Algorithms and Software for Delaunay Interpolation and Multiobjective Optimization

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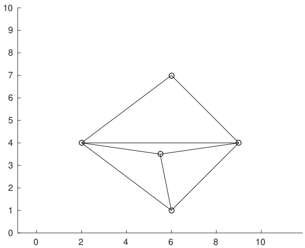
About me

- Ph.D. candidate at Virginia Tech
- Advisor: Dr. Layne Watson
- Interests: Analysis! (Numerical, Functional, Stochastic)
- Skills: Algorithms, Parallel Computing, Low-Level Languages
- Application areas: Data Science, Engineering Design, Quantum Computing

Table of Contents

- The *Delaunay triangulation* is an unstructured simplicial mesh defined by an arbitrary vertex set $P = \{p_1, \ldots, p_n\} \subset \mathbb{R}^d$
- The defining property of the Delaunay triangulation $DT(P)$ is that for every simplex $S \in DT(P)$, the circumball B_S must have empty intersection with P: $B_S \cap P = \emptyset$.



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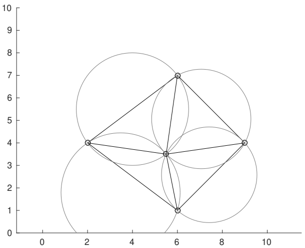

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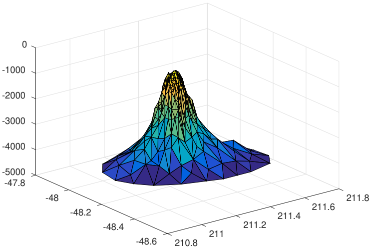
Applications of Delaunay Triangulations

- Interpolation mesh for
  - Finite element method,
  - data science,
  - GIS, and
  - computer graphics
- Topology – alpha shapes
- Delaunay graph



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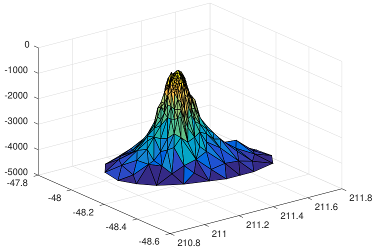

Piecewise linear interpolation: Let $f : \mathbb{R}^d \to \mathbb{R}$, and let $q \in S \in DT(P)$. S has vertex set $\{s_1, \ldots, s_{d+1}\}$ and there exist convex weights $\{w_1, \ldots, w_{d+1}\}$ such that $q = \sum_{i=1}^{d+1} w_i s_i$.

$$\hat{f}_{DT}(q) = \sum_{i=1}^{d+1} w_i f(s_i).$$

Properties of Delaunay Triangulations

- P is in *general position* when $DT(P)$ exists and is unique
  - If P does not lie in a $(d-1)$-dimensional affine subspace of $\mathbb{R}^d$, then $DT(P)$ exists
  - If at most $d+1$ points are cospherical, then $DT(P)$ is unique
- Globally Delaunay $\iff$ Locally Delaunay
- Oweing to Klee, the size of the Delaunay triangulation is

$$\mathcal{O}\left(n^{\lceil d/2 \rceil}\right)$$

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  - For $d > 4$, this is expensive!
  - For $d > 8$, this is not scalable!

Observation: For interpolation, we only need the vertices $(\{s_1, \ldots, s_{d+1}\})$ of $S \in DT(P)$ such that $q \in S$

$$\hat{f}_{DT}(q) = \sum_{i=1}^{d+1} w_i \, f(s_i).$$

Question: Can we find S containing q in polynomial time (without computing the whole mesh)?

