Measuring Sample Quality with Stein's Method

An attempt at quantifying Monte-Carlo efficiency by Gorham and Mackey (2015)

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Outline

Our goal is to calculate quantities of the form $\mathbb{E}_P[h(X)]$ where P is an unknown target distribution form the samples of Q as

$$\mathbb{E}_Q[h(X)] = \sum_{i=1}^{n} q(x_i)h(x_i).$$

We will be following (Gorham and Mackey, 2015).

- Revisiting Stein's Lemma
- Finding distances between distributions
- How Stein's method provides an answer
- Constructing Stein operators
- Calculating the discrepancies
- Experiments

Stein's Lemma

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$$X \sim \text{Gamma}(\alpha, \beta) \quad \Longleftrightarrow \quad \mathbb{E}[Xf'(X) + (\alpha - \beta X)f(X)] = 0$$
$$X \sim \text{Poisson}(\lambda) \quad \Longleftrightarrow \quad \mathbb{E}[\lambda f(X + 1) - Xf(X)] = 0$$
$$X \sim \text{Binomial}(n, p) \quad \Longleftrightarrow \quad \mathbb{E}[(1 - p)Xf(X) - p(n - X)f(X + 1)]$$

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$$X \sim P \quad \Longleftrightarrow \quad \mathbb{E}_P[(\mathcal{A}f)(X)] = 0.$$

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Target distribution P with open convex support $\mathcal{X} \subseteq \mathbb{R}^d$. We approximate P with Q.

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How to ensure that calculating this expression is tractable?

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Together, $\mathcal{T}, \mathcal{G}$ define the *Stein discrepancy*

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3. Upper bound $\mathcal{S}(Q, \mathcal{T}, \mathcal{G})$ to demonstrate convergence to zero (**Consistency**).

How to construct $\mathcal{T}$

Construct a generator (Barbour, 1988): for a Markov process $(Z_t)_{t \geq 0} \to P$:

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$$\mathcal{G}_{\|\cdot\|} = \left\{ g : \mathcal{X} \to \mathbb{R}^d \mid \sup_{x,y\in\mathcal{X}} \left(\|g\|^*, \|\nabla g\|^*, \frac{\|\nabla g(x) - \nabla g(y)\|^*}{\|x-y\|} \right) \leq 1 \right\}$$

Bounding the Stein Discrepancy

Lower bound:

Theorem (*Theorem 2*)

If $\mathcal{X} = \mathbb{R}^d$ and $\log p$ is strongly concave with continuous and bounded 3rd and 4th derivatives then for any measures $(\mu_m)_{m \geq 1}$, $\mathcal{S}(\mu_m, \mathcal{T}_P, \mathcal{G}_{\|\cdot\|}) \to 0$ only if $d_{\mathcal{W}}(\mu_m, P) \to 0$.

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Implies convergence of $\mathcal{S} \to 0$ whenever $X_m \sim Q_m \xrightarrow{L^2} Z \sim P$ and $\nabla \log p(X_m) \xrightarrow{L^1} \nabla \log p(Z)$.

Computing Stein Discrepancies

For observed sample values $\{x_i\}_{i=1}^n$, we want to solve the optimization problem

$$\mathcal{S}(Q, \mathcal{T}_P, \mathcal{G}_{\|\cdot\|}) = \sup_{g \in \mathcal{G}_{\|\cdot\|}} \sum_{i=1}^n q(x_i)(\langle g(x_i), \nabla \log g(x_i) \rangle + \nabla \cdot g_{x_i}),$$

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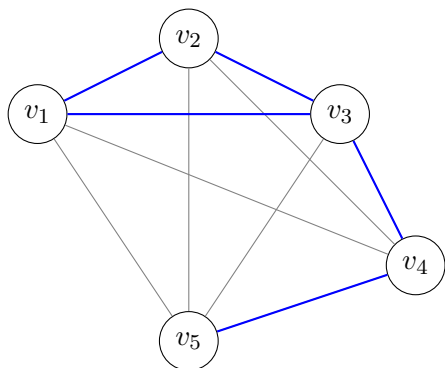
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$$\sup_{\gamma_j \in \mathbb{R}^n, \Gamma_j \in \mathbb{R}^{d \times n}} \sum_{i=1}^n q(x_i)(\langle \gamma_{ji}, \nabla \log \gamma_{ji}\rangle + \Gamma_{jji}),$$

for $\gamma_{ji} = g_j(x_i)$, $\Gamma_{jki} = \nabla_k g_j(x_i)$. An efficient way to define the constraints involves using *graph t-spanners* and an ℓ_1 norm.

