The secret role of undesired physical effects in accurate shape sensing with eccentric FBGs

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Abstract

Fiber optic shape sensors have enabled unique advances in various navigation tasks, from medical tool tracking to industrial applications. Eccentric fiber Bragg gratings (FBG) are cheap and easy-to-fabricate shape sensors that are often interrogated with simple setups. However, using low-cost interrogation systems for such intensity-based quasi-distributed sensors introduces further complications to the sensor’s signal. Therefore, eccentric FBGs have not been able to accurately estimate complex multi-bend shapes. Here, we present a novel technique to overcome these limitations and provide accurate and precise shape estimation in eccentric FBG sensors. We investigate the most important bending-induced effects in curved optical fibers that are usually eliminated in intensity-based fiber sensors. These effects contain shape deformation information with a higher spatial resolution that we are now able to extract using deep learning techniques. We design a deep learning model based on convolutional neural network that is trained to predict shapes given the sensor’s spectra. We also provide
a visual explanation, highlighting wavelength elements whose intensities are more relevant in making shape predictions. These findings imply that deep learning techniques benefit from the bending-induced effects that impact the desired signal in a complex manner. This is the first step toward cheap yet accurate fiber shape sensing solutions.

**Keywords:** Eccentric FBGs, fiber sensors, FBG sensors, polarization, bending loss, deep learning, shape sensing, curvature sensing

Fiber optic shape sensing is a game-changing technology with great potential in medical and industrial applications such as catheter navigation, surgical needle tracking, and continuum robot navigation. Compared to state-of-the-art navigation technologies [1–3], fiber shape sensing has many advantages, such as immunity to electromagnetic fields, bio-compatibility, and high flexibility. Fiber shape sensors are small in diameter, easily integrable into flexible instruments, require no line-of-sight, and provide high-resolution shape measurements in real-time.

Fiber shape sensors measure off-axis strain, which is then used to reconstruct the fiber’s shape [4]. Various fiber sensor configurations have been investigated in the literature for off-axis strain measurement, including multicore fibers with [5] or without [6] FBGs in their cores, fibers with cladding waveguide FBGs [7], and fiber bundles made from multiple single-mode fibers that contain FBG arrays [8–12]. Multicore fibers have been on the cutting edge of fiber-optic sensing and are commercially available. They can measure quasi-distributed or distributed off-axis strain [4].

In quasi-distributed sensors [5], the spatial resolution is limited by the minimum required distance between the FBGs inscribed inside the cores of a multicore fiber (usually around 1 cm [13]). Low spatial resolution and inaccuracies in strain measurement cause an accumulative error in shape reconstruction. Moreover, these sensors need a fan-out device for reading the signal from the cores and a multichannel FBG interrogator for monitoring the Bragg wavelengths, making them expensive navigation solutions.

In distributed sensors, off-axis strain is measured from Rayleigh or Brillouin scatterings. These scattering effects occur when there are refractive index fluctuations [14] or acoustic vibrations [14, 15] in the optical fiber. Multicore distributed sensors are intensity-based and need a fan-out and an optical reflectometer [16, 17]. Although such sensors can perform high-resolution strain measurements [17–19], their overall cost is high and yet are still limited by the accumulative error in shape reconstruction.

A suitable yet cheaper alternative to multicore sensors are the quasi-distributed eccentric FBG sensors (also known as edge-FBGs), which are highly localized FBGs, written off-axis in a single-mode fiber’s core (shown in Figure 1). In edge-FBG shape sensors, the directional bending is realized by placing three co-located edge-FBGs with 90° angular distance from each
Fig. 1 The FBG configuration and working principle of the edge-FBG sensor. As depicted in the cross-section view, each sensing plane of the edge-FBG sensor consists of three FBGs inscribed off-axis with 90° angular distance. (a) shows the mode-field distribution of a straight single-mode fiber and the expected signal from co-located edge-FBGs. As illustrated in (b), when the fiber is curved, the mode field distribution moves in the opposite direction of bending, which affects the relative intensity between the edge-FBGs.

other [20]. When a single-mode fiber is bent, the field distribution of the fundamental mode moves away from the core’s center [20–22] (see Figure 1 (b)). Dislocations in the mode field’s centroid cause intensity changes in the reflected signal from the edge-FBGs [20]. From the intensity ratio between the co-located edge-FBGs, the curvature and the bending direction can be calculated [20]. For simplification, this approach assumes that no other physical phenomena inside a bent optical fiber affect the intensity ratio between the co-located FBGs.

