Optimization of Advanced Marko Chain Monte Carlo Methods with Applications to Biological Systems

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Roadmap

- Experimentally assess optimal acceptance rates for model problems. Do theoretical results hold?
- How do non-identifiable dimensions affect the optimal acceptance rate and convergence?
- Combine Adaptive Metropolis with polytope samplers
- Is Adaptive Metropolis able to approximate optimal acceptances rates?
- Does Adaptive Metropolis work with non-identifiable dimensions?
- What other approaches exist there? Active subspaces [2]

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Optimal acceptance rates

- Performance measures:
  - Effective Sample Size (ESS):

$$N_{eff} = \frac{N}{1+\tau}, \quad \tau \dots \text{ autocorrelation time}$$

  - Expected Squared Jump Distance (ESJD):

$$\text{ESJD} = \frac{1}{N-1} \sum_{i=1}^{N-1} \|\theta_n - \theta_{n+1}\|_2^2$$

  - Upper bound on Expected Squared Jump Distance per second (ESJD/s):

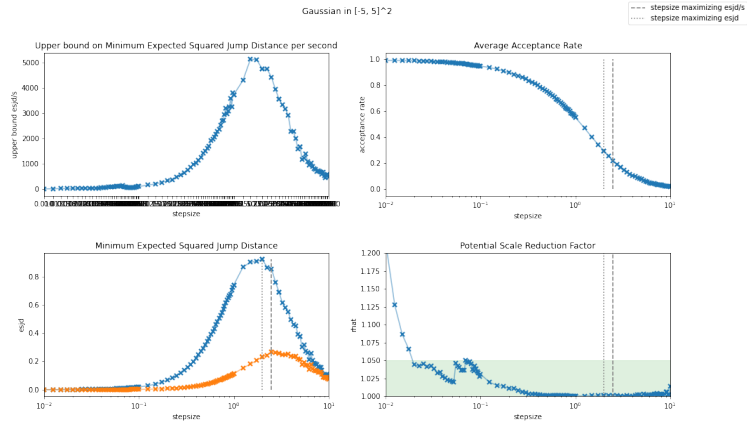
$$\text{ESJD/s} = \frac{\text{ESJD}}{t_\alpha r_\alpha + t_d}, \quad t_\alpha \dots \text{ time per simulation}, \quad r_\alpha \dots \text{ acceptance rate},$$
$$t_d \dots \text{ time per draw}$$

Optimal acceptance rates

- 4 chains where run until they hit convergence ($\widehat{R} < 1.05$) or maximal number of samples was exceeded
  - $\widehat{R}$ can be computed incrementally

Optimal acceptance rates

- Orange upper bound on the ESJD/s



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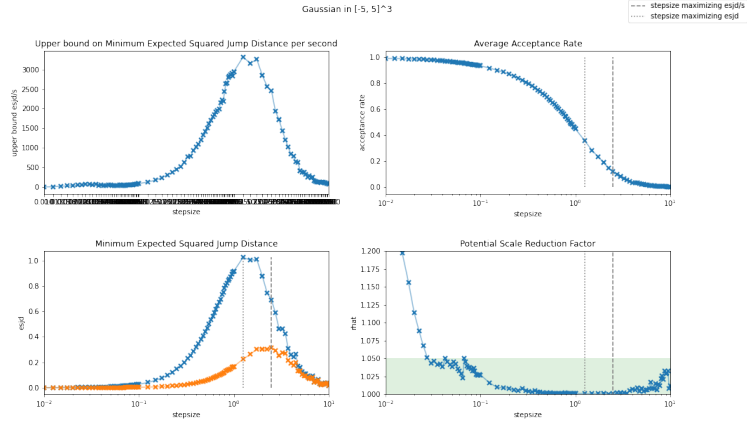

