

# Evolutionary Search and Fitness Landscapes of Pseudo-Boolean Problems

Doctoral dissertation

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# Slides available

<https://s.ntnu.no/phd-slides>



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# Outline

- 1 What this dissertation is about
- 2 How research was carried out
- 3 Summary of Publications
- 4 Concluding Remarks

## Section 1

# What this dissertation is about

# In this dissertation...

We deal with **descriptive theory** of **search landscapes** of **multimodal pseudo-Boolean** functions. We study these landscapes using **evolutionary computation**.

# What this dissertation is about

We deal with **descriptive theory** of **search landscapes** of **multimodal pseudo-Boolean** functions. We study these landscapes using **evolutionary computation**.

**Descriptive theory**: the use of mathematical notation to describe, measure, or quantify observations [Doe24].

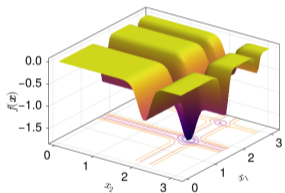
- ▶ Example: Fitness landscape analysis, schema theory...

We also use **experimentally guided theory**: setting up an artificial experiment, or experimentally analyse a particular question [Doe24].

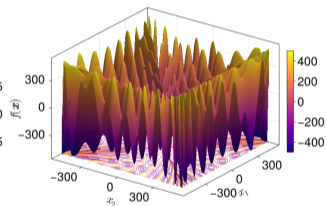
# What this dissertation is about

We deal with **descriptive theory** of **search landscapes** of **multimodal pseudo-Boolean** functions. We study these landscapes using **evolutionary computation**.

A **search landscape** is a visual representation of the solution space as it is navigated by a search method or optimisation algorithm [OM24].



(a) Michalewicz function



(b) Rana's function

Figure: Two optimisation landscapes: 2-dimensional continuous functions. The y-axis is used to plot the objective function, while the x- and z-axes are function parameters (shown here as  $x_1$  and  $x_2$ ).

# What this dissertation is about

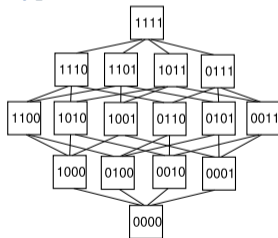
We deal with **descriptive theory** of **search landscapes** of **multimodal pseudo-Boolean** functions. We study these landscapes using **evolutionary computation**.

We focus on **pseudo-Boolean** functions (PBFs) [RS02].

- ▶ i.e. optimisation and search problems with objective functions of the form  $f: \mathbb{B}^n \rightarrow \mathbb{R}_{\geq 0}$

With a special interest in those with **multiple solutions** [LEDE17].

So search spaces look more like this →  
and usually contain many optima



# What this dissertation is about

We deal with **descriptive theory** of **search landscapes** of **multimodal pseudo-Boolean** functions. We study these landscapes using **evolutionary computation**.

We use **evolutionary algorithms** (EAs) as our heuristic search methods [Gol89]. Broadly, an EA can be defined as follows [Leh06]. Given a PBF  $f: \mathbb{B}^n \rightarrow \mathbb{R}_{\geq 0}$ ,

1. Initialise a population  $P$  with random elements from  $\mathbb{B}^n$
2. **While** stopping criterion is not met, **do**
  - 2.1 Select parents from  $P$  using fitness function  $f$
  - 2.2 Create a set of offspring  $C$  by recombining parents
  - 2.3 Stochastically mutate individuals in  $C$
  - 2.4 Select new individuals from  $P \cup C$  using  $f$  to form a new population  $P$
3. **return** the best individuals in  $P$  according to  $f$ .

## Section 2

# How research was carried out

# Research Context

## Research Structure

This dissertation encompasses research conducted from October 2021 to September 2025. The work was carried out in **two research directions**, comprising **three research objectives** and **six research questions** in total. Our results lead to **five publications**, all of which have been presented at both national and international venues.

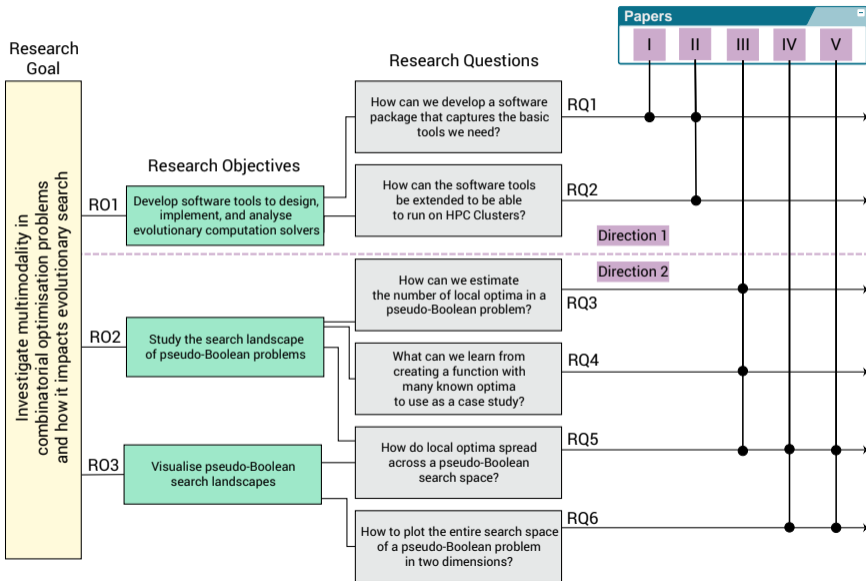
### Research Direction 1

Aimed at developing a code base for quick prototyping and testing of EAs.

### Research Direction 2

Focused on the analysis of search landscapes of multimodal PBFs.

# Overview of Research Structure



## Section 3

# Summary of Publications

# Paper I: EvoLP.jl: A Playground for Evolutionary Computation

Norwegian AI Society Symposium 2023 – Bergen, Norway



- ▶ Presents a Julia package for designing and implementing EAs through **building blocks**. *LP* comes from *Lekeplass*—“playground” in Norwegian.
- ▶ An **extensible computational unit** for each step in the evolution process
  - ▶ Initialisation → population **generator**:  $ind \rightarrow repr$
  - ▶ Selection → **selector**:  $P \rightarrow ind$
  - ▶ Crossover → **recombinator**:  $ind \times ind \rightarrow ind$
  - ▶ Mutation → **mutator**:  $ind \rightarrow ind$
  - ▶ Survival is usually algorithm dependent (but **selectors** can be used)
- ▶ It also includes test functions, results reporting, statistics computing, and a few built-in solvers for toy examples.

