

Simple, Effective, and General Regression and its Meta-analysis using Kernel Averages

Theory, Challenges, Solutions and Results

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Introductions

- The Problem Setting

 - Existing Methods

The Presented Solution's Theory

- Kernel Trickery

- Maximum Mean Discrepancy

- The Proposed Framework

 - Alquier and Gerber's Contribution

Next Steps

- Conditionalising

- Novel Kernel Mean Embeddings

Bibliography

The Problem Setting

$$x \in \mathcal{X} \subseteq \mathbb{R}^{d_x} \longrightarrow \boxed{Q(y|x)} \longrightarrow y \in \mathcal{Y} \subseteq \mathbb{R}^{d_y}$$

$$\exists \theta_0 \in \Theta : Q = P_{\theta_0} \in \mathcal{P}_\Theta$$

$$\mathcal{P}_\Theta = \{P_\theta \in \mathcal{P}(\mathcal{Y}|\mathcal{X})\}_{\theta \in \Theta}$$

An Example

$$x \in \mathcal{X} \subseteq \mathbb{R}^{d_x} \longrightarrow Q(y|x) \longrightarrow y \in \mathcal{Y} \subseteq \mathbb{Z}_{\geq 0}$$

$$\exists \theta_0 \in \Theta \subseteq \mathbb{R}^{d_x} : Q = P_{\theta_0} \in \mathcal{P}_{\Theta}$$

$$\mathcal{P}_{\Theta} = \left\{ P_{\theta} (y \in \mathcal{Y} | x \in \mathcal{X}) = \exp(-k(\theta^{\top} x)) \sum_{i \in \mathcal{Y}} \frac{k(\theta^{\top} x)^i}{i!} \right\}_{\theta \in \Theta}$$

Another Example

$$x \in \mathcal{X} \subseteq \mathbb{R}^{d_x} \longrightarrow \boxed{Q(y|x)} \longrightarrow y \in \mathcal{Y} \subseteq \mathbb{R}^{d_y}$$

$$\exists \theta_0 \in \Theta : Q = P_{\theta_0} \in \mathcal{P}_\Theta$$

$$\mathcal{P}_\Theta = \left\{ P_\theta(y \in \mathcal{Y} | x \in \mathcal{X}) = \frac{\int_{\mathcal{Y}} \exp\left(-\frac{1}{2}(y - m_\theta(x))^\top S_\theta^{-1}(x)(y - m_\theta(x))\right) \lambda(dy)}{\sqrt{2\pi \det(S_\theta(x))}^{d_y}} \right\}_{\theta \in \Theta}$$

Existing Methods

- ▶ **Highly-General Techniques**
 - ▶ Least Squares Estimation / Maximum Likelihood Estimation – [1].
 - ▶ Poor Performance under Misspecification.
 - ▶ Kolmogorov-Smirnov Testing – [2].
 - ▶ Suffers massively from the Curse of Dimensionality, as do most IPM-adjacent techniques.
- ▶ **Focused Techniques**
 - ▶ ‘Generalized Hosmer-Lemeshow Testing’ – [3].
 - ▶ Procedurally complex.
 - ▶ Cameron-Trivedi Testing – [4].
 - ▶ Assesses for data dispersion that isn’t unique to the Poisson Distribution.

Either heavily reliant on faulty heuristics or are overcomplex.

No generalisable direct comparison between measure allocation by the model and the measure underlying the observed data.

Examining something simpler

$$x \in \mathcal{X} \subseteq \mathbb{R}^{d_x} \longrightarrow \boxed{Q(y|x)} \longrightarrow y \in \mathcal{Y} \subseteq \mathbb{R}^{d_y}$$

$$\exists \theta_0 \in \Theta : Q = P_{\theta_0} \in \mathcal{P}_\Theta$$

$$\mathcal{P}_\Theta = \{P_\theta \in \mathcal{P}(\mathcal{Y}|\mathcal{X})\}_{\theta \in \Theta}$$

Examining something simpler

$$Q(y) \longrightarrow y \in \mathcal{Y} \subseteq \mathbb{R}^{d_Y}$$

$$\exists \theta_0 \in \Theta : Q = P_{\theta_0} \in \mathcal{P}_\Theta$$

$$\mathcal{P}_\Theta = \{P_\theta \in \mathcal{P}(\mathcal{Y})\}_{\theta \in \Theta}$$

