

Unsupervised source separation with deep priors

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July 15, 2020

Contents

Method	5
Modeling the priors	7
Sampling from the posteriors	10
Modeling the posteriors	11
Difficulties of this method	12

Method

IN THIS CHAPTER, we introduce the theoretical idea of our probability modelling of musical source separation. First, we explicitly state our chosen model of the problem, next derive a suitable optimization objective from it and then explain how we can optimize towards that.

We propose the graphical model as shown in Figure 1 as the generative story of music tracks being generated from separate source tracks. For each source, a sample is taken from the latent source distribution. The observed mix is generated deterministically from the full set of sources. Without loss of generality, we fix this function to be the mean.

Our stated task in ?? is to retrieve the sources $\{s_1, \dots, s_N\}$ from a given mix m . Our model is trained without using sample tuples

$$(m, \{s_1, \dots, s_N\}) : f(\{s_1, \dots, s_N\}) = m$$

which would show the relation between separate sources and mixes. The general idea is visualized in Figure 2.

Looking back at the graphical model in Figure 1, it implies the following factorization:

$$p(m) = \int^N p(s_1, \dots, s_N, m) d^N s \quad (1)$$

$$= \int^N p(m|s_1, \dots, s_N) \cdot p(s_1, \dots, s_N) d^N s \quad (2)$$

$$= \int^N p(m|s_1, \dots, s_N) \cdot p(s_1) \cdots p(s_N) d^N s \quad (3)$$

While the conditional $p(m|s_1, \dots, s_N)$ is not even probabilistic, as the mix is generated deterministically with the mean of the sources, the model posterior $p(s_1, \dots, s_N|m)$ is intractable and precisely what we are interested in. Again we want to make it clear that this setup changes the typical optimization target, as seen in other source separation approaches. We factorize the distribution $p(m)$ of mixed songs, only then to extract the most likely *latent* components that generate this mix, the sources. Therefore we are explicitly modelling the generative process of the mixed songs, and only implicitly the separation task.

Already with the graphical model we introduce a fairly big as-

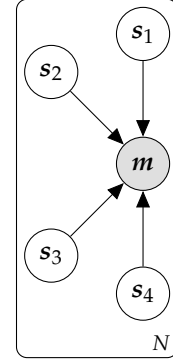


Figure 1: The used graphical model for the source separation task. We have the latent source channel variables s_k . Exemplary here, as in our data, we have four sources. The mix m is observed.

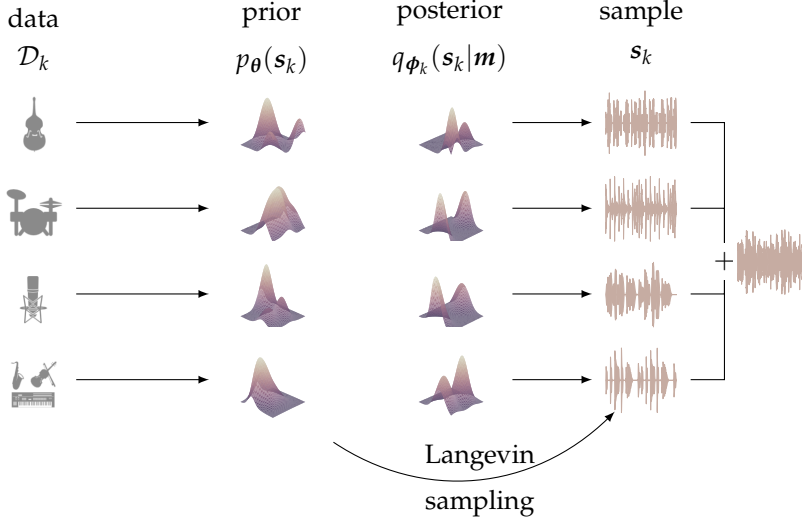


Figure 2: The method visualized

sumption, namely that we can model the source distributions independently from each other when modeling the joint:

$$p(\mathbf{m}, s_1, \dots, s_N) \equiv p(\mathbf{m} | s_1, \dots, s_N) \cdot \prod_k^N p(s_k) \quad (4)$$

Intuitively this assumption does not, in general, hold for the musical domain. We can expect a different behaviour for a *guitar* in a song involving a second source like a *percussion set*. The joint of those two models is different than their independent densities ¹. Nevertheless, this assumption is crucial to be able to model the prior instrumental models without needing the tuples (s_1, \dots, s_N) of co-occurring stems.

