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SMC-Guided Diffusion for General Optimisation

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Introduction

First Frame

Hello, world! Akyildiz et al. (2020), Anderson (1982), Del Moral (2011), Dou and Song (2023), and Ho et al. (2020)

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Experimental Results

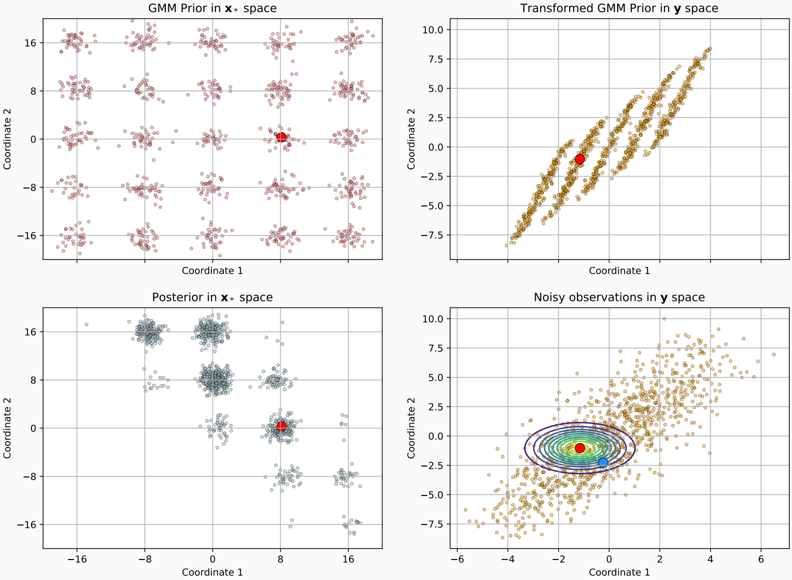
GMM Experiment — Setup

Consider a Gaussian mixture model (GMM), p_{data}, with 25 equally weighted ($\omega_{i,j} \propto 1$) d_x-dimensional Gaussian random variables with means $\mu_{i,j} := (8i, 8j, \ldots, 8i, 8j) \in \mathbb{R}^{d_x}$ for $(i,j) \in \{-2, \ldots, 2\}^2$ and unit variance. We generate some d_y-dimensional measurement, $\mathbf{y}$, according to the following process:

- Draw $\tilde{A} \sim \mathcal{N}(0,1)^{d_y \times d_x} \in \mathbb{R}^{d_y \times d_x}$ and compute its SVD decomposition, $USV^\top$.
- Sample $s_{i,j} \sim \mathcal{U}[0,1]$ for $(i,j) \in \{-2, \ldots, 2\}^2$.
- Set $A := U\, diag(\{s_{i,j}\})\, V^\top$.
- Draw $\mathbf{x}_* \sim p_{\text{data}}$ and set $\mathbf{y} := A\mathbf{x}_* + \sigma_y \epsilon,\ \epsilon \sim \mathcal{N}(\mathbf{0}_{d_y}, \mathrm{I}_{d_y})$.

The goal of the inverse problem is to take $\mathbf{y}$ (with A and σ_y known), and use it to infer $\mathbf{x}_*$. We consider $d_y < d_x$, making the problem ill-posed.

GMM Experiment — Setup Visualised



GMM Experiment — Prior Model and TMPD Guidance

GMM Experiment — `SMCDiffOpt`

GMM Experiment — Performance Comparison

d_x	d_y	SMCDiffOpt	DPS	ΠIGD	TMPD
8	1	**1.35 ± 1.0**	8.18 ± 7.5	3.16 ± 2.72	3.31 ± 2.86
	2	**0.55 ± 0.43**	2.72 ± 2.62	0.94 ± 0.89	1.34 ± 1.25
	4	0.19 ± 0.09	0.95 ± 0.9	**0.09 ± 0.03**	0.37 ± 0.33
80	1	**1.65 ± 1.41**	5.03 ± 4.63	3.08 ± 2.71	2.42 ± 1.71
	2	**1.19 ± 1.07**	3.14 ± 3.02	1.68 ± 1.62	1.35 ± 1.22
	4	1.11 ± 0.93	1.32 ± 1.21	**0.84 ± 0.79**	1.14 ± 0.9

Table 1: Sliced-Wasserstein distances of samples from particle samples.

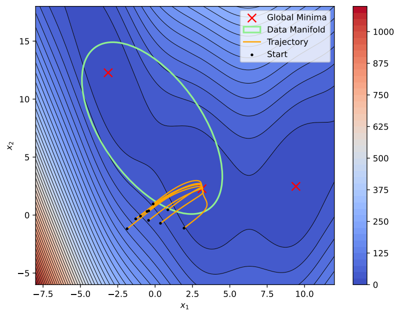
Branin Experiment — Setup

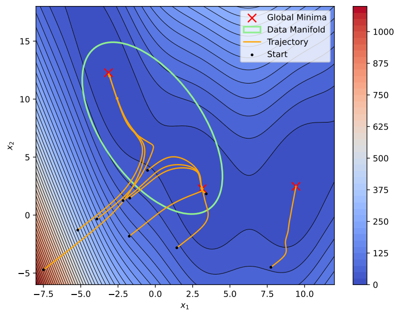
Consider optimising the Branin function as an objective over some constrained region (the data manifold) as detailed in Kong et al. (2024). The Branin function is defined by

$$f(x_1, x_2) = a(x_2 - bx_1^2 + cx_1 - r)^2 + s(1 - t)\cos(x_1) + s \tag{1}$$

where $a = 1$, $b = \frac{5.1}{4\pi^2}$, $c = \frac{5}{\pi}$, $r = 6$, $s = 10$, $t = \frac{1}{8\pi}$. It has three global minima located at $(-\pi, 12.275)$, $(\pi, 2.275)$ and $(9.42478, 2.475)$, with a value of 0.397887. We consider some uniform prior sampling distribution, p_{data}, over an ellipse region centred at $(-0.2, 7.5)$ with semi-axis lengths $(3.6, 8)$, tilted 25°. This region covers two of the global minima.

