Deep-Learned Broadband Encoding Stochastic Filters for Computational Spectroscopic Instruments

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Computational spectroscopic instruments with broadband encoding stochastic (BEST) filters allow the reconstruction of the spectrum at high precision with only a few filters. However, conventional design manners of BEST filters are often heuristic and may fail to fully explore the encoding potential of BEST filters. The parameter constrained spectral encoder and decoder (PCSED)—a neural network-based framework—is presented for the design of BEST filters in spectroscopic instruments. By incorporating the target spectral response definition and the optical design procedures comprehensively, PCSED links the mathematical optimum and practical limits confined by available fabrication techniques. Benefiting from this, a BEST-filter-based spectral camera presents a higher reconstruction accuracy with up to 30 times enhancement and a better tolerance to fabrication errors. The generalizability of PCSED is validated in designing metasurface- and interference-thin-film-based BEST filters.

Spectroscopic instruments such as spectrometers and spectral cameras are key drivers of many scientific discoveries in life and material sciences.[1–3] While different technical routes of spectroscopic instruments have been developed and commercially available, a commonly used configuration is that of a filter-based system.[4–6] To pursue a high spectral resolution, these instruments require many filters with sharp but contiguous passing bands, which are practically challenging due to the design and fabrication complexity. Worse still, the narrower passing band is followed by a higher risk of crosstalk and less luminous flux. These limits necessitate the tradeoffs between the spectral resolution and the signal-to-noise ratio (SNR).

To resolve this dilemma, researchers turned to an array of "broadband encoding stochastic (BEST) filters." Compared with conventional band-pass ones, BEST filters are advantageous, because they are naturally crosstalk-free, thereby improving the SNR. The production of these filters are also compatible with nearly all new materials, such as quantum dots,[7] plasmonic metasurfaces,[8] photonic crystals,[9] and nanowires.[10] Furthermore, the BEST-filter-based spectroscopic instruments (BEST-SIs), in tandem with advanced computational algorithms,[11] allow the reconstruction of the spectrum with fewer filter channels.[12] As a result, BEST-SIs stand out, for their cost-effectiveness, miniaturization, and portability.[13]

Unfortunately, irrespective of BEST-SI’s advantages, an easy-to-follow guideline for designing BEST-SIs is still wanting. The existing attempts always follow a sequential paradigm that includes two individual procedures—first, define the optimal spectral responses mathematically (“target response definition”), and then approach these optima in practice via certain production technique (“optical design”). However, there always lies a contradiction that a mathematically optimal spectral response usually converges to a white-noise-like one, whereas the optical design tends to create sufficiently smooth spectral curves to simplify the production. Regarding this predicament, many BEST-SIs[4,7–10] are instead built on a so-called “manufacturing-and-selection” strategy, i.e., a sufficient number of stochastic filters is produced to ensure randomness, and then the BEST filter set is selected via permutation and combination. However, this strategy de facto compromises the major advantages of BEST-SI because the number of filters needed as candidates can be orders of magnitude higher than that of the BEST-SI channels. Worse still, the encoding potential of BEST filters can never be fully explored.

Emerging deep learning-based solutions provide an alternative that might be conducive to the BEST-SI design. Aiming at the procedure of target response definition, several works[14,15] have added artificial priors, e.g., Gaussian-shaped or smoothness limit, to avoid converging to the white-noise-like spectral responses. The others[16–19] have enhanced the optical design...
precision under certain conditions. These methods work to some extent, but still, none of them comprehensively takes both procedures into account. As such, their results are compromised either by the productivity of the designed spectral responses or by the sensitivity to the fabrication error.

Inspired by the emerging data-driven computational imaging approaches,[20–23] we present a novel deep learned framework to comprehensively address both design procedures.

Given a continuous spectrum $S(\lambda)$ in a discrete form

$$s = [S_1, S_2, \ldots, S_N]^T$$

where $N$ is the sampling number, and $T$ denotes the transposition operation. When detecting $s$ using an $M$-channel BEST-SI, we have

