Gradient-based Training of Slow Feature Analysis by Differentiable Approximate Whitening

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Abstract
This paper proposes Power Slow Feature Analysis, a gradient-based method to extract temporally-slow features from a high-dimensional input stream that varies on a faster time-scale, and a variant of Slow Feature Analysis (SFA). While displaying performance comparable to hierarchical extensions to the SFA algorithm, such as Hierarchical Slow Feature Analysis, for a small number of output-features, our algorithm allows end-to-end training of arbitrary differentiable approximators (e.g., deep neural networks). We provide experimental evidence that PowerSFA is able to extract meaningful and informative low-dimensional features in the case of a) synthetic low-dimensional data, b) visual data, and also for c) a general dataset for which symmetric non-temporal relations between points can be defined.

1 Introduction
Finding meaningful representations in data is a core challenge in modern machine learning as the performance in many goal-directed frameworks such as reinforcement learning or supervised learning is directly and strongly influenced by the quality of the former. Usually, features are either provided (e.g. by expert knowledge) or acquired through learning. Most currently successful approaches for either deep supervised learning [1] or reinforcement learning [2] rely on a training signal, i.e., a classification label or reward signal, to provide sufficient indication which features of the input data should be extracted to increase performance. However, in most real-world scenarios labels have to be acquired by expert knowledge and reward signals are sparse. In unsupervised representation learning one tries to find and apply a principle by which to extract meaning from data without assuming the availability of any goal-driven metrics. Examples for such principles are based on reconstruction error (principal component analysis, autoencoder networks [3]), statistical dependence of extracted features
(independent component analysis [4]), indistinguishability of synthetically generated data from samples of the input distribution (generative adversarial nets [5]), fitting the probability distribution of input data (variational autoencoders [6]), (graph-)neighborhood preservation (locally-linear embedding [7], Laplacian eigenmaps [8]), and temporal coherence (slow feature analysis [9], regularized slowness optimization [10]). The latter is the focus of this work and has been shown to provide a useful proxy for extracting underlying causes from time-series data such as position, head direction, identity of spatial view similar to those observed in rodent brains [11] from ego-visual data, or object configuration (identity, position, angle) from a tabletop view of moving objects [12] when applied in the form of slow feature analysis (SFA) [9].

A graph-based generalization of SFA [13] has been used to achieve (at that time) state-of-the-art age estimation results on the MORPH dataset [14].

We propose a variant of SFA that approximately enforces the same constraints while being differentiable and thus allows training by gradient-descent-derived methods. This variant makes it possible to leverage the representational power of complex models such as deep neural networks as well as useful ideas from that domain (dropout, batch normalization, activation regularization) to extract slow and informative features from data. To demonstrate the applicability of this approach, we provide three distinct experimental evaluations.

1.1 Related work

1.1.1 Slowness-based Methods

While the original proposal of SFA [9] uses non-linear basis functions as a method to introduce non-linearity to the otherwise linear model, this classical approach has two limitations: a) The basis functions have to be chosen by expert knowledge or expensive trial-and-error, and b) as the resulting model is shallow, its expressivity tends to scale unfavorably in the dimension of the expansion [15] compared to hierarchical models. In the case of polynomial expansion, expanding to degree \(d\) on \(e\)-dimensional input data will result in \((d+e)\)-dimensional expanded data, e.g., quadratically expanding grayscale images of 180 × 90 pixels results in an output dimension > 131 · 10^6. Extracting a single feature with a linear model would thus require 5.7-times more parameters than the modern and powerful Xception network [16].

A classical way to circumvent this problem is to apply the kernel trick [17] that allows for implicit expansion of arbitrarily high (even infinite) dimension as long as the solution can be expressed in inner products of the input data. But while it is possible to formulate SFA in such a way [18] [19] and kernel-based methods are usually very expressive (universal approximators, they carry their own problems, as they a) still require a domain-specific choice of kernel, b) also require strong regularization to avoid over-fitting, and c) their memory- and evaluation complexity often scales linearly with the number of training points [20] [21]. These properties severely limit the applicability of kernel methods in domains with vast amounts of high-dimensional input data, e.g. in visual
An alternative approach to increase expressivity using expansions is to apply low-degree non-linearities repeatedly in a receptive-field fashion, interlacing them with projection steps. This has been done in Hierarchical SFA (HSFA) \cite{11, 22} and deep architectures \cite{1} in general. But while the latter are typically trained in an end-to-end fashion by variants of stochastic gradient-descent, HSFA is trained in a layer-wise procedure, solving the linear SFA problem consecutively for each layer as closed-form solution and thereby assuming that globally slow features can be composed of decreasingly-local slow features. This assumption can be partially relaxed by adding information by-passes to the model \cite{22}. Compared to HSFA, our method allows directly modifying parameters in different layers to optimize a global slowness objective.

