Q-FIT: The Quantifiable Feature Importance Technique for Explainable Machine Learning

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Abstract
We introduce a novel framework to quantify the importance of each input feature for model explainability. A user of our framework can choose between two modes: (a) global explanation: providing feature importance globally across all the data points; and (b) local explanation: providing feature importance locally for each individual data point. The core idea of our method comes from utilizing the Dirichlet distribution to define a distribution over the importance of input features. This particular distribution is useful in ranking the importance of the input features as a sample from this distribution is a probability vector (i.e., the vector components sum to 1), which provides a quantifiable explanation of how significant each input feature is to a model’s output. This quantifiable explainability differentiates our method from existing feature-selection methods, which simply determine whether a feature is relevant or not. Furthermore, a distribution over the explanation allows to define a closed-form divergence to measure the similarity between learned feature importance under different models. We use this divergence to study how the feature importance trade-offs with essential notions in modern machine learning, such as privacy and fairness. We show the effectiveness of our method on a variety of synthetic and real datasets, taking into account both tabular and image datasets.

1 Introduction
The European Union’s General Data Protection Regulation (GDPR) imposes several important requirements on algorithmic design [20]. Among them, explainability aims to protect the right of citizens to receive an explanation for algorithmic decisions [8]. With the goal of gaining such explainability, there has been a large number of methods developed for explaining why black-box machine learning models produce particular outputs (e.g., [19] and [13] among many). In this paper, the particular type of explainability we focus on is to explain which of the input features are relevant or important to a machine learning model for a given task.

Broadly speaking, there are two levels at which one could gain such input feature explainability. The first level is global, where the goal is to identify the most relevant features for a given task globally across all the data instances [10, 11, 6, 9, 12]. When the data exhibit a large variability, using global explanation methods is not suitable, as the learned feature importance at the global level is just the same for all data samples. Hence, these methods cannot provide the instance-wise, variable explanations. To overcome this limitation, the second level is local, where the goal is to identify the most relevant features for each data sample separately, resulting in instance-wise explanation [10].

In this paper, we propose a novel framework, the quantifiable feature importance technique (Q-FIT) for gaining the feature-additive explainability of complex machine learning models both globally and locally. Our method has the following benefits.

- Unlike existing feature selection methods, our method provides relative quantifiable feature importance. Our algorithm outputs a non-negative weight vector, which sums to 1, to express the significance of each feature.

- Unlike the previous methods which focus on either global or local explanations, we provide two explicit modes which respectively address each level of explainability.

- Our model is simple. For gaining global explanation, our model consists of just as many parameters as the input dimension. For gaining local explanation, we consider a simple multi-layer perceptron (MLP) to model the feature importance. Compared to INVASE [21] which requires three different neural networks, our model is significantly simpler and able to gain a similar level of quality in the instance-wise explanation as INVASE.

- Our method provides a distribution over the feature importance, which allows us to define a distance between feature importance distributions under different models. We showcase the usefulness of this aspect in quantifying the trade-offs between feature importance and fairness and privacy.

This paper is organised as follows. In Sec. 2 we introduce our method, Q-FIT. In Sec. 3 we highlight the similarity and dissimilarity between Q-FIT and other existing methods. In Sec. 4 we demonstrate the
effectiveness of our approach on several synthetic and real-world datasets.

2 Methods.
We first introduce the basic setup and our goal, then describe our method. We denote an $n$-element dataset $D = \{x_n, y_n\}_{n=1}^N$, where $x_n \in \mathbb{R}^D$ is an input datum and $y_n$ is its label (either discrete or continuous variables). The integer $D$ describes the number of features of the input data, and quantifying the importance of these features is the main subject of this work.

Our goal is to gain (a) global explanation: overall, which of the input features are important for the model to perform well in a classification task; and (b) local explanation: why the model $g$ outputs a particular class given an individual input $x$ and which of the input features for that piece of data are important to that decision.

2.1 The quantifiable feature importance technique (Q-FIT) for global explainability.
We introduce the feature importance vector $f \in \mathbb{R}^D$, a vector of random variables with the same dimension as the input features, as illustrated in the grey box (left half) in Fig. 1. We model the feature importance using the Dirichlet distribution with a parameter vector, $\alpha$:

$$f \sim \text{Dir}(\alpha).$$

Dirichlet distribution is a multivariate probability distribution which describes various multinomial distributions. In other words, it is a distribution over distributions. The motivation for this particular choice is that the sample of the distribution is a probability vector, where all elements of $f$ is non-negative and sum to 1, $\sum_{d=1}^D f_d = 1$. This property makes it natural to model a relative level of importance across different input features.

