Class-imbalanced Classifiers using Ensembles of Gaussian Processes and Gaussian Process Latent Variable Models

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Overview

❖ Motivation
❖ Problem Formulation
❖ Gaussian Process Latent Variable Model (GPLVM) for Ensemble Classification
❖ Experiments
❖ Conclusions
Motivation

Picture sources:
https://www.helcim.com/article/overview-credit-card-transaction-types/
Motivation

In our project, “Machine Learning Methods for Revealing the Wellbeing of Fetuses”, we face the severe imbalanced fetal heart rate (FHR) recordings.

Only 0.1% FHR tracings are classified into abnormal group.

Picture source:
https://www.stonybrook.edu/commcms/electrical/research/2021/djuric.php
Problem Formulation

The training set contains a majority class and a minority class:

\[ \mathcal{D} = \mathcal{C}_1 \cup \mathcal{C}_2 \]

\[ \mathcal{C}_1 = \{ (x_i, +1) | i = 1, 2, \ldots, n_{c_1} \} \]

\[ \mathcal{C}_2 = \{ (x_j, -1) | j = 1, 2, \ldots, n_{c_2} \} \quad n_{c_1} \gg n_{c_2} \]
Problem Formulation

The training set contains a majority class and a minority class:

Rewritten: \[ D = \{X, y\} \quad X \in \mathbb{R}^{dx \times n} \quad y \in \mathbb{R}^n \quad n = n_{c1} + n_{c2} \]

Similarly, the test set: \[ D^* = \{X^*, y^*\} \quad X^* \in \mathbb{R}^{dx \times n^*} \quad y^* \in \mathbb{R}^{n^*} \]
GPLVM for Ensemble Classification

One of the popular strategies to reduce the effect of performance distortion towards the majority class in the training process is ensemble clearing.
GPLVM for Ensemble Classification

Training data resampling
we under-sampled the majority class without replacement and oversampled the minority class by applying SMOTE*. 

*SMOTE: Synthetic Minority Over-sampling Technique
GPLVM for Ensemble Classification

Imbalanced training set D

Balanced training subset D1

GPC1

Balanced training subset D2

GPC2

...  

Balanced training subset Dk

GPCk

Data Resampling

Test set D*

$q(f^*|X^*, X_k, y_k)$

GPLVM

$p(y^* = 1|X^*, X, y)$
GPLVM for Ensemble Classification

For each branch

The posterior

\[ p(f|X_k, y_k) = \frac{p(y_k|f)p(f|X_k)}{p(y_k|X_k)} \]
GPLVM for Ensemble Classification

For each branch

The posterior

\[ p(f|X_k, y_k) = \frac{p(y_k|f)p(f|X_k)}{p(y_k|X_k)} \]

The predictive distribution

\[ p(f^*|X^*, X_k, y_k) = \int p(f^*|X^*, X_k, f)p(f|X_k, y_k)df \]
GPLVM for Ensemble Classification

For each branch

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\[ p(f|X_k, y_k) = \frac{p(y_k|f)p(f|X_k)}{p(y_k|X_k)} \]

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The Gaussian approximation

\[ q(f^*|X^*, X_k, y_k) = \mathcal{N}(f^*|\tilde{f}^*_k, \Sigma_{f^*, k}) \]
The Gaussian approximation

\[ q(f^* | X^*, X_k, y_k) = \mathcal{N}(f^* | \tilde{f}^*, \Sigma_{f^*}, k) \]

is the output of each Gaussian process classifier.
Let $F^* = [f_1^*, f_2^*, \ldots, f_K^*] \in \mathbb{R}^{n^* \times K}$ be an observation matrix and $f^* \in \mathbb{R}^{n^*}$ be an unknown true test latent vector.
GPLVM for Ensemble Classification

Let $F^* = [f_1^*, f_2^*, \ldots, f_K^*] \in \mathbb{R}^{n^* \times K}$ be an observation matrix and $f^* \in \mathbb{R}^{n^*}$ be an unknown true test latent vector.