Our algorithm is in line with recent work harnessing the temporal coherence prior \cite{23} in deep, self-supervised feature learning. This can be done by having a slowness term in the loss function. To avoid the trivial, constant solution, another term is usually added. For example, a reconstruction loss in an auto-encoder \cite{24} or one-step latent code prediction \cite{25}. Deep temporal coherence also been considered via the lens of similarity metric learning, for example by optimizing a contrastive loss \cite{26} \cite{27} or a triplet loss \cite{28} \cite{29}. These metric learning approaches manage to avoid degenerate solutions by pushing away points from each other (in feature space) that are not temporal neighbours. Our work differs from these approaches as we seek to directly approximate the optimization problem as originally posed by \cite{9} in a deep learning setting, automatically handling the constant solution and ensuring that different features code for different information.

1.1.2 Graph-based Methods

SFA has been generalized to graph-based SFA (GSFA) \cite{13} and generalized SFA \cite{30}. The former adapts only the objective function, while the latter additionally generalizes the constraints to D-orthogonality (D being the degree matrix of an underlying graph). Following generalized SFA, standard SFA can be shown (cf. \cite{30}) to be a special case of Laplacian Eigenmaps \cite{8}. Spectral Inference Networks (SpIN) \cite{31} utilize this connection to successfully derive a gradient-based SFA training as a special case and have been developed simultaneously to this work. SpINs are based on the correcting a biased gradient when directly optimizing the Rayleigh-Quotient with respect to the parameters that define the embedding. Similar to PowerSFA, this procedure allows for employing any differentiable architecture to find these embeddings. The generalization of PowerSFA proposed in section 5.3 is close to GSFA, assuming regularity in the graph for the orthogonality constraint.

It should be mentioned that as a special case of Laplacian eigenmaps, SFA could also be expressed as a variant of Kernel PCA using a data-dependent kernel \cite{21}. This requires the application of an explicit Kernel PCA projection \cite{32} or, equivalently, Nyström’s method for approximating eigenfunctions \cite{33} to embed out-of-sample points and is thus limited for large amounts of training.
data, suffering from similar limitations to those mentioned in 1.1.1.

1.1.3 Other Related Approaches

In section 5.3 we consider a generalization of PowerSFA’s loss similar to GSFA and apply it to the NORB dataset [34], a collection of photographs of toys on which pair-wise similarities based on rotation, elevation, and lighting conditions can be defined. We thereby loosely follow the experimental procedure in [35]. The authors use a siamese neural network architecture [36] for optimizing pair-wise distances of embedded points to reflect similarity and dissimilarity structure of the data. In particular, they do not enforce orthogonality of the embeddings but rely on the optimization procedure to maximize informativeness.

2 Slow Feature Analysis

Slow Feature Analysis (SFA) is based on the hypothesis that interesting high-dimensional streams of data that vary quickly in time are typically caused by a low number of underlying factors that vary comparably slow. Thus, slowness can be used as a proxy criterion by which to extract meaningful representations of these low-dimensional underlying causes even in the absence of labels.

There is strong evidence in favor of this hypothesis as it has been shown that features extracted by SFA tend to encode highly relevant information about the data-generating environments, e.g. slow features encode and disentangle object identity, rotation, and position in visual tasks [12] as well as agent position and orientation from visual first-person recordings of random movement similar to place cells in rodents or head-direction cells in primates [11].

