# Classification-based Violation Measurement for Constrained Efficient Global Optimization

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ABSTRACT

Efficient global optimization (EGO) [1] is an attractive method for optimizing expensive functions, but its application to constrained problems has significant scope for improvement. Several methods have been used for incorporating constraints, such as product of expected improvement (EI) with probability of feasibility ($P_{feasibility}$), $P_{feasibility}$ penalization, expected violation (EV) etc [2]. These methods, based on approximation of constraint violation probability or expectation, need to have a good model for predicting the violations. The task becomes especially challenging in the presence of multiple constraints, small feasible regions and binary or discontinuous responses [3,4].

Conventionally in EGO, both the objective and constraint response values are approximated using Kriging. However, classification methods have also been used recently for handling constraints, even for problems with only pass/fail data [3]. Based on the classification information (feasible/infeasible) of the samples ($\pm 1$), certain methods, such as support vector machines (SVM) [5] used in this work, define an explicit boundary of the feasible domain. Presence of binary or discontinuous responses is not a hindrance for these methods. Also, all the constraints can be combined into a single classification boundary, thus avoiding multiple approximations and associated error propagation [3].

However, use of classification methods in constrained EGO formulations requires probabilistic outputs, i.e. the probability of belonging to a certain class. This work will propose a new correlation-based probabilistic SVM (PSVM) model to improve the probability outputs, and compare the quantification of constraint violation probabilities based on existing probabilistic classification tools, such as a basic sigmoid-based PSVM [6], relevance vector machine (RVM) [7] and distance-based PSVM (DPSVM) [3].

The existing models such as the basic sigmoid PSVM and RVM models do not have any explicit term relating the probability with proximity to a sample belonging to certain category (feasible/infeasible). This poses an issue when using the probability for constrained EGO, as demonstrated for the basic PSVM [3]. DPSVM enforces P(+1|x) equal to 1 at +1 samples and 0 at -1 samples. However, the probability values away from the samples have scope for improvement, as it only takes into account the distance to nearest samples belonging to the two classes (+1/-1 or feasible/infeasible) [3]. It does not take into account the density of samples belonging to the classes in that region.

This article will investigate one or more modified PSVM model(s) in order to improve upon the previous model, while retaining its primary desirable quality (enforcement of zero misclassification probability at the evaluated samples). Instead of only the distances to the nearest samples of each class, a correlation metric containing the information about distances to all samples will be used. One of the possible models provides the probability of +1 class as:

$$P(+1|\mathbf{x}) = \frac{1}{1+e^{-As(\mathbf{x})+BR(\mathbf{x})+C}} \qquad A, B > 0$$

$$R(\mathbf{x}) = \sum_{i=1}^{N} y_i \tan\left(\frac{\pi}{2} r(\mathbf{x}, \mathbf{x}_i)\right)$$

$s$ : SVM value

$r$ : correlation function

$y_i$ : class label +1 or -1

$$\mathbf{x} \to \mathbf{x}_i \Rightarrow r(\mathbf{x}, \mathbf{x}_i) \to 1 \Rightarrow y_i \tan\left(\frac{\pi}{2} r(\mathbf{x}, \mathbf{x}_i)\right) \to y_i \cdot \infty \Rightarrow R(\mathbf{x}) \to y_i \cdot \infty$$

$$R(\mathbf{x}) \to \infty \Rightarrow P(+1|\mathbf{x}) \to 0 \quad \text{and} \quad R(\mathbf{x}) \to -\infty \Rightarrow P(+1|\mathbf{x}) \to 1$$

The full paper will provide a comparison of the proposed and existing probabilistic classification models and use them in constrained EGO formulations. The probability outputs are expected to improve compared to earlier models. Therefore, the efficiency of constrained EGO and its ability to locate the global optima is also expected to improve with the proposed method.

## REFERENCES


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