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:

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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 $Q(\boldsymbol{\theta}) : \mathbb{R}^D \to \mathbb{R}$.

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

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 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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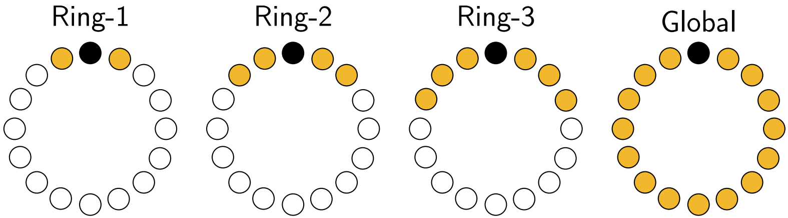
Easy to visualize example: Ring-k neighborhood topology.



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.
  $\rightarrow$ 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.

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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:

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

Mimics the behavior of standard PSO.

Easier to analyze, but tends to perform worse.

Adaptively Tuned BBPSO

Add flexibility to the scale parameter:

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

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

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

How to choose $\sigma^2(k)$'s progression?

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

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$$\log \sigma^2(k+1) = \log \sigma^2(k) + c\{R(k+1) - R^*\}$$

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

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

- ω is constant while ϕ_1 and ϕ_2 vary across time *and particle*.
- Can't use the same method to adapt ϕ_1 and ϕ_2.

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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- AT-PSO performs better than PSO on “hard enough” problems...
- ...but has trouble with many local optima.

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

Spatial Design — MSPE and Kriging

Sensible goal: choose new locations to minimize MSPE.

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When τ^2 and ϕ are known, the universal kriging predictor is:

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

(Cressie and Wikle, 2011) where

$$\begin{aligned}
\boldsymbol{X} &= (\boldsymbol{x}(\boldsymbol{s}_1), \ldots, \boldsymbol{x}(\boldsymbol{s}_{N_s}), \boldsymbol{x}(\boldsymbol{d}_1), \ldots, \boldsymbol{x}(\boldsymbol{d}_{N_d}))', \\
\boldsymbol{Y} &= (Y(\boldsymbol{s}_1), \ldots, Y(\boldsymbol{s}_{N_s}), Y(\boldsymbol{d}_1), \ldots, Y(\boldsymbol{d}_{N_d}))', \\
\boldsymbol{Z} &= (Z(\boldsymbol{s}_1), \ldots, Z(\boldsymbol{s}_{N_s}), Z(\boldsymbol{d}_1), \ldots, Z(\boldsymbol{d}_{N_d}))', \\
\boldsymbol{C}_Z &= \mathrm{Cov}(\boldsymbol{Z}) = \tau^2\mathbf{I} + \mathrm{Cov}(\boldsymbol{Y}), \\
\boldsymbol{c}_Y &= \mathrm{Cov}(Y(\boldsymbol{u}), \boldsymbol{Y}), \\
\widehat{\boldsymbol{\beta}}_{gls} &= (\boldsymbol{X}'\boldsymbol{C}_Z^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{C}_Z^{-1}\boldsymbol{Z}.
\end{aligned}$$

Spatial Design — Kriging Variances

Kriging MSPE: $\mathrm{E}\left\{Y(\boldsymbol{u}) - \widehat{Y}_{uk}(\boldsymbol{u})\right\}^2 = \sigma^2_{uk}(\boldsymbol{u};\boldsymbol{d}) =$

$$C_\phi(\boldsymbol{u},\boldsymbol{u}) - \boldsymbol{c}_Y(\boldsymbol{u})'\boldsymbol{C}_Z^{-1}\boldsymbol{c}_Y(\boldsymbol{u})$$
$$+ \{\boldsymbol{x}(\boldsymbol{u}) - \boldsymbol{X}'\boldsymbol{C}_Z^{-1}\boldsymbol{c}_Y(\boldsymbol{u})\}'(\boldsymbol{X}'\boldsymbol{C}_Z^{-1}\boldsymbol{X})^{-1}\{\boldsymbol{x}(\boldsymbol{u}) - \boldsymbol{X}'\boldsymbol{C}_Z^{-1}\boldsymbol{c}_Y(\boldsymbol{u})\}$$

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What about when τ^2 and ϕ are estimated?
$\rightarrow$ Parameter uncertainty universal kriging MSPE:

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

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

Spatial Design — Design Criteria

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

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

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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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- Highly multi-modal objective function (e.g. switch two locations).