The notion of extracting slow features from a time-series dataset has been formalized as a sequential optimization problem. Given a time-series \( \{ x_t \}_{t=0}^{\tau} \) with \( x_t \in \mathbb{R}^d \), sequentially find continuous functions \( g_i : \mathbb{R}^d \rightarrow \mathbb{R} \) with:

\[
\begin{align*}
\min_{g_i} & \quad \langle (g_i(x_{t+1}) - g_i(x_t))^2 \rangle_t \\
\text{s.t.} & \quad \langle g_i(x_t) \rangle_t = 0, \quad (1b) \\
& \quad \langle g_i(x_t)^2 \rangle_t = 1, \quad (1c) \\
& \quad \langle g_i(x_t)g_j(x_t) \rangle_t = 0, \quad \forall j < i \quad (1d)
\end{align*}
\]

where \( \langle \cdot \rangle_t \) is the average over \( t \). The constraints ensure that each of the extracted features is informative (decorrelated to all others, equation (1d)) and non-trivial (unit variance, equation (1c)). Originally, solutions to SFA directly where only proposed for the space of affine functions \( g_i \in \mathcal{G} \), for which a closed-form solution exists, and in a kernelized version that requires strong regularization.
3 (Approximate) Whitening

While the standard implementation of linear SFA [37] is based on computing the
closed-form solution to a generalized eigenvalue problem [38], another approach
is to first whiten the time-series data followed a projection onto the minor
components of the difference time-series \(\{\dot{x}_t = x_{t+1} - x_t\}_{t=0,\ldots,\tau-1}\).

Whitened data has three important properties: a) it is mean-free (constraint (1b)), b) has unit variance if projected onto an arbitrary unit vector (constraint (1c)), and c) projections onto orthonormal vectors are decorrelated (constraint (1d)).

For a dataset \(\tilde{X} \in \mathbb{R}^{d \times N}\) with \(N\) and \(d\) being size of dimension of the dataset, respectively, the corresponding whitened dataset is defined as

\[
X = W\tilde{X}
\]

with \(W = D^{-\frac{1}{2}}U^T\) and \(C = UDU^T \in \mathbb{R}^{d \times d}\) being the whitening matrix and the canonical eigendecomposition of the covariance matrix, respectively. \(U\)'s columns contain the eigenvectors of \(C\) and \(D\) contains the corresponding eigenvalues on its diagonal. As \(C\) is typically assumed to be positive definite, \(D^{-\frac{1}{2}}\) is well-defined.

One widely used method to extract eigenvector/-value pairs is power iteration. Starting from a random vector \(u_0 \in \mathbb{R}^d\), repeatedly applying:

\[
u_{t+1} = \frac{Cu_t}{\|Cu_t\|}
\]

will converge to the eigenvector \(u\) corresponding to the largest (absolute) eigenvalue \(\lambda\). The eigenvalue can then be extracted as

\[
\lambda = \|Cu\|
\]

and the spectral component corresponding to this eigenvector can be removed as

\[C \leftarrow C - \lambda uu^T.\]

Repeating the procedure will converge to the eigenvector corresponding to the next largest eigenvalue and so on. We use a previously fixed number of iterations for this method as experiments have shown that approximate whitening is enough to take meaningful optimization steps. In practice, a relatively small number of iterations results in acceptable whitening for most non-degenerate cases.
Data: covariance matrix C, number of iterations $N_{\text{iter}}$, data dimension $d$

Result: whitening matrix $W$

$W \leftarrow \{0\}^{d \times d}$

for $i = 0; i < d; i++$ do
    Sample $r \sim U[-1, 1]^d$
    for $j = 0; j < N_{\text{iter}}; j++$ do
        $r \leftarrow \frac{Cr}{\|Cr\|}$
    end
    $\lambda \leftarrow \|Cr\|$
    $C \leftarrow C - \lambda rr^T$
end

return $W$

Algorithm 1: Constructing $W$ by power iteration

Note that in algorithm 1 each operation is differentiable with respect to $C$.