Kernel Trickery, pt. 1

For more information – [5], [6], [7]

- ▶ Reproducing Kernel Hilbert Space $\mathcal{H}$ (RKHS)
 - ▶ Hilbert Space of functions $h : \mathcal{X} \rightarrow \mathbb{R}$ equipped with $\Phi_{\mathcal{H}} : \mathcal{X} \rightarrow \mathcal{H}$ such that:

$$\langle h, \Phi_{\mathcal{H}}(x) \rangle_{\mathcal{H}} = h(x) \forall x \in \mathcal{X}$$

- ▶ Reproducing Kernel of $\mathcal{H}$
 - ▶ $K : \mathcal{X}^2 \rightarrow [0, \infty)$ with:

$$K(x, y) = \langle \Phi_{\mathcal{H}}(x), \Phi_{\mathcal{H}}(y) \rangle_{\mathcal{H}} \forall x, y \in \mathcal{X}$$

[8] proves that you can pick a K first and that as long as K is ‘Symmetric and Positive Semi-Definite’ then there is a RKHS with Reproducing Kernel $\mathcal{H}$.

- ▶ Kernel Mean Embedding (KME)
 - ▶ For $P \in \mathcal{P}(\mathcal{H}) = \{Q \mid -\infty < \int h(x)dQ(x) < \infty \forall h \in \mathcal{H}\}$, μ_P is given by:

$$\mu_P = \int \Phi_{\mathcal{H}}(y)dP(y) \in \mathcal{H}$$

$$\langle \mu_P, \Phi_{\mathcal{H}}(x) \rangle_{\mathcal{H}} = \mu_P(x) = \int \langle \Phi_{\mathcal{H}}(x), \Phi_{\mathcal{H}}(y) \rangle_{\mathcal{H}} dP(y) = \int K(x, y)dP(y) \forall x \in \mathcal{X}$$

Kernel Trickery, pt. 2

For more information – [5], [6], [7]

- ▶ Double Kernel Mean Embedding (DKME)

- ▶ For $P_1, P_2 \in \mathcal{P}(\mathcal{H}) = \{Q \mid -\infty < \int h(x)dQ(x) < \infty \forall h \in \mathcal{H}\}$:

$$\langle \mu_{P_1}, \mu_{P_2} \rangle_{\mathcal{H}} = \iint K(x, y) dP_1(x) dP_2(y) \forall x \in \mathcal{X}$$

- ▶ Characteristic Kernel

- ▶ If the KME is Injective, then the underlying K is 'Characteristic'. The following two kernels are always Characteristic for Positive-Definite R and $n \in \mathbb{Z}_{\geq 0}$:

$$(x, y) \mapsto \exp\left(-\frac{1}{2}(x-y)^\top R^{-1}(x-y)\right), \quad (x, y) \mapsto \frac{n! \left(\sum_{i=0}^n \frac{(n+i)!}{i!(n-i)!} \left(\sqrt{(8n+4)(x-y)^\top R^{-1}(x-y)}\right)^{n-i}\right)}{(2n)! \exp\left(\sqrt{(2n+1)(x-y)^\top R^{-1}(x-y)}\right)}$$

- ▶ Core Kernel of P over $\mathcal{H}$

- ▶ For $P \in \mathcal{P}(\mathcal{H})$, the SPSP $K_P : \mathcal{X}^2 \rightarrow [0, \infty)$ with $K_P(x, y) = \langle \Phi_{\mathcal{H}}(x) - \mu_P, \Phi_{\mathcal{H}}(y) - \mu_P \rangle_{\mathcal{H}} \forall x, y$ satisfies $\int K_P(x, y) dP(y) = 0 \forall x$ and:

$$K_P(x, y) = K(x, y) - \int K(x, b) dP(b) - \int K(a, y) dP(a) + \iint K(a, b) dP(a) dP(b) \forall x, y$$

Maximum Mean Discrepancy

- ▶ For some $\mathcal{F}$ with norm $\|\cdot\|_{\mathcal{F}}$ and $\mathcal{P}(\mathcal{F}) = \{Q \mid \int |f(x)| dQ(x) < \infty \forall f \in \mathcal{F}\}$:

$$\text{MMD}_{\mathcal{F}}(P, Q) = \sup_{f \in \mathcal{F} : \|f\|_{\mathcal{F}} \leq 1} \left| \int f(x) dP(x) - \int f(x) dQ(x) \right| \quad \forall P, Q \in \mathcal{P}(\mathcal{F})$$

