Design (and Implementation) of PDMP Monte Carlo Methods

BAMC 2022 Minisymposium

Nonreversible Processes: Analysis and Computations

Sam Power, 13 Apr 2022

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    - for simplicity: x_t memoryless, stationary (“MCMC”)

Dynamical Systems for Sampling

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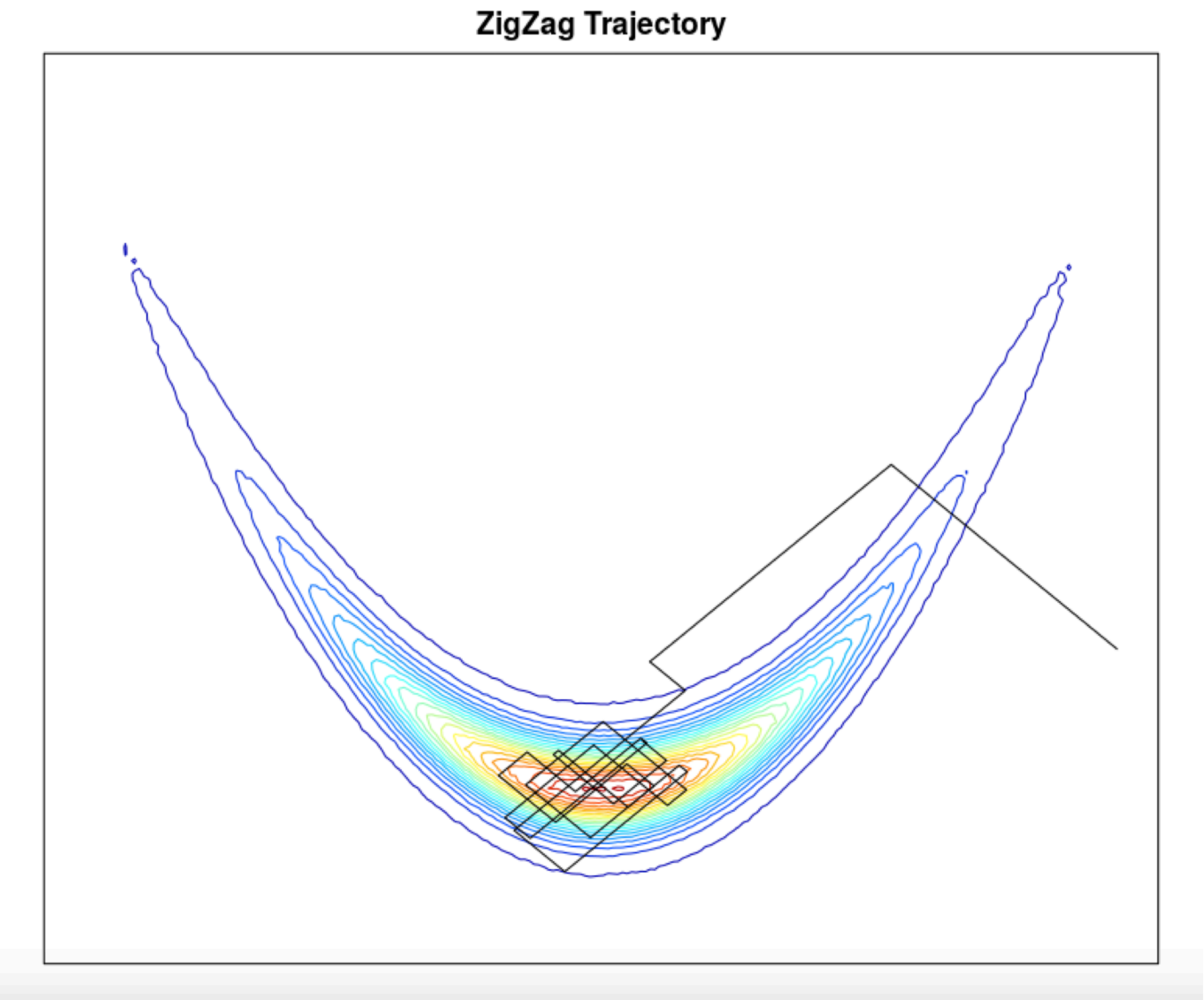
        - today: PDMPs = 1 + 3

