LECTURE 3
MULTI-OBJECTIVE OPTIMIZATION

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Pareto optimization
Multi-objective optimization

FIND THE PARETO SOLUTION SET IN A MULTI-DIMENSIONAL PARAMETER SPACE
TUNING THE PARAMETERS SO THAT CLOSEST FIT TO THE OBSERVED SYSTEM RESPONSE IS OBTAINED

HOWEVER, WHAT IS THE APPROPRIATE OBJECTIVE FUNCTION?
MULTI-OBJECTIVE OPTIMIZATION

Birds are trying to optimize multiple objectives simultaneously.

Trade-off between flight time and energy-use.

Need an optimization method that can identify ensemble of solutions that span the Pareto surface.

Vrugt et al. [J. Avian Biol., 2006]
Consider a two-dimensional optimization problem with two objectives:

\[ f_1(x) = x_1 + (x_2 - 1)^2; f_2(x) = x_2 + (x_1 - 1)^2 \] with \( x_1, x_2 \in [0,1] \)

We cannot find a single combination of \((x_1, x_2)\) for which \( f_1(x) \) and \( f_2(x) \) are both at their minimum.

Optimization problem with multiple optimal solutions.
MULTIPLE SOLUTIONS: THE PARETO FRONT

Consider a two-dimensional optimization problem with two objectives:
\[ f_1(x) = x_1 + (x_2 - 1)^2 \; ; \; f_2(x) = x_2 + (x_1 - 1)^2 \] with \( x_1, x_2 \in [0, 1] \)

1. Minimum value of \( f_1(x) \)?
   And for what value of \( x \)?

2. Minimum value of \( f_2(x) \)?
   And for what value of \( x \)?

3. Compromise: \( 0.5f_1(x) + 0.5f_2(x) \)?
   And for what value of \( x \)?

Red line defines the Pareto solution set
HOW TO OBTAIN MULTIPLE SOLUTIONS?

Aggregate the different objective functions to obtain a single scalar:

$$f_t(x) = w_1 f_1(x) + w_2 f_2(x) ; w_2 = 1 - w_1$$

By running multiple different optimization runs for different values of $w_1$, multiple different Pareto solutions are obtained.

INEFFICIENT SEARCH
Simultaneously identify multiple solutions that span the Pareto front / surface (more than 2 objectives)

Pareto ranking is a non-linear, multi-objective scoring technique. Procedure: Find non-dominated solutions with different ranks.

Don’t compare objective function values, but Pareto rank
HOW TO DO PARETO RANKING?

Objective Space

What are the best solutions (nondominated by others)

Pareto Rank 1

What are the next best solutions?

Pareto Rank 2

e tc.
POTENTIAL PROBLEM – CLUSTERING

Objective Space

$f_1$

$f_2$
HOW TO MAINTAIN DIVERSITY?

Solutions could cluster closely to each other – how to make sure to sample the entire front / surface?

Uniqueness of solution in multi-dimensional objective space is somehow taken into account. Extreme solutions are more unique!
STRENGTH PARETO APPROACH

Objective Space

Start with Pareto Rank 1 solutions
How many solutions do they dominate?

Extreme solutions are more unique and will always be maintained
EVENLY SAMPLES THE PARETO FRONT
Improved evolutionary optimization from genetically adaptive multimethod search

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In the last few decades, evolutionary algorithms have emerged as a revolutionary approach for solving optimization problems involving multiple conflicting objectives. Beyond their ability to search incredibly large spaces for multiple solutions, these algorithms are able to maintain a diverse population of solutions and exploit similarities of solutions by recombination. However, existing theory and numerical experiments have demonstrated that it is impossible to develop a single algorithm for population evolution that is always efficient for a diverse set of optimization problems. Here, we show that significant improvements in the efficiency of evolutionary search can be achieved by running multiple optimizers simultaneously using new concepts of global information sharing and genetically adaptive optimization. We call this approach a multiobjective, genetically adaptive, multiobjective, or AMALGAM, method, to evoke the image of a procedure that merges the strengths of different optimization algorithms. Benchmark results on a set of well-known test problems show that AMALGAM approaches a factor of 10 improvement over current optimization algorithms for the same sample, higher dimensional, multimodal problems. The AMALGAM method provides new opportunities for solving previously intractable optimization problems.