The general process is as follows:

First, because we assumed in our graphical model the latent sources to be independent, there exists a probability distribution $p(s_k)$ for each source k . Thereout we need to choose a model which gives the parametrized approximated prior $p_\theta(s_k)$ with the parameters θ which we optimize with the samples from \mathcal{D}_k .

Second, for each source, there exists a posterior given a mix $p(s_k | \mathbf{m})$ from which we want to draw samples. Here two approaches are possible. Either we can propose an approximate posterior $q_{\phi_k}(s_k | \mathbf{m})$, which is trained to minimize the divergence from the previously trained and fixed corresponding prior (VAE setting). Or, we can sample directly from the posterior using Stochastic Gradient Langevin Dynamics (SGLD)² without explicitly approximating the posterior distribution (sampling setting). Both optimization, either training or sampling, happen under the mixing constraint:

$$\sum_{k=1}^N s_k = \mathbf{m} \quad (5)$$

¹ A practical counter-example: If learning the behaviour of drums, only from solo drum recordings, one will encounter complex rhythms and sounds. In many rock genres drums often exhibit simpler sounds, providing beat and tempo. These two distributions are not the same.

² Welling and Teh, “Bayesian Learning via Stochastic Gradient Langevin Dynamics”, 2011.

When using the VAE setting we then can sample from each posterior to retrieve a set of (approximately) correct source tracks. In the case of using Langevin dynamics, the iterative sampling will directly give this set from the prior distributions.

Thinking in the common terms of the VAE we need to choose:

1. a parametrization $p_\theta(s_k)$ of the *prior* distribution
2. a parametrized approximate posterior distribution $q_{\phi_k}(s_k|\mathbf{m})$ with parameters η
3. a parametrized *encoder* which gives the parameters for the posterior distribution $\text{Encoder}_\phi(\mathbf{m}) = \eta$
4. a *decoder* which returns the input \mathbf{m} from the latents $\text{Decoder}(\{s_1, \dots, s_N\}) = \mathbf{m}$

As stated before the decoder in our case is the mean function, thus not probabilistic and without parameters. It is certainly possible to parametrize the decoder with trainable parameters. This would imply though that the latent samples are not in the *direct form* of the source sounds but under an (unknown) transformation.

Modeling the priors

The first step in the training procedure is the training of the independent source priors $p(s_k)$. We have to choose a model for estimating the density that results in smooth, tight densities but also is capable enough to capture the complex data space of audio data. We choose to estimate the priors, with flow models for which we gave an overview in ???. The invertibility of the flow gives us the ability to sample from the priors, which is necessary for the sampling-based approach. For the variational-based approach sampling is not necessary, nevertheless we utilize the same generative priors for both experiments. For different representations of the input, different network architectures are more suited. We experiment both with using directly the time-domain wave but also modelling on top of a spectral transformation of the time-domain data.

The two main variants of normalizing flows we build our priors from are the RealNVP and Glow. Their most important difference is the different formulation of the coupling layers. For the coupling layers, we have to split the layer input into two equally sized subsets, one of whom will be transformed using an invertible transformation parametrized by the other. The RealNVP masks the data spatially or over the channels. When done spatially a checkerboard binary mask is used (same for all channels), for the channel variant the channels are assigned in an even-odd switching. Glow, on the other hand, learns a 1×1 -convolution which permutes the data channel-wise and then just splits the data along the channel dimension into two. For both RealNVP and Glow prior work exists specifically adapting

the architecture to the time-series domain by integrating WaveNet modules, FloWaveNet³ and WaveGlow⁴, respectively.

Remove Glow if no experiment will use it

For the case of the time-domain representation, the data has only one channel (mono-audio). Therefore a Glow-like shuffling of channels is not possible and we resort to using spatial masking for the coupling layers. A one-dimensional mask is used over the time dimension. In the case of using a spectral representation of the audio data, the input samples have a lower time resolution but instead the frequency distribution over a deeper channel dimension. Therefore we can also experiment with channel-shuffling.