$$y = W \cdot s$$

where $y = [Y_1, Y_2, \ldots, Y_M]^T$ is the intensity vector recorded by all BEST filter channels, and each row of the matrix $W$, $w_j^T = [w_{j1}, w_{j2}, \ldots, w_{jN}]$ is the discretized spectral response of the filter in the $j$th channel ($j = 1, 2, \ldots, M$). Note that here in BEST-SI, the filter number $M$ can be smaller than $N$. While it represents the sensing matrix in the context of compressive sensing, from deep learning’s perspective, the matrix $W$ in Equation (2) acts as a fully connected (FC) layer in an artificial neural network.[24,25] Each entry $w_{ji}$ in the matrix $W$ corresponds exactly to the connection weighting coefficient from the $i$th unit in the prior layer to the $j$th unit in the following layer. Regarding this evidence, the BEST filters form an encoding network (encoder) constructed by a single FC layer (Figure 1). By attaching a decoder after it, the whole network, namely, the “spectral encoder and decoder” (SED) captures and reconstructs the input spectrum. Training the SED grants us access to the value of each $w_{ji}$ and equivalently, the optimized spectral responses. Accordingly, the training process solves the following optimization problem

$$(\hat{W}, \hat{\theta}) = \arg \min_{\hat{W}, \hat{\theta}} \|s - D_{p}(W \cdot s)\|_2^2$$

where $D_p(\cdot)$ represents the mapping function of the decoder, $\theta$ corresponds to the network parameters of the decoder, and $\hat{W}$ represents the optimized spectral responses.

Solving Equation (3) allows a co-design of filter spectral responses $W$ and the decoder parameters $\theta$. On this basis, considering the target response definition and the optical design procedures comprehensively, we aim to add a constraint to the trained SED during the training, where the constraint explicitly describes the mapping from the filter structure to its spectral response $w_j$. We observe that a forward modeling network (FMN)[16,19] can work perfectly for this task. Notably, it is possible to realize this mapping with other numerical algorithms in specific cases, such as finite difference time domain (FDTD),[26] rigorous coupled-wave analysis,[27] or the transfer matrix method.[28] However, FMN is more general and has an advantage in calculating speed ($\approx 10^6$ faster), which is crucial for improving the SED training efficiency (refer to Section S1, Supporting Information). Besides, as both FMN and SED are artificial neural networks with well-defined gradients, rendering FMN stable and efficient during the SED training. We use a $K$-dimensional vector $p_j = [p_{j1}, p_{j2}, \ldots, p_{jK}]^T$ to represent $K$ structure parameters (e.g., geometrical sizes of the structures). After training the FMN, the mapping from $p_j$ to $w_j$ can be written as

$$w_j = F_M (p_j)$$

where $F_M(\cdot)$ denotes the forward mapping carried out by the pre-trained FMN. With $p_j$ arranged into a $K$-by-$M$ matrix $P = [p_1, p_2, \ldots, p_M]$, Equation (4) can be written as

$$W = F_M (P)$$

By substituting Equation (5) into Equation (3), we have

$$(\hat{P}, \hat{\theta}) = \arg \min_{\hat{P}, \hat{\theta}} \|s - D_p[F_M(P)^T \cdot s]\|_2^2$$

Figure 1. Schematic of our parameter constrained spectral encoder and decoder (PCSED) design framework. The broadband encoding stochastic (BEST) filters act as an encoding neural network (encoder), whose connection weights (corresponding to the BEST filters’ responses) are constrained by the filters’ structure parameters through a pre-trained forward modeling network (FMN). During each training epoch, a batch of spectrums is fed into the encoder and the decoder gives the corresponding output, such as the reconstructed spectrums. The loss function, such as the mean square error (MSE) for the reconstructed spectrum is evaluated and the errors are back-propagated to the structure parameters (e.g., geometrical parameters of metasurface or thin-film structures). Under this framework, the BEST filters and the decoder are jointly designed.
We further add regularizations to explicitly limit the desired structure parameter range, which is beneficial for making the design robust to fabrication errors. Hence, Equation (6) becomes

$$\hat{P}, \hat{\theta} = \text{argmin} \| s - D_s [F \cdot M(P) \cdot \theta] \|^2 + R(P)$$

(7)

where $R(P)$ is the regularization term. The above procedure gives birth to a parameter constraining the spectral encoder and decoder (PCSED) neural network (Figure 1). This framework allows the structure parameters of BEST filters to be directly trained, which is impossible in the sequential design paradigm. Therefore, PCSED allows a full exploration of the optical designing flexibility. Furthermore, the PCSED leverages back-propagation through an FMN to obtain the learned structure parameters. Because the forward modeling mapping is injective (where there is a one-to-one mapping between one physical system and its corresponding response), PCSED is better convergent than the sequential inverse design methods\(^\text{[16]}\) for the same task.