However, positioning FBGs away from the core axis breaks the cylindrical symmetry of the fiber, which increases coupling from core mode to cladding modes [23, 24]. The strength of such mode coupling varies when the fiber is bent, as it affects the overlap integral between the interacting modes [23, 25]. Bending an optical fiber causes strain-induced refractive index changes and dislocates the intensity distribution of the propagating light [21, 26, 26], which directly affects the coupling efficiency. Therefore, the intensity of the cladding modes changes when the fiber is bent. In off-axis FBGs, the formation of cladding-mode resonances in fiber gratings provides highly sensitive full directional bending response with a simple power level measurement [27]. Although cladding modes are often stronger in stripped fibers or in fibers coated with lower refractive index material than the cladding layer [23, 24], they have also been observed in standard fibers coated with higher refractive index materials [28]. Any recoupling between the excited cladding resonances
and the fundamental mode, affects the relative intensity values between the edge-FBGs.

FBG interrogators for quasi-distributed sensors often consist of a broadband light source, like a super luminescent diode (SLED), and a grating-based spectrometer. The emitted light from SLEDs is partially polarized, meaning that it undergoes wavelength-dependent polarization changes [29] in a birefringence medium (e.g., bent fiber) [30–33]. On the other hand, the efficiency of gratings inside spectrometers is polarization-dependent, and therefore, the spectrum profile will be affected by polarization-dependent losses. This effect further modifies the measured intensity ratio between the Bragg peaks. The polarization effect in intensity-based fiber sensors is often kept at a minimum by using a polarization scrambler to change the polarization state randomly or by using polarization-insensitive spectroscopy instruments (e.g., optical spectrum analyzer).

As is well known, optical fibers lose power if their axes are curved [34]. Macro bending loss usually shows wavelength-dependent modulations caused by coherent coupling between the core propagating field and the radiated field reflected by the cladding-coating and the coating-air interfaces (also known as whispering gallery modes) [35, 36]. The reflected field, at the coating-air boundary, causes short-period modulations as the re-injection path is longer [35, 36]. Whereas, the reflections at the closer cladding-coating interface cause long-period resonances [36–39]. These bending attenuation losses further depend on temperature variations. Temperature variations affect the refractive index of the coating layer and consequently influence the coupling between the core and the cladding whispering gallery modes [40]. Many models have been proposed in the literature to evaluate bending loss peak positions and shapes ([37, 38, 41]). The strong wavelength dependence of bending losses is an additional complicating factor in designing intensity-based sensors [36] as it modulates the spectrum profile and affects the intensity ratio at the Bragg peaks between the co-located edge-FBGs.

Modelling all the aforementioned bending-related phenomena for accurate shape sensing is impossible, as their relevant parameters can not be estimated during calibration. Thus, in practice, one tries to minimize the impact of these phenomena such that the intensity ratio between the edge-FBGs is only influenced by the mode field dislocations. However, we developed in this paper a data-driven modeling technique based on deep learning that can indeed find a meaningful pattern in the signal affected by bending-sensitive mode coupling, polarization-dependent losses, and wavelength-dependent bending losses. These additional sources of information considerably improve the shape prediction accuracy by a factor of 50.

Concept

In this section, we explain the designing and the training process of a deep neural network for our edge-FBG shape sensor. The 30 cm long edge-FBG fiber sensor used in this paper features five sensing planes that are 5 cm apart.
Fig. 2  The architecture of the best performing configuration after hyperparameter tuning. It includes five 1D convolutional layers (Conv1D), six fully connected layers, five max pooling layers, four batch normalization, and two dropout steps. The designed network receives three consecutive spectral scans as the input and predicts the relative coordinates of 20 discrete points over the sensor’s curve. More detail on the channel, kernel, and pooling sizes is available in the Methods section.

