Bidirectional Recurrent Neural Networks as Generative Models

Anonymous Author(s) Affiliation Address email

Abstract

Bidirectional recurrent neural networks (RNN) are trained to predict both in the positive and negative time directions simultaneously. They have not been used commonly in unsupervised tasks, because a probabilistic interpretation of the model has been difficult. Recently, two different frameworks, GSN and NADE, provide a connection between reconstruction and probabilistic modeling, which makes the interpretation possible. As far as we know, neither GSN or NADE have been studied in the context of time series before. As an example of an unsupervised task, we study the problem of filling in gaps in high-dimensional time series with complex dynamics. Although unidirectional RNNs have recently been trained successfully to model such time series, inference in the negative time direction is non-trivial. We propose two probabilistic interpretations of bidirectional RNNs that can be used to reconstruct missing gaps efficiently. Our experiments on text data show that both proposed methods are much more accurate than unidirectional reconstructions, although a bit less accurate than a computationally complex bidirectional Bayesian inference on the unidirectional RNN. We also provide results on music data for which the Bayesian inference is computationally infeasible, demonstrating the scalability of the proposed methods.

033 034 035

036

000 001 002

003

005

007 008 009

010

011

016

018

019

021

022

023

024

025

026

027

028

029

030

031

1 Introduction

Recurrent neural networks (RNN) have recently been trained successfully for time series modeling, and have been used to achieve state-of-the-art results in supervised tasks including handwriting
recognition (Graves *et al.*, 2009) and speech recognition (Graves *et al.*, 2013). RNNs have also been used successfully in unsupervised learning of time series (Sutskever *et al.*, 2011; Boulanger-Lewandowski *et al.*, 2012).

Recently, RNNs have also been used to generate sequential data (Bahdanau *et al.*, 2015) in a machine translation context, which further emphasizes the unsupervised setting. Bahdanau *et al.* (2015) used a bidirectional RNN to encode a phrase into a vector, but settled for a unidirectional RNN to decode it into a translated phrase, perhaps because bidirectional RNNs have not been studied much as generative models. Even more recently, Maas *et al.* (2014) used a deep bidirectional RNN in speech recognition, generating text as output.

Missing value reconstruction is interesting in at least three different senses. Firstly, it can be used to cope with data that really has missing values. Secondly, reconstruction performance of artificially missing values can be used as a measure of performance in unsupervised learning (Raiko and Valpola, 2001). Thirdly, reconstruction of artificially missing values can be used as a training criterion (Brakel *et al.*, 2013; Goodfellow *et al.*, 2013; Uria *et al.*, 2014). While traditional RNN training criterion corresponds to one-step prediction, training to reconstruct longer gaps can push the model towards concentrating on longer-term predictions. Note that one-step prediction criterion is typically



Figure 1: Structure of the simple RNN (left) and the bidirectional RNN (right).

used even in approaches that otherwise concentrate on modelling long-term dependencies (see e.g. Mikolov et al., 2014; Koutník et al., 2014).

067 When using unidirectional RNNs as generative models, it is straightforward to draw samples from 068 the model in sequential order. However, inference is not trivial in smoothing tasks, where we want 069 to evaluate probabilities for missing values in the middle of a time series. For binary data, inference 070 with gap sizes of one is feasible - however, inference with larger gap sizes becomes exponentially 071 more expensive. Even sampling can be exponentially expensive with respect to the gap size.

One strategy used for training models that are used for filling in gaps is to explicitly train the model 073 with missing data (see e.g. Brakel et al., 2013). However, such a criterion has not to our knowledge 074 yet been used and thoroughly evaluated compared with other inference strategies for RNNs. 075

076 In this paper, we compare different methods of using RNNs to infer missing values for binary time series data. We evaluate the performance of two generative models that rely on bidirectional 077 RNNs, and compare them to inference using a unidirectional RNN. The proposed methods are very 078 favourable in terms of scalability. 079

2 **Recurrent Neural Networks**

Recurrent neural networks (Rumelhart et al., 1986; Haykin, 2009) can be seen as extensions of the standard feedforward multilayer perceptron networks, where the inputs and outputs are sequences instead of individual observations.

