Adaptively Tuned Particle Swarm Optimization for Spatial Design

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Overview of the Talk

1. What is particle swarm optimization (PSO)?
   (Blum and Li, 2008; Clerc, 2010, 2012)

2. New adaptively-tuned PSO algorithms.

3. Using (adaptively-tuned) PSO for spatial design.

4. Example adding locations to an existing monitoring network.

Particle Swarm Optimization — Intuition

Put a “swarm” of particles in the search space:

> Don’t search alone, pay attention to what your neighbors are doing!

Click!

Best for complex objective functions which are cheap to compute, and when near-optimal solutions are useful.

Particle Swarm Optimization

Goal: minimize some objective function $Q(\boldsymbol{\theta}) : \mathbb{R}^D \to \mathbb{R}$.

Populate $\mathbb{R}^D$ with n particles. Define particle i in period k by:

- a location $\boldsymbol{\theta}_i(k) \in \mathbb{R}^D$;
- a velocity $\boldsymbol{v}_i(k) \in \mathbb{R}^D$;
- a personal best location $\boldsymbol{p}_i(k) \in \mathbb{R}^D$;
- a neighborhood (group) best location $\boldsymbol{g}_i(k) \in \mathbb{R}^D$.

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Basic PSO: update particle i from k to $k+1$ via:

- For $j = 1, 2, \ldots, D$:

$$\begin{aligned} v_{ij}(k+1) &= \omega v_{ij}(k) + \mathrm{U}(0, \phi_1) \times \{p_{ij}(k) - \theta_{ij}(k)\} \\ &\qquad + \mathrm{U}(0, \phi_2) \times \{g_{ij}(k) - \theta_{ij}(k)\} \\ &= \text{inertia} + \text{cognitive} + \text{social}, \\ \theta_{ij}(k+1) &= \theta_{ij}(k) + v_{ij}(k+1), \end{aligned}$$

- Then update personal and group best locations.

PSO — Parameters

$$v_{ij}(k+1) = \omega v_{ij}(k) + \mathrm{U}(0,\phi_1) \times \{p_{ij}(k) - \theta_{ij}(k)\} \\ + \mathrm{U}(0,\phi_2) \times \{g_{ij}(k) - \theta_{ij}(k)\}$$

Inertia parameter: ω.

- Controls the particle's tendency to keep moving in the same direction.

Cognitive correction factor: ϕ_1.

- Controls the particle's tendency to move toward its personal best.

Social correction factor: ϕ_2.

- Controls the particle's tendency to move toward its group best.

Default choices:

- $\omega = 0.7298$, $\phi_1 = \phi_2 = 1.496$ (Clerc and Kennedy, 2002).
- $\omega = 1/(2\ln 2) \approx 0.721$, $\phi_1 = \phi_2 = 1/2 + \ln 2 \approx 1.193$ (Clerc, 2006).

PSO — Neighborhood Topologies

Sometimes it is useful to restrict the flow of information across the swarm — e.g. complicated objective functions with many local optima.

Particles are only informed by their neighbors for their group best $\boldsymbol{g}_i(k)$.
$\rightarrow$ *No matter where they are in the search space*.

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We use the stochastic star neighborhood topology (Miranda et al., 2008).

- Each particle informs itself and m random particles.
  $\rightarrow$ informants sampled with replacement once during initialization.
- On average each particle is informed by m particles.
- A small number of particles will be informed by many particles.

Many variants on basic PSO exist

See e.g. Clerc (2012), Simpson et al. (2017, appendix).

- Handling search space constraints.
- Coordinate free velocity updates.
- Parallelization.
- Asynchronous updates.
- Redraw neighborhoods.
- Bare-bones PSO (BBPSO) — no velocity term.

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$\rightarrow$ slowly decrease $\omega(k)$ over time (Eberhart and Shi, 2000).

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AT-PSO: tune $\omega(k)$ using an analogy with adaptively tuned random walk Metropolis (Andrieu and Thoms, 2008).

Can also create AT-BBPSO algorithms.

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c denote an adjustment factor.

Update $\omega(k)$ via:

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Defaults: $R^* \in [0.3, 0.5]$, $c = 0.1$.

AT-PSO/AT-BBPSO Simulation Study Results

Intuition: tuning $\omega(k)$ allows the swarm to adjust the exploration / exploitation tradeoff on the fly based on current swarm conditions.

- This has a tendency to speed up convergence.
- ...but convergence may be premature in multi-modal problems.

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Overview of results from a simulation study:

- AT-PSO performs better than PSO on "hard enough" problems...
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Overview of results from a simulation study:

- AT-PSO performs better than PSO on "hard enough" problems...
- ...but has trouble with many local optima.
- AT-BBPSO is often the best performing algorithm for complex, multimodal objective functions...
- ...but is less competitive for easier objective functions.