4 Gradient-based Slow Feature Analysis

The key idea for gradient-based SFA is that a whitening layer can be applied subsequently to any differentiable architecture (such as deep neural networks) to enforce outputs that approximately obey the SFA constraints while still being a differentiable architecture. As such, it can be trained using gradient-descent-like training procedures allowing for hierarchical architectures where every parameter is modified iteratively towards optimizing a global slowness objective as opposed to assuming a local-to-global slowness as in HSFA. To formalize, if 

$$\tilde{g}_\theta : \mathbb{R}^{N \times d} \rightarrow \mathbb{R}^{N \times e}$$

is a differentiable function approximator parameterized by $\theta$ such as a neural network and

$$W : \mathbb{R}^{N \times e} \rightarrow \mathbb{R}^{N \times e}$$

denotes the approximate whitening procedure, then for 

$$g_\theta = W \circ \tilde{g}_\theta : \mathbb{R}^{N \times d} \rightarrow \mathbb{R}^{N \times e}$$

is an approximator whose outputs will approximately obey the SFA constraints. As a loss function, we define a general loss as 

$$L_\theta(X) = \frac{1}{N} \sum_i \sum_j w_{ij} \|g_i - g_j\|^2$$ (2)  

with $g_i$ being the $i$-th row of $g_\theta(X)$ and $w_{ij}$ being the strength of the connection between two points $x_i$ and $x_j$ similar to weights in spectral graph embeddings.

For the slowness objective, we define the weight as 

$$w_{ij} = \delta_{i,j+1}$$
with $\delta$ being the Kronecker delta. This connects consecutive steps in the time-series and disconnects the others.

The approximator can then be trained to minimize the objective by following the negative gradient estimate of $L$ with respect to $\theta$, $-\nabla_\delta L$ for (mini-)batches of data as in any gradient-descent procedure. In our experiments, we used the ADAM optimizer [39] with Nesterov-accelerated momentum [40] to train the approximator. Learning rate and additional hyperparameters were left at default values as implemented in the popular Keras-package [41].

\footnote{Note that this is not exactly the same as the SFA objective as it does not include an ordering of the features, but instead might rather be called a \textit{slow subspace loss}. Any rotation of the data will obey the constraints and any optimal solution will just be a rotated version of the solution of an ordered objective.}
5 Experiments

5.1 Synthetic Trigonometric Data

To show the general feasibility of this approach, we first demonstrate that PowerSFA finds near-optimal solutions in the linear case for synthetic data. Since standard SFA is a linear method that relies on a) non-linear basis function expansion and b) hierarchical processing to induce non-linearity, this means that PowerSFA could hypothetically be used in a similar fashion (even though a gradient-based approach allows for more complex models in a natural way).

The data is generated by trigonometric polynomials of degree $N$ as:

$$x(t) = \epsilon_t + \sum_{n=1}^{N} \alpha_n \cos(nt) + \beta_n \sin(nt)$$

with $x, \epsilon, \alpha, \beta \in \mathbb{R}^D$, coefficients $\alpha_{in}, \beta_{in} \sim N(0,1)$. A noise term $\epsilon_{it} \sim N(0,0.01)$ is added for numerical stability when computing the closed form solution.

We implemented a temporal step-size of $\frac{2\pi}{100}$, and generate $T = 5000$ steps with maximum degree $N = 30$ and dimension $D = 100$. The data is whitened with $N_{\text{iter}} = 60$.

Figure 1 shows the extracted features for different variants of SFA. If the slowness loss is optimized without any constraints on the output features, the
model finds the optimal solution to collapse all signals to a constant \( \Delta = 0 \), while if unit variance is enforced only the features with slowness very close to the smallest \( \Delta \) are extracted multiple times and thus the representation becomes highly redundant. When using the approximate whitening, the quality of the solutions if comparable to the closed form solution acquired by solving a generalized eigenvalue problem. The ordering was achieved for representational purposes by weighting the output features with a monotonically decreasing weight. In Figure 2, the covariance matrices of the extracted signals are visualized.

Figure 2: Covariance matrices for five outputs in different settings. 1) slowness loss without constraints leads to nearly constant signals with (co)variances close to zero, 2) unit variance enforced leads to highly correlated output signals, 3 & 4) (approximate) whitening and the closed form solution show fully decorrelated output signals (identity covariance).

Note that it is not a sensible approach to use PowerSFA to optimize a linear model for such low-dimensional data as the closed-form solution is easily attainable. Thus, this experiment should be understood as a proof-of-concept and a general demonstration of applicability rather than a recommendation for a use-case.
5.2 Pose Estimation from Visual Data

SFA can be used to extract slowly-varying underlying causes from high-dimensional data, such as object position, identity, and rotation from visual simulations. In [12], textured three-dimensional fish-objects that change in x- and y-position as well as in-depth rotation $\phi$ have been used and it has been shown that HSFA features encode position and angle well. Since the code used to generate the stimulus data was outdated and could not be executed anymore, we re-implemented a similar scenario with a 3D model of an anvil (Figure 3, [42]) using the random walk procedure described in [12] to generate the configurations.

