

# Adaptively Tuned Particle Swarm Optimization for Spatial Design

Matthew Simpson

Department of Statistics, University of Missouri  
SAS Institute, Inc.

July 29, 2018

Simpson, M., Wikle, C. K., and Holan, S. H. (2017). Adaptively tuned particle swarm optimization with application to spatial design. *Stat.*

Joint work with Christopher Wikle and Scott H. Holan

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: optimize 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  $g_i(k) \in \mathbb{R}^D$ .

# Particle Swarm Optimization

Goal: optimize 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  $g_i(k) \in \mathbb{R}^D$ .

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.

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

## 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  $\mathbf{g}_i(k)$ .  
→ *No matter where they are in the search space.*

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.

# Adaptively Tuning PSO

In PSO larger  $\omega \implies$  more exploration, smaller  $\omega \implies$  more exploitation.

# Adaptively Tuning PSO

In PSO larger  $\omega \implies$  more exploration, smaller  $\omega \implies$  more exploitation.

Idea: deterministic inertia PSO (DI-PSO)

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

- Hard to set appropriately for any given problem.

# Adaptively Tuning PSO

In PSO larger  $\omega \implies$  more exploration, smaller  $\omega \implies$  more exploitation.

Idea: deterministic inertia PSO (DI-PSO)

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

- Hard to set appropriately for any given problem.

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

Can also create AT-BBPSO algorithms.

## Adaptively Tuned PSO — $\omega(k)$ 's progression

Define the improvement rate of the swarm in period  $k$ :

$R(k) =$  proportion of particles that improved  
on their personal best last period.

## Adaptively Tuned PSO — $\omega(k)$ 's progression

Define the improvement rate of the swarm in period  $k$ :

$R(k) =$  proportion of particles that improved  
on their personal best last period.

Let  $R^*$  denote a target improvement rate, and  
 $c$  denote an adjustment factor.

Update  $\omega(k)$  via:

$$\log \omega(k+1) = \log \omega(k) + c\{R(k+1) - R^*\}$$

## Adaptively Tuned PSO — $\omega(k)$ 's progression

Define the improvement rate of the swarm in period  $k$ :

$R(k) =$  proportion of particles that improved  
on their personal best last period.

Let  $R^*$  denote a target improvement rate, and  
 $c$  denote an adjustment factor.

Update  $\omega(k)$  via:

$$\log \omega(k+1) = \log \omega(k) + c\{R(k+1) - R^*\}$$

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.

# 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.

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-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.

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  $Y(\mathbf{u})$ ,  $\mathbf{u} \in \mathcal{D} \subset \mathbb{R}^2$ .

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

# Spatial Design

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

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

Usual solution: grid up the space and use an exchange algorithm.  
(Nychka and Saltzman, 1998; Wikle and Royle, 1999, 2005)

# Spatial Design

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

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

Usual solution: grid up the space and use an exchange algorithm.  
(Nychka and Saltzman, 1998; Wikle and Royle, 1999, 2005)

In principle, *any* location is a valid design point, not just the grid.  
⇒ why not use PSO?

# Spatial Design

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

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

Usual solution: grid up the space and use an exchange algorithm.  
(Nychka and Saltzman, 1998; Wikle and Royle, 1999, 2005)

In principle, *any* location is a valid design point, not just the grid.  
⇒ 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).

# Spatial Design

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

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

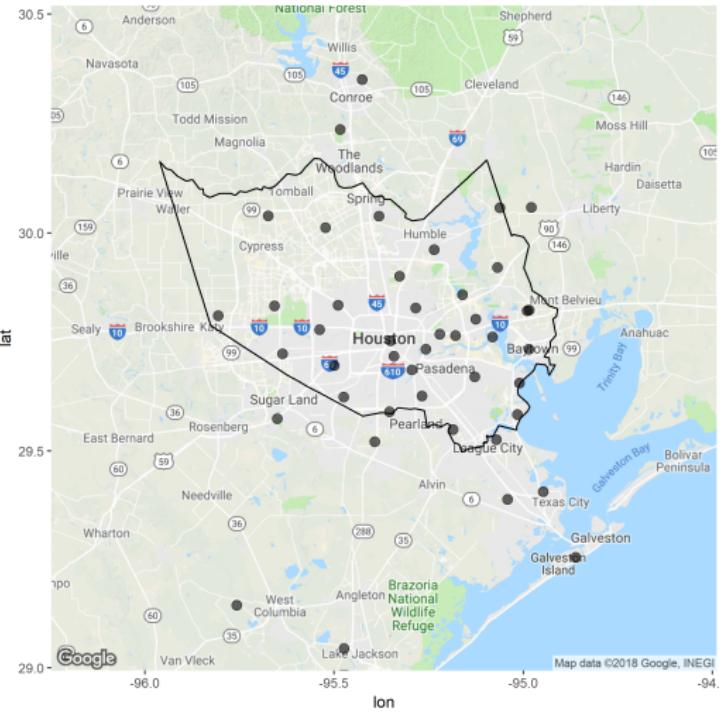
Usual solution: grid up the space and use an exchange algorithm.  
(Nychka and Saltzman, 1998; Wikle and Royle, 1999, 2005)

In principle, *any* location is a valid design point, not just the grid.  
⇒ 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).