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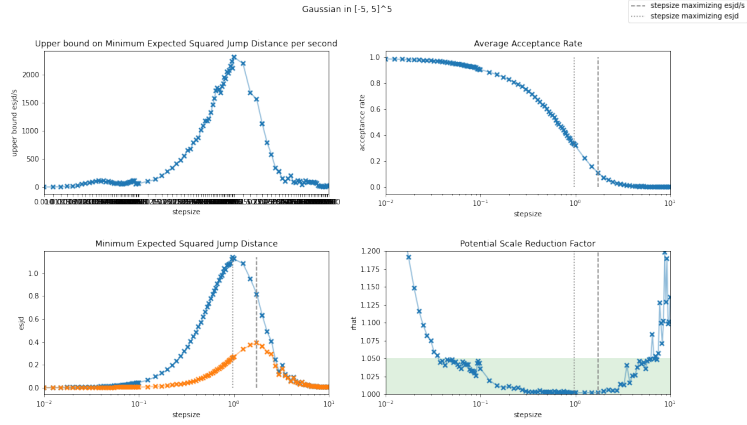

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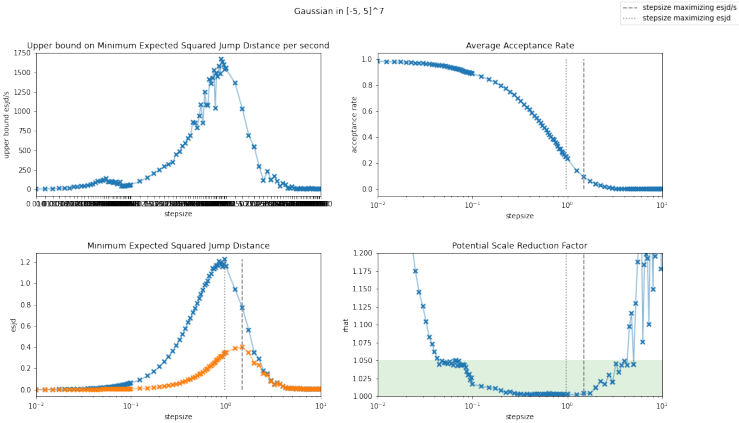

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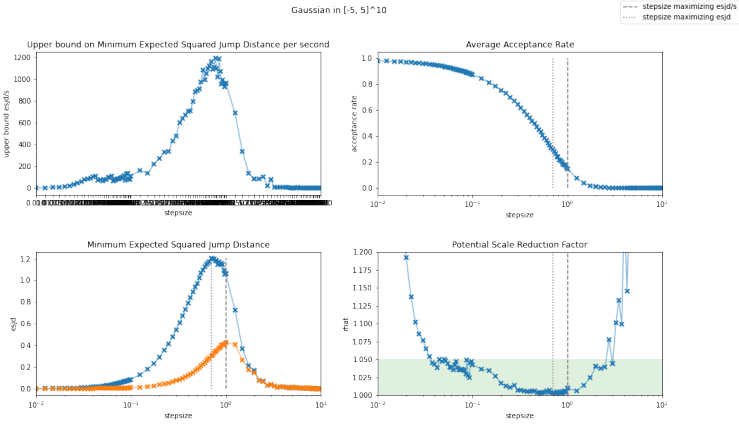

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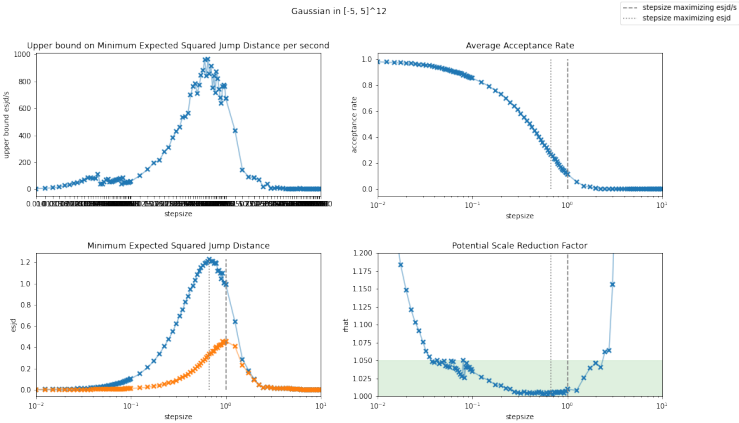

