Representer Point Selection via Local Jacobian Expansion for Classifier Explanation of Deep Neural Networks and Ensemble Models

Anonymous Author(s)
Affiliation
Address
email

Abstract

Explaining the influence of training data on machine learning model predictions is a critical tool for debugging models through data curation. A recent appealing and efficient approach for this task was provided via the concept of Representer Point Selection (RPS), i.e. a method the leverages the dual form of l_2 regularized optimization in the last layer of the neural network to identify the contribution of training points to the prediction. However, two key drawbacks of RPS-l_2 are that they (i) lead to disagreement between the originally trained network and the RPS-l_2 regularized network modification and (ii) often yield a static ranking of training data for test points in the same class, independent of the test point being classified. Inspired by the RPS-l_2 approach, we propose an alternative method based on a local Jacobian Taylor expansion (LJE). We empirically compared RPS-LJE with the original RPS-l_2 on image classification (with ResNet), text classification recurrent neural networks (with Bi-LSTM), and tabular classification (with XGBoost) tasks. Quantitatively, we show that RPS-LJE slightly outperforms RPS-l_2 and other state-of-the-art data explanation methods by up to 3% on a data debugging task. More critically, we qualitatively observe that RPS-LJE provides stable and individualized explanations that are more coherent to each test data point. Overall, RPS-LJE represents a novel approach to RPS-l_2 that provides a powerful tool for sample-based model explanation and debugging.

1 Introduction

Deep learning as well as ensemble methods such as XGBoost [2] have revolutionized the field of machine learning and led to unprecedented levels of accuracy in a variety of data-driven prediction applications. However, it can be extremely challenging to debug these complex methodologies when they make incorrect predictions. The first step in this debugging process is *explaining* the prediction, which can stem from a variety of interpretive processes. For example, we may seek to understand the key features [9, 12] or salient regions [14, 15] that led to a prediction, or in a more recent line of work, we make seen to understand the influence of the training data on test data predictions [1, 7, 11, 17].

In this paper we focus on a particularly appealing (and efficient) method for understanding the impact of training data on test predictions, namely Representer Points Selection (RPS) [17], which leverages an application of the representer theorem [13] to deep neural networks. Specifically, it uses the dual form of l_2 regularized optimization in the last layer of the neural network to identify the contribution of training data to the test prediction. Compared to model-agnostic approaches [1, 5, 6] that estimate data influence after optimization, the RPS approach directly integrates with the prediction model to provide a high-fidelity white-box interpretation of the prediction. Compared to the influence

Submitted to 35th Conference on Neural Information Processing Systems (NeurIPS 2021). Do not distribute.

(a) Same test image, different l_2 weight.

(b) Different test image, same l_2 weight.

Figure 1: **Drawbacks of Current Representer Point Selection Explanation (RPS-l_2) on CIFAR-10 Dataset.** The target model is ResNet [4]. (a) Explanations vary when the l_2 regularized fine-tune is conducted with different hyperparameter weightings. (b) RPS produces *identical* explanations (and rankings) for different test samples that belong to the same predicted class.

function-based approach [7], the RPS is computationally more efficient as it focuses on the last layer of a neural network instead of *all* parameters.

While holding many advantages, we note the existing RPS approach faces two key drawbacks. First, as the RPS approach requires fine-tuning the last layer of the neural network with l_2 regularization, it leads to a disagreement between the originally trained network and the l_2 regularized network and is furthermore highly sensitive to l_2 regularization strength (cf. Figure 1(a)). Thus, it is hard to justify if the explanation produced by RPS is for the original model or the modified model. Second, we observe that the explanations produced by RPS are nearly identical for all test samples that are classified into the same category, which provides more of a class-level rather than instance-level explanation for RPS (cf. Figure 1(b)). While the RPS approach is appealing in principle, both of these drawbacks significantly harm the utility of the RPS explanation approach in practice.

To address these issues, this paper presents an alternative derivation for Representer Point Selection (RPS) based on a Local Jacobian Taylor expansion (LJE), which corrects for both aforementioned problems. We empirically compared RPS-LJE to the original RPS-l_2 on image classification (with ResNet [4]), text classification (with Bi-LSTM), and credit analysis (with XGBoost [2]) tasks. Quantitatively, we show that RPS-LJE outperforms RPS-l_2 and other state-of-the-art data explanation methods by to up 3% on a data debugging task. Qualitatively — and perhaps most importantly — the RPS-LJE provides stable and diverse explanations that are more coherent to each test data point.

2 Representer Points Selection for Explaining Deep Neural Networks

2.1 Preliminary

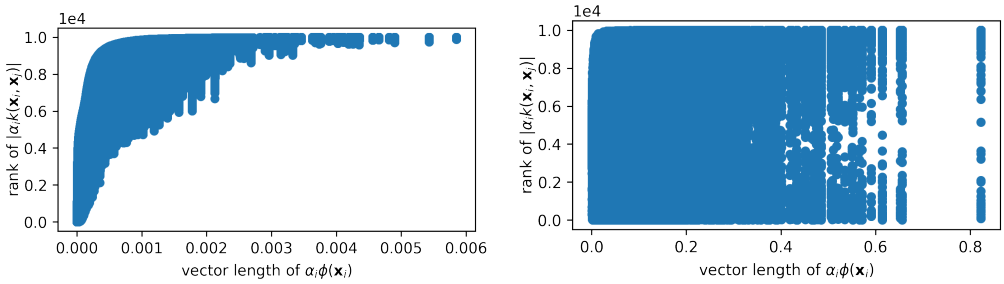
In a machine learning context, representer theorems [13] loosely state that under certain conditions, model prediction $\hat{\mathbf{y}}_t$ of a test sample x_t can be expressed as a linear combination of kernel evaluations $\mathcal{K}(\mathbf{x}_i, \mathbf{x}_t)$ between each training point $\mathbf{x}_i$ and the test sample $\mathbf{x}_t$ such that

$$\hat{\mathbf{y}}_t = \sum_i^n \boldsymbol{\alpha}_i \mathcal{K}(\mathbf{x}_i, \mathbf{x}_t) \,, \tag{1}$$

where $\boldsymbol{\alpha}_i$ is the weight of the training data point i that is independent from the test point t.