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?

Note: nearby locations outside of the county still useful for estimation.

# 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?

Note: nearby locations outside of the county still useful for estimation.

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.

# 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?

Note: nearby locations outside of the county still useful for estimation.

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.

Let  $Y(\mathbf{u})$  denote DM8 and  $Z(\mathbf{u})$  denote measured DM8 at  $\mathbf{u}$ .

# Ozone Monitoring Model

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

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

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

# Ozone Monitoring Model

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

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

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

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

$$\delta(\mathbf{u}) \sim \text{GP}(0, C_\phi(\cdot, \cdot))$$

where  $\mathbf{x}(\mathbf{u})$  is a vector of covariates known at all locations  $\mathbf{u} \in \mathcal{D}$ .

# Ozone Monitoring Model

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

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

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

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

$$\delta(\mathbf{u}) \sim \text{GP}(0, C_\phi(\cdot, \cdot))$$

where  $\mathbf{x}(\mathbf{u})$  is a vector of covariates known at all locations  $\mathbf{u} \in \mathcal{D}$ .

Details:

- 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.

# Spatial Design — MSPE and Kriging

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

# Spatial Design — MSPE and Kriging

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

With  $\tau^2$  and  $\phi$  known, universal kriging MSPE is (Cressie and Wikle, 2011):

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

# Spatial Design — MSPE and Kriging

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

With  $\tau^2$  and  $\phi$  known, universal kriging MSPE is (Cressie and Wikle, 2011):

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

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

# Spatial Design — MSPE and Kriging

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

With  $\tau^2$  and  $\phi$  known, universal kriging MSPE is (Cressie and Wikle, 2011):

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

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

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

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

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

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

Use a grid of 1229 points in Harris County.

| Algorithm      | $\bar{Q}_{puk}$ | $Q_{puk}^*$  |
|----------------|-----------------|--------------|
| 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        |
| AT1-PSO2-CF    | 15.60           | 24.02        |
| AT2-PSO1       | <b>14.42</b>    | <b>21.13</b> |
| 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        |
| AT1-BBPSOxp-CF | 14.84           | 22.34        |
| AT2-BBPSO      | 14.65           | 23.49        |
| AT2-BBPSOxp    | 15.21           | 23.25        |
| AT2-BBPSO-CF   | 14.63           | 21.92        |
| AT2-BBPSOxp-CF | 14.52           | 22.76        |
| GA-11          | <b>14.40</b>    | 21.19        |
| GA-21          | 15.20           | 23.21        |
| GA-12          | 14.45           | <b>20.84</b> |
| GA-22          | 15.26           | 22.61        |

Results:

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

| 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        |
| AT1-PSO2-CF    | 15.60                | 24.02        |
| AT2-PSO1       | <b>14.42</b>         | <b>21.13</b> |
| 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        |
| AT1-BBPSOxp-CF | 14.84                | 22.34        |
| AT2-BBPSO      | 14.65                | 23.49        |
| AT2-BBPSOxp    | 15.21                | 23.25        |
| AT2-BBPSO-CF   | 14.63                | 21.92        |
| AT2-BBPSOxp-CF | 14.52                | 22.76        |
| GA-11          | <b>14.40</b>         | 21.19        |
| GA-21          | 15.20                | 23.21        |
| GA-12          | 14.45                | <b>20.84</b> |
| GA-22          | 15.26                | 22.61        |

## Results:

- Uniform: uniformly sample new monitoring locations.
- GA: genetic algorithm.
- Bolded: top 5 for that design criterion (column).
- Objective function is simple enough that robustness of AT-BBPSO variants is unnecessary.

