

# 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:

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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  $p_i(k) \in \mathbb{R}^D$ ;
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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

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 neighborhood 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.

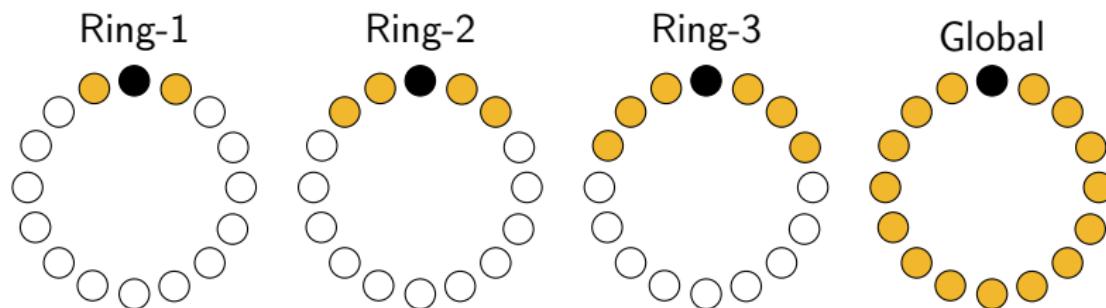
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Easy to visualize example: Ring- $k$  neighborhood topology.



Each particle is informed by  $k$  neighbors to the left and  $k$  to the right,  
*no matter where they are in the search space.*

# Stochastic Star Topology, and Other Bells and Whistles

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

- Each particle informs itself and  $m$  random particles.  
→ sampled with replacement once during initialization.
- On average each particle is informed by  $m$  particles.
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Many variants available (Clerc, 2012), (Simpson et al., 2017, appendix).

- Handling search space constraints.
- Coordinate free velocity updates.
- Parallelization.
- Asynchronous updates.
- Redraw neighborhoods.

## Bare Bones PSO (BBPSO)

Developed by Kennedy (2003).

Strips out the velocity term:

$$\theta_{ij}(k+1) \sim N\left(\frac{p_{ij}(k) + g_{ij}(k)}{2}, |p_{ij}(k) - g_{ij}(k)|^2\right).$$

Mimics the behavior of standard PSO.

Easier to analyze, but tends to perform worse.

# Adaptively Tuned BBPSO

Add flexibility to the scale parameter:

$$\theta_{ij}(k+1) \sim T_{df} \left( \frac{p_{ij}(k) + g_{ij}(k)}{2}, \sigma^2(k) |p_{ij}(k) - g_{ij}(k)|^2 \right).$$

with e.g.  $df = 1$  by default.

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- Smaller  $\sigma^2(k)$ : more exploitation.

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Analogy with adaptively tuned random walk Metropolis.  
(Andrieu and Thoms, 2008)

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

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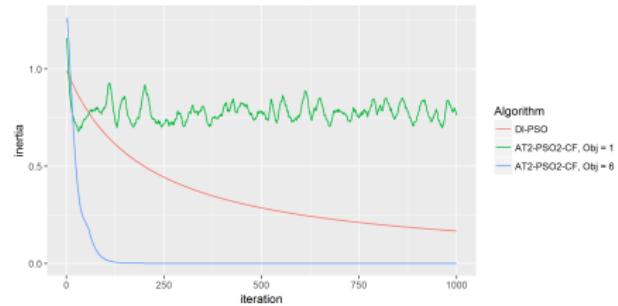
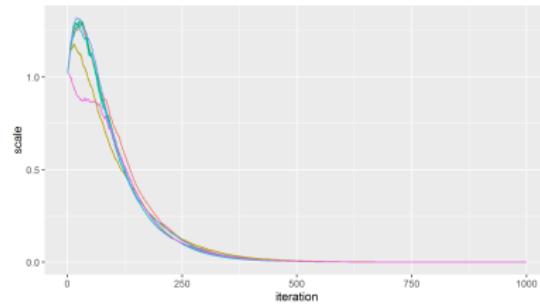
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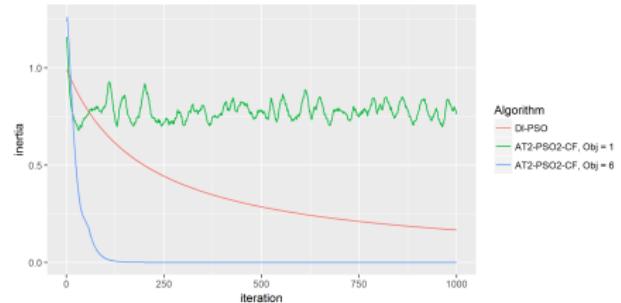
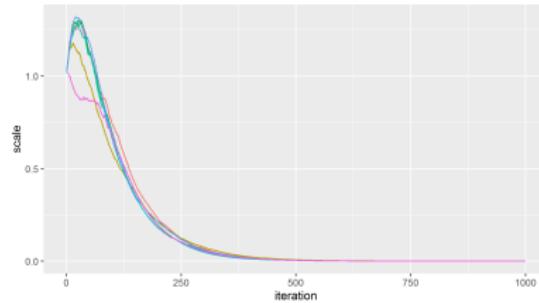
Similar PSO algorithm in spirit: Zhang et al. (2003).