- ▶ For a RKHS $\mathcal{H}$ with Characteristic Kernel $K : \mathcal{X}^2 \rightarrow (0, \infty)$, [7] show that:

$$\text{MMD}_{\mathcal{H}}(P, Q) = \|\mu_P - \mu_Q\|_{\mathcal{H}} = 0 \Leftrightarrow \mu_P = \mu_Q \Leftrightarrow P = Q$$

$$\text{MMD}_{\mathcal{H}}(P, R) = \|\mu_P - \mu_R\|_{\mathcal{H}} \leq \|\mu_P - \mu_Q\|_{\mathcal{H}} + \|\mu_Q - \mu_R\|_{\mathcal{H}} = \text{MMD}_{\mathcal{H}}(P, Q) + \text{MMD}_{\mathcal{H}}(Q, R)$$

- ▶ [9] show that:

$$\text{MMD}_{\mathcal{H}}^2(P, Q) = (\text{MMD}_{\mathcal{H}}(P, Q))^2 = \iint K_P(x, y) dQ(x) dQ(y)$$

MMD between model class $P_\theta \in \mathcal{P}(\mathcal{H})$ and data $p_i \sim P^\dagger : 1 \leq i \leq N$ for $P^\dagger \in \mathcal{P}(\mathcal{H})$

$$0 \leq \text{MMD}_{\mathcal{H}}(P_\theta, P^\dagger) \leq \text{MMD}_{\mathcal{H}}\left(P_\theta, \frac{1}{N} \sum_{i=1}^N \delta_{p_i}\right) + \underbrace{\text{MMD}_{\mathcal{H}}\left(\frac{1}{N} \sum_{i=1}^N \delta_{p_i}, P^\dagger\right)}_{\approx 0 \text{ as } N \rightarrow \infty \text{ from [10]}}$$

$$\text{MMD}_{\mathcal{H}}^2\left(P_\theta, \frac{1}{N} \sum_{i=1}^N \delta_{p_i}\right) = \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N K_{P_\theta}(p_i, p_j)$$

We can find $P_\theta \approx P^\dagger$ by taking $N \rightarrow \infty$ and minimising $\frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N K_{P_\theta}(p_i, p_j)$.

$$\text{Then set } T_N = \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N K_{P_\theta}(p_i, p_j)$$

Rundown of the Proposed Framework

$H : \mathbb{R} \rightarrow \{0, 1\}$ is the Heaviside Step Function, and $k > 0$ bounds K from above.

▶ Parametric Bootstrap Configuration.

1. Resample (x_i, y_i) from trained model M times.
2. For the m -th resample, swap out the old sample with the m -th resample in T_n and call it Δ_m .
3. Calculate $\frac{1}{M} \sum_{m=1}^M H(\Delta_m - T_N)$

▶ Wild Bootstrap Configuration, based off [11].

- ▶ Calculate the Gram Matrix of the Core at minimising parameters, then multiply it by N . Call this final matrix G_N .
- ▶ Sample M -many N -dimensional random variables $\{W_m\}_{m=1}^M$ from either $U(\{-1, 1\}^N)$ or $\mathcal{N}(0, \mathbf{1}_N)$. Must all be from the same distribution though!
- ▶ Calculate $\frac{1}{M} \sum_{m=1}^M H(W_m^\top G_N W_m - T_N)$

▶ Concentration Inequality Configuration, based off [12].

- ▶ Calculate $\exp \left(-1 - \frac{\max\{\frac{T_N}{k}, 2\}}{2} + \sqrt{2 \max\left(\left\{\frac{T_N}{k}, 2\right\}\right)} \right)$

Different performances due to different amounts of collected info. **All of them reject eventually.**

