DiPACE: Diverse, Plausible and Actionable Counterfactual Explanations

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Abstract: As Artificial Intelligence (AI) becomes integral to high-stakes applications, the need for interpretable and trustworthy decision-making tools is increasingly essential. Counterfactual Explanations (CFX) offer an effective approach, allowing users to explore "what if?" scenarios that highlight actionable changes for achieving more desirable outcomes. Existing CFX methods often prioritize select qualities, such as diversity, plausibility, proximity, or sparsity, but few balance all four in a flexible way. This work introduces DiPACE, a practical CFX framework that balances these qualities while allowing users to adjust parameters according to specific application needs. DiPACE also incorporates a penalty-based adjustment to refine results toward user-defined thresholds. Experimental results on real-world datasets demonstrate that DiPACE consistently outperforms existing methods Wachter, DiCE and CARE in achieving diverse, realistic, and actionable CFs, with strong performance across all four characteristics. The findings confirm DiPACE's utility as a user-adaptable, interpretable CFX tool suitable for diverse AI applications, with a robust balance of qualities that enhances both feasibility and trustworthiness in decision-making contexts.

1 INTRODUCTION

In recent years, the importance of interpretability in artificial intelligence (AI) has grown, especially in critical areas such as healthcare (Yagin et al., 2023; Shin et al., 2023), finance (Babaei et al., 2023; El Qadi et al., 2023; Zhu et al., 2023), cyber security (Kumar et al., 2023; Nadeem et al., 2023), disaster relief (Sanderson et al., 2023a; Sanderson et al., 2023b; Sanderson et al., 2024), and autonomous vehicles (Alatabani and Saeed, 2025; Starkey and Ezenkwu, 2023; Rawlley and Gupta, 2023), to name a few. Explainable AI (XAI) aims to provide transparency into AI models, fostering trust and supporting well-informed decisions (Mirzaei et al., 2023). Within XAI, counterfactual explanations (CFX) have become essential for exploring "what if?" scenarios, allowing users to understand how slight modifications to input features could lead to more desirable outcomes (Jiang et al., 2024). This approach not only provides insights into cause-and-effect relationships but also suggests actionable changes that can help users achieve different model outputs.

Effective counterfactual explanations should have at least four key qualities: diversity, plausibility, proximity, and sparsity (Guidotti, 2022). Diversity offers a range of alternative paths for achieving a desired outcome, providing users with different options (Mothilal et al., 2020). Plausibility ensures that counterfactuals are realistic and feasible, aligning with known data distributions and practical constraints (Del Ser et al., 2024). Proximity and sparsity further support actionable results by limiting counterfactuals to minimal, realistic changes that remain close to the original instance, making them more achievable and understandable (Wachter et al., 2018; Tsiourvas et al., 2024). These qualities are crucial for CFX to be practically valuable and applicable across diverse scenarios.

Despite recent advancements in CFX, most methods focus on only a subset of these attributes, often sacrificing one or more qualities. Wachter et al. (Wachter et al., 2018) introduced counterfactuals focused on proximity, ensuring minimal changes to the input but without addressing diversity or plausibility. DiCE (Mothilal et al., 2020) enhanced diversity by generating multiple counterfactuals that differ significantly from each other, providing users with options but often at the expense of plausibility and sparsity. DECE (Cheng et al., 2021) emphasized sparsity by limiting feature changes to the most influen-

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tial ones, but this restriction can hinder diversity and plausibility. Finally, Tsiourvas et al. (Tsiourvas et al., 2024) prioritized plausibility by aligning counterfactuals with real-world data, though this approach may reduce diversity and actionability. These approaches, while valuable for specific applications, lack a framework to balance all four qualities, limiting their adaptability to different real-world contexts where priorities may vary.

The choice of optimization technique also affects counterfactual generation. Gradient-based methods are popular due to their precision, as they can efficiently navigate complex loss landscapes and leverage gradient information for fine-tuned adjustments. However, these methods face two main limitations: they require access to model gradients, which limits them to differentiable models, and they are prone to getting stuck in local optima. To address these issues, researchers have explored alternative optimization techniques such as genetic algorithms (Schleich et al., 2021), shortest path algorithms (Poyiadzi et al., 2020), and mixed-integer programming (Carrizosa et al., 2024). While these methods are model-agnostic and can help avoid local minima, they often sacrifice precision due to the lack of direct gradient information. This trade-off between precision and adaptability restricts the effectiveness of existing CFX methods, which often cannot meet the needs of users who require both accuracy and a balanced combination of qualities.

To address these limitations, we propose DiPACE (Diverse, Plausible, Actionable Counterfactual Explanations), a practical and adaptable framework designed to optimize diversity, plausibility, proximity, and sparsity simultaneously. Unlike most existing methods, DiPACE allows users to adjust the emphasis on each quality according to specific application needs, making it highly suitable for real-world contexts where the priorities for counterfactual qualities may vary. DiPACE overcomes key limitations of current methods by making the following contributions:

(i) DiPACE's loss function is explicitly designed to balance diversity, plausibility, proximity, and sparsity. By allowing users to adjust the weights of each quality, it offers flexibility across different applications, addressing the issue of limited adaptability in existing methods.

(ii) To address the local optima challenges associated with gradient-based optimization, DiPACE integrates a perturbation mechanism that enables exploration beyond local minima. This retains the precision benefits of gradient-based methods while reducing the risk of suboptimal solutions, bridging the gap between gradient-based precision and model-agnostic flexibility.