Let us denote the input to a recurrent neural network by $\mathbf{X} = {\mathbf{x}_t}$ where $\mathbf{x}_t \in \mathbb{R}^N$ is an input vector for each time step t. Let us further denote the output as $\mathbf{Y} = {\mathbf{y}_t}$ where $\mathbf{y}_t \in \mathbb{R}^M$ is an 088 output vector for each time step t. Our goal is to model the distribution $P(\mathbf{Y}|\mathbf{X})$. Although RNNs map input sequences to output sequences, we can use them in an unsupervised manner by letting the RNN predict the next input. We can do so by setting $\mathbf{Y} = {\mathbf{y}_t = \mathbf{x}_{t+1}}$.

2.1 Unidirectional Recurrent Neural Networks

The structure of a basic RNN with one hidden layer is illustrated in Figure 1, where the output y_t is determined by

> $P\left(\mathbf{y}_{t} \mid \{\mathbf{x}_{d}\}_{d=1}^{t}\right) = \phi\left(\mathbf{W}_{v}\mathbf{h}_{t} + \mathbf{b}_{v}\right)$ (1)

where 100

054 055

064 065

066

080 081

082 083

084

085

087

089

090

091 092

094

095

096 097

101

$$\mathbf{h}_{t} = \tanh\left(\mathbf{W}_{h}\mathbf{h}_{t-1} + \mathbf{W}_{x}\mathbf{x}_{t} + \mathbf{b}_{h}\right)$$
(2)

102 and \mathbf{W}_{v} , \mathbf{W}_{h} , and \mathbf{W}_{x} are the weight matrices connecting the hidden to output layer, hidden to 103 hidden layer, and input to hidden layer, respectively. \mathbf{b}_{v} and \mathbf{b}_{h} are the output and hidden layer bias vectors, respectively. Typical options for the final nonlinearity ϕ are the softmax function 104 for classification or categorical prediction tasks, or independent Bernoulli variables with sigmoid 105 functions for other binary prediction tasks. In this form, the RNN therefore evaluates the output y_t 106 based on information propagated through the hidden layer that directly or indirectly depends on the 107 observations $\{\mathbf{x}_d\}_{d=1}^t = \{\mathbf{x}_1, \dots, \mathbf{x}_t\}.$

108 2.2 Bidirectional Recurrent Neural Networks

Bidirectional RNNs (BRNN) (Schuster and Paliwal, 1997; Baldi *et al.*, 1999) extend the unidirectional RNN by introducing a second hidden layer, where the hidden to hidden connections flow in opposite temporal order. The model is therefore able to exploit information both from the past and the future.

114 The output \mathbf{y}_t is traditionally determined by

$$P\left(\mathbf{y}_{t} \mid \{\mathbf{x}_{d}\}_{d \neq t}\right) = \phi\left(\mathbf{W}_{y}^{f}\mathbf{h}_{t}^{f} + \mathbf{W}_{y}^{b}\mathbf{h}_{t}^{b} + \mathbf{b}_{y}\right),$$

but we propose the use of

$$P\left(\mathbf{y}_{t} \mid \{\mathbf{x}_{d}\}_{d \neq t}\right) = \phi\left(\mathbf{W}_{y}^{f}\mathbf{h}_{t-1}^{f} + \mathbf{W}_{y}^{b}\mathbf{h}_{t+1}^{b} + \mathbf{b}_{y}\right)$$
(3)

119 where

115

118

120 121 122

129

130

131 132

146

$$\mathbf{h}_{t}^{\mathrm{f}} = \tanh\left(\mathbf{W}_{\mathrm{h}}^{\mathrm{f}}\mathbf{h}_{t-1}^{\mathrm{f}} + \mathbf{W}_{\mathrm{x}}^{\mathrm{f}}\mathbf{x}_{t} + \mathbf{b}_{\mathrm{h}}^{\mathrm{f}}\right) \tag{4}$$

$$\mathbf{h}_{t}^{\mathrm{b}} = \tanh\left(\mathbf{W}_{\mathrm{b}}^{\mathrm{b}}\mathbf{h}_{t+1}^{\mathrm{b}} + \mathbf{W}_{\mathrm{x}}^{\mathrm{b}}\mathbf{x}_{t} + \mathbf{b}_{\mathrm{b}}^{\mathrm{b}}\right).$$
(5)

The structure of the BRNN is illustrated in Figure 1 (right). Compared with the regular RNN, the forward and backward directions have separate non-tied weights and hidden activations, and are denoted by the superscript f and b for forward and backward, respectively. Note that the connections are acyclic. Note also that in the proposed formulation, y_t does not get information from x_t . We can therefore use the model in an unsupervised manner to predict one time step given all other time steps in the input sequence simply by setting Y = X.