Experiments in $\mathcal{P}(\mathcal{Y})$

Model class : $\mathcal{N}(\mu, 1)$ for $\mu \in \mathbb{R}$

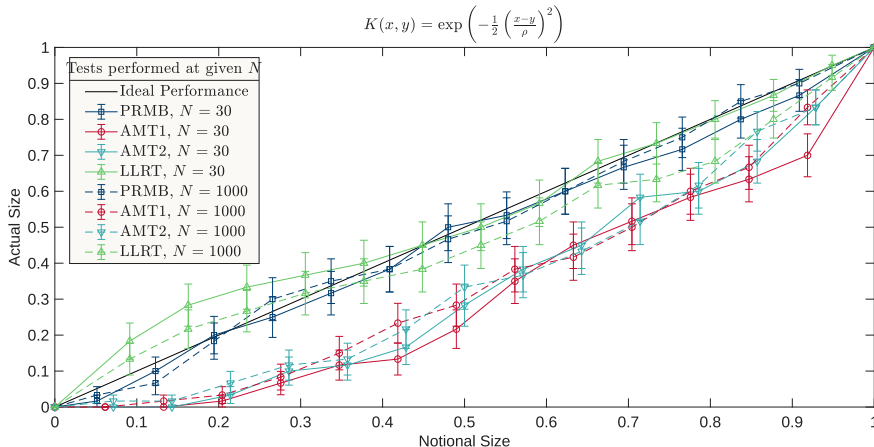
Experiment 1 : Simulate N data i.i.d. according to $\mathcal{N}(1, 1)$. Plot ECDF of calculated significances.

Experiment 2 : Simulate N data i.i.d. according to $\mathcal{N}(1, (1 + c)^2)$ for many $c > 0$. Plot Rejection Probability against c for $p = 0.1$.

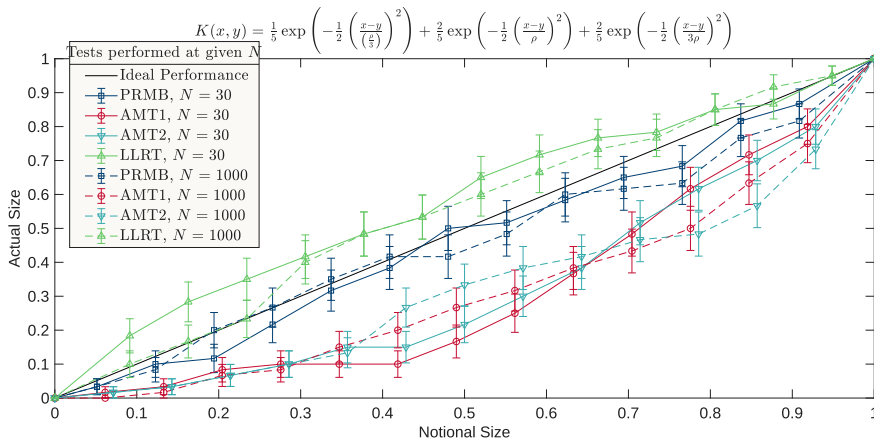
Experiment 3 : Simulate N data i.i.d. according to Skew Normal with mean 1, variance 1 and skew $c > 0$. Plot Rejection Probability against c for $p = 0.1$.

Likelihood Ratio Test will fail Experiment 3. The framework...?