**Optimization framework.** How can we learn this distribution? What we aim is to identify the parameters of the Dirichlet distribution that maximize the data likelihood. We treat the feature importance vector as latent variables and integrate them out when computing the data likelihood under the model $g$.

\begin{equation}
\log p_g(D) = \log \int p_g(D, f) df.
\end{equation}

However directly integrating out the latent variables is intractable under complex models. We instead use an approximate distribution $q(f)$, which is supposed to mimic the distribution $p_g(f|D)$. Then we can rewrite the data log-likelihood as

$$\log p_g(D) = \int q(f) \log \frac{p_g(D, f)}{q(f)} df + D_{KL}[q(f)||p_g(f|D)],$$

where the second term on RHS is defined by $D_{KL}[q(f)||p(f|D)] = - \int q(f) \log \frac{p_g(f|D)}{q(f)} df$. Note that this term is intractable as we do not know the true posterior distribution over the latent variables $p_g(f|D)$. But this term is non-negative, so maximizing the first term on RHS, the so-called variational lower bound $L$, with respect to the distribution $q(f)$ also maximizes the data log-likelihood:

\begin{equation}
L := \int q(f) \log p_g(D|f) df - D_{KL}[q(f)||p(f)].
\end{equation}

Figure 1: **Global explanation** (in grey box, left half). To gain global explanation, we define an importance vector, assumed to be Dirichlet distributed. To learn the parameters of this distribution, we element-wise multiply the sample of this distribution by input features, which is fed into the model in question. The model’s prediction and the target determine the loss, used to update the parameters of Dirichlet distribution through back-propagation (grey dotted line). **Local explanation** (in blue box, right half). To gain instance-wise, local explanation, we define an importance network (blue box) whose output follows Dirichlet distributions, and learn the parameters via back-propagation (blue dotted line). Note that the back-propagation does not affect the model in question. Also, note that we do not train the importance vector and the importance network simultaneously.
**Parameterization.** Each of the terms in $L$ is defined as follows. We model the approximate posterior $q(f) = \text{Dir}(f|\alpha)$, and the prior over $f$ by $p(f) = \text{Dir}(f|\alpha_0)$. While using the Dirichlet distribution for the posterior is our modelling choice as mentioned earlier, using another Dirichlet distribution for prior is to obtain a closed-form KL divergence. We model the conditional distribution $p_y(D|f)$ by the model $g_\theta$ of our interest, where $\theta$ is fixed and the model input is now weighted by the feature importance.

**Sampling vs. point estimate.** As illustrated in Fig. 1 (grey box), we generate samples for the feature importance $\{\hat{f}_i\}_{i=1}^I$, and multiply the samples with the input features, which we feed into the trained model $g$. The prediction made by $g_\theta$ and the target variable are then used for computing our loss, which is negative $L$. Using the samples, we express $L$ via Monte Carlo approximation

$$L_{MC} \approx \frac{1}{I} \sum_{i=1}^I \log p(D|\hat{f}_i) - D_{KL}[q(f)||p(f)].$$

In the case of classification, the log conditional probability becomes $\log p(D|f_i) \approx \sum_{n=1}^{N} \sum_{k=1}^{K} y_{n,k} \log \tilde{y}_{n,k,i}(\alpha)$, where the prediction from the trained model $g$ is denoted by $\tilde{y}_{n,k,i}(\alpha) = g_k(\hat{f}_i \circ x_{n_i})$, with $k$ being the index for target (or output of $g$) dimension, $i$ being the index for the Dirichlet samples, and $n$ being the index of datapoints.

A computationally cheap approximation to eq. 2.3 is using the analytic mean expression of the Dirichlet random variables, resulting in

$$L_M \approx \log p(D|\overline{f}) - D_{KL}[q(f)||p(f)],$$

where $\overline{f} = \frac{\overline{\alpha} \circ \alpha}{\sum_{k=1}^d \alpha_k}$.

Computing this does not require sampling and propagating gradients through the samples, which significantly reduces the run time. In our experiments, we use both approximations to $L$, where the specifics on each approximation are included in the Supplementary material.

**2.2 Local instance-wise explainability via the importance network**

Local explainability differs from the global one in that feature importance is evaluated for each data sample. Then in contrast to the global explanations, in the local setting we introduce a vector of random variable of feature importance for each datapoint $n$, i.e., $f_n \in \mathbb{R}^D$.

We model the feature importance using the Dirichlet distribution with parameters $\alpha$,

$$f_n \sim \text{Dir}(\alpha_n).$$

To account for the individual predictions, we extend the approach from the previous section to introduce an importance network. Importance network takes a data point as an input and outputs the Dirichlet parameter vector, $\alpha_n$, for the particular data point. Subsequently, we sample a multinomial distribution which becomes an importance vector for the data point. Subsequent steps are the same as in the global case, that is we perform scalar product of the importance vector with the data and feed it to the original model. Graphical depiction of this process is shown in the Fig. 1.