3 Probabilistic Interpretation for Unsupervised Modelling

Probabilistic unsupervised modeling for sequences using a unidirectional RNN is straightforward, as the joint distribution for the whole sequence is simply the product of the individual predictions:

$$P_{\text{unidirectional}}(\mathbf{X}) = \prod_{t=1}^{l} P(\mathbf{x}_t \mid \{\mathbf{x}_d\}_{d=1}^{t-1}).$$
(6)

For the BRNN, the situation is more complicated. The network gives predictions for individual outputs given all the others, and the joint distribution cannot be written as their product. We propose two solutions for this, denoted by *GSN* and *NADE*.

GSN Generative Stochastic Networks (GSN) (Bengio *et al.*, 2013) use a denoising auto-encoder to estimate the data distribution as the asymptotic distribution of the Markov chain that alternates between corruption and denoising. The resulting distribution is thus defined only implicitly, and cannot be written analytically. We can define a corruption function that masks x_t as missing, and a denoising function that reconstructs it from the others. It turns out that one feedforward pass of the BRNN does exactly that.

Our first probabilistic interpretation is thus that the joint distribution defined by a BRNN is the asymptotic distribution of a process that replaces one observation vector \mathbf{x}_t at a time in \mathbf{X} by sampling it from $P_{\text{BRNN}}(\mathbf{x}_t | \{\mathbf{x}_d\}_{d \neq t})$. In practice, we will start from a random initialization and use Gibbs sampling.

NADE The Neural Autoregressive Distribution Estimator (NADE) (Uria *et al.*, 2014) defines a probabilistic model by reconstructing missing components of a vector one at a time in a random order, starting from a fully unobserved vector. Each reconstruction is given by an auto-encoder network that takes as input the observations so far and an auxiliary mask vector that indicates which values are missing.

We extend the same idea for time series. Firstly, we concatenate an auxiliary binary element to input vectors to indicate a missing input. The joint distribution of the time series is defined by first drawing a random permutation o_d of time indices $1 \dots T$ and then setting data points observed one by one in that order, starting from a fully missing sequence:

$$P_{\text{NADE}}(\mathbf{X} \mid o_d) = \prod_{d=1}^{I} P(\mathbf{x}_{o_d} \mid \{\mathbf{x}_{o_e}\}_{e=1}^{d-1}).$$
(7)

162 In practice, the BRNN will be trained with some inputs marked as missing, while all the outputs are 163 observed. See Section 5.1 for more training details.

164 165

166 167

168

169

170

171

4 Filling in gaps with Recurrent Neural Networks

The task we aim to solve is to fill in gaps of multiple consecutive data points in high-dimensional binary time series data. The inference is not trivial for two reasons: firstly, we reconstruct multiple values in a row, which are likely to depend on each other, and secondly, we fill in data in the middle of a time series and hence need to consider the data both before and after the gap.

172 For filling in gaps with the GSN approach, we first train a bidirectional RNN to estimate $P_{\text{BRNN}}(\mathbf{x}_t \mid$ $\{\mathbf{x}_d\}_{d \neq t}$). In order to achieve that, we use the structure presented in Section 2.2. At test time, 173 the gap is first initialized to random values, after which the missing values are sampled from the 174 distribution $P_{\text{BRNN}}(\mathbf{x}_t \mid {\mathbf{x}_d}_{d \neq t})$ one by one in a random order repeatedly to approximate the 175 stationary distribution. For the RNN structures used in this paper, the computational complexity of 176 this approach at test time is $\mathcal{O}((dc+c^2)(T+gM))$ where d is the dimensionality of a data point, c 177 is the number of hidden units in the RNN, T is the number of time steps in the data, g is the length 178 of the gap and M is the number of Markov chain Monte Carlo (MCMC) steps used for inference. 179