- $\omega$  is constant while  $\phi_1$  and  $\phi_2$  vary across time *and particle*.
- Can't use the same method to adapt  $\phi_1$  and  $\phi_2$ .

# Example progressions of $\sigma^2(k)$ (left) and $\omega(k)$ (right):

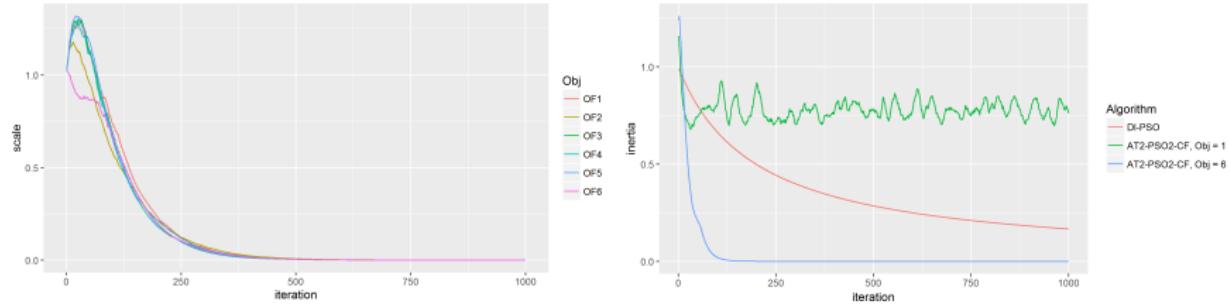


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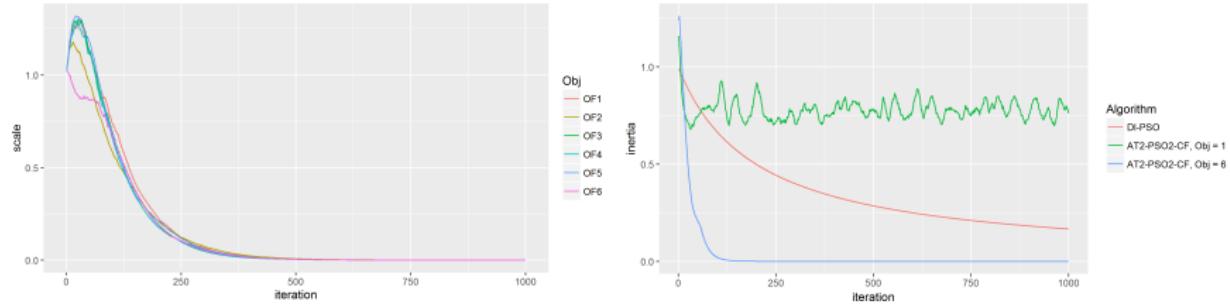
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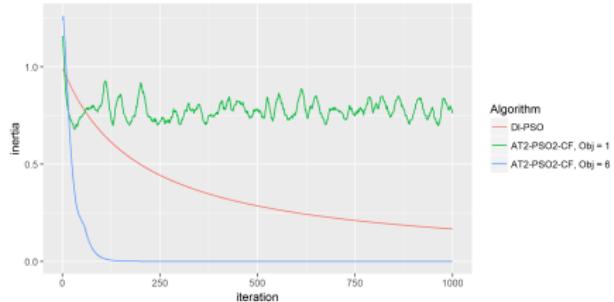
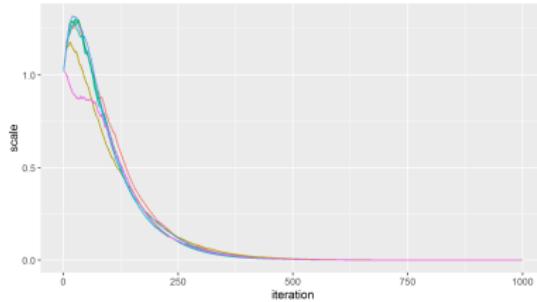
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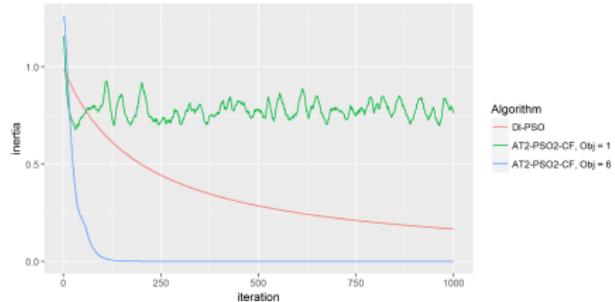
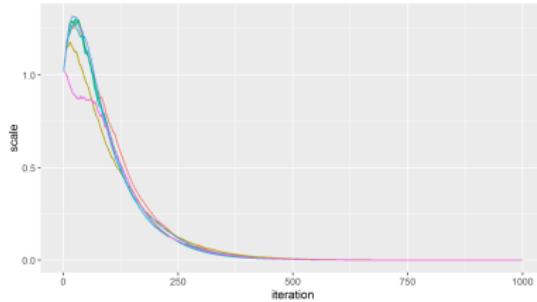
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- AT-PSO's inertia typically bounces around a flat trendline.  
→ Alternating between *relative* exploration and exploitation.
- AT-PSO's inertia crashes to zero when it converges.  
→ May be premature local convergence.

# Comparing AT-PSO/BBPSO to PSO/BBPSO

Tuning  $\omega(k)/\sigma^2(k)$  allows the swarm to adjust the exploration / exploitation tradeoff based on local conditions.

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Overview of results from a simulation study with a variety of objective functions:

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→ The  $T_{df}$  makes it fairly robust to many local optima.
