Neural Networks

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Neural Networks have the remarkable property that they are able to improve their performance with more data. In many other methods more data certainly helps, but the performance of the algorthms tends to achieve a plateau upon a certain amount of data. Furthermore nowadays more complex MM architectures can be run. So NN benefit from enhanced computer power because we are able to 1) handle more data 2)build more complex architectures, and 3) NN particularily benefit from more data. A summary of historic as well as recent developments and achievement of NN can be found in Ref. [57].

NN are typically used for supervised learning problem. They had quite some success for unstructured data (images, audio). So we can roughly say that there are the following main architectures:

- Standard NN (classification)
- Convolutional NN (image data)
- Recurrent NN (time series, sequence data)

1 Notation

We start with the notation for a classification. Todo: generalize this

- m Number of training examples
- x^i i-th feature, $x^i \in \mathbb{R}^{n_x}$
- with n_x the number of features
- y^i i-th label, $y^i \in \mathcal{Y}$
- $\tilde{y}^i$ i-th predicted label $\tilde{y}^i \in \mathcal{Y}$
- with $\mathcal{Y}$ the individual target classes.
- Feature Matrix $\mathbb{R}^{m \times n_x} \ni M = (x^1, \dots x^m)$
- Label vector $\mathbb{R}^m \ni Y = (y^1, \dots y^m)$

So the columns of the feature Matrix are the individual training features. Note that in other frameworks the feature matrix is defined as the transpose

2 Activation Functions

Non-linear activation functions

- Sigmoid function

$$f(x) = \frac{1}{1 + e^{-x}} \tag{1}$$

- tanh activation function

$$f(x) = \tanh(x) \tag{2}$$

- Rectified linear unit (Relu)

$$f(x) = \begin{cases} x & x \geq 0 \\ 0 & x < 0 \end{cases} \tag{3}$$

- Leaky Relu

$$f(x) = \begin{cases} x & x \geq 0 \\ \alpha x & x < 0 \end{cases} \quad \alpha \geq 0 \tag{4}$$

In practice the sigmoid function is not used, except for output layers in classification tasks. The tanh function outperforms the sigmoid function, since it symmetrizes the sigmoid function and thus has mean of zero. Currently the gold standard is the Relu function, which ameliorates problems with very small derives of the tanh activation function. Since the Relu function is 0 for $z < 0$ and thus gives zero derivatives, the leaky relu function avoids this by setting a very small constant negatve slope for $z < 0$. In practice there does not seem to be much of a difference between relu and leaky relu.

Note that all these activation functions are non-linear.

Non-linear activation functions In principle there are also linear activation $a = Mz + b$ functions thinkable. These include the identity function. However note, that these destroy the advantage of hidden layers because the linear combination of linear functions is linear. The only useful usecase is to use e.g. the identity activation in the output layer in a regression problem.

Output-layer activation functions Typically in a deep neural network the Relu activation function is used. Only the output layer plays a special role as it needs to reflect the problem structure.

- Binary classification
- Multi-class classification

3 Loss and cost functions

Definition 1 (Loss function) *Let there be the true label $y \in \mathcal{Y}$ and the predicted label $\tilde{y} \in \mathcal{Y}$ for feature x. Then a loss function is a map*

$$L : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$$

Note that the loss function depends on the problem at hand and should be defined appropriately.

Definition 2 (Cost function)

$$J = \frac{1}{m} \sum_{i=1}^{m} L(y^i, \tilde{y}^i)$$

Examples

- Quadratic loss function: $L(y, \tilde{y}) = \frac{1}{2}(y - \tilde{y})^2$

- Logistic regression loss function: $L(y, \tilde{y}) = -y \ln \tilde{y} - (1 - y) \ln(1 - \tilde{y})$

Eventually the cost function needs to be minimized. Numerically this is done by using optimizers such as gradient descent. However, these are local optimizers and a **convex** loss function is essential in order to find the global optimum.

Logistic regression The Logistic Regression is given

$$\tilde{y} = \sigma(w^T x + b) \tag{5}$$

$$\sigma(z) = \frac{1}{1 + e^{-x}}, \tag{6}$$

where σ is the logist function, x the training features, and w the model parameters to be learned. $\tilde{y}$ is interpreted as the probability of beeing in class 1 (and $1 - \tilde{y}$ as the probability of beeing in class 0). Summarizing, we get

$$p(y = 1|x) = \tilde{y} \tag{7}$$

$$p(y = 0|x) = 1 - \tilde{y}, \tag{8}$$

which can be expressed more compactly as

$$p(y|x) = \tilde{y}^y (1 - \tilde{y})^{1-y} \tag{9}$$

Taking the negative logartithm of this expression just gives the logistic regression loss function. The negative because just the logarithm would yield an objective function to be maximised and the loss function is a quantity we would like to minimize. The associated cost function may be obtained by assuming iid of training data. The total probability then $p(\{y_n\}|\{x_n\}) = \prod_n p(y_n|x_n)$. Using the same argument as for the loss function gives the logistic cost function.

4 Predicting and training

Once a NN is specified (architecture, definition of units and activation functions), it needs to be trained and eventually used to compute predictions. A NN may be understood as a computational graph. Together with the the concepts of forward and backward propagation training and predicting is done on this computational graph.

Predicting. Forward propagation is used to compute the output of the NN and thus is equivalent to the prediction step.

Training. Backward propagation is used to compute the gradients. This is the basic ingredient for computing the parameters of a NN, i.e. the training step. This is achieved by minimizing the cost function. Once the gradients are computed by back propagation algorithm [54] of the NN corresponds to minimizing the cost function with respect to the parameter space of the NN. As in the specification step of the NN the gradients need to be computed individually.

Gradient descent. Gradient descent is a common method to train the NN. Note that the parameters should be **initialized randomly** in order to achieve symmetry breaking. Furthermore for these parameters should be chosen to be small in order to avoid too small gradients, which eventually results in slow learning. Strictly speaking this only holds true for activation functions such as the sigmoid or tanh, which exhibit very small gradients for large input values (that is why we want to keep the input values small upon initialization).
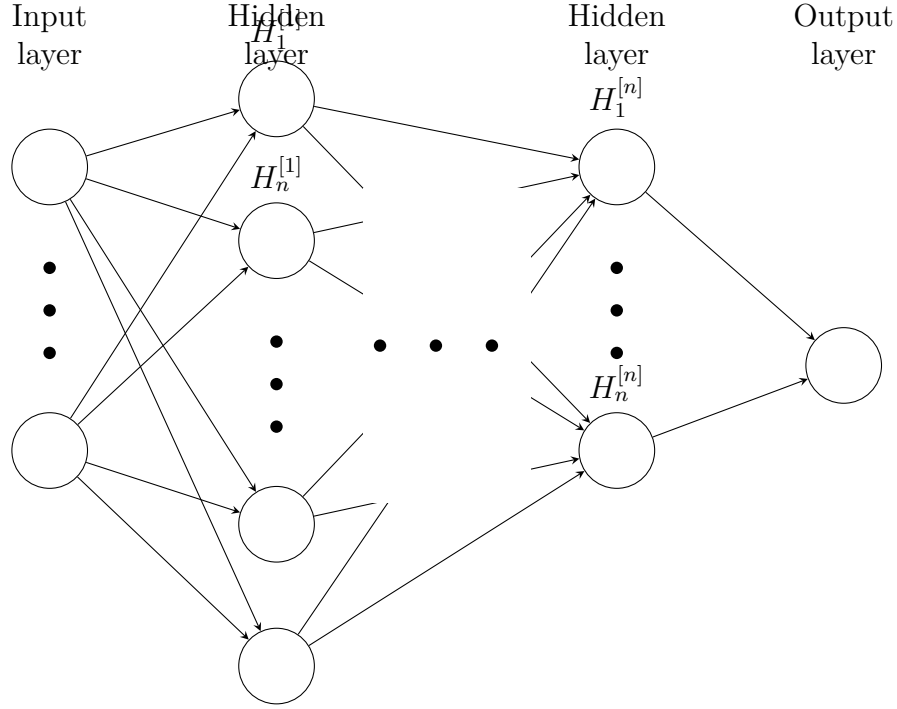
6

Figure 1: Illustration of a deep neural network with a single output unit.

5 Deep neural Networks

Deep neural networks have several hidden layers (Figure 1). The intuition behind this is, that the first layer finds very local details of the input (simple functions of the input). The ensuing layers then add more complex representations of the overall output (compositional representation). There are several motivations behind such a layered architecture:

- Universal approximation theorem

- Circuit theory: one may compute functions with a small (i.e., not many hidden units per layer) deep neural network that would require exponentially many hidden units in a shallow NN [42]. The infamous example is computing XOR on (all) the features (note that XOR itself with AND and OR functions itself already needs a deep neural network).

- An exhausitve list of arguments can be found in [22] Chap 6.4

Definition and Conventions

- $W^{[l]}, b^{[l]}$: Weights of layer l

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- $g^{[l]}$: Activation function of layer l
- $n^{[l]}$: Number of units in layer l

Note that the structure depicted in the graphical representation refers to a **single** training example. In implementations we usually work with vectorized formulars.

Parameters vs Hyperparameters. Parameters are just the weights $W^{[l]}, b^{[l]}$. These are the quantity to be trained. All other quantities (Number of layers l, number of units in layer l, activation function of layer l, learning rate, ...) are called Hyperparameters. These quantities must be set empirically.

Forward and Backpropagation

Vectorized version

Initialization

6 Optimizing Neural Networks

The predictive performance of a neureal network depends on the hyperparameters and its architecture. First the necessary concepts for judging the predictive power are presented. Based on that, concepts to improve the prediction accuracy are summarized.

6.1 Train, development and test set.

It's common practice to split the Data in 3 Sets: Training set, Hold-out crossvalidation (or development) set, and Test set. The Training set is used to train the model. The development set is used to test specific models and based on that develop better models. Once the choice for the best model is made the test set is used to get an *unbiased* estimate of the model performance. If no unbiased estimate on the model is needed sometimes only train and dev sets are used. How to split the data depends on the amount of data:

- **Conventionally** the splitting was made in the order of $70\% - 30\%$ (omitting the test set) or $60\% - 20\% - 20\%$. This applies $\approx 10^5$ datapoints on order to make sure to have enough test examples.

model	M1	M2	M3	M4
Training set error [%]	1	15	15	0.5
Development set error [%]	11	16	30	1
Problem diagnosis	high variance	high bias	high bias high variance	low bias low variance

Table 1: Illustration of bias and variance for 4 models M1 ... M4. .

- **Big data** usecases with $> 10^6$ datapoints typically have splittings in the order $98\% - 1\% - 1\%$ because there are still enough samples for the test statistics.

Since neural networks need a lot of data some applications use mismatched data distributions between the training set and development and test distributions. E.g., the training data come from webcrawling and the develpment and test sets come from the specific application at hand. However, in this case it is necessary that the development and the test set come from the same distribution.

6.2 Bias and Variance.

The **bias** of a model describes the complexity of the model. A model with high bias has a (too) simple decision boundary (e.g., linear regression). The bias may be assessed by the model performance on the training set. The **variance** describes the generalization property of model. A model with high variance tends to perform worse for new data (development set). High variance is also called **over-fitting**.

An example is given in Table 6.2. The worst case is model M3 (high bias and high variance). The ideal case is model M4 (low bias and low variance). Note that the model assessment in Table 6.2 is based on the assumption that the true labeling contained in train and development set are known without error (the Bayesian error is 0%). A counterexample to this assumption would be blurry images, where even humans make errors in labeling. Bias and variance are important quantities upon improving the model performance:

Strategies to reduce bias:

- Bigger network (number of layers / units / hyperparameter search)
- Train longer
- Use other optimization algorithm
- Different NN architecture

Strategies to reduce variance:

- More training data
- Regularization
- Different NN architecture

By iteration through bias reduction and variance reduction one can systematically improve the model performance. Note that in the case of neural networks reducing the bias and reducing the variance can be done relatively independently. This is a further advantage of neural networks. In the 'old days' one needed to find a bias variance trade off as these two quantities could not be improved independently. Probably the main reason is that nowadays there are much more data at hand. Also note that regularization also affects the bias.

The purpose of the test set is to judge the final performance of the algorithm. Ideally development set and test set error are very similar. However, if the test set error is much larger than the training set error then the development set should be increased.