Primer on PDMPs



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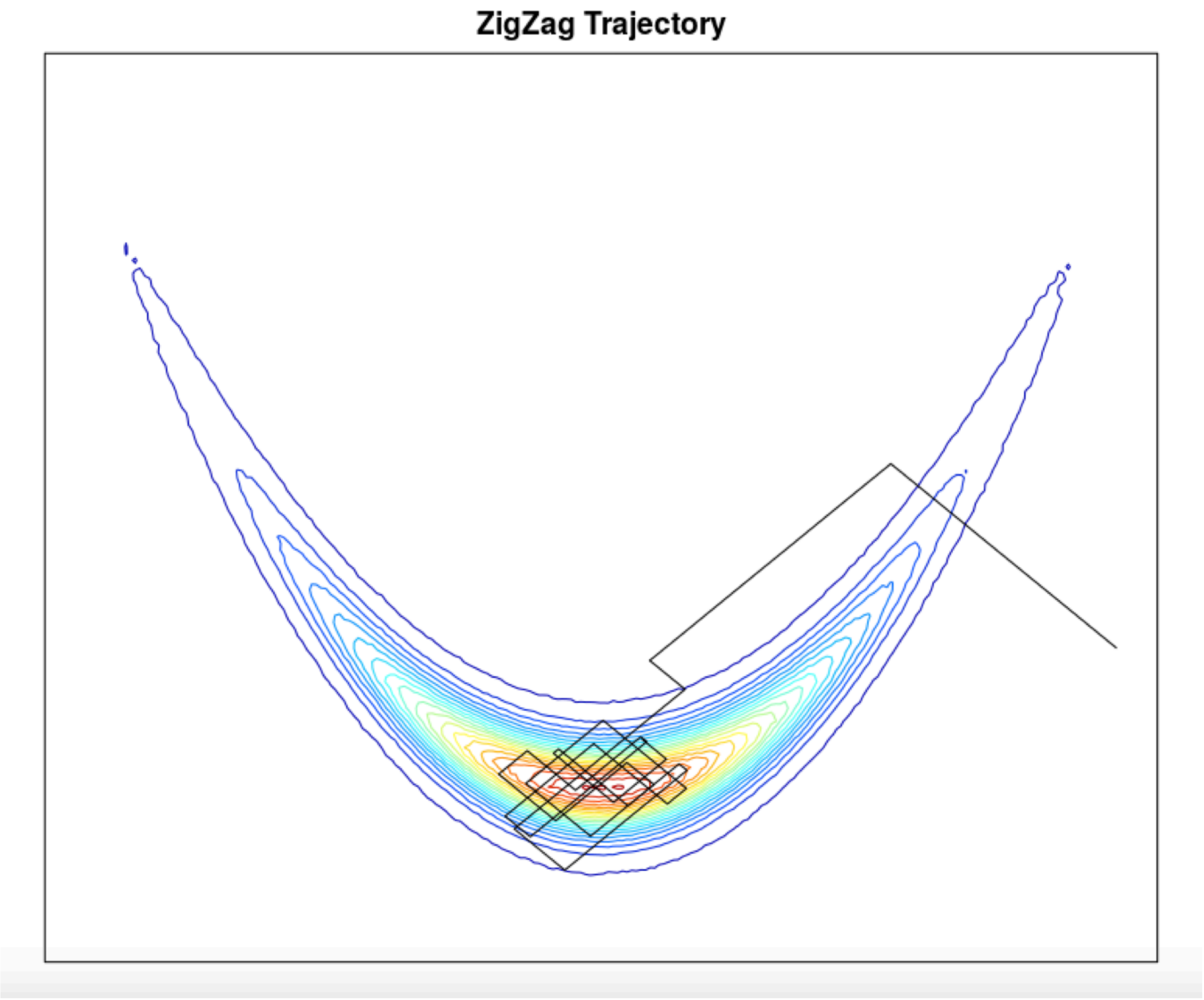

