Approaches for Engineering Design as Mixed Discrete Non-Linear Programming Problems

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Why Engineering Design as MDNLP Problems?

- Many engineering design problems combine “selection” and “sizing” – aircraft design is one of them
  - Selection
    - Choosing from a set of discrete options
    - Categorical (e.g. engine cycle choice, primary structural material, other technologies) and integer (e.g. number of engines)
  - Sizing
    - Finding appropriate / best values of continuous values
    - Wing area, engine thrust, aspect ratio
- Sizing can usually be posed as continuous optimization problem and solved with gradient-based solver
- Combining selection and sizing becomes Mixed Discrete Non-Linear Programming (MDNLP) problem
  - Usually with constraints; may have multiple objectives

A Constrained Mixed Discrete Nonlinear Programming Problem Formulation

- Optimization Formulation

minimize	$f(\mathbf{x}_C, \mathbf{x}_D)$
subject to	$\mathbf{g}(\mathbf{x}_C, \mathbf{x}_D) \leq \mathbf{0}$
with respect to	$\mathbf{x}_C$ (continuous variables) and
	$\mathbf{x}_D$ (discrete variables)

- MDNLP problems are hard to solve (NP- hard):
  - Every combination of discrete variable values could be optimal
  - Every combination of discrete variable values has different continuous variable values that specify the optimum design
  - Genetic Algorithm one possible solver, but computationally expensive
  - Gradient-based methods only useable for continuous variables (without modification of the problem)

Two Approaches for Engineering Design as MDNLP

- Both approaches discussed here involve the genetic algorithm as a major component
- Approach 1:
  - Using GA's population-based search in a multi-fidelity approach (using sequential Kriging models as the low-fidelity analysis) to reduce the number of high-fidelity fitness evaluations for MDNLP problems
- Approach 2:
  - A hybrid approach combining a multi-objective GA with a gradient-based optimizer to solve constrained, multi-objective MDNLP problems

Multi-Fidelity Optimization Strategies using Genetic Algorithms and Sequential Kriging Surrogates

Summary of Multi-Fidelity GA Effort

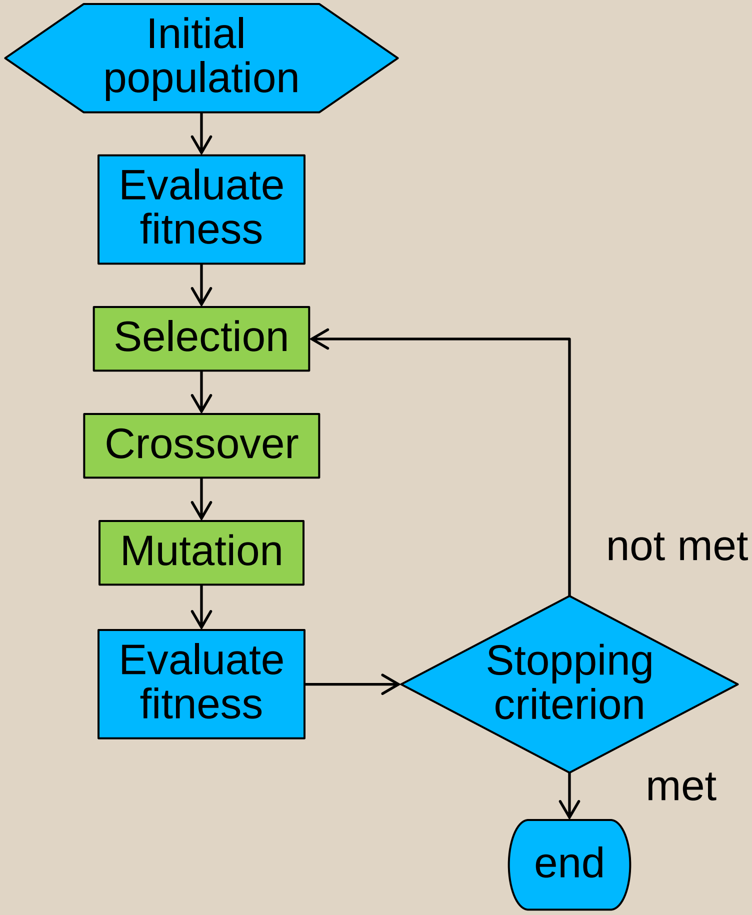
- Engineering problems with discrete variables, discontinuous functions
  - Genetic algorithm (GA) one possibility for design search
  - High number of analyses
- High-fidelity analyses
  - Analysis with substantial representation of underlying physics
  - Long compute time
- Formulate and demonstrate two strategies
  - GA provides framework for search strategy
  - Sequentially-updated Kriging models for low-fidelity analyses
  - Evolving GA population determines in-fill points for Kriging models
- Results
  - Both strategies obtain solutions comparable with baseline GA
  - Significant reduction in number of high-fidelity analyses
  - Space-filling Latin Hypercube Sampling (LHS) for initial population
  - Analyses used not expensive enough to reduce run time

Motivation and Goals

- Motivation
  - Combining non-gradient search algorithm with high-fidelity analyses is largely impractical
    - Non-gradient search allows for discontinuous functions, discrete variables
    - GA for CFD problem with four design variables (Obayashi, et al. 1998)
      - 100 individuals, 100 generations; 3 minutes per function evaluation leads about 21 days of run time (in serial)
  - Much recent multi-fidelity (or variable-fidelity) work using an approximation (typically Kriging) as a low-fidelity analysis
- Goals
  - Formulate and demonstrate multi-fidelity approaches
    - Genetic Algorithm as a global search framework
    - Sequentially update Kriging models throughout search
    - Evolving GA population provides infill points for Kriging model
  - Effective global search with reduced number of high-fidelity analyses

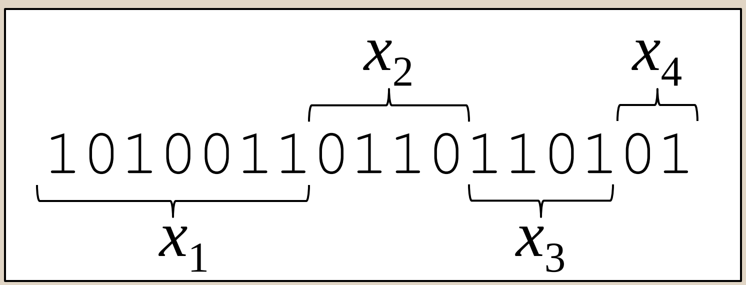
Genetic Algorithm

- Population-based search / optimization method based on "Theory of Natural Selection"
  - Three operators guide evolution of population: selection, crossover and mutation
  - Zero-order method: No gradient information required
- Wide applications in engineering design
  - Advantages for multi-objective and combinatorial (mixed discrete-continuous) problems
  - Can handle multi-modal, "noisy" or discontinuous functions



