b), where the Markov chain can be iteratively sampled from:

$$X_t \sim P_{\Theta}(X|\tilde{X}_{t-1}) \quad (1)$$

$$\tilde{X}_t \sim C(\tilde{X}|X_t) \quad (2)$$

As long as the learned distribution $P_{\Theta_n}(X|\tilde{X})$ is a consistent estimator of the true conditional distribution $P(X|\tilde{X})$ and the Markov chain is ergodic, then as $n \rightarrow \infty$, the asymptotic distribution $\pi_n(X)$ of the generated samples from the denoising auto-encoder converges to the data-generating distribution $P(X)$ (Bengio et al., 2013b).

2.2. Easing restrictive conditions on the denoising auto-encoder

A few restrictive conditions are necessary to guarantee ergodicity of the Markov chain - requiring $C(\tilde{X}|X) > 0$ everywhere that $P(X) > 0$. Particularly, a large region V containing any possible X is defined such that the probability of moving between any two points in a single jump $C(\tilde{X}|X)$ must be greater than 0. This restriction requires that $P_{\Theta_n}(X|\tilde{X})$ has the ability to model every mode of $P(X)$, which is a problem this model was meant to avoid.

To ease this restriction, Bengio et al. (Bengio et al., 2013a) prove that using a $C(\tilde{X}|X)$ that only makes small jumps allows $P_{\Theta}(X|\tilde{X})$ to model a small part of the space V around each \tilde{X} . This weaker condition means that modeling the reconstruction distribution $P(X|\tilde{X})$ would be easier since it would probably have fewer modes.

However, the jump size σ between points must still be large enough to guarantee that one can jump often enough between the major modes of $P(X)$ to overcome the regions of low probability: σ must be larger than half the largest distance of low probability between two nearby modes, such that V has at least a single connected component between modes. This presents a tradeoff between the difficulty of learning $P_{\Theta}(X|\tilde{X})$ and the ease of mixing between modes

separated by this low probability region.

2.3. Generalizing to GSN

While denoising auto-encoders can rely on X_t alone through a deterministic procedure for the state of the Markov chain, GSNs introduce a latent variable H_t that acts as an additional state variable in the Markov chain along with the visible X_t (Bengio et al., 2013a):

$$H_{t+1} \sim P_{\Theta_1}(H|H_t, X_t) \quad (3)$$

$$X_{t+1} \sim P_{\Theta_2}(X|H_{t+1}) \quad (4)$$

The latent state variable H can be equivalently defined as $H_{t+1} = f_{\Theta_1}(X_t, Z_t, H_t)$, a learned function f with an independent noise source Z_t such that X_t cannot be reconstructed exactly from H_{t+1} . If X_t could be recovered from H_{t+1} , the reconstruction distribution would simply converge to the Dirac at X . Denoising auto-encoders are therefore a special case of GSNs, where f is fixed instead of learned.

GSNs also use the notion of walkbacks to aid training. Walkbacks are the process of generating samples by iteratively sampling from $P_{\Theta_1}(H|H_t, X_t)$ and $P_{\Theta_2}(X|H_{t+1})$ for a given input. By using walkbacks, the model is more likely to seek out spurious modes in the data distribution and correct for them (Bengio et al., 2013b). The resulting Markov chain of a GSN is inspired by Gibbs sampling, but with stochastic units at each layer that can be backpropagated (Rezende et al., 2014).

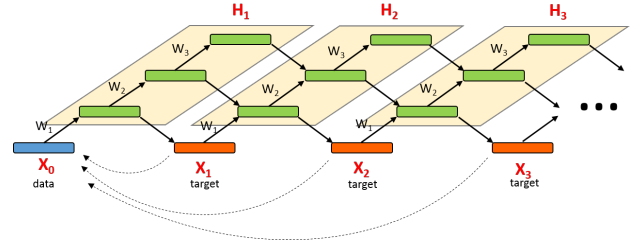


Figure 1. Unrolled GSN Markov chain.

Experimental results with GSNs show that their latent states mix well between the major modes of the data - mixing faster at higher layers in the model (Bengio et al., 2013a). Using this property, we tested a simple temporal GSN model to predict sequences of inputs. The temporal GSN uses a linear transformation $H \rightarrow H$ to predict $P(H_t|H_{t-1}, \dots, H_{t-n})$ with an input history of size n . Using this predicted H_t , an expected input x_t was sampled from the model's learned reconstruction distribution $P_{\Theta_2}(X|H)$.