Algorithm outline

- Grow an initial simplex (greedy algorithm)
- "Flip" accross a facet from which q is visible
- This "visibility walk" converges to q in finite steps (Edelsbrunner's acyclicity theorem)

Full algorithm published in *Tyler H. Chang, et al. "A polynomial time algorithm for multivariate interpolation in arbitrary dimension via the Delaunay triangulation." In the ACMSE 2018 Conf.*

Growing the first simplex

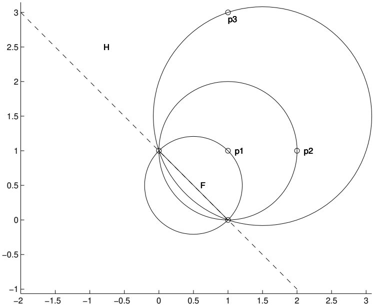
- Start with ϕ containing just the nearest neighbor to q in P;
- For all $p \in P \setminus \phi$, compute the radius r_{min} of the smallest circumball about $\{p\} \cup \phi$ and select the p^* that minimizes r_{min};
- $\phi \leftarrow \phi \cup \{p^*\}$;
- Repeat until $|\phi| = d + 1$;

Lemma

Let P be in general position, and let F be a Delaunay k-face with vertices $\phi \subset P$ where $k < d$. Let $p^* \in P \setminus \phi$ minimize the radius of the smallest $(d-1)$-sphere through the points in $\phi \cup \{p\}$, over all $p \in P \setminus \phi$. Then $F^* =$ ConvexHull$(\phi \cup \{p^*\})$ is a Delaunay $(k+1)$-face. **Proof by continuity.**

Flipping

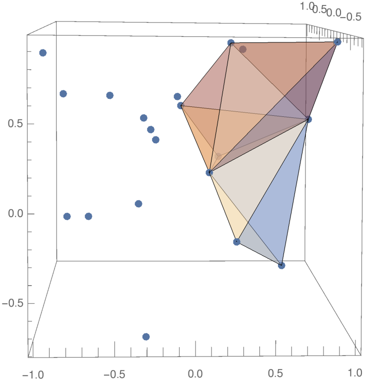
- Let ϕ be the vertices for a facet of a Delaunay simplex;
- Let F be the facet with vertices in ϕ;
- Let H be the halfspace containing q, w.r.t. the hyperplane containing F
- Unless F is a facet of the convex hull, there exists $p^* \in P \setminus \phi$ such that $\phi \cup \{p^*\}$ is the vertex set for a Delaunay simplex;



Visibility walk

- Grow an initial simplex S_0;
- While $q \notin S$, generate S_{k+1} by flipping across a facet of S_k from which q is "visible";
- Terminate when $q \in S_k$;

By *Edelsbrunner's Acyclicity Theorem* this process terminates in finite iterations.



Algorithm Complexity

- To grow the first simplex: $\mathcal{O}(nd^3)$ to apply n rank-1 updates to the QR factorization of $d \times j$ matrix for $j = 1, \ldots, d$
- To compute a flip: $\mathcal{O}(nd^2)$ to apply n rank-1 updates to the QR factorization of a $d \times d$ matrix
- k flips

	$n = 2K$	$n = 8K$	$n = 16K$	$n = 32K$
$d = 2$	3.05	2.90	3.25	3.10
$d = 8$	23.75	24.75	24.30	23.10
$d = 32$	95.25	125.60	131.85	150.10
$d = 64$	171.95	221.85	248.35	280.60

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Overall complexity: $\mathcal{O}(nd^2k)$

Linear programming interpretation

$$\max \tilde{c}^T \tilde{x} \text{ such that } \tilde{A}\tilde{x} \preceq \tilde{b}.$$

$$\tilde{A} = \begin{bmatrix} -p_1^T & 1 \\ -p_2^T & 1 \\ \vdots & \vdots \\ -p_n^T & 1 \end{bmatrix}, \tilde{b} = \begin{bmatrix} \|p_1\|_2^2 \\ \|p_2\|_2^2 \\ \vdots \\ \|p_n\|_2^2 \end{bmatrix}, \text{ and } \tilde{c} = \begin{bmatrix} -q \\ 1 \end{bmatrix}.$$

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Primal feasible basis $\Rightarrow \tilde{A}_B\tilde{x} = \tilde{b}_B$ and $\tilde{A}_K\tilde{x} \preceq \tilde{b}_K$ ($\tilde{A}_B$ is full-rank)

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Let $x = [\text{circumcenter}/2, r^2 - \|\text{circumcenter}\|_2^2]^T \Rightarrow$ Delaunay simplex

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$\Rightarrow q$ is a conv comb of columns in $A_B \Rightarrow$ Simplex contains q

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Primal + dual feasible basis $\Rightarrow$ Delaunay simplex containing q!