Formally, we treat the feature importance vector as latent variables and integrate them out when computing the data log-likelihood under the model $g$,

$$\log p_y(D) = \log \int_{\hat{f}} \cdots \int_{f_N} p_y(D, f_1, \cdots, f_N) df_1 \cdots df_N.$$

As in the global feature learning, we use an approximate distribution $q(f_1, \cdots, f_N)$, with which we rewrite the data log-likelihood as

$$\log p_y(D) = \int q(f_1, \cdots, f_N) \log \frac{p_y(D, f_1, \cdots, f_N)}{q(f_1, \cdots, f_N)} df_1 \cdots df_N + D_{KL}[q(f_1, \cdots, f_N)||p_y(f_1, \cdots, f_N|D)]$$

For the sake of tractability, we assume both the posterior and prior distributions are factorizing: $q(f_1, \cdots, f_N) = q(f_1) \cdots q(f_N)$ and $p(f_1, \cdots, f_N) = p(f_1) \cdots p(f_N)$. Under this assumption together with the assumption that our data is i.i.d., the variational lower bound becomes:

$$L := \sum_{n=1}^{N} \bigg[ \int q(f_n) \log p_y(D_n|f_n) df_n - D_{KL}[q(f_n)||p(f_n)] \bigg].$$

As in the global feature learning, we model the approximate posterior $q(f_n) = \text{Dir}(f_n|\alpha_n)$, and the prior over $f$ by $p(f_n) = \text{Dir}(f_n|\alpha_0)$ where the parameters are $\alpha_0$ same for all $n$. We model the conditional distribution $p_y(D_n|f_n)$ by the model $g_\theta$ of our interest, where $\theta$ is fixed and the model input is now weighted by the feature importance different for each input.

For each $n$, we generate samples for the feature importance $\{\hat{f}_{n,i}\}_{i=1}^I$, and multiply the samples with the input features, which we feed into the trained model $g$. The prediction made by $g_\theta$ and the target variable are then used for computing our loss, which is negative $L$. Using the samples, we express $L$ via Monte Carlo approximation

$$L_{MC} \approx \sum_{n=1}^{N} \bigg[ \frac{1}{I} \sum_{i=1}^I \log p(D_n|\hat{f}_{n,i}) - D_{KL}[q(f_n)||p(f_n)] \bigg].$$
In the case of classification, the log conditional probability becomes \( \log p(D_n | f_{n,i}) \approx \sum_{k=1}^{K} y_{n,k} \log \hat{y}_{n,k,i}(\alpha) \), where the prediction from the trained model \( g \) is denoted by \( \hat{y}_{n,k,i}(\alpha) = \hat{y}_k(f_{n,i} \circ x_n) \), with \( k \) being the index for target (or output of \( g \)) dimension, \( i \) being the index for the Dirichlet samples, and \( n \) being the index of datapoints.

Similarly to the global case, we test both evaluating the full posterior and using the analytic mean.

2.3 Divergence for measuring similarity under Q-FIT

The Q-FIT’s output, the Dirichlet distribution is an exponential family distribution, which we can write in terms of an inner product between the sufficient statistic:

\[
D \left( \alpha \right) = \langle \eta | \alpha \rangle - \alpha \cdot \beta, E_p[T(f)]
\]

where \( \eta(\alpha) = \log \int h(f) \exp((\eta(\alpha), T(f))) df \) is the log-partition function, and \( h(f) \) is the base measure. In case of the Dirichlet distribution, the natural parameter equals the parameter \( \eta(\alpha) = \alpha \), yielding a canonical form.

We are interested in measuring how similar feature importance is under two different models. We denote the two Dirichlet distributions for feature importance obtained under the two models by \( p \) and \( q \), respectively, where \( p \)'s parameters are \( \alpha = [\alpha_1, \ldots, \alpha_D] \) and \( q \)'s are \( \beta = [\beta_1, \ldots, \beta_D] \). The good news is that under the exponential family distribution, popular divergence definitions such as the KL divergence \( D_{KL}(p||q) \) and the Bregman divergence \( B(q||p) \) can be expressed in terms of the log-partition function, its parameter, and the expected sufficient statistic:

\[
D_{KL}(p||q) = B(q||p) := E_p[T(f)] = A(\eta(\alpha)) - A(\eta(\beta)) - \langle \alpha - \beta, E_p[T(f)] \rangle,
\]

where \( E_p[T(f)] \) is the expected sufficient statistic under the distribution \( p \). Under the Dirichlet distribution, all of the three terms are in closed-form, where the log-partition function is defined by \( A(\eta(\alpha)) = \log \Gamma(\alpha_0) - \sum_{d=1}^{D} \log \Gamma(\alpha_d), A(\eta(\beta)) = \log \Gamma(\beta_0) - \sum_{d=1}^{D} \log \Gamma(\beta_d), \) and each coordinate of the expected sufficient statistic is defined by \( E_p[T(f_d)] = \psi(\alpha_d) - \psi(\sum_d \alpha_d), \) where \( \psi \) is the digamma function. This allows us to evaluate the KL divergence conveniently. We demonstrate how we take advantage of having this easy-to-evaluate divergence in practice and examine the results under Q-FIT and INVASE.

