Sparse Surrogate Model for Optimization: Example of the Bus Stops Spacing Problem

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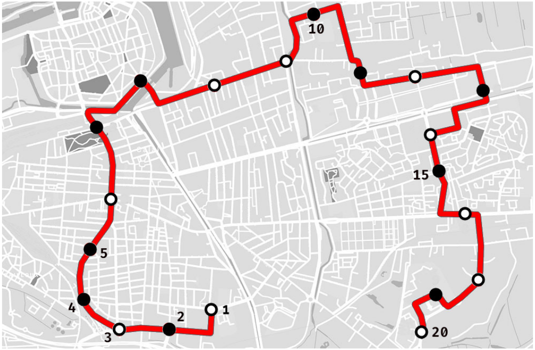
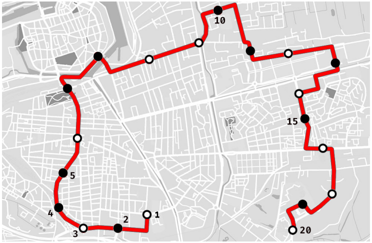
Motivation : bus stops in a city



Find the "optimal" positions of bus stops :

travel time, economic cost, service quality, number of people, etc.

Motivation for the simulated-based approach



- Algebraic expression of a global cost :
  - Expert knowledge, formal model, aggregated variables, etc.
  - Use exact, or heuristic algorithms
  - *But* : model design
- Simulation-based approach :
  - Low level models based on data, complex interactions
  - Use heuristic algorithms
  - *But* : expensive comp. time, and "black-box" optimization

Surrogate-assisted opt. for combinatorial optimization

Surrogate-Assisted Optimization

$X \leftarrow$ initial sample
repeat
  $M \leftarrow$ Build model of f from X
  $x^\star \leftarrow$ Optimize *w.r.t.* an acquisition function based on M
  $y^\star \leftarrow f(x^\star)$ using the numerical simulation
  $X \leftarrow X \cup \{(x^\star, y^\star)\}$
until time limit

Principle : guide the search toward better candidate solutions using surrogate

For numerical optimization :

Gaussian Process, polynomial chaos, NN, RBF net., deep$*$, etc.

For combinatorial optimization :

- BOCS [ICML18] multi. polynomial of Bool var, Bayesian estimation
- COMBO [ICML19] Cartesian product of graphs, Bayesian estimation
- COMEX [ICKDD20] polynomial/Walsh model, reinforcement learning
- WSaO [PPSN18] Fourier/Walsh surrogate, sparse linear reg.

Objectives of this work

Fourier/Walsh surrogate : multivariate polynomial model

Pros : Explicit model, easy to understand
Cons : Number of terms increases exponentially with degree
Challenge for an expert to select degree, terms, etc.

Goals

- Design a sparse surrogate model (Walsh/Fourier expansion) based on expert knowledge, dynamic programming algorithm.
- Spectral Fourier/Walsh analysis of the real-world problem to support expert hypothesis

First spectral analysis of a real-world combinatorial problem :
New tools to explore algebraic properties

Walsh/Fourier basis

Definition (see [O'Donnell,14])

Orthogonal, normal, and finite basis of $\{f : \{0,1\}^n \to \mathbb{R}\}$

$$\forall x \in \{0,1\}^n,\ f(x) = \sum_{I \subset [n]} \beta_I \varphi_I(x) \ \text{ with } \ \varphi_I(x) = \prod_{i \in I} (-1)^{x_i}$$

$\beta_I \in \mathbb{R}$: coefficient of Walsh function φ_I
Order of φ_i : size of the set of indices $I \subset [n]$

Multilinear polynomial expression in variable $\{-1,1\}^n$

$$f(\sigma) = \beta_\emptyset + \sum_{i \in [n]} \beta_i \sigma_i + \sum_{i<j \in [n]} \beta_{i,j} \sigma_i \sigma_j + \sum_{i<j<k \in [n]} \beta_{i,j,k} \sigma_i \sigma_j \sigma_k + \ldots$$

with $\sigma_i = (-1)^{x_i}$

Interpretation of Walsh expansion

$$f(\sigma) = \beta_\emptyset + \sum_{i \in [n]} \beta_i \sigma_i + \sum_{i<j \in [n]} \beta_{i,j} \sigma_i \sigma_j + \sum_{i<j<k \in [n]} \beta_{i,j,k} \sigma_i \sigma_j \sigma_k + \dots$$

- $\mathbb{E}_x[f] = \beta_\emptyset$: average of f
- $\mathrm{Var}_x[f] = \sum_{J \neq \emptyset} \beta_J^2$: variance of f
- $\beta_I \prod_{i \in I} \sigma_i$: interaction between the binary variables :
  β_I^2 part of the variance explained