Each sensing plane consists of three FBGs inscribed $\sim 2 \mu m$ away from the fiber’s axis, on the core’s top, left, and right side (see the cross-section view in Figure 1).

The dataset used for developing the deep learning-based model is collected using a similar setup reported in our previous work [42]. We use three normalized consecutively measured spectral scans with 190 wavelength elements from 800 nm to 890 nm as the input data to our deep learning model. The target data are the relative coordinates of the 20 measured discrete points over the sensor’s length. The total number of samples in this dataset, collected in 30 min, is roughly 58000. To evaluate the predictive performance of the trained model in an unbalanced way, the samples are first shuffled and then split into Train-Validation-Test subsets: 80% for training, 10% for validating, and 10% for testing. We refer to this testing data set as Test$^1$ in the remainder of this paper. The second set of data (Test$^2$) with a size of $\sim 5800$ samples is recorded separately to evaluate the performance of the trained model at unseen shapes from a continuous movement. We also collected 320 samples, as Test$^3$, when only certain sensor areas are bent (see Methods section for more detail).
A deep learning model needs an especially designed network architecture to extract essential features from the sensor’s spectra and to predict its corresponding shape. To do so, we ran an optimization algorithm similar to the Hyperband optimizer [43] to search for the best set of model hyperparameters that are essential parameters whose values cannot be estimated from the data during training (e.g., training learning rate). Figure 2 shows the architecture of the best performing configuration after hyperparameter tuning.

To understand which part of the spectra is vital for feature extraction, we calculate the forward finite difference of the network’s output with respect to the input spectral elements. The resultant heat map provides an influence evaluation for each wavelength element of the input spectra to decode the model’s predictions. More information is provided in the Methods section.

As a baseline for evaluating the shape prediction using the proposed deep learning approach, we use the state-of-the-art mode field dislocation method, applied to the same test sets. We refer to this method as BL in the remainder of the paper. Following the same process explained in our previous work [20], we calibrate the sensor by estimating the exact angular and radial position of each edge-FBG. The calibrated sensor can then calculate the curvature and the bending direction from the estimated mode field centroid [20].

Results and Discussion

Shape prediction evaluation. We prepared three testing datasets to evaluate the performance of the deep learning model (DL) and to compare it with the baseline (BL), the mode field dislocation method. Table 1 shows the shape error metrics when comparing both methods with the three test sets. These metrics include the tip error, that is, the Euclidean distance between the true and the predicted coordinate of the sensor’s tip, and the root-mean-square of the Euclidean distance (RMSE) between the true and the predicted coordinates of the discrete points along the sensor’s length. The BL approach, when using the Test1 dataset, shows median and interquartile (IQR) tip error values of 111.3 mm and 121.5 mm, respectively. These values are reduced to 98.5 mm and 46 mm when using Test2 dataset. The reason for such performance difference is that the dataset Test1 contains more diverse shapes, as the samples are randomly selected from a larger dataset compared to Test2, which is a continuous sensor movement in a short period.