For filling in gaps with the NADE approach, we first train a bidirectional RNN where some of the 180 inputs are set to a separate missing value token. At test time, all data points in the gap are first 181 initialized with this token, after which each missing data point is reconstructed once until the whole 182 gap is filled. Computationally, the main difference to GSN is that we do not have to sample each 183 reconstructed data point multiple times, but the reconstruction is done in as many steps as there 184 are missing data points in the gap. For the RNN structures used in this paper, the computational 185 complexity of this approach at test time is $\mathcal{O}((dc+c^2)(T+q))$ where d is the dimensionality of a 186 data point, c is the number of hidden units in the RNN, g is the length of the gap and T is the number 187 of time steps in the data. 188

In addition to the two proposed methods, one can use a unidirectional RNN to solve the same task. 189 We call this method *Bayesian MCMC*. Using a unidirectional RNN for the task of filling in gaps is 190 not trivial, as we need to take into account the probabilities of the values after the gap, which the 191 model does not explicitly do. We therefore resort to a similar approach as the GSN approach, where 192 we replace the $P_{\text{BRNN}}(\mathbf{x}_t \mid {\mathbf{x}_d}_{d \neq t})$ with a unidirectional equivalent for the Gibbs sampling. As 193 the unidirectional RNN models conditional probabilities of the form $P_{\text{RNN}}(\mathbf{x}_t \mid {\mathbf{x}_d}_{d=1}^{t-1})$, we can 194 use Bayes' theorem to derive: 195

 $P_{\text{RNN}}\left(\mathbf{x}_{t}=\mathbf{a}\mid\{\mathbf{x}_{d}\}_{d\neq t}\right)$

196

201 202

215

$$\propto P_{\text{RNN}}\left(\mathbf{x}_{t} = \mathbf{a} \mid \{\mathbf{x}_{d}\}_{d=1}^{t-1}\right) P_{\text{RNN}}\left(\{\mathbf{x}_{e}\}_{e=t+1}^{T} \mid \mathbf{x}_{t} = \mathbf{a}, \{\mathbf{x}_{d}\}_{d=1}^{t-1}\right)$$
(9)

$$= \prod_{\tau=t}^{T} P_{\text{RNN}}(\mathbf{x}_{\tau} \mid \{\mathbf{x}_{d}\}_{d=1}^{\tau-1})\Big|_{\mathbf{x}_{t}=\mathbf{a}}$$
(10)

(8)

203 where $P_{\text{RNN}}(\mathbf{x}_{\tau} | \{\mathbf{x}_d\}_{d=1}^{\tau-1})$ is directly the output of the unidirectional RNN given an input sequence **X**, where one time step t, i.e. the one we Gibbs sample, is replaced by a proposal **a**. The 204 205 problem is that we have to go through all possible proposals a separately to evaluate the probability 206 $P(\mathbf{x}_t = \mathbf{a} | \{\mathbf{x}_d\}_{d \neq t})$. We therefore have to evaluate the product of the outputs of the unidirectional 207 RNN for time steps $t \dots T$ for each possible a.

208 In some cases this is feasible to evaluate. For categorical data, e.g. text, there are as many possible 209 values for \mathbf{a} as there are dimensions¹. However, for other binary data the number of possibilities 210 grows exponentially, and is clearly not feasible to evaluate. For the RNN structures used in this 211 paper, the computational complexity of this approach at test time is $\mathcal{O}((dc+c^2)(T+aTM))$ where 212 a is the number of different values a data point can have, d is the dimensionality of a data point, c is the number of hidden units in the RNN, T is the number of time steps in the data, and M is 213 the number of MCMC steps used for inference. The critical difference in complexity to the GSN 214

¹For character-based text, the number of dimensions is the number of characters in the model alphabet.

216 approach is the coefficient a, that for categorical data takes the value d, for binary vectors 2^d and for 217 continuous data is infinite. 218

As a simple baseline model, we also evaluate the *one-gram* log-likelihood of the gaps. The one-gram 219 model assumes a constant context-independent categorical distribution for the categorical task, or a 220 vector of factorial binomial probabilities for the structured prediction task: 221

$$P_{\text{one-gram}}\left(\mathbf{y}_{t}\right) = \mathbf{f}\left(\mathbf{b}_{y}\right).$$

This can be done in $\mathcal{O}(dg)$. 224

We also compare to *one-way inference*, where the data points in the gap are reconstructed in order 226 without taking the future context into account, using Equations (1) and (2) directly. The computational complexity is $\mathcal{O}((dc + c^2)T)$.

