Minimum Enclosing Ball for Anomaly Detection on Biological Data using Frank-Wolfe based algorithms

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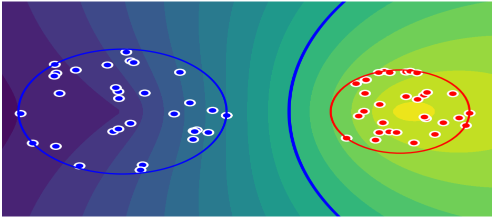
Introduction

- The **Minimum Enclosing Ball** (MEB) is a problem with a wide range of applications, of which anomaly detection is a prominent one.
- **Objective**: To understand and implement the MEB problem through three different variants of the Frank-Wolfe algorithm: the Pairwise Frank-Wolfe, the Blended Pairwise Conditional Gradient and a variant of the Away-Steps.
- **Application**: To find anomalies in the context of four different biological problems.

Minimum Enclosing Ball Problem

The problem is to find the smallest n-sphere that contains a given set of points in a Euclidean space. This sphere is called the minimum enclosing ball (MEB) of the point set.

- **Applications** in clustering, data classification, machine-learning and facility location, anomaly detection, among others.
- **Advantages**: Robustness, geometric interpretability and high-dimensionality



Minimum Enclosing Ball Problem

Formal definition

Given $\mathcal{A} := \{a^1, \ldots, a^m\} \subset \mathbb{R}^n$, the Minimum Enclosing Ball (MEB) problem consists in finding the smallest Euclidean n-ball

$$\mathcal{B}_{c,\rho} := \{x \in \mathbb{R}^n : ||x - c||_2 \leq \rho\}$$

that contains every point in $\mathcal{A}$, considering c as the center and ρ as the center and radius of the ball, respectively.

Minimum Enclosing Ball Problem

Primal MEB formulation

The optimization problem of the MEB is formulized as

$$\begin{aligned} \min_{c,\rho} \quad & \rho \\ \text{subject to} \quad & \\ & ||a^i - c|| \leq \rho, \quad i = 1, ..., m, \end{aligned}$$

By applying the transformation $\gamma := \rho^2$, we obtain

$$\begin{aligned} (\mathcal{P}) \quad \min_{c,\gamma} \quad & \gamma \\ \text{subject to} \quad & \\ & (a^i)^T a^i - 2(a^i)^T c + c^T c \leq \gamma, \\ & \qquad i = 1, ..., m. \end{aligned}$$

Minimum Enclosing Ball Problem

The Dual MEB

In high-dimensional spaces, transforming the MEB problem into its dual form can help reduce dimensionality and simplify the optimization process.

$$(\mathcal{D}1) \quad \max_{\mu} \qquad \phi(\mu) := \sum_{j=1}^{m} \mu_j (a^j)^T a^j - \left(\sum_{j=1}^{m} \mu_j a^j \right)^T \sum_{j=1}^{m} \mu_j a^j$$

$$\text{subject to}$$

$$\sum_{j=1}^{m} \mu_j = 1$$

$$\mu_i \geq 0, \quad i = 1, ..., m \quad ,$$

where vector μ contains the Lagrangian multipliers respective to the constraints of problem $(\mathcal{P})$.

Minimum Enclosing Ball Problem

The Dual MEB: Convex Formulation

We can express the dual formulation of the MEB ($\mathcal{D}1$) as a simplified convex version:

$$(\mathcal{D}2) \quad \min_{\mu \in \triangle^{m-1}} -\phi\left(\mu\right) \quad ,$$

where the Unit Simplex

$$\triangle^{m-1} = \left[\mu \in \mathbb{R}^m \middle| \sum_{i=1}^{m} \mu_i = 1 \quad \wedge \quad \mu_j \geq 0, \quad j = 1, ..., m \right]$$

satisfies the previous constraint of non-negativity and sum-to-one of the lagrangian multipliers.

Anomaly Detection Problem

Anomaly detection is the task of identifying data points that deviate significantly from the normal behavior of the data.