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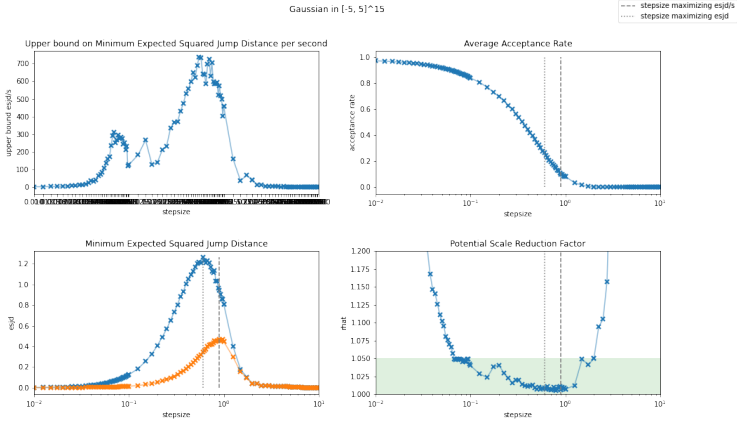

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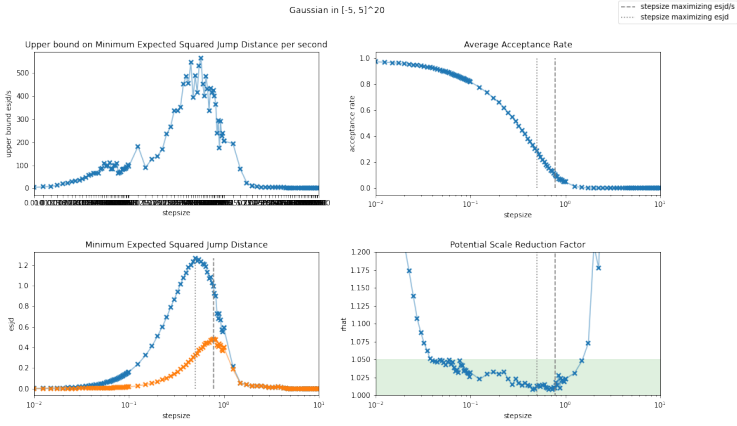

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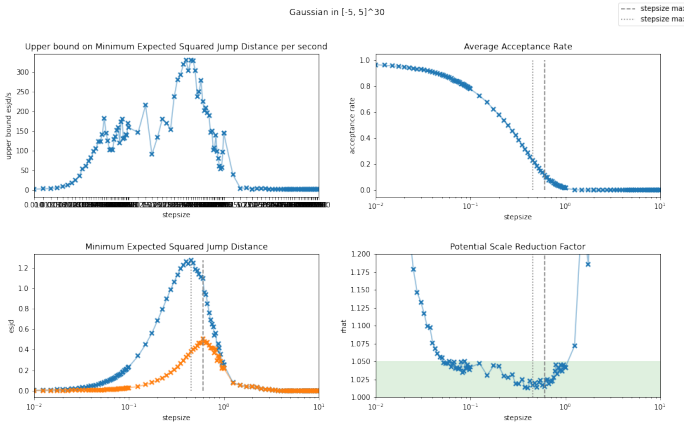

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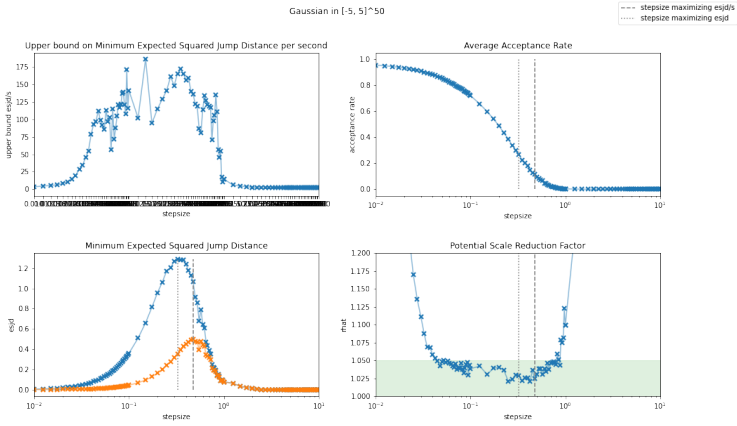