# Why Julia?

Paper I: EvoLP.jl: A Playground for Evolutionary Computation

- ▶ It is fast!
  - ▶ Type-inference and JIT compilation using LLVM
  - ▶ **1.54 petaFLOPs** on 1.3M threads over 9K KNL Nodes [Jul17]
- ▶ Solves the *two-language* problem [BEKS17]—one language instead of:
  - ▶ a simple language for scripting
  - ▶ another performant language for production
- ▶ Multiple dispatch allows for a **natural mapping** of evolutionary computation concepts to code

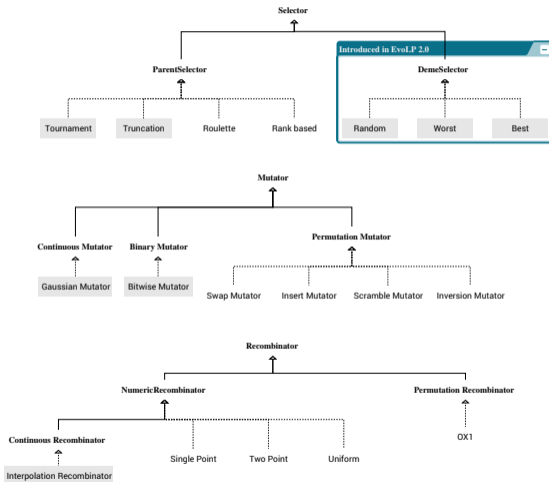
A high-level, high-performance programming language for scientific computing

# Paper I: EvoLP.jl: A Playground for Evolutionary Computation

Norwegian AI Society Symposium 2023 – Bergen, Norway

RQ1: How can we develop a software package that captures the basic tools we need?

- ▶ By **formalising** a type hierarchy [KW19] that closes the gap between modelling and implementation.
- ▶ Taking advantage of Julia's multiple dispatch—one function, several implementations depending on parameter types [Kwo].



# Paper II: Evolutionary Computation with Islands: Extending EvoLP.jl for Parallel Computing

Norsk IKT-konferanse for forskning og utdanning 2023 – Stavanger, Norway



# NIKT

Norwegian ICT conference  
for research and education  
**NIKT2023**

- ▶ Presents an extension for EvoLP.jl to run island models on **HPC systems** [SM23b]
  - ▶ Uses the Message Passing Interface (MPI) communication scheme [Mes21]
- ▶ Based on the **generalised island model** of Izzo et al. [IRB12]. Given an archipelago (set of islands and their topology), each island will:
  1. Run an EA with its parameters
  2. Select a deme  $\mathbb{M}$  from  $P$  using a selection policy
  3. **Send**  $\mathbb{M}$  to adjacent islands w.r.t the topology
  4. **Receive**  $\mathbb{M}'$  individuals from adjacent islands
  5. **Reinsert**  $\mathbb{M}'$  into the island's  $P$  using a replacement policy
  6. Continue running until termination/sync

Steps 3 and 4 are mapped directly with MPI directives!

# Paper II: Evolutionary Computation with Islands: Extending EvoLP.jl for Parallel Computing

Norsk IKT-konferanse for forskning og utdanning 2023 – Stavanger, Norway

RQ2: How can the software tools be extended to be able to run on HPC Clusters?

- ▶ By **formalising** the communication and **implementing** appropriate blocks [SM23a].
- ▶ Exploiting convergence and **diversity preservation** benefits from communication [ES15].
- ▶ Tested on both **local** hardware and NTNU's **HPC system**, Idun [SJTR22]

## drift operator

Send individuals from one island to another

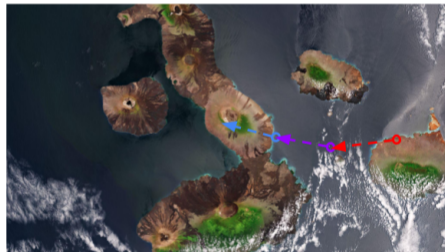
## strand operator

Receive individuals from another island

## reinsert! operator

Reinsert individuals into population according to a given policy

## The island model



The Galapagos Islands, Copernicus Sentinel (2020), ESA

# Paper II: Evolutionary Computation with Islands: Extending EvoLP.jl for Parallel Computing

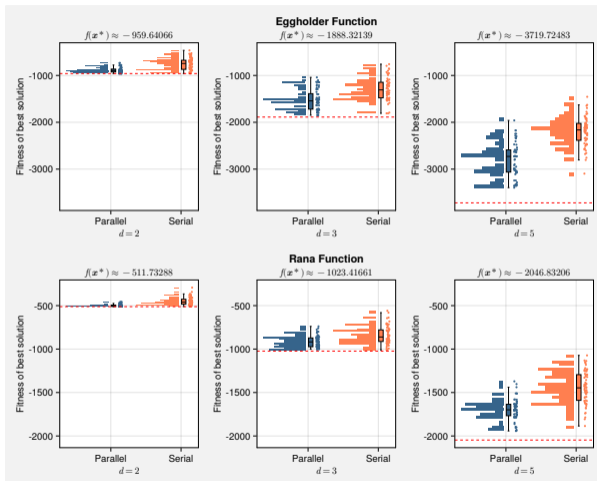
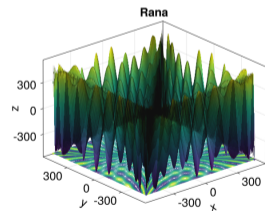
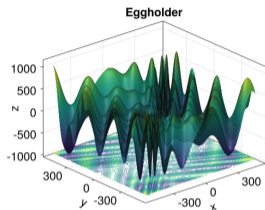
Norsk IKT-konferanse for forskning og utdanning 2023 – Stavanger, Norway

- ▶ **Test 1:** Empirical comparison of serial vs parallel island model approaches, using a unidirectional ring topology with 64 islands. Each island with a steady state GA with random deme selection policy, and replace-worst policy.
  - ▶ Ackley, Rosenbrock, and Michalewicz test functions, for dimensions  $d \in \{2, 5, 10\}$
  - ▶ Migration every 10 iterations (5 for Michalewicz)
  - ▶ Results hint at **better convergence** to the known optima when run **on parallel**.
  
- ▶ **Test 2:** Empirical comparison of the impact of exploration on island models on highly multimodal test functions. Same topology.
  - ▶ Eggholder and Rana test functions, for dimensions  $d \in \{2, 3, 5\}$
  - ▶ Migration every 10 generations
  - ▶ Results show **smaller spread of fitnesses** across populations.

Implemented as an **extension** in EvoLP.jl in Oct. 2025:

<https://ntnu-ai-lab.github.io/EvoLP.jl/stable/man/islands.html>

# Paper II: Test 2



► Higher median of best solutions on **serial approach**

► *Better exploration* overall using the **parallel approach**

## Subsection 2

# Research Direction II — Landscape Analysis

# Paper III: Estimating the Number of Local Optima in Multimodal Pseudo-Boolean Problems: Validation via Landscapes of Triangles

Genetic and Evolutionary Computation Conference 2024 – Melbourne, Australia

Introduces Triangle, a synthetic PBF with an **adjustable number of optima**.

- ▶ Dependent on the interaction of its parameters [SM24]
- ▶ We use it to estimate the number of optima in landscapes with different structures
- ▶ The estimation procedure is based on the **Birthday Paradox** [Mat91]
  - ▶ First studied by Caruana and Mullin [CM00] for continuous optimization
  - ▶ Later studied by Hernando et al. [HML13] for TSP



Given 365 days in a year, how many people in a room do we need to find a repeated birthday with  $p \geq 0.5$ ?