We have a nonlinear mapping

$$F^* = G(f^*) + E$$
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We have a nonlinear mapping

$$\mathbf{F}^* = \mathbf{G}(f^*) + \mathbf{E}$$

Function $\mathbf{G}(\cdot)$ defines $K$ independent GPs

$$f^*_k = g_k(f^*) \sim \mathcal{GP}(\mathbf{m}(f^*), K(f^*, f^*))$$
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We have a nonlinear mapping
\[
F^* = G(f^*) + E
\]

Function \( G(*) \) defines \( K \) independent GPs
\[
f^*_k = g_k(f^*) \sim \mathcal{GP}(\mu(f^*), K(f^*, f^*))
\]

\( E \) contains i.i.d. zero-mean Gaussian noises
\[
\epsilon \sim \mathcal{N}(0, \sigma^2)
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GPLVM for Ensemble Classification

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$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

Then, the likelihood function is

$$p(F^*|f^*) = \prod_{k=1}^{K} p(f_k^*|f^*)$$

$$= \prod_{k=1}^{K} \int \int p(f_k^*|\bar{f}_k^*)p(\bar{f}_k^*|v_k, f^*)p(v_k|f^*)d\bar{f}_k^*dv_k$$
GPLVM for Ensemble Classification

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Considering the outputs from GPCs

$$q(f^*|X^*, X_k, y_k) = \mathcal{N}(f^*|\bar{f}_k^*, \Sigma_{f^*, k})$$
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Considering the outputs from GPCs

\[
q(f^*|X^*, X_k, y_k) = \mathcal{N}(f^*|\tilde{f}_k^*, \Sigma f^*, k)
\]

The likelihood is a product of Gaussian distributions

\[
p(F^*|f^*) = \prod_{k=1}^{K} \mathcal{N}(f_k^*|0, \Sigma_k)
\]

\[
\Sigma_k = K_k + \Sigma f^*, k + \sigma^2 I
\]
GPLVM for Ensemble Classification

Then, the likelihood function is

\[
p(F^*|\mathbf{f}^*) = \prod_{k=1}^{K} p(f^*_k|\mathbf{f}^*)
\]

\[
= \prod_{k=1}^{K} \int \int p(f^*_k|\mathbf{f}^*)p(\mathbf{f}^*_k|\mathbf{v}_k, \mathbf{f}^*)p(\mathbf{v}_k|\mathbf{f}^*)d\mathbf{f}^*_k d\mathbf{v}_k
\]

Considering the outputs from GPCs

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GPLVM for Ensemble Classification

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p(F^* | f^*) = \prod_{k=1}^{K} \mathcal{N}(f_k^* | 0, \Sigma_k)
\]

\[
\Sigma_k = K_k + \Sigma_{f^*,k} + \sigma^2 I
\]

\(K_k\) is the covariance matrix computed by evaluating the kernel of the kth GP.

If the prior

\[
p(f^*) = \prod_{i=1}^{n^*} \mathcal{N}(0, 1)
\]
GPLVM for Ensemble Classification

Then, the likelihood function is

$$p(F^*|f^*) = \prod_{k=1}^{K} p(f_k^*|f^*)$$

$$= \prod_{k=1}^{K} \int \int p(f_k^*|\vec{f}_k^*) p(\vec{f}_k^*|\mathbf{v}_k, f^*) p(\mathbf{v}_k|f^*) d\vec{f}_k^* d\mathbf{v}_k$$

Considering the outputs from GPCs

$$q(f^*|X^*, X_k, y_k) = \mathcal{N}(f^*|\vec{f}_k^*, \Sigma_f^{*,k})$$

The likelihood is a product of Gaussian distributions

$$p(F^*|f^*) = \prod_{k=1}^{K} \mathcal{N}(f_k^*|0, \Sigma_k)$$

$$\Sigma_k = K_k + \Sigma_{f^*,k} + \sigma^2 I$$

$K_k$ is the covariance matrix computed by evaluating the kernel of the kth GP.