We make it clear that the success of this method depends strongly on the expressiveness and smoothness of the learned prior models. In the case of learning the posterior, variational learning will fit the posterior distribution under the prior distribution. If the prior does not contain enough variation of the actual data distribution, the de-mixing model cannot fit a conditional posterior similar to the sample in the mixed song. In the case of the sampling approach, this constraint is even more stressed. The mixed is generated by iteratively sampling from the set of prior distributions, any possible source sample, therefore, has to be found on the manifold of the prior. If any of the priors does not capture the full variations of the data distributions, neither method will be able to extract the correct separated sources.

More practically we again point out the high difficulty of modelling audio data. As laid out in ?? audio consists of information at greatly different resolutions. A generative model of an instrument has to model the low-range components, e.g. pitch, timbre, tremolo and high-range components, e.g. notes and rhythm.

Prior architecture

See the visualization of the prior model's architecture in Figure 3. We construct normalizing flow models, following the description in Kim et al.⁵.

The flow network, at the highest level, consists of n_b context blocks, each of whom contain one squeeze operation and n_f flows. The squeeze operation halves the length of the signal by doubling the number of channels. By doing so, we effectively double the receptive field of the WaveNet operators in the affine couplings. One flow contains one affine coupling layer after which the masking for the coupling (*even/odd*) is inverted. Before the coupling layer, we apply activation normalization⁶. The affine coupling is applying an affine transformation on the *odd* set of the input, with scale s and translation t coming from the *even* input put through a *non-causal* WaveNet.

The *even/odd* masking for the coupling layer is simply achieved by splitting the channel dimension into two equal parts. Flipping the masking exchanges the top half of channels with the bottom half.

³ Kim et al., "FloWaveNet : A Generative Flow for Raw Audio", 2019.

⁴ Prenger et al., "WaveGlow: A Flow-Based Generative Network for Speech Synthesis", 2018.

⁵ Kim et al., "FloWaveNet : A Generative Flow for Raw Audio", 2019.

⁶ Kingma and Dhariwal, "Glow: Generative Flow with Invertible 1x1 Convolutions", 2018.

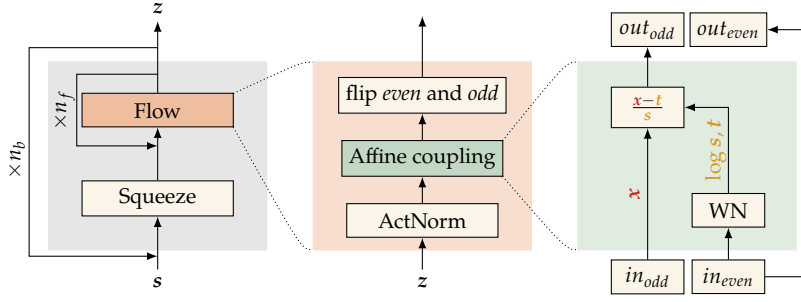


Figure 3: The building blocks for the prior model. The model consists of n_b blocks (left). Each block consists of n_f flows (middle). In each flow we apply activation normalization, followed by the affine coupling (right), after which the binary mask for the even/odd mapping is inverted. The affine coupling layer uses a WaveNet with the *even* set as the input to output scaling $\log s$ and translation t which the *odd* set is transformed.



Figure 4: Flip and squeeze operation for the coupling layers. The squeeze operation doubles the channels and halves the length while the flip operation inverts the tensor along the channel dimension.

No channel transformation of the channels is learned as in Glow. Further observe that through the repeated squeeze operation the masking implicitly includes a checkerboard pattern on the temporal dimension, similar to the explicit pattern used in RealNVP.