As the representer theorem linearly separates the contribution of training data points to the prediction, it has been introduced into the model interpretation research [17] as a convenient method for tracking the influence of training data on deep learning model predictions. Concretely, the current Representer Points Selection (RPS) approach [17] introduces an l_2 regularization term (for the parameters of last layer $\Theta_L \subset \boldsymbol{\Theta}$) into a model's original objective function, which facilities its derivation such that it fulfills Equation 1 by setting

$$\boldsymbol{\alpha}_i = -\frac{1}{2\lambda n} \frac{\partial \mathcal{L}(\mathbf{x}_i, y_i, \boldsymbol{\Theta})}{\partial \Theta_L \phi(\mathbf{x}_i)} \quad \textit{and} \quad \mathcal{K}(\mathbf{x}_i, \mathbf{x}_t) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_t) \,, \tag{2}$$



(a) RPS-l_2 (b) RPS-LJE

Figure 2: **Correlation between the Rank of Explanations ($\boldsymbol{\alpha}_i \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_t)$) and term $\boldsymbol{\alpha}_i \phi(\mathbf{x}_i)$.** (a) RPS-$l_2$'s explanation rank heavily depends on $\boldsymbol{\alpha}_i \phi(\mathbf{x}_i)$, which shows strong dominance that suppressed information of test example. (b) Proposed RPS-LJE does not encounter this issue. This demo is produced on a binary classification task (horses vs. cars), where we only look at α_i of the positive class.

where λ denotes the hyper-parameter of l_2 regularization term, and $\phi(\mathbf{x}_i)$ and $\phi(\mathbf{x}_t)$ are the representations of input $\mathbf{x}_i$ and $\mathbf{x}_t$ at layer L. As this explanation approach works on the last layer of a network and is efficient to compute, it demonstrates a significant advantage over influence function-based approaches [7] in terms of computational efficiency.

2.2 Caveats of Current Representer Points Selection

As mentioned previously, to facilitate the its derivation, the current RPS approach introduces an l_2 regularization term into the computation, which inevitably violates the saddle point assumption its derivation relies on. To address this problem, the RPS conducts fine-tuning on the trained model with the new objective function

$$\Theta_L^* = \arg\min_{\Theta_L} \left\{ \frac{1}{n} \sum_i^n \mathcal{L}(\Phi(x_i, \boldsymbol{\Theta}), \Phi(x_i, \boldsymbol{\Theta}_{given})) + \lambda \|\Theta_L\|^2 \right\}, \tag{3}$$

where $\Phi(x_i, \boldsymbol{\Theta}_{given})$ and $\Phi(x_i, \boldsymbol{\Theta})$ represents the post-activation prediction of x_i of the given model and fine-tuned model, respectively. Correspondingly, the kernel weights in the expression of Equation 2 are updated as

$$\boldsymbol{\alpha}_i = -\frac{1}{2\lambda n} \frac{\partial \mathcal{L}(\mathbf{x}_i, y_i, \boldsymbol{\Theta}^*)}{\partial \Theta_L^* \phi(\mathbf{x}_i)}. \tag{4}$$

As the data importance factor $\boldsymbol{\alpha}_i$ is computed with respect to the l_2-modified parameter set $\boldsymbol{\Theta}^*$, the explanations correspond to the modified model instead of the original model. Indeed, the gap between the two sets of parameters is sensitive to the hyper-parameter setting of the l_2 regularizer. This reflects our previous observation in Figure 1(a) showing that prediction explanations can vary *significantly* based on different l_2 regularizer weightings.

Also, by inspecting the expression of training data contribution

$$\begin{aligned} \Theta_L^* \phi(\mathbf{x}_t) = \boldsymbol{\alpha}_i \mathcal{K}(\mathbf{x}_i, \mathbf{x}_t) &= -\frac{1}{2\lambda n} \frac{\partial \mathcal{L}(\mathbf{x}_i, y_i, \boldsymbol{\Theta}^*)}{\partial \Theta_L^* \phi(\mathbf{x}_i)} \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_t) \\ &= -\frac{1}{2\lambda n} \frac{\partial \mathcal{L}(\mathbf{x}_i, y_i, \boldsymbol{\Theta}^*)}{\partial \Theta_L^* \phi(\mathbf{x}_i)} \frac{\partial \Theta_L^* \phi(\mathbf{x}_i)}{\partial \Theta_L^*} \phi(\mathbf{x}_t) = \underbrace{-\frac{1}{2\lambda n} \frac{\partial \mathcal{L}(\mathbf{x}_i, y_i, \boldsymbol{\Theta}^*)}{\partial \Theta_L^*}}_{\textit{dominant term}} \phi(\mathbf{x}_t), \end{aligned} \tag{5}$$

we note the first-order derivative of the loss of a single training example is the dominant term that suppresses a small difference of test example representation $\phi(\mathbf{x}_t)$ among test samples in the same class. Figure 2(a) shows the strong positive correlation between the dominant term and the relevant order of the training data contribution. This supports our observation in Figure 1(b) that explanations tend to be identical for the test samples being classified into the same category making RPS more of a class-level than instance-level explanation that defeats the intent of uncovering instance-level prediction errors!