Graph Spanners

Graph $G = K_n$ (Original)

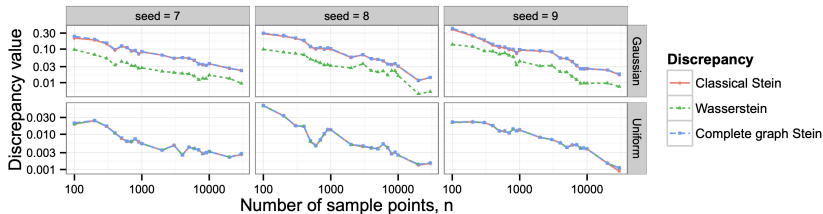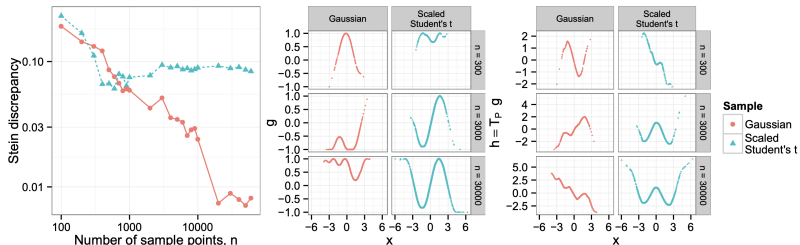|	
——	t-Spanner Edges (G')
——	Original Edges (G)

Graph G' (t-Spanner for $t \geq 1$)

Algorithm Multivariate Spanner Stein Discrepancy (Algorithm 1 in Gorham & Mackey 2015)

1: **input:** Q, coordinate bounds $(\alpha_1, \beta_1), \ldots, (\alpha_d, \beta_d)$
2: $G_2 \leftarrow$ Compute sparse 2-spanner of $\mathrm{supp}(Q)$
3: **for** $j = 1$ to d **do** (**parallelizable**)
4:     $r_j \leftarrow$ Solve the j-th coordinate from linear program $(\star)$
5: **end for** $\sum_{j=1}^{d} r_j$

Experiments

Target distribution $P = \mathcal{N}(0, 1)$.

Extensions

- Change the diffusion process to generate $\mathcal{T}_P$.
- Replacing the calculation of $\mathcal{S}$ with a Kernel Approach (Gorham and Mackey, 2017).
- Consider general diffusion operators (Gorham et al., 2019).
- If $\mathcal{T}_P$ is too expensive to calculate, use *stochastic Stein discrepancies* (SSDs) (Gorham et al., 2020).
- And many others... (Anastasiou et al., 2023)

References

A. Anastasiou, A. Barp, F.-X. Briol, B. Ebner, R. E. Gaunt, F. Ghaderinezhad, J. Gorham, A. Gretton, C. Ley, Q. Liu, L. Mackey, C. J. Oates, G. Reinert, and Y. Swan. Stein's method meets computational statistics: A review of some recent developments. *Statistical Science*, 38(1):120–139, 2023. doi: 10.1214/22-STS863. URL https://projecteuclid.org/journals/statistical-science/volume-38/issue-1/Steins-Method-Meets-Computational-Statistics--A-Review-of-Some/10.1214/22-STS863.full.

A. D. Barbour. Stein's method and poisson process convergence. *Journal of Applied Probability*, 25A:175–184, 1988.

J. Gorham and L. Mackey. Measuring sample quality with stein's method. In *Advances in Neural Information Processing Systems*, volume 28, 2015.

J. Gorham and L. Mackey. Measuring sample quality with kernels. In D. Precup and Y. W. Teh, editors, *Proceedings of the 34th International Conference on Machine Learning*, volume 70 of *Proceedings of Machine Learning Research*, pages 1292–1301. PMLR, Aug 06–11 2017. URL https://proceedings.mlr.press/v70/gorham17a.html.

J. Gorham, A. B. Duncan, S. J. Vollmer, and L. W. Mackey. Measuring sample quality with diffusions. *Annals of Applied Probability*, 29(5):2884–2928, 2019. doi: 10.1214/19-AAP1467.

J. Gorham, A. Raj, and L. W. Mackey. Stochastic stein discrepancies. In *Advances in Neural Information Processing Systems 33 (NeurIPS 2020)*, pages 17931–17942. Curran Associates, Inc., Dec. 2020. URL https://proceedings.neurips.cc/paper/2020/file/d03a857a23b5285736c4d55e0bb067c8-Paper.pdf.

C. Stein. A bound for the error in the normal approximation to the distribution of a sum of dependent random variables. In *Proceedings of the Sixth Berkeley Symposium on Mathematical Statistics and Probability, Volume II: Probability Theory*, pages 583–602. University of California Press, 1972.