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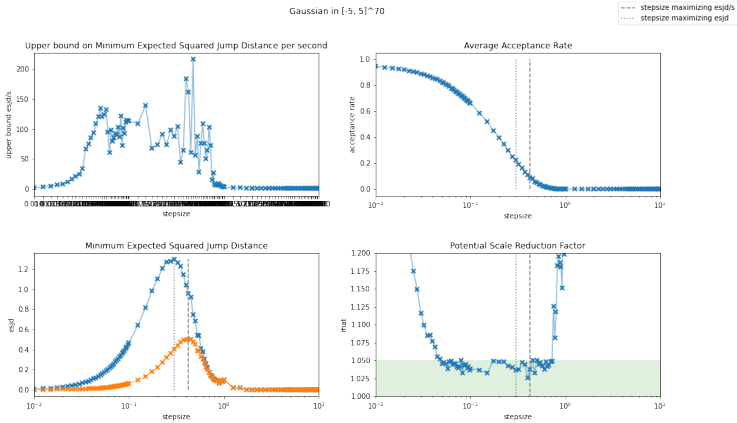

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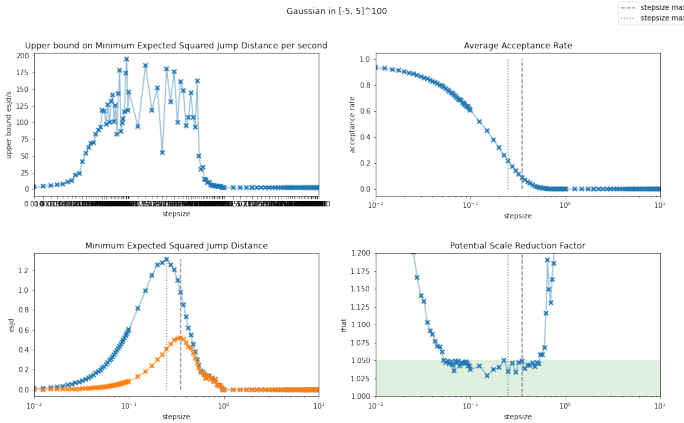
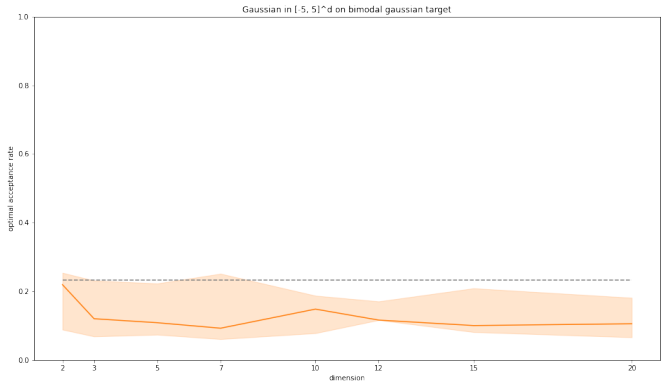


Optimal acceptance rates

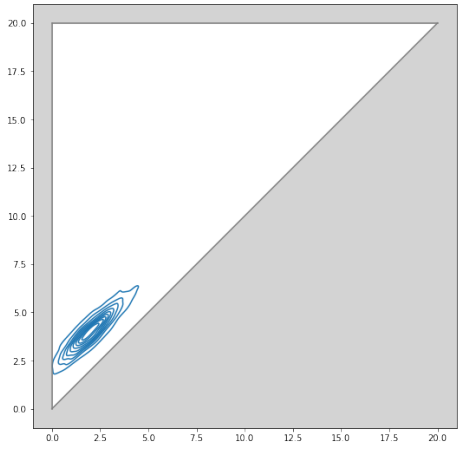
- Optimal acceptance rate per dimension



Optimal acceptance rates

- Justifies two things:
  - Use ESJD instead of ESS, as it is more robust, cheaper and seems like a good estimator
  - Tuning to theoretically optimal 0.234 does not hold, if we consider time costs & costly simulations
- Motivates: Offline tuning of the stepsize using ESJD

Offline tuning using ESJD



- First Approach:
  - Objective function draws N samples using stepsize s and compute ESJD.
  - Plug objective function in general-purpose optimizer
- Issue: Objective function is time-inhomogeneous and/or noisy
  - Low probability starting point errorneously favors large step sizes

$\rightarrow$ Possibly calls for *Bayesian optimization* approaches?