To support our claim, we applied the PCSED to the design of BEST filter-based spectroscopic instruments. In our first demonstration, we designed a metasurface BEST filter-based spectral camera. We set the number of BEST filters as 4, an extension of a Bayer filter unit\(^\text{[29]}\) over the imaging sensor. In this way, the PCSED simulates the working stream of a metasurface spectral camera—the four adjacent metasurface BEST filters construct a macro-pixel and encode the spectrum of the incident light, and the detected intensity data are decoded by the decoder to reconstruct a spectrum. We used both CAVE\(^\text{[30]}\) and ICVL\(^\text{[31]}\) datasets for training the PCSED, by which the spectral range of interest is 400–700 nm. The training and the test sets, respectively, include 10\(^4\) and 10\(^3\) spectral samples, which are randomly selected from the pixels of CAVE and ICVL hyperspectral images. The spectral images in the original CAVE and ICVL datasets have 31 spectral channels, corresponding to a spectral step size of 10 nm. Because the sampling number of each BEST filter’s response must be the same as the spectral channel number of the dataset, we interpolated them into 151 channels, corresponding to a spectral step size of 2 nm. The interpolation is essential, because only in this way, the spectral responses of the deeply learned filters can be finely defined, and the network simulates the physical world accurately. Notably, the spectral resolution of the whole network is not improved, because the interpolation does not introduce additional information, thus the spectral step of the output data does not represent the spectral resolution.

As shown in Figure 2a, we synthetically built the metasurface BEST filters with a basic structure of silicon nanobricks on a two-layer substrate, which is constructed by coating a Si$_3$N$_4$ thin layer on a SiO$_2$ block. The structure parameters that potentially influence the spectral responses involve the edge length (L), the height (H) of the nanobricks, the thickness (T) of the Si$_3$N$_4$ layer, and the unit period (D). Each parameter varies in a range of 100–200 nm (L), 50–200 nm (H), 200–400 nm (T), and 300–400 nm (D), respectively. Tuning the structure parameters enables us to obtain diverse spectral responses\(^\text{[12,13]}\). (For the training details of FMN and PCSED, see Sections S2.1 and S2.2, Supporting Information.)

For comparison, we also applied a sequential design paradigm for the same task. In detail, we built an SED and added an $l_1$-norm-based smoothness regularization to the single-FC-layered encoder (method in ref. [15]). After training the SED, we fed the trained target spectral responses into an inverse design network to derive the structures of metasurface BEST filters (method in ref. [19]). For brevity, we denote this method “SED-inv.” (For details of SED-inv, see Section S2.3, Supporting Information.)

After running both PCSED and SED-inv, we fed the output structure parameters into the FDTD simulation to generate the spectral responses of the designed BEST filters. We further added the random structure variance within the range of ±3 nm to evaluate the possible fabrication error. By taking the target, the designed BEST filters, and those added with fabrication errors as the encoder, the spectrum reconstructed by the decoder and the corresponding reconstruction error level are assessed using the mean square error (MSE).

Figure 2b,c presents the spectral responses of all four BEST filters generated by PCSED (Figure 2b) and SED-inv (Figure 2c), respectively. While two curves from PCSED roughly match on the shape, the spectral responses (dashed orange) designed by SED-inv present strong fluctuations around the target responses (solid orange). Applying PCSED can effectively reduce the MSE between the target and the design responses by a factor of 2–10. Not surprisingly, lower MSE in design induces higher precision of spectral reconstruction. Table 1 highlights the average spectral reconstruction MSE on the test set, using the metasurface spectral camera designed by both methods. In particular, the MSE values in the “Target” row are extremely small (<10$^{-3}$), suggesting that both methods are applicable for training the BEST filters and the decoder. However, the producibility of the trained BEST filters differs. When taking the designed BEST filters as the encoder, the reconstruction MSE of the PCSED still maintains at a low level (≈10$^{-5}$), while that of the SED-inv is ≈30 times higher (“Designed” row). On the other hand, the MSE contributed by the fabrication error is minute. For the PCSED, the fabrication error only increases the MSE by ≈10%, while for the SED-inv, the MSE is even smaller after we introduced the artificial fabrication error (“W. fab. error” row). As the mismatch between the target and the designed spectral responses dominates the reconstruction MSE, employing PCSED instead of SED-inv becomes critical.