| dataset | method | tip error [mm] | RMSE [mm] |
|---------|--------|----------------|-----------|
|         |        | median | IQR | median | IQR |
| Test1   | BL     | 111.3  | 121.5 | 61.6  | 74.2 |
|         | DL     | 2.1    | 2.6  | 1.5   | 1.6  |
| Test2   | BL     | 98.5   | 46.0  | 53.8  | 29.1 |
|         | DL     | 19.5   | 11.7  | 9.8   | 7.0  |
| Test3   | BL     | 39.5   | 34.7  | 17.1  | 18.3 |
|         | DL     | 6.0    | 9.0   | 5.1   | 6.6  |
However, the predicted shapes when using the DL method on Test$_1$ samples show considerably lower values of 2.1 mm and 2.6 mm for the median and the IQR tip error. These values go up to 19.5 mm and 11.7 mm on less diverse Test$_2$ samples. To understand such behavior, we need to consider that a deep learning model can only learn to extract the most general/relevant features from the input signal if the training dataset is representative of expected signals from the sensor. Investigating the Test$_2$ dataset, we realized that less than 2% of the samples have at least 100 similar examples in the training data (a maximum RMSE of 5 mm is chosen as the similarity measure after evaluating several thresholds). This shows that 30 min of manual shape manipulation is insufficient to cover the sensor’s working space and create a representative training dataset for the model to generalize properly. However, in the Test$_1$ dataset, almost 20% of the samples have at least 100 similar examples in the training dataset. Therefore, Test$_1$ can mimic the situation where the training dataset represents the expected sensor’s shapes, as it challenges the DL method with samples that the model has learned how to handle.

The shape evaluation results of the Test$_1$ dataset define the performance of our model’s lower limit. Such performance difference also suggests that the deep learning model is better to be trained application-specific, as it can better focus on relevant features when learned from the expected sensor’s shape distribution. On the other hand, one challenge, when the training data covers most of the expected behaviors from the sensor, is that the deep learning model only memorizes the corresponding shape for each signal without searching for relevant features in the sensor’s spectrum. For this reason, we compare the performance of the method DL with a dictionary-based algorithm. In this approach, all the training and validation samples create a pre-defined dictionary. The shape prediction is made by looking for the closest spectrum to the test sample and presenting its corresponding shape. The median tip errors on datasets Test$_1$ and Test$_2$ are 5.9 mm and 50.0 mm with IQR values of 3.9 mm and 43.3 mm, respectively, which are higher than error values when using our deep learning technique. This shows that the deep learning model generalizes and is indeed beneficial for predicting more accurate shapes.

Two essential factors to consider when working with dictionaries are the dictionary size and the execution time, required to find the best matching example. To get an accurate shape estimation for a given sample, the number of stored samples in the dictionary should be high enough to cover all possible examples, which leads to a long execution time. Therefore, this approach has a trade-off between accuracy and execution time. However, extensive training data do not affect these two factors negatively in deep learning, as the resulting model size is independent of the training data size.

Our observations showed that the designed deep learning model can spot deformations even between the sensing planes. To further investigate this astonishing finding, we evaluated the shape predictions using the Test$_3$ dataset, in which the deformations are only applied between the sensing planes. The Test$_3$ dataset contains four deformation examples, each repeated twice
and measured 40 times. The classical BL method is not able to accurately predict the sensor’s shape for such deformations, as the deformed area is not at the sensing planes. However, when using the DL method, we achieve a median tip error of 6 mm which is $\sim$ six times smaller than the median tip error using BL on this dataset. The precision of the predicted tip position in the Test$_3$ dataset is 1.9 mm on average.

**Fig. 3** An example from Test$_3$ samples in which the sensor is bent in the area between the sensing planes 3 and 4. In (a) the true shape (ground truth) is shown with green circles. The five sensing planes of the sensor are shown with $\times$ signs. The predicted shapes using the mode field dislocation method (BL) and the deep learning method (DL) are shown with orange and purple solid lines, respectively. (b) shows the finite difference of the loss value with respect to the input spectral elements. Wavelength elements shown with colors closer to yellow contribute more to the model’s decision on this particular example. (c) highlights the importance of input spectral elements in relative coordinate prediction of all 20 markers based on the magnitude of the Euclidean distance between the predicted relative coordinates of each marker, before and after spectral modification. The position of the sensing planes with respect to the markers are indicated with dashed blue lines.