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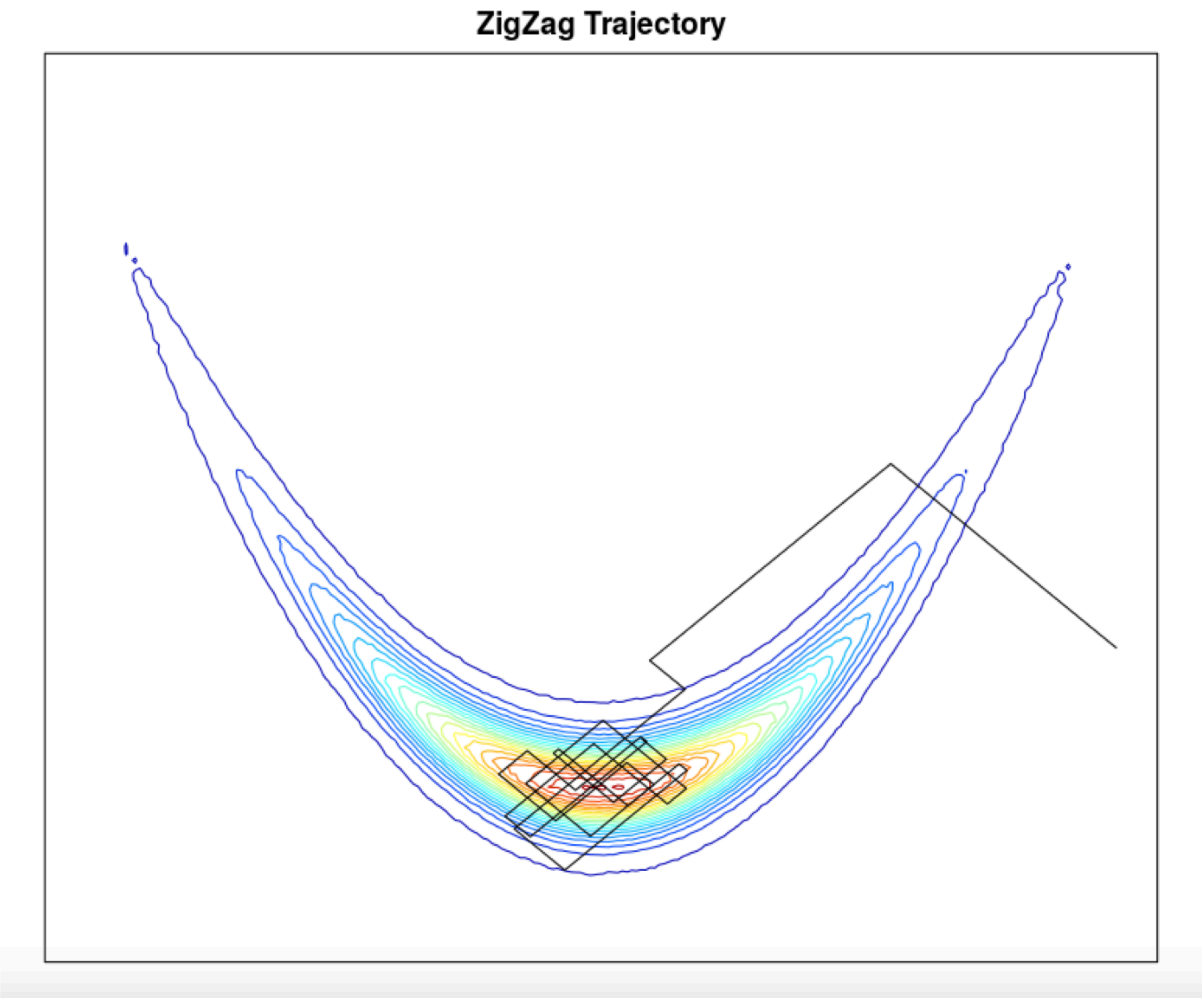

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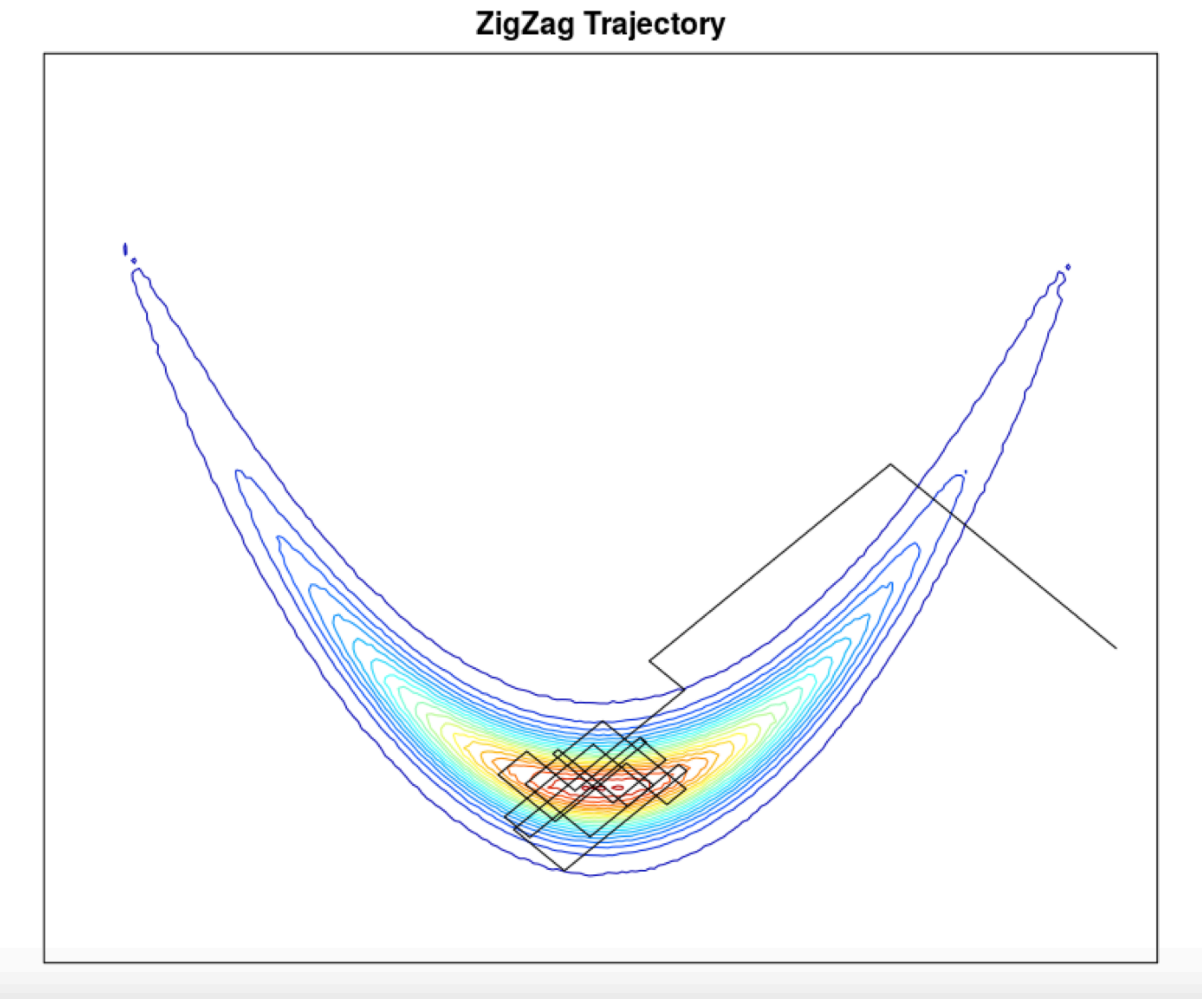

