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 to an existing monitoring network.

Particle Swarm Optimization — Intuition

Click!

Put a "swarm" of particles in the search space:

> Don't search alone, pay attention to what your neighbors are doing!

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

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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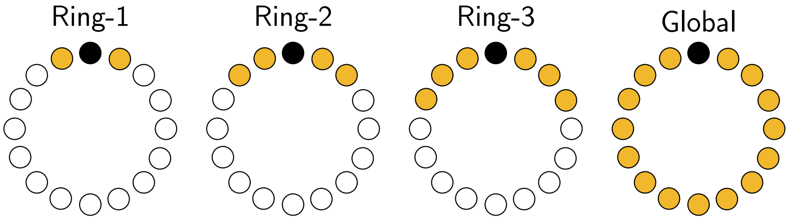
Easy to visualize example: Ring-k neighborhood topology.



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

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c denote an adjustment factor.

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

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

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

- Hard to set appropriately for any given problem.

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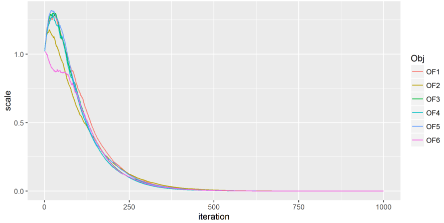
Similar PSO algorithm in spirit: Zhang et al. (2003).

- 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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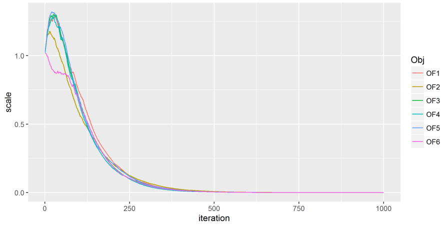

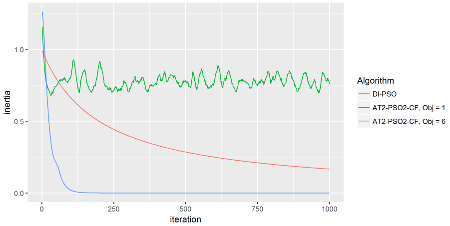

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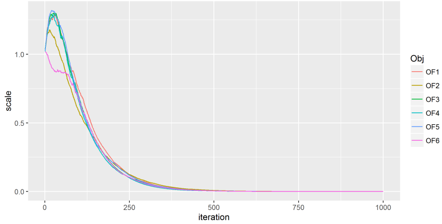

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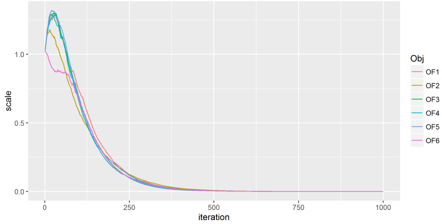

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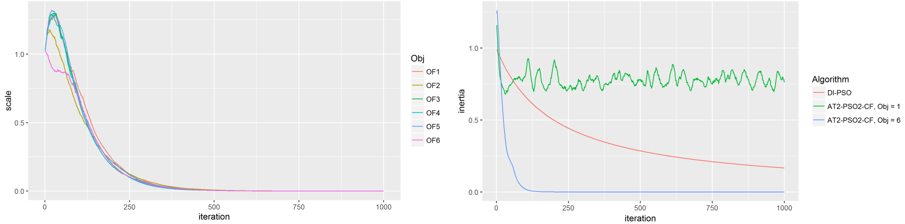

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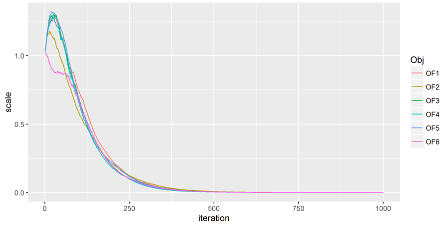

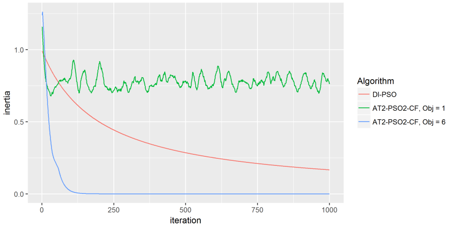

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- AT-PSO's inertia typically bounces around a flat trendline.
  $\rightarrow$ Alternating between *relative* exploration and exploitation.
- AT-PSO's inertia crashes to zero when it converges.
  $\rightarrow$ May be premature local convergence.

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:

- BBPSO tends to perform poorly, but AT-BBPSO performs quite well.
- AT-BBPSO often the best for complex objective functions.
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- AT-PSO performs better than PSO on "hard enough" problems...
- ...but has trouble with many local optima.

Spatial Design — Problem Setup

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

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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 τ^2, $\boldsymbol{\beta}$, and $C(\cdot, \cdot)$ are unknown?

Spatial Design — MSPE and Kriging

Sensible goal: minimize MSPE in some sense.

When τ^2 and $C(\cdot,\cdot)$ are known, the universal kriging predictor is:

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

(Cressie and Wikle, 2011) where

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

Spatial Design — Kriging Variances

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

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

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What about when τ^2 and/or $C(\cdot,\cdot)$ 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 Fisher information matrix and the MLE of all parameters, denoted by $\widehat{\boldsymbol{\theta}}$ (Zimmerman and Cressie, 1992; Abt, 1999).

Spatial Design — Design Criteria

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

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

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

- Minimize $\sum_{i=1}^{N_t} \sigma^2(\boldsymbol{r}_i)$
- Minimize $\max_{i=1,2,\ldots,N_t} \sigma^2(\boldsymbol{r}_i)$

Thank you!

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