3 Representer Point Selection via Local Jacobian Expansion

In an effort to preserve the conceptual and computational advantages of the previously discussed RPS-l_2 methodology while improving fidelity of the explanations to the original model and encouraging test instance-level explanation, we now present a novel derivation of Representer Point Selection through a Local Jacobian Expansion (RPS-LJE). Similar to RPS-l_2, RPS-LJE also expresses the pre-activation prediction outcome of a well-trained classification model (near the saddle point) as a linear combination of kernel evaluations between the test sample and the training points. Specifically, we use a first-order Taylor expansion on the Jacobian matrix in our derivation, which avoids the problems introduced by imposing the additional l_2 regularization term in RPS-l_2. First, we begin the formal problem definition.

Consider a classifier $\mathcal{M}_{\mathbf{\Theta}^\dagger}$ (the target model in the following context) that has learned to map input observation $\mathbf{x}_t \in \mathbb{R}^d$ to an output space $y_t \in \{1 \cdots k\}$, whose pre-activation prediction [1] $\bar{\mathcal{M}}_{\mathbf{\Theta}^\dagger}$ could be formulated as

$$\hat{\mathbf{y}}_t = \bar{\mathcal{M}}_{\mathbf{\Theta}^\dagger}(\mathbf{x}_t) = \Theta_L^\dagger \phi(\mathbf{x}_t), \tag{6}$$

where bold $\mathbf{y}_i \in \mathbb{R}^k$ represents the prediction vector (one element for a class). Our goal of prediction explanation is to reformulate Equation 6 into the format of Equation 1 such that the contribution of each training data point on the prediction is linearly separable.

While the above setting appears restricted, it represents a large group of machine learning models commonly used in practice; many well-known models, such as ResNet [4] for images, Transformers [16] for text, and even XGBoost [2] for tabular classification tasks, can be expressed in this simple formulation leveraging a feature embedding stage followed by a pre-activation linear prediction stage.

3.1 First-order Taylor Expansion on Jacobian Matrix

We begin by presuming we are given a well-trained target model $\mathcal{M}_{\mathbf{\Theta}^\dagger}$, whose loss derivative with respect to the decision making parameter Θ_L is close to a saddle point such that

$$0 \approx \sum_{i=1}^{n} \frac{\partial \mathcal{L}(\mathbf{x}_i, y_i, \mathbf{\Theta})}{\partial \Theta_L}\bigg|_{\Theta_L = \Theta_L^\dagger}. \tag{7}$$

With any parameter assignment Θ_L^* close to the model parameter $\Theta_L^\dagger$, we can further rewrite Equation 7 via a first-order Taylor expansion such that

$$0 \approx \frac{1}{n}\sum_{i=1}^{n} \underbrace{\frac{\partial \mathcal{L}(\mathbf{x}_i, y_i, \mathbf{\Theta})}{\partial \Theta_L}\bigg|_{\Theta_L = \Theta_L^*}}_{\nabla_{\Theta_L}\mathcal{L}(\mathbf{x}_i, y_i, \mathbf{\Theta}^*)} + (\Theta_L^\dagger - \Theta_L^*) \underbrace{\left[\frac{1}{n}\sum_{i=1}^{n} \frac{\partial \mathcal{L}^2(\mathbf{x}_i, y_i, \mathbf{\Theta})}{\partial \Theta_L^2}\bigg|_{\Theta_L = \Theta_L^*}\right]}_{\mathcal{H}_{\Theta_L^*} \stackrel{\text{def}}{=} \frac{1}{n}\sum_{i=1}^{n} \nabla^2_{\Theta_L}\mathcal{L}(\mathbf{x}_i, y_i, \mathbf{\Theta}^*)}. \tag{8}$$

This expansion yields the model parameter $\Theta_L^\dagger$ as a linear combination of functions of each training data point

$$\Theta_L^\dagger = \Theta_L^* - \sum_{i=1}^{n} \frac{1}{n}\mathcal{H}_{\Theta_L^*}^{-1} \nabla_{\Theta_L}\mathcal{L}(\mathbf{x}_i, y_i, \mathbf{\Theta}^*) + \xi, \tag{9}$$

where ξ is a negligible error term. Intuitively, this equation shows the model parameter $\Theta_L^\dagger$ could be reconstructed through a one-step gradient descent from the nearby parameter assignment Θ_L^* with a dynamic learning rate $\frac{1}{n}\mathcal{H}_{\Theta_L^*}^{-1}$ (as a matrix).

We remark that the expression in Equation 9 represents the contribution of each data point as a linearly separable function, which is fundamentally different from recording gradients at training time as a data importance score [11]. That is, the gradients during model training are sensitive to both training order and optimizer settings.

For Equation 9 to hold after the Taylor expansion, Θ_L^* has to be close to the model parameter $\Theta_L^\dagger$. Therefore, we propose to estimate Θ_L^* through a one-step stochastic gradient ascent from the trained

[1] For the trained classifier, the predictions before and after activation are consistent.

model using any optimizer (Adam, RMSProp, etc), such that

$$\sum_{i=1}^{n} \mathcal{L}(\mathbf{x}_i, y_i, \mathbf{\Theta}^*) > \sum_{i=1}^{n} \mathcal{L}(\mathbf{x}_i, y_i, \mathbf{\Theta}^\dagger) \tag{10}$$

and Θ_L^* is maintained close to the original model parameter $\Theta_L^\dagger$ with a small loss shift.