Spatial Design — Problem Setup

Goal: want to learn about the spatial field $Y(\boldsymbol{u})$, $\boldsymbol{u} \in \mathcal{D} \subset \mathbb{R}^2$.

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$$Z(\boldsymbol{u}) = Y(\boldsymbol{u}) + \varepsilon(\boldsymbol{u})$$

for all $\boldsymbol{u} \in \mathcal{D}$, and $\varepsilon(\boldsymbol{u}) \overset{iid}{\sim} \mathrm{N}(0, \tau^2)$.

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Assume $Y(\boldsymbol{u}) = \boldsymbol{x}(\boldsymbol{u})'\boldsymbol{\beta} + \delta(\boldsymbol{u})$ with

$$\delta(\boldsymbol{u}) \sim \mathrm{GP}(0, C_{\phi}(\cdot, \cdot))$$

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Where should we put additional monitoring locations, $\boldsymbol{D} = \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_{N_d}\}$?

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$$\sigma^2_{uk}(\boldsymbol{u}; \boldsymbol{D}, \widehat{\boldsymbol{\theta}}) = C_{\widehat{\phi}}(\boldsymbol{u}, \boldsymbol{u}) - \boldsymbol{c}_Y(\boldsymbol{u}; \boldsymbol{D})' \boldsymbol{C}_Z^{-1}(\boldsymbol{D}) \boldsymbol{c}_Y(\boldsymbol{u}; \boldsymbol{D}) +$$
$$\left\{\boldsymbol{x}(\boldsymbol{u}) - \boldsymbol{X}' \boldsymbol{C}_Z^{-1}(\boldsymbol{D}) \boldsymbol{c}_Y(\boldsymbol{u}; \boldsymbol{D})\right\}' \left\{\boldsymbol{X}' \boldsymbol{C}_Z^{-1}(\boldsymbol{D}) \boldsymbol{X}\right\}^{-1} \left\{\boldsymbol{x}(\boldsymbol{u}) - \boldsymbol{X}' \boldsymbol{C}_Z^{-1}(\boldsymbol{D}) \boldsymbol{c}_Y(\boldsymbol{u}; \boldsymbol{D})\right\}$$

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What about when τ^2 and ϕ are estimated?

Parameter uncertainty universal kriging MSPE:

$$\approx \sigma^2_{puk}(\boldsymbol{u};\boldsymbol{D},\widehat{\boldsymbol{\theta}}) = \sigma^2_{uk}(\boldsymbol{u};\boldsymbol{D},\widehat{\boldsymbol{\theta}}) + \text{ stuff},$$

depending on the FI matrix and gradient of predictor wrt $\boldsymbol{\theta}$ (Zimmerman and Cressie, 1992; Abt, 1999).

Spatial Design — Design Criteria

Ideal design criteria: choose design points to minimize...

- Mean/total MSPE: $\overline{Q}_{puk}(\boldsymbol{D}) = \int_{\mathcal{D}} \sigma^2_{puk}(\boldsymbol{u}; \boldsymbol{D}, \widehat{\boldsymbol{\theta}}) d\boldsymbol{u}$
- Maximum MSPE: $Q^*_{puk}(\boldsymbol{D}) = \max_{\boldsymbol{u}\in\mathcal{D}} \sigma^2_{puk}(\boldsymbol{u}, \boldsymbol{D}, \widehat{\boldsymbol{\theta}})$

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This is computationally infeasible.

Realistic criteria: approximate with a grid of target points $\boldsymbol{r}_1, \dots, \boldsymbol{r}_{N_t}$:

- Minimize $\overline{Q}_{puk}(\boldsymbol{D}) = \sum_{i=1}^{N_t} \sigma^2_{puk}(\boldsymbol{r}_i; \boldsymbol{D}, \widehat{\boldsymbol{\theta}})$
- Minimize $Q^*_{puk}(\boldsymbol{D}) = \max_{i=1,2,\dots,N_t} \sigma^2_{puk}(\boldsymbol{r}_i; \boldsymbol{D}, \widehat{\boldsymbol{\theta}})$

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$\Longrightarrow$ why not use PSO? Other points in its favor:

- Near-optimal solutions are nearly as valuable as optimal solutions.
- Objective function is cheap in universal kriging.
- More expensive in kriging with parameter uncertainty, but doable.
- Highly multi-modal objective function (e.g. switch two locations).

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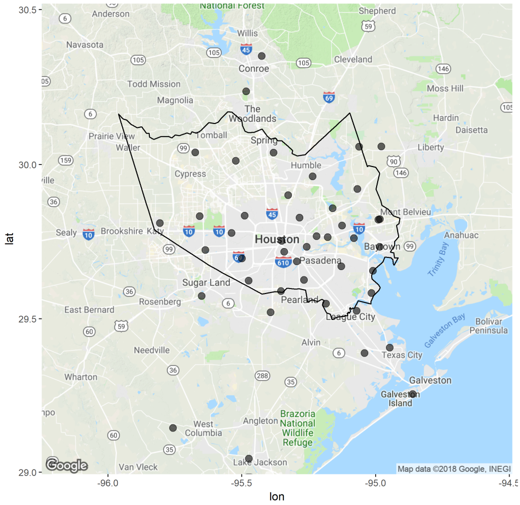
Genetic algorithms also reasonable, e.g. Hamada et al. (2001).

