

# 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  $Q(\theta) : \mathbb{R}^D \rightarrow \mathbb{R}$ .

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

- a **location**  $\theta_i(k) \in \mathbb{R}^D$ ;
- a **velocity**  $v_i(k) \in \mathbb{R}^D$ ;
- a **personal best** location  $p_i(k) \in \mathbb{R}^D$ ;
- a **neighborhood (group) best** location  $g_i(k) \in \mathbb{R}^D$ .

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

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

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

$$\theta_{ij}(k+1) = \theta_{ij}(k) + v_{ij}(k+1),$$

- Then update personal and group best locations.

## PSO — Parameters

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

Inertia parameter:  $\omega$ .

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

Cognitive correction factor:  $\phi_1$ .

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

Social correction factor:  $\phi_2$ .

- 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.

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

- Each particle informs itself and  $m$  random particles.  
→ 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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$$\log \omega(k+1) = \log \omega(k) + c\{R(k+1) - R^*\}$$

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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 — Problem Setup

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

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

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

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

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Where should we put additional monitoring locations,  $\mathcal{D} = \{\mathbf{d}_1, \dots, \mathbf{d}_{N_d}\}$ ?

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$$\begin{aligned}\sigma_{uk}^2(\mathbf{u}; \mathbf{D}, \widehat{\boldsymbol{\theta}}) = & C_{\widehat{\phi}}(\mathbf{u}, \mathbf{u}) - \mathbf{c}_Y(\mathbf{u}; \mathbf{D})' \mathbf{C}_Z^{-1}(\mathbf{D}) \mathbf{c}_Y(\mathbf{u}; \mathbf{D}) + \\ & \{x(\mathbf{u}) - \mathbf{X}' \mathbf{C}_Z^{-1}(\mathbf{D}) \mathbf{c}_Y(\mathbf{u}; \mathbf{D})\}' \{ \mathbf{X}' \mathbf{C}_Z^{-1}(\mathbf{D}) \mathbf{X} \}^{-1} \{x(\mathbf{u}) - \mathbf{X}' \mathbf{C}_Z^{-1}(\mathbf{D}) \mathbf{c}_Y(\mathbf{u}; \mathbf{D})\}\end{aligned}$$

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What about when  $\tau^2$  and  $\phi$  are estimated?

Parameter uncertainty universal kriging MSPE:

$$\approx \sigma_{puk}^2(\mathbf{u}; \mathbf{D}, \hat{\boldsymbol{\theta}}) = \sigma_{uk}^2(\mathbf{u}; \mathbf{D}, \hat{\boldsymbol{\theta}}) + \text{stuff},$$

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:  $\bar{Q}_{puk}(\mathbf{D}) = \int_{\mathcal{D}} \sigma_{puk}^2(\mathbf{u}; \mathbf{D}, \hat{\theta}) d\mathbf{u}$
- Maximum MSPE:  $Q_{puk}^*(\mathbf{D}) = \max_{\mathbf{u} \in \mathcal{D}} \sigma_{puk}^2(\mathbf{u}, \mathbf{D}, \hat{\theta})$

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- Maximum MSPE:  $Q_{puk}^*(\mathbf{D}) = \max_{\mathbf{u} \in \mathcal{D}} \sigma_{puk}^2(\mathbf{u}, \mathbf{D}, \hat{\theta})$

This is computationally infeasible.

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

- Minimize  $\bar{Q}_{puk}(\mathbf{D}) = \sum_{i=1}^{N_t} \sigma_{puk}^2(\mathbf{r}_i; \mathbf{D}, \hat{\theta})$
- Minimize  $Q_{puk}^*(\mathbf{D}) = \max_{i=1,2,\dots,N_t} \sigma_{puk}^2(\mathbf{r}_i; \mathbf{D}, \hat{\theta})$