Genetic Algorithm Implementation

- Binary chromosomes
  - Gray coding
  - All variables discretized



  - Encountering same good designs likely

- Fitness function
  - Constraint violations handled via exterior penalty

$$\Phi(\mathbf{x}) = f(\mathbf{x}) + r_p \sum_{j=1}^{n_{con}} P_j(\mathbf{x})$$

- Stopping Criteria
  - Bit-String Affinity
  - Maximum generations

GA Operator Implementation

- Tournament selection

00110011010 → $f(\mathbf{x}) = 358$

11010011011 → $f(\mathbf{x}) = 273$

→ tournament → 11010011011

- Uniform crossover

11010011011 → 10000001001

00100101000 → 01110111010

- Bit mutation using $P_{\text{mutation}} = (l+1)/(2Nl)$

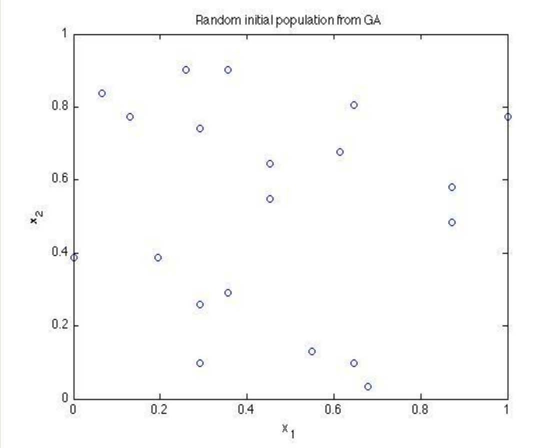
00110011010 → 00110111010

Surrogate Modeling

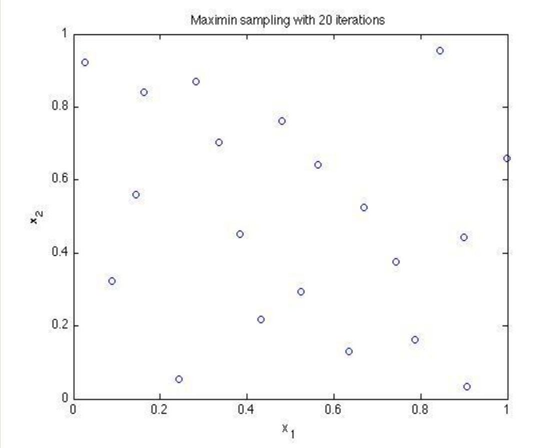
- Surrogate models are inexpensive approximations of expensive functions or simulations
- Approximations are used to model the design space for optimization with reduced computational resources
- Kriging was used as a surrogate model of the high-fidelity deterministic simulation or analysis
  - Global metamodel (handles local minima)
  - Spatial Correlation method
  - Uses a stochastic approach to building the approximation
  - Uses a MATLAB-based toolbox to generate Kriging model, including GA to determine the correlation parameters*
  - One shot Kriging vs. Sequential Kriging for simulation optimization

*Forrester, Alexander I. J., Keane, A. and Sóbester, A.,*Engineering Design Via Surrogate Modelling: a Practical Guide*, Chichester, West Sussex, England: J. Wiley, 2008.

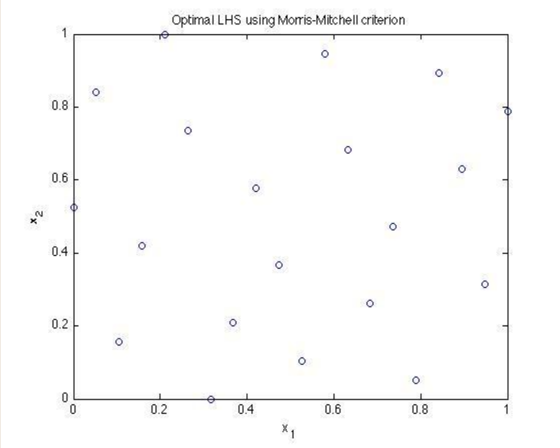
Sampling Methods



Random sampling



LHS

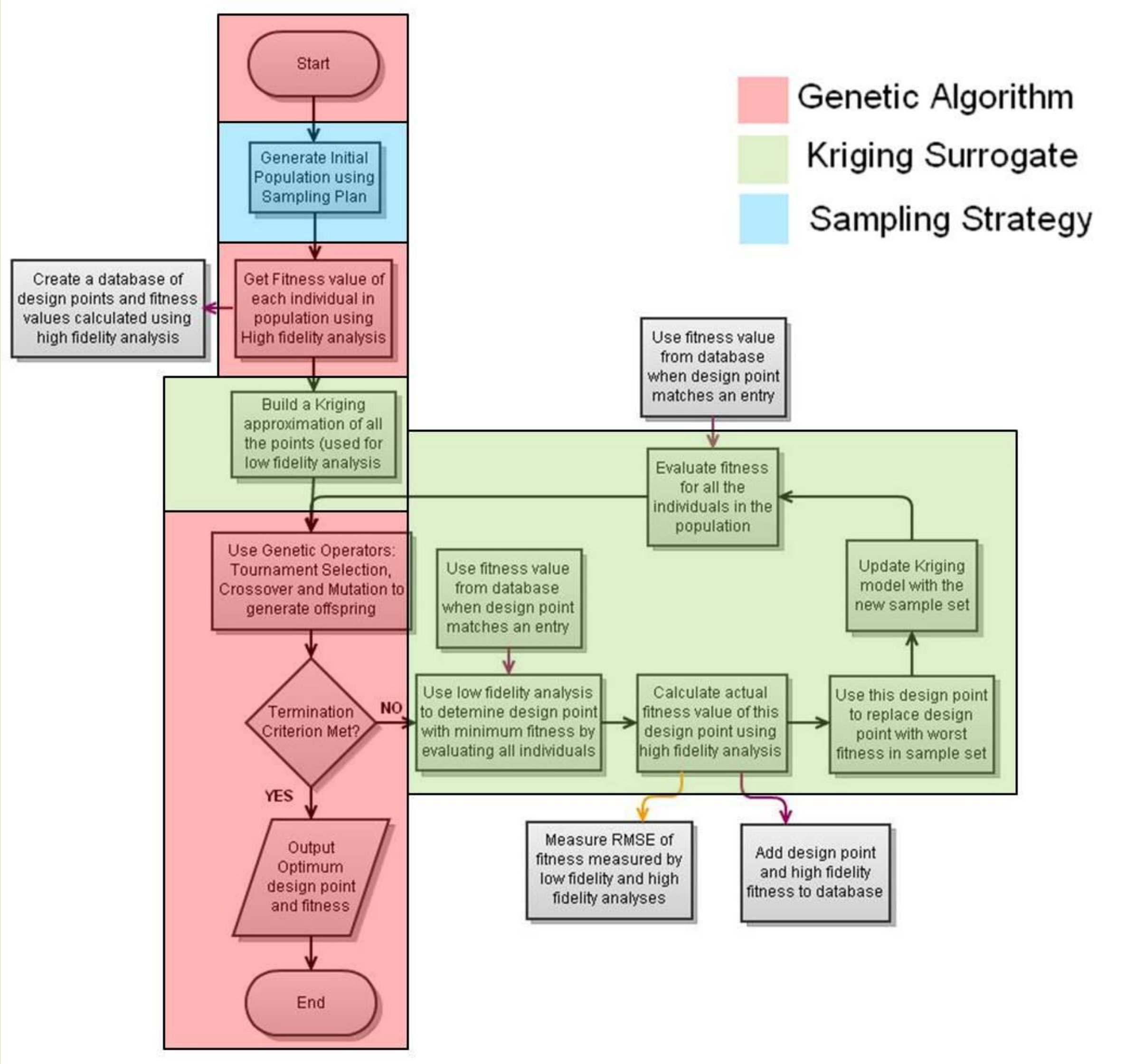


OLH

- Latin Hypercube Sampling(LHS) is a stratified sampling technique for multiple variables. The sample is made of components of each of the variables randomly matched together.
- Effect of the initial sampling on the final solution was examined:
  - Best space-filling by the Optimal Latin Hypercube (OLH)* sampling
  - Good option for one-shot solution approach
  - Has an optimization problem inbuilt, increasing complexity of the approach