(iii) DiPACE supports the specification of mutable and immutable features, acceptable ranges, and directional constraints for feature changes. These configurable options ensure that counterfactuals are not only feasible but also aligned with real-world requirements, overcoming the practical limitations of current methods that lack flexible constraint handling.

Additionally, we introduce DiPACE+, an enhanced version of DiPACE that incorporates penalty terms to further refine counterfactuals based on user-defined thresholds. By enforcing penalties for deviations from these thresholds, DiPACE+ enables more aggressive optimization tailored to specific application needs, making it suitable for scenarios where particular qualities are prioritized.

Through experiments on real-world datasets, we demonstrate that DiPACE offers a flexible, balanced solution for counterfactual explanations, making it a valuable tool for applications in AI where interpretability and practical adaptability are critical.

2 METHODOLOGY

2.1 DiPACE Framework

The primary goal of the DiPACE framework is to generate a set of counterfactual (CF) instances that differ in their predicted outcome from a given query instance while balancing multiple desirable qualities: diversity, plausibility, proximity, and sparsity. These qualities ensure that the CFs are realistic, provide a range of actionable options, and are feasible to implement in real-world applications. To achieve this balance, DiPACE optimizes a loss function that is a weighted combination of terms for each quality.

Let n denote the number of features in the query instance x^q, and let the CF set C represent a set of candidate counterfactuals. The loss function combines the following components:

- **Prediction Loss (L_{pred}).** Ensures that each CF in C results in the desired change in model outcome from that of the query instance.
- **Diversity Loss (L_{di}).** Promotes diversity among CF instances by maximizing the differences between them, offering users multiple actionable options.
- **Plausibility Loss (L_{pl}).** Encourages CFs to stay close to the distribution of the observed data, enhancing their feasibility and trustworthiness.

- **Proximity Loss** (L_{pr}). Minimizes the magnitude of change required to transform the query instance into each CF, ensuring interpretability.
- **Sparsity Loss** (L_{sp}). Limits the number of feature changes, making each CF more actionable by keeping modifications minimal.
- **Categorical Loss** (L_{cat}). Maintains the integrity of categorical features, ensuring that one-hot encoded variables sum to 1 for valid CF representation.

DiPACE uses gradient descent to optimize the weighted sum of these losses, requiring access to the model gradients. To mitigate the common issue of local optima in gradient-based optimization, DiPACE incorporates a perturbation mechanism, allowing CFs to explore a wider solution space when stuck at suboptimal points. DiPACE+ further refines this approach by applying penalty adjustments for CFs that do not meet user-defined thresholds for plausibility, proximity, or sparsity, enabling more aggressive optimization when specific qualities are prioritized.

Algorithm 1 outlines the steps for generating CFs in DiPACE and DiPACE+.

Algorithm 1: DiPACE and DiPACE+.

Input: Query Instance x^q, Model f, Hyperparameters θ
parameter : Learning rate α, Weights λ, Thresholds τ, Scale Factors γ, Maximum Iterations μ, Maximum Perturbation Attempts δ
Output: Counterfactual Set C
Let iteration count $t = 0$, perturbation count $p = 0$, counterfactual set $C \leftarrow \mathcal{N}(0,1)^{n \cdot len(x^q)}$.
while $t < \mu$ *or* $ld \geq \tau_{ld}$ **do**
  Compute loss components L_{pred}, L_{di}, L_{pl}, L_{pr}, L_{sp}, L_{cat}.
  if *DiPACE+* **then**
    if $L_i \in L_{pl}$, L_{pr}, $L_{sp} > \tau_i$ **then**
      $L_i \leftarrow L_i(1+\gamma_i)$;
    end
    if $L_{di} < \tau_{di}$ **then**
      $L_{di} \leftarrow L_{di}(1-\gamma_{di}$
    end
  end
  Compute total loss $L \leftarrow L_{pred} + \lambda_1 \cdot (1 - L_{di}) + \lambda_2 \cdot L_{pl} + \lambda_3 \cdot L_{pr} + \lambda_4 \cdot L_{sp} + L_{cat}$.
  Compute gradients of L w.r.t C.
  Update C with gradient descent with learning rate α.
  Apply user-defined constraints.
  Compute loss difference $ld \leftarrow L_t - L_{t-1}$.
  if $t \geq \theta$ *or* $ld < \tau_{ld}$ **then**
    break
  end
  Increment t.
end
while $L < \tau_{pert}$ *and* $p < \delta$ **do**
  Perturb C by adding $\mathcal{N}(0, \gamma_{pert})$.
  Go to step 2.
  if $L \leq \tau_{pert}$ **then**
    return C
  end
  Increment p.
end
return *C with lowest L*

2.2 Loss Function

The DiPACE loss function is designed to balance diversity, plausibility, proximity, and sparsity, ensuring feasible and realistic counterfactual explanations (CFX). Additionally, it includes terms for prediction loss to ensure valid counterfactuals and categorical loss to handle categorical variables accurately. Recognizing that users may prioritize certain characteristics depending on the application, we introduce a set of weights λ for each characteristic, allowing for customizable tuning of the results. The overall loss function for DiPACE is given by Equation 1.

$$L = L_{pred}(f(c_i), y) + \lambda_1 \cdot (1 - L_{di}(C)) + \lambda_2 \cdot L_{pl}(C, X) + \lambda_3 \cdot L_{pr}(C, x^q) + \lambda_4 \cdot L_{sp}(C, x^q) + L_{cat}(C) \tag{1}$$

where $c_i \in C$ is a counterfactual instance in the set C of generated counterfactuals, and $x_i \in X$ is an observed instance in the original dataset. The query instance is represented by x^q.