# Paper III: Estimating the Number of Local Optima in Multimodal Pseudo-Boolean Problems: Validation via Landscapes of Triangles

Genetic and Evolutionary Computation Conference 2024 – Melbourne, Australia

- ▶ RQ3: How can we estimate the number of local optima in a PBF?
- ▶ RQ4: What can we learn from creating a function with many known optima to use as a case study?
- ▶ RQ5: How do local optima spread across a pseudo-Boolean search space?

By using the *reverse* birthday paradox:

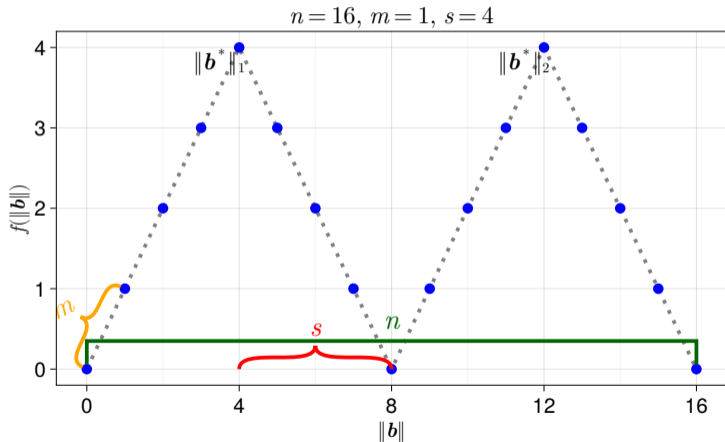
Given this many **people** in a room with a repeated birthday, how many **days** are there in a *year*?

- ▶ **Sampling procedures** are essential for landscape analysis
- ▶ The size and distribution of **basins of attraction** affect algorithm behaviour

# Paper III: Estimating the Number of Local Optima in Multimodal Pseudo-Boolean Problems: Validation via Landscapes of Triangles

Genetic and Evolutionary Computation Conference 2024 – Melbourne, Australia

- ▶  $n$  is the bitstring length
  - ▶ There are  $nCk$  bitstrings at  $\|b\| = k$
- ▶  $s$  is a segmenting factor
  - ▶ or *the step*
  - ▶ number of bit flips to optimum
  - ▶ determines peak width
- ▶  $m$  is a scaling factor
  - ▶ or *the slope*
  - ▶ scales fitness
  - ▶ can introduce deception



Triangle( $\mathbf{b}$ ,  $m = 1$ ,  $s = 2$ ),  $\mathbf{b} \in \mathbb{B}^4$

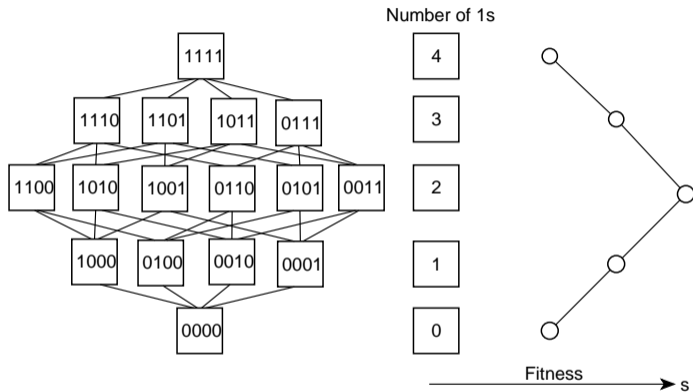
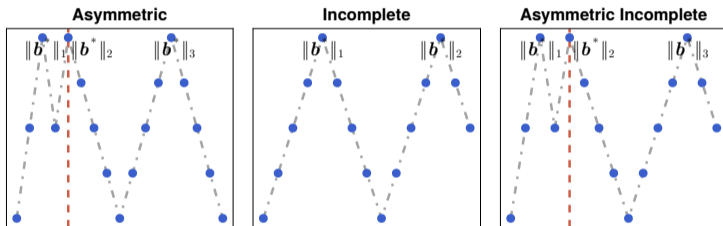


Figure: The search space of a Triangle function with  $n = 4$ ,  $m = 1$ , and  $s = 2$ , and how each state relates to its objective function. Note no edge exists between two states with the same fitness.

# Paper III: Estimating the Number of Local Optima in Multimodal Pseudo-Boolean Problems: Validation via Landscapes of Triangles

Genetic and Evolutionary Computation Conference 2024 – Melbourne, Australia



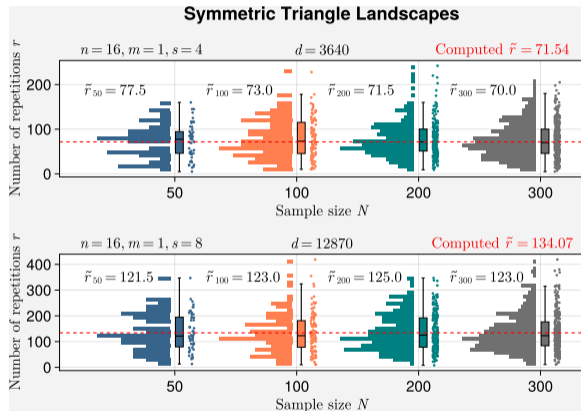
- ▶ We can create several landscape structures using parameter interaction
- ▶ One landscape from several Triangle functions
  - ▶ piecewise definition
  - ▶ different *Region of attraction* sizes

Two experiments using a 1+1-EA for sampling, using random initialisation:

- 1) **Symmetric** landscapes
- 2) **Asymmetric, Incomplete**, and **Asymmetric Incomplete** landscapes

# Symmetric Landscapes

## Paper III: Experiment 1 — Estimating Local Optima in Symmetric Landscapes



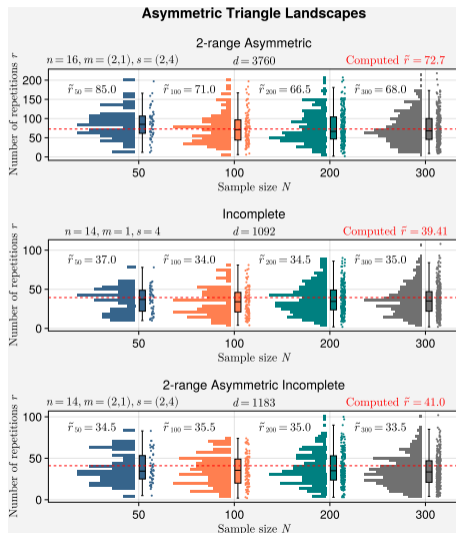
- ▶ The estimation procedure is noticeably accurate on **symmetric landscapes** (with uniformly distributed optima)
  - ▶ Even with a small number of samples  $N$ , empirical estimates (medians) are close to the **computed estimate**
  - ▶ Large landscapes are naturally more difficult to sample evenly

# Asymmetric Landscapes

## Paper III: Experiment 2 — Estimating Local Optima in Asymmetric Landscapes

- ▶ **Incomplete** landscapes ( $n \text{ div } s \notin \mathbb{Z}$ ) have larger difference in the size of their regions of attraction
  - ▶ Estimates are still relatively accurate, although not as in symmetric landscapes
- ▶ Estimates on **asymmetric** landscapes are more accurate than those in incomplete landscapes
  - ▶ Less accurate than symmetric landscapes

Useful for **budgeting** purposes!