- AT-PSO performs better than PSO on “hard enough” problems...
- ...but has trouble with many local optima.

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

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What if  $\theta = (\tau^2, \boldsymbol{\beta}, \phi)$  is unknown?

# Spatial Design — MSPE and Kriging

Sensible goal: choose new locations to minimize MSPE.

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When  $\tau^2$  and  $\phi$  are known, the universal kriging predictor is:

$$\hat{Y}_{uk}(\mathbf{u}; \mathbf{d}) = \mathbf{x}(\mathbf{u})' \hat{\boldsymbol{\beta}}_{gls} + \mathbf{c}_Y(\mathbf{u})' \mathbf{C}_Z^{-1} (\mathbf{Z} - \mathbf{X} \hat{\boldsymbol{\beta}}_{gls})$$

(Cressie and Wikle, 2011) where

$$\mathbf{X} = (\mathbf{x}(\mathbf{s}_1), \dots, \mathbf{x}(\mathbf{s}_{N_s}), \mathbf{x}(\mathbf{d}_1), \dots, \mathbf{x}(\mathbf{d}_{N_d}))',$$

$$\mathbf{Y} = (Y(\mathbf{s}_1), \dots, Y(\mathbf{s}_{N_s}), Y(\mathbf{d}_1), \dots, Y(\mathbf{d}_{N_d}))',$$

$$\mathbf{Z} = (Z(\mathbf{s}_1), \dots, Z(\mathbf{s}_{N_s}), Z(\mathbf{d}_1), \dots, Z(\mathbf{d}_{N_d}))',$$

$$\mathbf{C}_Z = \text{Cov}(\mathbf{Z}) = \tau^2 \mathbf{I} + \text{Cov}(\mathbf{Y}),$$

$$\mathbf{c}_Y = \text{Cov}(Y(\mathbf{u}), \mathbf{Y}),$$

$$\hat{\boldsymbol{\beta}}_{gls} = (\mathbf{X}' \mathbf{C}_Z^{-1} \mathbf{X})^{-1} \mathbf{X}' \mathbf{C}_Z^{-1} \mathbf{Z}.$$