What about extrapolation?

- Project q on to the convex hull of P
- Interpolate the projection (if the residual is small)
- Note, the project is a quadratic program (requires more time and space than interpolation algorithm (an LP))

Let W be a $d \times n$ matrix whose columns are points in P, and let z be an extrapolation point (outside convex hull of P).

$$x^* = \arg\min_{x \in \mathbb{R}^n} \|Wx - z\| \quad \text{subject to} \quad x \geq 0 \quad \text{and} \quad \sum_{i=1}^{n} x_i = 1.$$

Projection: $\hat{z} = Wx^*$

DELAUNAYSPARSE Package

Standalone software package `DELAUNAYSPARSE`:

- Robust against degeneracy
- Runs in $\mathcal{O}(kmnd^2)$ time, where k is the number of "flips", n is the numer of data points, m is the number of interpolation points, and d is the input dimension
- Typically, $k \approx \mathcal{O}(d \log d)$
- Parallel and serial implementations

Under review: *Tyler H. Chang, et al. "Algorithm XXX: DELAUNAYSPARSE: Interpolation via a sparse subset of the Delaunay triangulation in medium to high dimensions." Submitted to ACM Transactions on Mathematical Software (2019).*

Serial performance

Runtime in seconds for interpolating a single point $(m = 1)$ with n points in d dimensions

n	d: 2	8	32	64	128
100	0.001	0.004	0.060	0.820	n/a
500	0.021	0.042	0.325	6.479	59.511
2000	0.344	0.583	2.230	28.984	242.066
8000	5.580	9.027	26.210	151.177	905.711
16,000	22.086	35.725	109.448	386.596	2190.362
32,000	82.915	145.115	421.934	1097.060	slow

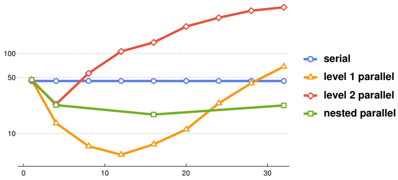
Parallel implementation

Distributed memory: Trivial, for $m > 1$, just run the serial algorithm with multiple batches of interpolation points $Q = Q_1 \cup Q_2 \cup \dots$

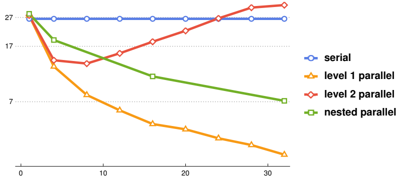
Shared memory: Multiple levels

- Level 1: shared memory loop over multiple interpolation points (just like the distributed case) – Add a few locks in order to "check ahead" if the current simplex contains future interpolation points
- Level 2: loop(s) over data points – results in additional work to reduce multiple solutions; preferrable only when m is small and n is large

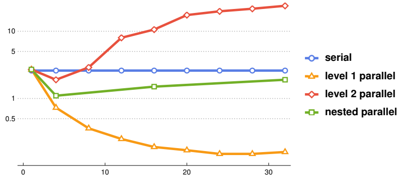
Parallel performance



$d = 10,\ n = 1000,\ m = 1024$



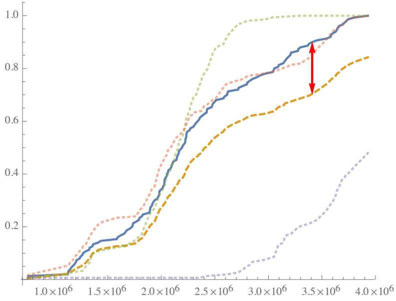
$d = 10,\ n = 10,000,\ m = 64$



$d = 20,\ n = 200,\ m = 64$

Applications of DELAUNAYSPARSE

- HPC system data interpolation
- Aerospace engineering surrogate model
- Nonparametric distribution interpolation
- Data science applications
- Delaunay graph