MEB Approach

To find the smallest hypersphere that contains all the data points used for training, i.e., points that are known to not be anomalies *a priori*. From there, new data points that lie outside of the hypersphere obtained in the training stage are considered to be anomalies.

Algorithms

In this work we present three algorithms:

- Pairwise Frank Wolfe (Lacoste-Julien and Jaggi (2015) and Mitchell, Dem'yanov, and Malozemov (1974))
- Blended Pairwise Conditional Gradients (BPCG) (Tsuji, Tanaka, and Pokutta (2022))
- $(1+\epsilon)$-approximation to the MEB($\mathcal{A}$) algorithm (Yildirim (2008))

Algorithm 1: Pairwise Frank Wolfe

- The direction chosen in every step is based on a weight change from the away atom a_t to the FW atom w_t, while keeping all the other weights unchanged.
- Cons: Swap steps.

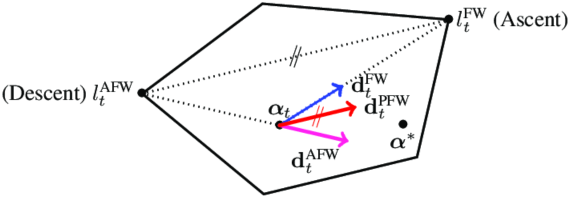


Figure 1: Illustration of Frank-Wolfe towards, away and pairwise directions

Algorithm 2: Blended Pairwise Conditional Gradients (BPCG)

- A blending criterion is added that favors local steps made over the convex hull of the current active vertex set, offering a sparser solution without swap steps.
- The only reason for new atoms being added to S_t is a sufficient decrease in the local pairwise gap.

Algorithm 1 and 2: MEB adaptation of PFW and BPCG

Gradient

Finding the step direction in algorithms PFW and BPCG, requires the computation of the gradient of $-\phi$ to compute:

$$\nabla_i(-\phi(\mu)) = 2\left(a^i\right)^T \sum_{j=1}^{m} a^j \mu_j - (a^i)^T a^i.$$

Algorithm 1 and 2: MEB adaptation of PFW and BPCG

In the case of Frank-Wolfe iterations on the PFW and BPCG algorithms, we compute w_t as:

$$w_t = argmin_{w \in \triangle^{m-1}} w^T \nabla\big(-\phi(\mu_t)\big) \tag{1}$$

From the Fundamental Theorem of Linear Programming the solution should be a vertex of $\triangle^{m-1}$. Since the vertices of $\triangle^{m-1}$ correspond to the standard basis vectors $e_j \in \mathbb{R}^m$, $j = 1, ..., m$, equation (1) obtains the same result as

$$w_t = argmin_{e_j \in \mathbb{R}^m} e_j^T \nabla\big(-\phi(\mu_t)\big)$$

So, if we take $i = i_t^w := argmin_{j \in \{1,\ldots,m\}} \Big(\nabla\big(-\phi(\mu_t)\big)\Big)_j$, we see that $w_t = e_i$.

Algorithm 1 and 2: Short step rule

For the line search we chose to use the short-step rule suggested by Tsuji:

$$\lambda_t = \frac{\langle \nabla - \phi(\mu), d_t \rangle}{L \| d_t \|^2} \quad .$$

To determine L, we start by calculating the Hessian matrix, H, where each component is determined as:

$$h_{ij} = \frac{\partial^2 \left(-\phi(\mu) \right)}{\partial \mu_i \partial \mu_j} = 2 \left(a^j \right)^T a^i$$

We can then obtain the Lipschitz constant as

$$L = \lambda_{\text{max}}(H),$$

where $\lambda_{\text{max}}(H)$ is the largest eigenvalue of H and it needs to be positive.