# Paper IV: Regularized Feature Selection Landscapes: An Empirical Study of Multimodality

Parallel Problem Solving from Nature XVIII, 2024 – Hagenberg, Austria

Studies the effect of **regularisation** on the search landscape of **feature selection** (a real-world, highly multimodal PBF [MMOE19]).



- ▶ We study 10 classification datasets from UCI [KRK]
  - ▶ Paper IV focuses on two of them: *Glass identification* [Ger87] and *Heart Disease (Cleveland)* [And89]
  - ▶ Here we show only a subset of the results for brevity
- ▶ Introduces the **Hinged-Bitstring Map (HBM)** [SMM24]
  - ▶ Visual overview of the entire pseudo-Boolean landscape
  - ▶ Highlights the **distribution of optima** across the landscape
  - ▶ Works in combination with **Local-Optima Networks** [SMM24; MSM25]

# Paper IV: Regularized Feature Selection Landscapes: An Empirical Study of Multimodality

Parallel Problem Solving from Nature XVIII, 2024 – Hagenberg, Austria

- ▶ RQ5: How do local optima spread across a pseudo-Boolean search space?
- ▶ RQ6: How to plot the entire search space of a PBF in two dimensions?

Precomputing the entire landscape to **count** the optima and **visualise** their distribution using HBMs [SMM24], LONs [OTVD08; OVDT14], and fitness-distance correlation [SM25].

Three experiments:

1. Impact of varying regularisation
2. Visualising regularisation
3. Visualising connectedness and optima distribution

# Paper IV: Regularized Feature Selection Landscapes: An Empirical Study of Multimodality

Parallel Problem Solving from Nature XVIII, 2024 – Hagenberg, Austria

## Feature selection [SMM24]

Consider a bitstring  $\mathbf{b} = b_1, \dots, b_n$  indicating which features are included ( $b_i = 1$ ) or not ( $b_i = 0$ ). We model the feature selection problem as an *energy* function to **minimize**:

$$h(\mathbf{b}) = h_E(T(\mathbf{b})) + \epsilon \cdot h_P(\mathbf{b}),$$

where  $h_E(T(\mathbf{b}))$  is the **classification error** over a given dataset using a model  $T$ ,  $h_P(\mathbf{b})$  is a penalty depending on the number of features used for training with feature subset  $\mathbf{b}$ , and  $\epsilon$  controls the degree of regularisation.

For this paper,  $T$  is a **decision tree** trained on all  $2^n$  feature subsets.

# Paper IV: Regularized Feature Selection Landscapes: An Empirical Study of Multimodality

Parallel Problem Solving from Nature XVIII, 2024 – Hagenberg, Austria

## Exhaustive enumeration - landscape precomputing

1. Enumerate all bitstrings  $\mathbf{b}_i, i \in \{1, 2, \dots, 2^n - 1\}$ 
  - ▶ e.g., bitstring  $\mathbf{b}_7 = 00000111$ , with  $n = 8$
  - ▶ i.e., «using the first three features, not using the remaining five»
2. Train a decision tree using  $T(\mathbf{b}_i)$  and store its classification error
  - ▶ using 70% of the data for training
  - ▶ testing on the remaining 30%
3. Use the classification error as a surrogate for the *fitness*
4. Calculate regularisation with varying degrees of  $\epsilon \in \{0, 1/8, 1/16, 1/32\}$

Massive amounts of parallel compute provided by NTNU's **HPC system**, Idun [SJTR22].  
The surrogate tables are available in UiT's Dataverse.NO [Sán24].

# Data

## Paper IV — Experiment 1: Impact of Varying Regularisation

Table: Datasets used in Paper IV, sorted by number of features ( $n$ ). We show the number of examples  $m$ , and the number of local  $|\mathbf{L}|$  and global optima  $|\mathbf{G}|$  for various values of the regularization term  $\epsilon$ .

Name	$n$	$m$	Number of optima							
			$\epsilon = 0$		$\epsilon = 1/32$		$\epsilon = 1/16$		$\epsilon = 1/8$	
			$ \mathbf{L} $	$ \mathbf{G} $	$ \mathbf{L} $	$ \mathbf{G} $	$ \mathbf{L} $	$ \mathbf{G} $	$ \mathbf{L} $	$ \mathbf{G} $
1-seeds	7	210	20	5	14	1	6	1	7	1
2-e-coli	7	336	17	1	7	1	7	1	6	1
3-breast-w	9	699	65	2	6	1	9	1	9	1
<b>4-glass</b>	9	214	65	1	51	2	22	2	7	2
<b>5-heart-c</b>	13	303	700	1	407	1	117	1	13	1
6-wine	13	178	976	58	286	2	29	3	14	3
7-credit-a	15	690	2511	4	351	1	18	1	15	1
8-zoo	16	101	10862	8275	3003	1	134	1	16	1
9-letter-r	16	20000	3964	1	16	1	16	1	16	1
10-hepatitis	19	155	50985	2284	23577	3	7621	3	133	3

# The Hinged-Bitstring Map (HBM)

Paper IV — Experiment 2: Visualising Regularisation

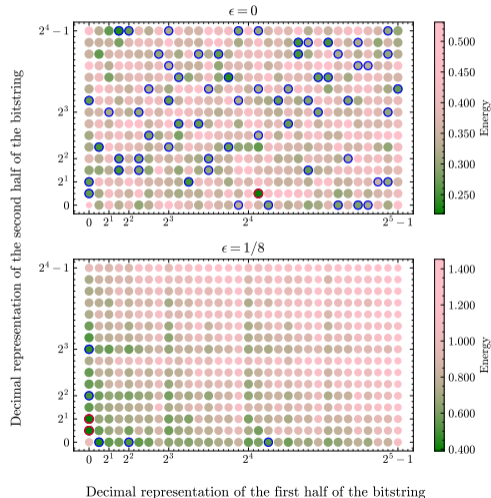
## HBM construction

For each bitstring  $\mathbf{b}_i \in \mathbb{B}^n$

1. Split  $\mathbf{b}_i$  into halves<sup>a</sup>  $\mathbf{b}_{i_1} \parallel \mathbf{b}_{i_2}$ 
  - ▶ e.g.,  $\mathbf{b}_{167} = 1010 \parallel 0111$
2. Use  $\text{Dec}(\mathbf{b}_{i_1})$ , as the  $x$ -coordinate
3. Use  $\text{Dec}(\mathbf{b}_{i_2})$  as the  $y$ -coordinate
4. Plot  $\mathbf{b}_i$  at  $(x, y)$  as a scatter plot, using colour for fitness
  - ▶ i.e.,  $\mathbf{b}_{167} \mapsto (10, 7)$
5. Highlight **global** and **local** optima