A current limitation of our model (cf. section 6.1) is that it does not scale well in the number of output features, rendering the relatively high number of 512 output features used in [12] infeasible. We used an output dimension of 10 with a comparable architecture that replaces quadratic expansion by ELU-nonlinearities (a Keras-summary is provided in Appendix A). Due to the low
number of output features, we were not able to successfully extracted the rotational angle $\Phi$.

In line with the original publication, we computed linear regression to predict $\cos(\pi x)$ and $\cos(\pi y)$ and used the inverse transformation to extract the object position. The results are shown in Figure 4 and are comparable to those presented in [12] as they were able to achieve a RMSE of 9% for $x$-position and 7% for $y$-position.
5.3 NORB

While gradient-based SFA is the main contribution of this work, previous work on generalizing SFA [30] has shown that the SFA optimization problem is just a special case of a more general spectral embedding method, i.e. Laplacian Eigenmaps [8], or, with small differences, graph-based SFA [13]. For this reason, we defined a more general loss function in equation 2.

Figure 5: The embedded object from the NORB dataset. Samples differ in azimuth, elevation and lighting.

In fact, weights $w_{ij}$ can be defined between any two points $x_i$ and $x_j$ of a given dataset, not just consecutive ones, thus allowing to optimize neighborhood-respecting embeddings for general graphs. This is similar (but not fully equivalent) to spectral embeddings on graph data, as used in algorithms such as Laplacian eigenmaps. Our approach exhibits four significant differences:

1. It does not find ordered features, but a rotation of an optimal embedding,
2. the found solution should be assumed to be only local optima (or saddle points),
3. it does ignore the graph regularity when enforcing the orthogonality constraint, and
4. it allows a natural and scalable way to embed unseen points.

Computing an out-of-sample embedding will require the same forward-pass through the differentiable architecture as the training embeddings. In particular, its complexity does not scale with the number of observed points used for training as is usually the case in other approximations, such as Nyström approximation [33].

We demonstrate the usefulness of such an approach by embedding an object of the NORB dataset [34], a collection of photographs of toys taken at different elevations, azimuths, and under different lighting conditions. Following the experimental procedure of [35], we embedded photographs of a toy plane (Figure 5) in 972 configurations (18 azimuths × 6 lighting conditions × 9 elevations angles) that were randomly split into a train- and test-set of sizes 660 and 312 respectively and the connection weights $w_{ij}$ were chosen as 1 if $x_i$ and $x_j$ differed...
only in one step either in rotation (i.e., one azimuth) or elevation (i.e., one level) and 0 otherwise. The weights were independent of lighting condition.

The convolutional neural network architecture used was the MobileNet [43] scaled with $\alpha = 0.25$.

Figures 6 and 7 show the three-dimensional embedding that was found in this setting. The data was embedded in a cylindrical shape in which the circumference encodes the rotation angle of the embedded object and the length along the cylinder encodes the elevation configuration of the object for the train-set as well as in the out-of-sample case of the test-set. In [35], a similar cylindrical encoding was found, however, their results exhibit a more clean-cut embedding. We assume that this is due to DrLIM’s maximization of distance for dissimilar samples that our model does not implement.

6 Discussion

We propose a new way of extracting informative slow features from quickly varying inputs based on differentiable whitening of processed batches of the
input data. To experimentally demonstrate the feasibility of the method, we
trained a linear model to extract slowly varying output signals from synthetic
time-series by gradient-descent and showed that the differentiable whitening
ensures informativeness of the extracted features when optimizing a slowness
loss function. Furthermore, the features corresponded to those found by closed-
form SFA.

To show applicability to visual time-series data, we trained a convolutional
neural network on an input stream of an object randomly rotating in-depth and
moving in a 2-dimensional plane. Gradient-based SFA preserves the position of
the object in a low-dimensional representation as does a hierarchical version of
closed-form SFA. Rotation was not extracted successfully due to computational
costs in the naive implementation for a large number of output features (cf. [6.1]).