3 Related Work

In terms of perspectives on explanations, there are broadly two categories: feature-additivity and feature-selection. Feature additivity methods provide importance attributions per dimension, such that the sum of attributions matches the model output. Attribution-based methods such as Integrated Gradient, SmoothGrad, and LIME, as well as the game-theoretic approach, SHAP fall into this category. Feature selection methods select a subset of input features which produces a similar result to the case when the full set of input features is used. The size of the subset can be set in advance as in L2X, or chosen by balancing loss terms for sparsity and similarity of output (e.g. INVASE). Feature selection can be done globally or locally (instance-wise).

In terms of feature-additivity, the most closely related method is SHAP. We in fact found that the performance of our method and SHAP is very similar for gaining global explanations. This outcome is expected: if there exists a true feature importance, both methods will uncover it similarly if the characteristic function in SHAP uses the same objective function as ours (i.e., maximum likelihood). However our method not just outputs the point estimate of feature importance as in the SHAP case, but also outputs the distribution over the importance, which we can utilize for a further study using the learned feature importance as shown in Sec. [4]. The relative importance weight under Q-FIT method is also better captured as depicted as Fig. [4].

As the Q-FIT method measures instance-wise feature importance, it shares the goal with the L2X and INVASE. Unlike L2X, we do not require to know the number of important features per instance. This is particularly useful in the case of real-world datasets, as in practice we usually do not know how many features per instance a model relies on. Another difference is that L2X learns a distribution over the set of features by maximizing the mutual information between subsets of features and the response variable, while we learn the distribution over the feature importance by maximizing the variational lower bound. Compared to INVASE that consists of selector, predictor, and baseline networks, our method can be as simple as a vector of unknowns for global explainability. For local explainability, our method does need a neural network to learn the parameters of the Dirichlet distribution instance-wise, while the model complexity in this case is still far lower than that in INVASE.

Compared to L2X and INVASE, we output the level of importance rather than selecting features being important or not. INVASE outputs the probability for Bernoulli variables, but once \( p > 0.5 \), all the features are equally important. On the other hand, in our case, every value of \( \alpha \) matters, and these values allow us to quantify the importance. Also, our learned importance
of each feature is a function of other features’ importance (due to the sum-to-1 property), while each feature’s selection is independent of other feature’s selection in L2X and INVASE, as illustrated in Fig. 2.

The idea of using the Dirichlet distribution for learning the level of importance is previously presented in [2], where the Dirichlet distribution models the significance of the neurons in neural network models and the learned significance is used for a compression task. In this paper we use this distribution to provide the feature-additive explanation on the input features both globally and locally to understand the model at hand.

4 Experiments

4.1 Synthetic data We first test our method on six synthetic datasets. The first three binary synthetic datasets [7] are generated by an 11-dimensional input feature \( x \sim N(0, 1) \) and the associated label \( p(y = 1|x) = \frac{1}{1 + 10^x} \) and \( p(y = 0|x) = \frac{1}{1 + 10^{-x}} \) where the particular \( r \) is defined by

- Syn1: \( \exp(X_1X_2) \)
- Syn2: \( \exp(\sum_{i=3}^{11} X_i^2 - 4) \)
- Syn3: \( \exp(-100 \sin (2X_7) + 2|X_8| + X_9 + \exp(-X_{10})) \)

In the remaining three datasets, a label \( y \) depends on an alternating set of features:

- Syn4: if \( x_{11} < 0 \), a sample is generated from Syn1, and otherwise from Syn2.
- Syn5: if \( x_{11} < 0 \), a sample is generated from Syn1, and otherwise from Syn3.
- Syn6: if \( x_{11} < 0 \), a sample is generated from Syn2, and otherwise from Syn3.

Notice that the features of the two datasets do not overlap and we can uniquely distinguish the features which generated a given sample. We generate 10,000 samples for each dataset, using 80% for training and the rest for testing. Note that in case of Syn1-3, these features are static, while in the case of Syn4-6, the features are alternating. To make the evaluation holistic in terms of capturing all the aspects of the binary classification, we use the Matthews correlation coefficient (MCC) \[14\]. The key advantage of MCC is that it produces a high score only if the high percentage of negative data instances and a high percentage of positive data instances is correctly classified, regardless of the size of each class. While measures such as TPR (true positive rate) or FDR (false discovery rate) capture only some aspects of the confusion matrix, MCC includes all elements (TP, TN, FP, FN) with equal weight, thus removing the class imbalance problem.

In Table 1, we include three variations of the proposed method, global selection described in Sec. 2.1 and two ways to compute local explanations described in Sec. 2.2. The first one evaluates the full integral through sampling (which we denote by samp), while the second one uses a point estimate (which we denote by pe) computed analytically as a mean of the Dirichlet distribution parameters. In all of these variants, we first train a model, and then feed it to our framework where we freeze the model parameters, and only optimize Q-FIT’s parameters.