To visualize the spectral reconstruction results, we simulated the imaging process of the designed camera and analyzed the reconstructed spectrums of the hyperspectral images. Figure 2d–h displays the results when we used the designed BEST filters (dashed curves in Figure 2b,c) as the encoder. For the results using the BEST filters with artificial fabrication errors, refer to the Section S2.4 in the Supporting Information. For all seven images randomly selected from CAVE and ICVL datasets (Figure 2d), while the SED-inv fairly reconstructs the spectrum (Figure 2f), the PCSED strikingly increases the overall peak signal-to-noise ratio (PSNR) for more than 10 dB (Figure 2e). In contrast to Figure 2e in which the purple color is almost uniformly distributed, Figure 2f includes more components with larger MSEs (highlighted with bright colors). Even for the positions where the MSEs of both methods are relatively low (marked by red and green patches), our method is superior in that it offers a higher spectral reconstruction precision (Figure 2g,h).

Remarkably, PCSED is not limited to optimizing metasurfaces. In principle, it applies to any production techniques whose spectral response is theoretically predictable via a well-defined
Figure 2. Schematic and synthetic performance of the metasurface BEST-filter-based hyperspectral camera. a) Schematic of BEST filter’s nanostructures. The structure parameters include the edge length ($L$) and height ($H$) of nanobricks, the thickness ($T$) of the $\text{Si}_3\text{N}_4$ layer, and the period ($D$) of the repeating units. b,c) Spectral responses of the target (solid curves) and designed (dashed curves) BEST filters generated by b) PCSED and c) SED-inv. d–j) Synthetic hyperspectral reconstruction by using the designed cameras. For each row, there are d) hyperspectral images in RGB form, chosen from CAVE (first four) and ICVL (last three); e,f) the reconstructed hyperspectral images in RGB form; g,h) the pixel-wise spectral reconstruction MSE of each hyperspectral image, the value on top of each figure stands for the peak signal-to-noise ratio (PSNR) of the whole image; i,j) the reconstructed spectrum from the red and green patches in (d)–(h).

Table 1. Spectral reconstruction MSE of the metasurface spectral camera designed by PCSED and SED-inv.

|                | PCSED   | SED-inv  |
|----------------|---------|----------|
| Target         | 0.00015 | 0.00009  |
| Designed       | 0.0011  | 0.0358   |
| W. fab. error  | 0.0013  | 0.0342   |

In summary, we have proposed a novel deep-learned co-design of the BEST filters and the decoder in computational spectroscopic instruments. By representing the array of BEST filters as an FC layer of an artificial neural network, it is viable to optimize the BEST filters’ spectral responses by training the entire network. Furthermore, using the FMN to conduct the mapping from structure parameters to the spectral responses enables us to improve the design convergence. In the meanwhile, the design procedure is simplified by evading the further inverse mathematical model. In our second example, we aimed to design the thin-film interference BEST filters. We assumed that these filters have five layers of TiO$_2$ and five layers of SiO$_2$ alternatively coated on a glass substrate. In PCSED, the FMN enabled us to conveniently limit the thickness of each layer to a range of 100–300 nm, approximately a quarter wavelength if the light is visible. Such a scale is also desirable in avoiding super-thin layers that are challenging for fabrication.\textsuperscript{[34]} Similarly, we have also developed the SED-inv networks and then compared the results with those from our PCSED method (Sections S3.1–S3.3, Supporting Information). Intuitively, the designed spectral responses from both methods roughly match the target ones (“designed” column in Table S3, Supporting Information), but still, PCSED is significantly better. In addition to an ≈50% smaller MSE of the BEST filters’ spectral responses, PCSED also exhibits a better tolerance to fabrication errors. Specifically, the BEST filters designed by PCSED decrease the MSE by a factor of ≈7.5 when taking those from SED-inv for reference (see Section S3.4, Supporting Information).
design, irrespective of the filter production methods. Simulation results prove that our design paradigm bridges the gap between the target response definition and the optical design procedures, thereby enabling more flexibility in design space. Although the current output of the PCSED involves only the reconstructed spectrum where we foresee an urgent application demand, we envision the proposed method applies to alternative visual tasks such as spectral recognition or classification.

**Supporting Information**

Supporting Information is available from the Wiley Online Library or from the author.

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**Conflict of Interest**

The authors declare no conflict of interest.

**Data Availability Statement**

Open-source codes and data for this study can be downloaded from our Github repository (https://github.com/Hao-Laboratory/PCSED). The datasets generated and/or analyzed during the current study are available from X.H. on reasonable request.

**Keywords**

computational spectroscopy, deep learning, hyperspectral imaging, optical inverse design

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