In an experiment on a non-time-series image dataset on which symmetric
similarity relations between the data can be defined, we show that a generaliza-
tion of gradient-based SFA in the spirit of graph-based SFA is able to find a low-
dimensional representation that preserves and disentangles the configuration-
parameters used to define the similarity, in this case, azimuth and elevation of
a photographed toy. This representation generalizes well to previously unseen
configurations of the object.

While the algorithm is still in a prototypical state, the proof-of-concept re-
sults presented in this paper show promise for gradient-based SFA by differen-
tiable whitening to extract meaningful representations for goal-oriented learning
while leveraging the expressive power of modern architectures, such as convolu-
tional neural networks.

More research has to be dedicated to explore the computational limitations
of this method and possibly lower the complexity for a larger number of output
features. Furthermore, closed-form SFA has a strong theoretical framework
describing the optimal responses in an idealized setting. At this point, we are
unclear how well this framework translates to the proposed method of slowness
extraction as the used models typically suffer from local optima when being
iteratively trained.

6.1 Limitations

PowerSFA does currently not scale favorably in the number of output features e.
We see two main reasons for this: the necessary batch size to get a meaningful
estimate of the batch-covariance estimate and its calculation. The latter is due
to the complexity of a naive $\mathbb{R}^{e \times N_{\text{batch}}} \cdot \mathbb{R}^{N_{\text{batch}} \times e}$ matrix-multiplication being
$O(N_{\text{batch}} e^2)$, while the former is due to the whitening procedure expecting a
covariance matrix of full rank and thus $N_{\text{batch}} \geq e$ samples.

To reduce the lower bound on the batch-size at batch $t$, a convex mixture
with the covariance matrix of the previous batch might be applicable:

$$ C_t = (1 - \gamma) C_0 + \gamma C_{t-1} $$
Note, that only the current batches covariance matrix $C_\theta$ is considered parameter-dependent and allows to propagate a gradient for training. Thus, large values for $\gamma$ might cause a significant bias in the gradient-estimate. This has not been implemented in the proof-of-concept algorithm for this paper.

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## Appendices

### A  Keras Description (HSFA-like Architecture)

| Layer (type)      | Output Shape          | Param # |
|-------------------|-----------------------|---------|
| input_1 (InputLayer) | (None, 156, 156, 1)   | 0       |
| conv2d_1 (Conv2D)  | (None, 147, 147, 32)  | 3232    |
| activation_1 (Activation) | (None, 147, 147, 32) | 0       |
| dropout_1 (Dropout) | (None, 147, 147, 32)  | 0       |
| conv2d_2 (Conv2D)  | (None, 28, 28, 32)    | 102432  |
| activation_2 (Activation) | (None, 28, 28, 32) | 0       |
| dropout_2 (Dropout) | (None, 28, 28, 32)    | 0       |
| conv2d_3 (Conv2D)  | (None, 25, 25, 32)    | 16416   |
| activation_3 (Activation) | (None, 25, 25, 32) | 0       |
| dropout_3 (Dropout) | (None, 25, 25, 32)    | 0       |
| conv2d_4 (Conv2D)  | (None, 11, 11, 32)    | 16416   |
| activation_4 (Activation) | (None, 11, 11, 32) | 0       |
| dropout_4 (Dropout) | (None, 11, 11, 32)    | 0       |
| conv2d_5 (Conv2D)  | (None, 8, 8, 32)      | 16416   |
| activation_5 (Activation) | (None, 8, 8, 32) | 0       |
| dropout_5 (Dropout) | (None, 8, 8, 32)      | 0       |
| conv2d_6 (Conv2D)  | (None, 3, 3, 32)      | 16416   |
| activation_6 (Activation) | (None, 3, 3, 32) | 0       |
| dropout_6 (Dropout) | (None, 3, 3, 32)      | 0       |
| flatten_1 (Flatten) | (None, 288)           | 0       |
| dense_1 (Dense)    | (None, 10)            | 2890    |
| power_whitening_1 (PowerWhit) | (None, 10) | 0       |

Total params: 174,218
Trainable params: 174,218
Non-trainable params: 0