To summarize the results, all proposed and benchmark methods perfectly discover the features that generated Syn1 and Syn2. Q-FIT and L2X also perform well on the more challenging Syn3. The proposed method excels particularly in the local setting, on a more challenging datasets, where in all three datasets outperforms the existing methods by a substantial margin, 10-20 percentage points.

In selecting feature selection method, it is worth considering their advantages and disadvantages. The Q-FIT global is a method whose number of parameters is linear in the number of features, however it works only in the global setting. The local variants require an additional network which may however work better, also in the global setting (by averaging the importance over all the data points). In terms of performance, the sampling and point estimate Q-FIT produce similar results, however the shortcoming of the point estimate is that it produces the results with relatively high variance (please see Supplementary materials for summary results). On the other hand, sampling is more time-consuming due to evaluations required for each sample.

Notice also that in this experiment we test whether a feature is important or not but not how important it is. In the case of Syn1 and Syn2, each of the relevant features has the same weight. This is not the case for Syn3. However, it is clear that some features have higher weight than others. Unlike the previous methods, Q-FIT naturally and explicitly finds an importance of a feature as described in Fig. 2. We further demonstrate this strength in the real-world dataset experiment.

4.2 Real-world data In the experiments we consider both tabular and image data which come from real-world datasets.

Tabular Data We consider credit and adult datasets with tabular input features and binary labels. Adult dataset predicts whether income exceeds $50K a year based on census data, and credit dataset classi-
Learned importance
Shapley value
Selection probability
Q-FIT (global) 1.000 1.000 0.850 - - -
Q-FIT (inst, samp) 1.000 1.000 0.936 0.819 0.860 0.852
Q-FIT (inst, pe) 1.000 1.000 0.829 0.840 0.790 0.856
L2X 1.000 1.000 0.951 0.660 0.645 0.738
INVASE 1.000 1.000 0.810 0.573 0.500 0.361

Table 1: Synthetic datasets to detect ground truth features. The Syn1-3 datasets consists of a fixed set of globally invariant important features, while Syn 4-6 consists of varying sets of important features instance-wise. The average over 5 runs is reported. The higher MCC (Matthews correlation coefficient), the better. In Q-FIT, (inst, samp) means instance-wise explanation with sampling, while (inst, pe) means that with point estimate. Our method outperforms L2X and INVASE in 5 out of 6 synthetic datasets.

Figure 2: Learned feature importance using a dataset with input features $x \sim N(0, I)$ where $x \in \mathbb{R}^{10}$ and $p(y = 1|x) \propto \exp[-100\sin(2X_0) + 2|X_1| + X_2 + \exp(-X_3)]$, following [7]. Top: Our method uncovered the ground truth correctly with a different level of importance for the four features. Middle: SHAP performed similarly as ours. Bottom: INVASE’s selection probability (the probability of Bernoulli random variables) is all equal for selected features, giving less information about the feature importance than our method.

fies applicants for credit availability. This experiment consists of two parts. In the first part, we aim to find globally important features in the entire dataset. In the second part, we perform local feature search in a similar way to the experiment done on the synthetic datasets. As there is no known ground truth about the features, we evaluate the effectiveness of each method by selecting top $k$ features which are deemed most significant, and then performing the post-hoc classification task given these $k$ input features with removing the rest. In the global setting, $k$ features are fixed for the entire dataset, while in the local setting each sample can select a different set of $k$ features.

Q-FIT outputs a probability distribution which directly allows to identify top $k$ features. On the other hand, INVASE and L2X output binary decisions for feature importance. For global explanations, we average the output for all data points, thus creating global ranking of features in INVASE and L2X. For local explanations, in case of L2X we can specify $k$ relevant features. INVASE has no such option and thus, for the fairest comparison, we use the selection probability given by the selector network as a proxy of importance score. For a global explanation part, we also include SHAP. As shown in Table 2 (classification accuracy averaged over five independent runs), Q-FIT performs well in both tasks, with a bigger edge in global search. We found that local explanation search is significantly more challenging than the global one, which is reflected in the lower classification accuracy.

**MNIST Data** Following [7], we construct a binary dataset by gathering the 3 and 8 digit samples from MNIST. We then train Q-FIT, as well as L2X and INVASE models to select 4x4 pixel patches as relevant features. As the inputs have a dimensionality of 28x28, there are 49 features to choose from. To evaluate the quality of the selection, we first mask the test set by setting all non-selected patches to 0 and then use a classifier which was trained on unmasked data to compute the posthoc accuracy on this modified test set. The post-hoc accuracies averaged over 5 runs are shown in Table 3 for different numbers of $k$ selected features.