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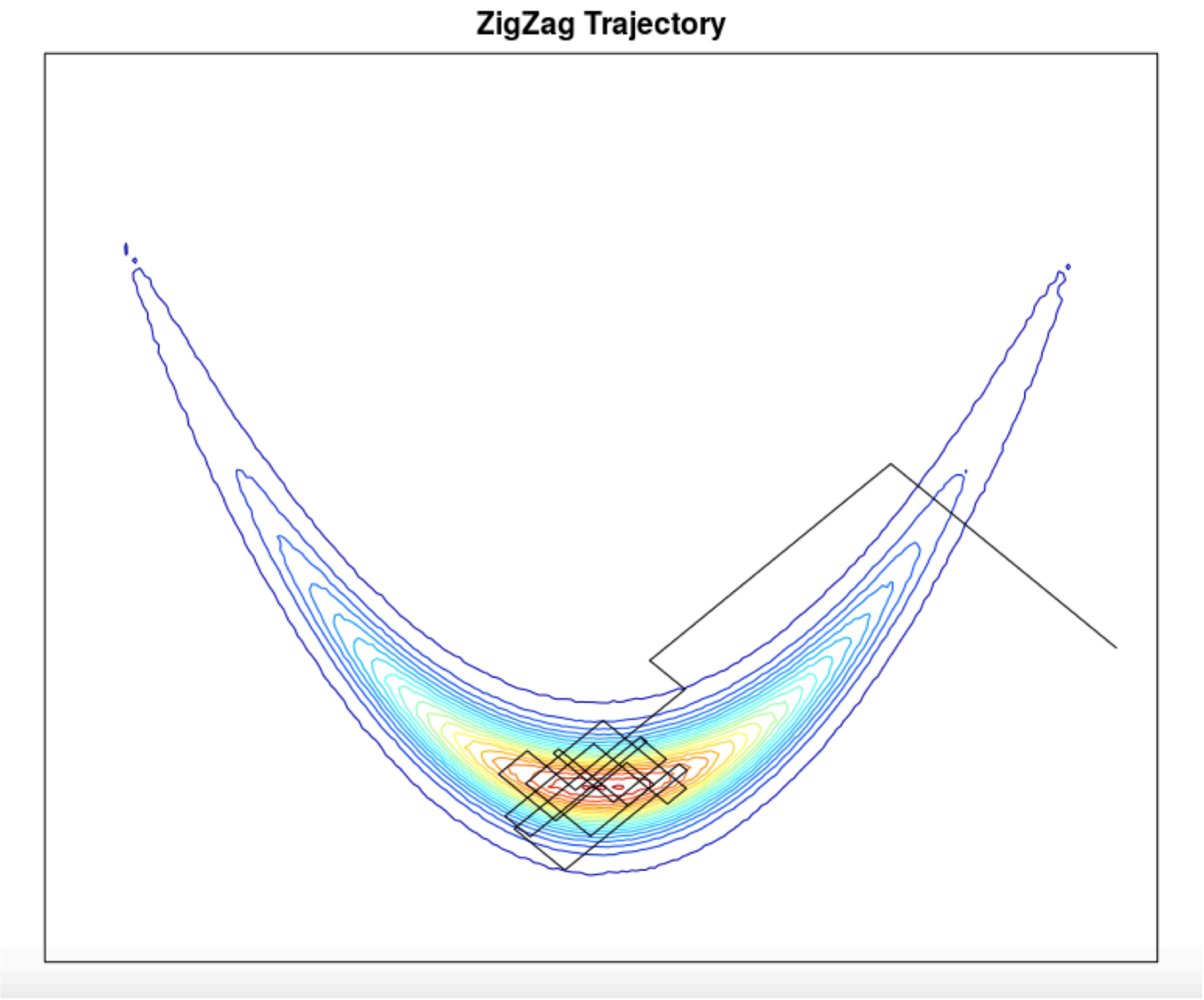