Algorithm 1: Pairwise Frank Wolfe

Algorithm 1 Pairwise Frank-Wolfe algorithm for the MEB problem: `PFW_MEB`$(x^{(0)}, \mathcal{A}, \epsilon)$

```
Require: point $x_0 \in \mathcal{A}$
  $S_0 \leftarrow \{x_0\}$
  for $t = 0$ to $T$ do
      $i_t^w \leftarrow_{j\in\{1,\dots m\}} (-\nabla\phi(\mu_t))_j$
      $d_t^{FW} = e_{\mu_t} - e_{i_t^w}$                    ▷ FW direction
      $i_t^a \leftarrow_{\substack{j\in\{1,\dots,m\}\\ e_j\in S_t}} (-\nabla\phi(\mu_t))_j$
      $d_t^A = e_{\mu_t} - e_{i_t^a}$                      ▷ Away direction
      $g_t^{FW} \leftarrow \langle \nabla - \phi(\mu_t), d_t^{FW} \rangle$
      if $g_t^{FW} \leq \epsilon$ then                    ▷ FW gap is small enough
          return $x^t$
      end if
      $d_t \leftarrow e_{i_t^w} - e_{i_t^a}$
      $\lambda_{max} \leftarrow \alpha_v^t$
      $\lambda_t \leftarrow \max\left(0, \min\left(\lambda_{max}, \frac{\langle -\nabla\phi(\mu_t), d_t \rangle}{L||d_t||_2^2}\right)\right)$
      $\mu_{t+1} \leftarrow \mu_t + \lambda_t d_t$
      $\alpha_{i_t^a}^{(t+1)} = \alpha_{i_t^a}^{(t)} - \lambda_t$
      $\alpha_{i_t^w}^{(t+1)} = \alpha_{i_t^w}^{(t)} + \lambda_t$
      $S_{t+1} \leftarrow \{e_{i_t^w} \in A \text{ s.t. } \alpha_v^{t+1} > 0\}$
  end for
```

Algorithm 2: Blended Pairwise Conditional Gradients (BPCG)

Algorithm 2 Blended Pairwise Conditional Gradients (BPCG) for the MEB problem

```
Require: convex smooth function $f$, start vertex $\mu_0 \in \triangle^{m-1}$.
Ensure: points $\mu_1, \dots, \mu_T$ in $P$. Weights Initialization: $\alpha_t^v = 1$ for
  $v = \mu_0$, and 0 otherwise.
  $\mu_0 \leftarrow \frac{1}{m} * 1$                                  ▷ Feasible initialization
  $S_0 \leftarrow \{\mu_0\}$
  $\lambda_t \leftarrow \frac{2}{t+2}$                                  ▷ Fixed step size
  for $t = 0$ to $T - 1$ do
      $i_t^a \leftarrow_{\substack{j \in \{1,\dots,m\} \\ e_j \in S_t}} (-\nabla\phi(\mu_t))_j$          ▷ away vertex
      $i_t^s \leftarrow_{\substack{j \in \{1,\dots,m\} \\ e_j \in S_t}} (-\nabla\phi(\mu_t))_j$          ▷ local FW
      $i_t^w \leftarrow_{j \in \{1,\dots m\}} (-\nabla\phi(\mu_t))_j$               ▷ global FW

      if $\langle \nabla - \phi(\mu_t), e_{i_t^a} - e_{i_t^s} \rangle \geq \langle \nabla - \phi(\mu_t), \mu_t - e_{i_t^w} \rangle$ then
          $d_t = e_{i_t^a} - e_{i_t^s}$
          $\Lambda_t^* \leftarrow c[\mu_t](e_{i_t^a})$
          $\lambda_t \leftarrow \max\left(0, \min\left(\Lambda_t^*, \frac{\langle \nabla\phi(\mu_t), d_t \rangle}{L||d_t||_2^2}\right)\right)$

          if $\lambda_t < \Lambda_t^*$ then
              $S_{t+1} \leftarrow S_t$                                ▷ descent step
              $\alpha^{e_{i_t^a}} = \alpha^{e_{i_{t-1}^a}} - \lambda_t$
              $\alpha^{e_{i_t^s}} = \alpha^{e_{i_{t-1}^s}} + \lambda_t$
          else
              $S_{t+1} \leftarrow S_t \setminus \{e_{i_t^a}\}$                        ▷ drop step
              $\alpha^{e_{i_t^a}} = 0$
              $\alpha^{e_{i_t^s}} = \alpha^{e_{i_{t-1}^s}} + \lambda_t$
          end if
      else
          $d_t = \mu_t - e_{i_t^w}$                                ▷ FW step
          $\lambda_t \leftarrow \max\left(0, \min\left(1, \frac{\langle \nabla\phi(\mu_t), d_t \rangle}{L||d_t||_2^2}\right)\right)$
          $S_{t+1} \leftarrow S_t \cup \{w_t\}$ (or $S_{t+1} \leftarrow i_t^w$ if $\lambda_t = 1$)
          $\alpha_t = \alpha_{t-1}(1 - \lambda_t)$
          $\alpha^{e_{i_t^w}} = \alpha^{e_{i_t^w}} + \lambda_t$
      end if
      $\mu_{t+1} \leftarrow \mu_t - \lambda_t d_t$
  end for
```