$\rightarrow$ Log-uniform sampling of stepsize parameters?

Starting point selection

- We want to optimize step size for the "interesting bits", so we first need to get there

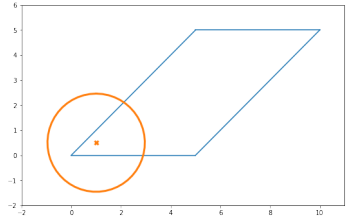
→ Typical warm start procedure is *burn in*

- Charles Geyer:
  "Any point you don't mind having in a sample is a good starting point."[1]

→ Use *maximum a posteriori/maximum likelihood* estimator by first optimizing the target distribution

[1] http://users.stat.umn.edu/ geyer/mcmc/burn.html

Proposal Preconditioning: Polytope Rounding

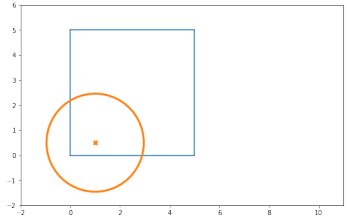


Polytope:

$$\mathcal{P} = \{x : Ax \leq b\}$$

Proposal:

$$x'_n = x_n + z, \quad z \sim \mathcal{N}(0, I)$$

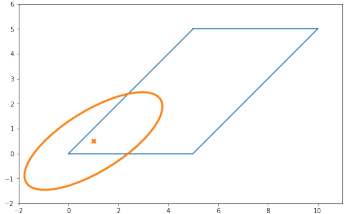


Polytope:

$$\mathcal{P} = \{x : ATx \leq b\}$$

Proposal:

$$x'_n = x_n + z, \quad z \sim \mathcal{N}(0, I)$$



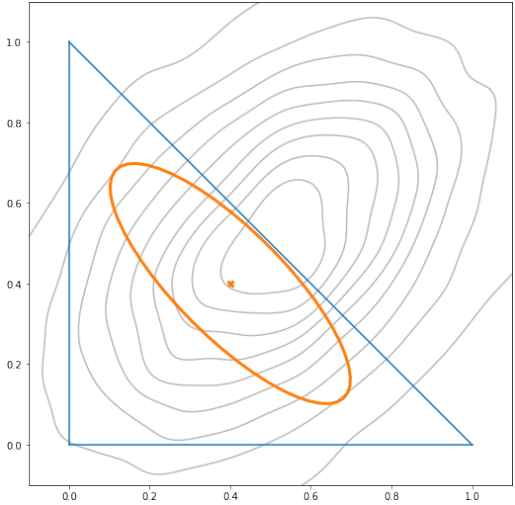
Polytope:

$$\mathcal{P} = \{y : Ay \leq b\}, \quad y = Tx$$

Proposal:

$$y'_n = y_n + Tz, \quad z \sim \mathcal{N}(0, I)$$

Proposal Preconditioning: Dikin Ellipsoid and/or Fisher Matrix



Dikin Walk [3]:

$$x'_n = x_n + \frac{r}{\sqrt{d}} D^{-1/2} z, \quad z \sim \mathcal{N}(0, I)$$

with

$$D = \sum_i \frac{a_i a_i^\top}{(b_i - a_i^\top x)^2}$$

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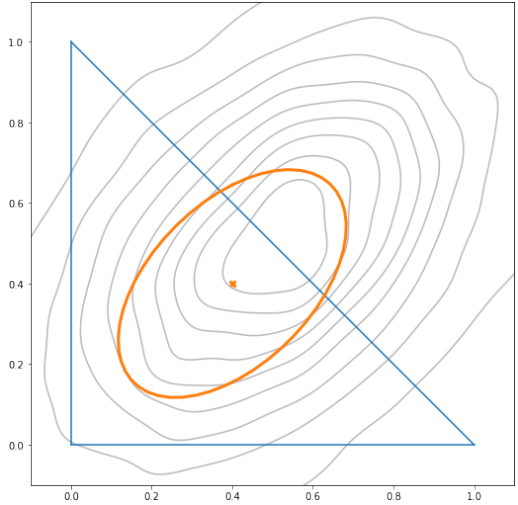