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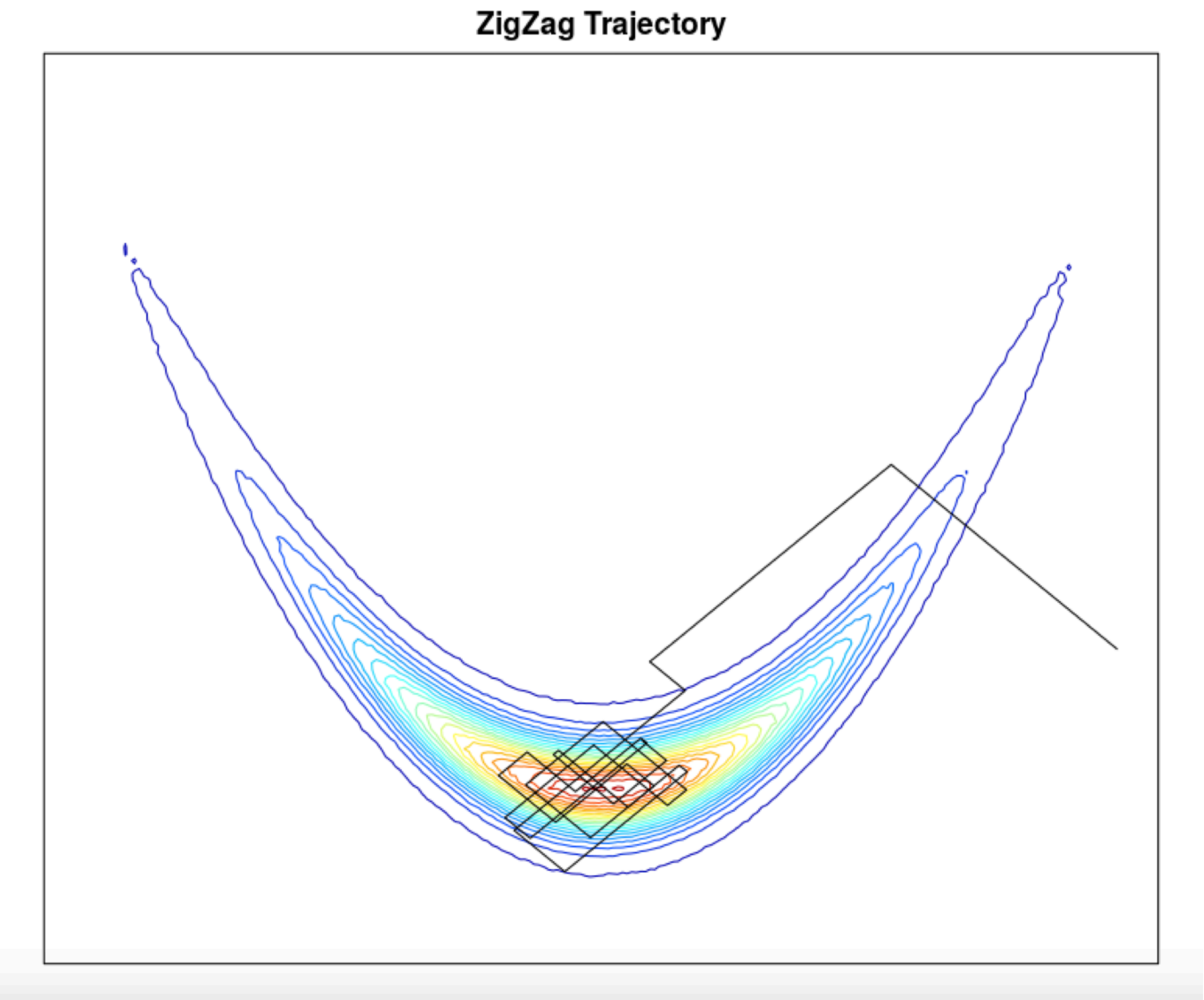