6.3 Regularization

Regularization aims to reduce the variance, i.e., reduce generalization errors. There are several regularization strategies for neural networks [63, 22]:

Parameter norm penalties. This procedure is also called weight decay and follows the same ideas as standard regularization. Then this regularization scheme adds to the cost function $J(\theta)$ a penalty term

$$\tilde{J}(\theta) = J(\theta) + \lambda \Omega(\theta), \tag{10}$$

where λ is an additional hyperparameter and θ are model parameters, which are determined by minimizing the cost function. $\tilde{J}$ is then used instead of J as objective function in order to determine the modelparmeters within an optimization algorithm. In the specific case of a deep neural network a common regularization scheme is

$$\tilde{J}(\{w^{[l]}, b^{[l]}\}) = J(\{w^{[l]}, b^{[l]}\}) + \frac{\lambda}{2m} \sum_{i=1}^{L} \|w^{[i]}\|_F^2, \tag{11}$$

where $w^{[l]}, b^{[l]}$ are the weights of layer l, $\|w\|_F$ is the Frobenius norm ($\|w\|_F^2 = \sum_{i,j} w_{ij}^2$,) and m is the number of training examples. This procedure is also

called weight decay. Note that in this scheme only the $w^{[l]}$ are regularized - probably because there are much more parameters than in the $b^{[l]}$ and the assumption that this leads to a sufficient regularization.

Remark: The disadvantage of this approach is the scaling properties are lost. These can be recovered by regularizing not all layers [63] ?!?

Dropout. In dropout regularization nodes and its edges are removed at random for each training example. This introduces a new hyperparamter the "survival" probability of a node. This probability can be layer dependent. In particular layers with many units that are suspicious to overfitting may be assigned lower survival probabilities than layers with only a few units. In principle dropout can be also used in the input layer. Dropout has been successful in particular in computer vision. Dropout is implemented by masking the activation with a boolean random draw of of a Bernoulli experiment with given survival probability. In practice "inverse dropout" is used, which additionally divides the activations by the the survival probability.

Remark: With dropout the cost function J is no longer well defined. So the convergence behaviour of J as monotonically decreasing function during iteration is lost.

Data augmentation. Reduces the variance by artificially creating more data via e.g., random rotations, distortions, flips, crops of images. This approach does *not* introduce new hyper parameters.

Early stopping. This approach tries to reduce over fitting by "tweaking" the optimization step. Instead of ensuring, that the cost function w.r.t to the training data is minimized, additionally the cost function or error w.r.t the development set is monitored (optimization is still performed with the training set). One then stops at the optimization step where the cost function of the development data is minimized. This approach roots in the observation, that typically the development set error decreases with increasing optimization steps but then starts to increase again. This approach does *not* introduce new hyperparameters.

Further regularization techniques[63]:

- Parameter tying and sharing
- Bagging/ensemble methods
- Tangent methods
- Adversarial training

7 Optimization algorithms

Given an objective function $J(\theta)$ an optimization algorithm tries to find a local minimizer $\theta^* = \arg\min_\theta J(\theta)$ [43]. To this end an optimization algorithm generates a sequence of iterates $\{\theta_k\}_{k=0}^\infty$ that (ideally) terminate at the minimizer. Different algorithms differ the process of generating these iterates. θ_0 is often called initialization. For brevity we will use the notation $\nabla J_k \equiv \nabla_\theta J(\theta)|_{\theta_k}$.

7.1 Algorithms used for neural networks

Gradient descent. The update in gradient descent is given by

$$\theta_{k+1} = \theta_k - \alpha \nabla J_k, \tag{12}$$

where α is called learning rate (hyper parameter).

Exponentially moving average (EMA). This is not an optimization algorithm itself but a very common ingredient. Exponentially moving average is a comutationally efficient method to approximate moving averages. Gradient descent may produce oscillating gradients, which induce a reduced learning rate in order to achieve convergence. Many alogrithmic improvements of gradient descent are based on the first and second moment of the gradient.

For example, in order to soften oscillations one could use the moving average over the last m computed derivatives, $\bar{\nabla} J_k := 1/m \sum_{i=k-m}^k \nabla J_k$ instead of the current gradient in Equation 12. However, this would require storing $m-1$ additional gradients. Instead, the moments are approximated by the exponentially moving average.

Assume a series of data $\{q_k\}$. Then the exponentially moving average is defined iteratively as

$$\langle q \rangle_0^{\text{EMA}} = 0 \tag{13}$$

$$\langle q \rangle_k^{\text{EMA}} = \frac{1}{1-\beta^k} \left(\beta \langle q \rangle_{k-1}^{\text{EMA}} + (1-\beta) q_k \right) \tag{14}$$

There is also refined version of exponentially moving average that includes bias correction,

$$\langle q \rangle_0^{\text{cEMA}} = 0 \tag{15}$$

$$\langle q \rangle_k^{\text{cEMA}} = \frac{1}{1-\beta^k} \left(\beta \langle q \rangle_{k-1}^{\text{EMA}} + (1-\beta) q_k \right) \tag{16}$$

The term $1/\left(1 - \beta^k\right)$ is called *bias correction.* It corrects detoriations for the first few data points.

Gradient descent with momentum. Gradient descent with momentum replaces the gradient by its first moment (expectation value) obtained by the exponentially weighted average 14. The update procedure of 12 gets then modified to:

$$\langle \nabla J \rangle_0^{\text{EMA}} = 0 \ (\text{initialization}) \tag{17}$$

$$\langle \nabla J \rangle_k^{\text{EMA}} = \beta \langle \nabla J \rangle_{k-1}^{\text{EMA}} + (1 - \beta)\nabla J_k \tag{18}$$

$$\theta_{k+1} = \theta_k - \alpha \langle \nabla J \rangle_k^{\text{EMA}}. \tag{19}$$

The term $\langle \nabla J \rangle_{k-1}^{\text{EMA}}$ is called momentum, which lends the algorithm it's name. β describes how many past gradients are used and is in principle an other hyper parameter. In practice it is often set to $\beta = 0.8$. Gradient descent with momentum converge typically faster than gradient descent.

RMSprop [65]. Gradient descent with momentum damps gradient oscillations by using the approximate averages over the previous gradients. RMSprop ("Root mean square propagation") tries to damp oscillation in a complementary fashion. It weights the gradient by the inverse of the root mean square of the previous gradients – again using as exponentially moving averages as approximations to the average.

$$\langle \nabla J \odot \nabla J \rangle_0^{\text{EMA}} = 0 \ (\text{initialization}) \tag{20}$$

$$\langle \nabla J \odot \nabla J \rangle_k^{\text{EMA}} = \beta \langle \nabla J \odot \nabla J \rangle_{k-1}^{\text{EMA}} + (1 - \beta)\nabla J_k \odot \nabla J_k, \tag{21}$$

$$\theta_{k+1} = \theta_k - \alpha \nabla J_k \oslash \left(\sqrt{\langle \nabla J \odot \nabla J \rangle_k^{\text{EMA}}} + \epsilon \right), \tag{22}$$

where the square rood is taken elementwise $(\sqrt{A})_{ij} = \sqrt{A_{ij}}$, and the elementwise (Hadamard) product $(A \odot B)_{ij} = A_{ij}B_{ij}$ and division $(A \oslash B)_{ij} = A_{ij}/B_{ij}$ is used. The matrix ϵ prevents division by zero and it's components are typically set to 10^{-8}. The expression $\langle \nabla J \odot \nabla J \rangle_k^{\text{EMA}}$ is the element wise second moment of the gradient within the EMA approximation. Thus, the RMSprop update 22 scales the gradients by the element wise RMS (root mean square) using EMA. As with gradient descent with momentum, β introduces a new hyper paramter but it's typically set to $\beta = 0.8$.

Adam [32]. Adaptive moment estimation (Adam) combines gradient descent with momentum with RMSprop. It takes the averaged gradients as in 19 and scales them according to RMSprop 22. However, instead of using EMA the bias corrected EMA is used. Adam then updates the optimization steps according to

- Initialize θ and first and second moments of gradients

$$\langle \nabla J \rangle_0^{\text{cEMA}} = 0$$
$$\langle \nabla J \odot \nabla J \rangle_0^{\text{cEMA}} = 0$$

- Update Update moments

$$\langle \nabla J \rangle_k^{\text{cEMA}} = \frac{1}{1 - \beta_1^k} \left(\beta_1 \langle \nabla J \rangle_{k-1}^{\text{EMA}} + (1 - \beta_1) \nabla J_k \right)$$

$$\langle \nabla J \odot \nabla J \rangle_k^{\text{cEMA}} = \frac{1}{1 - \beta_2^k} \left(\beta_2 \langle \nabla J \odot \nabla J \rangle_{k-1}^{\text{EMA}} + (1 - \beta_2) \nabla J_k \odot \nabla J_k \right)$$

- Update optimization step

$$\theta_{k+1} = \theta_k - \alpha \langle \nabla J \rangle_k^{\text{cEMA}} \oslash \left(\sqrt{\langle \nabla J \odot \nabla J \rangle_k^{\text{cEMA}}} + \epsilon \right), \qquad (23)$$

Apart from the learning rate α there are in principle three additional hyper parameters: $\beta_1, \beta_2, \epsilon$. In practice these are not tuned but set to the values $\beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}$ [32].

7.2 Problems of optimizers for neural networks

We briefly judge the optimization strategies for neural networks

- Neural networks pose a **non-convex optimization problem**. However, the algorithms above are modifications of established algorithms for convex optimization problems. So it would be desirable to have non-convex optimization algorithms.

- In principle neural networks may have **many local minima** and the optimization algorithm finds one of them (of course one would like to find the global minimum). This problem has been debated intensively in the community. However, there is an interesting counterargument: in order to have a local minimum θ^* *all* components of the second derivative at the minimum must be greater than zero $\partial_\theta^2 J|_{\theta^*} > 0$.

Howver, for a very large NN where θ is high dimensional (several thousand components) this is very unlikely. So extremal points are most probably saddle points, which don't pose a problem to the the above optimizers. This is a consequence, that low dimensional intuition does not necessarily carry over to high dimensional neural networks.

- **Flat regions** of the cost functions may lead to very slow learning. Algorithms like Adam tend to reduce this problem, but it can still be severe.

- All algorithms of section 7 only use the first derivative of the cost function (and it's first and / or second moments). However in the literature the most powerful standard algorithms also use the second derivative (**Hessian**).

- Mind the paradigm: "In practice, it is more important to choose a model family that is easy to optimize than to use a powerful optimization algorithm" [22].

In summary, there seems to be quite some room for improving optimization algorithms [72].

7.3   Speed up the learning process

Training a NN is optimizing the cost function with respect ot the parameters. In practice this can be a tricky task for several reasons:

- Algorithm specific problems: learning rate

- NN architecture specific problems: vanishing or exploding gradients for (very) deep neural networks.

- Large training data (slow computations).

For these reasons optimization in neural networks is yet not well understood. We summerize some heuristics often used in the community.

Data normalization.   When data are in the same numerical range a larger learning rate can be chosen.

Weight initialization.   The problem of vanishing or exploding gradients can be partially reduced by carefully initializing the weights. The weights are initialized by drawing from samples from the unit normal distribution, $\mathcal{N}(1, 0)$ followed by a calibration transformation. The latter depends on the activation function but it's main rational is to account for different number

of nodes per layer via a variance argument. Popular initialization schemes are:

- Reilu activation: $w_{ij}^{[l]} = \mathcal{N}(1,0)\sqrt{\frac{2}{n^{[l-1]}}}$

- Tanh activation: $w_{ij}^{[l]} = \mathcal{N}(1,0)\sqrt{\frac{1}{n^{[l-1]}}}$ (Xavier initialization),

where $n^{[l-1]}$ is the number of nodes in layer $n-1$. The aim of these initialization schemes is to reduce the tendency of gradients to explode or vanish for very deep neural networks.

Mini-batch gradient descent. For moderately many training data a vectorized implementation of gradient descent may have an acceptable speed. In this version all training examples are passed into a single optimization step, which is also called batch (gradient descent). However, for many training examples (larger than $\sim 10^3$) this may become slow. Mini-batch gradient descent splits the data in mini batches of size. Each optimization step then only sees one mini batch (including the labels and cost function).

An **epoch** is an entire pass through the training set. While batch gradient descent allows only one optimization step per epoch, mini-batch gradient descent allows for batch size over mini-batch size many optimization steps in one epoch.