Experiment 1

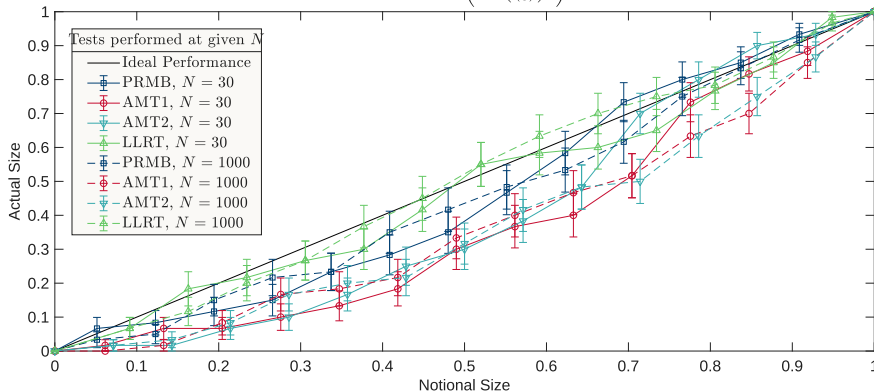


Experiment 1

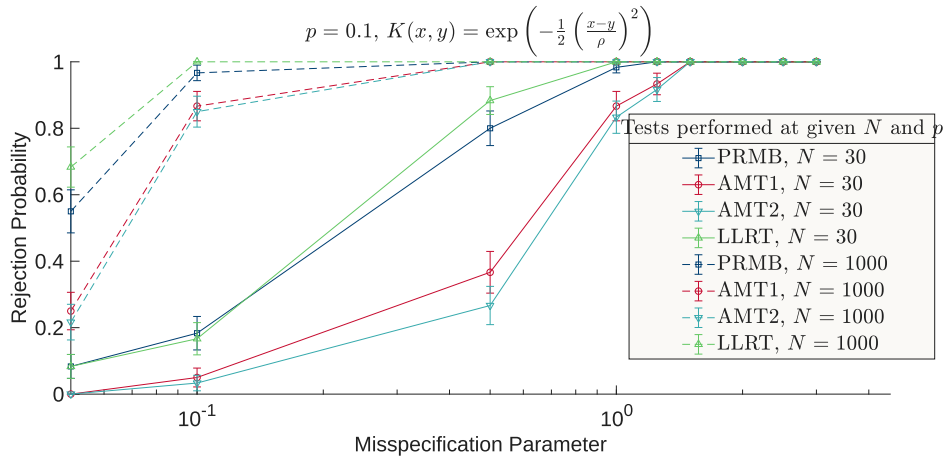


Experiment 1

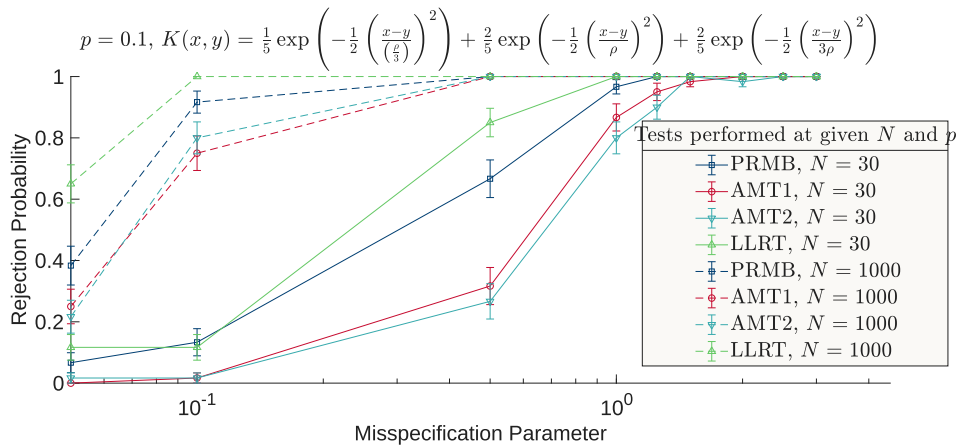
$$K(x, y) = \exp\left(-\frac{1}{2}\left(\frac{x-y}{\left(\frac{\rho}{3}\right)}\right)^2\right)$$