Algorithm 3: $(1+\epsilon)$-approximation to the MEB($\mathcal{A}$) algorithm

Some notions

Given $\epsilon > 0$, a ball $\mathcal{B}_{\boldsymbol{c},\rho}$ is said to be a $(1+\epsilon)$-approximation to the MEB($\mathcal{A}$), $\mathcal{B}_{\boldsymbol{c}_{\mathcal{A}},\rho_{\mathcal{A}}}$, if

$$\mathcal{A} \subset \mathcal{B}_{\boldsymbol{c},\rho} \quad \wedge \quad \rho \leq (1+\epsilon)\rho_{\mathcal{A}}.$$

A subset $\mathcal{X} \subseteq \mathcal{A}$ is said to be an ϵ-core set (or a core set) of $\mathcal{A}$ if

$$\rho_{\mathcal{X}} \leq \rho_{\mathcal{A}} \leq (1+\epsilon)\rho_{\mathcal{X}},$$

where $\mathcal{B}_{\boldsymbol{c}_{\mathcal{X}},\rho_{\mathcal{X}}} :=$ MEB($\mathcal{X}$).

Algorithm 3: $(1+\epsilon)$-approximation to the MEB$(\mathcal{A})$ algorithm

- This algorithm is closely related to the Away-Steps variant of the Frank–Wolfe algorithm.
- With a proper initialization applied to the dual formulation of the MEB problem and the possibility of "dropping" points from the working core set at each iteration.
- Core sets allow for a compact representation of the input set, and as such are of great importance when working with large-scale problems.

Algorithm 3: $(1+\epsilon)$-approximation to the MEB($\mathcal{A}$) algorithm

Algorithm 3 $(1+\epsilon)$-approximation to MEB($\mathcal{A}$)

```
Require: Input set of points $\mathcal{A} = \{a^1, \ldots, a^m\} \subset \mathbb{R}^n, \epsilon > 0$.
  $\alpha \leftarrow_{i=1,\ldots,m} \|a^i - a^1\|^2$
  $\beta \leftarrow_{i=1,\ldots,m} \|a^i - a^\alpha\|^2$
  $u^0_\alpha \leftarrow 1/2,\ u^0_\beta \leftarrow 1/2$
  $\mathcal{X}_0 \leftarrow \{a^\alpha, a^\beta\}$
  $c^0 \leftarrow \sum_{i=1}^m u^0_i a^i$
  $\gamma^0 \leftarrow \Phi(u^0)$
  $\kappa \leftarrow_{i=1,\ldots,m} \|a^i - c^0\|^2$
  $\xi \leftarrow_{i:a^i \in \mathcal{X}_0} \|a^i - c^0\|^2$
  $\delta^+_0 \leftarrow (\|a^\kappa - c^0\|^2/\gamma^0) - 1$
  $\delta^-_0 \leftarrow 1 - (\|a^\xi - c^0\|^2/\gamma^0)$
  $\delta_0 \leftarrow \max\{\delta^+_0, \delta^-_0\}$
  $k \leftarrow 0$
```