$SP_i$: $i$th Sensing Plane.
An example from Test$^3$ samples in which the sensor is bent in the area between the sensing planes 3 and 4 is depicted in Figure 3 (a). As explained in the Introduction section, the intensity ratio of the Bragg wavelength between the co-located edge-FBGs can also be affected by bending loss oscillations, polarization-dependent losses, and the cladding modes. When a bending occurs between the sensing planes, the base-line approach (BL) cannot correctly interpret the signal’s changes, as it does not consider the bending loss, the cladding mode coupling, and polarization-dependent loss effects. On the other hand, the deep learning model manages to accurately predict the sensor’s shape as it looks at the full spectrum profile, including the minute changes at the wavelengths outside of the Bragg resonances. Figure 3 (b) shows the finite difference analysis of the loss value with respect to the 190 wavelength elements of the input spectra. The higher the difference, the more important the corresponding wavelength element is for shape prediction in this example. Figure 3 (c) gives a deeper insight into this investigation. For all 190 wavelength elements, the Euclidean distance between the predicted relative coordinates of each marker before and after the spectral modification is depicted with a color map. The contribution of each wavelength element to the relative coordinate prediction of all 20 markers can be realized from the presented color map in Figure 3 (c).

Another remaining question is, whether the deep learning model can also detect deformations after the last sensing plane where changes in spectrum profile no longer affect the edge-FBG spectra. Figure 4 shows an example in which, a 3 cm long segment, 1 cm after the last sensing plane, is deformed. Similar to the example in Figure 3, the BL method is not able to accurately predict the sensor’s shape in such deformations. The deep learning model, in contrast, learned to employ relevant features in the side slopes of the FBG spectra to, nevertheless, accurately predict the correct shape, see Figure 4 (b and c). A possible explanation for such astonishing performance is that in the area after the sensing plane, wavelength-dependent interference occurs between the back-reflected signal from the air-glass interface at the fiber’s exit end (Fresnel reflection) and the downstream incident light. Deformations in this area affect interferences in two ways. First, the spectrum profile of the downstream signal changes due to the bending, which means that the back-reflected signal from the fiber’s end interface also has a modified spectrum profile. Second, the coupling conditions between the upstream and the downstream signals changes. Consequently, the measured spectra from the fiber sensor show small changes, as the deformations affect the interference pattern.

**Optimum number of sensing planes.** An important factor in edge-FBG sensors, similar to all other quasi-distributed shape sensors, is the number of sensing planes for detecting shape deformations. The distance between the sensing planes determines the sensor’s spatial resolution in shape measurements. Depending on the complexity level of the shape deformations, a limited number of sensing planes in the sensor (low spatial resolution) can lead to large tip errors in methods that include shape reconstruction (e.g., the BL method). In this section, we present a theoretical analysis for realizing the optimum
number of sensing planes required in edge-FBG sensors for an accurate shape prediction when using the BL method. Then, we compare the results with our deep learning approach, which includes no shape reconstruction step and directly predicts the spatial curve of the sensor containing only five sensing planes.

We simulated the shape reconstruction error when different spatial resolutions were employed. To do so, we first interpolate the discrete curve points over the sensor’s true shape, measured by the motion capture system, using a Spline with a resolution of 0.1 mm (this value was selected by trial and error). We then calculated the curvature and the torsion, the curve’s deviation from the osculating plane, at the query points. Finally, we use the calculated curvatures and bending directions at the sensing planes to reconstruct the spatial curve and compare it with the true shape. For a 25 cm long sensor with 50 mm spatial resolution (five sensing planes), the median tip error of the reconstructed

![Graph](image.png)

Fig. 4 An example from Test samples in which a 3 cm long segment, 1 cm after the last sensing plane, is deformed. Refer to the caption of Figure 3 for more details.
shapes, tested on Test\textsubscript{1} and Test\textsubscript{2} datasets, is $\sim 50\text{mm}$, which is almost 16 times higher as compared to what the DL approach achieved (see Table 1). The median tip error of reconstructed shapes dropped to $\sim 10\text{mm}$ when the sensing planes are 10\text{mm} apart. In order to get a median tip error of 3\text{mm}, the spatial resolution of the sensor should also be in a similar range, which is technically not possible, as a minimum distance of $\sim 10\text{mm}$ is required in laser-inscribed FBG arrays [13].