The extreme case of mini-batch size one is called **stochastic gradient descent**. The mini-batch size is another hyper parameter – in practice typical values are powers of two in the range 64, 128, ... 512.

Learning rate decay The algorithms in section 7 use a fixed learning rage α. Intuitively, near the optimum the learning rate should be smaller and larger at areas far away from the optimum. There are several heuristics that adapt the learning rate in terms of epochs n_e

- $\alpha = \frac{\alpha_0}{1+dn_e}$, with hyper parameters α_0 (initial learning rate) and d (decay rate).

- $\alpha = \alpha_0 \, 0.95^{n_e}$, with hyper parameters α_0 (initial learning rate).

- $\alpha = \frac{\alpha_0 \, d}{\sqrt{n_e}}$, with hyper parameters with hyper parameters α_0 (initial learning rate) and d.

8 Convolutional neural networks

Convolutional neural networks come from computer vision (image classification, object detection, neural style transfer, ...). If a forward deep neural

network was used for such tasks it would yield a very high dimensional input space and thus parameter space. As a consequence, there would not be enough data to prevent overfitting[1].

Continuous case. Let $f, g : \mathbb{R}^n \to \mathbb{C}$, then

$$(f * g)(t) = \int f(t')g(t - t') \, dt' \quad \textbf{(convolution)} \tag{24}$$

$$(f \star g)(t) = \int \overline{f(t')}g(t + t') \, dt' \quad \textbf{(cross correlation)}, \tag{25}$$

While these quantities look innocently similar the interpretation is different. Cross correlation is interpreted as the similarity of the functions f and g (shifted by t). As special case, the *auto correlation* at lag τ is just the cross correlation with itself $R_f(\tau) = (f \star f)(\tau)$. Convolution is interpreted as f being "smeared out" by a g: $(f * g)(t)$ is the weighted "mean" of $f(t')$ by a function $g(t - t')$. The convolution satisfies the following properties:

- Commutative $f * g = g * f$

- Associative

- Distributive

- Identity $f * \delta = f$. And therefore the inverse convolution (if exisits) is defined as

- Translational equivariance. $\tau_x(f * g) = (\tau_x f) * g = f * (\tau_x g)$, with the translation operator $(\tau_x(f))(y) = f(y - x)$ (convolution commutes with translation).

Introducing the mirror operater $Pf(t) = f(-t)$ these convolution and cross correlation are related by [2]

$$f \star g = \overline{Pf} * g. \tag{26}$$

So, if f is hermitian (symmetric for real valued functions), $\overline{f}(t) = f(-t)$, then $f \star g = f * g$. And if both, f and g are hermitian then the cross correlation is commutative, $f \star g = g \star f$. Convolution and Cross correlation is translational equivariant.

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[1]For example a 1000×1000 pixel input image with 1000 units in the first hidden layer would lead to a $3 \cdot 10^6 \times 1000$ dimensional weight matrix just for the first hidden layer (the factor of 3 comes from the 3 RGB channels).

[2]Because $\overline{Pf} * g = \int \overline{f(-t')}g(t - t') \, dt' = \int \overline{f(t')}g(t + t') \, dt' = f \star g$

In practice, these quantities are often calculated using the convolution theorem. Consider the Fourier transform of a function $f \in L^1(\mathbb{R}^n)$

$$(\mathcal{F}f)(y) = \frac{1}{\sqrt{2\pi}^n} \int f(x)e^{-iy \cdot x} \, dx \tag{27}$$

$$(\mathcal{F}^{-1}\hat{f})(x) = \frac{1}{\sqrt{2\pi}^n} \int \hat{f}(y)e^{iy \cdot x} \, dy, \tag{28}$$

where $\mathcal{F}^{-1}$ is the inverse Fourier transform and $y \cdot x$ is the standard scalar product $(x, y \in \mathbb{R}^n)$. The *convolution theorem* states that,

$$f * g = \mathcal{F}^{-1}(\mathcal{F}f \cdot \mathcal{F}g), \tag{29}$$

$$f \star g = \mathcal{F}^{-1}(\overline{\mathcal{F}f} \cdot \mathcal{F}g). \tag{30}$$

with the pointwise product $(f_1 \cdot f_2)(x) = f_1(x) \, f_2(x)$. The expression follows from (26) and $\mathcal{F}\{\overline{Pf}\} = \overline{\mathcal{F}f}$. Thus, convolution and cross correlation may be computed from (inverse) Fourier transforms.

Discrete convolution. Let $F : \mathbb{Z}^d \to \mathbb{R}$ be a discrete function. Let $\Omega_r = [-r, r]^d \cap \mathbb{Z}^d$ and $\omega : \Omega_r \to \mathbb{R}$ be a $(2r + 1)^d$ dimensional filter kernel. Then the discrete convolution operator $*$ is defined as [73, 15]

$$(F * k)(p) = \sum_{s+t=p} F(s) \, \omega(t), \tag{31}$$

where in the context of neural networks F is called input feature map and the convolution is called output feature map. The filter kernel size $(2r + 1)^d$ determines the size a given filter locally looks at the input feature map. For neural networks this is also called *receptive field*.

For example, in image processing there are well known edge detection filter kernels,

$$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}, \quad \begin{bmatrix} 0 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 0 \end{bmatrix}, \quad \begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}. \tag{32}$$

Deconvolution and transposed convolution [74]

Dilated and causal convolutions [73, 9]

Convolutions in neural networks. There are several tweaks in the application of convolutions to neural networks

- Filters are learned by back propagation.

- Activation function and bias.

- Discrete correlation instead of convolution.

- Several Filters in parallel (filterbanks)

- Dimensions

- Padding and strides

- Pooling

- https://cs231n.github.io/convolutional-networks/
- https://arxiv.org/pdf/1511.07122.pdf - http://torch.ch/blog/2016/02/04/resnets.html
- https://cs231n.github.io/optimization-2/

9   Sequence Models

Sequence models are largely motivated from natural language processing but also find application in time series modeling [17, 38, 49, 69, 39].

Recurrent neural nets suffer from vanishing / exploding gradient problem. Furthermore they are not easily capable of considering events in the long past. Eventually they suffer from big memory requirement and need long training. One reason is that they use the last hidden state in the encoder step. Gated recurrent units (GRU) ans long-short-term-memory (LSTM) try to incorporate more information from the past by a more sophisticated activation unit. However, NLP tasks still suffer from the last hidden state approach in the encoder step. One could heuristically incorporate more hidden encoder states and pass them into the decoder.

A more sound approach is the attention mechanism[4, 40], which weights the hidden states and passes them into the decoder. Incorporating the attention mechanism also in the encoder step is called self-attention. This leads to the concept of transformers [68, 3] and state of the art NLP models like BERT [13] or GPT2 [48, 2].
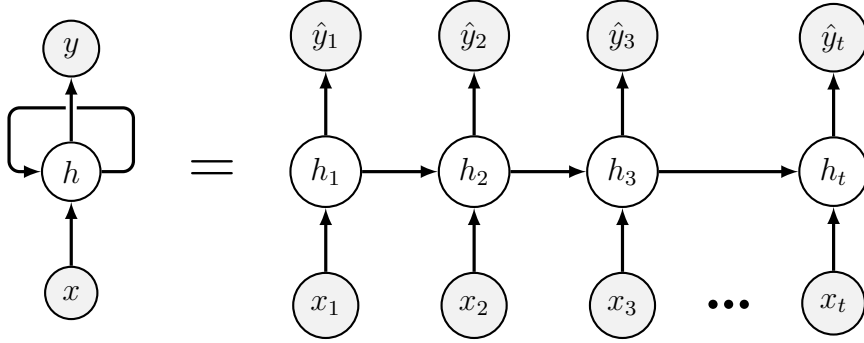
Figure 2: Illustration of a RNN. The right hand side shows the time unfolded structure, which explicitly depends on time.

9.1 Recurrent Neural Networks (RNN)

In contrast to feed forward neural networks RNNs are *in principle* capable of looking at the whole time sequence. The basic idea is that, RNN cells contain an internal memory state $h_t \in \mathbb{R}^{d_h}$ which acts as a compact summary of past information. At each time step the memory state is updated with new observations [55, 38]. Furthermore, RNNs are related to Bayesian filtering in discrete state Markov models [39, 6].

Assume that we have temporarily ordered features $\{x_t\}$ and labels $\{y_t\}$, with $x_t \in \mathbb{R}^{d_x}$ and $y_t \in \mathbb{R}^{d_y}$. There are many formulations of RNNs. One of the simplest RNNs, the Eilman RNN, takes as internal memory state h_t the expression [16, 22]

$$h_t = \gamma_h \left(W_{h_1} h_{t-1} + W_{h_2} x_t + b_h \right) \tag{33}$$

$$y_t = \gamma_y \left(W_y h_t + b_y \right), \tag{34}$$

where $W_{h_1} \in \mathbb{R}^{d_h \times d_h}, W_{h_2} \in \mathbb{R}^{d_h \times d_x}, b_h \in \mathbb{R}^{d_h}$ and $W_y \in \mathbb{R}^{d_y \times d_h}, b_y \in \mathbb{R}^{d_y}$. Training corresponds to learning these weights. Together with their usual demand for initialization the initial state is taken as $h_0 = 0$. γ_h and γ_y are activation functions (a common choics is $\gamma_h(\cdot) = \text{thanh}(\cdot)$ and $\gamma_y(\cdot) = \text{softmax}(\cdot)$ for classification). The **advantages** of RNN are

- They can process input sequences of any length. As a consequence RNNs do not require the explicit specification of a lookback window.

- The model size is invariant with respect to input size.

- The computation for step t in principle uses information from many steps back.

The **disadvantage** are

- Slow computation.

- Very limited temporal memory in practice [7, 36], which is implied by the exploding and vanishing gradient problem. [22]. One can show that the matrix norm of the partial derivatives necessary for back propagation is of the form $\|\partial h_t / \partial h_k\| \leq \beta_1 \beta_2^{t-k}$, which can easily explode or vanish for large time differences $t - k$.

There are several RNN **design patterns**,

- RNN that produce at time step an output and have recurrent connections between hidden units. (E.g., decoder part in sequene to sequence models)

- RNN that have recurrent connections between hidden units and only produce an output at the final time step. (E.g., encoder part in sequene to sequence models)

- *Bi-directional* RNN that use future information for predictions. This can be usesful in NLP tasks. The construction of bi-directional essentially doubles the number of weights and ist straight forward. It constructs forward and backward memory cells and then concatinates them. For the Eilmann RNN e.g., this yields

$$\overrightarrow{h}_t = \gamma_h \left(\overrightarrow{W}_{h_1} \overrightarrow{h}_{t-1} + \overrightarrow{W}_{h_2} x_t + \overrightarrow{b}_h \right) \tag{35}$$

$$\overleftarrow{h}_t = \gamma_h \left(\overleftarrow{W}_{h_1} \overleftarrow{h}_{t-1} + \overleftarrow{W}_{h_2} x_t + \overleftarrow{b}_h \right) \tag{36}$$

$$h_t = \overrightarrow{h}_t \oplus \overleftarrow{h}_t \tag{37}$$

$$y_t = \gamma_y \left(W_y h_t + b_y \right), \tag{38}$$

where $\oplus$ is the direct sum (i.e., concatinate vectors).

Long-Short-Term Memory (LSTM)   LSTMs [27, 21] try to overcome the limitations in learning long-range dependencies in the data by improving "gradient flow" within the network [58]. This is achieved by a more complex memory state. LSTMs introduce an additional cell state c_t, which stores long-term information with additional temporal modulations conducted by so called gates,

$$\text{\textit{Input gate:}} \quad i_t = \sigma \left(W_{i_1} h_{t-1} + W_{i_2} x_t + b_i \right) \tag{39}$$

$$\text{\textit{Output gate:}} \quad o_t = \sigma \left(W_{o_1} h_{t-1} + W_{o_2} x_t + b_o \right) \tag{40}$$

$$\text{\textit{Forget gate:}} \quad f_t = \sigma \left(W_{f_1} h_{t-1} + W_{f_2} x_t + b_f \right), \tag{41}$$

where $W_{i_1}, W_{o_1}, W_{f_1} \in \mathbb{R}^{d_h \times d_h}$, $W_{i_2}, W_{o_2}, W_{f_2} \in \mathbb{R}^{d_h \times d_x}$, and $b_i, b_o, b_f \in \mathbb{R}^{d_h}$. h_t is called hidden state and $\sigma(\cdot)$ is the sigmoid activation function. The gates modify hidden state h_t and cell state c_t at time t according to

$$\text{Cell state} \quad c_t = f_t \odot c_{t-1} + i_t \odot (W_{c_1} h_{t-1} + W_{c_2} x_t + b_c) \quad (42)$$

$$\text{hidden state:} \quad h_t = o_t \odot \tanh(c_t), \quad (43)$$

where $W_{c_1} \in \mathbb{R}^{d_h \times d_h}, W_{c2} \mathbb{R}^{d_h \times d_x}, b_c \in \mathbb{R}^{d_h}$, and $\odot$ is the component wise (Hademard) product. The initial states are set to $h_0 = c_0 = 0$. As with simple RNNs there are many kinds of LSTMs [23], in particular peephole LSTMs [20, 19] and peephole convolutional LSTMs [59].