Algorithm 3: $(1+\epsilon)$-approximation to the MEB($\mathcal{A}$) algorithm

Algorithm 4 $(1+\epsilon)$-approximation to MEB($\mathcal{A}$)

```
Require: Input set of points $\mathcal{A} = \{a^1, \dots, a^m\} \subset \mathbb{R}^n, \epsilon > 0$.
  while $\delta_k > (1+\epsilon)^2 - 1$ do
      if $\delta_k > \delta_k^-$ then
          $\lambda^k \leftarrow \delta_k / [2(1+\delta_k)]$
          $k \leftarrow k+1$
          $u^k \leftarrow (1-\lambda^{k-1})u^{k-1} + \lambda^{k-1}e^{\kappa}$
          $c^k \leftarrow (1-\lambda^{k-1})c^{k-1} + \lambda^{k-1}a^{\kappa}$
          $\mathcal{X}^k \leftarrow \mathcal{X}^{k-1} \cup \{a^k\}$
      else
          $\lambda^k \leftarrow \min\left\{\frac{\delta_k^-}{2(1-\delta_k^-)}, \frac{u_\xi^k}{1-u_\xi^k}\right\}$
          if $\lambda^k = u_\xi^k/(1-u_\xi^k)$ then
              $\mathcal{X}_{k+1} \leftarrow \mathcal{X}_k \setminus \{a^\xi\}$
          else
              $\mathcal{X}_{k+1} \leftarrow \mathcal{X}_k$
          end if
          $k \leftarrow k+1$
          $u^k \leftarrow (1+\lambda^{k-1})u^{k-1} - \lambda^{k-1}e^{\xi}$
          $c^k \leftarrow (1+\lambda^{k-1})c^{k-1} - \lambda^{k-1}a^{\xi}$
      end if
      $\gamma^0 \leftarrow \Phi(u^k)$
      $\kappa \leftarrow_{i=1,\dots,m} \|a^i - c^0\|^2$
      $\xi \leftarrow_{i:a^i \in \mathcal{X}_0} \|a^i - c^k\|^2$
      $\delta_k^+ \leftarrow (\|a^\kappa - c^k\|^2/\gamma^k) - 1$
      $\delta_k^- \leftarrow 1 - (\|a^\xi - c^k\|^2/\gamma^k)$
      $\delta_k \leftarrow \max\{\delta_k^+, \delta_k^-\}$
  end while
  Output $c^k, \mathcal{X}_k, u^k, \sqrt{(1+\delta_k)\gamma^k}$
```

Convergence Analysis

- All of the algorithms presented enjoy linear convergence when applied to the MEB problem.
- The MEB problem is a case of the Non-Strongly Convex generalization of the results in Lacoste [1], where global linear convergence is still guaranteed.
- BPCG is expected to perform at least as good as the PFW, if not better due to the lack of swap steps.
- The $(1+\epsilon)$-approximation to the MEB algorithm converges in $O(1/\epsilon)$ iterations.

Metrics

In the anomaly detection problem, we want to assess how well the model predicts the anomaly data in a new dataset.We report the following measures:

$$Recall = \frac{TP}{TP+FN}, \ Precision = \frac{TP}{TP+FP}, \ Accuracy = \frac{TP+TN}{TP+FP+TN+FN},$$

- As we focus on the anomaly points, we use recall as the benchmark measure. Recall measures the fraction of true anomalies detected by the model.

Datasets

1. Breast Cancer: 569 samples of women with breast tumors and 30 features of the tumor, and a dichotomous variable with the diagnosis (malignant or benign). The objective is to detect malignant tumors (anomalies).

2. Breast cancer gene expression: 801 instances and 20,531 features. The focus is placed on breast cancer samples identified with the gen BRCA (Breast invasive carcinoma).

Datasets

3. Vertebral column pathology: 310 instances of patients with 6 biomechanical features and a variable indicating different vertebral column diseases. The goal is to detect if a patient has vertebral column pathology (anomaly).