As explained in ?? the invertible flow $f(\cdot)$ network directly maps the data space into a prior distribution $p(z)$. Through the invertibility we can directly optimize the log probability with the change of variable formula:

$$\log p(x) = \log p(f(x)) + \log \det \left(\frac{\partial f(x)}{\partial x} \right) \quad (6)$$

Our network consists of n_b blocks with each n_f flows each with one activation normalization layer f_{AN} and an affine coupling layer f_{AC} . Therefore the log-determinant becomes:

$$\log \det \left(\frac{\partial f(x)}{\partial x} \right) = \sum_i^{n_b \cdot n_f} \log \det \frac{\partial f_{AN}(x)}{\partial x} + \log \det \frac{\partial f_{AC}(x)}{\partial x} \quad (7)$$

The activation normalization layer f_{AN} learns an affine transformation per channel i :

$$f_{AN}^i(x_i) = s_i \cdot x_i + t_i \quad (8)$$

The log-determinant is easily computed with⁶:

$$\log \det \frac{\partial f_{AN}(x)}{\partial x} = T \cdot \sum_i^C \log |s_i| \quad (9)$$

where C is the number of channels and T is the length of the signal.

For the affine coupling layer, the log-determinant is made tractable by only transforming half the elements in each application. The coupling transforms the *odd* part as follows:

The inverse is:

$$f_{AN}^{-1}(y_i) = \frac{y_i - t_i}{s_i}$$

$$\log \mathbf{s}, \mathbf{t} = \text{WN}(\text{in}_{\text{odd}}) \quad (10)$$

$$\text{out}_{\text{odd}} = f_{\text{AC}}(\text{in}_{\text{odd}}) = \frac{\text{in}_{\text{odd}} - \mathbf{t}}{\mathbf{s}} \quad (11)$$

where $\text{WN}(\cdot)$ is a WaveNet. The Jacobian of the coupling function is a lower triangular matrix⁷ because of which the log-determinant becomes the product of the diagonal elements:

$$\log \det \frac{\partial f_{\text{AC}}(\mathbf{x})}{\partial \mathbf{x}} = -\sum \mathbf{s} \quad (12)$$

The purpose of the invertible flow is it to project the complex data distribution into a tractable defined prior distribution. In most cases, as in this, the prior $p(\mathbf{z})$ is set to be a factorized Gaussian distribution with zero mean and variance of one. As such the likelihood of $f(\mathbf{x}) \sim p(\mathbf{z})$ can be evaluated with:

$$\log p(f(\mathbf{x})) = -\frac{1}{2}(\log(2 \cdot \pi)) + f(\mathbf{x})^2 \quad (13)$$

To train the model we maximize the likelihood in Equation (6) which we is the sum of the parts in Equations (9), (12) and (13). Optimization is done in mini-batches with the Adam optimizer⁸ and a decaying learning rate scheme.

It is noted that the likelihood under the prior is computed “pixel”-wise⁹. While for the optimization the actual loss on which the optimizers performs update steps is the mean likelihood, we can use the trained prior flow to assign a likelihood map to an input signal where each log-likelihood value is depending on this values receptive field.

WaveNet

In the affine coupling layer we utilize a *non-causal* WaveNet for generating the scale $\log \mathbf{s}$ and translation \mathbf{t} values. The WaveNet is non-causal because the filters are centred, as such the receptive field of an output value is symmetrically in the past and future input space. The kernel size is fixed to 3. The WaveNet is using the original gated convolution scheme described in ???. Appended to the last skip connection output are two additional one-dimensional convolutional layers, each preceded by a ReLU. The last convolutional layer is initialized to zero. By that we initialize the affine transformation of the coupling layer to the identity at the beginning of training, helping to stabilize optimization. The last layer outputs both scaling and translation factors. Learning those factors with weight sharing does not change the formulation of the coupling layer, as the log-determinant does not depend on the network. Learning them in the same network might increase efficiency, as well as, increasing implementation simplicity. The WaveNet completely consists of convolutional operations. As such it can be applied to one-dimensional signals of variable length.

The inverse is:

$$f_{\text{AC}}^{-1}(\text{out}_{\text{odd}}) = \text{out}_{\text{odd}} \cdot \mathbf{s} + \mathbf{t}$$

⁷ Dinh, Sohl-Dickstein, et al., “Density Estimation Using Real NVP”, 2017.

⁸ kingmaAdam2017.