Future work

- Delaunay interpolation in an arbitrary metric space
- Other sparse subsets, such as umbrella neighborhood
  Tyler H. Chang, et al. "Computing the umbrella neighbourhood of a vertex in the Delaunay triangulation and a single Voronoi cell in arbitrary dimension." In IEEE SoutheastCon 2018.

Questions about Delaunay interpolation?

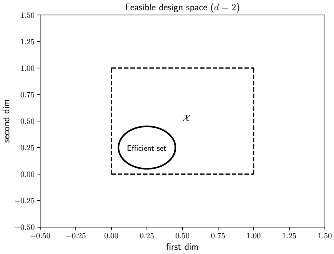
What is a MOP?

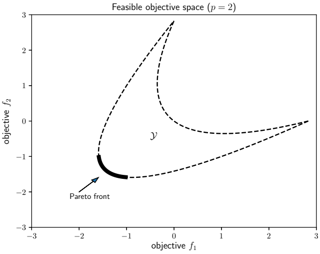
- The Multiobjective Optimization Problem (MOP) generalizes the Single Objective (Scalar) Optimization Problem (SOP);
- The MOP attempts to balance the tradeoff between multiple conflicting objectives;
- Whereas the SOP generally has a unique solution, the solution to a MOP is a *set* of *Pareto optimal* solutions;

- The objective/cost function is $F : \mathbb{R}^d \to \mathbb{R}^p$
- $\mathbb{R}^d$ is the *design space* and $\mathbb{R}^p$ is the *objective space*;
- $\mathcal{X} = [L, U]$ is the feasible design space;
- $\mathcal{Y} = F(\mathcal{X})$ is the feasible objective space;
- x, y will denote arbitrary points in the design space;
- X, Y will denote arbitrary points in the objective space;
- $X \preceq Y$ if X is componentwise less than or equal to Y;
- $X \leq Y$ if $X \preceq Y$ and $X_i < Y_i$ for some $1 \leq i \leq p$. This is read "X dominates Y";

The Objective Space and Pareto Front

- The objective space is a poset under the relation "$\preceq$";
- The solution to a MOP is a set of *nondominated* or *Pareto optimal* solutions;
- x^* is Pareto optimal if for all $x \in \mathcal{X}$, $F(x) \npreceq F(x^*)$;





Goals:

Find a discrete set of approximately nondominated objective points that describes the Pareto front, and the corresponding efficient designs

Types of MOPs

functions are "cheap" to evaluate derivative info is available	functions are "cheap" to evaluate no derivative info is available
functions are costly to evaluate derivative info is available	functions are costly to evaluate no derivative info is available

Focus on bottom right: **expensive blackbox MOPs**!

Motivating Example: VarSys

VarSys: Managing performance variance

- For multiple runs of the same I/O task on the same HPC system, we get varying throughputs
- This presents issues for load balancing and performance guarantees
- Needs to be balanced against other concerns such as energy consumption and mean throughput
- Evaluation expense: 1+ minutes to build distributions