Qualitatively, this model appears to predict temporal dependencies well within its history window n (Figure 3).

This result provided motivation to use the latent state H as the emitted parameter in a better-suited temporal model, such as an RNN.

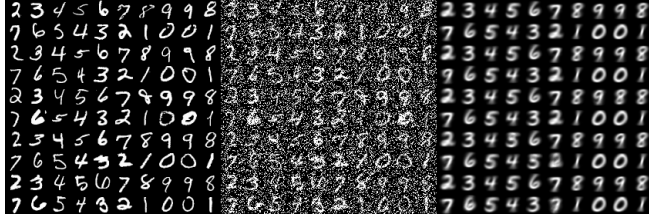


Figure 2. Temporal GSN with history $n = 2$ trained on an arbitrary MNIST sequence. Original input sequence is on the left, a noisy version of the input fed into the model is in the middle, and the predicted input based on the history is on the right.

3. Recurrent Neural Networks

Traditional RNNs simulate a discrete-time system that has an input sequence $\{x_1 \dots x_t\}$ and a hidden state sequence $\{h_1 \dots h_t\}$ that map to an output sequence $\{y_1 \dots y_t\}$. The network is defined for timestep t in the sequence by the hidden and output equations:

$$h_t = \Phi_h(W^T h_{t-1} + U^T x_t + b_h) \quad (5)$$

$$y_t = \Phi_y(V^T h_t + b_y) \quad (6)$$

where Φ_h and Φ_y are element-wise nonlinear functions and W , U , V , b_h , and b_y are the network parameters Θ . The hidden state h contains all information about the sequence for a given timestep t .

RNNs can be trained via backpropagation over a set number of time steps, which is known as backpropagation through time. However, due to the exploding gradient problem, backpropagation through time has difficulty training the parameters for long-term temporal dependencies. To fix the exploding gradient problem, long short-term memory units (LSTM) (Hochreiter & Schmidhuber, 1996) can be introduced as the hidden units that contain extra parameters to learn a gated memory for storing the unit's activation value for a period of time steps. With this architecture, normal backpropagation through time can train the model to learn much longer temporal dependencies. Alternatively, Hessian-free optimization (Martens & Sutskever, 2011) can learn the model parameters for long-term temporal dependencies without needing to introduce specialized hidden units.

3.1. Extension to deep RNN

While traditional RNNs can be seen as deep networks over multiple timesteps due to the hidden connections $h_{t-1} \rightarrow h_t$, they suffer from being shallow, meaning they only contain a single nonlinear layer, at each individual timestep.

This property limits the complexity of inputs RNNs can realistically represent. When analyzing RNNs in a single timestep, there are four areas where depth can be added: input-to-hidden function $x_t \rightarrow h_t$, hidden-to-output function $h_t \rightarrow y_t$, hidden-to-hidden function $h_{t-1} \rightarrow h_t$, and stacking hidden layers h_t (Pascanu et al., 2013).

Adding depth to the input-to-hidden function $x_t \rightarrow h_t$ exploits the non-temporal structure of the input. Because higher-level representations tend to better disentangle the underlying factors of variation in the original input (Bengio et al., 2012), using a deep input-to-hidden function should reduce complexity of the input to the RNN. With a less complex input, the RNN can model the temporal structure between successive timesteps more easily, rather than wasting parameters to also model the input complexity.

Similarly, adding depth to the hidden-to-output function $h_t \rightarrow y_t$ reduces the complexity of the recurrent hidden state, which makes predicting the output easier. This also allows the hidden state to use less parameters for modeling output complexity, which allows it to devote more resources for modeling temporal structure; the hidden state learns a more efficient temporal representation. This is the structure used by the RNN-RBM/NADE variants, as well as the RNN-GSN used for experiments in Section 5.

A deep hidden-to-hidden transition function $h_{t-1} \rightarrow h_t$ is slightly different, where multiple layers are added between each timestep. By increasing the number of layers in the hidden states, the RNN can adapt more quickly to changing modes of the input data distribution. However, introducing depth in the recurrent hidden state creates difficulty for performing backpropagation through time, as the gradient has to traverse through more nonlinear steps. This increases the difficulty of capturing longer-term temporal dependencies. The deep hidden-to-hidden transition structure has been used successfully as a recurrent convolutional neural network (RCNN), which uses a convolutional neural network to model the transition between consecutive RNN hidden states (Pinheiro & Collobert, 2013).