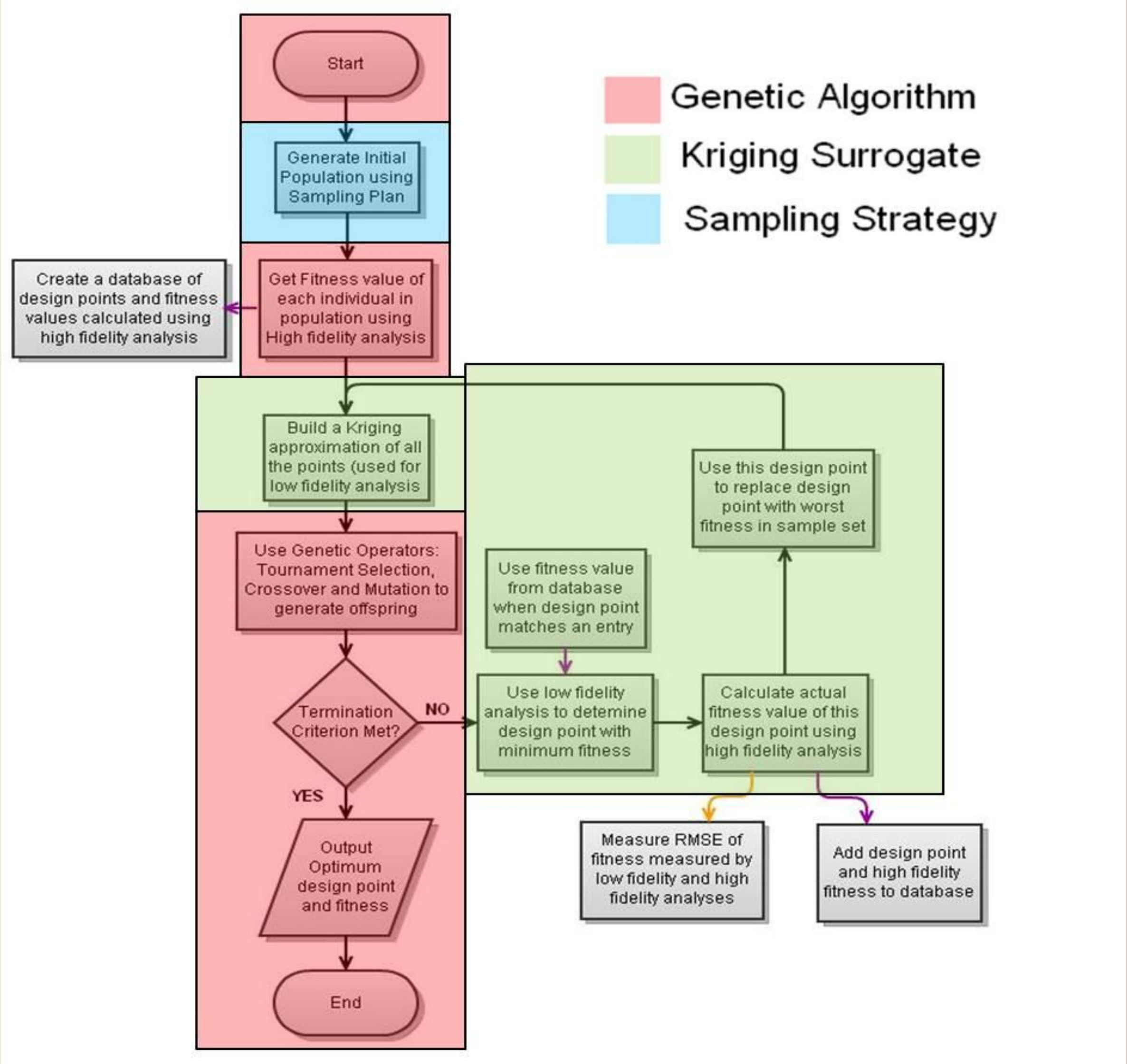
*Forrester, Alexander I. J., Keane, A. and Sóbester, A.,*Engineering Design Via Surrogate Modelling: a Practical Guide*, Chichester, West Sussex, England: J. Wiley, 2008.

Strategy I



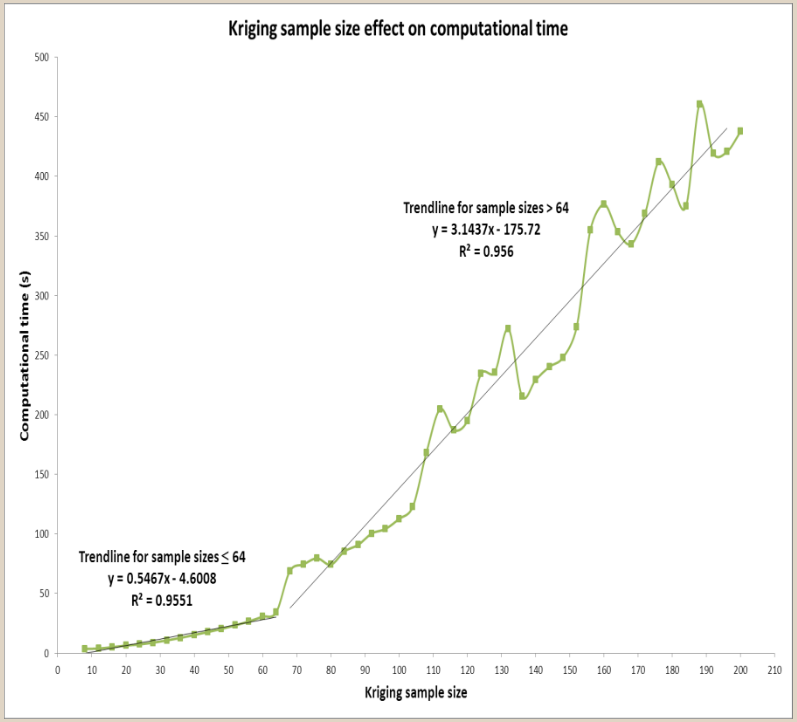
- Fitness values for selection will mix high-fidelity results with low-fidelity, Kriging model results
- Best available information, but potentially inconsistent comparisons

Strategy II



- Fitness values for selection use only most recent Kriging model results
- Consistent comparison, but selection ignores high-fidelity information when available

Limitation on Kriging Sample Size



This appears to be an issue with how the Kriging toolbox uses available CPU resources on our compute server

Kriging Sample Size Fixed on Test Problem

	Yes	No
Median # of hi-fi evaluations	127.5	126
Median Fitness	0.8419	0.8419
Computational time (s)	2123.35	3799.27

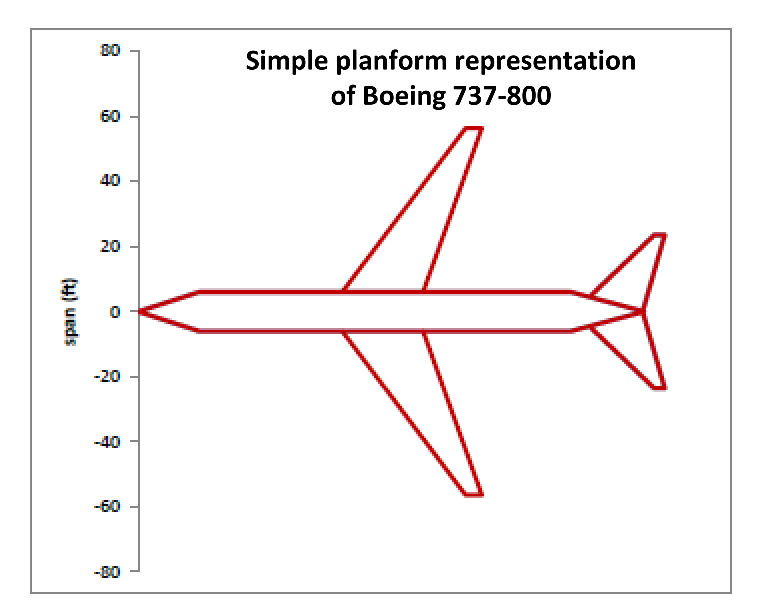
Effect of Initial Population on Test Problem

	64	4 × *l**
Median # of hi-fi evaluations	124	193
Median Fitness	0.1771	0.1487
Computational time (s)	2144.07	9826.88

*** *l* = length of the chromosome**

Aircraft Design Problem

- Multidisciplinary Simulation Optimization problem (one analysis code handles multiple disciplines)
- Problem: Design of a medium range, two-wing mounted engine, single-aisle commercial aircraft similar to Boeing 737-800
- Objective: Minimize the total fuel weight for the sizing mission
  - Reduced ticket prices
  - Reduced CO_2 emissions
- Constraints on performance and geometry
- Simulation: sizing analysis using FLOPS#
- Used two CFM-56 like engine performance models



#Flight Optimization System, McCullers, L. A., Software Package, Ver. 8.12, NASA Langley Research Center, Hampton, VA, 2010.