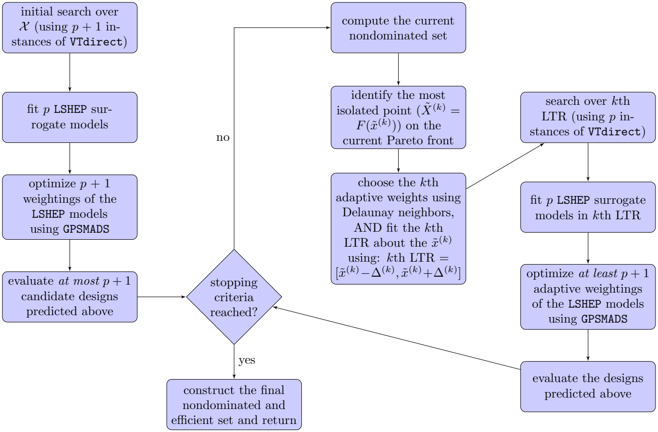
VTMOP

VTMOP is a Fortran 2008 blackbox MOP solver and framework, based on an algorithm by *Shubhangi Deshpande, et al. "Multiobjective optimization using an adaptive weighting scheme." Optimization Methods and Software 31.1 (2016): 110-133.*

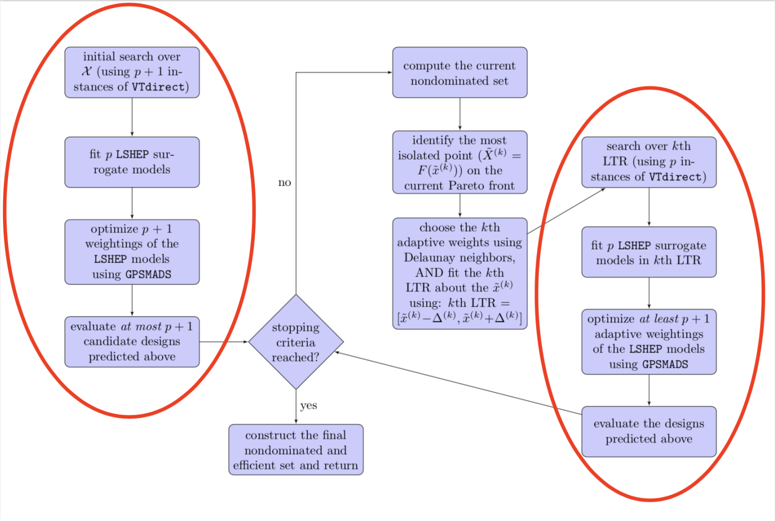
VTMOP is meant to be flexible, scalable, portable, robust, and efficient for solving expensive blackbox MOPs

Combines adaptive weighting scheme, response surface modeling, and trust region methods