3.2 Representer Point Selection with Local Jacobian Expansion (RPS-LJE)

With the derivation of Equation 9, we can now reformulate the pre-activation prediction of a test point $\mathbf{x}_t$ as a weighted linear combination of kernels leading to our key result of the final form of RPS-LJE:

$$\begin{aligned}\Theta_L^\dagger \phi(\mathbf{x}_t) &= \sum_{i=1}^{n} \left[\frac{1}{n}\Theta_L^* - \frac{1}{n}\mathcal{H}_{\Theta_L^*}^{-1} \nabla_{\Theta_L} \mathcal{L}(\mathbf{x}_i, y_i, \mathbf{\Theta}^*) \right] \phi(\mathbf{x}_t) \\ &= \sum_{i=1}^{n} \underbrace{\left[\frac{1}{\phi(\mathbf{x}_i)n}\Theta_L^* - \frac{1}{n}\mathcal{H}_{\Theta_L^*}^{-1} \frac{\partial \mathcal{L}(\mathbf{x}_i, y_i, \mathbf{\Theta}^*)}{\partial \Theta_L^* \phi(\mathbf{x}_i)} \right]}_{\boldsymbol{\alpha}_i} \underbrace{\phi(\mathbf{x}_i)^T \phi(\mathbf{x}_t)}_{\mathcal{K}(\mathbf{x}_i, \mathbf{x}_t)} .\end{aligned} \tag{11}$$

Similar to the claim of the original RPS using an l_2 norm (RPS-l_2), when a training data $\mathbf{x}_i$ is close to the test point $\mathbf{x}_t$ in the representation space with a large positive value α_{ik} , the prediction score for class k is increased. On the other hand, when the α_{ik} is a large negative value, the prediction score for class k is then decreased.

The first notable difference between our derivation of RPS-LJE and the original RPS-l_2 is that the $\boldsymbol{\alpha}_i$ term now contains an inverse of second-order derivative that estimates the correlation among the parameter entries in $\Theta_L^\dagger$. This modification mitigates the risk of over-weighting training data points with a large predictive error that causes a small number of data points to dominate the explanations as discussed in Section 2.2 and Figure 1(b). Figure 2(b) illustrates the effects of correction.

The second difference is that the prediction explanation of our derivation of RPS-LJE is faithful w.r.t. the original model $\mathcal{M}_{\mathbf{\Theta}^\dagger}$ instead of the l_2-regularized model $\mathcal{M}_{\mathbf{\Theta}^*}$. To clarify, the left hand side of of Equation 11 is different with that of RPS-l_2 in Equation 5. In addition, data importance factor $\boldsymbol{\alpha}_i$ in the new derivation no longer depends on the l_2 regularization hyper-parameter. Hence, the changes in the RPS-LJE framework directly address the problem described in Figure 1(a).

3.3 Relation to Influence Function-based Interpretation

The influence function method [7] estimates the prediction importance of each training data point by up-weighting the data points with small perturbation ϵ that results in the following final expression

$$\mathcal{I}_{up,loss}(\mathbf{x}_i, \mathbf{x}_t) = -\nabla_{\Theta_L} \mathcal{L}(\mathbf{x}_t, y_t, \mathbf{\Theta}^\dagger)^T \underbrace{\mathcal{H}_{\Theta_L^\dagger}^{-1} \nabla_{\Theta_L} \mathcal{L}(\mathbf{x}_i, y_i, \mathbf{\Theta}^\dagger)}_{\mathcal{I}_{up,params}(\mathbf{x}_i) \stackrel{\text{def}}{=} \frac{d\mathcal{L}(\mathbf{x}_t, y_t, \mathbf{\Theta}^\dagger)}{d\epsilon}\Big|_{\epsilon=0}} . \tag{12}$$

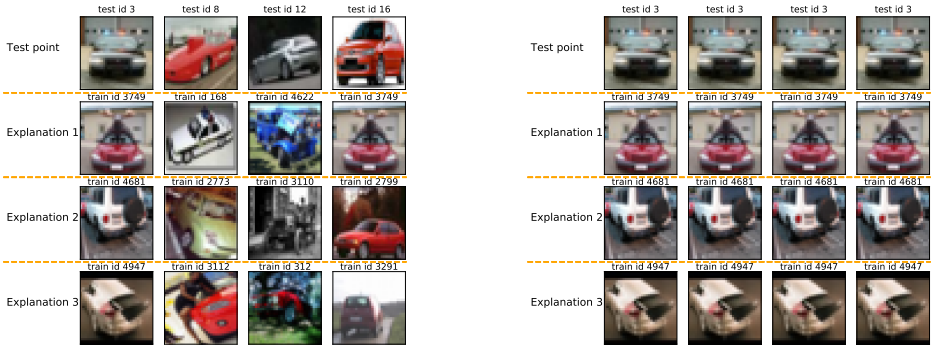
If we rewrite the above equation by expanding the first-order derivatives with chain rule such that

$$\mathcal{I}_{up,loss}(\mathbf{x}_i, \mathbf{x}_t) = -\frac{\partial \mathcal{L}(\mathbf{x}_t, y_t, \mathbf{\Theta}^\dagger)}{\partial \Theta_L^\dagger \phi(\mathbf{x}_t)} \mathcal{H}_{\Theta_L^\dagger}^{-1} \frac{\partial \mathcal{L}(\mathbf{x}_i, y_i, \mathbf{\Theta}^\dagger)}{\partial \Theta_L^\dagger \phi(\mathbf{x}_i)} \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_t), \tag{13}$$

we note the expression is very similar to RPS-LJE proposed in this work (as described in Equation 11) except two subtle differences:

- The influence function includes a multiplicative factor $\frac{\partial \mathcal{L}(\mathbf{x}_t, y_t, \mathbf{\Theta}^\dagger)}{\partial \Theta_L^\dagger \phi(\mathbf{x}_t)}$ that is relevant to the test point, whereas the RPS-LJE has an additive factor $\frac{1}{n}\Theta_L^* \phi(\mathbf{x}_t)$ that is also only relevant to the test point.
- The derivative in the influence function respects the original model parameters $\Theta^\dagger$, whereas RPS-LJE's derivatives apply to Θ^*.