<sup>a</sup>in favour of  $\mathbf{b}_{i_1}$  if  $n$  is odd

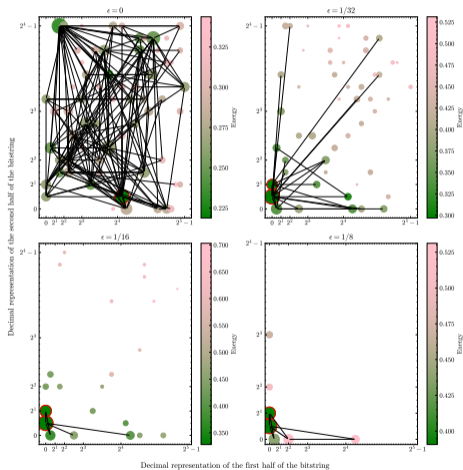
Figure: *Glass Identification* ( $\epsilon \in \{0, 1/8\}$ )



# LONs and HBMs

## Paper IV — Experiment 3: Connectedness and Optima Distribution

Figure: *Glass identification* ( $\epsilon \in \{0, 1/32, 1/16, 1/8\}$ )



## Local Optima Network (LON)

A graph representation of a **multimodal** landscape [OTVDo8; OVDT14].

- ▶ Nodes are **local optima**
- ▶ Edges represent connections (or the *probability of a connection*) between basins
- ▶ Node size is proportional to basins of attraction size

Regularisation transforms the landscape:

- ▶ Optima disappear, basins are split, and connectivity decreases

# Paper V: Visualizing Pseudo-Boolean Functions: Feature Selection and Regularization for Machine Learning

25th European Conference on Evolutionary Computation in Combinatorial Optimization, 2025 – Trieste, Italy

Delves further into visualisation of PBFs through both synthetic and **feature selection** problems.



- ▶ We study four additional datasets from UCI [KRK]
  - ▶ Paper V highlights *Dry Bean* [KÖ20] and *Bank Marketing* [MRC12]
  - ▶ In contrast to Paper IV, here we use a **random forest classifier** (with `n_trees= 10`)
- ▶ This paper also formalises the **Hinged-Bitstring Map (HBM)** [SMM24]
  - ▶ Proof of the impossibility of keeping neighbourhood structure in  $\mathbb{R}^2$ 
    - ▶ Based on the work by Masson [Mas24]
  - ▶ Introduces the LON+HBM [MSM25; SM25]

# Paper V: Visualizing Pseudo-Boolean Functions: Feature Selection and Regularization for Machine Learning

25th European Conference on Evolutionary Computation in Combinatorial Optimization, 2025 – Trieste, Italy

- ▶ RQ5: How do local optima spread across a pseudo-Boolean search space?
- ▶ RQ6: How to plot the entire search space of a PBF in two dimensions?

In a similar fashion to Paper IV, we precompute the entire landscape to **count** the optima and **visualise** their distribution using HBMs [SMM24] and LONs [OTVD08; OVDT14].

Two case studies:

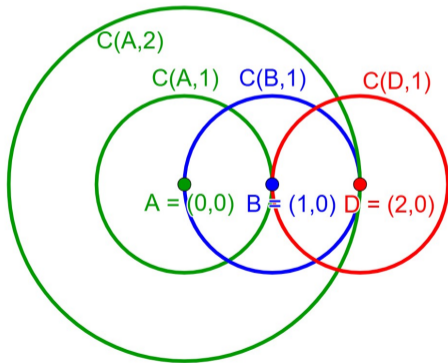
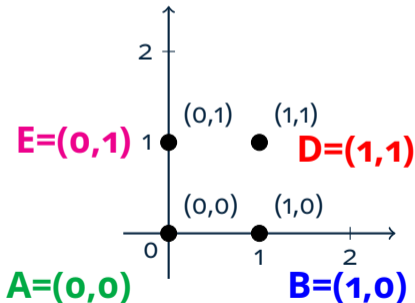
1. Toy problem in  $\mathbb{B}^6$
2. Real-world case: **feature selection** with regularisation

# Preserving Neighbourhood Structure

Paper V — Analysis of Visualisation

## Lemma

*There is no isometric embedding from  $\mathbb{B}^2$  into  $\mathbb{R}^2$  that preserves the Hamming distance as the Euclidean distance [Mas24].*



# Enhancing the HBM

Paper V — Analysis of Visualisation

Since there is no way around the neighbourhood distortion in 2D, we may as well enhance our visualisation. An HBM can be enhanced by combining it with a LON [SM25]:

- ▶ Using **arrows** to show connectedness between optima (like a LON)
- ▶ Using **size** to convey the size of **basin of attraction** (like a LON)
- ▶ Using the **position** resulting from the coordinate system of the HBM

Using the **aesthetic** and **geometric elements** of both visualisations [Wil05], they can be merged by superimposing one on top of the other [JE12].

# HBM+

Paper V — Case Study 1: A toy problem in  $\mathbb{B}^6$ :  $\sin(2\text{Dec}(b))$

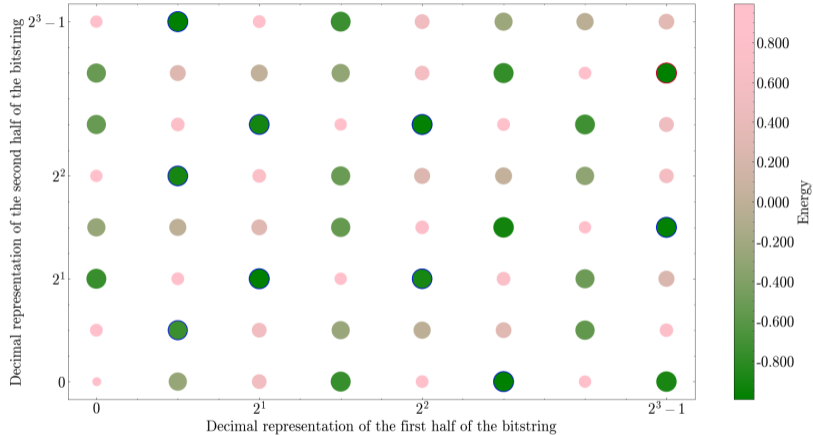


Figure: An HBM for  $\sin(2\text{Dec}(b))$ , altering the **size** of local and global optima.

# HBM+Arrows

Paper V — Case Study 1: A toy problem in  $\mathbb{B}^6$ :  $\sin(2\text{Dec}(b))$

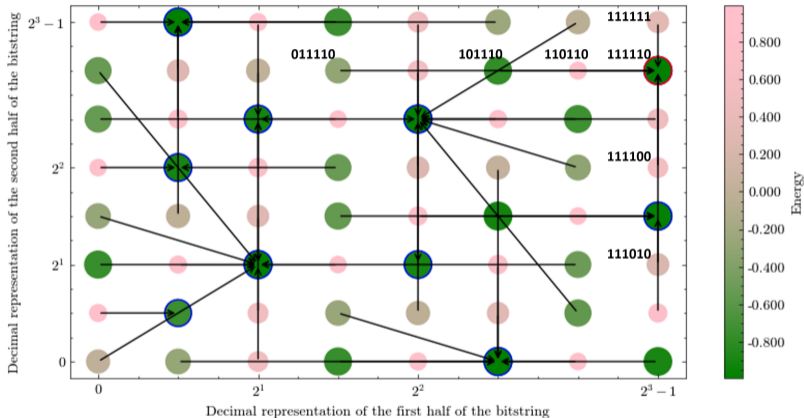


Figure: An HBM for  $\sin(2\text{Dec}(b))$ , altering the **size** aesthetic and adding **arrow** geometries for connectivity between basins.