5 Experiments

We run two sets of experiments: one for a categorical prediction task, and one for a binary structured prediction task. In the categorical prediction task we fill in gaps of five characters in Wikipedia text, while in the structural prediction task we fill in gaps of five time steps in different polyphonic music data sets.

235 236 237

222 223

225

227

228 229

230 231

232

233

234

5.1 Training details for categorical prediction task

238 For the categorical prediction task, we test the performance of the two proposed methods, GSN and 239 NADE. In addition, we compare the performance to MCMC using Bayesian inference and one-way 240 inference with a unidirectional RNN. We therefore have to train three different RNNs, one for each 241 method 242

Each RNN is trained as a predictor network, where the character at each step is predicted based 243 on all the previous characters (in the case of the RNN) or all the previous and following characters 244 (in the case of the BRNNs). We use the same data set as Sutskever et al. (2011), which consists 245 of 2GB of English text from Wikipedia. For training, we follow a similar strategy as Hermans and 246 Schrauwen (2013). The characters are encoded as one-hot binary vectors with a dimensionality of 247 d = 96 characters and the output is modelled with a softmax distribution. We train the unirectional 248 RNN with string lengths of T = 250 characters, where the error is propagated only from the last 200 249 outputs. In the BRNN we use string length of T = 300 characters, where the error is propagated 250 from the middle 200 outputs. We therefore avoid propagating the gradient from predictions that lack 251 long temporal context.

252 For the BRNN used in the NADE method, we add one dimension to the one-hot input which cor-253 responds to a missing value token. During training, in each minibatch we mark q = 5 consecutive 254 characters every 25 time steps as a gap. During training, the error is propagated only from these 255 gaps. For each gap, we uniformly draw a value from 1 to 5, and set that many characters in the gap 256 to the missing value token. The model is therefore trained to predict the output in different stages of 257 inference, where a number of the inputs are still marked as missing.

258 For all the models, the weight elements are drawn from the uniform distribution: $w_{i,j} \sim \mathcal{U}[-s,s]$ 259 where s = 1 for the input to hidden layer, and following Glorot and Bengio (2010), where 260 $s = \sqrt{6/(d_{in} + d_{out})}$ for the hidden-to-hidden and the hidden-to output layers. The biases are 261 initialized to zero. 262

We use c = 1000 hidden units in the unidirectional RNN and c = 684 hidden units in the two hidden 263 layers in the BRNNs. The number of parameters in the two model types is therefore roughly the 264 same. In the recurrent layers, we set the recurrent activation connected to the first time step to zero. 265

266 The networks are trained using stochastic gradient descent and the gradient is calculated using backpropagation through time. We use a minibatch size of 40, i.e. each minibatch consists of 40 ran-267 domly sampled sequences of length 250. As the gradients tend to occasionally "blow up" when 268 training RNNs (Bengio et al., 1994; Pascanu et al., 2013), we normalize the gradients at each up-269 date to have length one. The step size is set to 0.25 for all layers in the beginning of training, and it is linearly decayed to zero during training. As training the model is very time-consuming², we
 do not optimize the hyperparameters, or repeat runs to get confidence intervals around the evaluated
 performances.

5.2 Training Details for the Binary Structured Prediction Task

In the other set of experiments, we use four polyphonic music data sets (Boulanger-Lewandowski *et al.*, 2012). The data sets consist of at least 7 hours of polyphonic music each, where each data point is a binary d = 88-dimensional vector that represents one time step of MIDI-encoded music, indicating which of the 88 keys of a piano are pressed. We test the performance of the two proposed methods, but omit training the unidirectional RNNs as the computational complexity of the Bayesian MCMC is prohibitive ($a = 2^{88}$).