| 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        |
| AT1-PSO2-CF    | 15.60                | 24.02        |
| AT2-PSO1       | <b>14.42</b>         | <b>21.13</b> |
| 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        |
| AT1-BBPSOxp-CF | 14.84                | 22.34        |
| AT2-BBPSO      | 14.65                | 23.49        |
| AT2-BBPSOxp    | 15.21                | 23.25        |
| AT2-BBPSO-CF   | 14.63                | 21.92        |
| AT2-BBPSOxp-CF | 14.52                | 22.76        |
| GA-11          | <b>14.40</b>         | 21.19        |
| GA-21          | 15.20                | 23.21        |
| GA-12          | 14.45                | <b>20.84</b> |
| GA-22          | 15.26                | 22.61        |

## Results:

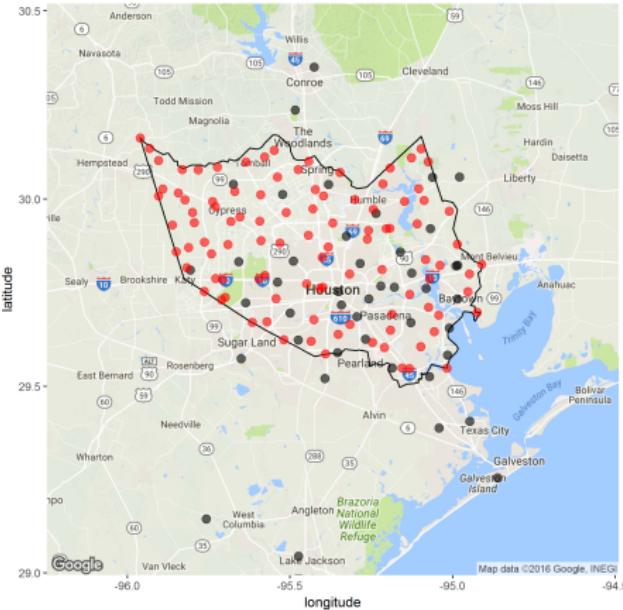
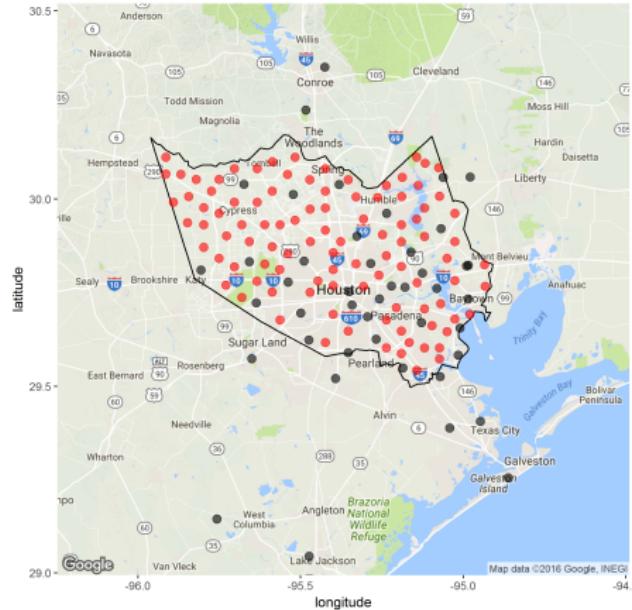
- Uniform: uniformly sample new monitoring locations.
- GA: genetic algorithm.
- Bolded: top 5 for that design criterion (column).
- Objective function is simple enough that robustness of AT-BBPSO variants is unnecessary.
- PSO and AT-PSO variants tend to be the best.
- GAs are competitive.

| 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        |
| AT1-PSO2-CF    | 15.60                | 24.02        |
| AT2-PSO1       | <b>14.42</b>         | <b>21.13</b> |
| 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        |
| AT1-BBPSOxp-CF | 14.84                | 22.34        |
| AT2-BBPSO      | 14.65                | 23.49        |
| AT2-BBPSOxp    | 15.21                | 23.25        |
| AT2-BBPSO-CF   | 14.63                | 21.92        |
| AT2-BBPSOxp-CF | 14.52                | 22.76        |
| GA-11          | <b>14.40</b>         | 21.19        |
| GA-21          | 15.20                | 23.21        |
| GA-12          | 14.45                | <b>20.84</b> |
| GA-22          | 15.26                | 22.61        |

## Results:

- Uniform: uniformly sample new monitoring locations.
- GA: genetic algorithm.
- Bolded: top 5 for that design criterion (column).
- Objective function is simple enough that robustness of AT-BBPSO variants is unnecessary.
- 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).

# Conclusions

- Introduced new classes of adaptively tuned PSO and BBPSO algorithms.

# Conclusions

- Introduced new classes of adaptively tuned PSO and BBPSO algorithms.
- AT-BBPSO performed well on very difficult problems — quite robust to extreme multimodality.