Ultimately, these differences help explain the comparative performance of these methods in our experiments (cf. Section 4.3), but — because they are also subtle – they help explain the similarity of explanations produced by RPS-LJE and influence functions for image classification explanation.



(a) (b)

Figure 3: **Sanity Check of Representer Point Selection with Local Jacobian Expansion (RPS-LJE) on CIFAR-10 Dataset.** (a) RPS-LJE can correctly produce individualized explanations. (b) Explanation maintains consistency as the gradient hyperparameter setting changes.

4 Experimental Evaluation

We perform a range of experiments with multiple datasets (and corresponding model architectures) and evaluate the performance of RPS-LJE against the original RPS-l_2 as well as influence function-based approaches. Note that all three methods do not specifically require access to the training history, which is rarely available in deployment settings. In contrast, TracIn [11], which requires access to training checkpoints, is not in the scope of our comparison. The goal of these experiments is to demonstrate that the alternative derivation of RPS described in this work, RPS-LJE, successfully addresses the two critical drawbacks of RPS-l_2 and leads to substantial performance improvement on multiple use cases, including data debugging and model behavior explanation.

4.1 Sanity Check of Representer Point Selection with Local Jacobian Expansion

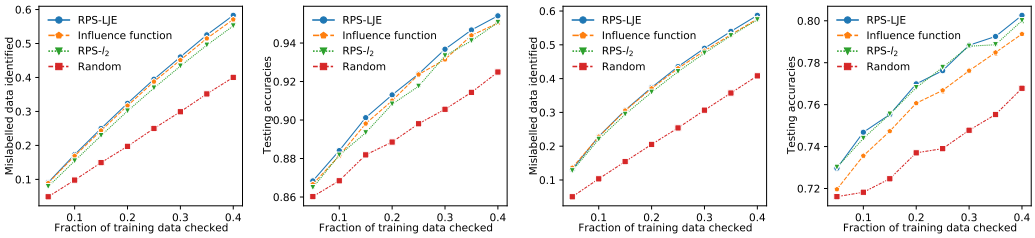
Before describing our quantitative analysis, we first start with a sanity check to show the proposed RPS-LJE approach indeed addresses the problem we highlighted earlier in Section 2.2 and Figure 1. Concretely, we repeat our showcase in Figure 3 using RPS-LJE with the same test examples and target model. Here, we highlight the following observations:

- As shown in Figure 3(a), the RPS-LJE can produce an individualized explanation for test samples in the same category. This observation reflects our previous description in Figure 2(b), where the term $\boldsymbol{\alpha}_i \phi(\mathbf{x}_i)$ in RPS-LJE no longer dominates the explanation ranking.
- To test the sensitivity of one-step gradient descent in RPS-LJE (used to search Θ_L^* as described in Section 3.1), we experimented with multiple learning rates γ in a large range $\gamma \in \{5e-4 \cdots 1e-3, 5e-3 \cdots 1e-2\}$. As shown in Figure 3(b), the explanations vary little with the learning rate.

4.2 Fixing Mislabeled Training Examples (Data Debugging)

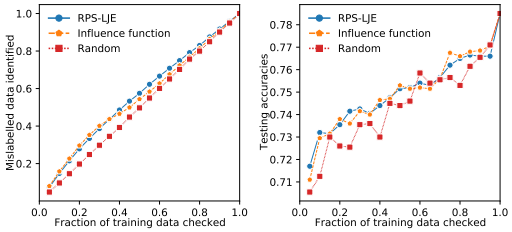
In this experiment, we simulate an application scenario where human experts need to inspect the data annotation quality of the training set that directly impacts the model performance on the test samples.

We simulate data debugging on three classification tasks, including 1) binary image classification with ResNet [4] on CIFAR-10 [8] dataset (horses vs. cars) presented in the RPS-l_2 paper [17], 2) sentiment analysis with LSTM on IMDB [10] dataset, and 3) credit risk identification with XGBoost on German Credit dataset [3]. The datasets are intentionally corrupted by randomly flipping 20-30 percent of the data points' labels, naturally resulting in low test accuracy. Our goal is to identify which data points' label corruption are more harmful and correct them as early as possible. With the partially corrected dataset (after each 5% of checking), we retrain the models and record the test accuracies for each task. Experiments are repeated for ten random split and corruptions on CNN and XGBoost and five random split and corruptions on RNN; we report the average result. For RPS approaches (LJE and l_2), we pick data points that have the largest self-prediction contribution



(a) CIFAR-10 Image Classification with ResNet

(b) IMDB Sentiment Analysis with LSTM



(c) German Credit Risk Analysis with XGBoost

Figure 4: **Performance Comparison on Dataset Debugging Tasks.** For each sub-figure group, we show data correction rate vs. fraction of data checked (left) and how such a correction would impact performance (right). RPS-LJE shows slightly better performance than influence functions and marginally better than the original RPS with l_2 norm injection.