CSmMALA (s=1) without drift [5]:

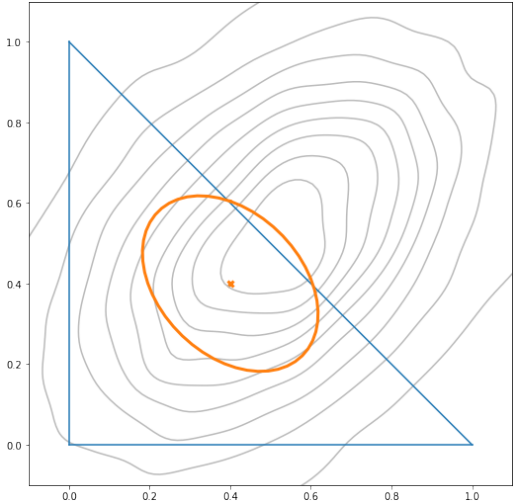
$$x'_n = x_n + rF^{-1/2}z, \quad z \sim \mathcal{N}(0, I)$$

with

$$F = -\mathbb{E}\Big[\frac{\partial^2}{\partial x^2}\log \mathcal{L}(d|x)\Big|x\Big],$$

with $\mathcal{L}$ being the likelihood function

Proposal Preconditioning: Dikin Ellipsoid and/or Fisher Matrix



CSmMALA (s=0.5) without drift [5]:

$$x'_n = x_n + rG^{-1/2}z, \quad z \sim \mathcal{N}(0, I)$$

with

$$G = sF + (1-s)D$$

with $\mathcal{L}$ being the likelihood function

Proposal Preconditioning: Dikin Ellipsoid and/or Fisher Matrix

- CSmMALA(s=0.5) 40 times higher ESS as the second best algorithm for a Gaussian target [5]
- CSmMALA takes two orders of magnitude more time for real ^{13}C data

$\rightarrow$ **Gradients of ^{13}C too expensive**

Local Approximations and Gradient Esimation

- Idea: Use local approximations of the target function, that are easy to evaluate
- *How do we construct such approximations?*

→ Conrad et al. have the answer! [1]

Local Approximations and Gradient Esimation

- Maintain set $\mathcal{S}$ of samples and their values, independently from chain samples
- Choose $N_L = \sqrt{d}(d+1)$ or $N_Q = \sqrt{d}(d+1)(d+2)/2$ points for linear or quadratic model respectively which are nearest to current state
- Fit model and cross-validate it on the N samples
- If error threshold is exceeded, add new point to $\mathcal{S}$

- Conrad et al. [1] replace exact target function with approximate one, thus sample the "wrong" distribution
- We only want to estimate the local gradient by using the fitted model's gradient
- Try updating the quadratic model with less points than N_Q by using least Frobenius norm update [4]

What to do with the Gradient Esimate?

- Accelerate CSmMALA
- Precondition Hit & Run algorithm with Fisher information estimate

What to do with the Gradient Esimate?

- Accelerate CSmMALA
- **Precondition Hit & Run algorithm with Fisher information estimate**

Fisher-preconditioned Hit & Run?

- CSmMALA takes convex combination of Dikin & Fisher information to remain inside polytope & adapt to target function
- Hit & Run is guaranteed to remain inside polytope!

→ Precondition it with Fisher information matrix to adapt to target function

- Hit & Run works best in rounded polytopes

→ **Pitfall:** Take care to *round* target function, i.e. evaluate it at the correct position

Roadmap

- Experimentally assess optimal acceptance rates for model problems. Do theoretical results hold?
- Offline stepsize tuning starting from MAP estimate
- Local approximation and gradient estimates for cheap preconditioning

Postponed:

- How do non-identifiable dimensions affect the optimal acceptance rate and convergence?
- Combine Adaptive Metropolis with polytope samplers
- Is Adaptive Metropolis able to approximate optimal acceptances rates?
- Does Adaptive Metropolis work with non-identifiable dimensions?
- What other approaches exist there? Active subspaces [2]

Thanks!

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