In DiPACE+, additional penalties are introduced for greater control over how strictly the generated counterfactuals adhere to user-defined thresholds for plausibility, proximity, and sparsity. For each characteristic $L_i \in \{L_{pl}, L_{pr}, L_{sp}\}$, if its computed value exceeds a user-defined threshold τ, a penalty is applied to enforce a stronger emphasis on this characteristic, as shown in Equation 2.

$$L_i = \begin{cases} L_i, & \text{if } L_i \leq \tau \\ L_i\,(1+\gamma), & \text{otherwise.} \end{cases} \tag{2}$$

For diversity, since we aim to maximize this characteristic rather than minimize it, the penalty is applied by subtracting from the diversity term when it falls below the threshold, as in Equation 3.

$$L_{di} = \begin{cases} L_{di}, & \text{if } L_{di} \geq \tau \\ L_{di}\,(1-\gamma), & \text{otherwise.} \end{cases} \tag{3}$$

where γ is the penalty scale factor, and L_i refers to the loss term for each component. This penalty mechanism in DiPACE+ allows for more aggressive optimization when specific qualities—like proximity, sparsity, or plausibility—are prioritized, enhancing DiPACE's flexibility for real-world applications.

2.2.1 Diversity

Diversity encourages a range of unique, actionable counterfactuals by maximizing the differences between CF instances. We follow the diversity measurement proposed by Mothilal et al. (Mothilal et al., 2020), calculating diversity as the negative determinantal point process (DPP) of a matrix of pairwise distances D_{ij} between CF instances $c_i \in C$. This DPP approach promotes a broad set of possible outcomes by increasing the average pairwise distance among instances.

$$L_{di} = dpp\left(\frac{1}{1+\sum_{l=1}^{n}\left|c_{il}-c_{jl}\right|}\right) \tag{4}$$

2.2.2 Plausibility

Plausibility ensures that counterfactuals resemble realistic data points by keeping them close to instances in the observed dataset X. Following the approach of Dandl et al. (Dandl et al., 2020), we compute plausibility as the normalized average distance between each CF instance and its nearest k observed instances, encouraging CFs that align with the data distribution.

$$L_{pl} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{1}{k}\sum_{j=1}^{k}\frac{|c_i - x_j| - d_{min}}{d_{max}-d_{min}+\varepsilon}\right) \tag{5}$$

where m is the number of CFs in the set, d_{min} and d_{max} are the minimum and maximum distances among the k nearest observed instances, and ε is a small constant to avoid division by zero.

2.2.3 Proximity

Proximity promotes interpretability by keeping CFs close to the query instance, minimizing the changes needed to achieve the desired outcome. We calculate proximity as the mean element-wise absolute difference between each feature of the query instance x^q and the CF instances $c_i \in C$, following the approach of Wachter et al. (Wachter et al., 2018).

$$L_{pr} = \frac{1}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}\frac{\left|c_{ij}-x_j^q\right|}{w} \tag{6}$$

where w is a weighting vector to control the influence of each feature on proximity based on the inverse median absolute deviation (MAD).

2.2.4 Sparsity

Sparsity encourages minimal changes between the query instance and each CF, promoting actionable and interpretable results. We measure sparsity as the count of features in each CF instance c_i that differ from the query instance x^q, averaged across the set C.

$$L_{sp} = \frac{1}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}\mathbb{1}(|c_{ij}-x_j^q| \leq \varepsilon) \tag{7}$$

where $\mathbb{1}(\cdot)$ is an indicator function that equals 1 when c_{ij} differs from x_j^q by more than ε and 0 otherwise.

2.2.5 Handling Categorical Variables

Handling categorical variables in counterfactual explanations is challenging due to their discrete nature. To maintain the validity of one-hot encoded categorical features, we enforce a linear equality constraint in the loss function, ensuring that all levels of each categorical variable sum to 1. This constraint iterates over each categorical variable and penalizes any deviation from a valid one-hot encoded representation.

$$L_{cat} = \sum_{v \in cat}\sum_{i=1}^{m}\left(\left(\sum_{j=v_{start}}^{v_{end}} c_{ij}\right)-1\right)^2 \tag{8}$$

where $v \in cat$ represents the range of indices for each categorical variable, and v_{start} and v_{end} indicate the first and last indices in the one-hot encoding of each categorical feature.

2.3 Optimization

To minimize our loss function, we employ the Adam gradient descent optimizer, chosen for its efficiency in navigating complex, high-dimensional loss landscapes and its ability to incorporate user-defined constraints. Adam allows for adaptive learning rates, which enhances the precision and stability of the optimization process in finding high-quality CFX.

However, gradient-based optimization is prone to becoming trapped in local optima, especially in high-dimensional spaces. To address this, we introduce a perturbation mechanism. If the overall loss exceeds a user-defined threshold after a certain number of iterations, we perturb the CF by adding random noise to each feature that significantly deviates from the original instance. This noise is sampled from a normal distribution and scaled by a user-defined factor, encouraging exploration of alternative solutions that may escape local minima.