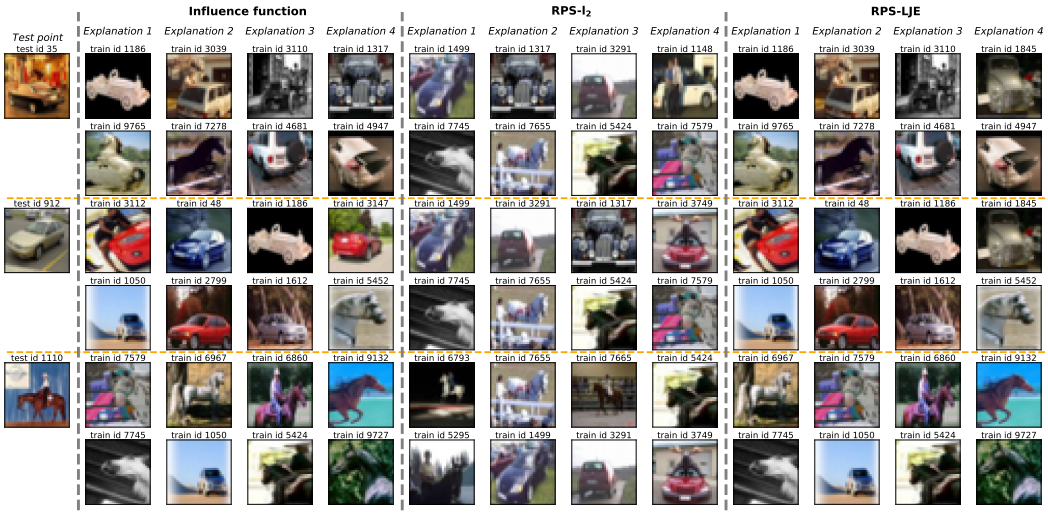


Figure 5: **Comparison of Top-4 Influential Training Images for Three Test Samples.** For each test sample, the upper row shows positive influential points, whereas the bottom row shows negative influential points. Examples are randomly selected from 2000 test samples in our experiment setting.

$|\alpha_i \mathcal{K}(\mathbf{x}_i, \mathbf{x}_i)|$ [2] as suspicious corrupted data points. For influence functions, we use self-influence (see Equation 12) as the score of ranking.

Figure 4 shows the experimental results. Here, we highlight the following observations:

- RPS-LJE either slightly dominates RPS-l_2 or performs comparably to it. This demonstrates that it is an effective data debugging tool comparable to as RPS-l_2, since both show a significant performance gap to the random baseline on all three tasks.
- RPS-LJE shows slightly better performance than both influence function and RPS-l_2 on all tests. For the image classification task, the RPS-LJE shows 3% better performance (around 60 more mislabelled data identified) than original RPS-l_2 after searching through 40% of all training data.

[2] We note that, for RPS-l_2, there is no difference on using $|\alpha_i|$ or $|\alpha_i \mathcal{K}(\mathbf{x}_i, \mathbf{x}_i)|$ to select corrupt data points.

Table 1: **Explanation Comparison among RPS-LJE, RPS-l_2 and Influence Function on IMDB sentiment analysis data.** Column "Sentiment" is the target (label) column, and raw review is the input of Bi-LSTM network. Examples are randomly selected from the test set.

		ID	Sentiment	Raw Reviews
Sample 1	Test point	41	positive	This movie is good for entertainment purposes, but it is not historically reliable. If you are look···
RPS-LJE	Explanation 1	741	positive	This movie is about sexual obsession.Bette Davis plays Mildred. This is a woman who men are···
	Explanation 2	14701	positive	This is a very memorable spaghetti western.It has a great storyline, interesting characters,and some···
	Explanation 3	3159	positive	This movie was featured on a very early episode of Mystery Science Theater 3000,but when I see···
RPS-l_2	Explanation 1	9112	positive	Tim Krabbe is the praised author of 'Het Gouden Ei' , a novel that was put on the screen twice···
	Explanation 2	3704	positive	THE DEVIL'S PLAYTHING is my second attempt at a Joseph Sarno production-and although I ···
	Explanation 3	4000	positive	So , Todd Sheets once stated that he considers his 1993 , shot-on-video Z - epic, Zombie Bloodbath···
Influence function	Explanation 1	14701	positive	This is a very memorable spaghetti western.It has a great storyline, interesting characters,and some···
	Explanation 2	741	positive	This movie is about sexual obsession.Bette Davis plays Mildred. This is a woman who men are···
	Explanation 3	669	positive	Did you ever wonder how far one movie could go?Schizophreniac relentlessly explores the world···
Sample 2	Test point	525	positive	I can think of no movie that better captures the concept of grace, in a theological sense.The well-···
RPS-LJE	Explanation 1	14109	positive	I can tell you just how bad this movie is.I was in the movie and I haven't seen it yet,but I cringe at···
	Explanation 2	2300	positive	I am one of Jehovah's Witnesses and I also work in an acute care medical facility.Over the years I···
	Explanation 3	6372	positive	I think the film is educational. However,it fails to treat the issue which sparked so much controversy···
RPS-l_2	Explanation 1	9112	positive	Tim Krabbe is the praised author of 'Het Gouden Ei' , a novel that was put on the screen twice···
	Explanation 2	3704	positive	THE DEVIL'S PLAYTHING is my second attempt at a Joseph Sarno production-and although I ···
	Explanation 3	4000	positive	So , Todd Sheets once stated that he considers his 1993 , shot-on-video Z - epic, Zombie Bloodbath···
Influence function	Explanation 1	2394	negative	A memorable line from a short lived show.After viewing the episode where that line was introduced···
	Explanation 2	14109	positive	I can tell you just how bad this movie is.I was in the movie and I haven't seen it yet,but I cringe at···
	Explanation 3	2300	positive	I am one of Jehovah's Witnesses and I also work in an acute care medical facility.Over the years I···
Sample 3	Test point	13087	negative	I really tried to like this film about a doctor who has the possibility of a new life with a young···
RPS-LJE	Explanation 1	3064	negative	I'm sorry but I didn't like this doc very much I can think of a million ways it could have been better···
	Explanation 2	4622	negative	I have to be completely honest in saying first that I fell asleep somewhere in the middle, so I can···
	Explanation 3	9777	negative	I recently viewed Manufactured Landscapes at the Seattle International Film Festival.I was drawn···
RPS-l_2	Explanation 1	4801	negative	A so common horror story about a luxury building at Brooklyn which hides the gates to hell . It is···
	Explanation 2	11015	negative	The thing that stands out in my mind in this film (sadly) is the introduction , where John Berlin···
	Explanation 3	12446	negative	Taped this late night movie when I was in grade 11 , watched it on fast forward . I sugest you do···
Influence function	Explanation 1	3064	negative	I'm sorry but I didn't like this doc very much I can think of a million ways it could have been better···
	Explanation 2	4622	negative	I have to be completely honest in saying first that I fell asleep somewhere in the middle, so I can···
	Explanation 3	16805	positive	After viewing several episodes of this series,I have come to the conclusion that television producers···