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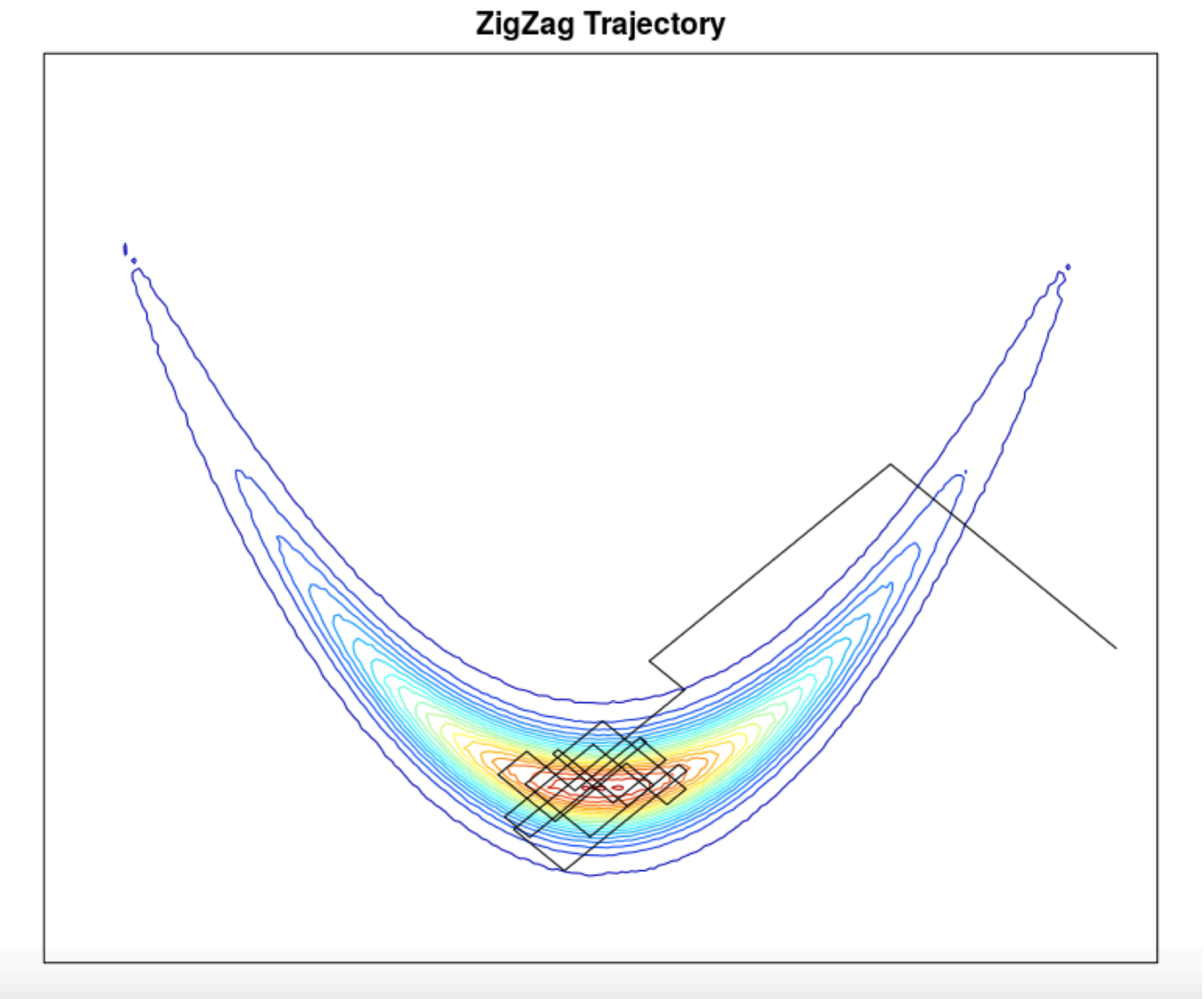