Finally, RNNs can be made deeper by stacking the hidden layers h_t . This approach differs from deep hidden-to-hidden transitions because each stacked hidden layer would take input from the previous timestep's hidden layers and pass output to the next timestep's hidden layers. This architecture might allow the RNN to represent multiple time scales in the input sequence.

These deeper architectures for RNNs serve the purpose of increasing the efficiency with which the recurrent hidden states H can model the temporal structure of the inputs. We explore adding depth per static frame with the hidden-to-output function, as well as theoretically combining it with a deep input-to-hidden function. This way, the recurrent

hidden states can work exclusively on modeling the temporal relationships in the data in a less complex space.

4. The RNN-GSN

The recurrent GSN (RNN-GSN)

$$\hat{H}_t = \Phi_h(A^T U_t + b_h) \quad (7)$$

$$\hat{X}_t \sim GSN(X, \hat{H}) \quad (8)$$

$$U_{t+1} = \Phi_u(B^T X_t + C^T U_t + b_u) \quad (9)$$

where Φ_h and Φ_u are element-wise nonlinear functions, A , B , C , b_h , and b_u are the recurrent network parameters, and $GSN(X, \hat{H})$ is a GSN from Section 2 trained with parameters Θ_1 and Θ_2 .

This architecture retains separation between the recurrent part and the deep GSN part.

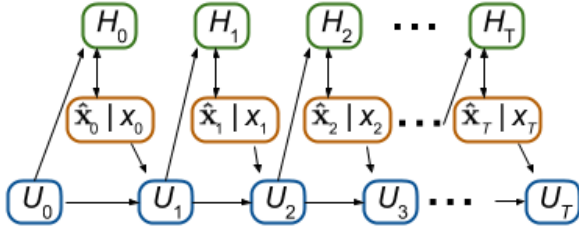


Figure 3. RNN-GSN architecture. Input distribution is X , GSN hidden layers are H , and recurrent hidden units are U .

$$\hat{H}_t = \Phi_h(A^T U_t + b_h) \quad (10)$$

$$\hat{X}_t \sim GSN(X, H) \quad (11)$$

$$H_t \sim GSN(X, H) \quad (12)$$

$$U_{t+1} = \Phi_u(B^T H_t + C^T U_t + b_u) \quad (13)$$

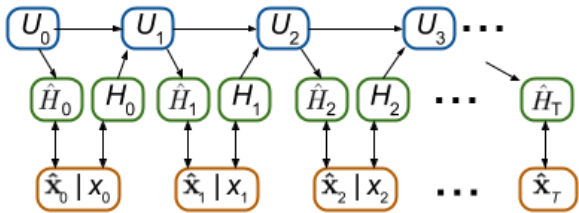


Figure 4. Extension of the RNN-GSN to use both deep input-to-hidden and hidden-to-output functions with a GSN.

4.1. Initialization strategies

5. Experiments

This is the experiments section. Each RNN-GSN was first initialized with GSN parameters and trained with noise scheduling, which has been shown to help the network learn appropriate features during stochastic gradient descent (Geras & Sutton, 2014).

5.1. Sequences of MNIST digits

arbitrary sequences of images.

- Sequence1 is a simple linear sequence of digits 0-9 repeating.
- Sequence2 introduces one bit of parity by alternating sequences 0-9 and 9-0 repeating, where the next value depends on whether the sequence is ascending or descending.
- Sequence3 creates a longer, more complex sequence by introducing a second bit of parity. It is formed by:

Log-likelihoods are estimated by a Parzen density estimator, which is biased. Further validation can be seen qualitatively by the predicted samples produced from the model.

5.2. Sequences of polyphonic music

midi stuff.

- Piano-midi.de
- Nottingham
- MuseData
- JSB chorales

Log-likelihoods estimated by the Parzen density estimator are biased and cannot be compared to the AIS estimation used by Boulanger-Lewandowski et al. However, accuracies as computed by Bay et al. are provided for comparison (Bay et al., 2009).

6. Conclusion

We presented the RNN-GSN, a generative, non-probabilistic model for learning deep sequence representations. We validated its efficacy as a deep recurrent model on complex inputs with sequences of MNIST images and MIDI representations of polyphonic music. The RNN-GSN works as well as other deep recurrent models, such as the RNN-RBM, but is an easier framework

to perform inference over and sample from due to its non-probabilistic nature.