For the sentiment analysis task, the performance improvement is about 1% (around 35 more mislabelled data found than the others).

4.3 Understand Model Behavior through Prediction Explanation

In this section, we qualitatively analyze the prediction explanation ability of candidate sample-based explanation models on the three tasks mentioned in Section 4.2. While we compare the explanation results in this experiment, we only intend to compare and contrast the three explanation approaches.

CIFAR-10 Image Classification with ResNet

In Figure 5, we visualize the top-4 training points (both positively and negatively) that have the strongest influence on the prediction of test samples from Influence function, RPS-l_2, and the proposed RPS-LJE approaches on the image classification model. Here, we make the following key observations:

- The explanation produced by RPS-LJE is more similar to that of influence function than RPS-l_2 but with some differences in explanation order. This observation aligns with our previous conjecture in Section 3.3 that the RPS-LJE's formula of computing training data importance appears similar to that of influence functions.
- Explanations produced by RPS-l_2 contain a lot of repetition. Training example ID-3291 and ID-7655 are in all three test samples' explanation lists.

IMDB Sentiment Analysis with LSTM

Table 1 shows the top-3 explanations produced by the candidate explanation approaches on the IMDB sentiment analysis model (Bi-LSTM). Here, we make the following key observations:

Table 2: **Explanation Comparison between RPS-LJE and Influence Function on German Credit Data.** Column "Risk" is the target (label) column, and all columns after it are feature columns. Examples are randomly selected from the test set.

		ID	Risk	Checking Account	Credit History	Savings Account	Other Debtors	Employment
Sample 1	Test point	318	low	none	critical account/ other credits existing	little	none	1 to 4 years
RPS-LJE	Explanation 1	210	low	none	critical account/ other credits existing	unknown/none	none	1 to 4 years
	Explanation 2	526	low	none	critical account/ other credits existing	moderate	none	1 to 4 years
	Explanation 3	294	low	none	critical account/ other credits existing	unknown/none	none	more than 7 years
Influence function	Explanation 1	668	high	poor	critical account/ other credits existing	little	co-applicant	more than 7 years
	Explanation 2	747	high	poor	existing credits paid back duly till now	little	none	less than 1 year
	Explanation 3	611	high	moderate	existing credits paid back duly till now	moderate	none	more than 7 years
Sample 2	Test point	414	high	poor	existing credits paid back duly till now	unknown/none	none	1 to 4 years
RPS-LJE	Explanation 1	828	high	poor	existing credits paid back duly till now	unknown/none	none	more than 7 years
	Explanation 2	796	high	poor	existing credits paid back duly till now	unknown/none	none	more than 7 years
	Explanation 3	918	high	poor	existing credits paid back duly till now	moderate	none	unemployed
Influence function	Explanation 1	828	high	poor	existing credits paid back duly till now	unknown/none	none	more than 7 years
	Explanation 2	252	high	little	existing credits paid back duly till now	little	guarantor	1 to 4 years
	Explanation 3	796	high	poor	existing credits paid back duly till now	unknown/none	none	more than 7 years
Sample 3	Test point	951	high	poor	delay in paying off in the past	little	none	4 to 7 years
RPS-LJE	Explanation 1	174	high	poor	delay in paying off in the past	little	none	less than 1 year
	Explanation 2	466	high	poor	delay in paying off in the past	little	none	less than 1 year
	Explanation 3	862	high	poor	existing credits paid back duly till now	little	none	less than 1 year
Influence function	Explanation 1	174	high	poor	delay in paying off in the past	little	none	less than 1 year
	Explanation 2	172	high	little	delay in paying off in the past	little	none	unemployed
	Explanation 3	534	low	none	existing credits paid back duly till now	unknown/ none	none	less than 1 year

- Among the three explanation approaches, RPS-LJE's explanation is more coherent to the properties of the test points. For instance, the explanations of RPS-LJE for Sample 1 all start with "This", which is more intuitive to the model auditor on why such prediction is made. Similarly, for Sample 1 and 3, we see the explanations follow the same narrative style by starting with "I".
- Explanations provided by influence functions generate similar explanations (2 out of the top 3) with RPS-LJE. But influence functions sometimes produce confusing explanations. For example, Sample 2 has a positive comment, but Explanation 1 provided by the influence function has a negative sentiment. Similarly, Sample 3 and its Explanation 3 have the opposite sentiment.