9.2   Attention mechanism

The attention mechanism [5, 10, 41]. Assume a sequence $\{x_1, \ldots, x_T\}$ with $x_i \in \mathbb{R}^{d_x}$. Then the attention mechanism is of the form

$$x'_t = \sum_i f(x_i) \, \lambda_{it} \quad (44)$$

$$\lambda_{it} = \lambda(x_i, x_t) = \text{softmax} \, g(x_i, x_t), \quad (45)$$

where f and g are potentially trainable functions. Different choices for them yield different attention mechanisms. The transformed $x'_t \in \mathbb{R}^{d_h}$ is sometimes called context vector or attention. It is common to parametrize the weights λ_{it} with the softmax function (45), [3] and call g similarity function.

Hard vs. soft attention   The softmax parametrization enables a probabilistic interpretation of the weights $\lambda_{it} = p(i|t)$ with respect to i for a given t. The most common approach to obtain a attention function is given in (44) as a weighted linear combination over vectors $f(x_i)$. This approach is called *soft attention* and can be directly incorporated with back propagation.

However, one could also sample an ℓ of the λ-distribution $p(i|t)$ and then use $x'_t = f(x_\ell)$ as attention function instead of averaging (44). This approach is called *hard attention* and thus pays attention only to a specific part of the sequence (for example think of x_ℓ as a glimpse of a figure). Hard attention is harder to train as back propagation is not feasible and one has to resort to methods from reinforcement learning.

---

[3]$\text{softmax} \, g(x_i, x_t) = \frac{e^{g(x_i, x_t)}}{\sum_i e^{g(x_i, x_t)}}$

Self Attention   Self attention computes a transformed x_t' with respect to every element in the sequence $\{x_1, \ldots, x_T\}$ - in particular there is also a contribution to (44) from x_t it*self*. Specifically [68] parametrizes the functions f and g with three matrices W_q, W_k, W_v, with $W_v \in \mathbb{R}^{d_h \times d_x}$ and $W_q, W_k \in \mathbb{R}^{d_s \times d_x}$. Now, define

$$q_t := W_q x_t, \quad k_i := W_k x_i, \quad v_i := W_v x_i, \tag{46}$$

and identify the functions f and g in (44) - (45) with

$$f(x_i) := v_i \tag{47}$$

$$g(x_i, x_t) := \frac{k_i^T q_t}{\sqrt{d_s}} = \frac{q_t^T k_i}{\sqrt{d_s}}, \tag{48}$$

gives as attention $x_t' = \sum_i v_i \lambda_{it}$ with $\lambda_{it} = \mathrm{softmax}(q_t^T k_i / \sqrt{d_s})$. The vectors $v_i \in \mathbb{R}^{d_h}$, $q_i \in \mathbb{R}^{d_s}$ and $k_i \in \mathbb{R}^{d_s}$ are called value, query and key in analogy with database retrieval systems.

So for a fixed point in time t the weights are essentially obtained by a scaled dot product of the query vector q_t at t with the key vectors *at all times* $k_i, i \in \{1, \ldots, T\}$ (including t itself). The attention is then the weighted sum over the value vectors v_i.

The formulation can be readily extended to all points in time. Define the matrices

$$X := [x_1, \ldots, x_T] \in \mathbb{R}^{d_x \times T} \tag{49}$$

$$Q := W_q X \in \mathbb{R}^{d_s \times T}, \tag{50}$$

$$K := W_k X \in \mathbb{R}^{d_s \times T}, \tag{51}$$

$$V := W_v X \in \mathbb{R}^{d_h \times T}, \tag{52}$$

which gives

$$X' =: \mathcal{A}(Q, K, V) = V\lambda, \quad \lambda = \mathrm{softmax}\left(\frac{Q^T K}{\sqrt{d_s}}\right), \tag{53}$$

where the softmax function is component wise and the normalization w.r.t to rows. This formulation computes the attention for all times simultaneously ($X' := [x_1', \ldots, x_T'] \in \mathbb{R}^{d_h \times T}$). Note that in practice rather a dual (i.e., transposed) formulation is used as it is more compatible with sequence conventions (time as leading index). Either way, **training corresponds to computing the matrices W_q, W_k, W_v** via back propagation.

Multi-head attention   The idea is to perform self attention in parallel on different subspaces for increased performance. Each individual attention computation within this approach is called *head*.

Specifically for each h (*head*) in $1, \ldots H$ introduce "projection" - Matrices $P_{h,q}, P_{h,k}, P_{h,v}$, where $P_{h,q}, P_{h,k} \in \mathbb{R}^{d_{s'} \times d_s}$ and $P_{h,v} \in \mathbb{R}^{d_{h'} \times d_h}$. Now define

$$Q_h = P_{h,q} W_q X = W_{h,q} X \in \mathbb{R}^{d_{s'} \times T}, \tag{54}$$

$$K_h = P_{h,k} W_k X = W_{h,k} X \in \mathbb{R}^{d_{s'} \times T}, \tag{55}$$

$$V_h = P_{h,v} W_v X = W_{h,v} X \in \mathbb{R}^{d_{h'} \times T}, \tag{56}$$

and compute the matrix multiplications, which yield effective weight matrices $W_{h,q}, W_{h,k} \in \mathbb{R}^{d_{s'} \times d_x}$ and $W_{h,q} \in \mathbb{R}^{d_{h'} \times d_x}$. The multi-head attention is then the direct sum[4] of the individual attentions together with an additional matrix multiplication by a matrix W,

$$X' = W \oplus_{h=1}^{H} \mathcal{A}(Q_h, K_h, V_h), \tag{57}$$

where $X' \in \mathbb{R}^{H d_{h'} \times T}$ and $W \in \mathbb{R}^{H d_{h'} \times H d_{h'}}$. Training corresponds to learning the $3H$ matrices $\{W_{h,q}, W_{h,k}, W_{h,v}\}$ and the matrix W via back propagation.

Dual formulation   While the the above formulations seem natural if the weight matrices are thought of linear operators in the it is common to use the dual formulation (because conventionally the time index is the first index). This can be achieved by transposing the design matrix X all subsequent expressions and then rename the Matrices. So consider matrices of the form $W_v \in \mathbb{R}^{d_x \times d_h}$ and $W_q, W_k \in \mathbb{R}^{d_x \times d_s}$. Then, in the matrix formulation the attention is given by

$$X := [x_1, \ldots, x_T]^T \in \mathbb{R}^{T \times d_x} \tag{58}$$

$$Q := X W_q \in \mathbb{R}^{T \times d_s}, \tag{59}$$

$$K := X W_k \in \mathbb{R}^{T \times d_s}, \tag{60}$$

$$V := X W_v \in \mathbb{R}^{T \times d_h}, \tag{61}$$

$$X' =: \mathcal{A}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_s}}\right) V, \tag{62}$$

where $\mathcal{A}(Q, K, V) \in \mathbb{R}^{T \times d_h}$ and the element-wise softmax is now normalized with respect to columns. For the multi-head attention choose matrices

---

[4]The direct sum is with respect to columns $\mathcal{A}(Q_i, K_i, V_i) \oplus \mathcal{A}(Q_j, K_j, V_j) \in \mathbb{R}^{2 d_{h'} \times T}$

$P_{h,q}, P_{h,k} \in \mathbb{R}^{d_s \times d_{s'}}$ and $P_{h,v} \in \mathbb{R}^{d_h \times d_{h'}}$ and

$$Q_h = XW_q P_{h,q} = XW_{h,q} \in \mathbb{R}^{T \times d_{s'}}, \tag{63}$$

$$K_h = XW_k P_{h,k} = XW_{h,k} \in \mathbb{R}^{T \times d_{s'}}, \tag{64}$$

$$V_h = XW_v P_{h,v} = XW_{h,v} \in \mathbb{R}^{T \times d_{h'}}, \tag{65}$$

$$X' = \oplus_{h=1}^{H} \mathcal{A}(Q_h, K_h, V_h)W, \tag{66}$$

where the direct sum is now with respect to columns.

Causal attention   So far there was no notion auf causality. For a given point in time t the attention ranges over the whole time period and thus also w.r.t to future events. In order to introduce temporal causality contributions from future events should vanish in (44): $\lambda_{it} = 0$ for $i > t$. In the parametrization of self attention this can be achieved by masking

$$\mathcal{A}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_s}} + M\right) V, \tag{67}$$

where M is $-\infty$ in the upper triangular and 0 elsewhere.

9.3   Sequence to sequence models and transformers

The problem with RNNs are i) long range dependencies ii) vanishing and exploding gradients, iii) large number of training steps and iv) the recurrence prevents from parallel training. *All* of these problems are improved by transformer networks. Transformers are entirely based on attention. They just look at contextual similarity and thus inherently neglect temporal ordering. Therefore the temporal ordering (positions) is incorporated by adding positional encoding to the input features.

- compare methods: https://jalammar.github.io/illustrated-bert/

- http://jalammar.github.io/illustrated-word2vec/

- https://www.youtube.com/watch?v=5vcj8kSwBCY

10   Normalizing flows

Baysian methods allow to model uncertainties. While there are methods of its own for Bayesian modeling via a Baysian belief network there are approaches that incorporate these ideas into neural network architectures [31].

In principle there are two sources for uncertainty. **Epistemic uncertainty** is inherent to the model due to the likelihood function, which is of the general $p(y|x, \theta)$ form for a supervised problem for a target random variable Y given covariates X and model parameters θ. **Aleotoric uncertainty** is the uncertainty on the model parameters coming from limited training data D, $p(\theta|D)$.

For likelihood functions, and hence epistemic uncertainty the traditional approach is to parametrize the likelihood function by some analytic pdf. In the context of neural networks these parameters are learned by a neural network with suitable activation functions in the output layer to fit the domain of definitions of these parameters. While this allows to incorporate features into the likelihood function in a non-linear fashion this may still limit the expressiveness of the model as it hinges on the particular choice of the likelihood function. In order to overcome this limitation recent attempts aim to learn the likelihood function in a parameter free fashion via normalizing flows [46, 35], diffusion models [25], or implicit quantile regression [11]

10.1 Transformation of random variables

Consider two random variables $X, Y \in \mathbb{R}^d$ with probability distributions p_X, p_Y. Let f be an **bijective** function such that $f(X) = Y$. Then the two probability distributions are linked by the change of variable formular.

$$p_Y(y) = p_X(f^{-1}(y))|\det Df^{-1}(y)| \tag{68}$$

where $Df^{-1}(y) = \partial f^{-1}/\partial y$ is the Jacobian evaluated at point y. The density p_Y is also sometimes called *push forward* of p_X by the function f, $f_* p_X$. So, given f and p_X one can compute the pdf p_Y. As f is bijective then the inverse transformation is

$$p_X(x) = p_Y(f(x))|\det Df(x)|. \tag{69}$$

Now we ask a more complicated question. Let there be given two probability distributions p_X, p_Y - does there exist a bijective function f that transforms these distributions into each other? However, from a practical point of view the mere existence is not enough as (68) dictates that the inverse and the Jacobi determinant should be cheap to compute. [8, 30]. Fortunately there is theoretical support,

Definition 3 *(Triangular map) A map $T = (T_1, \ldots, T_d) : \mathbb{R}^d \to \mathbb{R}^d$ is called triangular if T_1 is a function of x_1, T_2 a function of (x_1, x_2), and so on: T_i is a function of $(x_1, \ldots, x_i)$. A triangular map is called (strictly) increasing if every component T_i is (strictly) increasing with respect to the variable x_i (keeping the other variables $(x_1, \ldots, x_{i-1})$ fixed).*

Theorem 1 *[8, 30] For any two densities p_X, p_Y over $X = Y = \mathbb{R}^d$ there exists a unique increasing triangular map $T : X \to Y$ such that $p_Y = T_* p_X$.*

Triangular maps are in fact rather intuitive. Each multi variate pdf can be decomposed in d univariate conditional pdfs $p(x_i|x_{1:i-i})$, $i = 1, \ldots, d$,

$$p(x) = p(x_1)p(x_2|x_1) \ldots p(x_d|x_{1:d-1}) \tag{70}$$

Triangular maps then map each of this conditional pdf individually, which can be always done as guaranteed by the theorem.