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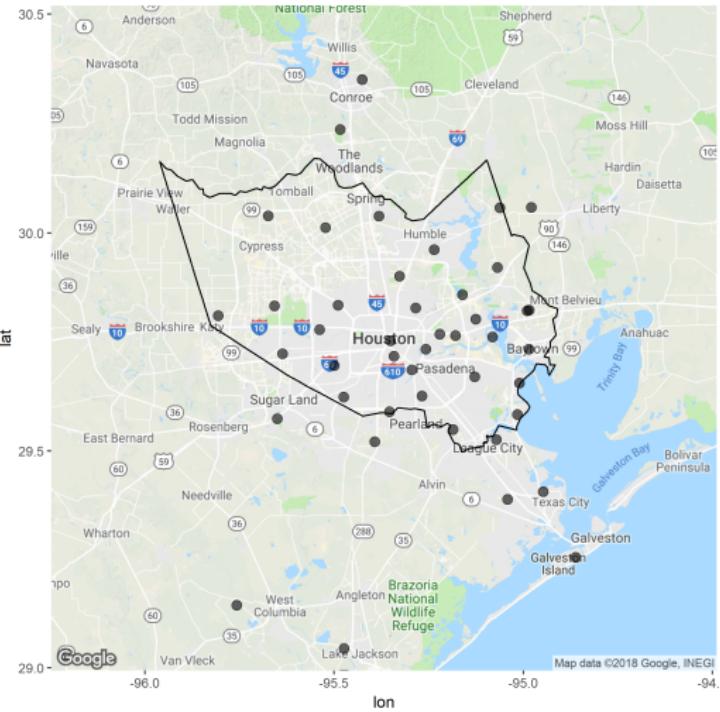
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Genetic algorithms also reasonable, e.g. Hamada et al. (2001).

# 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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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.
  - 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:  $\mathbf{x}(\mathbf{u})' = (u_1, u_2)$ .
- Exponential covariance function:

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

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

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Design Criteria:

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

Algorithm	$\overline{Q}_{puk}$	$Q_{puk}^*$
Uniform	16.40	26.80
PSO1	<b>14.40</b>	<b>20.63</b>
PSO2	14.45	<b>21.03</b>
PSO1-CF	15.53	23.54
PSO2-CF	15.77	23.16
AT1-PSO1	<b>14.38</b>	<b>20.57</b>
AT1-PSO2	14.56	23.18
AT1-PSO1-CF	15.96	23.33
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AT2-PSO2	<b>14.32</b>	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
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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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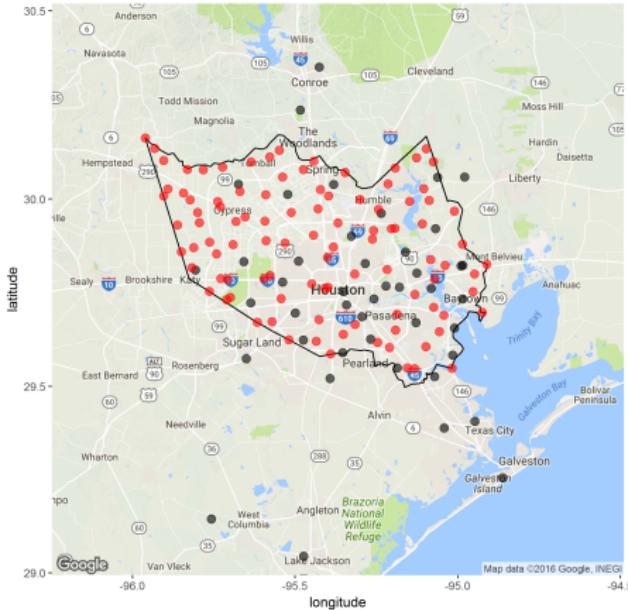
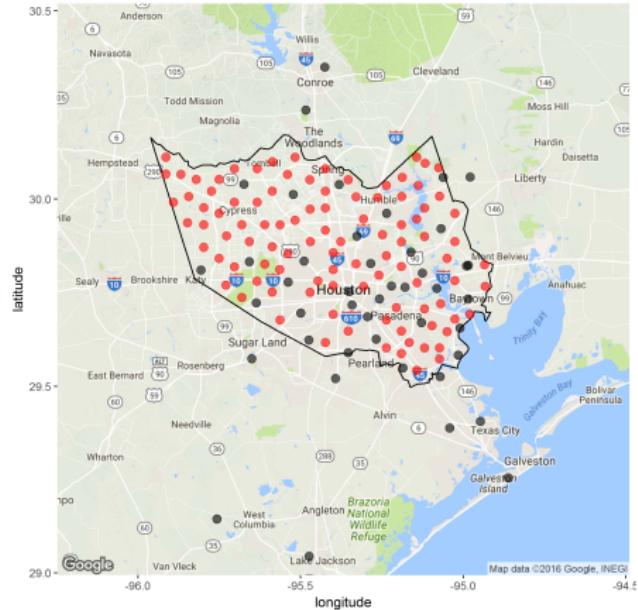
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- PSO and AT-PSO variants tend to be the best.
- GAs are competitive.
- With significantly fewer monitoring locations, PSO variants are the best.

# Best designs found according to $\bar{Q}_{puk}$ (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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