# Spatial Design — Kriging Variances

Kriging MSPE:  $E \left\{ Y(\mathbf{u}) - \hat{Y}_{uk}(\mathbf{u}) \right\}^2 = \sigma_{uk}^2(\mathbf{u}; \mathbf{d}) =$

$$\begin{aligned} & C_\phi(\mathbf{u}, \mathbf{u}) - \mathbf{c}_Y(\mathbf{u})' \mathbf{C}_Z^{-1} \mathbf{c}_Y(\mathbf{u}) \\ & + \{ \mathbf{x}(\mathbf{u}) - \mathbf{X}' \mathbf{C}_Z^{-1} \mathbf{c}_Y(\mathbf{u}) \}' (\mathbf{X}' \mathbf{C}_Z^{-1} \mathbf{X})^{-1} \{ \mathbf{x}(\mathbf{u}) - \mathbf{X}' \mathbf{C}_Z^{-1} \mathbf{c}_Y(\mathbf{u}) \} \end{aligned}$$

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

→ Parameter uncertainty universal kriging MSPE:

$$E \left\{ Y(\mathbf{u}) - \hat{Y}_{uk}(\mathbf{u}) \right\}^2 \approx \sigma_{puk}^2(\mathbf{u}; \mathbf{d}, \hat{\boldsymbol{\theta}}) = \sigma_{uk}^2(\mathbf{u}; \mathbf{d}, \hat{\boldsymbol{\theta}}) + \text{stuff},$$

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

# Spatial Design — Design Criteria

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

- Mean/total MSPE:  $\overline{Q}_{(p)uk}(\mathbf{d}) = \int_{\mathcal{D}} \sigma_{(p)uk}^2(\mathbf{u}) d\mathbf{u}$
- Maximum MSPE:  $Q_{(p)uk}^*(\mathbf{d}) = \max_{\mathbf{u} \in \mathcal{D}} \sigma_{(p)uk}^2(\mathbf{u})$

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This is computationally infeasible.

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

- Minimize  $\bar{Q}_{(p)uk}(\mathbf{d}) = \sum_{i=1}^{N_t} \sigma_{(p)uk}^2(\mathbf{r}_i)$
- Minimize  $Q_{(p)uk}^*(\mathbf{d}) = \max_{i=1,2,\dots,N_t} \sigma_{(p)uk}^2(\mathbf{r}_i)$

# Spatial Design — Design Criteria

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

- Mean/total MSPE:  $\bar{Q}_{(p)uk}(\mathbf{d}) = \int_{\mathcal{D}} \sigma_{(p)uk}^2(\mathbf{u}) d\mathbf{u}$
- Maximum MSPE:  $Q_{(p)uk}^*(\mathbf{d}) = \max_{\mathbf{u} \in \mathcal{D}} \sigma_{(p)uk}^2(\mathbf{u})$

This is computationally infeasible.

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

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- Minimize  $Q_{(p)uk}^*(\mathbf{d}) = \max_{i=1,2,\dots,N_t} \sigma_{(p)uk}^2(\mathbf{r}_i)$