The optimization process stops under two conditions: (1) when the overall loss reaches the user-defined threshold, indicating a sufficiently optimized solution, or (2) when a maximum number of perturbation attempts have been made without further reduction in the loss. This approach ensures that the optimization converges efficiently while retaining flexibility in finding realistic, actionable CFs.

2.4 User Constraints

While optimizing for proximity, sparsity, plausibility, and diversity helps ensure that counterfactuals (CFs) are realistic and feasible, additional real-world restrictions may apply in specific contexts. The DiPACE framework allows users to define these custom constraints, tailoring CF generation to meet application-specific needs and making the explanations more actionable.

In the DiPACE framework, users can specify the following constraints:

- **Features to Vary.** Specifies which features may be adjusted. This is useful in cases where only certain features can feasibly be changed (e.g., adjusting financial inputs while leaving demographic data constant). *Default: all features are allowed to vary.*
- **Immutable Features.** Specifies which features must remain unchanged, accommodating scenarios where some features are fixed (e.g., legal or physical constraints). *Default: no features are set as immutable.*
- **Feature Ranges.** Defines acceptable value ranges for certain features, ensuring that CFs remain within realistic boundaries. *Default: features can range between the minimum and maximum value in the observed data.*
- **Feature Directions.** Specifies if a feature can only increase or decrease. This constraint is useful for features where only unidirectional change is feasible (e.g., increasing years of experience but not decreasing it). *Default: features are allowed to vary in both directions.*

These constraints empower users to generate CFs that are not only realistic but also contextually relevant, enhancing the practical utility of the DiPACE framework.

2.5 Datasets

To evaluate the DiPACE framework, we use two datasets from the UCI Machine Learning Repository, each representing a real-world scenario where actionable interventions could realistically influence the outcome. These datasets cover distinct problem domains, allowing us to demonstrate DiPACE's effectiveness across different types of data and decision contexts.

Table 1: Description of the Heart Disease Dataset.

Feature	Type	Values
Age	Cont	29-77
Resting Blood Pressure (RBP)	Cont	94-200
Cholesterol (Chol)	Cont	126-564
Maximum Heart Rate (MHR)	Cont	71-202
ST Depression (STD)	Cont	0-6.2
Sex	Cat	1 or 0
Chest Pain Type (CP)	Cat	1-3
Fasting Blood Sugar (FBS)	Cat	1 or 0
Rest ECG (RECG)	Cat	0-3
Exercise Induced Angina (EA)	Cat	1 or 0
Slope	Cat	1-3
Major Vessels Coloured By Flourosopy (CA)	Cat	0-3
Thal	Cat	0-3
Class	Cat	1 or 0

The selected datasets are as follows:

- **Heart Disease Dataset** (Janosi et al., 1988)**.** This dataset contains 303 instances with 13 features, of which 5 are continuous and 8 are categorical, as described in Table 1. The target variable is binary, indicating the presence or absence of heart disease. This dataset is well-suited for counterfactual analysis, as many features (e.g., cholesterol level, blood pressure) represent factors that can be modified to reduce disease risk.
- **Credit Approval Dataset** (Quinlan, 2014)**.** This dataset consists of 690 instances with 14 features, 4 of which are continuous and 10 are categorical, as described in Table 2. The binary target variable indicates whether a credit application is approved or denied. This dataset provides a relevant test case for counterfactual explanations, as certain features (e.g., income, debt-to-income ratio) can feasibly be adjusted by applicants to improve their approval chances.

Our selection prioritizes datasets that provide realistic examples of CFX applications, over concerns with dataset dimensionality or size. DiPACE is minimally affected by dataset size, as it requires only the query instance and the k nearest instances for evaluating plausibility, reducing dependency on the full dataset. Additionally, each of DiPACE's metrics is normalized by the number of features, ensuring that

Table 2: Description of the Credit Approval Dataset.

Feature	Type	Values
Age	Cont	13.75-80.25
Debt	Cont	0-28
Years Employed (YE)	Cont	0-28.5
Income (Inc)	Cont	0-100k
Sex	Cat	1 or 0
Marital Status (MS)	Cat	1 or 0
Bank Customer (BC)	Cat	1 or 0
Industry (Ind)	Cat	0-13
Prior Default (PD)	Cat	1 or 0
Employed (Emp)	Cat	1 or 0
Credit Score (CS)	Cat	0-6
Driving License (DL)	Cat	1 or 0
Citizen (Cit)	Cat	0-2
Class	Cat	1 or 0

performance remains consistent regardless of the dimensionality or size of the data. This focus on realistic applications allows us to demonstrate DiPACE's utility in real-world scenarios, particularly its ability to deliver actionable counterfactuals in scenarios where meaningful changes to outcomes can be achieved.

2.6 Experimental Setup

We conducted our experiments on a 1.4 GHz Quad-Core Intel Core i5 CPU with 8GB of RAM, using Python 3.9 and PyTorch 2.2.2 on macOS Sonoma 14.4. To ensure reproducibility, we set a random seed of 42 for both NumPy and PyTorch.

2.6.1 Predictive Model

The predictive model used in our experiments is a fully connected neural network with an input layer, a 64-neuron hidden layer, a 32-neuron hidden layer, and an output layer with sigmoid activation. This specific architecture was selected for simplicity, as any differentiable model could function similarly within the DiPACE framework.

2.6.2 Evaluation Metrics

We quantitatively evaluate DiPACE+ using four core metrics—diversity, plausibility, proximity, and sparsity—without MAD weighting, providing insight into how well DiPACE+ balances these qualities relative to alternative approaches. Additionally, we measure counterfactual prediction confidence to assess the likelihood of correctly reversing the classification, offering further perspective on counterfactual quality.