Consider some properties of triangular maps. First, the Jacobian of a triangular map is triangular because $\partial T_i/\partial x_j = 0$ for $j > i$ and therefore the Jacobian determinant can be computed from the diagonal elements $\det DT = \prod_i \partial T_i/\partial x_i$. The inverse strictly increasing triangular map is also a triangular map.

$$T^{-1} = (T_1^{-1}, \ldots, T_d^{-1}) : \mathbb{R}^d \to \mathbb{R}^d \tag{71}$$

Consider the scalar map $t_i : x_i \mapsto T_i(x_1, \ldots x_i)$, for fixed $x_1, \ldots x_{i-1}$. The inverse t_i^{-1} exists because this map is strictly increasing. This establishes the components of T^{-1}

$$
\begin{aligned}
&T_1^{-1}(y_1) = t_1^{-1}(y_1) \\
&T_2^{-1}(y_1, y_2) = t_2^{-1}(T_1^{-1}(y_1), y_2) \\
&\ldots \\
&T_d^{-1}(y_1, \ldots, y_d) = t_d^{-1}(T_1^{-1}(y_1), \ldots, T_{d-1}^{-1}(y_1, \ldots, y_{d-1}), y_d) \tag{72}
\end{aligned}
$$

Apparently this is a triangular map[5]. We need to show that it is indeed the inverse map $T^{-1} \circ T = T \circ T^{-1} = id$. We show this by induction in d. For $d = 1$ this is apparently true. Assume that the statment holds fof $d - 1$. Pick $x \in \mathbb{R}^d$, the components of $T(x)$ are given by $y_1 = T_1(x_1), y_2 = T_2(x_1, x_1), \ldots y_d = T_d(x_1, \ldots, x_d)$. By the induction assumption we have $T_1^{-1}(y_1) = x_1 \ldots, T_{d-1}^{-1}(y_1, \ldots y_{d-1}) = x_{d-1}$. For the last component we have $T_d^{-1}(y_1, \ldots, y_d) = t_d^{-1}(T_1^{-1}(y_1), \ldots, T_{d-1}^{-1}(y_1, \ldots, y_{d-1}), y_d) = t_d^{-1}(x_1, \ldots x_{d-1}, y_d)$ for fixed $x_1, \ldots x_{d-1}$. But this is a scalar function and its value at y_d is by construction x_d. Thus $T^{-1} \circ T = id$. And similar for $T \circ T^{-1} = id$

From a computational point of view the inverse T^{-1} needs to be computed iteratively as T_i^{-1} relies on $T_1^{-1}, \ldots, T_{i-1}^{-1}$. Therefore it cannot be computed in a parallel fashion (as opposed to T), which can be a limiting factor for models

---

[5]Note that abuse of notation for $d = 1$: t_1^{-1} is the inverse of T_1. But T_1^{-1} is also denoted as the first component of the inverse map

with high dimensions. However, the good news is that each component of this recursion is just the inverse of a scalar function, which can be computed fairly easy also numerically (if necessary).

The composition of triangular maps is again a triangular map. Consider two triangular maps T with $x_i' = T_i(x_1, \ldots, x_i)$ and T' then $(T' \circ T)_i = T_i'(x_1', \ldots, x_i') = T_i'(T_1(x_1), \ldots, T_i(x_1, \ldots, x_i))$ only depends in $x_1, \ldots, x_i$. $T' \circ T$ is (strictly) increasing if T and T' are.

In summary,

- The Jacobian of a triangular map is triangular and the Jacobian Determinant can be computed from the diagonal entries only

$$\det DT = \prod_i \partial T_i / \partial x_i. \tag{73}$$

- The inverse of a strictly increasing triangular map is triangular and given by Eqs. (71) and (72).

- The composition of triangular maps $T = T^n \circ \cdots \circ T^2 \circ T^1$ is triangular and the Jacobian factorizes $DT = \prod_{i=1}^n DT^i$. If the T^i are strictly increasing then the inverse of T is given by $T = T^{1^{-1}} \circ \cdots \circ T^{n^{-1}}$.

10.2 Normalizing Flows: basic idea

Let p_X be a complicated distribution and p_Y a known, tractable pdf (uniform or normal distribution). Further assume that we only have samples of p_X $\mathcal{D} = \{x^{(i)}\}_{i=1}^N$ exists, but is unknown otherwise. We would like to learn a tringular map $f : X \to Y$ by a neural network (Fig. 3).

If we could succeed in learning f then we can use it in two fold manner. We could use it for density estimation and data generation by drawing samples from the known base distribution $y \sim p_Y$ and then obtain new samples in the target distribution p_X from $f^{-1}(y)$. From this samples all relevant statistical properties can be computed. Furthermore this approach can be also used to construct flexible test distributions for the approximate posterior in variational inference [52].

Let the base distribution be parametrized by parameters ϕ, such that $p_Y(y) = p_Y(y|\phi)$ and denote the neural network parameters of f by θ, $f_\theta(x) = f(x|\theta)$. The training (inference) task is to estimate the parameters of the base distribution and the function (ϕ, θ) from $\mathcal{D}$.

In order to learn the parameters θ of f one needs to define a loss function, which shall be minimized. This loss function should "compare" the pdfs from the inverse transformation induced by f from (103) $p_X(x|\phi, \theta)$ and the true,
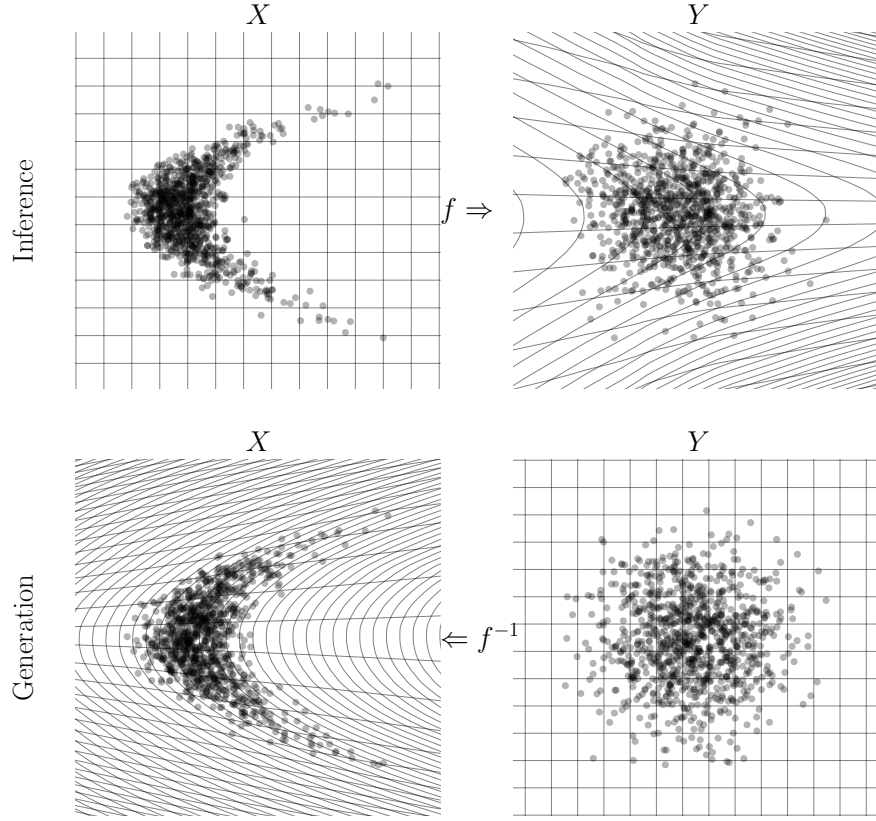
Figure 3: Illustration of normalizing flow.

unknown distribution $p_X(x)$ (of which, we only have samples) in some sense. There are several possible loss functions and the Kullback-Leibler[6] divergence

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[6] $\mathrm{KL}(q||p) = \int q(x) \ln \frac{q(x)}{p(x)} \, dx = \langle \ln q \rangle_q - \langle \ln p \rangle_q$

is an obvious one:

$$
\begin{aligned}
\mathcal{L}(\phi, \theta, \mathcal{D}) &= \mathrm{KL}(p_X(x) \,||\, p_X(x|\phi, \theta)) \\
&= -\langle \ln p_X(x|\phi, \theta) \rangle_{p_X} + const. \\
&\approx -\frac{1}{N} \sum_i^N \ln p_X(x^{(i)}|\phi, \theta) + const. \\
&= -\frac{1}{N} \sum_i^N \left\{ \ln p_Y(f(x^{(i)}|\theta) \,|\, \phi) + \ln |\det Df(x^{(i)}|\theta)| \right\} + const.,
\end{aligned}
$$
(74)

where the constant terms are contributions independent of the paramters to optimize (ϕ, θ). In the second line the expectation value w.r.t. the unknown exact pdf is approximated by the empirical mean (Monte-Carlo approximation) given samples from $\mathcal{D}$. So (74) can be used to determine gradients on the function $\partial_\theta \mathcal{L}(\phi, \theta)$ and on the base distribution $\partial_\phi \mathcal{L}(\phi, \theta)$ needed to minimize the Kullback-Leibler divergence. Note however, that in some implementations only the parameters θ of f are learned keeping the parameters of the base distribution ϕ fixed.

Alternatively we could aim to determine the parameters (ϕ, θ) in order maximize the log-likelihood, $\ln p_X(\mathcal{D}|\phi, \theta)$, and thus minimize the negative of it,

$$
\begin{aligned}
\mathcal{L}(\phi, \theta, \mathcal{D}) &= -\ln p_X(\mathcal{D}|\phi, \theta) \\
&= -\ln \prod_{i=1}^N p_X(x^{(i)}|\phi, \theta) \\
&= -\sum_i^N \left\{ \ln p_Y(f(x^{(i)}|\theta) \,|\, \phi) + \ln |\det Df(x^{(i)}|\theta)| \right\},
\end{aligned}
$$
(75)

which eventually gives up to the constant $1/N$ the same gradients as the KL divergence. Therefore, both versions share the same minimizer[7]. There are several other possible loss functions like the Wasserstein metric as reviewed in [46].

This is summarized in the basic normalizing flow algorithm for inference and data generation in algorithms 1 and 2, respectively.

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[7]However, when using an optimizer with given step length the optimal step length could be different as the computed gradients differ by $1/N$. On the other hand it ist most common to optimize the average of the log likelihood, which gives the same result as the KL approach.

Algorithm 1: Inference of a normalizing flow model using stochastic gradient descent (SGD)

Input:
  Data $\mathcal{D}$
  A base distribution $p_Y(\cdot|\phi)$
  A function f_θ
Result: Learned parameters ϕ, θ
Initialize: ϕ, θ
while *SGD not converged* **do**
  $\quad$ $\mathcal{M} \sim \mathcal{D}$ (Random minibatch of data)
  $\quad$ Compute loss $\mathcal{L}(\theta, \phi, \mathcal{M})$ from Eq. (74)
  $\quad$ Compute gradients $\partial_\theta \mathcal{L}(\theta, \phi, \mathcal{M})$, $\partial_\phi \mathcal{L}(\theta, \phi, \mathcal{M})$
  $\quad$ Udate θ, ϕ using SGD optimizer
end

Algorithm 2: Data generation with a normalizing flow

Input:
  A base distribution $p_Y(\cdot|\phi)$
  A function f_θ
Result: Sample $x \sim p_X(\cdot|\theta)$
$y \sim p_Y(\cdot|\phi)$
$x = f_\theta^{-1}(y)$

10.3 Constructing f

So far no statement of how to construct f has been made. Theorem 1 suggests to construct f as a triangular map. The theorem only guarantees that there is an increasing triangular map. However, as we wish to generate samples from the inverse map in practice strictly increasing triangular maps are constructed. Surprisingly some of these have been shown to be universal [30, 28][8]. While most of the normalzing flows are triangular maps, there are exceptions. In either case a common strategy to construct more complex normalizing flows is composition. It is illustrative to start with some simple transformations $f : \mathbb{R}^d \to \mathbb{R}^d$.