Problem Setup

Continuous Design Variables	Wing area (ft^2)	$1000 \le SW \le 2000$
	Wing taper ratio	$0.1 \le TR \le 0.3$
	Wing thickness-to-chord (%)	$0.08 \le TCA \le 0.16$
	Aspect Ratio	$6 \le AR \le 16$
	Thrust (lb)	$16{,}000 \le Thrust \le 30{,}000$
Discrete Design Variables	Wing Sweep (degrees)	-5, 0, 5 10, 15, 20, 25, 30
	Cruise Mach Number	0.7, 0.72, 0.74, 0.76, 0.78, 0.8

Variables:

The problem had 7 design variables

- 5 Continuous variables
- 2 Discrete variables (Continuous variables with coarse resolution)

Constraints:

Problem had 10 constraints

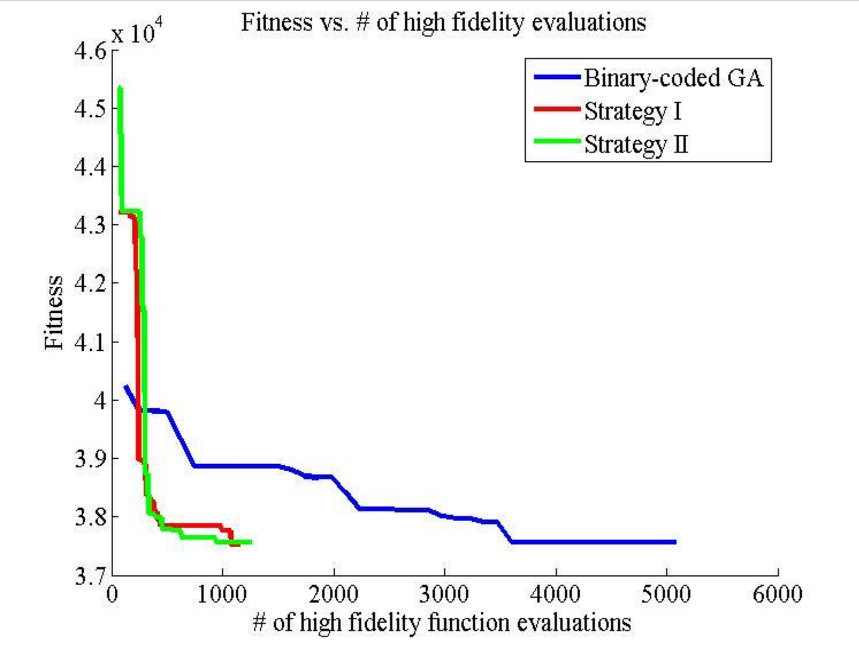
- Operational constraints
- Geometry constraints
- Ensure feasible designs

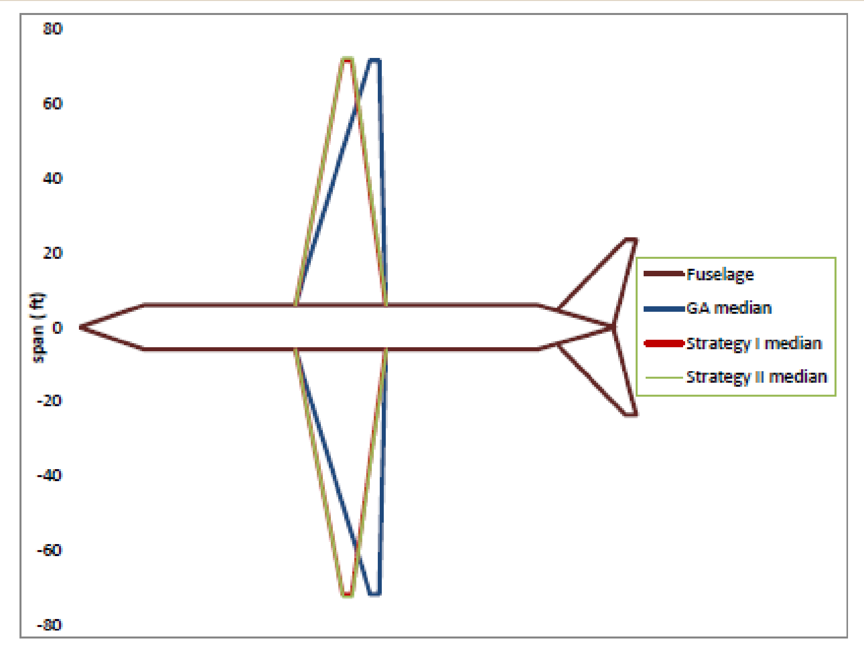
Design Range	=	3000	nm
Ceiling	=	42,000	ft
MTOW	≤	180,000	lb
Takeoff field length	≤	7500	ft
Landing field Length	≤	5000	ft
Wing Span	≤	130	ft
Approach Velocity	≤	150	kts
Missed Approach	≥	0	lb
Second Segment Climb	≥	0	lb
Excess Fuel Capacity	≥	0	lb

Optimization Run

GA SETUP	Binary Coded GA	Strategy I	Strategy II
Termination Criterion	90% BSA		
Maximum # of Generations	200	600	
Initial Population	124	64	
Probability of Mutation	.0041	.0080	
Probability of Crossover	0.5		

- Kriging model built for fitness function
- Quadratic penalty function with penalty multiplier $r_p = 10^5$





Aircraft Design Problem – Initial Runs

	GA	Strategy I		Strategy II	
Median # of hi-fi evaluations	4960	1238	75%	1250.5	74.8%
Median fitness	37590.8	37523.3	1.7%	37501.8	2.4%
Median total fuel weight (lb)	35247	35202.3	0.13%	35170.6	0.22%
Median Runtime (s)	13103.2	22641.8	73%	22369.7	71.7%

- Both multi-fidelity strategies reduce median number of high-fidelity evaluations by about 75%
- Slightly better median fitness and total fuel weight values from multi-fidelity strategies
- Median fitness values > median objective function suggests constraint violations
- Median run time increased for multi-fidelity strategies (by over 70%)

Aircraft Design Problem – Follow-on Runs

- Quadratic penalty function and selected penalty multiplier gave slightly infeasible designs in initial runs
  - Landing field length (LFL) and wing span constraints violated by 10%
  - Quadratic penalty function changed to linear penalty function
  - Penalty multiplier increased to $r_p = 10^6$
- Bit String Affinity value reduced to 80% to reach stopping criterion sooner and 10 runs conducted for repeatability in follow-on runs

	Linear Penalty w/ 80% BSA and $r_p = 10^6$ (median values from 10 runs)				
	LFL	Span	Total Fuel Weight (lb)	# of hi-fi evaluations	Maximum # of generations
	% Violation				
GA	5.24	0	43288	3968	31
Strategy I	5.12	0	41866	644	296
Strategy II	6.36	0	43955	584	260

Observations about Multi-fidelity Strategy

- Both multi-fidelity strategies reduced the number of high-fidelity evaluations with near approximate solutions to that of the binary-coded GA
- Strategies handled mixed discrete non-linear optimization problems
  - Kriging model fit as through discrete variables were continuous, but GA only required evaluation at specified discrete values
- In some cases, the multi-fidelity optimization strategies, with a smaller initial population, scanned the design space better than the binary-coded GA
- LHS using 'maximin' criterion with 20 iterations, from the MATLAB Statistical Toolbox, provided good design space coverage for the initial population
- Sequential surrogate modeling is associated with long runtimes, but this can be addressed using processors in parallel and by limiting the sample space used for the Kriging model
- Using separate Kriging surrogate models for the objective function and for the constraint functions may improve constraint handling

Multi-Objective Optimization using a Hybrid Approach for Constrained Mixed Discrete Non-Linear Programming Problems

Motivation

- Features of a typical engineering design problem
  - Discrete & continuous design variables
  - Multi-objective
  - Constrained
- Several optimization algorithms address some of these features - only a few can handle all of these
- Approach here combines Two-Branch Genetic Algorithm (GA) with gradient-based local search algorithm using a multi-objective formulation
- Ensures tight constraint satisfaction while solving the multi-objective MDNLP problems
  - We have not seen this in other hybrid approaches

Multi-Objective Problem

- Competing objectives, no single optimal solution.
- A set of optimal solutions called Pareto-optimal set (or set of non-dominated designs)