# Conclusions

- Introduced new classes of adaptively tuned PSO and BBPSO algorithms.
- AT-BBPSO performed well on very difficult problems — quite robust to extreme multimodality.
- AT-PSO performed well on difficult, but not too difficult problems.

# Conclusions

- Introduced new classes of adaptively tuned PSO and BBPSO algorithms.
- AT-BBPSO performed well on very difficult problems — quite robust to extreme multimodality.
- AT-PSO performed well on difficult, but not too difficult problems.
- For spatial design problems, standard PSO works well.

# Conclusions

- Introduced new classes of adaptively tuned PSO and BBPSO algorithms.
- AT-BBPSO performed well on very difficult problems — quite robust to extreme multimodality.
- AT-PSO performed well on difficult, but not too difficult problems.
- For spatial design problems, standard PSO works well.
- For large enough spatial design problems, AT-PSO is attractive.

# Conclusions

- Introduced new classes of adaptively tuned PSO and BBPSO algorithms.
- AT-BBPSO performed well on very difficult problems — quite robust to extreme multimodality.
- AT-PSO performed well on difficult, but not too difficult problems.
- 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!

## References |

- Abt, M. (1999). Estimating the prediction mean squared error in Gaussian stochastic processes with exponential correlation structure. *Scandinavian Journal of Statistics*, 26(4):563–578.
- Andrieu, C. and Thoms, J. (2008). A tutorial on adaptive MCMC. *Statistics and Computing*, 18(4):343–373.
- Blum, C. and Li, X. (2008). Swarm intelligence in optimization. In Blum, C. and Merkle, D., editors, *Swarm Intelligence: Introduction and Applications*, pages 43–85. Springer-Verlag, Berlin.
- Clerc, M. (2006). Stagnation analysis in particle swarm optimisation or what happens when nothing happens. 17 pages.  
<https://hal.archives-ouvertes.fr/hal-00122031>.
- Clerc, M. (2010). *Particle swarm optimization*. John Wiley & Sons.
- Clerc, M. (2012). Standard particle swarm optimisation. 15 pages.  
<https://hal.archives-ouvertes.fr/hal-00764996>.

## References II

- Clerc, M. and Kennedy, J. (2002). The particle swarm—explosion, stability, and convergence in a multidimensional complex space. *Evolutionary Computation, IEEE Transactions on*, 6(1):58–73.
- Cressie, N. and Wikle, C. K. (2011). *Statistics for Spatio-Temporal Data*. John Wiley & Sons, Hoboken, NJ.
- Eberhart, R. C. and Shi, Y. (2000). Comparing inertia weights and constriction factors in particle swarm optimization. In *Evolutionary Computation, 2000. Proceedings of the 2000 Congress on*, volume 1, pages 84–88. IEEE.
- Ensor, K. B., Raun, L. H., and Persse, D. (2013). A case-crossover analysis of out-of-hospital cardiac arrest and air pollution. *Circulation*, 127(11):1192–1199.
- Hamada, M., Martz, H., Reese, C., and Wilson, A. (2001). Finding near-optimal Bayesian experimental designs via genetic algorithms. *The American Statistician*, 55(3):175–181.

## References III

- Kahle, D. and Wickham, H. (2013). ggmap: Spatial visualization with ggplot2. *The R Journal*, 5(1):144–161.
- Miranda, V., Keko, H., and Duque, A. J. (2008). Stochastic star communication topology in evolutionary particle swarms (EPSO). *International journal of computational intelligence research*, 4(2):105–116.
- Nychka, D. and Saltzman, N. (1998). Design of air-quality monitoring networks. In Nychka, D., Piegorsch, W. W., and Cox, L. H., editors, *Case Studies in Environmental Statistics*, pages 51–76. Springer, New York.
- Simpson, M., Wikle, C. K., and Holan, S. H. (2017). Adaptively tuned particle swarm optimization with application to spatial design. *Stat*, 6(1):145–159.
- Wikle, C. K. and Royle, J. A. (1999). Space-time dynamic design of environmental monitoring networks. *Journal of Agricultural, Biological, and Environmental Statistics*, 4(4):489–507.

## References IV

- Wikle, C. K. and Royle, J. A. (2005). Dynamic design of ecological monitoring networks for non-Gaussian spatio-temporal data. *Environmetrics*, 16(5):507–522.
- Zimmerman, D. L. (2006). Optimal network design for spatial prediction, covariance parameter estimation, and empirical prediction. *Environmetrics*, 17(6):635–652.
- Zimmerman, D. L. and Cressie, N. (1992). Mean squared prediction error in the spatial linear model with estimated covariance parameters. *Annals of the Institute of Statistical Mathematics*, 44(1):27–43.