2.6.3 Hyperparameter Tuning

Hyperparameters were optimized via grid search to identify the best-performing configurations. We used consistent λ values of 0.5 for both datasets after testing values in the range of 0.3–1.0. The optimized values for other hyperparameters are as follows:

- γ_{pen} set at 0.1 (range: 0.1–0.5)
- γ_{pert} set at 0.5 (range: 0.3–0.7)
- τ_{div} set at 0.9 (range: 0.7–1.0)
- τ_{plaus} set at 1.5 for heart disease and 1.0 for credit approval (range: 0.6–2.0)
- τ_{prox} set at 0.5 for heart disease and 0.2 for credit approval (range: 0.1–0.7)
- τ_{spars} set at 0.4 for heart disease and 0.2 for credit approval (range: 0.1–0.7)
- τ_{pert} set at 1.0 for heart disease and 0.8 for credit approval (range: 0.5–1.5)

The learning rate was set to 0.005 after testing values from 0.001 to 0.1, and the maximum number of iterations was set to 100,000. The actual number of iterations required is shown in Fig. 1.

2.6.4 Comparative Algorithms

In our final experiment, we compare DiPACE+ with the original DiPACE and three state-of-the-art algorithms: Wachter (Wachter et al., 2018), DiCE (Mothilal et al., 2020), and CARE (Rasouli and Chieh Yu, 2024). Wachter is included as a foundational baseline in counterfactual generation, DiCE as a widely used CFX tool, and CARE as a recent multi-objective genetic optimization approach. Each algorithm is implemented using its respective published Python library.

3 RESULTS AND ANALYSIS

3.1 Loss Function Ablation Study

To evaluate the effectiveness of the proposed loss function in achieving balanced CFX, we conduct an ablation study of the four key characteristics: diversity, plausibility, proximity, and sparsity, as well as the confidence of the model in its counterfactual classification. The results, shown in Table 3, explore combinations of these characteristics to demonstrate their individual and collective impact on CF quality. Proximity is included in every combination, as it is fundamental to any CFX algorithm. We consider the

Table 3: Ablation Study of Loss Function Terms for Each Dataset.

	Div.	Plaus.	Prox.	Spars.	Conf.
			Heart Disease		
1	0.61	0.84	0.19	**0.23**	0.67
2	0.87	0.67	**0.15**	**0.23**	0.75
3	0.88	0.22	0.32	0.36	0.84
4	0.70	0.81	0.18	0.29	0.64
5	0.89	**0.20**	0.43	0.41	0.84
6	0.92	0.97	0.47	0.46	0.57
7	0.91	0.26	0.43	0.43	0.87
8	**0.95**	0.44	0.36	0.39	**0.88**
			Credit Approval		
1	0.79	0.47	0.14	0.19	0.70
2	0.84	0.74	0.17	0.23	0.74
3	0.93	0.16	0.22	0.26	0.77
4	0.01	0.54	**0.09**	**0.12**	0.66
5	0.91	0.21	0.17	0.21	0.68
6	**0.95**	0.93	0.27	0.28	0.57
7	0.91	0.10	0.22	0.26	**0.81**
8	0.92	**0.06**	0.18	0.20	0.73

following combinations: (1) Proximity, (2) Proximity and Diversity, (3) Proximity and Plausibility, (4) Proximity and Sparsity, (5) Proximity, Diversity, and Plausibility, (6) Proximity, Diversity, and Sparsity, (7) Proximity, Plausibility, and Sparsity, and (8) Proximity, Diversity, Plausibility, and Sparsity.

The results indicate that including all four characteristics (combination 8) achieves the most balanced CF set. For the heart disease dataset, this configuration yields a high diversity score of 0.95, a low plausibility score of 0.44, and relatively low proximity and sparsity scores of 0.36 and 0.39, respectively, along with a high confidence score of 0.88. Similarly, for the credit approval dataset, combination 8 achieves high diversity of 0.92, low plausibility of 0.06, and suitably low proximity and sparsity scores of 0.18 and 0.20, with a confidence score of 0.73.

The ablation study also reveals interactions between the different characteristics. For example, excluding certain characteristics often results in higher values for others, illustrating the flexibility of the proposed approach. In particular, plausibility is weakest in combination 6 (Proximity, Diversity, and Sparsity), where the lack of plausibility optimization can lead to less alignment with the data distribution. Additionally, proximity and sparsity scores tend to be lower when both characteristics are included, as sparsity generally supports closer CFs by reducing feature modifications. However, the inclusion of diversity can increase both proximity and sparsity scores due to the conflicting goals of promoting variation while keeping CFs similar to the original instance.

Notably, the proximity and sparsity values are generally lower and less variable for the credit approval dataset compared to the heart disease dataset. This difference may be attributed to the higher proportion of continuous features in the heart disease dataset, which can result in more pronounced changes in CFs. This finding highlights the importance of tuning hyperparameters, such as τ and δ, to suit the specific characteristics of each dataset.