⁹ time-points in our sound case

Sampling from the posteriors

After having estimated the N prior distributions the first possibility for retrieving sample estimates \mathbf{s}_k is sampling from the posterior using Langevin dynamics¹⁰. With Stochastic Gradient Langevin Dynamics (SGLD) we can sample from $\mathbf{s}_i \sim p(\cdot|\mathbf{m})$ without computing, explicitly, the posterior $p(\mathbf{s}_i|\mathbf{m})$. For an overview of SGLD see ??.

Starting with the update step in SGLD we reformulate the update with our problem constraint:

$$\mathbf{s}_k^{(t+1)} = \mathbf{s}_k^{(t)} + \eta \cdot \nabla_{\mathbf{s}_k} \log p(\mathbf{s}_k^{(t)}|\mathbf{m}) + 2\sqrt{\eta}\epsilon_t \quad (14)$$

$$= \mathbf{s}_k^{(t+1)} + \eta \cdot \nabla_{\mathbf{s}_k} [\log p(\mathbf{m}|\mathbf{s}_k) + \log p(\mathbf{s}_k) - \log p(\mathbf{m})] + 2\sqrt{\eta}\epsilon_t \quad (15)$$

$$= \mathbf{s}_k^{(t+1)} + \eta \cdot \nabla_{\mathbf{s}_k} [\log p(\mathbf{m}|\mathbf{s}_k) + \log p(\mathbf{s}_k)] + 2\sqrt{\eta}\epsilon_t \quad (16)$$

$$= \mathbf{s}_k^{(t+1)} + \eta \cdot \left[\|\mathbf{m} - \frac{1}{N} \sum_j \mathbf{s}_j^{(t)}\| + \nabla_{\mathbf{s}_k} \log p(\mathbf{s}_k) \right] + 2\sqrt{\eta}\epsilon_t \quad (17)$$

η is the update step size and $\epsilon_t \sim \mathcal{N}(0, \mathbb{I})$.

Note that the final formulation of the update step is simply a constrained greedy hill-climb under the prior model with added Gaussian noise. Intuitively the artificially noised update makes it harder for the greedy optimization to get stuck in local minima of the prior surface.

```

1: for  $t = 1 \dots T$  do
2:   for  $k = 1 \dots N$  do
3:      $\epsilon_t \sim \mathcal{N}(0, \mathbb{I})$ 
4:      $\Delta \mathbf{s}_k^t \leftarrow \mathbf{s}^t + \eta \cdot \nabla \log p(\mathbf{s}^t) + 2\sqrt{\eta}\epsilon_t$ 
5:   end for
6:   for  $k = 1 \dots N$  do
7:      $\mathbf{s}_k^{t+1} \leftarrow \Delta \mathbf{s}_k^t - \frac{\eta}{\sigma^2} \cdot [\mathbf{m} - \frac{1}{N} \sum_i \mathbf{s}_i^t]$ 
8:   end for
9: end for

```

The idea of using SGLD in combination with deep parametrized priors was, concurrently to this work, introduced in Jayaram and Thickstun¹¹. The authors empirically show that

$$\mathbb{E} [\|\nabla_s \log p_\sigma(\mathbf{s})\|^2] \propto 1/\sigma^2$$

They argue that this surprising proportionality is stemming from the severe non-smoothness of the prior model. If the prior model, in the extreme case, exhibits a Dirac delta peak as the probability mass, then the estimation of the gradient with added Gaussian noise will itself be proportional to the Gaussian. From there the authors argue, that the prior models have to be trained with noised samples, where the added noised is proportional to later used estimator noise.

¹⁰ Welling and Teh, “Bayesian Learning via Stochastic Gradient Langevin Dynamics”, 2011.

$\log p(\mathbf{m})$ is independent from \mathbf{s}_k therefore no gradient.

Algorithm 1: The Langevin sampling procedure for source separation is fairly straight forward. For a fixed number of steps T we sample we take a step into the direction of the gradient under the priors and the gradient of the mixing constraint while adding Gaussian noise ϵ_t .

¹¹ Jayaram and Thickstun, “Source Separation with Deep Generative Priors”, 2020.