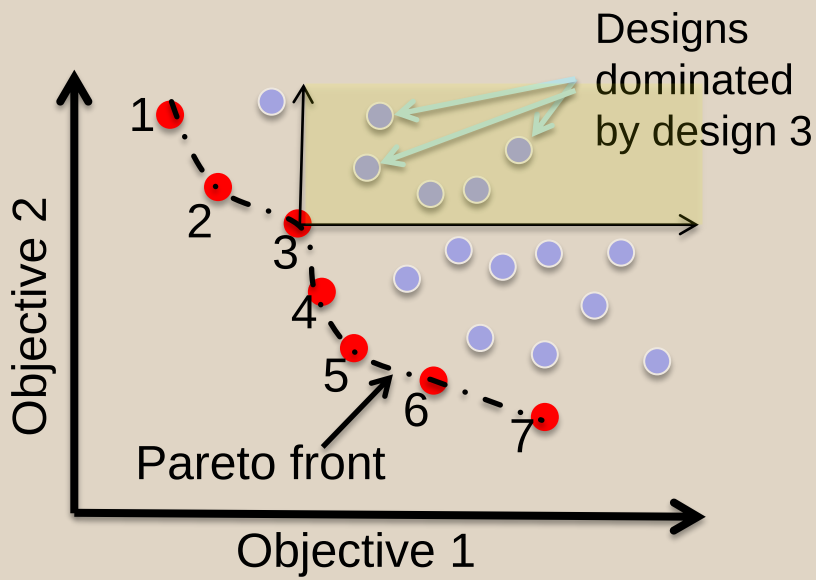
For minimization problem,
a design $\mathbf{x}^i$ dominates $\mathbf{x}^j$ iff,

$\forall_k: f_k(\mathbf{x}^i) \leq f_k(\mathbf{x}^j)$

and

$\exists: f_k(\mathbf{x}^i) \leq f_k(\mathbf{x}^j)$

for at least one $k \in [1,K]$



Multi-Objective Formulation

- Handling multiple objectives using gradient based methods
  - Converts multi-objective into a single-objective formulation
  - Need certain sets of user-supplied input
- Some common gradient-based multi-objective formulations:
  - Weighted Sum Approach
    - Uses a weight vector to indicate relative importance of each objective
  - ε-Constraint Approach
    - Chooses a primary objective function
    - Converts the other objectives into a set of inequality constraints
  - Goal Attainment Approach
    - Minimizes an attainment factor
    - Converts all the objectives into a set of inequalities that include the attainment factor

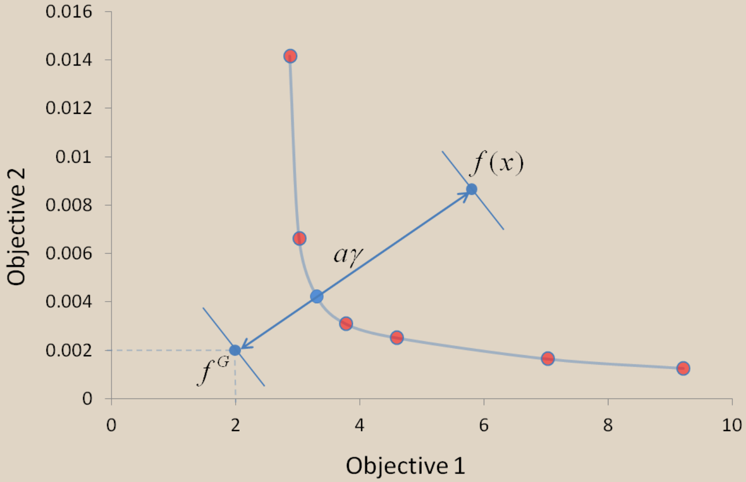
Goal Attainment Approach

- Minimizes the goal attainment factor γ
- Multiple objectives appear as a set of inequality constraints
- Needs user-specified goal values

Minimize γ

Subject to:

$$f_k(\mathbf{x}) - \alpha\gamma \leq f_k^G,\ k = 1,2,\ldots,K$$
$$g_j(\mathbf{x}) \leq 0,\ j = 1,2,\ldots,J$$
$$h_l(\mathbf{x}) = 0,\ l = 1,2,\ldots,L$$



Hybrid Optimization

- Combine two (or more) different search / optimization algorithms
  - Improve search performance by using advantages of each algorithm
- Requires information exchange between algorithms
  - Framework to allow easy integration of different algorithms and facilitate information exchange

Comparison of Optimizers

Global Optimizer

Genetic Algorithm
Searches the entire design space
Requires many function evaluations
Can handle discrete and continuous problems
No guarantee to find an actual optimum

Local Optimizer

Sequential Quadratic Programming
Starts from an initial guess and converges to an optimum
Efficient constrained NLP method
Can only handle continuous problems
Optimization result satisfies optimality condition

Overview of Multi-Objective Hybrid Approach

- Two-branch tournament selection GA handles discrete variables, and evolves population into a representation of the Pareto set
  - Performs global search
  - GA fitness values are unconstrained
- SQP solution obtained for each GA fitness evaluation
  - Addresses continuous variables
  - Uses Goal Attainment formulation
  - Enforces constraints
  - For the local search, each individual in the population is assigned a goal point based on their spatial location

Hybridization Approach

- Problem statement has two levels:
  - Top Level: solved by two-branch GA

Minimize $\begin{Bmatrix} f_1(\mathbf{x}_d, \mathbf{x}_c) \\ f_2(\mathbf{x}_d, \mathbf{x}_c) \end{Bmatrix}$

$f_1(\mathbf{x}_d, \mathbf{x}_c^*)$, $f_2(\mathbf{x}_d, \mathbf{x}_c^*)$ are the fitness values associated with each individual; these come from solving the sub-level SQP problem

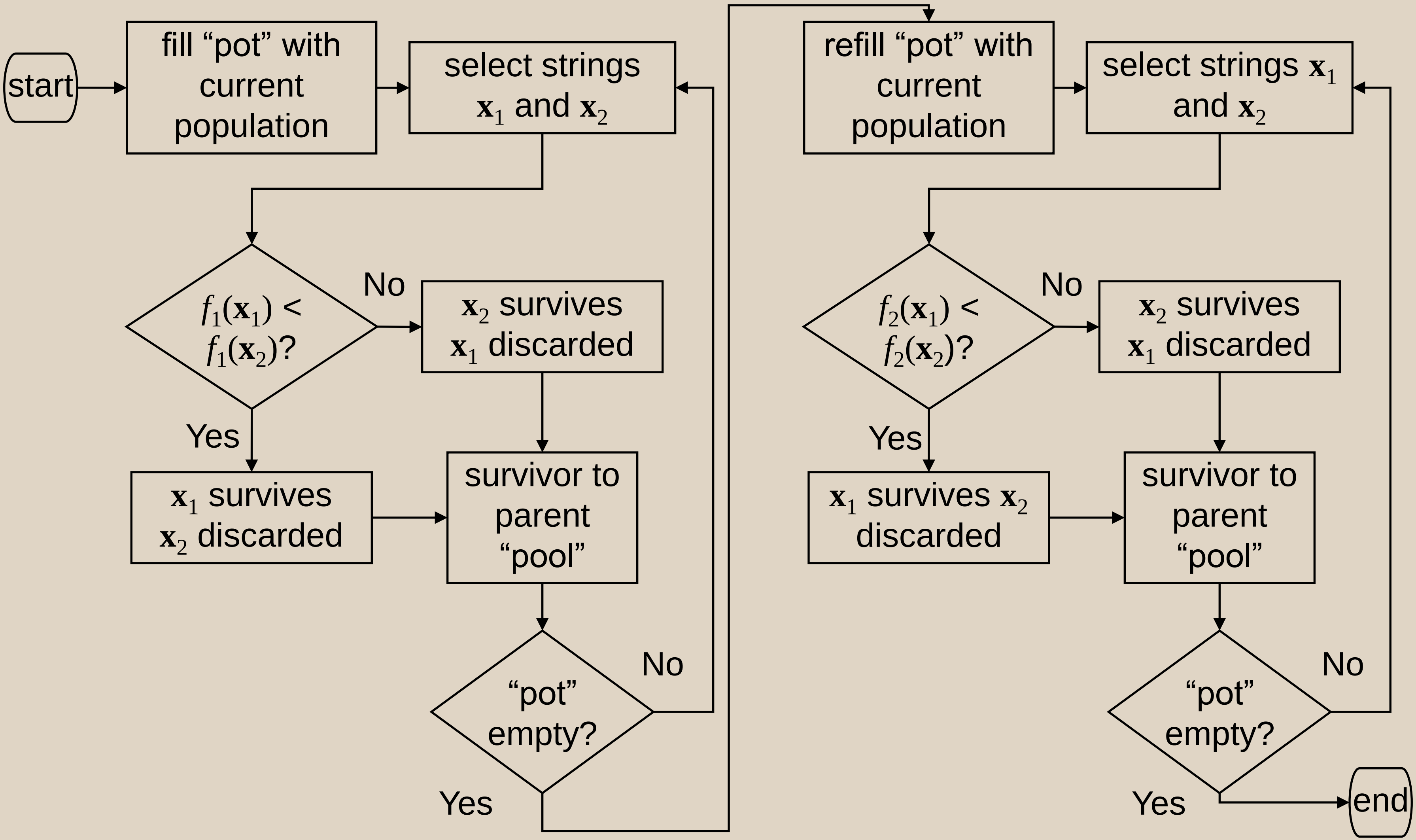
Subject to: $(\mathbf{x}_c)_i^L \leq (\mathbf{x}_c)_i \leq (\mathbf{x}_c)_i^U$ (Continuous variables)