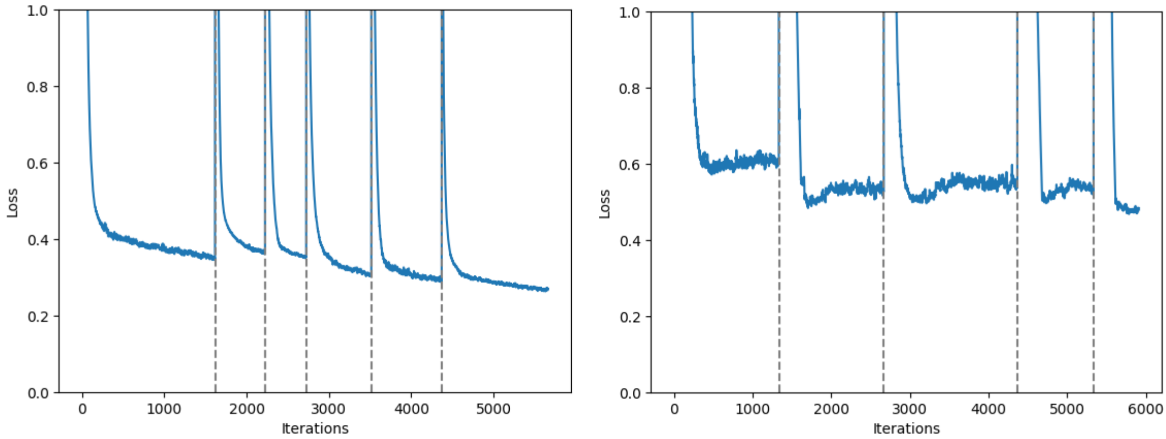
Overall, the results show that the inclusion of all four characteristics best promotes a balanced set of counterfactuals, reinforcing the versatility of DiPACE+ in generating feasible, actionable, and diverse CFs across datasets.

3.2 Optimization Strategy

Fig. 1 shows the loss curves for both datasets throughout the optimization process, illustrating the impact of perturbation on reaching a lower loss. The vertical dashed lines indicate points of perturbation. Following each perturbation, the loss values generally show a marked reduction, demonstrating the effectiveness of this approach in escaping local optima and progressing towards a more globally optimal solution. Without perturbation, the loss tends to plateau early, as observed in the convergence at the first perturbation point in each subfigure, highlighting the limitations of standard gradient descent.

Table 4 presents the values for diversity, plausibility, proximity, sparsity, and confidence for the CFs generated with and without perturbation. The results show that including perturbation consistently yields improved values for most metrics across both datasets. For instance, the diversity and confidence scores are higher with perturbation, which indicates that the CFs generated are both more varied and more likely to meet the desired outcome. Additionally, lower proximity and sparsity values are achieved, demonstrating that CFs are closer to the original instance and involve fewer feature changes, thus enhancing interpretability and feasibility. Furthermore, lower plausibility scores demonstrate that the inclusion of perturbations drives the optimization towards a CF outcome that is closer to existing instances in the dataset, and so are more realistic for potential implementation.

These results emphasize the impact of including perturbation in the gradient descent process for achieving a more globally optimal solution. By perturbing instances that show signs of converging prematurely, the optimization escapes local optima and continues to improve. This process allows DiPACE+ to achieve a desirable balance across key metrics,



(a) . (b) .

Figure 1: Loss Curves for (a) heart disease, and (b) credit approval. The vertical dashed lines represent points of perturbation.

Table 4: Results with and without Perturbation in the Optimization Strategy for Each Dataset.

	Div.	Plaus.	Prox.	Spars.	Conf.
			Heart Disease		
W/	**0.95**	**0.44**	**0.36**	**0.39**	**0.88**
W/o	0.92	0.63	0.49	0.45	0.83
			Credit Approval		
W/	**0.93**	**0.35**	**0.18**	**0.20**	**0.73**
W/o	0.91	0.44	0.20	0.22	0.71

yielding counterfactuals that are both feasible and actionable.

In contrast, existing methods of CF generation often rely on gradient-based optimization alone, which can result in suboptimal solutions due to convergence at local optima. Alternatively, some methods use model-agnostic optimization techniques like genetic algorithms or shortest-path algorithms, which avoid the pitfalls of local optima but sacrifice precision due to the lack of access to model gradients. Our approach demonstrates that gradient information can be leveraged effectively while mitigating convergence issues, achieving a solution that balances diversity, plausibility, proximity, and sparsity with improved confidence in the counterfactual outcome.

Overall, the perturbation-enhanced optimization strategy in DiPACE+ enables a more refined exploration of the solution space, combining the precision of gradient-based methods with the flexibility to escape local optima, as evidenced by the improved metrics observed in Table 4.

3.3 Qualitative Analysis

An example CF set generated by DiPACE+ is presented in Table 5 for heart disease and Table 6 for credit approval. These results illustrate how DiPACE+ adjusts key features to achieve the desired shift in prediction outcome. For heart disease, blood pressure (F2) is consistently reduced across most counterfactuals, reflecting its critical role in improving cardiovascular health. Maximum heart rate (F4) shows varied adjustments, suggesting an interaction with other health indicators to optimize the outcome. Cholesterol (F3) levels generally show slight increases, implying that the original values may be within acceptable limits, or that improvements in other features offset these changes. Adjustments to age (F1) are varied, indicating the model's adaptive approach based on the holistic health profile. Categorical features such as sex (F6) and cardiac conditions (F7–F12) show minimal changes, suggesting they may already be optimized or constrained due to limited flexibility.

Table 5: Example CF Set for Heart Disease.