Spectral analysis

- β_I^2 : Fourier weight • $\bar{\beta}_I^2 = \frac{\beta_I^2}{\mathrm{Var}_x[f]}$: Normalized Fourier weight
- $\{\frac{\beta_I^2}{\mathrm{Var}_x[f]} \mid I \subset [n]\}$: Spectral sample, prob. distribution on $I \subset [n]$
- $\deg_\beta(f) = \frac{1}{\sum_{I \in [n]} \beta_I^2} \sum_{I \in [n]} \beta_I^2 |I|$: Weighted degree

Walsh surrogate : complexity, and quality

$$f(\sigma) = \beta_\emptyset + \sum_{i \in [n]} \beta_i \sigma_i + \sum_{i<j \in [n]} \beta_{i,j} \sigma_i \sigma_j + \sum_{i<j<k \in [n]} \beta_{i,j,k} \sigma_i \sigma_j \sigma_k + \ldots$$

- Number of terms of order n : $\binom{n}{k}$
  ex. for degree 3, $1 + n + \frac{n(n-1)}{2} + \frac{n(n-1)(n-2)}{6} = \mathcal{O}(n^3)$
- Mean square error of a surrogate function $\hat{f}$:

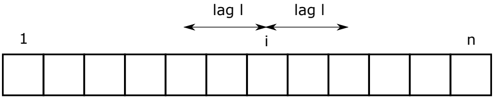
$$\text{mse}(\hat{f}) = \mathbb{E}_x[(\hat{f}(x) - f(x))^2] = \sum_{I \subset [n]} (\hat{\beta}_I - \beta_I)^2$$

- As a consequence, optimal surrogate with p non-zero terms :
  $\hat{f}(x) = \sum_{i=1}^{p} \beta_{I_i} \varphi_{I_i}(x)$ s.t. I_i terms with the p highest $\beta_{I_i}^2$ values.

with mean square error $\sum_{I \subset [n] \setminus \{I_1, \ldots, I_p\}} \beta_I^2$

Sparse Walsh surrogate

- Keep important terms based on expert knowledge, checked with spectral analysis
- Hypothesis : variable are not randomly distributed, main interactions between the closest variables



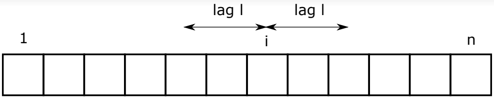
Definition : Sparse Walsh model of degree d, and lag ℓ

Maximum degree d, and bounded interactions

$$\hat{f}_{d,\ell}(x) = \sum_{\substack{I \subset [n] \\ \text{s.t. } |I| \leqslant d, D(I) \leqslant \ell}} \hat{\beta}_I \varphi_I(x)$$

with $D(I)$: maximum difference of variable indices

Sparse Walsh surrogate : properties



Example degree $d = 2$, lag $\ell = 2$

$$
\begin{aligned}
\hat{f}_{d,\ell}(\sigma) \quad & = \beta_{\emptyset} + \beta_1\sigma_1 + \ldots + \beta_n\sigma_n + \ldots \\
\ldots \quad & + \beta_{i-2,i}\sigma_{i-2}\sigma_i + \beta_{i-1,i}\sigma_{i-1}\sigma_i + \beta_{i,i+1}\sigma_i\sigma_{i+1} + \beta_{i,i+2}\sigma_i\sigma_{i+2} + \\
\ldots \quad & + \beta_{n-2,n}\sigma_{n-2}\sigma_n + \beta_{n-1,n}\sigma_{n-1}\sigma_n
\end{aligned}
$$

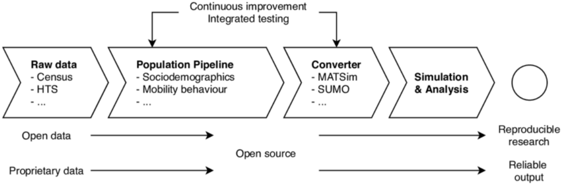
Properties

- Limited number of terms : $(n-\ell)\binom{d-1}{\ell} + \sum_{k=d-1}^{\ell-1}\binom{d-1}{k}$
  for degree 2, $1 + n + (n-\ell)\ell + 1$ terms (linear in dim. n)
- Bonus : exact algorithm to find global optimum :

$$
\begin{aligned}
f_n(x_1, \ldots, x_{n-\ell}, \ldots, x_n) = \quad & f_{n-1}(x_1, \ldots, x_{n-\ell}, \ldots, x_{n-1}) \\
& + F_n(x_{n-\ell}, \ldots, x_{n-1}, x_n)
\end{aligned}
$$