However, in the DL method, the sensor’s low spatial resolution is no longer the major limitation, as the model learned to also make use of other parts of the edge-FBG spectrum, including the side slopes of the Bragg resonances, for shape prediction. These sensitive side slopes provide the deep learning model with the missing information from the area without sensing planes, compensating for the sensor’s low spatial resolution.

**Conclusion**

In this paper, we investigated the most important limiting factors, including cladding mode coupling, bending loss oscillations, and polarization-dependent losses, in intensity-based edge-FBG shape sensors. It is achievable but not cost-effective to minimize the impact of such bending-induced phenomena by adapting the sensor’s design and the interrogation system. Moreover, calculating the exact influence of these effects on the edge-FBGs spectrum is not practically possible. Therefore, these effects are not considered in the commonly used sensor modeling method based on mode-field dislocation measurement (the BL method). We proposed a novel data-driven technique (the DL method) for modeling edge-FBG sensors, in which a specially designed deep learning algorithm directly learns from the sensor’s spectra to estimate their corresponding shapes. We compared the shape prediction accuracy of our designed model with the mode field dislocation method as a baseline. We showed that the maximum spatial resolution of 1 cm in edge-FBG sensors is the main limitation when the sensor’s modeling method includes the shape reconstruction step (e.g., the BL approach). This leads to large shape prediction errors in complex shapes, as the deformations between the edge-FBG sensing planes are not detected. The deep learning technique uses the sensor’s full spectrum, including the Bragg resonance’s side slopes, as the model’s input. These additional sources of information, which are sensitive to bending, help to overcome the spatial resolution limitation and detect complex deformations (in a curvature range of 0.58 m\textsuperscript{-1} to 33.5 m\textsuperscript{-1}) with a low prediction error, reduced by a factor of $\sim 50$. We also showed that the designed deep learning model generalizes nicely, as the performance is twice as good compared to a dictionary-based algorithm. The proposed shape sensing solution is 30 times less expensive than the commercially available distributed fiber shape sensor with a similar level of accuracy.
Fig. 5  The data acquisition experimental setup. The motion capture system includes five tracking cameras (Oqus 7+). For protection purposes, the fiber sensor is inserted in a Hytrel furcation tubing with an inner diameter of 425 µm and an outer diameter of 900 µm. Two v-clamps are used to hold the protection tubing and to fix the optical fiber before the insertion. The reflective markers are 6.4 mm in diameter with an 1 mm opening (X12Co., Ltd, Bulgaria). A thermocouple is placed close to the sensor’s base to monitor the temperature during the data acquisition, ensuring no sudden thermal fluctuation affects the sensor’s signal.

Methods

Setup. The data acquisition setup used for developing the deep learning-based model is shown in Figure 5. We used a low-cost FBG interrogator (MIOPAS GmbH, Goslar, Germany) consisting of an uncooled TOSA module SLED and a NIR micro-spectrometer with 0.5 nm resolution to cover all 15 Bragg wavelengths from 813 nm to 869 nm. We recorded the sensor’s spectra at random curvatures and orientations (in a curvature range of 0.58 m⁻¹ to 33.5 m⁻¹) while monitoring the reflective markers attached to the 30 cm long sensor using a motion capture system (Qualisys AB, Sweden). The data acquisition time period was 30 min for the Test₁ and 3 min for the Test₂ datasets. The update rates in the FBG interrogator and the motion capture system were 75 Hz and 200 Hz, respectively. The sensor’s spectra and the coordinate values corresponding to its shape were synchronized with a tolerance of less than 3 ms.

We also used a laser-cut curvature template (Figure 5) to collect 320 samples of the Test₃ dataset, when only certain sensor areas should be bent. The curvature template has four grooves allowing the sensor to be bent at the middle 30 mm area between the sensing planes 2 and 3, 3 and 4, 4 and 5, and 5, and 10 mm after the last sensing plane with a bending radius of 50 mm.