	Query	CF Values				
Age	52	60	45	44	52	53
RBP	172	128	122	140	132	144
Chol	199	229	222	257	255	226
MHR	162	130	186	156	168	111
STD	0.5	2.6	0.0	0.5	0.0	0.8
Sex	1	1	1	1	1	1
CP	2	0	0	2	0	0
FBS	1	0	0	0	0	0
RECG	1	0	0	0	1	0
EA	0	1	0	0	1	1
Slope	2	1	2	2	2	2
CA	0	2	0	0	0	0
Thal	3	3	2	2	3	3
Class	1	0	0	0	0	0

For credit approval, age (F1) is generally in-

Table 6: Example CF Set for Credit Approval.

	Query	CF Values				
Age	23.5	48.1	27.7	42.2	24.8	37.4
Debt	2.75	3.0	2.4	5.0	6.0	2.5
YE	4.5	1.01	1.97	9.0	1.63	1.16
Inc	25	27	35	22	24	30
Sex	1	0	1	1	1	1
MS	1	1	1	1	1	1
BC	1	1	1	1	1	1
Ind	6	1	7	9	4	7
Race	2	0	4	1	4	4
PD	0	1	1	1	1	1
Emp	0	0	0	0	1	0
CS	0	0	0	0	3	0
DL	0	0	0	1	0	1
Cit	0	0	1	0	0	0
Class	0	1	1	1	1	1

creased, suggesting a preference for older applicants, possibly indicating financial stability. Debt levels (F2) vary, suggesting that it can be acceptable in certain cases depending on other factors. Years employed (F3) is mostly reduced, except for one instance with a significant increase, indicating that while employment stability is important, it interacts with other features in determining creditworthiness. Income (F4) is slightly adjusted, implying that it was initially near an acceptable threshold. Prior default (F10) consistently switches to 1, highlighting its significant importance in reversing predictions. Variations in industry (F8) and ethnicity (F9) indicate their potential influence on approval outcomes, with the variations in ethnicity indicating potential bias learned by the underlying model.

3.4 User Constraints

User constraints are applied to reflect realistic, domain-specific restrictions for both datasets. These constraints ensure that generated CFs remain feasible, relevant, and ethically aligned with real-world scenarios.

For the heart disease dataset, certain attributes are immutable as they are inherent to the patient or part of their medical history. Specifically:

- Sex, chest pain type (cp), and exercise-induced angina (exang) are immutable due to their fixed nature in a patient's medical profile.
- Age can only increase, as it is not realistic to decrease it in counterfactual analysis.
- Since maximum heart rate (thalach) is dependent on age (calculated as $200 - \text{age}$), its upper bound is set to 168 $(200 - 52)$ and lower bound to the dataset's minimum value of 94.
- Other lifestyle-related features (e.g., blood pressure, cholesterol) are mutable, reflecting the potential for modification through lifestyle changes or medical interventions.

Table 7: Quantitative Results of Applying User Constraints with Heart Disease Data.

	Div.	Plaus.	Prox.	Spars.	Conf.
Heart Disease					
Con.	0.75	0.73	**0.29**	**0.34**	0.80
Uncon.	**0.95**	**0.44**	0.36	0.39	**0.88**
Credit Approval					
Con.	0.16	0.78	**0.11**	**0.12**	0.62
Uncon.	**0.93**	**0.35**	0.18	0.20	**0.73**

For the credit approval dataset, specific features are constrained based on inherent or historical characteristics of the individual:

- Gender, ethnicity, and citizenship are immutable as they represent fixed personal attributes.
- Prior default is also immutable, as it reflects past financial behavior.
- Age and years employed can only increase, as these values realistically grow over time.
- For demonstration, we hypothetically constrain income to a maximum value of 100, reflecting a plausible earning limit based on qualifications and experience.

Table 7 shows quantitative performance comparisons with and without user constraints.

Applying these constraints impacts the quantitative results, as shown in Table 7. Notably, proximity and sparsity improve across both datasets when constraints are applied, as fewer features are allowed to change, leading to CFs that remain closer to the original instance. Diversity and plausibility decrease, especially in the credit approval dataset, where diversity drops from 0.93 to 0.16 and plausibility rises significantly to 0.78. This is due to the restricted range of changes, which limits variation and makes it challenging for CFs to align with typical instances in the data distribution. Confidence is slightly reduced in the constrained CFs, as fewer features are able to shift, making it harder for the CFs to meet all desired conditions for class reversal. For example, in the heart disease dataset, confidence drops from 0.88 to 0.80, reflecting that restricted features may limit the classifier's certainty in outcome changes.

Example CFs with the described user constraints applied are shown in Tables 8 and 9. In the heart disease example, immutable attributes (sex, chest pain

Table 8: Example CF Set for Heart Disease with User Constraints.

	Query	CF Values				
Age	52	57	52	58	52	54
RBP	172	150	138	140	138	124
Chol	199	196	196	211	256	258
MHR	162	163	163	157	156	150
STD	0.5	1.6	0.1	1.2	0.4	0.4
Sex	1	1	1	1	1	1
CP	2	2	2	2	2	2
FBS	1	0	0	1	0	0
RECG	1	1	0	0	0	0
EA	0	0	0	0	0	0
Slope	2	2	2	2	2	1
CA	0	0	0	0	0	0
Thal	3	2	2	2	2	3
Class	1	0	0	0	0	0

Table 9: Example CF Set for Credit Approval with User Constraints.