4. Maternity risk: 1013 instances of pregnant women with 5 features of biomedical indicators and a categorical variable with the risk of maternal mortality during pregnancy. The objective is to identify pregnant women with high-risk levels during pregnancy (anomaly).

Dataset Preprocessing (I)

- We divided the dataset into two sets: *training* and *test*, with a proportion of 70/30.
- Training set to get the radius and center of the non-anomalous points.
- Test set uses as input the radius and center to identify the anomalies. We relied on recall to assess goodness of fit.
- On the Breast cancer dataset, we apply the Standard Scaler technique that transforms the features of a dataset to have zero mean and unit variance.

Dataset Preprocessing (II)

We reduce the number of features for each dataset, except for the Breast cancer gene expression, for which we wish to keep it large-scale for later comparison purposes.

Dataset	Features	Optimal K
Breast Cancer	30	4
Vertebral Column	6	2
Maternity Risk	6	3

Table 1: Optimal K search

Results

- In all the experiments, we set a maximum number of iterations of $T = 100,000$, and a *tolerance* of 10^{-4}.
- In the case of PFW and BPCG we use the same initial point and stopping condition.

Results

Dataset 1

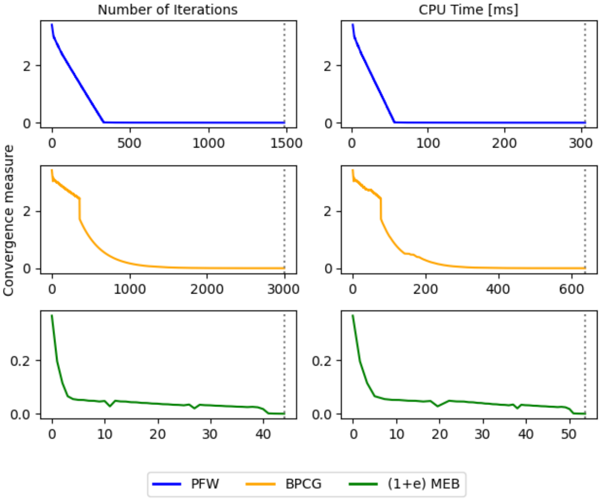


Figure 2: Convergence measure for Breast cancer dataset

Results

Dataset 2

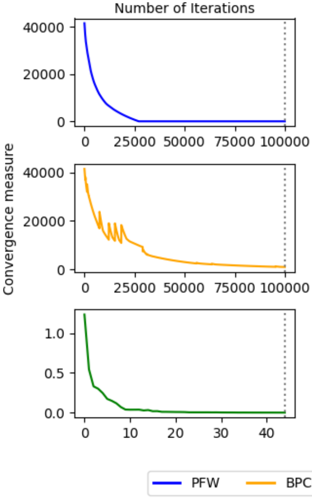


Figure 3: Convergence measure for Breast cancer gene expression dataset

Results

Dataset 3

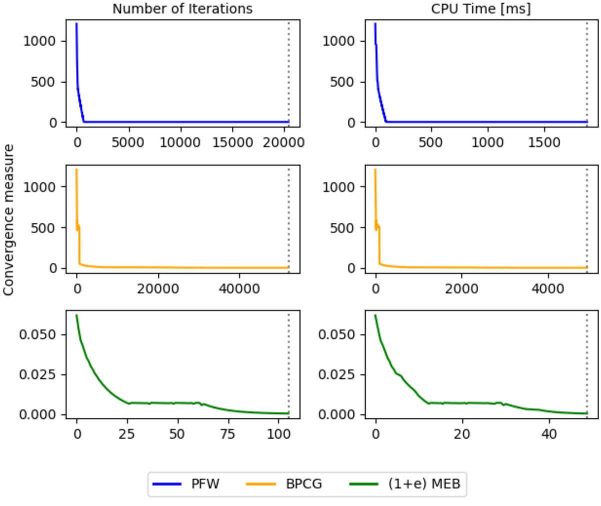


Figure 4: Convergence measure for Vertebral column dataset

Results

Dataset 4

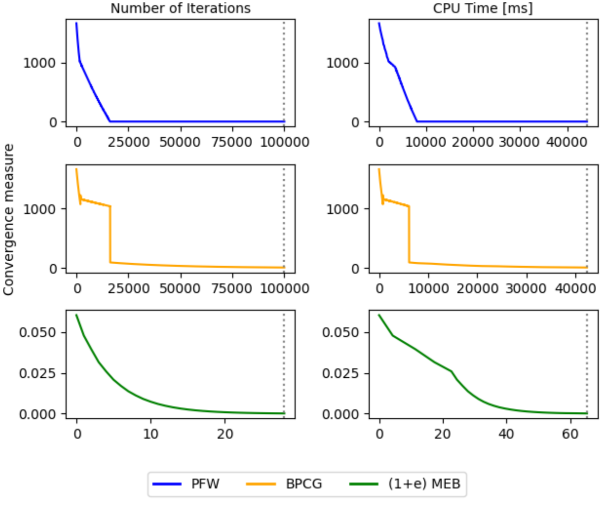


Figure 5: Convergence measure for Maternity risk dataset

Results

Dataset 4

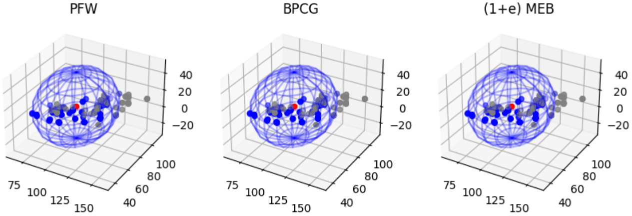


Figure 6: MEB for Maternity risk dataset

Results