The selection method differs between models. For Q-FIT, we select the $k$ most highly weighted patches and for L2X, $k$ is set in advance. INVASE is treated differently, as the number of selected features varies and can only be modified implicitly through the strength of the regularizer. So we tune the regularizer strength $\lambda$ to different values such that the average number of selected features equals $k$. The $\lambda$ values we use are 100, 50, 23, 18.5 and 15.5 for $k = 1,...,5$. 
Table 2: **Tabular datasets.** Classification accuracy as a function of \( k \) selected features. **Left:** For gaining global explainability. Same features are selected for all the datapoints. **Right:** For gaining local (instance-wise) explainability. A set of \( k \) features is selected for each data point separately.

|      | Adult | Credit | Adult | Credit |
|------|-------|--------|-------|--------|
|      | 1 | 3 | 5 | 1 | 3 | 5 | 1 | 3 | 5 | 1 | 3 | 5 |
| Q-FIT | 78.2 | 76.5 | 82.4 | 96.1 | 94.9 | 94.9 | 77.9 | 78.5 | 80.1 | 89.8 | 91.5 | 93.5 |
| INVASE | 65.5 | 82.3 | 82.4 | 95.5 | 90.7 | 94.6 | 73.5 | 78.6 | 82.1 | 81.4 | 90.9 | 91.5 |
| L2X | 65.5 | 77.2 | 80.0 | 82.6 | 92.2 | 95.2 | 78.6 | 81.7 | 83.1 | 86.5 | 89.1 | 92.8 |
| SHAP | 76.6 | 79.7 | 83.1 | 96.1 | 94.3 | 96.4 |

Table 3: Post-hoc accuracy of **MNIST** classifier distinguishing digits 3 and 8 based on \( k \) number of (4x4) selected patches. Q-FIT outperforms other methods.

|      | k = 1 | k = 2 | k = 3 | k = 4 | k = 5 |
|------|-------|-------|-------|-------|-------|
| Q-FIT | 0.788 | 0.937 | 0.973 | 0.981 |
| L2X | 0.633 | 0.761 | 0.84 | 0.871 | 0.864 |
| INVASE | 0.584 | 0.780 | 0.901 | 0.915 | 0.905 |

**Figure 3:** Fairness vs feature importance on modified Adult data. (1) Trade-off between accuracy and fairness of a classifier. (2) We evaluate the KL divergence of selection probabilities between the baseline (unfair) classifier and varying levels of fair classifiers (44, 57, 82 and 96%). The 2nd and 3rd dots show the selected features by INVASE being identical while their KL divergence values differ. (3) The KL divergence between the Q-FIT’s importance distributions at varying levels of fair classifiers and the baseline classifier. (4) The difference in KL divergence under Q-FIT is well reflected in the learned importance at different levels of fairness.

**Figure 4:** Privacy vs feature importance on Adult data. (1) Trade-off between accuracy and privacy. (2) KL divergence under INVASE remains similarly at different noise levels (1, 2, 4, 8), while the selected features at those levels are not identical. (3) KL divergence under Q-FIT quantifies the trade-off between the feature importance and privacy. (4) The difference in KL divergence under Q-FIT is consistent with the learned importance. Additionally, many features get equal importance at a very high level of noise (17), giving an insight on the behaviour of the private classifier.
4.3 Divergence for comparing feature importance distributions.

As described in Sec. 2, our method outputs the Dirichlet distribution over the feature importance. The existence of probability distribution allows naturally to incorporate probability distance definitions to quantify the difference between distributions over feature importance. With the deliberate choice of Dirichlet distribution, we obtain a closed-form KL divergence between two Q-FIT’s learned Dirichlet distributions. Subsequently, we apply KL-divergence as a metric to describe the level of explainability sacrificed at the cost of increase in fairness and privacy of the classifier.

Fairness vs feature importance. First, we show the usefulness of our method to study the trade-off between explainability in terms of feature importance and fairness. We consider a fair classifier introduced in [19], and the Adult data to train a fair classifier in terms of Race. For this experiment, we modify the dataset, such that it only consists of 12 features by excluding the Race and Sex features as done in [19]. As shown in (1) in Fig. 3 the classifier loses accuracy measured in terms of the area under the curve as we increase the fairness measured in terms of the percentage rule [19], which is a well-known phenomenon, but we aim to show that Q-FIT allows to measure well the loss in explainability when increasing the fairness of the classifier.

In this case, as shown in (2) and (3) of Fig. 3, both INVASE and Q-FIT demonstrate gradual loss of explainability as the KL divergence between the feature distribution under the classifier trained without any fairness constraint and that at different levels of fairness (44%, 57%, 82% and 96% fair) increases as the fairness constraint increases. However, the vanilla INVASE by outputting just a set of important features does not distinguish between the level of 57% and 82% (by outputting [0, 4, 5, 8, 10] for both levels). Meanwhile, under Q-FIT, the difference in the KL divergence is well reflected in the learned importance as shown in (4). By virtue of assigning continuous importance weights, Q-FIT is able to account for smaller changes in the trained model than a discrete method like INVASE.