	Query	CF Values				
Age	23.5	50.8	31.3	69.2	50.8	35.2
Debt	2.8	2.3	1.1	5.0	2.3	3.4
YE	4.5	4.8	4.5	6.5	4.5	8.2
Inc	25	11	25	22	51	29
Sex	1	1	1	1	1	1
MS	1	1	1	1	1	1
BC	1	1	1	1	1	1
Ind	6	13	13	6	13	13
Race	2	2	2	2	2	2
PD	0	0	0	0	0	0
Emp	0	0	1	1	0	0
CS	0	0	3	7	0	7
DL	0	0	0	0	0	1
Cit	0	0	0	0	0	0
Class	0	1	1	1	1	1

type) remain unchanged, and age is adjusted only upward. Similarly, in the credit approval example, immutable attributes (gender, ethnicity, citizenship, and prior default) are preserved, and features such as age and years employed increase in line with this real world constraint.

Overall, these results demonstrate that DiPACE+ effectively balances the need for actionable counterfactuals with user-defined constraints. While diversity and plausibility may be weaker due to fixed attributes, the model retains flexibility in generating CFs that meet realistic constraints, demonstrating its applicability for real-world, constraint-based scenarios.

Table 10: Comparison of DiPACE+ and DiPACE with Previous Work.

	Div.	Plaus.	Prox.	Spars.	Conf.
Heart Disease					
DiPACE+	**0.95**	**0.44**	0.36	0.39	0.88
DiPACE	0.88	0.58	0.44	0.43	0.83
Wachter	0.31	0.83	**0.02**	**0.17**	0.75
DiCE	0.82	0.96	0.16	0.25	0.88
CARE	0.77	0.85	0.44	0.48	**0.89**
Credit Approval					
DiPACE+	**0.93**	**0.35**	0.18	0.20	0.73
DiPACE	0.92	0.57	0.18	0.21	**0.75**
Wachter	0.35	0.74	**0.03**	**0.10**	0.56
DiCE	0.84	0.69	0.12	0.28	0.64
CARE	0.68	0.63	0.18	0.56	0.66

3.5 Comparison of Algorithms

To evaluate the quality of DiPACE+, we benchmark its performance against DiPACE and three state-of-the-art CFX algorithms: Wachter, DiCE, and CARE. The comparative results are presented in Table 10. Across both datasets, DiPACE+ achieves the highest scores in diversity and plausibility, with strong performance in proximity and sparsity, indicating a balanced generation of CFs that are diverse, realistic, and reasonably close to the original instance.

The Wachter algorithm obtains the lowest diversity scores but outperforms all other methods in proximity and sparsity. This result is consistent with Wachter's design, which optimizes only for proximity, resulting in highly similar CFs that minimize feature changes. However, this focus on proximity limits diversity and, as observed, leads to weaker plausibility, as the generated CFs may not align well with realistic instances in the observed data distribution.

DiCE and CARE perform moderately well in diversity and proximity, though both score lower than DiPACE+ in diversity. DiCE achieves higher proximity values than CARE, but both perform less effectively in plausibility, yielding CFs that are less similar to observed instances. This highlights the importance of explicitly incorporating plausibility into the loss function for generating realistic CFs. DiPACE+'s enhanced plausibility indicates a greater alignment with real-world data patterns, making its CFs more actionable and relevant for practical applications.

For all metrics except confidence, DiPACE+ consistently outperforms DiPACE, demonstrating the effectiveness of its additional penalty term in balancing key characteristics, resulting in CFs that are both realistic and close to the query instance. However, the inclusion of this penalty term introduces a slight trade-off in confidence, as observed by a modest decrease compared to DiPACE. This suggests that DiPACE+ prioritizes CF diversity and feasibility over prediction certainty, which may be desirable depending on application needs.

Overall, DiPACE+ achieves the most balanced performance across the metrics, illustrating its ability to generate CFs that are diverse, realistic, and feasible, while maintaining reasonable confidence in the outcome. These results highlight DiPACE+ as a robust solution for CF generation in real-world contexts where multiple qualities, including plausibility and diversity, are essential for actionable insights.

4 CONCLUSION

This study introduces DiPACE and DiPACE+, novel algorithms for generating counterfactual explanations that achieve a balanced optimization of diversity, plausibility, proximity, and sparsity, advancing the field of counterfactual explanation (CFX). By integrating these characteristics into the loss function and using an optimization strategy that combines gradient descent with perturbations, our approach successfully escapes local optima, producing CF sets that are both realistic and actionable. Experimental results on heart disease and credit approval datasets demonstrate that DiPACE+ consistently outperforms existing CFX algorithms in achieving diverse and plausible CFs, particularly excelling in scenarios with complex interactions among features. The practical applications of DiPACE+ extend to various fields where actionable and realistic CFs are essential, such as healthcare, finance, and user-focused AI systems. For stakeholders like data scientists and machine learning engineers, DiPACE+ provides deeper insights into model behavior and potential biases, enhancing transparency and interpretability in critical decision-making applications.

Future work should aim to improve the convergence efficiency of the optimization strategy. While perturbations are effective for escaping local optima, they can increase convergence time; thus, exploring adaptive or hybrid optimization approaches may yield faster results. Additionally, extending DiPACE+ to handle more complex data types, such as time series and high-dimensional image data, would broaden its applicability. Future research could also focus on developing evaluation metrics that more precisely capture the trade-offs among diversity, plausibility, proximity, and sparsity, as well as assessing DiPACE+'s impact on user trust and understanding in interactive settings.

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