Example: Ozone Monitoring in Harris County, TX



Map via ggmap (Kahle and Wickham, 2013).

- Ozone concentration is associated with increased risk of cardiac arrest (Ensor et al., 2013).
- In August 2016, there were 44 active monitoring locations near Houston, TX.
- Harris County, TX, contains 33 of these locations.

Hypothetical Design Problem and Data

Want to learn more about ozone concentrations in Harris County.

Where to put 100 new monitoring locations within the county?

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Data from the Texas Commission on Environmental Quality (TCEQ)

- Monitoring locations measure several air quality indicators.
- Ozone: daily maximum eight-hour ozone concentration (DM8) in parts per billion.
  $\rightarrow$ maximum of all contiguous 8-hour means for that day.
- Some locations have missing data.

Model and Design Criteria

Model:

- Linear mean function in spatial coordinates: $\boldsymbol{x}(\boldsymbol{u})' = (u_1, u_2)$.
- Exponential covariance function:

$$C(\boldsymbol{u}, \boldsymbol{v}) = \sigma^2 \exp(-||\boldsymbol{u} - \boldsymbol{v}||/\psi)$$

- Estimate $(\boldsymbol{\theta}, \boldsymbol{\delta})$ via maximum likelihood.

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Design Criteria:

- Mean MSPE w/ parameter uncertainty $\overline{Q}_{puk}(\boldsymbol{d})$.
- Maximum MSPE w/ parameter uncertainty $Q^*_{puk}(\boldsymbol{d})$.
- Approximate each with a grid of 1229 points in Harris County.

Algorithm	$\overline{Q}_{puk}$	Q^*_{puk}
Uniform	16.40	26.80
PSO1	**14.40**	**20.63**
PSO2	14.45	**21.03**
PSO1-CF	15.53	23.54
PSO2-CF	15.77	23.16
AT1-PSO1	**14.38**	**20.57**
AT1-PSO2	14.56	23.18
AT1-PSO1-CF	15.96	23.33
AT1-PSO2-CF	15.60	24.02
AT2-PSO1	**14.42**	**21.13**
AT2-PSO2	**14.32**	22.11
AT2-PSO1-CF	15.85	24.00
AT2-PSO2-CF	15.95	23.63
AT1-BBPSO	14.53	22.28
AT1-BBPSOxp	15.87	22.19
AT1-BBPSO-CF	14.65	21.33
AT1-BBPSOxp-CF	14.84	22.34
AT2-BBPSO	14.65	23.49
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GA-11	**14.40**	21.19
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Results:

- Uniform: uniformly sample new monitoring locations.
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- Bolded: top 5 for that design criterion (column).

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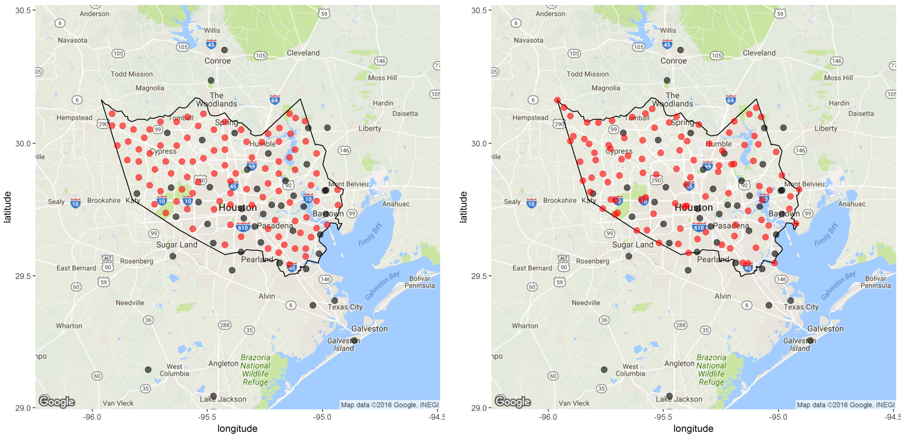
- PSO and AT-PSO variants tend to be the best.
- GAs are competitive.
- With significantly fewer monitoring locations, PSO variants are the best.

Best designs found according to $\overline{Q}_{puk}$ (left) and Q^*_{puk} (right)



Optimal design is highly dependent on the mean function (Zimmerman, 2006).

Background map via ggmap (Kahle and Wickham, 2013).

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- For spatial design problems, standard PSO works well.
- For large enough spatial design problems, AT-PSO is attractive.
- Approach can easily be extended to spatio-*temporal* design.

Thank you!

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