We train all models for 10000 updates in minibatches of ≈ 3000 individual data points³. As the data sets are small, we select the initial learning rate on a grid of $\{0.0001, 0.0003, \dots, 0.3, 1\}$ based on the lowest validation set cost. We use no "burn-in" as several of the scores are fairly short, and therefore do not specifically mask out values in the beginning or end of the data set as we did for the text data.

For the NADE method, we use an additional dimension as a missing value token in the data. For the missing values, we set the missing value token to one and the other dimensions to zero.

290 Other training details are similar to the categorical prediction task.

5.3 Evaluation of Models

- 291 292
- 293

274

275

At test time, we evaluate the models by calculating the mean log-likelihood of the correct value of gaps of five consecutive missing values in test data.

296 In the GSN and Bayesian MCMC approaches, we first set the five values in the gap to a random value 297 for the categorical prediction task, or to zero for the structured prediction task. We then sample all 298 five values in the gap in random order, and repeat the procedure for $M = 100 \text{ MCMC steps}^4$. For 299 evaluating the log-likelihood of the correct value for the string, we force the last five steps to sample 300 the correct value, and store the probability of the model sampling those values. We also evaluate the probability of reconstructing correctly the individual data points by not forcing the last five time 301 steps to sample the correct value, but by storing the probability of reconstructing the correct value 302 for each data point separately. We run the MCMC chain 100 times and use the log of the mean of 303 the likelihoods of predicting the correct value over these 100 runs. 304

When evaluating the performance of one-directional inference, we use a similar approach to MCMC. However, when evaluating the log-likelihood of the entire gap, we only construct it once in sequential order, and record the probabilities of reconstructing the correct value. When evaluating the probability of reconstructing the correct value for each data point separately, we use the same approach as for MCMC and sample the gap 100 times, recording for each step the probability of sampling the correct value. The result for each data point is the log of the mean of the likelihoods over these 100 runs.

On the Wikipedia data, we evaluate the GSN and NADE methods on 50 000 gaps on the test data. On the music data, all models are evaluated on all possible gaps of g = 5 on the test data, excluding gaps that intersect with the first and last 10 time steps of a score. When evaluating the Bayesian MCMC with the unidirectional RNN, we have to significantly limit the size of the data set, as the method is highly computationally complex. We therefore run it on 1 000 gaps on the test data.

For NADE, we set the five time steps in the gap to the missing value token. We then reconstruct them one by one to the correct value, and record the probability of the correct reconstruction. We repeat this process for all possible permutations of the order in which to do the reconstruction, and therefore acquire the exact probability of the correct reconstruction given the model and the data.

³²¹ 322

²We used about 8 weeks of GPU time for the reported results.

³A minibatch can therefore consist of e.g. 100 musical scores, each of length T = 30.

 $^{^{4}}M = 100$ MCMC steps means that each value in the gap of g = 5 will be resampled M/g = 20 times

Table 1: Negative Log Likelihood (NLL) for gaps of five time steps using different models (lower is better). In the experiments, GSN outperforms NADE.

327	Inference strategy	Wikipedia	Nottingham	Piano	Muse	JSB
328	GSN	4.60	17.7	39.0	36.4	43.4
329	NADE	4.86	19.9	40.5	36.9	45.0
330	Bayesian MCMC	4.41	NA	NA	NA	NA
331	One-way inference	5.79	NA	NA	NA	NA
333 333	One-gram	23.3	145	138	147	118



Figure 2: Average NLL per data point using different methods with the Wikipedia dataset (left) and the Piano dataset (right) for different positions in a gap of 5 consecutive missing values. The middle data point is the most difficult to estimate for the most methods, while the one-way inference cannot take future context into account making prediction of later positions difficult. For the leftmost position in the gap, the one-way inference performs the best since it does not require any approximations such as MCMC.

We also evaluate the individual character reconstruction probabilities by recording the probability of sampling the correct value given all other values in the gap are set to missing.

5.4 Results

From Table 1 we can see that the results follow the same order as the computational complexity of the methods. The Bayesian MCMC method seems to yield the best results, followed by GSN and NADE. Qualitative examples of the reconstructions obtained with the GSN and NADE on the Wikipedia data are shown in Table 3 (supplementary material).