Example: Component wise affine linear flow. Consider the compo-

---

[8]A flow is called universal if it can learn any target density to any required precision given sufficient capacity and data. The existence of such a map is guaranteed by Theorem 1

---

nent wise map $y_i = e^{\alpha_i} x_i + \beta_i$. This is a trivial triangular map because $T_i(x_1, \ldots, x_i) = T_i(x_i)$. It's inverse is given by $x_i = e^{-\alpha_i}(y_i - \beta_i)$. Its Jacobian is given by $Df = \mathrm{diag}(e^{\alpha_1}, \ldots, e^{\alpha_d})$ and therefore $\ln |\det Df| = \ln |\prod_i e^{\alpha_i}| = \ln \prod_i e^{\alpha_i} = \sum_i \alpha_i$. This is essentially a affine linear map with the additional exponential map that ensures invertibility for any α_i.

Example: Permutation. A permuation $f_\pi : y = P_\pi x$ is given by an orthogonal permutation matrix $P_\pi^{-1} = P_{\pi^{-1}} = P_\pi^T$. It has Jacobi determinant $\det Df = \mathrm{sgn}(\pi)$ and therefore $\ln |\det Df| = \ln 1 = 0$. This is *not* a triangular map. However it is commonly used as "intertwiner" in a composition. This has been shown to be beneficial in practice. The reason is that triangular maps inherently depend on the ordering of the random variables (think of factorization of a joint pdf in terms of conditional pdfs). While this is in the limit of infinitely many training data probably not a problem, in practice changing the order of the variables may improve performance (in particular when triangular maps are composed). A generalization of the permutation groups are so called *linear normalizing flows*, which aim to determine the best ordering.

Example: batch normalization. Batch normalization [29] is used to speed up training can be understood as normalizing flow. It is of the adapted form [47]

$$y_i = \frac{x_i - \tilde{\mu}_i}{(\tilde{\sigma}_i^2 + \varepsilon)^{\frac{1}{2}}} \, e^{\alpha_i} + \beta_i, \ i = 1 \ldots d, \tag{76}$$

where α_i, β_i are the trainable parameters and ε is a small constant (hyperparameter) to ensure numerical stability ($\varepsilon = 10^{-5}$). $\tilde{\mu}_i$ and $\tilde{\sigma}_i$ are the empirical means and standard deviations derived from data $\mathcal{D} = \{x_i^n\}_{n=1}^N$ along dimension i for a minibatch (during training) and for test data (during prediction). Different choices for the choice of sampling space for training and prediction phase exist. As the map is defined component wise it is also triangular. It's inverse is given by

$$x_i = (y_i - \beta_i)\left(\tilde{\sigma}_i^2 + \varepsilon\right)^{\frac{1}{2}} e^{-\alpha_i} + \tilde{\mu}_i, \ i = 1 \ldots d, \tag{77}$$

and the Jacobian is diagonal $Df = \mathrm{diag}(e^{\alpha_1}/(\tilde{\sigma}_1^2 + \varepsilon)^{\frac{1}{2}}, \ldots, e^{\alpha_d}/(\tilde{\sigma}_d^2 + \varepsilon)^{\frac{1}{2}})$, and therefore

$$\ln |\det Df| = \sum_{i=1}^d \left(\alpha_i - \frac{1}{2} \ln\left(\tilde{\sigma}_i^2 + \varepsilon\right)\right). \tag{78}$$

Autoregressive flows. The affine linear flow extends to a more general form, which is still triangular, $y_i = e^{\alpha_i(x_{1:i-1})} x_i + \beta_i(x_{1:i-1})$, where α_i and β_i are now functions of $x_{1:i-1} = x_1, \ldots, x_{i-1}$.

More generally, let $\tau_i(\cdot\,;\alpha_i) : \mathbb{R} \to \mathbb{R}$ be bijections parametrized by $\theta_i \in \mathbb{R}^{|\theta_i|}$. Then a triangular map is called autoregressive flow if it is of the form

$$y_i = T_i(x_1, \ldots, x_i) = \tau_i(x_i; \gamma_i(x_{1:i-1})), \quad i = 1, \ldots, d, \tag{79}$$

with $\alpha_i = \gamma_i(x_{1:i-1})$. The function τ_i is called coupling function or transformer and γ_i is called conditioner function. For $i = 1$ the conditioner does not depend on x. So, the conditioner "learns" the parameters for the univarite coupling function τ_i.

As autoregressive flows are triangular, all properties hold – and they further simplify. In particular for the diagonal element of the Jacobian (73), $\partial y_i / \partial x_i$ only the derivative of the coupling functions needs to be comupted (keeping the conditioner fixed) in (79). And similar, the inverse needs to be computed only with respect to the coupling function: from (72)

$$\begin{aligned} T_d^{-1}(y_1, \ldots, y_d) &= t_i^{-1}(T_1^{-1}(y_1), \ldots, T_{i-1}^{-1}(y_1, \ldots, y_{i-1}), y_i) \\ &= t_i^{-1}(x_1 \ldots x_{i-1}, y_i) \\ &= \tau_i^{-1}(y_i; \gamma_i(x_1 \ldots x_{i-1})), \end{aligned} \tag{80}$$

where in the last line the specific form of (79) was used. The inverse has still a recursive form as $\tau_i^{-1}(y_i; \gamma_i(x_1, \cdots, x_{i-1}))$ can only be computed once the $x_1, \ldots x_{i-1}$ (i.e. the inverses $\tau_1^{-1}, \tau_{i-1}^{-1}$) are known.

The property that the Jacobian and the inverse need not be evaluated for the conditioner functions is exploited in constructing autoregressive flows: the conditioner can be any "crazy" function (neural network) and only the coupling function needs fine tuning in order to be strictly increasing (bijective). From a theoretical point of view this is also beneficial as one can exploit the universal approximation theorem for the conditioner part and the universality property needs to shown only for the univariate coupling functions. [30, 70, 28]

Real NVP [14]. Fix $\ell < d$ then the real NVP normalzing flow is defined as

$$\begin{aligned} y_{1:\ell} &= x_{1:\ell} \\ y_{\ell+1:d} &= x_{\ell+1:d} \odot \exp(\alpha(x_{1:\ell})) + \beta(x_{1:\ell}), \end{aligned} \tag{81}$$

where the pair of conditioner functions $\gamma = (\alpha, \beta)$ with $\alpha, \beta : \mathbb{R}^\ell \to \mathbb{R}^{d-\ell}$ are neural networks with appropriate dimensions (whose parameters are op-

timized by e.g. algorithm 1). This kind of block parametrizations of normalizing flows are also called *coupling layers*. The inverse of real NVP is given by

$$
\begin{aligned}
x_{1:\ell} &= y_{1:\ell} \\
x_{\ell+1:d} &= (y_{\ell+1:d} - \beta(x_{1:\ell})) \odot \exp(-\alpha(y_{1:\ell})),
\end{aligned}
\tag{82}
$$

and the diagonal elements of the Jacobian

$$
\begin{pmatrix} 1_\ell & 0 \\ \cdot & \mathrm{diag}\left(e^{\alpha(x_{1:\ell})}\right) \end{pmatrix}
\tag{83}
$$

and therefore $\ln|\det Df| = \sum_{i=1}^{d-\ell} \alpha_i(x_{1:\ell})$, that is the sum over all components of the vector-valued function α.

To see that this is indeed an autoregressive flow write equivalently

$$
y_i = T(x_{1:i}) = \begin{cases} T(x_i) = x_i & \text{for } i \le \ell \\ T(x_{1:\ell}, x_i) = x_i \exp(\alpha_i(x_{1:\ell})) + \beta_i(x_{1:\ell}) & \text{for } i > \ell, \end{cases}
\tag{84}
$$

where α_i, β_i are the i-th components of $\alpha, \beta \in \mathbb{R}^{d-\ell}$, respectively. As $x_{1:\ell}$ in (85) are not transformed, in practice compositions with alternative permutations are used, $f = \dots f_\pi \circ f_{NVP} \circ f_\pi \circ f_{NVP}$. After the permutation f_π untouched x parts enter a non trivial map. The coupling function in 85 is affine linear. The unusual exponential map ensures invertiblity for any $\alpha(x_1 : \ell)$. Therefore there are no constraints on the underlying neural network for the conditioner.

Masked autoregressive flow (MAF)[47]. The conditioners α, β in real-NVP are all the same for $i > \ell + 1$ as the take as input $x_{1:\ell}$ and therefore are not of the most general form of (79). MAF generalizes the parametrization of the conditioners in this direction:

$$
y_i = x_i \exp(\alpha_i(x_{1:i-1})) + \beta_i(x_{1:i-1}),
\tag{85}
$$

where for each component there is now a pair of conditioner functions $\gamma_i = (\alpha_i, \beta_i)$, $i = 1 \dots d$, with $\alpha_i, \beta_i : \mathbb{R}^{i-1} \to \mathbb{R}$ for $i > 1$ (and constants for $i = 1$). The logarithm of the Jacobian determinant is $\ln|\det Df| = \sum_{i=1}^{d} \alpha_i(x_{1:i-1})$. The inverse follows from (80) recursively,

$$
x_i = (y_i - \beta_i(x_{1:i-1})) \exp(\alpha_i(x_{1:i-1})).
\tag{86}
$$

While MAF is a straightforward extension of the conditioner over real-NVP, it requires to set up $2d$ neural networks for the conditioner functions $\gamma_i =$

(α_i, β_i), $i = 1 \ldots d$ as opposed to only two in real-NVP (α, β)[9]. So for a single function evaluation of (86) one needs $2d$ neural network forward passes, which can be cumbersome for large d. However, one can combine these $2d$ neural networks into a *single* masked conditioner neural network.

Masked conditioner neural networks [18]. The following method is sometimes called MADE after the title of [18] although it is used in the context of normalizing flows.

The aim is to construct a conditioner network for all functions $\gamma = (\gamma_1, \ldots, \gamma_d)$ in one forward pass of a single neural network. For simplicity consider first the case where the coupling function only requires one scalar parameter from the conditioner network, $\gamma_i : \mathbb{R}^{i-1} \to \mathbb{R}$ (the map γ_1 is interpreted as constant parameters). And therefore we the vector valued function assumes the form[10] $\gamma = (\gamma_1, \ldots, \gamma_d) : \mathbb{R}^d \to \mathbb{R}^d$ with image $\alpha = \gamma(x) = (\gamma_1, \gamma_2(x_1), \gamma_3(x_1, x_2) \ldots, \gamma_d(x_{1:d-1})) = (\alpha_1, \ldots, \alpha_d)$.

A deep neural network (multi layered perceptron, MLP) is of the form

$$\gamma : \begin{array}{ccccccccc} \mathbb{R}^d & \xrightarrow{f^1} & \mathbb{R}^{d_1} & \xrightarrow{f^2} & \mathbb{R}^{d_2} & \xrightarrow{f^3} & \ldots & \xrightarrow{f^L} & \mathbb{R}^d \\ \cup & & \cup & & \cup & & & & \cup \\ x & & h^1 & & h^2 & & & & \alpha \end{array}$$

$$f^\ell : h^\ell = a^\ell \left((M^\ell \odot W^\ell) h^{\ell-1} + b^\ell \right), \tag{87}$$

where $h^\ell \in \mathbb{R}^{d_\ell}$ is called hidden layer and a component of it h_i^ℓ is called neuron. a^ℓ is the activation function, $W^\ell \in \mathbb{R}^{d_\ell \times d_{\ell-1}}$ the weights, and $b^\ell \in \mathbb{R}^{d_\ell}$ the biases of layer ℓ. Identify $x \equiv h^0$ (and its $d \equiv d_0$) and $\alpha \equiv h^L$ (and its $d \equiv d_L$) and thus the final activation a^L must match the requirements of the coupling functions. Note that d_0 is dictated by the feature dimension and d_L by the coupling function, so the free dimesional hyperparameters are $d_1, \ldots, d_{L-1}$. The aim is to construct a binary Matrix (*mask*) $M^\ell \in \{0, 1\}^{d_\ell \times d_{\ell-1}}$, which satisfies the autoregressive property [18],

$$\alpha_i = h_i^L = h_i^L(x_{1:i-1}), \tag{88}$$

---

[9]One could express the pair of neural networks $\alpha, \beta : \mathbb{R}^\ell \to \mathbb{R}^{d-\ell}$ by doubling the output dimension and compute one neural network $\gamma : \mathbb{R}^\ell \to \mathbb{R}^{2(d-\ell)}$ and then use slicing in the coupling function (which can be computed vectorized). Typically one enlarges the network in this case to have a similar amount of parameters as when working with two networks in order to ensure similar expressiveness. Similar for MAF $\gamma_i : \mathbb{R}^{i-1} \to \mathbb{R}^2$. But then there are still d of such combined networks.