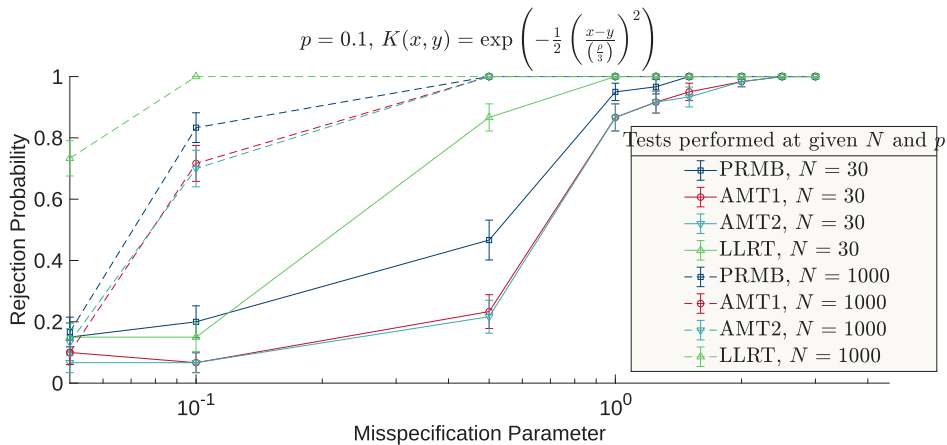
Experiment 2



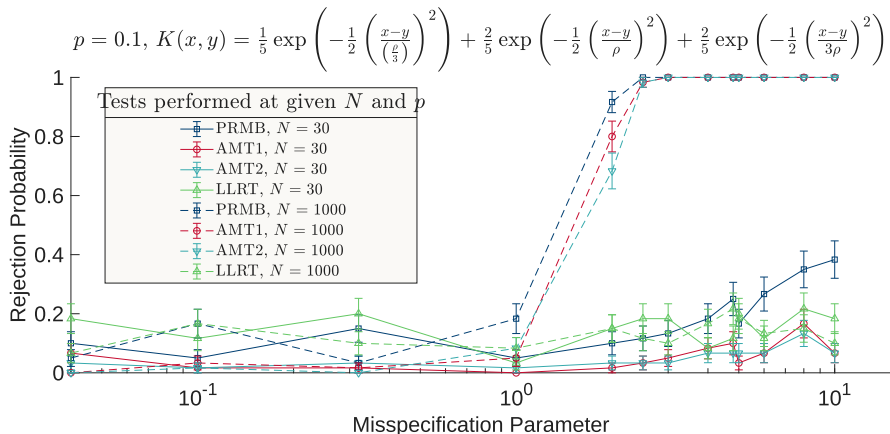
Experiment 2



Experiment 2

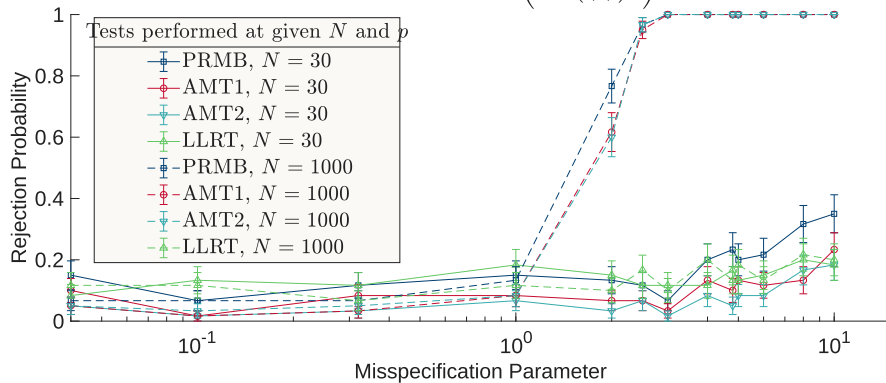


Experiment 3



Experiment 3

$$p = 0.1, K(x, y) = \exp \left(-\frac{1}{2} \left(\frac{x-y}{\left(\frac{p}{3}\right)} \right)^2 \right)$$



MMD between model class $P_\theta \in \mathcal{P}(\mathcal{H})$ and data $p_i \sim P^\dagger : 1 \leq i \leq N$ for $P^\dagger \in \mathcal{P}(\mathcal{H})$

$$0 \leq \text{MMD}_{\mathcal{H}}(P_\theta, P^\dagger) \leq \text{MMD}_{\mathcal{H}}\left(P_\theta, \frac{1}{N} \sum_{i=1}^N \delta_{p_i}\right) + \underbrace{\text{MMD}_{\mathcal{H}}\left(\frac{1}{N} \sum_{i=1}^N \delta_{p_i}, P^\dagger\right)}_{\approx 0 \text{ as } N \rightarrow \infty \text{ from [10]}}$$

$$\text{MMD}_{\mathcal{H}}^2\left(P_\theta, \frac{1}{N} \sum_{i=1}^N \delta_{p_i}\right) = \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N K_{P_\theta}(p_i, p_j)$$

- The Presented Solution's Theory
- The Proposed Framework
- Alquier and Gerber's Contribution

MMD between $P_\theta \in \mathcal{P}(\mathcal{Y}|\mathcal{X})$ and $(x_i, y_i) \sim P^\dagger|P_\mathcal{X} : 1 \leq i \leq N$ for $P^\dagger \in \mathcal{P}(\mathcal{Y}|\mathcal{X})$ using [13].

