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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$$X \text{ standard Gaussian} \quad \Longrightarrow \quad \mathrm{Cov}(X, g(X)) = \mathbb{E}[g'(X)],$$

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

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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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2. Lower bound $\mathcal{S}$ by some familiar IPM $d_{\mathcal{H}}$. **Reliability**: for $\{\mu_m\}_{m \geq 1}$
$$d_{\mathcal{H}}(\mu_m, P) \to 0 \quad \Longrightarrow \quad \mathcal{S}(\mu_m, \mathcal{T}, \mathcal{G}) \to 0.$$

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$$d_{\mathcal{H}}(\mu_m, P) \to 0 \quad \implies \quad \mathcal{S}(\mu_m, \mathcal{T}, \mathcal{G}) \to 0.$$
3. Upper bound $\mathcal{S}(Q, \mathcal{T}, \mathcal{G})$ to demonstrate convergence to zero (**Consistency**).

How to construct $\mathcal{T}$

Construct a generator for a Markov process $(Z_t)_{t\geq 0} \to P$ (Barbour, 1988). Consider a semigroup of operators $(\mathcal{A}_t f)(x) = \mathbb{E}[f(X_t) \mid X_0 = x]$. P is a limiting distribution if

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Stein Set

$$\mathcal{G}_{\|\cdot\|} = \Big\{ g : \mathcal{X} \to \mathbb{R}^d \mid \sup_{x,y \in \mathcal{X}} \left(\|g\|^*, \|\nabla g\|^*, \frac{\|\nabla g(x) - \nabla g(y)\|^*}{\|x - y\|} \right) \leq 1, \\ \langle g(x), \hat{n}(x) \rangle = 0,\ \forall x \in \partial \mathcal{X} \Big\},$$

where

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Observation

This imposes conditions for all pairs of points in $\mathcal{X}$.

Bounding the Stein Discrepancy

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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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Upper bound:

Theorem (*Proposition 3*)

If $X \sim Q$ *and* $Z \sim P$ *with* $\nabla \log p(Z)$ *integrable, then*

$$\mathcal{S}(Q, \mathcal{T}_P, \mathcal{G}_{\|\cdot\|}) \leq \mathbb{E}\|X - Z\| + \mathbb{E}\|\nabla \log p(X) - \nabla \log p(Z)\| \\ + \mathbb{E}\|\nabla \log p(Z)(X - Z)^\top\|.$$

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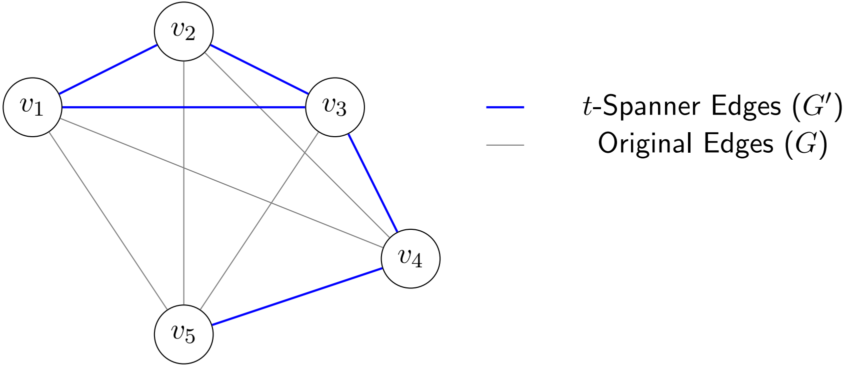
$$\sup_{\gamma_j \in \mathbb{R}^n, \Gamma_j \in \mathbb{R}^{d \times n}} \sum_{i=1}^{n} q(x_i)(\langle \gamma_{ji}, \nabla \log \gamma_{ji} \rangle + \Gamma_{jji}),$$

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)



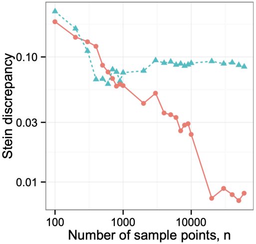
Graph G' (t-Spanner for $t \geq 1$)

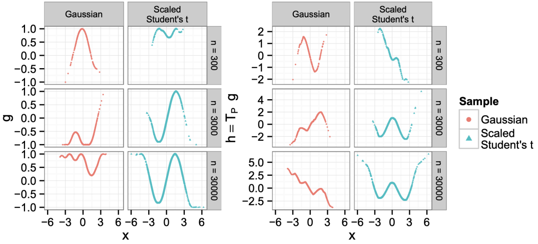
Algorithm Multivariate Spanner Stein Discrepancy (`Algorithm 1` in Gorham & Mackey 2015)

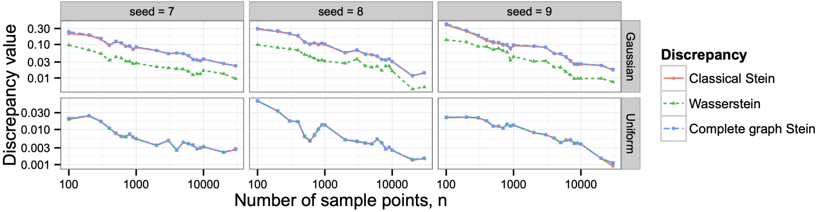
1: **input:** Q, coordinate bounds $(\alpha_1, \beta_1), \ldots, (\alpha_d, \beta_d)$
2: $G_2 \leftarrow$ Compute sparse 2-spanner of $\mathrm{supp}(Q)$
3: **for** $j = 1$ to d **do** (**parallelizable**)
4: $\quad r_j \leftarrow$ Solve the j-th coordinate from linear program $(\star)$
5: **end for**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

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)

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