[10]Strictly speaking $\gamma : \mathbb{R}^{d-1} \to \mathbb{R}^d$, because γ_d only depends on $x_{1:d-1}$. However, we will the more general map $\mathbb{R}^d \to \mathbb{R}^d$ (as this eventually allows for order agnostic training). This implies that it must be ensured that x_d does note contribute.

that is to ensures that each neuron output i only depends (implicitly) on $x_{1:i-1} = h^0_{1:i-1}$.

First, each neuron $1 \ldots d_\ell$ of layer ℓ is assign an integer number ($\ell = 0, \ldots \ldots L$; the input layer $\ell = 0$ is included). For each layer this can be written as

$$
\begin{aligned}
m^0 &= (1, \ldots, d), \\
m^\ell &= (m^\ell(0), \ldots, m^\ell(d_\ell)), \quad 1 \leq \ell \leq L - 1, \\
&\quad m^\ell(i) \in \{\min(m^{\ell-1}), \ldots, d - 1\}, \\
m^L &= (1, \ldots, d).
\end{aligned}
\tag{89}
$$

This assignment rules are also called *connectivity constraints*. The mask is then constructed as

$$
\begin{aligned}
M^\ell_{i,j} &= \begin{cases} 1 & \text{if } m^\ell(i) \geq m^{\ell-1}(j) \\ 0 & \text{else,} \end{cases} \qquad \ell = 1, \ldots, L - 1, \\[2mm]
M^L_{i,j} &= \begin{cases} 1 & \text{if } m^L(i) > m^{L-1}(j) \\ 0 & \text{else,} \end{cases}
\end{aligned}
\tag{90}
$$

where the mask for the output layer $\ell = L$ requires a strict inequality sign.

The assigment rule (89) for the input layer $\ell = 0$ (consisting of $x \in \mathbb{R}^d$) maps each neuron to its index $m^0(i) = i$, $i = 1, \ldots, d$. And similar for the output layer (which will be generalized later on for more complex coupling functions). For each hidden layer ℓ, $1 \leq \ell \leq L - 1$ the assignment per neuron $m^\ell(i)$, $i = 1, \ldots, d_\ell$ is typically randomly sampled from a uniform distribution. It takes values $m^\ell(i) \in \{\min(m^{\ell-1}), \ldots, d - 1\}$. The choice of the lower limit $\min(m^{\ell-1})$ with respect to the previous layer avoids unconnected units[11]. The choice of of the upper limit ensures that only components $x_{1:d-1}$ and not x_d propagate through the network necessary for the autoregressive property[12].

We need to show that this construction indeed fulfills the autoregressive

---

[11]If there was a neuron k at layer ℓ such that $m^\ell(k) < \min(m^{\ell-1})$ then the corresponding mask $M^\ell_{k,i} = 0$, $i = 1, \ldots, d_{\ell-1}$. And thus there is no connection from the previous layer $\ell - 1$ to that neuron.

[12]The first mask $M^1_{i,d} = 0$, $i = 1, \ldots, d_1$ has no connection to x_d and thus M^1 already filters out all contributions from x_d and therefore the whole NN does not depend on x_d. This can be seen from $m^0(d) = d$ and $m^1(i) < d$ for any i by construction. Therefore $m^1(i) < m^0(d) = d$. Thus the requirements of footnote 10 are met.

property (88). Consider the output of neuron i of the output layer

$$h_i^L = a^L \left(\sum_{j=1}^{d_{L-1}} (M^L \odot W^L)_{i,j} h_j^{L-1} + b_i^L \right)$$

$$= a^L \left(\sum_{j=1}^{d_{L-1}} M_{i,j}^L W_{i,j}^L h_j^{L-1} + b_i^L \right) \tag{91}$$

First consider the compontent $i = 1$. From (89) it follows that $m^L(1) = 1$, and together with the strict inequality of (90) the corresponding mask $M_{1,j}^L = 0$, $j = 1 \ldots, d_{L-1}$. Therefore $h_i^L = a_L(b_1^L)$ does not depend on x and only the constant (yet trainable parameter for a neural network) contributes.

Now pick an $2 \leq i \leq d_L$ with $m^L(i) = i$. Assume that there is an x_k, $k \geq i$, which contributes to h_i^L. So there must be an unmasked path in the neural network from h_i^L to x_k. Therefore there is a sequence of neurons $i_{L-i}, i_{L-2}, \ldots, i_1$ on the intermediate layers $L-1, L-2, \ldots, 1$ for which

$$i = m^L(i) > m^{L-1}(i_{L-1}) \geq m^{L-2}(i_{L-2}) \cdots \geq m^1(i_1) \cdots \geq m^0(k) = k.$$

And thus $i > k$, which contradicts the assumption $k \geq i$. Therefore h_i^L can at most depend on $x_{1:i-1}$.

So far the assumption was made that each coupling function only a scalar output from the conditioner network $\gamma_i : \mathbb{R}^{i-1} \to \mathbb{R}$, and thus the network is a map $\gamma = (\gamma_1, \ldots, \gamma_d) : \mathbb{R}^d \to \mathbb{R}^d$. This **generalizes to any number of parameters** of the coupling function. Require that $\gamma_i : \mathbb{R}^{i-1} \to \mathbb{R}^{p_i}$, where p_i is the number of parameters provided by the conditioner function i to coupling function i. Then, the joint masked conditioner neural network is a map

$$\gamma = (\gamma_1, \ldots, \gamma_d) : \mathbb{R}^d \to \mathbb{R}^{p_1} \times \cdots \times \mathbb{R}^{p_d} \tag{92}$$

This can be easily achieved by adapting the assignment rules of the output layer in (89)

$$m^L = (\underbrace{1, \ldots, 1}_{\times p_1}, \underbrace{2, \ldots, 2}_{\times p_2} \ldots, \underbrace{d, \ldots, d}_{\times p_d}) \tag{93}$$

and use the output together with appropriate slicing in the coupling function.

Example MAF: MAF requires two parameters for the coupling function in (86), $\gamma_i(x_{1:i-1}) = (\alpha_i(x_{1:i-1}), \beta_i(x_{1:i-1})) \in \mathbb{R}^2$. Thus the conditioner network for MAF can be constructed by setting $p_i = 2$, $i = 1, \ldots, d$ in (93).

There are two extensions to masked conditioner networks [18],

- **Order agnostic training**. As with normalizing flows in general the natural ordering of the input $x_{1:d}$ is a constraint to the result. One could therefore in change the assignment rule for the input layer in (89) and randomly sample $m^0 = \left(m^0(1), \ldots, m^0(d)\right)$. [18] suggest to randomly sample *at each minibatch iteration*, which essentially gives an ensemble of models (as many models as there are orderings).

- **Connectivity agnostic training**. In this approach also the assignment rules for the hidden layers m^ℓ in (89) are re sampled *at each minibatch iteration*.

Technical note: the networks hyperparameters are the depth of the network (number of hidden layers $L - 1$) and the with of the hidden layers d_ℓ, $\ell \in 1, \ldots, L - 1$. In particular if the with $d_\ell < d - 1$ together with the randomly assigned connectivity constraints not all x propagate to the output layer. Thus it seems to be important that the hidden layers should be wide enough (with respect to the input dimension d).

Neural autoregressive flow (NAF) [28]. So far only affine coupling functions were used. NAF constructs a more expressive coupling function by a neural network. While in practice this model is hard to train (which can be improved [12]) it is conceptually interesting and is most importantly universal. As the coupling function needs to be strictly increasing (to be invertible), the neural network needs to satisfy constraints:

Proposition 1 *[28] Using strictly positive weights and strictly monotonic differentiable activation functions for h_ℓ is sufficient for the entire network to be strictly increasing.*

First note that the composition of strictly increasing functions is again strictly increasing. Specifically for a neural network with layer $h^\ell, \ell = 1, \ldots, L$ with $h^0 = x$ and $h^L = y$ we have for the derivative of the components

$$\frac{\partial y_i}{\partial x_j} = \frac{\partial h_i^L}{\partial h_l^{L-1}} \frac{\partial h_l^{L-1}}{\partial h_m^{L-2}} \cdots \frac{\partial h_k^1}{\partial x_j} \tag{94}$$

(using einstein sum convention). If $h^\ell = a^\ell(W^\ell h^{\ell-1} + b^\ell)$ with some strictly monotonic activation function a^ℓ and strictly positive weights $W_{i,k}^\ell > 0$. Then $\partial h^\ell / \partial h^{\ell-1} > 0$. But then each term in the sum of (94) is greater zero and thus $\partial y_i / \partial x_j > 0$. The following networks assume different parametrizations but the proof remains valid.

NAF proposes two versions for the couping functions $\tau_i(x_i, \gamma_i(x_{1:i-1}))$. *Deep sigmoidal flows* (DSF)

$$\tau_i : y_i = \sigma^{-1}\left(w_i^T \cdot \sigma\left(W_i x_i + b_i\right)\right), \tag{95}$$

where the parameters are obtained from the conditioner (e.g. by a masked conditioner network), $\gamma_i(x_{1:i-1}) = (w_i, W_i, b_i)$, with $w_i, W_i, b_i \in \mathbb{R}^{d_1}$, with d_1 beeing a hidden dimension. The neural network assumes the form of a standard affine linear function together with a attention-like [5] linear combination induced by $w_i, 0 < w_{k,i} < 1, \sum_k w_{k,i} = 1, \ k = 1 \ldots d_1, \ i = 1 \ldots d$. The strict inequality sign rather comes from the requirement on the network to ensure strict increasing the from the convex sum. This requirement also puts the constraint $W_{k,i} > 0$. These constraints must be satisfied by the conditioner via a suitable choice for the activation function in the output layer (by applying e.g. softmax or softplus functions). σ and σ^{-1} is the sigmoid function and its inverse (logit function), which are evaluated component wise. Both are strictly increasing and the logit function is used to assure that y_i can take any value over the real line.

The component wise definition of $\tau_i, i = 1, \ldots, d$ can be combined (vectorized) into one single neural network[13],

$$\tau : y = \sigma^{-1}\left(w^T \cdot \sigma\left(W x + b\right)\right), \tag{96}$$

with $w_i, W_i, b_i \in \mathbb{R}^{d_1 \times d}$. The individual conditioner outputs, $\gamma_i(x_{1:i-1}) = (w_i, W_i, b_i)$ are stacked in to matrices $W = (W_1, \ldots W_d), w = (w_1, \ldots w_d), b = (b1, \ldots, b_d)$ and a vector[14].

Note that this neural network for the coupling function has *no* trainable parameters (these are trained only in the conditioner network).

The diagonal element of the Jacobian is given by

$$\frac{\partial y_i}{\partial x_i} = \left\{ \sigma^{-1\prime}\left(\sum_{k=1}^{d_1} w_{k,i}\sigma\left(W_{k,i}x_i + b_{k,i}\right)\right) \right\} \left\{ \sum_{k=1}^{d_1} w_{k,i}\sigma'\left(W_{k,i}x_i + b_{k,i}\right) W_{k,i} \right\} \tag{97}$$

However the inverse cannot be computed analytically. It needs to be computed numerically for each y_i on the real line[15] together with the general formular (80).

---

[13]In practice the vectorized version is not used as it is more tedious to construct the matrices from the conditioner than calling one function d times. Furthermore, vectorization is less important as there are no parameters to optimize for this coupling function neural network.

[14]Note that we there is indeed a rather unorthodox "bias matrix", $b_i \in \mathbb{R}^{d_1 \times d}$ from incorporating attention.