The Algorithm Outline

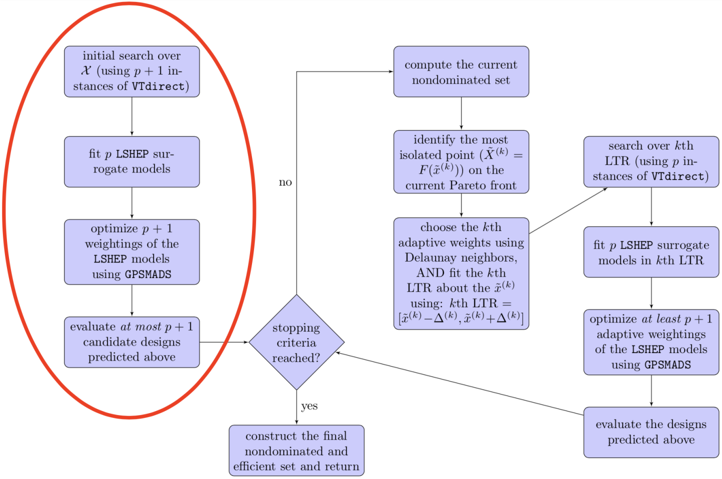


RSM phases

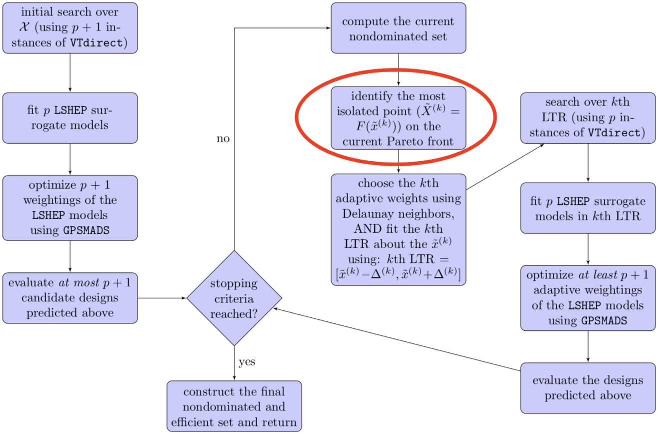


initial search over $\mathcal{X}$ (using $p+1$ instances of VTdirect)
fit p LSHEP surrogate models
optimize $p+1$ weightings of the LSHEP models using GPSMADS
evaluate *at most* $p+1$ candidate designs predicted above
stopping criteria reached?
no
yes
construct the final nondominated and efficient set and return
compute the current nondominated set
identify the most isolated point ($\tilde{X}^{(k)} = F(\tilde{x}^{(k)})$) on the current Pareto front
choose the kth adaptive weights using Delaunay neighbors, AND fit the kth LTR about the $\tilde{x}^{(k)}$ using: kth LTR $= [\tilde{x}^{(k)} - \Delta^{(k)}, \tilde{x}^{(k)} + \Delta^{(k)}]$
search over kth LTR (using p instances of VTdirect)
fit p LSHEP surrogate models in kth LTR
optimize *at least* $p+1$ adaptive weightings of the LSHEP models using GPSMADS
evaluate the designs predicted above

0th iteration



Key component



Identifying an Isolated Point

Let $P^{(k)}$ be the kth set of nondominated objective points $P^{(k)} = \{X^{(1,k)}, \ldots, X^{(N_k,k)}\}$. Define the projected set

$$H^{(k)} = \left\{ \left(\frac{X_1^{(n,k)}}{X_p^{(n,k)}}, \ldots, \frac{X_{p-1}^{(n,k)}}{X_p^{(n,k)}} \right) \;\middle|\; n = 1, \ldots, N_k \right\}$$

The most isolated point is identified by considering the average Euclidean distance to all neighbors in the Delaunay graph of $H^{(k)}$

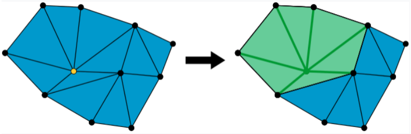


Image from Wikipedia

Compute the Delaunay neighborhood of $X^{(1,k)}$, …, $X^{(N_k,k)}$ with respect to the projected set $H^{(k)}$.

- Only need the Delaunay graph G_{DT}
- Number of connections in G_{DT} is upper bounded by $N_k(N_k-1)/2$
- Can recover G_{DT} by interpolating the midpoint between each pair of points in $H^{(k)}$
- Using `DELAUNAYSPARSE`, requires $\mathcal{O}(N_k^3 p^3 \log p)$ time

Sources of Parallelism

1. The function F (left to the user)
2. Iteration complexity (assumed to not offer much improvement)
3. The exploration phase
    - `VTDIRECT95` offers a parallel implementation `pVTdirect`, which distributes function evaluations across a network using MPI.
    - `VTDIRECT95` is called p times per iteration (or $p+1$ times in the 0th iterations).
    - An experimental design could be evaluated in parallel
4. Evaluating candidate designs (from MADS output)

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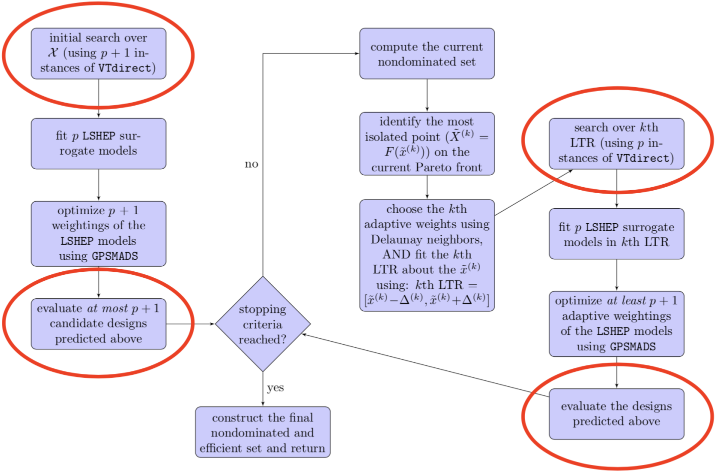
Focus on items 3 & 4!