	Time (ms)			Iterations		
Dataset	**PFW**	**BPCG**	**MEB(A)**	**PFW**	**BPCG**	**MEB(A)**
1	664.50	647.54	49.15	1,484	2,998	44
2	369,959.76	397,067.57	2,116.30	100,000	100,000	44
3	2,049.54	5,462.73	48.56	20,411	52,194	105
4	44,272.91	45,906.90	65.50	100,000	100,000	28

Table 2: Computational results with short step rule for BPCG and PFW

	Time (ms)		Iterations	
Dataset	**PFW**	**BPCG**	**PFW**	**BPCG**
1	65.40	31.50	396	163
2	125,779.36	130,001.06	100,000	100,000
3	18.76	115.47	158	2,155
4	62.19	70.12	168	292

Table 3: Computational results with diminishing step size

Results

	Recall Training			Recall Test		
Dataset	**PFW**	**BPCG**	**MEB(A)**	**PFW**	**BPCG**	**MEB(A)**
1	0.84	0.84	0.84	0.84	0.84	0.84
2	0.84	0.85	0.84	0.85	0.86	0.85
3	0.59	0.59	0.59	0.51	0.51	0.51
4	0.43	0.44	0.43	0.48	0.50	0.48

Table 4: Recall results with short step rule for BPCG and PFW.

	Recall Training			Recall Test		
Dataset	**PFW**	**BPCG**	**MEB(A)**	**PFW**	**BPCG**	**MEB(A)**
1	0.84	0.84	0.84	0.84	0.84	0.84
2	0.84	0.85	0.84	0.85	0.85	0.85
3	0.59	0.59	0.59	0.51	0.51	0.51
4	0.43	0.44	0.43	0.48	0.48	0.48

Table 5: Recall results with diminishing step size

Conclusion

- We presented the MEB problem approach to the anomaly detection task by means of three different algorithms related to the classical Frank-Wolfe.
- The three algorithms implemented allow drop steps, representing a significant improvement of the Frank-Wolfe algorithm, allowing sparser solutions.
- The $(1+\epsilon)$-approximation to the MEB algorithm outperformed the other methods on the datasets, showing faster convergence and lower computational cost.
- This is specially true when working with large-scale datasets.
- The initialization of the α and β as coreset points seems to give a good approximation of the optimal diameter from the very beginning
- Gradient computations are costly