with state : $(x_{n-\ell}, \ldots, x_{n-1})$

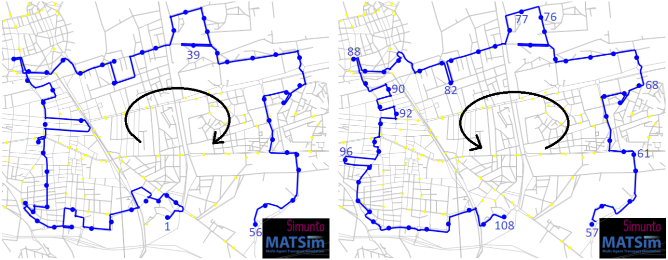
Bus stops spacing problem



Mobility system simulator : MatSim (cars, public transport, etc.)
Real-world scenario : eqasim pipeline [Hörl 21]
Based on open data sources : 15 data sources...
Candidate bus-stops positions : $1 =$ open / $0 =$ close,
Criterium : minimize travel time
$n = 108$ bus-stops, avg. computation time for 1 simu. = 30 min

"hard" work : memory issues, data, stability, reproducibility, etc.
Many thanks to Sebastian Hörl, SystemX, for his help !

Bus stops spacing problem



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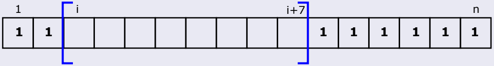
Methodology

1. Spectral analysis based on full enumeration of sub-spaces :
   for $i = 1, 5, 9, \dots, n-7$, enumerate $(x_i, \dots, x_{i+7})$

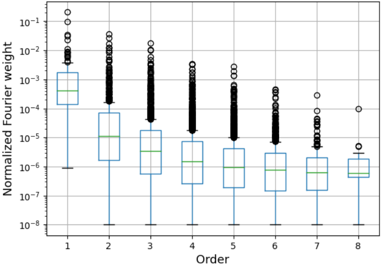


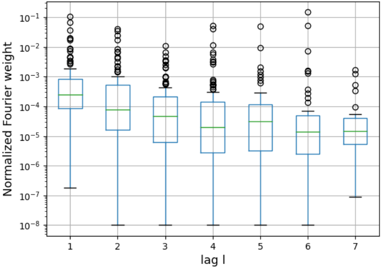
   $x_j = 1$ when $j \notin \{i, \dots, i+7\}$
2. Quality of the sparse model :
   from a random sample of $4,000$ solutions
3. Performance of optimization algorithm :
   Offline scenario, one single optimization

Code, data, scenario : `https://gitlab.com/vvendi/offline-wsao`

1. Spectral analysis : importance *vs.* order, and lag

Avg. value norm. Fourier weights (log scale) over all windows



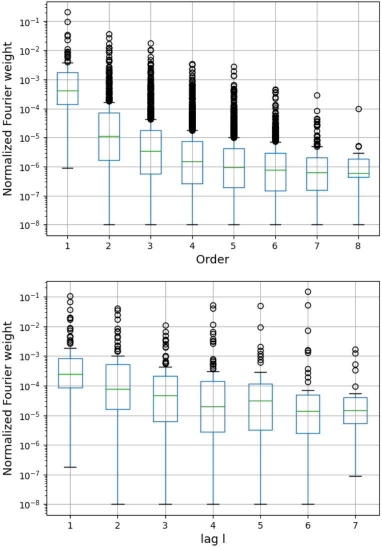


Weights *vs.* order

- Weights are heterogeneous, decreasing with order
- med. order 1 $\approx 17\times$ ord. 2 $\approx 1.7\times$ ord. 3
- 54% of variance explained by ord. 1, 79% by ord. 1, and 2
- Weighted degree is 1.6
- Suggest that Walsh degree 2 is relevant

1. Spectral analysis : importance *vs.* order, and lag

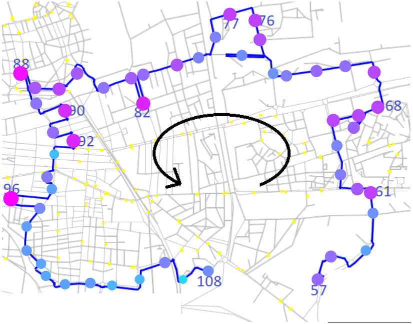
Avg. value norm. Fourier weights (log scale) over all windows

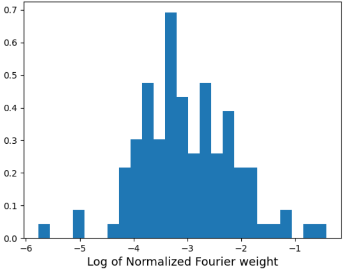


Degree 2 : weights *vs.* lag

- Weights decreasing with lag
- med. lag 1 $\approx 3.24\times$ lag 2 $\approx 1.67\times$ lag 3
- 51.4% variance explained of deg. 2 with lag 1 and 2
- Specific terms with lag 6 could have importance
- Suggest that moderate value of lag is relevant.