In order to get an indication of how the number of MCMC steps in the GSN approach affects performance, we plotted the difference in NLL of GSN and NADE of the test set as a function of the number of MCMC steps in Figure 3 (supplementary material). The figure indicates that the music data sets mix fairly well, as the performance of GSN quickly saturates. However, for the Wikipedia data, the performance could probably be even further improved by letting the MCMC chain run for more than M = 100 steps.

In Figure 2 we have evaluated the NLL for the individual characters in the gaps of length five. As expected, all methods except for one-way inference are better at predicting characters close to both edges of the gap.

As a sanity check, we make sure our models have been successfully trained by evaluating the mean test log-likelihood of the BRNNs for gap sizes of one. In Table 2 (supplementary material) we can see that the BRNNs expectedly outperform previously published results with unidirectional RNNs, which indicates that the models have been trained successfully.

³⁷⁸ 6 Conclusion and Discussion

379 380

402

416 417

418

422

423

424

425

426

427

428

Although recurrent neural networks have been used as generative models for time series data, it has not been trivial how to use them for inference in cases such as missing gaps in the sequential data.

In this paper, we proposed to use bidirectional RNNs as generative models for time series, with
 two probabilistic interpretations called GSN and NADE. Both provide efficient inference in both
 positive and negative directions in time, and both can be used in tasks where Bayesian inference of a
 unidirectional RNN is computationally infeasible. GSN reconstructions are a bit more accurate and
 computationally heavier than NADE reconstructions.

The model we trained for NADE differed from the basic BRNN in several ways: Firstly, we artifi-388 cially marked gaps of 5 consecutive points as missing, which should help in specializing the model 389 for such reconstruction tasks. It would be interesting to study the effect of the missingness pattern 390 used in training, on the learned representations and predictions. Secondly, we used as training signal 391 only the reconstructions of those missing values, rather than all outputs. This reduces the effec-392 tive amount of training that the model went through. Thirdly, the model had one more input (the 393 missingness indicator) that makes the learning task more difficult. We can see from Table 2 that 394 the model we trained for NADE has a worse performance than the BRNN for reconstructing single 395 values. This indicates that these differences in training have a significant impact on the quality of the 396 final trained probabilistic model. This might explain the performance difference in the experiments 397 between the two approaches.

We used the same number of parameters when training an RNN and a BRNN. The RNN can concentrate all the learning effort on forward prediction, and re-use the learned dependencies in backward inference by the computationally heavy Bayesian inference. It remains an open question which approach would work best given an optimal size of the hidden layers.

As future work, other model structures could be explored in this context, for instance the Long Short-Term Memory (Hochreiter and Schmidhuber, 1997). Specifically to our NADE approach, it might make sense to replace the regular additive connection from the missingness indicator input to the hidden activations in Eq. (4,5), by a multiplicative connection that somehow gates the dynamics mappings \mathbf{W}_{h}^{f} and \mathbf{W}_{h}^{b} . Another direction to extend is to use a deep architecture with more hidden layers.

The midi music data is an example of a structured prediction task: Components of the output vector depend strongly on each other. However, our model assumes independent Bernoulli distributions for them. One way to take those dependencies into account is to use stochastic hidden units \mathbf{h}_t^f and \mathbf{h}_t^b , which has been shown to improve performance on structured prediction tasks (Raiko *et al.*, 2015).

The proposed methods could be easily extended to continuous-valued data. As an example application, time-series reconstructions with a recurrent model has been shown to be effective in speech recognition especially under impulsive noise (Remes *et al.*, 2011).

References

- Bahdanau, D., Cho, K., and Bengio, Y. (2015). Neural machine translation by jointly learning to align and translate. In *Proceedings of the International Conference on Learning Representations* (*ICLR 2015*).
 - Baldi, P., Brunak, S., Frasconi, P., Soda, G., and Pollastri, G. (1999). Exploiting the past and the future in protein secondary structure prediction. *Bioinformatics*, **15**(11), 937–946.
 - Bengio, Y., Simard, P., and Frasconi, P. (1994). Learning long-term dependencies with gradient descent is difficult. *IEEE Transactions on Neural Networks*, **5**(2), 157–166.
 - Bengio, Y., Yao, L., Alain, G., and Vincent, P. (2013). Generalized denoising auto-encoders as generative models. In Advances in Neural Information Processing Systems, pages 899–907.
- Boulanger-Lewandowski, N., Bengio, Y., and Vincent, P. (2012). Modeling temporal dependencies in high-dimensional sequences: Application to polyphonic music generation and transcription. In *Proceedings of the 29th International Conference on Machine Learning (ICML 2012)*, pages 1159–1166.