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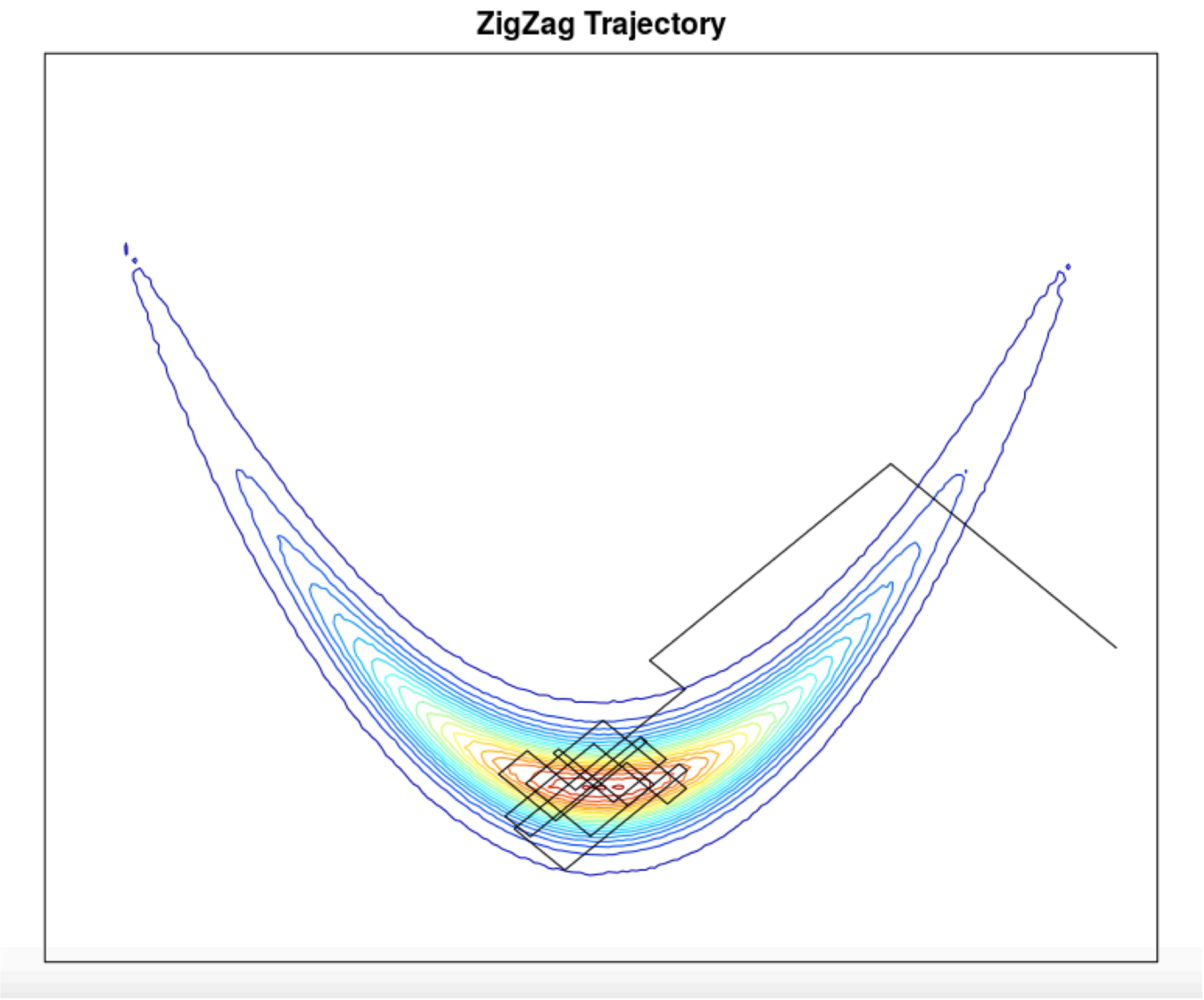