Branin Experiment — Pitfalls of Gradient Optimisation





Branin Experiment — SMCDiffOpt

Black-Box Experiment — Motivation

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Black-Box Experiment — Setup

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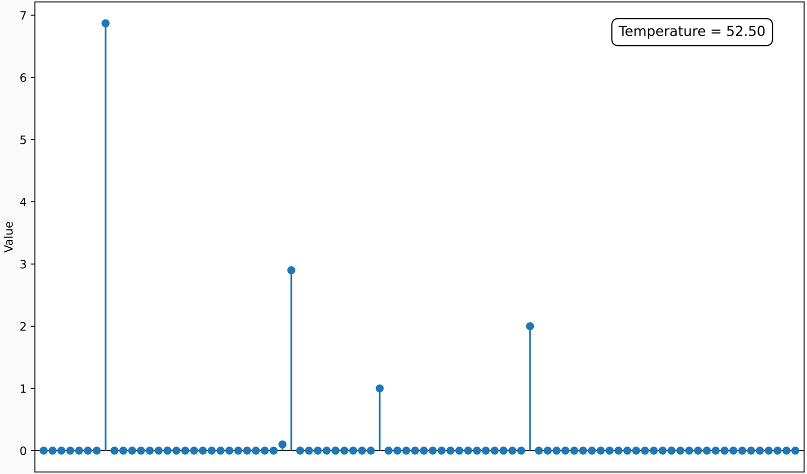
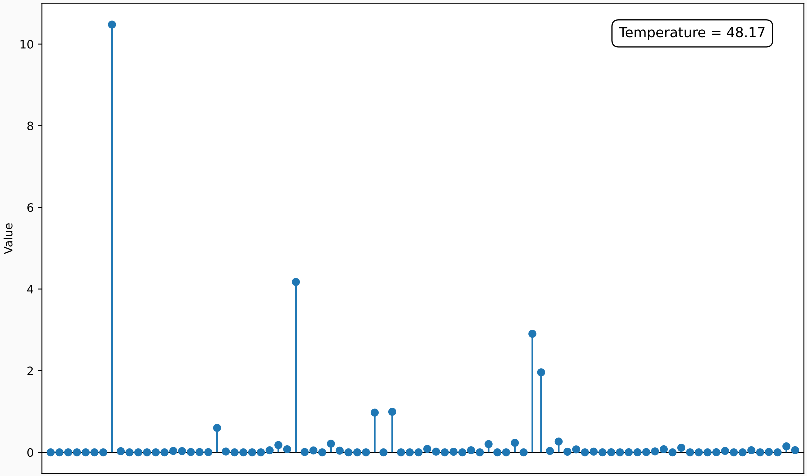
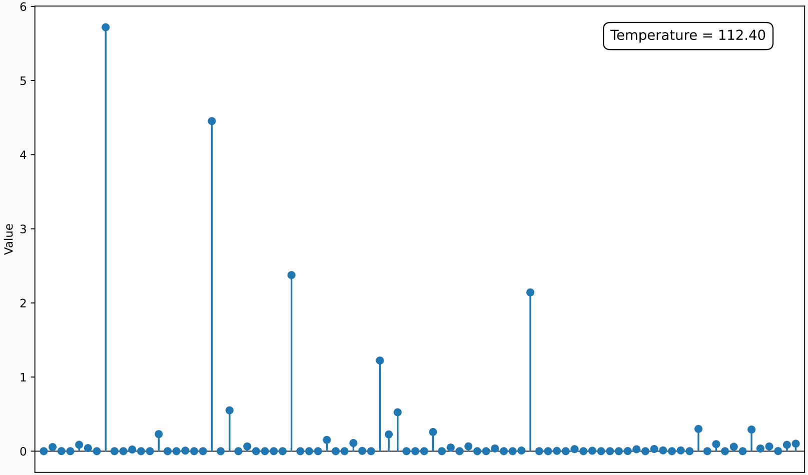
Black-Box Experiment — Real Sample



Black-Box Experiment — Generated Sample



Black-Box Experiment — Optimised Sample



Black-Box Experiment — Performance Comparison

CbAS	CMA-ES	Gradient Ascent	MINs	REINFORCE	DDOM	DiffOpt	**SMCDiffOpt**
0.433 ± 0.027	0.474 ± 0.021	0.510 ± 0.009	0.473 ± 0.003	0.483 ± 0.015	0.560 ± 0.044	0.614 ± 0.029	**0.644 ± 0.024**

Table 2: Normalised scores for SuperConductor experiment.

CbAS	CMA-ES	Gradient Ascent	MINs	REINFORCE	DDOM	DiffOpt	**SMCDiffOpt**
80.082 ± 4.933	87.774 ± 3.965	94.414 ± 1.719	87.483 ± 0.481	89.351 ± 2.708	103.600 ± 8.139	113.545 ± 5.322	**119.059 ± 4.497**

Table 3: Raw scores for SuperConductor experiment.

Conclusion

Future Work

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Final Remarks

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Thank you!

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