Evolutionary optimization is a subject of intense interest in many fields, including computational chemistry, biology, bioinformatics, economics, computational science, geophysics, and environmental science (1–8). The goal is to determine values for model parameters or parameters that provide the best possible solution to a predefined set of objectives or values of a set of optimal solutions in the case of two or more competing objectives. However, locating optimal solutions often turns out to be painstakingly slow, or even completely beyond current or projected computational capacity (9).

Here, we consider a multiobjective optimization problem, with a decision variable (parameter), and a cost function: $y(x) = f(x_1, ..., x_n)$, where $x$ denotes the decision vector, and $y$ is the objective value. We seek an algorithm to optimize problems in which the parameter space $X$, although perhaps quite large, is bounded to a finite set $X$. Under the presence of multiple objectives, the optimization problem has to fit into a set of Pareto-optimal solutions, instead of a single solution (10, 11). A Pareto-optimal solution is one in which one objective cannot be further improved without causing a simultaneous degradation in at least one other objective. As such, they represent globally optimal solutions to the tradeoff problem.

Numerous approaches have been proposed to efficiently find Pareto-optimal solutions for complex multiobjective optimization problems (12–15). In particular, evolutionary algorithms have emerged as the most powerful approach for solving search and optimization problems involving multiple conflicting objectives. Beyond their ability to search incredibly large spaces for multiple Pareto-optimal solutions, these algorithms are able to maintain a diverse set of solutions and exploit similarities of
(1) **Generate sample**: Sample \( N \) points, \( \{\theta_1, \ldots, \theta_N\} \) from the feasible parameter space, and compute the \( n \) objective function values of each of point. Store in matrix \( OF[1:N,1:n] \).

(2) **Create offspring**: Use \( K \) different search operators (GA, PSO, DE, AMS) to produce the offspring population, \( \{\theta^*_1, \ldots, \theta^*_N\} \). Each algorithm contributes \( N_k, k = \{1, \ldots, K\} \) points.

(3) **Calculate objective functions children**: Store information in \( OF^*[1:N,1:n] \)


(5) **Select new Population**: Select \( N \) points from children and parents according to \( R[1:2N,1:2] \).

(6) **Update Contribution Algorithms**: Update \( N_k, k = \{1, \ldots, K\} \) based on the number of points they contributed to the new population.

(7) **Check convergence**: If convergence criteria are satisfied, stop; otherwise return to step 2.
MUCH FASTER CONVERGENCE WITH MULTIPLE SEARCH OPERATORS

IMPORTANCE OF INDIVIDUAL SEARCH METHODS

DYNAMIC CHANGES IN CONTRIBUTION OF INDIVIDUAL ALGORITHMS

Pareto front analysis of flight time and energy use in long-distance bird migration

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Optimality models are frequently used in studies of long distance bird migration to help understand and predict migration routes, stopover strategies and fuelling behaviour in a spatially varying environment. These models typically evaluate bird behaviour by focusing on a single optimization currency, such as total migration time or energy-use, without explicitly considering trade-offs between the involved objectives. In this paper, we demonstrate that this classic single-objective approach downplays the importance of variability in bird behaviour. In the light of these considerations, we therefore propose to use a full multi-criteria optimization method to isolate the set of non-dominated, efficient or Pareto optimal solutions. Unlike single-objective optimization where there is only one combination of bird behaviour maximizing fitness, the Pareto solution set represents a range of optimal solutions to conflicting objectives. Our results demonstrate that this multi-objective approach provides important new ways of analyzing how environmental factors and behavioural constraints have driven the evolution of migratory behaviour.

One of the central goals in avian biology is to understand the behavioural strategies that birds adopt in real-world environments. Faced with the complexity and variability in nature, and the difficulty of performing controlled experiments, a variety of theoretical optimization models have been developed to help understand and examine migratory behaviour of birds. These models range from simple mathematical equations predicting the stopover duration at a given site when optimizing energy or time (Alerstam and Lindström 1990, Hedenström and Alerstam 1997, Weber and Houston 1997, Houston 1998) to spatially explicit individual-based models in which birds migrate over a simulated environment given a set of behavioural rules (Erni et al. 2002a, 2003). Irrespective of the dimensionality and complexity of these models, it is assumed that the bird’s behaviour can be understood and predicted by posing the migration problem into an optimality framework. In such a framework, the behavioural strategy of a bird is evaluated against some prior defined fitness measure (e.g. time, energy and risk of predation), given appropriate biological and environmental constraints. The behavioral strategy that maximizes (as appropriate) this predefined fitness measure is then compared with observed behaviour.

