Adaptively Tuned Particle Swarm Optimization for Spatial Design

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August 3, 2016

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Research supported by the NSF-Census Research Network

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!

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

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

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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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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Define the improvement rate of the swarm in period k:

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c denote an adjustment factor.

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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...
- ...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

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

Where should we observe $Y(\boldsymbol{u})$? Usual objective: minimize MSPE.

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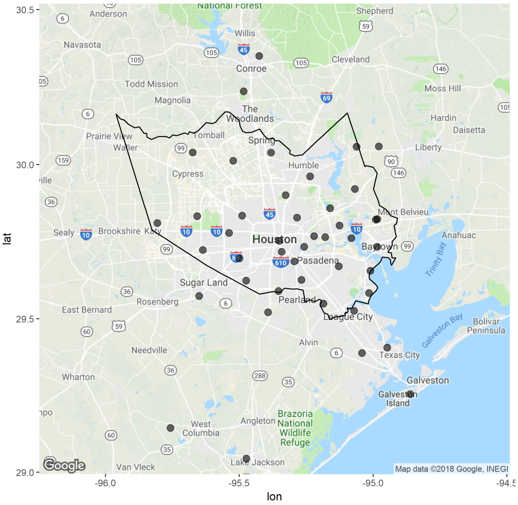
Genetic algorithms also reasonable, e.g. Hamada et al. (2001).

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

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- Ozone: daily maximum eight-hour ozone concentration (DM8) in parts per billion.
  $\rightarrow$ maximum of all contiguous 8-hour means for that day.
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Let $Y(\boldsymbol{u})$ denote DM8 and $Z(\boldsymbol{u})$ denote measured DM8 at $\boldsymbol{u}$.

Ozone Monitoring Model

Assume $Z(\boldsymbol{u})$ is a noisy signal of $Y(\boldsymbol{u})$:

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

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

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

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

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Details:

- 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.

Spatial Design — MSPE and Kriging

Goal: choose new locations $\boldsymbol{D} = \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_{100}\}$ to minimize MSPE.

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$$\sigma^2_{uk}(\boldsymbol{u}; \boldsymbol{D}, \widehat{\boldsymbol{\theta}}) = C_{\widehat{\phi}}(\boldsymbol{u}, \boldsymbol{u}) - \boldsymbol{c}_Y(\boldsymbol{u}; \boldsymbol{D})' \boldsymbol{C}_Z^{-1}(\boldsymbol{D}) \boldsymbol{c}_Y(\boldsymbol{u}; \boldsymbol{D}) +$$
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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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Realistic criteria: approximate with a grid of target points $\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{N_t}$:

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Use 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
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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
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GA-11	**14.40**	21.19
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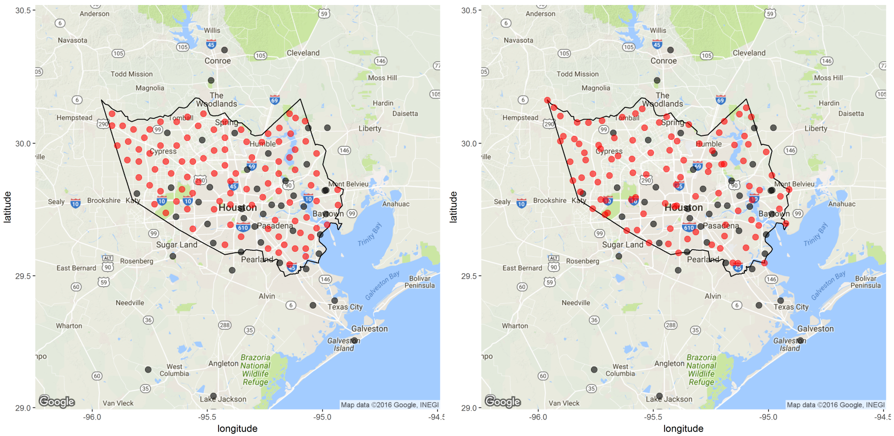
- GAs are competitive.
- With significantly fewer monitoring locations, PSO variants are the best.

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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- Approach can easily be extended to spatio-*temporal* design.

Thank you!

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