# HBM+LON

Paper V — Case Study 1: A toy problem in  $\mathbb{B}^6$ :  $\sin(2\text{Dec}(b))$

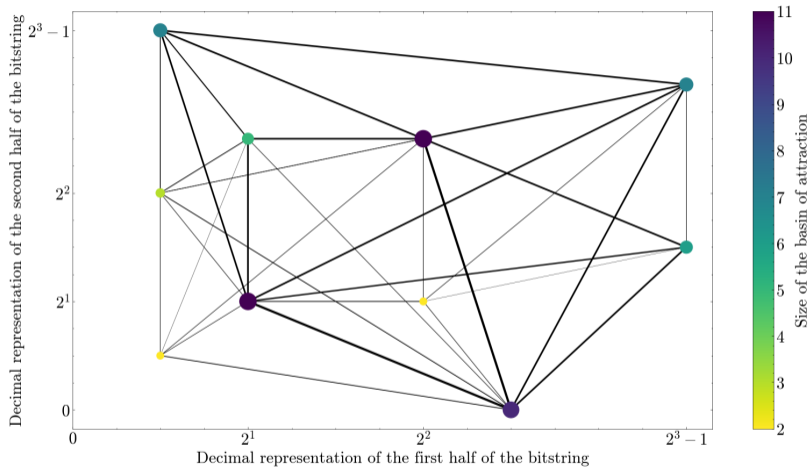


Figure: An HBM+LON for  $\sin(2\text{Dec}(b))$ . Nodes represent specific bitstrings.

# Data

## Paper V — Case Study 2: Feature Selection and Regularisation

Table: Datasets used in Paper V. We present number of features ( $n$ ), number of examples ( $m$ ) and number of classes.

Name	Subject Area	$n$	$m$	Number of Classes
Yeast [Nak96]	Biology	8	1484	10
HTRU2 [Ly017]	Physics and Chemistry	8	17898	2
Dry Bean [KÖ20]	Biology	16	13611	7
Bank Marketing [MRC12]	Business	16	45211	2

## Reminder: Feature Selection

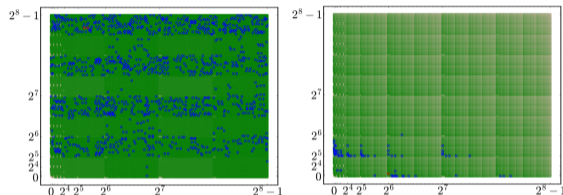
$$h(\mathbf{b}) = h_E(T(\mathbf{b})) + \epsilon \cdot h_P(\mathbf{b})$$

For this paper,  $T$  is a **random forest** classifier trained on all  $2^n$  feature subsets, 70%/30% train/test split, using the default parameters in scikit-learn.

# Visualising Regularisation

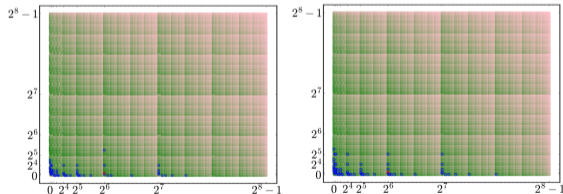
## Paper V — Case Study 2: Feature Selection and Regularisation

Figure: Classification error of  $T$  on *Dry Bean* with regularisation values  $\epsilon \in \{0, 1/32, 1/16, 1/8\}$ .



(a)  $\epsilon = 0$

(b)  $\epsilon = 1/32$



(c)  $\epsilon = 1/16$

(d)  $\epsilon = 1/8$

Similar findings as in Paper IV!

- ▶ **Number of optima** diminishes drastically
- ▶ The model prefers bitstrings with fewer 1s
- ▶ **Data preprocessing and treatment** affect the number and distribution of optima over the landscape
- ▶ Several repetitions are necessary when dealing with **stochastic** classifiers

## Section 4

# Concluding Remarks

# Contributions

## Concluding Remarks

Some of the contributions from our research include:

1. A **software framework**: EvoLP.jl
  - ▶ and its extension for HPC!
2. A **new multimodal PBF**: Triangle
3. A novel **visualisation technique** for PBFs: HBM
4. A series of **precomputed fitness landscapes** (*lookup tables*)

# Limitations and Future Work

## Concluding Remarks

...and there plenty of ways to continue our work!

### ▶ **Extending HBMs**

- ▶ Build *sparse* HBMs from samples
- ▶ HBMs and their mapping
- ▶ HBMs to visualise evolutionary operators
- ▶ HBMs to represent formulas or operators in propositional logics

### ▶ **Formal analysis** of Triangle

- ▶ Testing other **sampling procedures** for local optima estimation
- ▶ Using **different ML models** for feature selection landscapes
  - ▶ Computing repetitions and logging compute time
  - ▶ Consider regularisation as a multiple-objective problem

That's it.

# The thesis is available online

at the Norwegian Research Information Repository (NVA)

<https://s.ntnu.no/phd-thesis>



<https://s.ntnu.no/phd-thesis>

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## Section 6

# Additional Material

# Research Direction 1

## Research Structure

### Research Objective 1

Develop software tools to design, implement, and analyse evolutionary computation solvers.

- ▶ RQ1: How can we develop a software package that captures the basic tools we need?
  - ▶ **Paper I:** EvoLP.jl: A Playground for Evolutionary Computation in Julia (NAIS 2023)
- ▶ RQ2: How can the software tools be extended to be able to run on HPC Clusters?
  - ▶ **Paper II:** Evolutionary Computation with Islands: Extending EvoLP.jl for Parallel Computing (NIKT 2023)

# Research Direction 2

## Research Structure

### Research Objective 2

Study the search landscape of pseudo-Boolean problems.

### Research Objective 3

Visualise pseudo-Boolean search landscapes.