The advantages of this optimality approach are not difficult to enumerate: the fitness of any behavioural strategy, defined by a collection of decisions and actions can be directly evaluated in terms of the bird’s ability to reach the considered objectives, and perhaps most importantly, the strengths of modelling and measuring bird behaviour are combined in a natural way.

In the pioneering work by Alerstam and Lindström (1990) two main currencies were developed that birds might seek to optimize during a migratory episode. Minimizing energy cost of transport is one strategy that could be used by migrating birds, especially short-distance migrants. An alternative currency is the time spent on migration, a currency most likely to be important for long-distance migrants (Weber and Houston 1997). With some notable exceptions (Houston 1998) most optimality models used in avian biology generally obtain predictions assuming either time or energy minimization, without interpreting the range of
## PARAMETERS AND RANGES

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial fat amount</td>
<td>gram</td>
<td>0</td>
<td>20</td>
</tr>
<tr>
<td>Endogenous direction</td>
<td>degrees</td>
<td>150</td>
<td>230</td>
</tr>
<tr>
<td>Number of FlyDays</td>
<td>d</td>
<td>1</td>
<td>15</td>
</tr>
<tr>
<td>Number of RestDays</td>
<td>d</td>
<td>1</td>
<td>15</td>
</tr>
<tr>
<td>Minimum fat amount</td>
<td>gram</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>BarrierCrossFat</td>
<td>gram</td>
<td>0</td>
<td>20</td>
</tr>
</tbody>
</table>

**Additional parameters when wind influence is “On”**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wind Compensation</td>
<td>%</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>Min. NetSpeed to take off</td>
<td>m/s</td>
<td>0</td>
<td>10</td>
</tr>
</tbody>
</table>
PARETO SOLUTION SET

MODEL PREDICTED FLIGHT ROUTES

REAL WORLD PROBLEM: MRI DATASET

Concentration of MnCl₂ versus time at 53,248 voxels and 112 time snapshots. This results in 5,963,776 data points!!
1. Steady State Flow Simulation
   - Regular numerical grid at the scale of the concentration data
   - FEHM finite element simulation of steady state flow field through the heterogeneous system

2. Particle Tracking Transport Simulation
   - FEHM random walk particle tracking algorithm used to minimize numerical dispersion
   - 250,000 particles (~1 cpu-hr on 3.4GHz processor)
   - Particle tracking results converted to normalized concentration using a numerical convolution method

Many thanks to Bruce Robinson for setting up the forward model
1. Permeabilities of individual 5 zones

- Ranges assigned so that rank order of the permeabilities of the five sands is honored

2. Molecular diffusion

3. Longitudinal and transverse dispersivity

- Parameter ranges assigned based on literature estimates and scientific judgment
SOLUTION USING HYBRID PARALLELIZATION SCHEME

(AMALGAM) algorithm

I. Use population size $N = 25$

(TEHM) Flow and transport code

Each chain evolves on a different node
Each chain uses 10 other nodes for particle tracking

Computational time reduced with a factor of 250
OPTIMIZATION RESULTS WITH DREAM

12,000 model FEHM runs using hybrid parallelization with 250 processors

Original results with median parameter values

First inverse Run - 250,000 particles

Breakthrough curves in high-flow zones are well matched, but dispersion, diffusion, or advection into lower permeability zones under-represented.
RESULTS MULTIOBJECTIVE OPTIMIZATION

- $f_1$: Permeability zones 1 - 3
- $f_2$: Permeability zones 4 & 5

RED: Original formulation with 5 parameters
BLACK: SCE-UA solution
BLUE: Modified formulation with 15 parameters (each zone has its own dispersivity values)

TRADE-OFFS in MODEL BETWEEN HIGH AND LOW FLOW ZONES