Constraints needed for GA chromosome coding

$(\mathbf{x}_d)_i \in 1, 2, 3, 4 \ldots$ (Discrete variables)

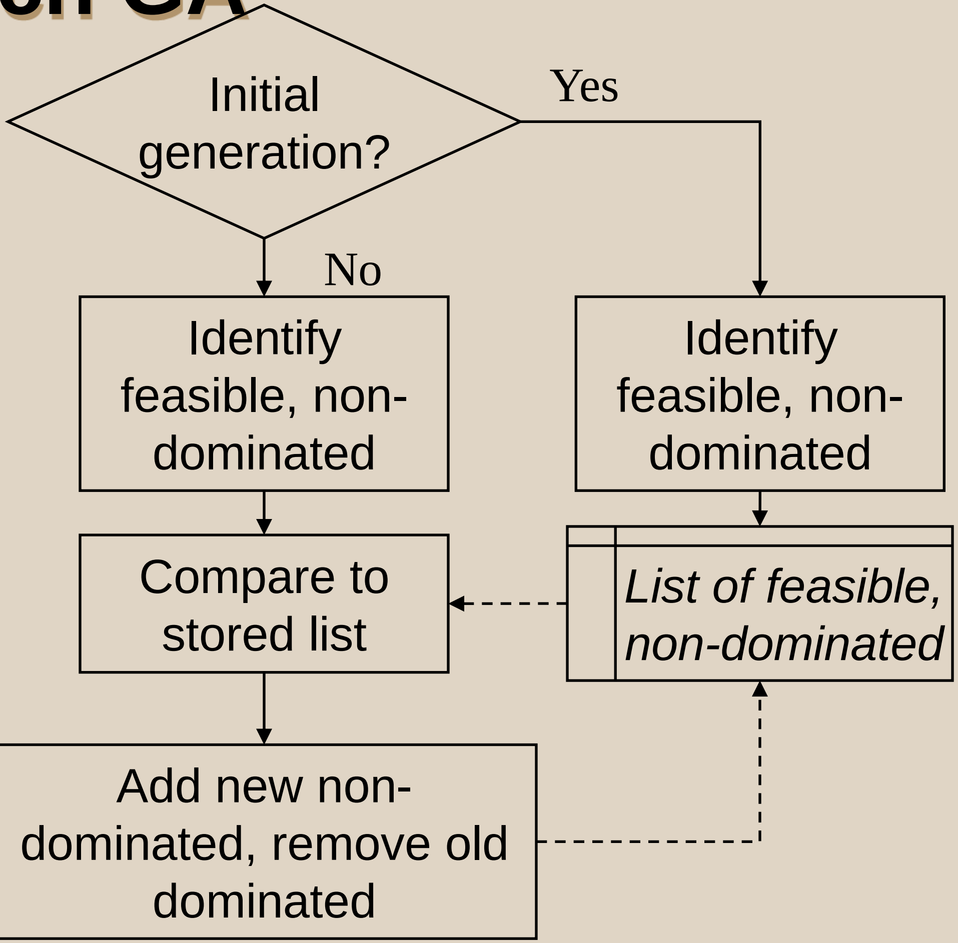
  - Chromosome describes $\mathbf{x}_d$, $\mathbf{x}_c^0$

Two-Branch GA Selection Mechanics



Collecting Non-Dominated Designs in Two-Branch GA

- Many designs evaluated
  - Approximate Pareto front over run
  - Any feasible, non-dominated design encountered is desired
- Collection scheme
  - Identify and store feasible, non-dominated individuals from initial generation
  - Subsequent generations, identify and compare
  - Update stored list as needed



Hybridization Approach

- Sub-level problem: solved by SQP using goal attainment strategy (here, MATLAB's `fgoalattain`)
  - For this problem, $\mathbf{x}_d$, $\mathbf{x}_c^0$, and f_l^G are parameters provided from the top-level problem

Minimize γ

Subject to:

$f_i(\mathbf{x}_c) - a_i\gamma \le f_i^G$	converted objective functions
$g_j(\mathbf{x}_c) \le 0$	inequality constraints
$h_k(\mathbf{x}_c) = 0$	equality constraints
$(\mathbf{x}_c)_i^L \le (\mathbf{x}_c)_i \le (\mathbf{x}_c)_i^U$	bounds on continuous variables

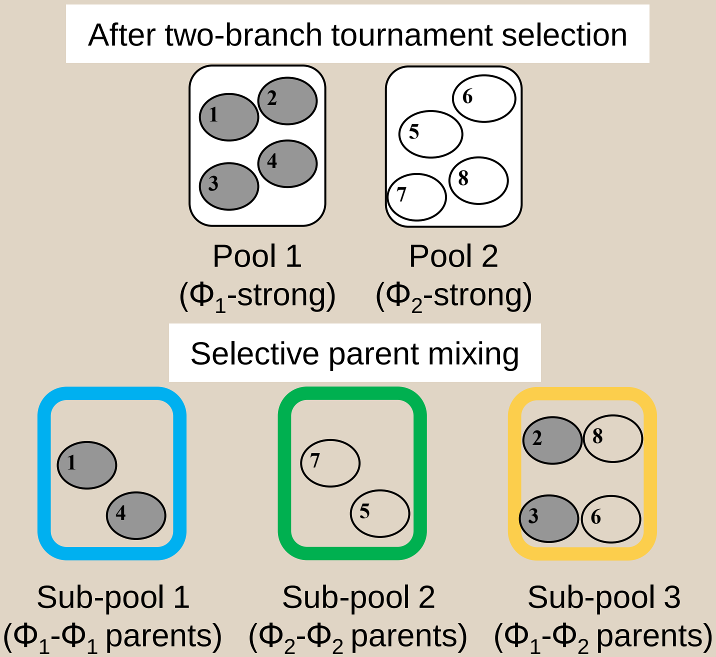
$f_1(\mathbf{x}_d, \mathbf{x}_c^*)$, $f_2(\mathbf{x}_d, \mathbf{x}_c^*)$ are returned to top-level as fitness values for two-branch GA

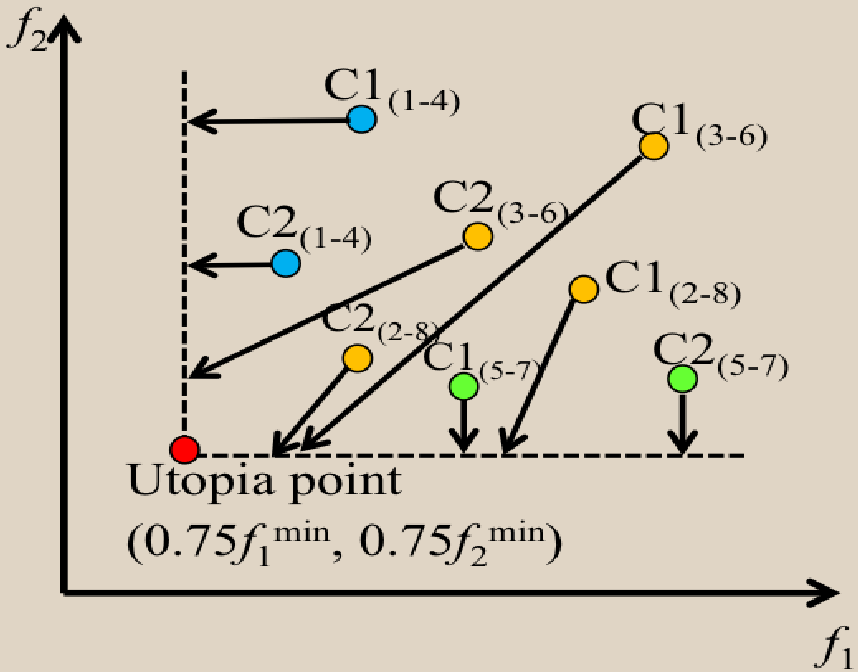
Determining Goal Points for Goal Attainment