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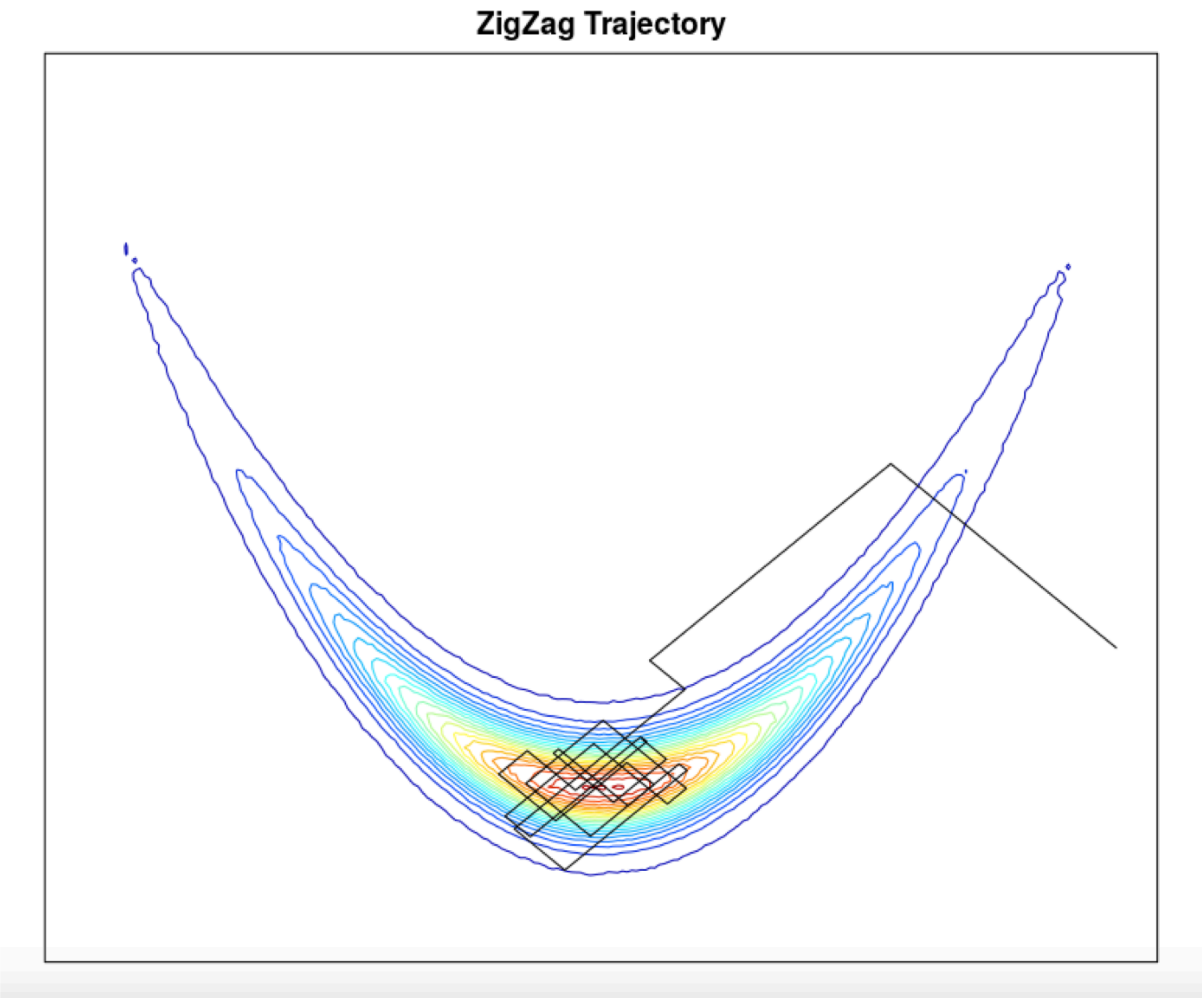

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    - events at rate $\lambda(x, v) = \max\left(0, \langle v, \nabla U(x) \rangle\right)$

    - jumps: specular reflection of v along contours of U

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2. ‘Zig-Zag Process’

- events at rate $\lambda_i(x, v) = \max\left(0, \langle v_i, \nabla_{x_i} U(x)\rangle\right)$
- jumps: flip v_i

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3. 'Local' Bouncy Particle Sampler

- assume structured target: $\pi(x) = \exp\left(-\sum_{a} U_a(x_{\partial a})\right)$
- events at rate $\lambda_a(x, v) = \max\left(0, \langle v_{\partial a}, \nabla U_a\left(x_{\partial a}\right)\rangle\right)$
- jumps: specular reflection of $v_{\partial a}$ along contours of U_a

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- skew-reversibility: backwards in time, process looks *almost* the same

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- generalisation: *split* time-enriched PDMP
  - dynamics: $\dot{x} = \sum_{\ell} \tau_\ell b_\ell(x),\ \tau_\ell \in \{\pm 1\}$
  - decompose $r(x, \tau) = \sum_j r_j(x, \tau)$
    - each term antisymmetric under a certain 'flip' $\mathscr{F}_j$ of τ variables
    - at 'j-jump', apply j^{th} flip operator

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  - structured { targets / dynamics / events } easier to analyse
  - simplifies design of new methods
- ongoing: simplifying implementation

thanks!

Design of Sampling Dynamics

(ODE, SDE case)

- bare minimum: dynamics should leave π invariant
  - linear condition on generator of process (simple to check, in principle)
- for pure ODE: specify skew-symmetric $Q(x)$, then define
  - $b(x) = Q(x)\,\nabla \log \pi(x) + \mathrm{div} Q(x)$
  - evolve by $\dot{x} = b(x)$
- for reversible SDE: specify PSD $D(x)$, then define
  - $b(x) = D(x)\,\nabla \log \pi(x) + \mathrm{div} D(x)$
  - evolve by $\mathrm{d}x = b(x)\,\mathrm{d}t + \sqrt{2D(x)}\mathrm{d}W$

Design of Sampling Dynamics

(ODE, SDE case)

- general SDE = (pure ODE) + (reversible SDE)
  - so: pick $\left(Q(x), D(x)\right)$, and you're good to go!
- result is ~ old:
  - versions known in stat phys since ~1970s
  - re-popularised by Ma-Chen-Wu-Fox in ML (stochastic gradients)
  - expanded by Barp-Betancourt-Takao-Arnaudon-Girolami (geometry)
- but … PDMPs?