- ▶ RQ3: How can we estimate the number of local optima in a PBF?
- ▶ RQ4: What can we learn from creating a function with many known optima to use as a case study?
  - ▶ **Paper III**: Estimating the Number of Local Optima in Multimodal Pseudo-Boolean Problems: Validation via Landscapes of Triangles (GECCO 2024)
- ▶ RQ5: How do local optima spread across a pseudo-Boolean search space?
- ▶ RQ6: How to plot the entire search space of a PBF in two dimensions?
  - ▶ **Paper IV**: Regularized Feature Selection Landscapes: An Empirical Study of Multimodality (PPSN 2024)
  - ▶ **Paper V**: Visualizing Pseudo-Boolean Functions: Feature Selection and Regularization for Machine Learning (EvoCOP 2025)

# Paper I: EvoLP.jl: A Playground for Evolutionary Computation

Norwegian AI Society Symposium 2023 – Bergen, Norway

- ▶ **Example 1:** a **Simple Genetic Algorithm** (GA) [Gol89] solving a continuous problem, the Rosenbrock test function.
  - ▶ Random initialisation:  $\mathbf{x} \in X \sim \mathcal{N}(\mu, \sigma^2)$  with  $\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$  and  $\sigma^2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
  - ▶ Rank-based selection
  - ▶ Interpolation crossover  $\lambda = 0.5$
  - ▶ Gaussian mutation  $\sigma = 0.5$
- ▶ **Example 2:** a **steady state GA** [Sim13] solving a combinatorial problem, the 8-queens problem [RN20].
  - ▶ Random initialization:  $\mathbf{x} \in X \sim \mathcal{U}(\mathcal{S}_8)$  where  $\mathcal{S}_8$  is the set of permutations of  $[8] = \{1, 2, \dots, 8\}$
  - ▶ Random tournament selection, with tournament size  $T_s = 5$
  - ▶ Order-one crossover
  - ▶ Swap mutation

Worked examples are available in the documentation: <https://ntnu-ai-lab.github.io/EvoLP.jl/>

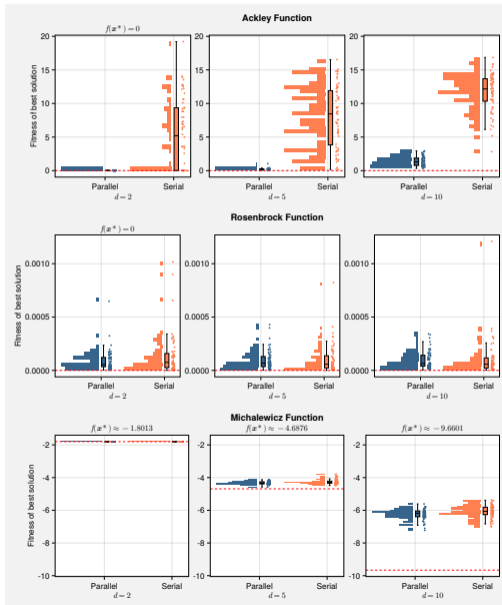
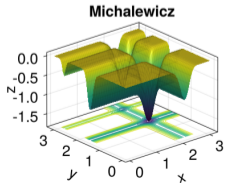
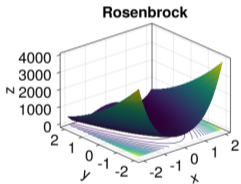
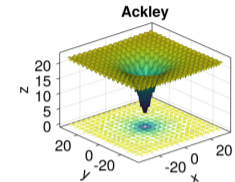
# The (1+1)-EA in EvoLP.jl

```
function oneplusone!(
    logger::Logbook, f::Function, ind::AbstractVector, k_max::Integer, M::Mutator
)
    fx = Inf # works only on minimisation problems
    runtime = @elapsed for _ in 1:k_max
        c = mutate(M, ind)
        fx, fc = f(ind), f(c)
        if fc <= fx #  $O(2 * k\_max)$  # minimisation problem
            ind = c
            fx = fc
        end
        compute!(logger, [fx])
    end

    n_evals = 2k_max

    return Result(fx, ind, [ind], k_max, n_evals, runtime)
end
```

# Paper II: Test 1



- ▶ Serial approach has higher spread
- ▶ Parallel approach has better convergence

# Paper III: Estimating the Number of Local Optima in Multimodal Pseudo-Boolean Problems: Validation via Landscapes of Triangles

Genetic and Evolutionary Computation Conference 2024 – Melbourne, Australia

## Definition

Let  $\|\mathbf{b}\|$  be the number of 1s in the bitstring  $\mathbf{b} \in \mathbb{B}^n$ . Then, the *triangular positive wave function*, or `Triangle` for short, is defined as:

$$\text{Triangle}(\mathbf{b}, m, s) = \begin{cases} g(\mathbf{b}), & \text{if } \left\lceil \frac{\|\mathbf{b}\|}{s} \right\rceil \bmod 2 = 1 \\ m \left( \left\lceil \frac{\|\mathbf{b}\|}{s} \right\rceil \cdot s - \|\mathbf{b}\| \right) & \text{otherwise} \end{cases} \quad (1)$$

where

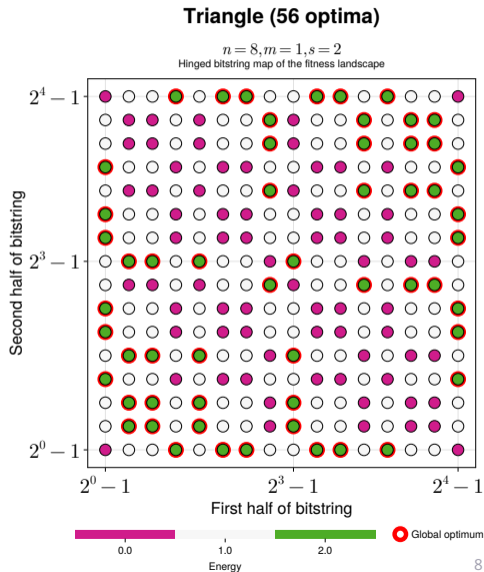
$$g(\mathbf{b}) = \begin{cases} m \cdot s, & \text{if } \|\mathbf{b}\| \bmod s = 0 \\ m(\|\mathbf{b}\| \bmod s) & \text{otherwise.} \end{cases} \quad (2)$$

Triangle( $\mathbf{b}$ ,  $m = 1$ ,  $s = 2$ ),  $\mathbf{b} \in \mathbb{B}^8$

► The search space can be partitioned into three levels according to fitness:

- Level 1:  $f(\mathbf{b}) = 0$  with 0 ones
- Level 2:  $f(\mathbf{b}) = 1$  with 1 one
- Level 3:  $f(\mathbf{b}) = 2$  with 2 ones

Easy to find any optima, not as easy to find all of them!