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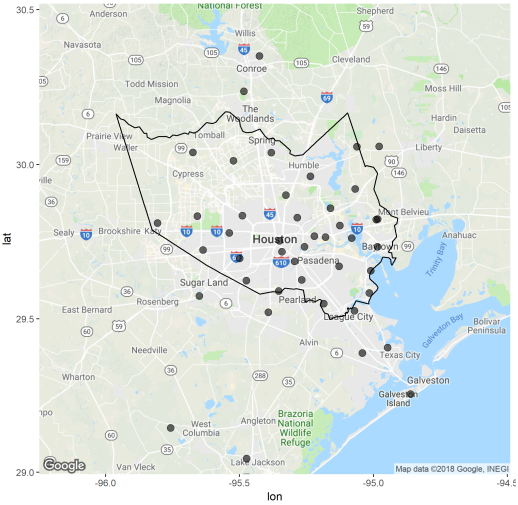
Genetic algorithms also reasonable, e.g. Hamada et al. (2001).

Example: Ozone Monitoring in Harris County, TX



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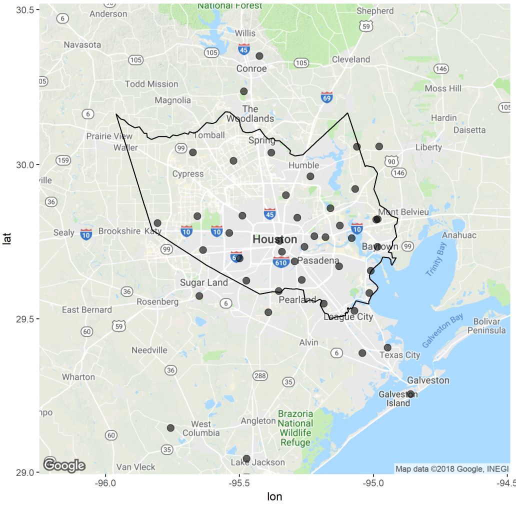

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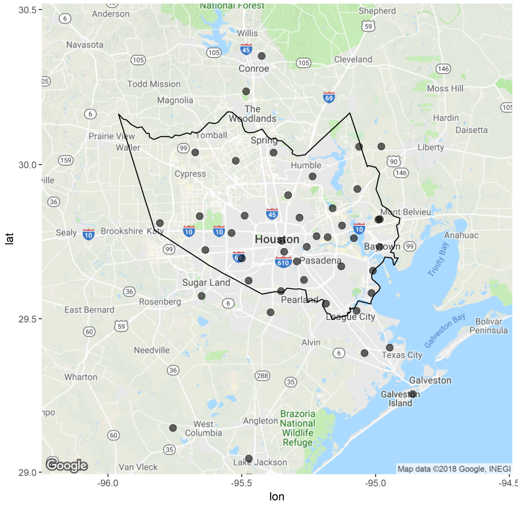

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- In August 2016, there were 44 active monitoring locations near Houston, TX.
- Harris County, TX, contains 33 of these locations.

Hypothetical Design Problem and Data

Want to learn more about ozone concentrations in Harris County.

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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.

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Design Criteria:

- Mean MSPE w/ parameter uncertainty $\overline{Q}_{puk}(\boldsymbol{d})$.
- Maximum MSPE w/ parameter uncertainty $Q^*_{puk}(\boldsymbol{d})$.

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 $\boldsymbol{\theta} = (\tau^2, \beta_0, \beta_1, \beta_2, \sigma^2, \psi)$ via maximum likelihood.

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
AT2-BBPSOxp	15.21	23.25
AT2-BBPSO-CF	14.63	21.92
AT2-BBPSOxp-CF	14.52	22.76
GA-11	**14.40**	21.19
GA-21	15.20	23.21
GA-12	14.45	**20.84**
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Results:

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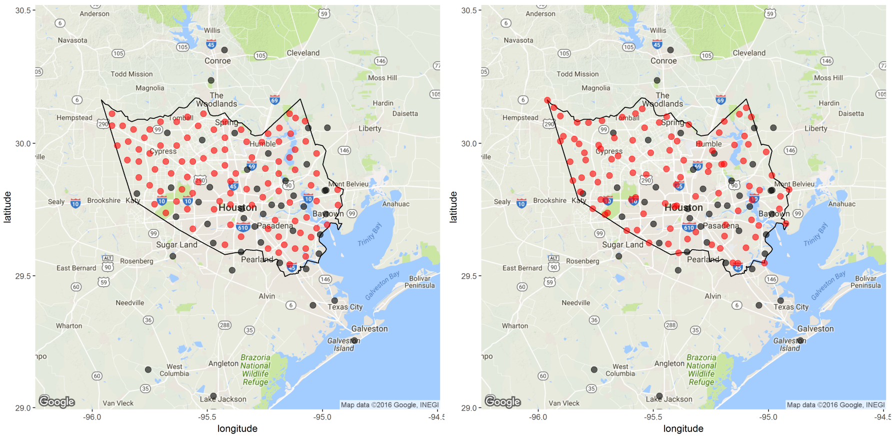
- PSO and AT-PSO variants tend to be the best.
- GAs are competitive.
- With significantly fewer monitoring locations, PSO variants are the best.

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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- AT-BBPSO performed well on very difficult problems.
- 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.

Thank you!

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