Privacy vs feature importance. Second, we show the usefulness of our method to study the trade-off between explainability and privacy. We consider a private classifier using the differentially private stochastic gradient descent (DP-SGD) technique [1], which perturbs the gradients during training to yield a classifier that guarantees a certain level of privacy. We use the Adult dataset to train a private classifier. The effect of adding noise to the gradients on the predictive accuracy is shown in (1) in Fig. 4. The figure shows how the classifier loses the accuracy measured in terms of the area under the curve as we increase the privacy level (the exact level of differential privacy at the different level of noise is given in the Supplementary material), expressed in terms of the level of noise we induced to the gradients during training. We compute the accuracy over 10 independent runs to obtain the error bars (grey). As the loss of accuracy is a known phenomenon, we aim to show a different effect, namely the impact of noise on the possibility to explain the data in form of the difference between the feature distribution without the noise and that when the noise is present at different levels.

For comparison, we examine how this effect can be described both by Q-FIT and INVASE [21]. For INVASE, we adjust the setup so that we jointly train the baseline network with a private classifier, then freeze the baseline network, and only update the selector and predictor networks. As INVASE is a method for instance-wise feature selection, once trained, we use INVASE to output the feature selection for the test datapoints, and average the selection probability (the Bernoulli distribution over the feature selection) across those test datapoints.

The plots (2) and (3) in Fig. 4 compare INVASE and Q-FIT. In the case of INVASE, the KL divergence is not necessarily informative as the divergence metric between the selection distribution under the non-private classifier and that at different levels of noise variance (1, 2, 4, 8 and 17) remains similar for the noise variance being 1, 2, 4, 8. In the case of Q-FIT, the KL divergence between the feature importance distribution under the non-private classifier and that at different levels of privacy increases as the privacy constraint increases. In addition, this difference in the KL divergence is again well reflected in the learned importance as shown in (4) which depicts gradual loss of feature importance differentiation as the noise levels increase.

Overall, both privacy and fairness experiments suggest that our method together with KL divergence is a suitable tool to study such trade-offs, giving additional insight on the behaviour of the respective classifiers in terms of the feature importance.

5 Conclusion

In this work, we attempt to address the pressing problem of interpretable machine learning, with focus on learning feature importance for individual data points, an issue which is relatively new in the literature. The method performs very competitively with other existing methods for providing both global and local (instance-wise) explanations. Moreover, by providing a probability distribution it intuitively and accurately weighs the relative importance of features, which can be additionally used as a measure of explainability.
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A Experiment details for synthetic data

Below we give details on the experimental setups for each of the results presented in the paper.

A.1 Methods

**Q-FIT.** We first train the network for 500 epochs, using stochastic gradient decent with learning rate: 0.001, momentum:0.9, and weight decay: $10^{-4}$. Then we freeze these weights are finetune the switch vector or switch network for 5-10 epochs with learning rate 0.05. In the experiment 1 we use analytic mean of Dirichlet distribution. We also tested the sampling but analytic mean proved to work faster and better.

**L2X.** We use the original code with minimal changes to load the additional datasets for 125 epochs (preserving number iterations due to the smaller dataset). On Syn4 and Syn5 where the number of relevant features is not fixed, we report results for $k=5$, which maximized $(TPR - FDR)$.

**INVASE.** We run the original code with minimal changes for 10k iterations. As suggested by the authors ([https://github.com/jsyoon0823/INVASE/issues/1](https://github.com/jsyoon0823/INVASE/issues/1)), we set $\lambda = 0.15$ for Syn5 and to 0.1 otherwise. We use SELU nonlinearities for Syn4-6 but not for Syn3, as we obtained better results with ReLUs on the first three datasets.

A.2 Standard deviation comparison. We compare here the standard deviation of the selected methods used in the main text.

|       | Syn 1 | Syn 2 | Syn 3 | Syn 4 | Syn 5 | Syn 6 |
|-------|-------|-------|-------|-------|-------|-------|
| Q-FIT (inst, samp) | 0     | 0     | 0.107 | 0.019 | 0.010 | 0.025 |
| Q-FIT (inst, pe)   | 0     | 0     | 0.201 | 0.015 | 0.061 | 0.093 |

Table 4: The comparison of the standard deviation of the MCC (Matthews correlation coefficient) (in 5 runs) presented in the Table 1 in the main text.

B Experiment details for real-world data

B.1 Tabular data

**Q-FIT.** We perform experiments on two real-world tabular datasets, adult and credit. The former can be found at [http://archive.ics.uci.edu/ml/datasets/kddcup99](http://archive.ics.uci.edu/ml/datasets/kddcup99) (we also include it in the repository), and the latter is available at [https://www.kaggle.com/mlg-ulb/creditcardfraud?select=creditcard.csv](https://www.kaggle.com/mlg-ulb/creditcardfraud?select=creditcard.csv). We use the same optimization settings as in the case of synthetic data. The details can me found at README file and the provided codabase.