Training Setup. The search space we defined for tuning the network’s hyperparameters consists of the number of 1D convolutional layers (Conv1D), the number of fully connected layers (FC), the layer settings, the choice of
Table 2 Search criteria for hyperparameter optimization.

| hyperparameter                          | search space               | selected values |
|-----------------------------------------|-----------------------------|-----------------|
| number of Conv1D layer                  | min: 1, max: 20, step: 1    | 5               |
| number of FC layer                      | min: 1, max: 20, step: 1    | 5               |
| BN after each layer                     | true, false                |                 |
| dropout after FC layer                  | true, false                |                 |
| dropout rate                            | min: 0.1, max: 0.8          |                 |
| stride                                  | min: 1, max: 2, step: 1     |                 |
| kernel size (max pooling layer)         | min: 2, max: 3, step: 1     |                 |
| distribution of initial weights          | Xavier_uniform, Xavier_normal, Kaiming_uniform, Kaiming_normal | Xavier_normal |
| learning rate                           | 0.01, 0.001, 0.0001, 0.00001 | 0.0001          |
| sorting Conv1D layers                   | true, false                | true            |
| L2 regularization                       | 0.1, 0.01, 0.001, 0.0001, 0.00001, 0 | 0               |
| threshold in SmoothL1                    | any values between 0.0 and 5.0 | 4.04           |

batch normalization and downsampling, training settings, and loss function parameters. Table 2 shows the search criteria.

In the designed network, the input samples with a batch size of 256 are first batch normalized and then fed into a Conv1D layer with 16 channels, followed by a max pooling layer with a kernel size of 3 and a stride of 2. The second Conv1D layer also has 16 channels, followed by a max pooling layer with a kernel size of 2. The third Conv1D layer has 32 channels, followed by a max pooling layer with a kernel size of 3 and a stride of 2. The fourth Conv1D layer also has 32 channels with a stride of 2, followed by a max pooling layer with a kernel size of 3. The last Conv1D layer has 256 channels, followed by batch normalization and a max pooling layer with a kernel size of 2 and a stride of 2. The extracted features are flattened to a 2048-long vector, fed into five FC layers, each with 2000 units. The first FC layer is followed by batch normalization and a dropout layer with a probability of 0.37, and two more FC layers. A batch normalization, an FC layer, a dropout layer with a probability of 0.16, and a fourth FC layer are the remaining layers before the final layer. The last layer is an FC layer that maps the output of the fourth FC layer into the target values, the relative coordinates. In all layers of this network architecture, the rectified linear unit (ReLU) serves as the activation function, and the kernel size for the Conv1D layers is 3. In this model, the Adam optimizer with a learning rate of 0.0001 minimizes the SmoothL1 loss function with a threshold of 4.04.

Decoding The Model’s Decisions. Inspired by Gradient-weighted Class Activation Mapping (Grad-CAM), we decode the decisions made by our CNN (convolutional neural network)-based model. Decoding our model’s decisions helps us understand which part of the input spectra contributes to coordinate predictions. Grad-CAM is a commonly used technique in image classification problems that generates visual explanations from any CNN-based model without any re-training or architectural changes required. Gradient is a measure
that shows the effect on the output caused by the input. In other words, we are looking for the part of the input with the highest effect on the model’s output. However, due to the small output dimension in each channel of the last Conv1D layer, its gradient heat map highlights the inputs’ important parts with a low resolution. Therefore, instead of the gradient of the Conv1D layers, we calculate the forward finite difference of the model’s loss with respect to the input spectral elements. The spacing constant is chosen 0.1, higher than the spectral intensity noise level. In this method, we modify the intensity value of one spectral element and monitor the changes of the model’s loss value. We repeat this process for all 190 spectral elements. The resultant color maps (shown in Figure 3 (b) and Figure 4 (b)) indicate the impact of the changes in each spectral element on the model’s SmoothL1 loss value. In order to investigate the contribution of each spectral element to the coordinate prediction of each individual marker, we calculated the Euclidean distance between the predicted coordinates of each marker before and after spectral modification. This way, we were able to highlight all the spectral elements contributing to the relative coordinate prediction of each marker.

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