[15]Given y_i, find numerically the root of the functon $x_i \mapsto y_i - \tau_i(x_i, \gamma_i(x_{1:i-1}))$ keeping $x_{1:i-1}$ fixed.

The *deep dense simoidal flow* network proposed in [28] assumes for a component of the coupling function the form

$$\tau_i : \begin{array}{ccccccccc} \mathbb{R} & \xrightarrow{f^1} & \mathbb{R}^{d_1} & \xrightarrow{f^2} & \mathbb{R}^{d_2} & \xrightarrow{f^3} & \dots & \xrightarrow{f^L} & \mathbb{R} \\ \cup\!\!\!| & & \cup\!\!\!| & & \cup\!\!\!| & & & & \cup\!\!\!| \\ x & & h^1 & & h^2 & & & & y \end{array}$$

$$f^\ell : h^\ell = \sigma^{-1} \left\{ \left(w^\ell \cdot \sigma \left(a^\ell \odot W^\ell h^{\ell-1} + b^\ell \right) \right) \right\}, \tag{98}$$

where $h^0 = x$ and $h^L = y$, and $w^\ell \in \mathbb{R}^{d_\ell \times d_\ell}$, $W^\ell \in \mathbb{R}^{d_\ell \times d_{\ell-1}}$, $a_\ell, b_\ell \in \mathbb{R}^\ell$. The requirement for strictly increasing are all parameters (except b^ℓ) to be strictly positive. For the attention mechanism to work: $\sum_j w_{i,j}^\ell = \sum_j w_{i,j}^\ell = 1$. Again these constraints must be assured by the conditioner. Note that this is not a mere stacking of a deep sigmoidal flow (95) as this would induce "bottlenecks". Because in (95) the output is a scalar.

The diagonal Jacobian elements are tedious but straight forward to compute (see Appendix C of [28]). As a technical note, they may become numerically unstable and one has to resort to the *Log-Sum-Exp* trick (see Appendix 111).

Sum-of-squares polynomial Flow (SOS) [30].   In order to obtain a flexible (strictly increasing) coupling functions SOS constructs one from polynomials. The basic idea is to obtain a positive function by squaring a polynomial (these squared polynomials can be again expanded with some coefficients) and then construct a strictly increasing function by integrating it. Generally,

Proposition 2 *[30] A univariate real polynomial is increasing iff it can be written as*

$$\tau(x; a, b) = b + \int_0^x \sum_{j=1}^k \left(\sum_{i=0}^r a_{i,j} u^i \right)^2 du, \tag{99}$$

with $b \in \mathbb{R}, a \in \mathbb{R}^{(r+1) \times (k)}$. It is strictly increasing iff it is not constant. Furthermore let C be the space of real univariate continuous functions, equipped with the topology of compact convergence. Then, the set of increasing polynomials is dense in the cone of increasing continuous functions.

The hyperparameter $r \in \mathbb{N}$ is called the degree of the polynomial, and $k \in \mathbb{N}$ is called number of polynomials A autoregressive flow can be readily constructed by

$$y_i = \tau_i(x_i, a_i, b_i) = \tau(x_i, a_i(x_{1:i-1}), b_i(x_{1:i-1})), \tag{100}$$

with the coupling function (99) and $\gamma_i(x_{1:i-1}) = (a_i(x_{1:i-1}), b_i(x_{1:i-1}))$ can be approximated by e.g., a masked conditioner network. That these polynomials are dense in the cone of increasing continuous function essentially shows the universality property of this flow.

In practice only small values for the hyper parameters k, r are used ($k = 5, r = 4$ or so). Further expressiveness can be achieved by composition (deep) or increasing r (wide), where the latter is theoretically more sound but introduces more parameters. Because there are just polynomials the integral can be performed analytically. The diagonal element of the Jacobian is given by[16]

$$\frac{\partial y_\ell}{\partial x_\ell} = \sum_{j=1}^{k} \left(\sum_{i=0}^{r} (a_\ell)_{i,j} \, x_\ell^i \right)^2. \tag{102}$$

However the inverse cannot be computed analytically. It needs to be computed numerically for each y_i on the real line together with the general formular (80).

SOS is easier to train than NAF as there are no constraints on parameters of the coupling function. Also note that for $r = 0$ SOS reduces to the affine couling function.

Summary. While there are several non-triagonal flows, autoregressive forms are a promising avenue to construct flows.

- By their definition they are triangular and thus Theorem 1 may be exploited.

- The **conditioning function** can be approximated efficiently by masked conditioners and accurately due to the universal approximation theorem for deep neural networks.

- For the **coupling function** it is enough to construct univariate (strictly) increasing functions. This can be achieved by care carefully designing a neural network as in NAF. More generally this can also achieved by integrating non-negative functions [70] as in the Sum-of-squares polynomial flow.

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[16]

$$\frac{\partial}{\partial x} \int_0^x f(u)\,du = \frac{\partial}{\partial x} \left(F(x) - F(0) \right) = \frac{\partial}{\partial x} F(x) = f(x) \tag{101}$$

- While such constructions are necessary to assure universality they have a drawback compared to affine coupling functions (or other simple, yet analytically invertible coupling functions): for sampling they typically need to be inverted numerically (for each y_i in one dimension respectively). If there are more sampling steps then inference steps, then one could also learn the f^{-1} rather than f like in the inverse autoregressive flow (IAF) [33]. If both, efficient sampling and density estimates is important then [45] train a student network for f^{-1} with f as a teacher network.

Alternatively, the coupling function may be constructed by a superposition of known cumulative distribution functions (CDF) to ensure strictly increasing For images or sound modeling the conditioner via masked autoregression is not appropriate. In this case conditioners based on convolutional neural networks are constructed [24, 67, 66, 45].

10.4   Conditional probabilities

Up until now we considered only transformations on the joint pdfs from one propability distribution p_X, to another (base) distribution p_Y via a function $f : X \to Y$ such that $p_X(x) = p_Y(f(x))|\det Df(x)|$.

In practice one would often learn such a map for conditional probabilities $p(x|x')$ of a random variables $x \in \mathbb{R}^d$ conditioned on random variables $x' \in \mathbb{R}^{d_c}$. So the aim is to learn a function $f : (X; X') \to Y$ such that

$$p_X(x|x') = p_Y(f(x; x'))|\det D_x f(x; x')|, \tag{103}$$

where the x' serve as function parameters and the jacobian is only evaluated with respect to x.

The extension of normalizing flows is straightforward [47]. Autoregressive flows (79) generalize

$$y_i = T_i(x_1, \ldots, x_i) = \tau_i(x_i; \gamma_i(x_{1:i-1}, x')), \quad i = 1, \ldots, d, \tag{104}$$

and the conditioner function is now allowed to depend on *all x'* in addition to the subset $x_{1:i-1}$ of x as demanded by the autoregressive (tringualar) property. Thus, one only needs to adapt the conditoner to allow more variables. In particular the masked conditioner networks generalize readily. The input layer (87) in is now of dimension $\mathbb{R}^{d_c+d}$ in and the connectivity constraints for the input layer (89) can be written e.g., as

$$m^0 = (\underbrace{0, \ldots, 0}_{\times d_c}, 1, \ldots, d), \tag{105}$$

in other words the conditioning set comes *before* the other random variables. The rest remains unchanged. More formally one could also extend the defintion of triangular maps keeping its properties [17].

10.5 Dequantization

The theory assumes continuous random variables. However, in practice often discrete data occur. Assume that the input data data are count data $x_i \in \mathbb{N}$. Instead of the real data one adds uniform noise, $x_i' = x_i + Unif(0, 1))$ and feeds that data into the flow algorithm. This process is called dequantization [64, 24].

11 Variational autoencoders

[34]
http://krasserm.github.io/2019/03/14/bayesian-neural-networks/

12 Generative autoregressive models

13 Diffusion models

[71, 60, 26, 53]

Note: Diffusion models can be understood as discrete state Markov models [6]. Diffusion models are closely related to so called score based generative models [62, 61]. This leads to stochastic differential equations (SDE) [44] using Langevin dynamics. There also seems to be a close relation to flow models, which also assume the form of an SDE in the limit of composing infinitely many flows [35].

14 Time Series Neural Network

Common practices for time series modelling

- **Split time** in context and prediction times

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[17]A map $T = (T_1, \ldots, T_d) : \mathbb{R}^{d_c+d} \to \mathbb{R}^d$ is called triangular if T_1 is a function of (x', x_1), T_2 a function of (x', x_1, x_2), and so on: T_i is a function of $(x', x_1, \ldots, x_i)$. A triangular map is called (strictly) increasing if every component T_i is (strictly) increasing with respect to the variable x_i

- **Scaling:** scale data over context time and rescale after prediction

- **Metrics for evaluation** *Continuous Ranked Probability Score* (CRPS) for probabilistic time series models

- **Dequantization:** corresponds to adding noise (e.g. from a uniform distribution) for disrecte data when using models that require contineous data (eg. normalizing flow models).

- **Categorical features:** use embeddings

- Use fourier components

Time series can be understood as subclass of sequence models. This section summarizes explicit time series models.

LSTNet. This network [37] aims to model long and short term patterns by combining neural net components with an autoregressive model. A prediction at time step t given by

$$\hat{y}_t = y_t^{AR} + y_t^{NN}, \tag{106}$$

where y_t^{NN} is the neural net component and y_t^{AR} is the auto regressive component. The auto regressive part is sensitive to the scale of the inputs (which is a hard for neural networks). This significantly improves model performance.

The neural network part models modulations with respect to this baseline model. It introduces a so called recurrent skip connection by adapting the formulae of e.g. LSTM (in the paper of GRU): LSTM uses hidden states at time $t-1$ as inputs for time t. The paper instead uses hidden states of time step $t-p$ as input for time step t. This adds a parameter p (the number of hidden states skipped through) and needs to be tuned. For periodic patterns p is obviously the periodicity. This method should increase the long term capacity of standard RNNs.

$$\text{Temporal convolution: } y_t \mapsto y_t' \tag{107}$$
$$\text{Gated recurrent network: } y_t' \mapsto y_t'' \tag{108}$$
$$\text{Recurrent-skip network: } y_t' \mapsto y_t''' \tag{109}$$
$$\text{Combination } y_t^{NN} = W^1 y_t'' + \sum_{i=0}^{p-1} W_i^2 y_{t-i}''' + b \tag{110}$$

The convolution shall capture short term dependencies and serves as input for following RNN. The RNN should capture long term time dependencies

and even more the recurrent skip network. Finally both recurrent units are combined by a small dense NN. As input serve only the last hidden state at time t of the RNN (context vector) and the last p hidden states of the recurrent-skip network. Instead of the last two steps also the attention mechanism can be used (which also increases the long term capacity). The authors find similar accuracy within these two approaches.

Modelling Uncertainties The principal idea is to model the temporal dependencies of a time series via an LSTM or Attention Network. Call this temporal network. The *temporal fusion transformer* then uses the output of the temporal network for point estimates (quantiles) of the uncertainties [1]. Alternatively one could model a distribution to reflect the uncertainties. *Deep Ar* uses the outputs of the temporal network as parameters of a fixed, parametrized distribution (e.g., the parameters of the negative Binomial distribution for count data) [56]. In order to overcome the limits of fixed distributions the outputs of the temporal network could be fed into a *normalizing flow* [51] or a *diffusion model* [50].

A Numerics

A.1 Log-sum-exponent trick.

The logarithm of sum of exponentials may suffer from numerical overflow (due to exponent) or underflow. A numerical stable equivalent is

$$\ln \sum_i e^{x_i} = \ln \sum_i e^{x_i - c} + c, \quad c = \max\{x_i\}, \tag{111}$$

which prevents the exponent to explode (numerical overflow). This idea may be put forward compute numerical stable logarithms of matrix multiplication. More generally, consider the logarithm of a Tensor contraction

$$\ln \sum_k A_{ikl} B_{ikl} = \ln \sum_k e^{\ln A_{ikl}} e^{\ln B_{ikl}} \tag{112}$$

$$= \ln \sum_k \exp(\ln A_{ikl} + \ln B_{ikl}) \tag{113}$$

As a special case the matrix product is given by

$$\ln AB_{ij} = \ln \sum_k A_{ik} B_{kj} = \ln \sum_k \exp(\ln A_{ik} + \ln B_{kj}), \tag{114}$$

both can be computed in a numerical stable fashion using (111). Furthermore the logarithm of a Matrix product can be written as a generalized sum of the individual Matrix logarithms.

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