Modeling the posteriors

Instead of formulating a sampling regime for approaching s_k we can also use the prior models to variationally train a model to estimate the parameters of an approximate posterior $q_{\phi_k}(s_k|\mathbf{m})$. While estimating the true posterior $p(s_k|\mathbf{m})$ is intractable, we choose a certain parametrized distribution as an approximation of the posterior and optimize the parameters to align with the true one.

We follow the same steps as previously shown generally for the latent variable models. First, we introduce an approximate posterior $q_{\phi_k}(s_k|\mathbf{m})$ for each source channel. Next, we express the mix density as the expectation over those posteriors:

$$\log p(\mathbf{m}) = \mathbb{E}_{q_{\phi_k}(s_k|\mathbf{m})}^N [\log p(\mathbf{m})] \quad (18)$$

From here we introduce the approximate posteriors in the expectation as before, just now for N separate priors:

$$\mathbb{E}_{q_{\phi_k}(s_k|\mathbf{m})}^N [\log p(\mathbf{m})] = \mathbb{E}_{q_{\phi_k}(s_k|\mathbf{m})}^N \left[\log \frac{p(\mathbf{m}, s_1, \dots, s_N)}{p(s_1, \dots, s_N|\mathbf{m})} \right] \quad (19)$$

$$= \mathbb{E}_{q_{\phi_k}(s_k|\mathbf{m})}^N \left[\log \frac{p(\mathbf{m}|s_1, \dots, s_N) \cdot \prod_k^N p(s_k)}{\prod_k^N q_{\phi_k}(s_k|\mathbf{m})} + \log \frac{\prod_k^N q_{\phi_k}(s_k|\mathbf{m})}{p(s_1, \dots, s_N|\mathbf{m})} \right] \quad (20)$$

Note that again we use the assumption in Equation (4) to factorize the joint. This assumption is not being used for the independent approximate posteriors. While the true posterior certainly is the posterior of the joint source model, we choose our approximate posteriors to be independent. The expectation in (18) over those is still correct. The error arising from the independence assumption is captured in the tightness of the ELBO.

We arrive at the ELBO by leaving out the divergence of the approximate posterior to the true posterior:

$$\mathbb{E}_{q_{\phi_k}(s_k|\mathbf{m})}^N [\log p(\mathbf{m})] \geq \sum_k^N \mathbb{E}_{q_{\phi_k}(s_k|\mathbf{m})} \left[\log \frac{p(s_k)}{q_{\phi_k}(s_k|\mathbf{m})} \right] + \mathbb{E}_{q_{\phi_k}(s_k|\mathbf{m})} [p(\mathbf{m}|s_1, \dots, s_N)] \quad (21)$$

The lower bound, as in the normal VAE, will be our optimization target for training the inference models that give the variational parameters ϕ_k . We can also formulate the objective for just one source, as the Encoders are trained independently¹². Thus we come to:

¹² While the optimization of the Encoders is independent, the training is, of course, concurrent as the mixing conditions depends on all N source samples.

$$\mathbb{E}_{q_{\phi_k}(s_k|\mathbf{m})} [\log p(\mathbf{m})] \geq \mathbb{E}_{q_{\phi_k}(s_k|\mathbf{m})} \left[\log \frac{p(s_k)}{q_{\phi_k}(s_k|\mathbf{m})} \right] + \mathbb{E}_{q_{\phi_k}(s_k|\mathbf{m})} [p(\mathbf{m}|s_1, \dots, s_N)] \quad (22)$$

$$= \mathbb{E}_{q_{\phi_k}(s_k|\mathbf{m})} \left[\log \frac{p(s_k)}{q_{\phi_k}(s_k|\mathbf{m})} \right] + \|\mathbf{m} - \frac{1}{N} \sum_j^N \mathbf{s}_j\| \quad (23)$$

The Kullback-Leibler divergence term is computationally expensive, therefore the divergence is the stochastic estimate using just one mini-batch.

With Equation (23) we have the optimization objective set up and now have to choose a fitting parametrized posterior for $q_{\phi_k}(s_k|\mathbf{m})$. In many recent

```

1: for  $x \in \mathcal{D}_k$  do
2: end for

```

Algorithm 2: Training of the approximate posterior.

Difficulties of this method

1. Good prior densities

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