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

Populate Θ 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

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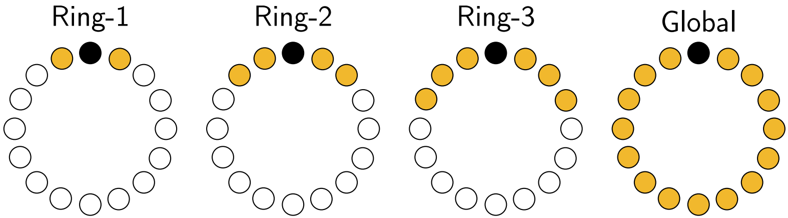
Easy to visualize example: Ring-k neighborhood topology.



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

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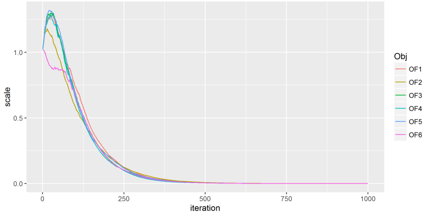
Similar PSO algorithm in spirit: Zhang et al. (2003).

- 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.

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



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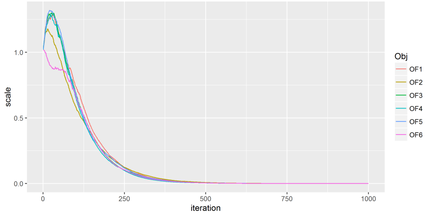

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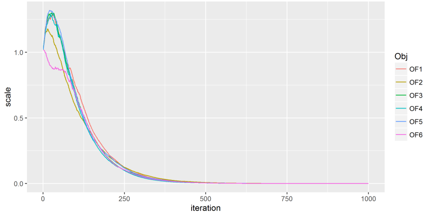

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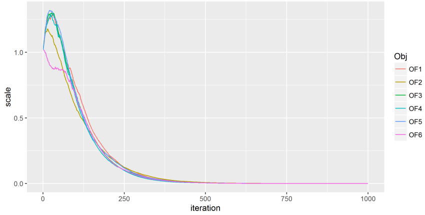

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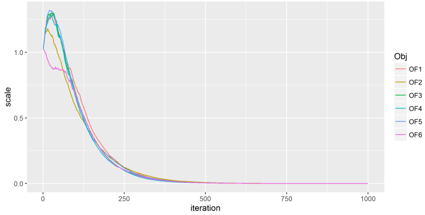

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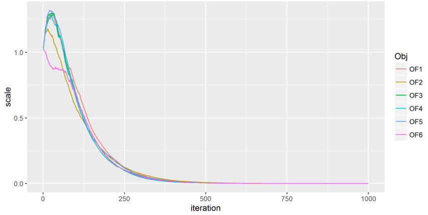

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- AT-PSO's inertia typically bounces around a flat trendline.
  $\rightarrow$ Alternating between *relative* exploration and exploitation.
- AT-PSO's inertia crashes to zero when it converges.
  $\rightarrow$ May be premature local convergence.

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.

- 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 with a variety of objective functions:

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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

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

Spatial Design — Kriging Variances

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

$$C_\phi(\boldsymbol{u},\boldsymbol{u}) - \boldsymbol{c}_Y(\boldsymbol{u})'\boldsymbol{C}_Z^{-1}\boldsymbol{c}_Y(\boldsymbol{u})$$
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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: $\overline{Q}_{(p)uk}(\boldsymbol{d}) = \int_{\mathcal{D}} \sigma^2_{(p)uk}(\boldsymbol{u})d\boldsymbol{u}$
- Maximum MSPE: $Q^*_{(p)uk}(\boldsymbol{d}) = \max_{\boldsymbol{u}\in\mathcal{D}} \sigma^2_{(p)uk}(\boldsymbol{u})$

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

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$\Longrightarrow$ why not use PSO?

- 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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The spatial design optimization problem cannot be solved in closed form.

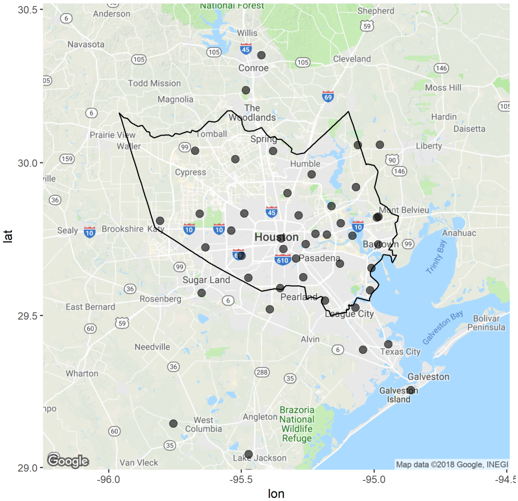
Usual solution: grid up the space and use an exchange algorithm. (Nychka and Saltzman, 1998; Wikle and Royle, 1999, 2005)

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

- 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



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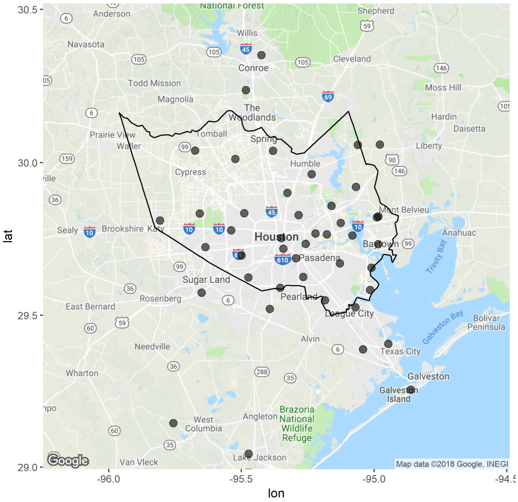

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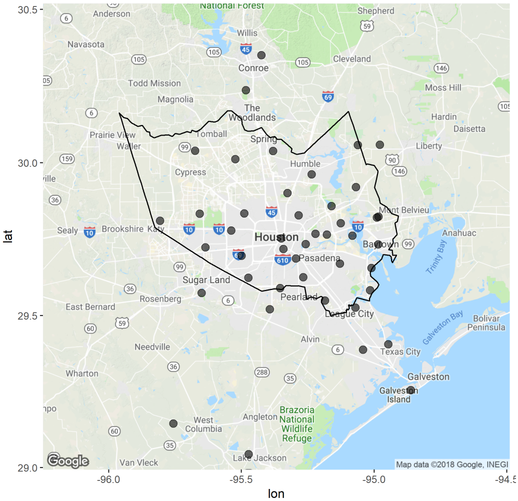

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- In August 2016, there were 44 active monitoring locations near Houston, TX.
- Harris County, TX, contains 33 of these locations.

Hypothetical Design Problem and Data

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Where to put 100 new monitoring locations within the county?

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

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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 $Q^*_{puk}(\boldsymbol{d})$.
- 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
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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.

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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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