# Fitness-Distance Correlation

Paper IV — Experiment 2: Visualising Regularisation

*Big valley*

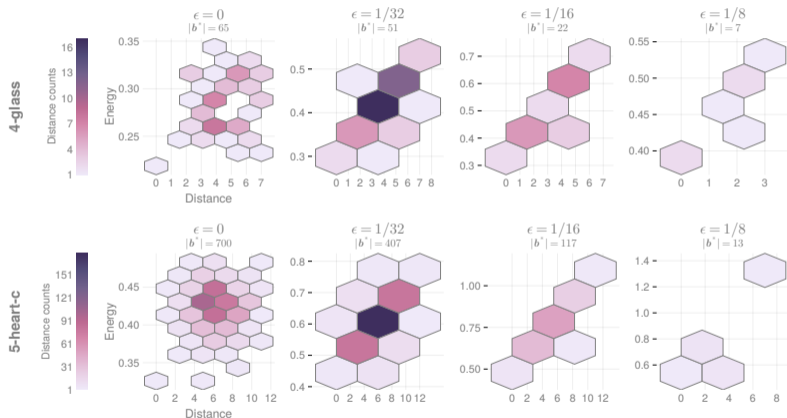
hypothesis [TO22]:

- ▶ Funnel structures
- ▶ Many local optima concentrated around a global optimum

Regularisation splits the big valley into **rings**

- ▶ Informally, we say that basin size is reduced

Hamming distance to closest global minimum



# Preserving Neighbourhood Structure

Paper V — Analysis of Visualisation

## Lemma

*There is no isometric embedding from  $\mathbb{B}^2$  into  $\mathbb{R}^2$  that preserves the Hamming distance as the Euclidean distance [Mas24].*

## Proof.

Let  $A, B, E$  and  $D$  be the bitstrings 00, 10, 01 and 11, respectively. Put  $A$  anywhere in Euclidean space, and draw its Hamming shell of radius 1 with a circle. Place  $B$  (a neighbour of  $A$ ) on this circle, such that  $H(A, B) = 1$ . Place  $D$  in space such that  $H(A, D) = 2$  and  $H(B, D) = 1$ . However, there is no point in Euclidean space for  $E$  other than on top of  $B$ . Hence, there is no isometric embedding between the two spaces that preserves the original distance. □

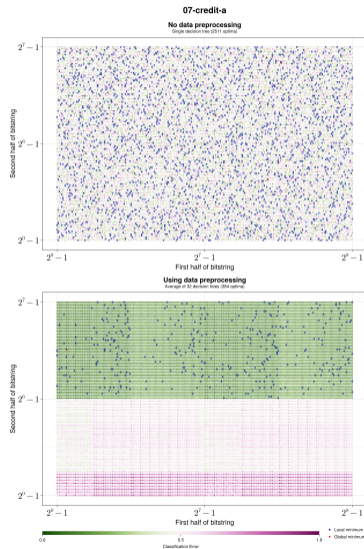
# Data preprocessing and treatment

Credit approval [Qui87], with  $n = 15$  features and  $m = 20000$  rows

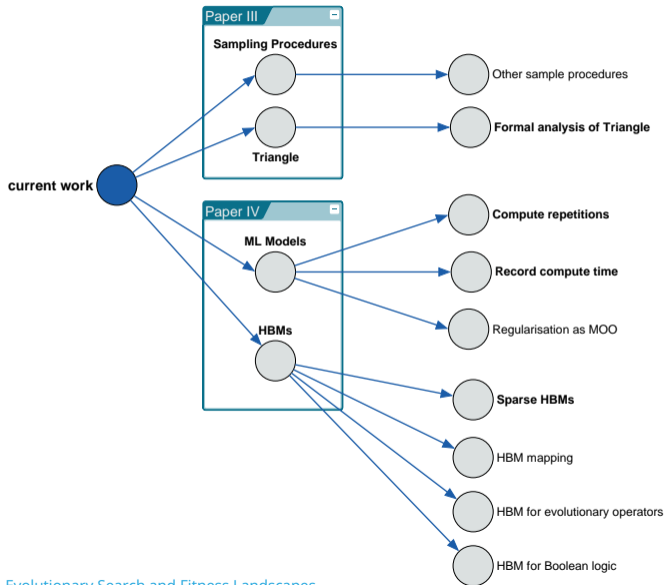
Data preprocessing reduces number of optima and generates *dense* landscapes. Informally:

- ▶ Dense landscapes are *easier* to optimise
- ▶ Learning occurs due to the presence of *some structure*

Landscapes depend on the data, the algorithm, and its hyperparameters!



# Future Work



## Subsection 6

### **Additional Research Contributions**

# Additional Research Contributions I

- ▶ **GECCO 2023: Comparing Metaheuristic Optimization Algorithms for Ambulance Allocation: An Experimental Simulation Study**
  - ▶ Schjøberg, M. E., Bekkevold, N. P., Sánchez-Díaz, X. F. C., & Mengshoel, O. J. (2023). Comparing Metaheuristic Optimization Algorithms for Ambulance Allocation: An Experimental Simulation Study. Proceedings of the Genetic and Evolutionary Computation Conference, 1454--1463. <https://doi.org/10.1145/3583131.3590345>
- ▶ **GECCO 2023: Controlling Hybrid Evolutionary Algorithms in Subset Selection for Multimodal Optimization**
  - ▶ Mengshoel, O. J., Foss, F., & Sánchez-Díaz, X. F. C. (2023). Controlling Hybrid Evolutionary Algorithms in Subset Selection for Multimodal Optimization. Proceedings of the Companion Conference on Genetic and Evolutionary Computation, 507-510. <https://doi.org/10.1145/3583133.3590545>

## Additional Research Contributions II

- ▶ **NorwAI Innovate 2024: Investigating the Ethical Dimensions of AI: An Interdisciplinary Approach Combining CBR and “It Could be Otherwise”**
  - ▶ Wang, S., Ecclesia, S., Sánchez-Díaz, X. F. C., Søraa, R. A. & Øztürk, P. (2024). Investigating the Ethical Dimensions of AI: An Interdisciplinary Approach Combining CBR and “It Could be Otherwise”. NorwAI Innovate Conference 2024. (Trondheim, Norway. Sep. 2024).
  
- ▶ **NAIS 2025: Multimodality in Combinatorial Search Landscapes**
  - ▶ Sánchez-Díaz, X. F. C., & Mengshoel, O. J. (2025). Visualizing Multimodality in Combinatorial Search Landscapes (No. arXiv:2510.06517). arXiv. <https://doi.org/10.48550/arXiv.2510.06517>

## Additional Research Contributions III

- ▶ **GECCO 2025: Empirical Studies of Multimodality in Feature Selection: Generalized Crowding for Genetic Algorithms**

- ▶ Masson, C., Mengshoel, O. J., & Sánchez-Díaz, X. F. C. (2025). Empirical Studies of Multimodality in Feature Selection: Generalized Crowding for Genetic Algorithms. Proceedings of the Genetic and Evolutionary Computation Conference Companion, 235–238. <https://doi.org/10.1145/3712255.3726535>

- ▶ **NorwAI Innovate 2025: Understanding Multimodality in Feature Selection Landscapes**

- ▶ Sánchez-Díaz, X. F. C., & Mengshoel, O. J. (2025). Understanding Multimodality in Feature Selection Landscapes. NorwAI Innovate Conference 2025. (Trondheim, Norway. Sep. 2025).

# Additional Research Contributions IV

- ▶ **GECCO 2026: Benchmarking Evolutionary and Machine Learning Algorithms: The SIREN Challenge of Emergency Medical Services**
  - ▶ Kallekleiv, T.A, Sánchez-Díaz, X. F. C., & Mengshoel, O. J. (2026). Benchmarking Evolutionary and Machine Learning Algorithms: The SIREN Challenge of Emergency Medical Services. *In Press*. Proceedings of the Genetic and Evolutionary Computation Conference. (San José, Costa Rica, Jul. 2026)