Function evaluations



For regular usage:

- Recall F is being distributed by user
- Use OpenMP *shared memory parallelism*, essentially for achieving asynchronous behavior
- Puts burden of distribution on user, but allows for flexibility in distributing many instances of F

The `libEnsemble` library from Argonne's Exascale computing project:

- Generator function
- Evaluator function
- Allocator function

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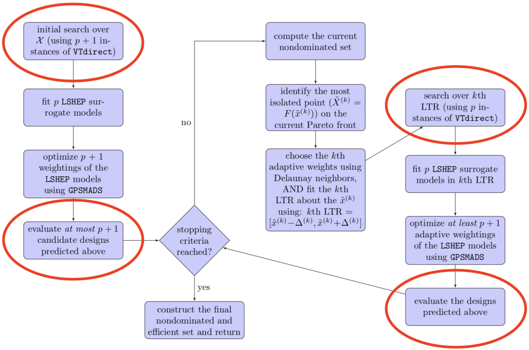
`VTMOP` is the *generator* for `libEnsemble`

- Each call to the *generator* runs a half-iteration and requests a design exploration or batch of candidate evaluations
- The *allocator* switches to evaluations
- The *evaluator* evaluates all the requested designs
- The *allocator* switches back to the *generator*

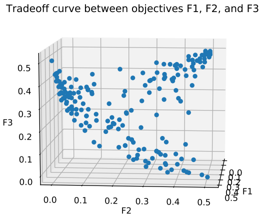
Integrating with libEnsemble

- Want nice big batches that match available resources
- Use a latin hypercube search during the search phase
- Pad out batches of candidates using additional weights

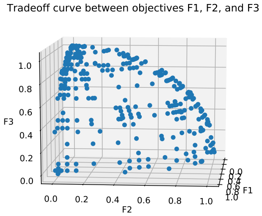


Test functions

- $F_c(x) = (\|x - e_1\|_2^2, \ldots, \|x - e_p\|_2^2)$
- Convex Pareto front $\Rightarrow$ "easier" problem



- `DTLZ2` from Deb et al.
- Concave Pareto front $\Rightarrow$ "harder" problem



Approximation results

Number of solutions, RMSE, and Delaunay discrepancy (respectively) for F_c and `DTLZ2`, after a budget of 2000 function evaluations, with $d = 5$ (Averaged over 5 runs).

Performance metrics:

1. the *cardinality* of the solution set (num pts)
2. the *convergence* of the solution points to the true Pareto front (RMSE)
3. the *relative spacing/coverage* of the solution set (Delaunay discrep)

Prob/Meth	$p=2$	$p=3$	$p=4$
F_c / `bVTdir`	73, .00100, .207	173, .0505, .579	288, .101, NA
F_c / `libE`	78, .0127, .158	189, .0560, .429	283, .104, .551
`DTLZ2` / `bVTdir`	139, .00713, .109	354, .0401, .230	658, .0443, NA
`DTLZ2` / `libE`	66, .103, .201	258, .175, .691	548, .201, .793

Runtime performance

Runtimes for `VTMOP` with 2000 function evaluations (either 1 second or in range [0.5 s, 1.5 s]), for `bVTdirect` and `libEnsemble` with $d = 5$. Shows CPU time / wall time in seconds, for 36 core machine.