- Sub-problem requires goal values for each objective
  - Scan current population for lowest value of f_1 and lowest value of f_2
  - Assign a "utopia" point at ($0.75\, f_1^{low}$, $0.75\, f_2^{low}$) to help avoid over-attainment
  - Determine goal point for each individual based upon parents and distance to goal references

Selective Parent Mixing and Unique Goal Assignment Technique

- Selective parent mixing leads to different sub-pool of populations
- Children from each sub-pools uses a different goal assignment strategy



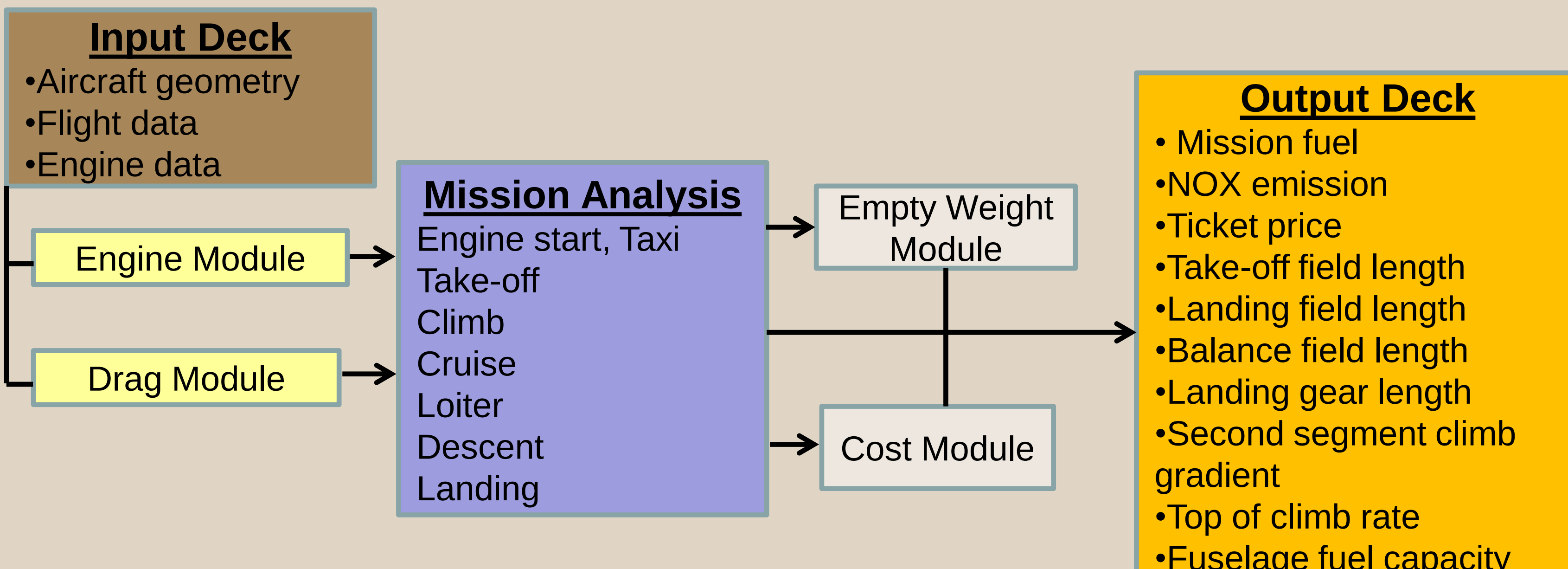


Aircraft Design Problem

- Builds on work from Lehner and Crossley for “greener aircraft”
  - Design a twin-engine 150-seat aircraft to fly 3000 nmi
  - Minimize combinations of:
    - Ticket price and fuel burn
    - Ticket price and NOx emissions
    - Fuel burn and NOx emissions
  - Constraints imposed on aircraft performance and geometry
  - Ten continuous variables describing wing and engine
  - Seven discrete variables describing technology choices for aerodynamics, engine cycle and primary structural material
    - 4,608 different combinations of discrete variables

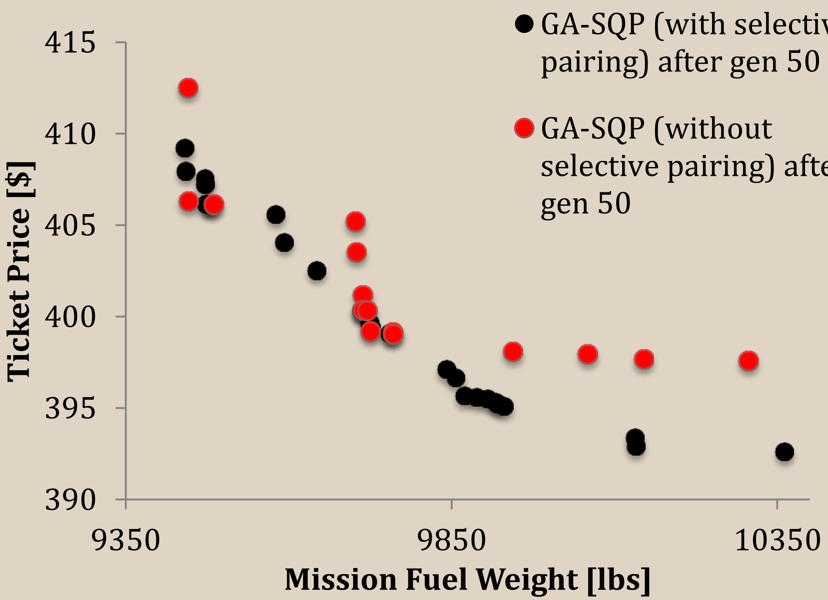
Sizing Code

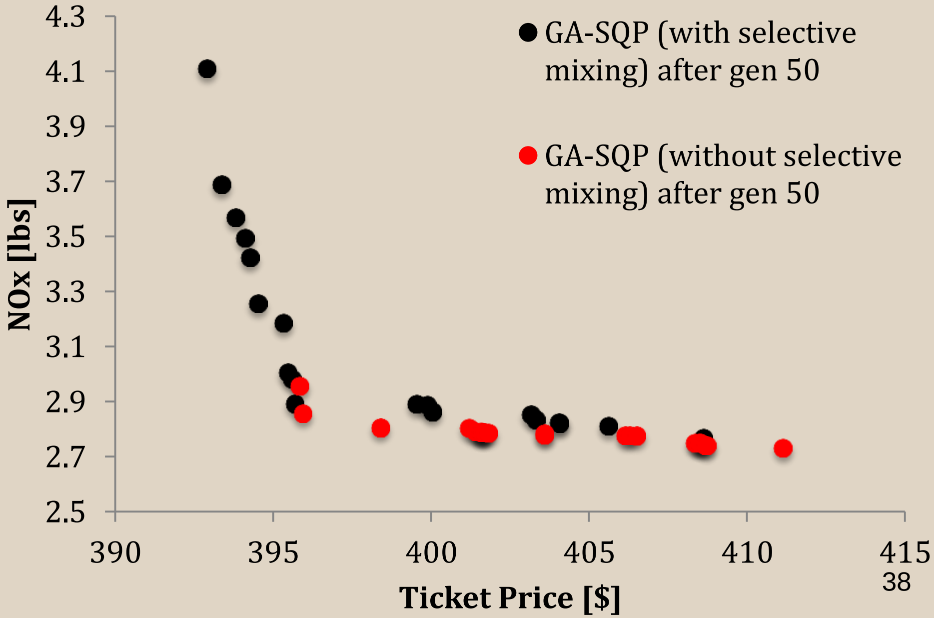
- Relatively simple sizing code performs mission analyses and weight estimation to estimate values needed in constraint and objective functions
- Developed for this effort ; requires (near) first-order continuity for SQP sub-problem