German Credit Risk Analysis with XGBoost

Table 2 lists the predictions of three test samples in the German Credit dataset through the XGBoost model with corresponding explanations produced by RPS-LJE and influence function. Here, we removed RPS-l_2 from the candidate list as it requires fine-tuning the model with l_2 normalization, which is incompatible with tree ensemble models. Here, we highlight the following observations:

- The explanation produced by RPS-LJE is more similar to the test point than that of influence function in the sense of sharing similar feature values. For instance, the "Checking Account" values of the RPS-LJE explanation always align with the test samples, but that of the influence function does not.
- Influence Function tends to provide diverse explanations for each sample case, where the explanations produced by it show more or fewer differences.

5 Conclusion and Discussion

We presented an approach for explaining the impact of training data on a test prediction, called Representer Point Selection via Local Jacobian Expansion (RPS-LJE). Our approach aimed to correct two drawbacks of the existing Representer Point approach (RPS-l_2) [17], namely that it often 1) produces identical explanations for different instances in the same class and 2) that it produces highly varying explanations based on the strength of an l_2 regularization modification to the original model being explained. We began by observing these problems empirically and then analyzing the RPS-l_2 derivation to reveal the technical source of these problems. We then proposed corrections to derive a novel form of RPS based on a local Jacobian Taylor expansion that addresses the technical limitations of the RPS-l_2 approach.

We conducted multiple experiments that quantitatively and qualitatively analyzed the proposed RPS-LJE against existing state-of-the-art approaches, RPS-l_2 and Influence Function. Our experiments empirically show that the proposed RPS-LJE fulfilled our expectation in terms of correcting RPS-l_2's problems. It produces individualized explanations instead of a class-level explanation and quantitatively performs comparably to, or outperforms, existing data-explanation approaches.

References

[1] J. Bien and R. Tibshirani. Prototype selection for interpretable classification. *The Annals of Applied Statistics*, pages 2403–2424, 2011.

[2] T. Chen, T. He, M. Benesty, V. Khotilovich, Y. Tang, H. Cho, et al. Xgboost: extreme gradient boosting. *R package version 0.4-2*, 1(4), 2015.

[3] D. Dua and C. Graff. UCI machine learning repository, 2017.

[4] K. He, X. Zhang, S. Ren, and J. Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 770–778, 2016.

[5] B. Kim, O. Koyejo, R. Khanna, et al. Examples are not enough, learn to criticize! criticism for interpretability. In *NIPS*, pages 2280–2288, 2016.

[6] B. Kim, C. Rudin, and J. A. Shah. The bayesian case model: A generative approach for case-based reasoning and prototype classification. In *Advances in neural information processing systems*, pages 1952–1960, 2014.

[7] P. W. Koh and P. Liang. Understanding black-box predictions via influence functions. In *Proceedings of the 34th International Conference on Machine Learning - Volume 70*, ICML'17, page 1885–1894. JMLR.org, 2017.

[8] A. Krizhevsky. Learning multiple layers of features from tiny images. Technical report, 2009.

[9] S. M. Lundberg and S.-I. Lee. A unified approach to interpreting model predictions. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems 30*, pages 4765–4774. Curran Associates, Inc., 2017.

[10] A. L. Maas, R. E. Daly, P. T. Pham, D. Huang, A. Y. Ng, and C. Potts. Learning word vectors for sentiment analysis.

[11] G. Pruthi, F. Liu, M. Sundararajan, and S. Kale. Estimating training data influence by tracing gradient descent, 2020.

[12] M. T. Ribeiro, S. Singh, and C. Guestrin. "why should I trust you?": Explaining the predictions of any classifier. In *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, San Francisco, CA, USA, August 13-17, 2016*, pages 1135–1144, 2016.

[13] B. Schölkopf, R. Herbrich, and A. J. Smola. A generalized representer theorem. COLT '01/EuroCOLT '01, page 416–426, Berlin, Heidelberg, 2001. Springer-Verlag.

[14] R. R. Selvaraju, M. Cogswell, A. Das, R. Vedantam, D. Parikh, and D. Batra. Grad-cam: Visual explanations from deep networks via gradient-based localization. *International Journal of Computer Vision*, 128(2):336–359, Oct 2019.

[15] K. Simonyan, A. Vedaldi, and A. Zisserman. Deep inside convolutional networks: Visualising image classification models and saliency maps, 2014.

[16] A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, u. Kaiser, and I. Polosukhin. Attention is all you need. In *Proceedings of the 31st International Conference on Neural Information Processing Systems*, NIPS'17, page 6000–6010, 2017.

[17] C.-K. Yeh, J. S. Kim, I. E. Yen, and P. Ravikumar. Representer point selection for explaining deep neural networks. NIPS'18, 2018.

Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] We include a discussion in the appendix(as supplementary material).
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] We include a discussion in the appendix(as supplementary material).
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] Section 3.1 states our assumptions.
   (b) Did you include complete proofs of all theoretical results? [Yes] Section 3.1 provides a full proof.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] All code to reproduce these results is publicly available on Github. URL suppressed for anonymous review.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] Details are provided in the appendix (as supplementary material).)
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [No] The only applicable experiment is section 4.2. However, since the exact numbers vary extensively based on the random corruption, a meaningful error bar will require too many runs and thus too computational extensive.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] Details are provided in the appendix.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes] Citations [8],[10], and [3].
   (b) Did you mention the license of the assets? [No] Not Applicable. All datasets used are public datasets.
   (c) Did you include any new assets either in the supplemental material or as a URL? [Yes] The code of our experiments is publicly available on Github.URL suppressed for anonymous review.
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [No] Not applicable.The dataset used in this paper are all public available for research purposes.
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? **[TODO]**
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? **[TODO]**
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? **[TODO]**