Further improvements and areas of study could be using LSTM units in the RNN or Hessian-free optimization, and combining depth at multiple stages of the RNN. We would like to look into using GSNs as both the input-to-hidden and hidden-to-output functions of the RNN, further reducing the complexity for representing the sequence. Finally, multimodal GSNs could provide benefits when the hidden representations of the input data distribution cannot be assumed as unimodal (Ozair et al., 2013).

References

- Bay, Mert, Ehmann, Andreas F, and Downie, J Stephen. Evaluation of multiple-f0 estimation and tracking systems. In *10th International Society for Music Information Retrieval Conference*, 2009.
- Bengio, Yoshua, Mesnil, Grégoire, Dauphin, Yann, and Rifai, Salah. Better mixing via deep representations. *CoRR*, abs/1207.4404, 2012.
- Bengio, Yoshua, Thibodeau-Laufer, Eric, and Yosinski, Jason. Deep generative stochastic networks trainable by backprop. *CoRR*, abs/1306.1091, 2013a.
- Bengio, Yoshua, Yao, Li, Alain, Guillaume, and Vincent, Pascal. Generalized denoising auto-encoders as generative models. *CoRR*, abs/1305.6663, 2013b.
- Boulanger-Lewandowski, Nicolas. *Modeling High-Dimensional Audio Sequences with Recurrent Neural Networks*. PhD thesis, Université de Montréal, april 2014.
- Boulanger-Lewandowski, Nicolas, Bengio, Yoshua, and Vincent, Pascal. Modeling temporal dependencies in high-dimensional sequences: Application to polyphonic music generation and transcription. In *Proceedings of the 29th International Conference on Machine Learning*, 2012.
- Geras, Krzysztof J. and Sutton, Charles A. Scheduled denoising autoencoders. *CoRR*, abs/1406.3269, 2014.
- Glorot, Xavier, Bordes, Antoine, and Bengio, Yoshua. Domain adaptation for large-scale sentiment classification: A deep learning approach. In *Proceedings of the Twenty-eight International Conference on Machine Learning, ICML*, 2011.
- Goodfellow, Ian, Lee, Honglak, Le, Quoc V., Saxe, Andrew, and Ng, Andrew Y. Measuring invariances in deep networks. In Bengio, Y., Schuurmans, D., Lafferty, J.D., Williams, C.K.I., and Culotta, A. (eds.), *Advances in Neural Information Processing Systems 22*, pp. 646–654. Curran Associates, Inc., 2009.
- Hochreiter, Sepp and Schmidhuber, Jürgen. Bridging long time lags by weight guessing and "long short term memory". In *Spatiotemporal models in biological and artificial systems*, pp. 65–72. IOS Press, 1996.
- Larochelle, Hugo and Murray, Iain. The neural autoregressive distribution estimator. *Journal of Machine Learning Research*, 15:29–37, 2011.
- Martens, James and Sutskever, Ilya. Learning recurrent neural networks with hessian-free optimization. In *Proceedings of the 28th International Conference on Machine Learning (ICML-11)*, pp. 1033–1040, 2011.
- Ozair, Sherjil, Yao, Li, and Bengio, Yoshua. Multimodal transitions for generative stochastic networks. *CoRR*, abs/1312.5578, 2013.
- Pascanu, Razvan, Gülçehre, Çağlar, Cho, Kyunghyun, and Bengio, Yoshua. How to construct deep recurrent neural networks. *CoRR*, abs/1312.6026, 2013.
- Pinheiro, Pedro H. O. and Collobert, Ronan. Recurrent convolutional neural networks for scene parsing. *CoRR*, abs/1306.2795, 2013.
- Rezende, Danilo J., Mohamed, Shakir, and Wierstra, Daan. Stochastic backpropagation and approximate inference in deep generative models. In *Proceedings of the 31st International Conference on Machine Learning*, 2014.
- Rumelhart, David E., Hinton, Geoffrey E., and Williams, Ronald J. Learning representations by back-propagating errors. In *Parallel Dist. Proc.*, pp. 318–362. MIT Press, 1986.
- Sutskever, Ilya, Hinton, Geoffrey E., and Taylor, Graham W. The recurrent temporal restricted boltzmann machine. In Koller, D., Schuurmans, D., Bengio, Y., and Bottou, L. (eds.), *Advances in Neural Information Processing Systems 21*, pp. 1601–1608. Curran Associates, Inc., 2009.
- Yao, Li, Ozair, Sherjil, Cho, Kyunghyun, and Bengio, Yoshua. On the equivalence between deep nade and generative stochastic networks. *CoRR*, abs/1409.0585, 2014.