Result and Analysis of Multi-objective MDNLP Performance

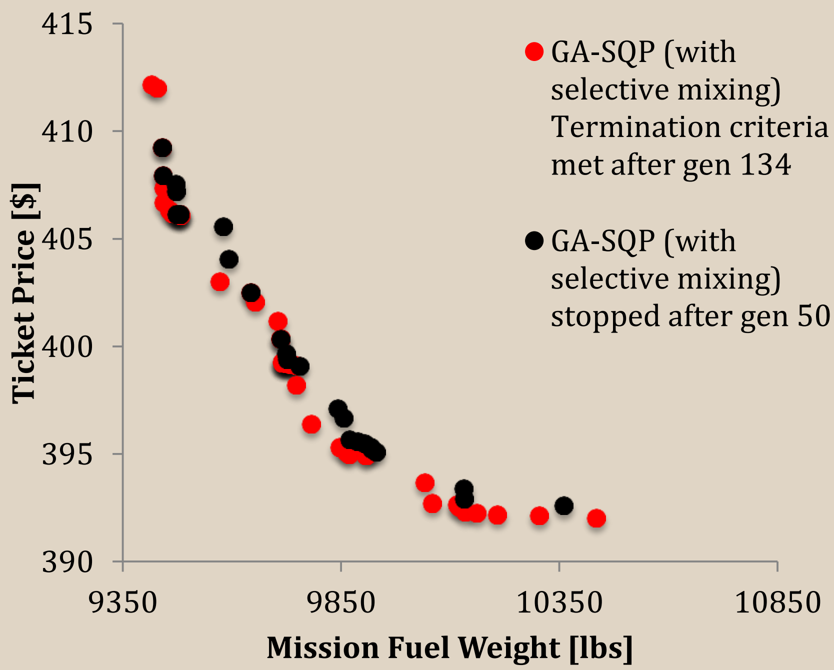
- Using selective parent mixing improves the spread and quality of the Pareto front
- The change in continuous variable with improved method of handling the goal attainment formulation refines the result.
- Improved spread for the objective pair: NOx and ticket price (Reduction in NOx is about 34%)

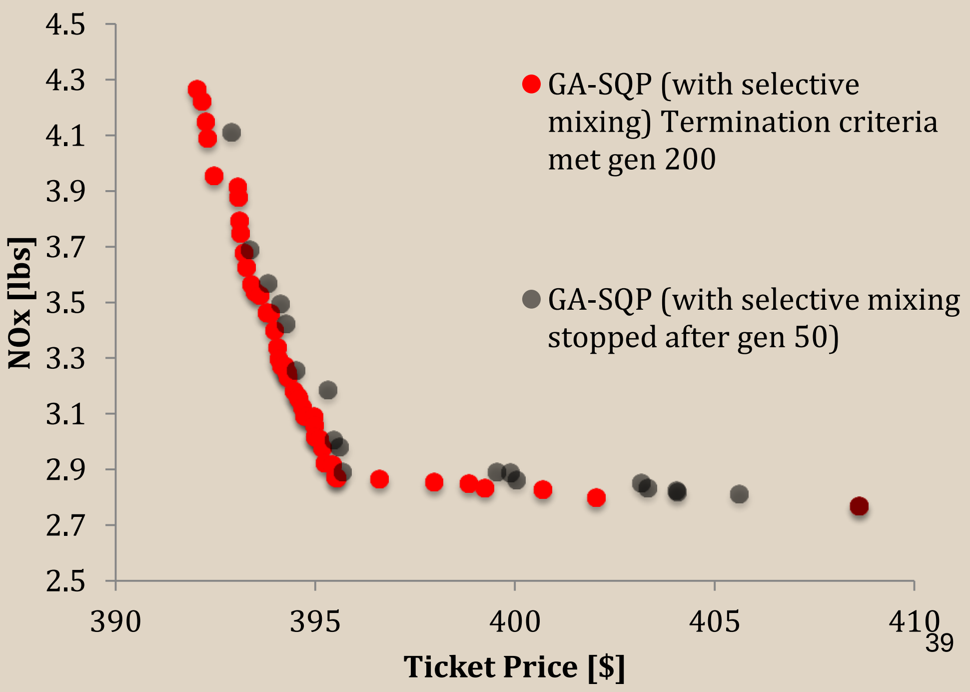




Effects on Termination Criteria

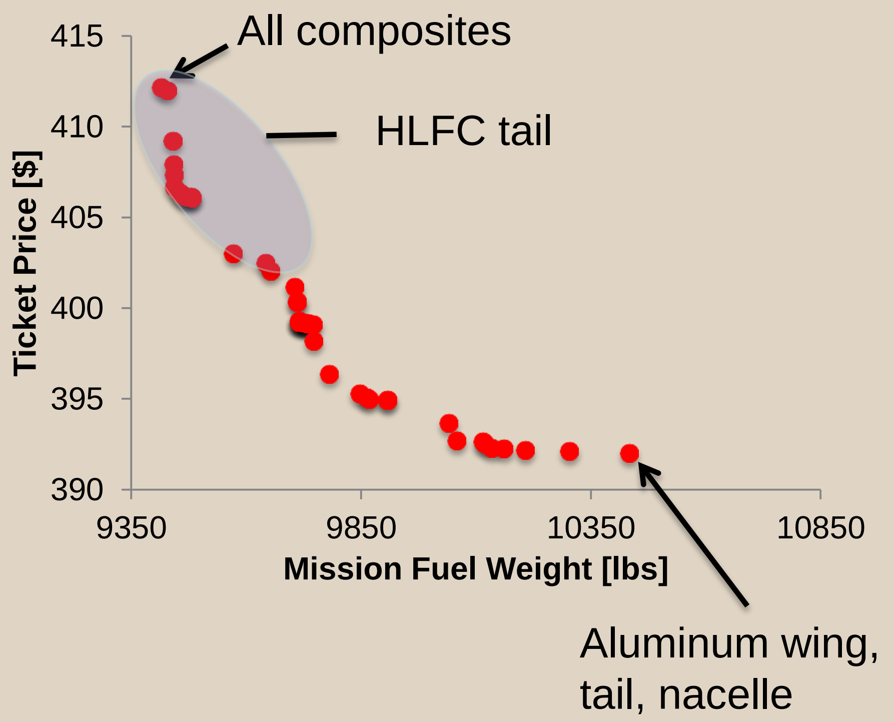
- Initial termination criterion stopped run after 50 generations
- New stopping criteria set the maximum generation to 200 or terminates the algorithm if there is no new inclusion/exclusion in the non-dominated set in last 10 generations.





Technology Considerations via Pareto Set

- Identifying a representation of the Pareto set enables technology consideration
  - Natural laminar flow wing and open rotor type engine are preferred for all the designs
  - Hybrid laminar flow control on tail surfaces appears on low fuel, but high price designs
  - High ticket price, low fuel designs have all composite structures
  - Higher fuel side designs have more aluminum structures
- Choices here are based upon our technology models, many rely upon expert opinion



Observations about Hybrid Approach for Constrained MO-MDNLP

- The hybrid combination allows the population to evolve in the direction of the Pareto front, while SQP refines the search and ensures satisfaction of the problem constraints
- Using the selective parent mixing concept and the unique goal assignment technique provides better spread and quality of Pareto frontier than previous approach
- Approach allows for technology consideration in context of best possible tradeoffs
  - Results shown here rely heavily on our technology models, which have low-fidelity

Potential Future Work for Hybrid Approach for Constrained MO-MDNLP

- Establish a basis of comparison with other MO algorithms (particularly population-based) in terms of computational cost, spread and quality of the Pareto front
- Termination criteria plays an important role; this would benefit from further study
- Extend to formulations with more than two objectives (although visualization of results becomes difficult)