If the prior

$$p(f^*) = \prod_{i=1}^{n^*} \mathcal{N}(0, 1)$$

the log of the posterior

$$\log p(f^*|F^*) \propto -\frac{(K+1)n^*}{2} \log(2\pi) - \frac{1}{2} \text{tr}(f^*f^{*T})$$

$$- \frac{1}{2} \sum_{i=1}^{n^*} \left( \log|\Sigma_k| + \vec{f}_k^{*T} \Sigma_k^{-1} \vec{f}_k^* \right)$$
GPLVM for Ensemble Classification

The log of the posterior

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GPLVM for Ensemble Classification

The log of the posterior
\[ \log p(f^*|F^*) \propto -\frac{(K + 1)n^*}{2} \log(2\pi) - \frac{1}{2} \text{tr}(f^*f^{*T}) - \frac{1}{2} \sum_{i=1}^{n^*} \left( \log|\Sigma_k| + \bar{f}_k^* \Sigma_k^{-1} \bar{f}_k^* \right) \]

The MAP estimation is
\[ \hat{f}_{MAP}^* = \arg\max_{f^*, \theta} \log p(f^*|F^*) \]
GPLVM for Ensemble Classification

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\]

The MAP estimation is
\[
\hat{f}_{MAP}^* = \arg \max_{f^*,\theta} \log p(f^*|F^*)
\]

The probabilistic output is
\[
p(y^* = 1|X^*, X, y) = \phi(\hat{f}_{MAP}^*)
\]
GPLVM for Ensemble Classification

The MAP estimation is

$$\hat{f}_{MAP} = \arg \max_{\hat{f}^*, \theta} \log p(f^* | F^*)$$

The probabilistic output is

$$p(y^* = 1 | X^*, X, y) = \phi(\hat{f}_{MAP})$$
GPLVM for Ensemble Classification

The MAP estimation is

$$\hat{f}_{\text{MAP}} = \arg \max_{f^* \theta} \log p(f^*|F^*)$$

The probabilistic output is

$$p(y^* = 1|X^*, X, y) = \phi(\hat{f}_{\text{MAP}})$$

We used the logistic function:

$$p(y_i|f_i) = \phi(y_i f_i) = \frac{1}{1 + \exp(-y_i f_i)}$$
GPLVM for Ensemble Classification

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\[
\hat{f}_{\text{MAP}} = \arg \max_{f, \theta} \log p(f^* | F^*)
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We used the logistic function:
\[
p(y_i | f_i) = \phi(y_i f_i) = \frac{1}{1 + \exp(-y_if_i)}
\]

We chose the popular radial basis function (RBF) as the kernel of GP models.
\[
k_{\text{RBF}}(x, x') = \sigma^2_f \exp\left(-\frac{||x - x'||^2}{2l^2}\right)
\]

And the automatic relevance determination (ARD) is applied for dimentionality reduction.
\[
k_{\text{RBF-ARD}}(x, x') = \sigma^2_f \exp\left(-\frac{1}{2} \sum_{d=1}^{D} \frac{(x_d - x'_d)^2}{l_d^2}\right)
\]
Experiments

Synthetic Binary Classification

We generated a two-moon dataset centered at (2.5,3) and (-2.5,-3).

majority class: \( n_{c_1} = 100 \)

minority class: \( n_{c_2} = 10 \)

test set: \( n^* = 2000 \)

# of branches: \( K=10 \)

# of data in training subset: 20
Experiments

Synthetic Binary Classification

EnGPC-GPLVM: newly proposed method

GPC: only using a GPC-based model on imbalanced dataset

EnGPC-Avg: ensemble of GPCs whose outputs are averaged

<table>
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<tr>
<th>Methods</th>
<th>TPR</th>
<th>FPR</th>
<th>TNR</th>
<th>FNR</th>
<th>ACC</th>
<th>F-score</th>
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<tr>
<td>GPC</td>
<td>0.9802</td>
<td>0.2341</td>
<td>0.7659</td>
<td>0.0115</td>
<td>0.8702</td>
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<td>EnGPC-Avg</td>
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Experiments

Test with real-world dataset

Based on the work in [1], we have a uterine contraction dataset annotated by experts.
Training set: 233 positive samples
46 negative samples
Test set: 41 samples per class

<table>
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<tr>
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<th>FNR</th>
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<tr>
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Conclusions

• We addressed the problem of binary classification with imbalanced dataset.

• An ensemble of Gaussian process classifiers with the Gaussian process latent variable model as a decision maker, is proposed.

• Experiments using both synthetic and real-world data show promise of the proposed approach.
Thank you very much for your attention!

Contacts

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