B.2 MNIST data We generate the binary classification dataset by selecting all samples of classes 3 and 8 from MNIST, keeping the separation between train and test set. For the evaluation we then train a fully connected classifier network with 2 hidden layers of size 300, batch-normalization and ReLU activations to a test accuracy of 99.6%. This model is later used to compute post-hoc accuracy on the feature-selected data. In all cases below, the feature selection models output 49 dimensions representing the patches, which are then copied over 4x4 pixel patches to a full output size of 784.

**Q-FIT.** We first train a classifier for 10 epochs with the same architecture as the post-hoc accuracy model, but without batch-norm, as this leads to more stable selector training. Following this, the selector is network is trained for 10 epochs and then we use the selector to generate feature importances for the full test-set. For each sample the $k$ most highly weighted patches are kept and the remaining features are set to 0.

**L2X.** Because the original released L2X code does not contain the setup for the MNIST experiment, we use our own implementation based on the released code for synthetic data. We increase hidden dimensions in the selector and classifier parts of the model from 100 & 200 to 250 & 500 due to the higher data complexity.
| noise level | privacy guarantee |
|------------|------------------|
| $\sigma = 0$ | $\epsilon = \infty$ |
| $\sigma = 1.35$ | $\epsilon = 8.07$ |
| $\sigma = 2.3$ | $\epsilon = 4.01$ |
| $\sigma = 4.4$ | $\epsilon = 1.94$ |
| $\sigma = 8.4$ | $\epsilon = 0.984$ |
| $\sigma = 17$ | $\epsilon = 0.48$ |

Table 5: Differential privacy guarantees based on noise levels

**INVASE.** We adapt the INVASE setup for synthetic data to mnist and tune the $\lambda$ parameter in order to produce feature selections with different average numbers $k$ of selected features. For $k$ ranging from 1 to 5, we use $\lambda$ values of 100, 50, 23, 18.5, 15.5. As the relationship between the value of $\lambda$ and average $k$ is not reliable, we discard results from random seeds that didn’t produce the desired $k$. The chosen random seeds are listed in the experiment code.

**C Experiment details for Trade-offs**

**C.1 Feature importance vs fairness**

**Dataset** We use the Adult data used in the earlier section, with a change of excluding sex and race from the input features. The resulting dataset has 12 input features: age(0), workclass(1), fnlwgt(2), education(3), education number (4), marital status(5), occupation(6), relationship(7), capital gain(8), capital loss(9), hours per week(10), native country(11).

**Fair classifiers** We use this modified dataset and train a classifier with different fairness constraints following code from [https://github.com/equialgo/fairness-in-ml/blob/master/fairness-in-ml.ipynb](https://github.com/equialgo/fairness-in-ml/blob/master/fairness-in-ml.ipynb).

**Q-FIT** Given a classifier at each level of fairness, 44, 57, 82, 96% in terms of percentage rule based on race, we learn the global feature importance vector for 400 epochs. When computing the variational lower bound, we used a single sample. We set the prior parameter to be $\alpha_0 = 0.1$. As shown in the main text, initially when the classifier is unfair, the marital status(5) is the most important, and the education number (4) is in the second place, and the capital gain (8) is in the third place. As we increase the fairness in training the classifier, while the importance of marital status remains almost the same, the education number and capital gain become less important, while the age starts appearing to be important.

**INVASE** We train the INVASE model by exchanging the classifier component with the pre-trained fair models and only optimize the selector component. This diverges from the standard way of training INVASE, but despite the frozen classifier the model achieves an accuracy of 83% by the end of training.

**C.2 Feature importance vs privacy**

**Dataset** We use the original Adult dataset, which contains 14 input features: age(0), workclass(1), fnlwgt(2), education(3), education number (4), marital status(5), occupation(6), relationship(7), race(8), sex(9), capital gain(10), capital loss(11), hours per week(12), native country(13).

**Private classifiers** Using this dataset, we train a classifier, a 3-layer feedforward network with 100 and 20 hidden units in each hidden layer for 20 epochs, using the differentially private stochastic gradient descent (DP-SGD), which adds appropriately adjusted amount of noise to the gradient during training for privacy. The amount of noise and the corresponding privacy guarantee of the classifier is summarized in Table 5. The highly nonlinear relationship between the noise level and the corresponding privacy level is calculated by using the autodp package: [https://github.com/yuxiangw/autodp](https://github.com/yuxiangw/autodp).

**Q-FIT** Under each of the classifier, we learn the global feature importance of the input features using Q-FIT for 400 epochs. When computing the variational lower bound, we used a single sample. We set the prior parameter to be $\alpha_0 = 0.01$. Under the non-private classifier, relationship(7) status is the most important, and education number (4) is second, and capital gain(10) is the third. As we increase the noise level for a stronger privacy guarantee, the importance of the relationship(7) feature gets lower and other features such as age(0) and marital status(5) become more important.

**INVASE** The setup here equals the setup for fair models, with the difference that privacy classifier models are loaded instead.