- Brakel, P., Stroobandt, D., and Schrauwen, B. (2013). Training energy-based models for time-series imputation. *The Journal of Machine Learning Research*, 14(1), 2771–2797.
- Glorot, X. and Bengio, Y. (2010). Understanding the difficulty of training deep feedforward neural networks. In *International conference on artificial intelligence and statistics*, pages 249–256.
- Goodfellow, I., Mirza, M., Courville, A., and Bengio, Y. (2013). Multi-prediction deep boltzmann machines. In *Advances in Neural Information Processing Systems*, pages 548–556.
- Graves, A., Liwicki, M., Fernández, S., Bertolami, R., Bunke, H., and Schmidhuber, J. (2009). A
 novel connectionist system for unconstrained handwriting recognition. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 31(5), 855–868.
- Graves, A., Mohamed, A.-r., and Hinton, G. (2013). Speech recognition with deep recurrent neural networks. *arXiv preprint arXiv:1303.5778*.
- 444 Haykin, S. (2009). *Neural networks and learning machines*, volume 3. Pearson Education.
- Hermans, M. and Schrauwen, B. (2013). Training and analysing deep recurrent neural networks.
 In C. Burges, L. Bottou, M. Welling, Z. Ghahramani, and K. Weinberger, editors, *Advances in Neural Information Processing Systems* 26, pages 190–198. Curran Associates, Inc.
- Hochreiter, S. and Schmidhuber, J. (1997). Long short-term memory. *Neural computation*, 9(8), 1735–1780.
 - Koutník, J., Greff, K., Gomez, F., and Schmidhuber, J. (2014). A clockwork RNN. In *Proceedings* of the 31 st International Conference on Machine Learning.
- Maas, A. L., Hannun, A. Y., Jurafsky, D., and Ng, A. Y. (2014). First-pass large vocabulary contin uous speech recognition using bi-directional recurrent dnns. *arXiv preprint arXiv:1408.2873*.
- Mikolov, T., Joulin, A., Chopra, S., Mathieu, M., and Ranzato, M. (2014). Learning longer memory
 in recurrent neural networks. *arXiv preprint arXiv:1412.7753*.
 - Pascanu, R., Mikolov, T., and Bengio, Y. (2013). On the difficulty of training recurrent neural networks. In *Proceedings of the 30th International Conference on Machine Learning (ICML* 2013), pages 1310–1318.
 - Raiko, T. and Valpola, H. (2001). Missing values in nonlinear factor analysis. In Proc. of the 8th Int. Conf. on Neural Information Processing (ICONIP01), (Shanghai), pages 822–827.
- Raiko, T., Berglund, M., Alain, G., and Dinh, L. (2015). Techniques for learning binary stochastic feedforward neural networks. In *International Conference on Learning Representations (ICLR 2015)*, San Diego.
 - Remes, U., Palomäki, K., Raiko, T., Honkela, A., and Kurimo, M. (2011). Missing-feature reconstruction with a bounded nonlinear state-space model. *IEEE Signal Processing Letters*, 18(10), 563–566.
 - Rumelhart, D. E., Hinton, G. E., and Williams, R. J. (1986). Learning representations by backpropagating errors. *Nature*, **323**, 533–536.
 - Schuster, M. and Paliwal, K. K. (1997). Bidirectional recurrent neural networks. *IEEE Transactions* on Signal Processing, 45(11), 2673–2681.
- Sutskever, I., Martens, J., and Hinton, G. E. (2011). Generating text with recurrent neural networks.
 In *Proceedings of the 28th International Conference on Machine Learning (ICML 2011)*, pages 1017–1024.
- Uria, B., Murray, I., and Larochelle, H. (2014). A deep and tractable density estimator. In *Proceed- ings of The 31st International Conference on Machine Learning*, pages 467–475.
- 478 479

451

452

457

458

459 460

461

466

467

468

469

470

471

472

- 481
- 482
- 483 484
- 405
- 485