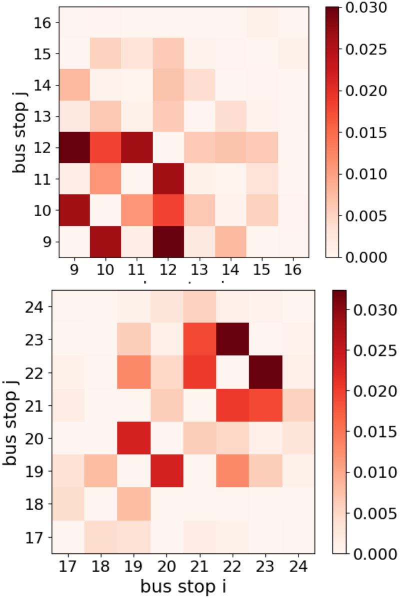
Importance of order 1 terms





- Median 0.7×10^{-3}
- Heterogeneous :
  "log-normal" shape
- Easy to interpret on a map, toward explained optimization ?

Importance of order 2 terms

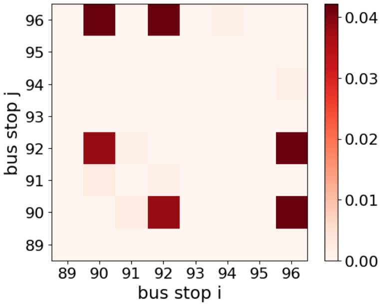


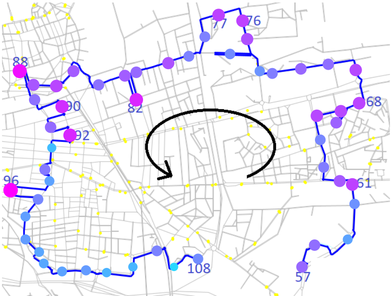
Matrix of norm. Fourier weights $\bar{\beta}_{ij}$

Examples of generic case :

- Highest weights :
  close to diagonal

Importance of order 2 terms



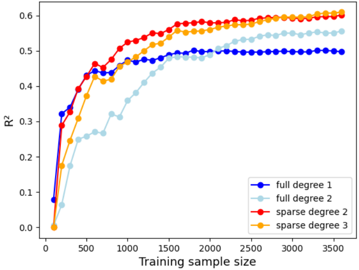


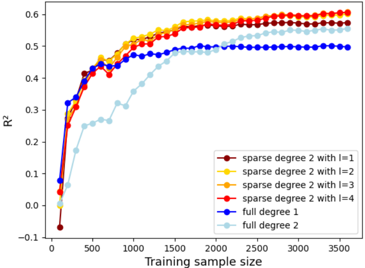
Matrix of norm. Fourier weights $\bar{\beta}_{ij}$

Specific "Exception" cases :

- Highest weights :
  out of the diagonal
- Easy to understand on the map

2. Quality of Walsh models





R^2 : variance explained by surrogate
train sample size $|X| \leq 3600$,
test sample size 400.

Sparse model with lag $\ell = 4$

- "full" linear better than "full" quadratic up to $2,000$
- Sparse deg. 2 slightly better than deg. 3 up to $3,000$
- Sparse models outperform "full" models

Sparse with deg. 2

- Different lags are very closed up to $2,000$
- Lag $\ell = 1$ slightly worst when $|X| \geq 2,000$

3. "Offline" optimisation with sparse model ($d = 2$, $\ell = 2$)

From the original sample of $4,000$ random solutions :

1. Select at random s_{train} solutions from the sample
2. Compute the surrogate (full or sparse)
3. $x =$ Opt. surrogate (DRILS or exact algo.)
4. Evaluate $f(x)$ with simulator

Repeat 30 times, Mann-Whitney test, min. travel time

s_{train}	Full Walsh model	Sparse Walsh model
540	$2,715$ (7.5)	**2,697** (4.8)
$1,080$	$2,704$ (4.5)	**2,694** (3.6)
$3,000$	**2,692** (3.7)	**2,691** (1.9)

- Sparse outperforms full surrogate at low budget
- Sparse, and full surrogates have similar perf. at high budget (notice lower std. dev.)

Conclusions

Summary

- Fourier/Spectral analysis of a real-world problem,
  Using enumeration of subspace, and random sample
  A new way to "see" a combinatorial optimization problem
- Propose a sparse model based on expert knowledge
- Approach : sparse model and an efficient algorithm together
  large dim. $n = 108$ compare to state of the art ($n \leq 50$)

Perspectives

- Extend to larger p.t. plan, larger cities, other criteria, etc.
- Anytime algorithm : update the sample during search (SaO)
- Fourier/Spectral analysis of others combinatorial problems

Code of simulator, and algorithms :

`https://gitlab.com/vvendi/offline-wsao`

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