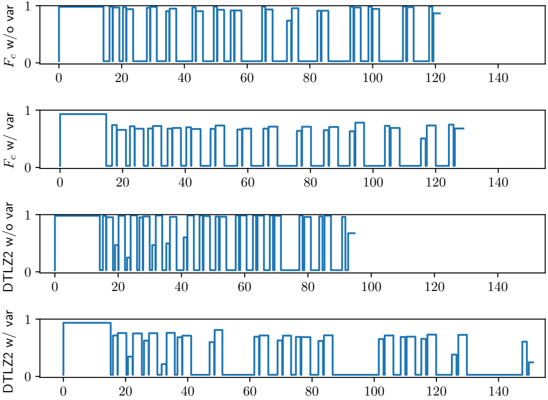
p	Method	F_c, no var	F_c, w/ var	DTLZ2, no var	DTLZ2, w/ var
2	`bVTdir`	2008 / 1037	2007 / 1039	2007 / 1093	2004 / 1082
	`libE`	2051 / 112	2070 / 142	2060 / 111	2064 / 143
3	`bVTdir`	2012 / 717	2012 / 719	2021 / 797	2018 / 797
	`libE`	2077 / 133	2066 / 144	2054 / 99	2057 / 126
4	`bVTdir`	2026 / 582	2029 / 586	2177 / 807	2149 / 782
	`libE`	2134 / 190	2124 / 186	2182 / 227	2185 / 257

Tyler H. Chang, et al. "Managing computationally expensive blackbox multiobjective optimization problems with libEnsemble." Submitted to SpringSim 2020, 28th HPC Symposium.

CPU usage

CPU usage (36 cores) when running `VTMOP` with `libE`.

Note the peaks and valleys



Spectrum of blackbox problems

Computationally cheap $\longrightarrow$ expensive

- Eval: ≈ 1 sec
- Budget: $\approx 10,000$
- Software: `NSGA-II`

- Eval: ≈ 1 min
- Budget: ≈ 1000
- Software: `VTMOP`

- Eval: ≈ 1 hr
- Budget ≈ 100 (at most)
- Software: `FUN3D`? `NASTRAN`?

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- **Future work!**

Summary of future works

For `DELAUNAYSPARSE`:

- Interpolation in arbitrary metric space
- Other subsets of the Delaunay triangulation

Extension of `VTMOP` to extremely expensive problems:

- Leveraging multifidelity data
- Quick low-fidelity approximation to Pareto front and efficient set based on only pure solutions

Various applications of interpolation and multiobjective optimization

Significant work

Peer-Reviewed:

T. H. Chang, et al. "Least-squares solutions to polynomial systems of equations with quantum annealing." Springer, QINP 18:374 (2019).

T. H. Chang, et al. "Computing the umbrella neighbourhood of a vertex in the Delaunay triangulation and a single Voronoi cell in arbitrary dimension." In IEEE SoutheastCon 2018.

T. H. Chang, et al. "A polynomial time algorithm for multivariate interpolation in arbitrary dimension via the Delaunay triangulation." In the ACMSE 2018 Conf.

T. H. Chang, et al. "Predicting system performance by interpolation using a high-dimensional Delaunay triangulation." In SpringSim 2018, 26th HPC Symp.

Under Review:

T. H. Chang, et al. "Algorithm XXX: DELAUNAYSPARSE: Interpolation via a sparse subset of the Delaunay triangulation in medium to high dimensions." Submitted to ACM TOMS (2019).

T. H. Chang, et al. "Managing computationally expensive blackbox multiobjective optimization problems with libEnsemble." Submitted to SpringSim 2020, 28th HPC Symp.

Major Awards:

Cunningham Fellow. Virginia Tech, Grad School. 2016–Present

SCGSR award. DOE, Office of Sci. Jun–Dec, 2019

Various CS/Eng. dept. fellowships. Virginia Tech. 2016–Present

Projects:

VarSys project at Virginia Tech. NSF grant #1565314

Professional:

Reviewer for *IEEE SoutheastCon* and *JMLR*