Zimmerman (2006): optimal design is highly dependent on the mean function

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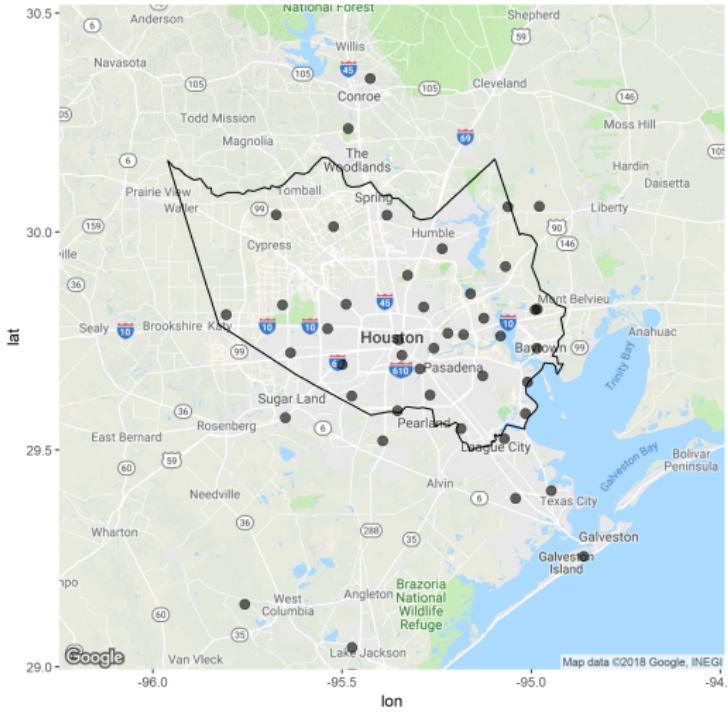
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Genetic algorithms also reasonable, e.g. Hamada et al. (2001).

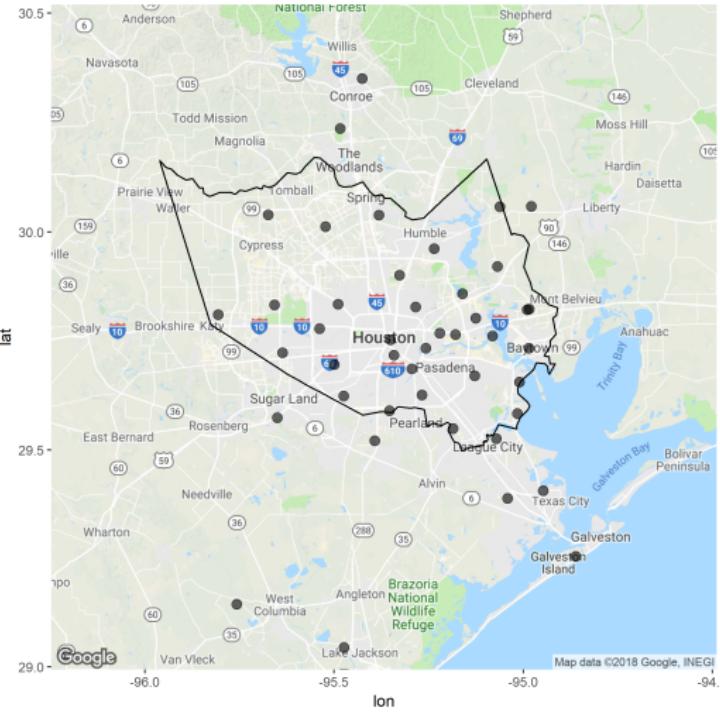
# Example: Ozone Monitoring in Harris County, TX



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Map via ggmap (Kahle and Wickham, 2013).

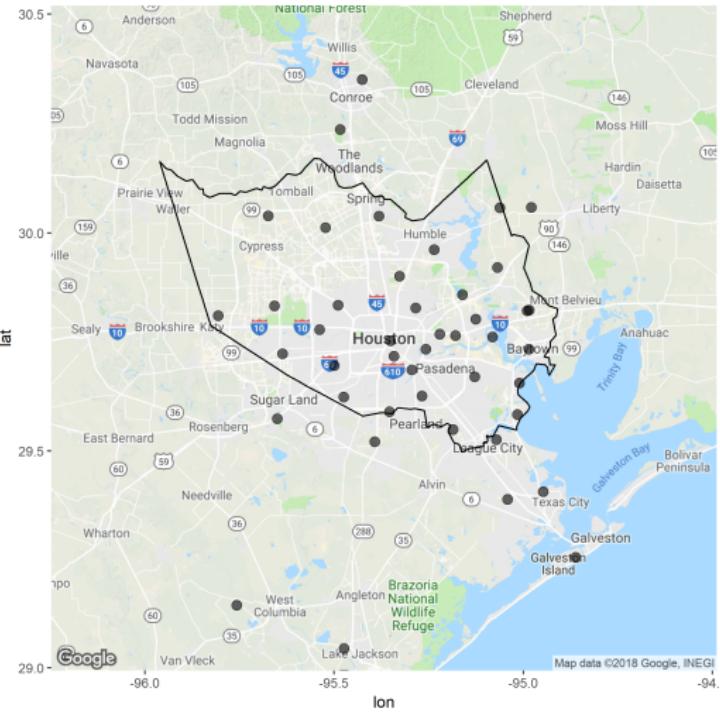
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- In August 2016, there were 44 active monitoring locations near Houston, TX.
- Harris County, TX, contains 33 of these locations.

