# 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

For $X$ mean-zero random variable and $g$ a weakly differentiable and $L_1$ integrable function, we have that

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

$$\mathbb{E}[g'(X) - Xg(X)] = 0, \qquad \longrightarrow \qquad \mathbb{E}[\mathcal{A}g(X)] = 0$$

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

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

# Quality Measures for samples

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

Goal: to have a measure of the quality of the samples $Q$:

- Detects convergence $Q_m \to P$
- Detects $Q$ not converging to $P$
- Is computationally feasible

A possible way to ensure these is by using an *integral probability metric*

$$d_{\mathcal{H}}(Q, P) = \sup_{h \in \mathcal{H}} |\mathbb{E}_Q[h(X)] - \mathbb{E}_P[h(X)]|$$

How to ensure that calculating this expression is tractable?

# Stein's Method

Characterizing convergence in distribution (Stein, 1972):

1. Find a real-valued operator $\mathcal{T} : \mathcal{G} \to \mathbb{R}$ characterizing $P$ in the sense that

$$\mathbb{E}_P[(\mathcal{T}g)(Z)] = 0 \quad \forall g \in \mathcal{G}.$$

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

$$\mathcal{S}(Q, \mathcal{T}, \mathcal{G}) := \sup_{g \in \mathcal{G}} |\mathbb{E}_Q[(\mathcal{T}g)(X)]| = d_{\mathcal{G}}(Q, P).$$

2. Lower bound $\mathcal{S}$ by some familiar IPM $d_{\mathcal{H}}$. **Reliability**: for $\{\mu_m\}_{m \geq 1}$

$$d_{\mathcal{H}}(\mu_m, P) \to 0 \quad \implies \quad \mathcal{S}(\mu_m, \mathcal{T}, \mathcal{G}) \to 0.$$

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

$$\int (\mathcal{A}_t f) d\mu = \int f d\mu \quad \forall t \geq 0,$$

$$\lim_{t \downarrow 0} \int \frac{\mathcal{A}_t f(x) - f(x)}{t} \, d\mu(x) = 0, ,$$

$$(\mathcal{A}u)(x) = \lim_{t \to 0} \frac{1}{t} \left( \mathbb{E}[u(x) \,|\, Z_0 = x] - u(x) \right).$$

With this we can take for a diffusion $dZ_t = \frac{1}{2} \nabla \log p(Z_t) dt + dW_t$ the *Stein operator*

$$(\mathcal{T}_P g)(x) \triangleq \langle g(x), \nabla \log p(x) \rangle + \nabla g(x)$$

# Stein Set

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

where

$$\|w\|^* = \sup_{\|v\|=1} \langle w, v \rangle \, .$$

**Observation**

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

# 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 $d_{\mathcal{W}}(\mu_m, P) \to 0$.*

- Sufficient but not necessary conditions for convergence.

**Upper bound:**

### Theorem (*Proposition 3*)

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

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

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

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

such that $g$ satisfies the conditions to be inside $\mathcal{G}_{\|\cdot\|}$.

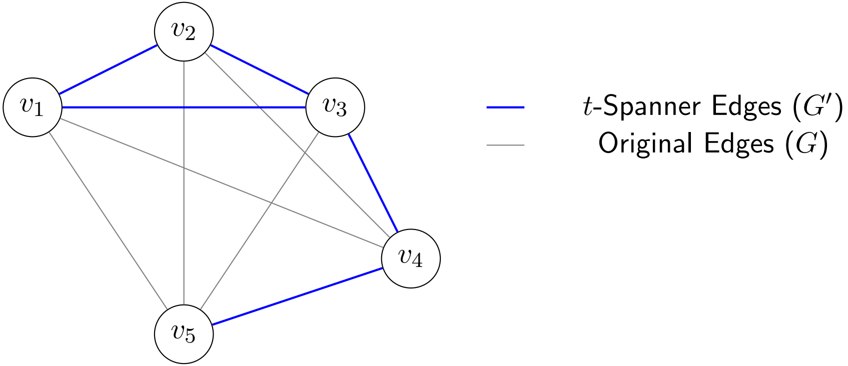
To make it feasible, Gorham and Mackey (2015) propose constraining the problem only on the values of $g$ on $\{x_i\}_{i=1}^n$.

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

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 $\ell_1$ norm.

# Graph Spanners

Graph $G = K_n$ (Original)

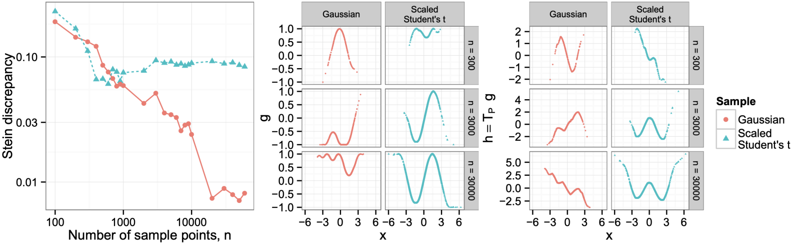


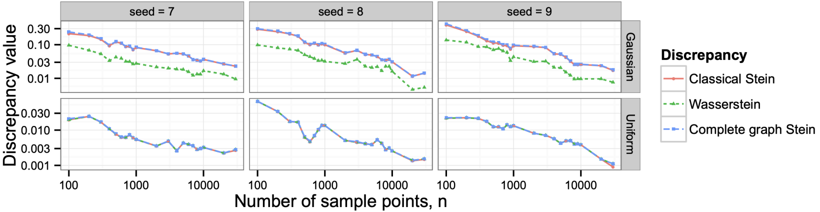

Graph $G'$ (t-Spanner for $t \geq 1$)

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

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

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

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