# 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.
  - maximum of all contiguous 8-hour means for that day.
- Some locations have missing data.

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- Mean MSPE w/ parameter uncertainty  $\overline{Q}_{puk}(\mathbf{d})$ .
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- Approximate each with 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        |
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| AT1-PSO2       | 14.56           | 23.18        |
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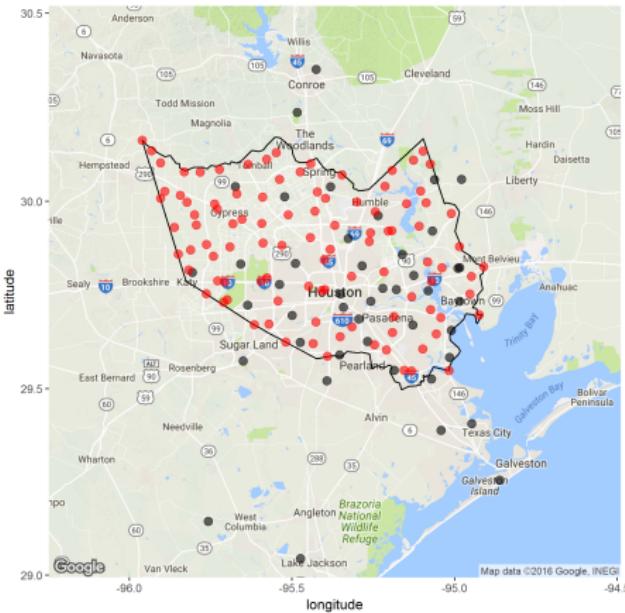
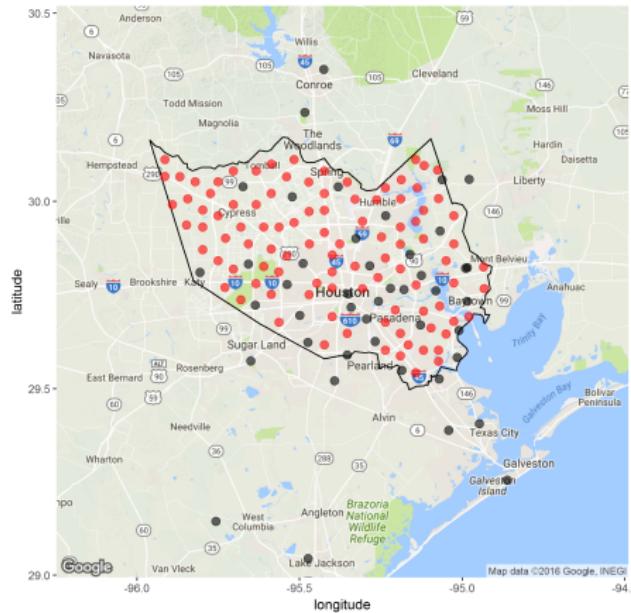
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# Best Designs for Both Criteria



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

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

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- For large enough spatial design problems, AT-PSO is attractive.

# 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.
- Kennedy, J. (2003). Bare bones particle swarms. In *Swarm Intelligence Symposium, 2003. SIS '03. Proceedings of the 2003 IEEE*, pages 80–87. IEEE.
- 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.

## References IV

- 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.
- 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.
- Zhang, W., Liu, Y., and Clerc, M. (2003). An adaptive PSO algorithm for reactive power optimization. In *IET Conference Proceedings*, pages 302–307. Institution of Engineering and Technology.
- 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.