$$\begin{aligned}
 0 \leq \text{MMD}_{\mathcal{H}_Z} \left(P_\theta | P_\mathcal{X}, P^\dagger | P_\mathcal{X} \right) &\leq \text{MMD}_{\mathcal{H}_Z} \left(P_\theta | \frac{1}{N} \sum_{i=1}^N \delta_{x_i}, \frac{1}{N} \sum_{i=1}^N \delta_{(x_i, y_i)} \right) + \underbrace{\text{MMD}_{\mathcal{H}_Z} \left(\frac{1}{N} \sum_{i=1}^N \delta_{(x_i, y_i)}, P^\dagger | P_\mathcal{X} \right)}_{\approx 0 \text{ as } N \rightarrow \infty \text{ from [10]}} \\
 &\left[\underbrace{\mathcal{X} \times \mathcal{Y} = \mathcal{Z}}_{\text{Joint Sample Space}} \mid \underbrace{K_\mathcal{X} \rightarrow \mathcal{H}_\mathcal{X}}_{\text{Covariate RKHS}} \mid \underbrace{K_\mathcal{X} \otimes K_\mathcal{Y} \rightarrow \mathcal{H}_\mathcal{X} \otimes \mathcal{H}_\mathcal{Y} = \mathcal{H}_Z}_{\text{Joint RKHS}} \right] + \underbrace{C_o \text{MMD}_{\mathcal{H}_\mathcal{X}} \left(\frac{1}{N} \sum_{i=1}^N \delta_{x_i}, P_\mathcal{X} \right)}_{\approx 0 \text{ as } N \rightarrow \infty \text{ from [10]}}
 \end{aligned}$$

$$\text{MMD}_{\mathcal{H}_Z}^2 \left(P_\theta | \frac{1}{N} \sum_{i=1}^N \delta_{x_i}, \frac{1}{N} \sum_{i=1}^N \delta_{(x_i, y_i)} \right) = \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N K_{P_\theta | \frac{1}{N} \sum_{k=1}^N \delta_{x_k}}((x_i, y_i), (x_j, y_j))$$

Next Steps

- ▶ Consistently calculating $\text{MMD}_{\mathcal{H}_{\mathcal{Z}}}^2 \left(P_{\theta} | \frac{1}{N} \sum_{i=1}^N \delta_{x_i}, \frac{1}{N} \sum_{i=1}^N \delta_{(x_i, y_i)} \right)$
 - ▶ $\int K(x, y) dP(y), \iint K(x, y) dP(x) dQ(y)$ range from difficult to calculate perfectly to impossible to calculate perfectly.
 - ▶ Novel contributions to the canon in tracking some of these down.
- ▶ Developing a conditional testing framework
 - ▶ Work with $T_N = N \min_{\theta \in \Theta} \text{MMD}_{\mathcal{H}_{\mathcal{Z}}}^2 \left(P_{\theta} | \frac{1}{N} \sum_{i=1}^N \delta_{x_i}, \frac{1}{N} \sum_{i=1}^N \delta_{(x_i, y_i)} \right)$.

$$P_{\theta} = \mathcal{N}(\theta_1 + \theta_2 x_1 + \theta_3 x_2, 1)$$

Rundown of the Conditional Framework

$H : \mathbb{R} \rightarrow \{0, 1\}$ is the Heaviside Step Function, and $k > 0$ bounds $K_{\mathcal{X}} \otimes K_{\mathcal{Y}}$ from above.

▶ Parametric Bootstrap Configuration.

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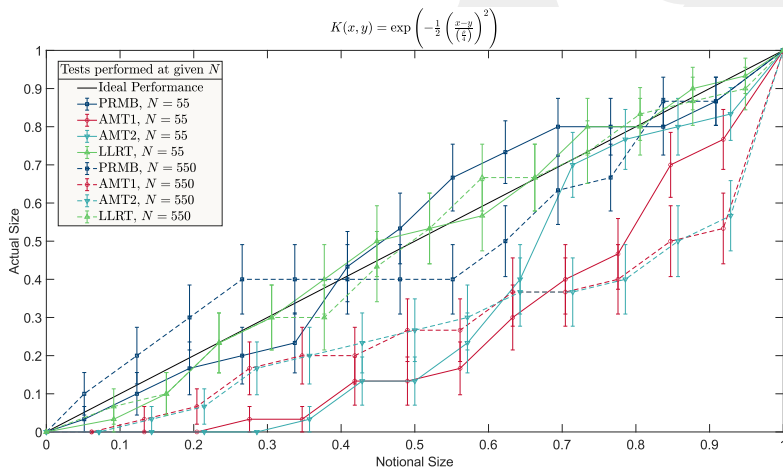
▶ Wild Bootstrap Configuration, based off [11].

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- ▶ Calculate $\frac{1}{M} \sum_{m=1}^M H(W_m^\top G W_m - T_N)$

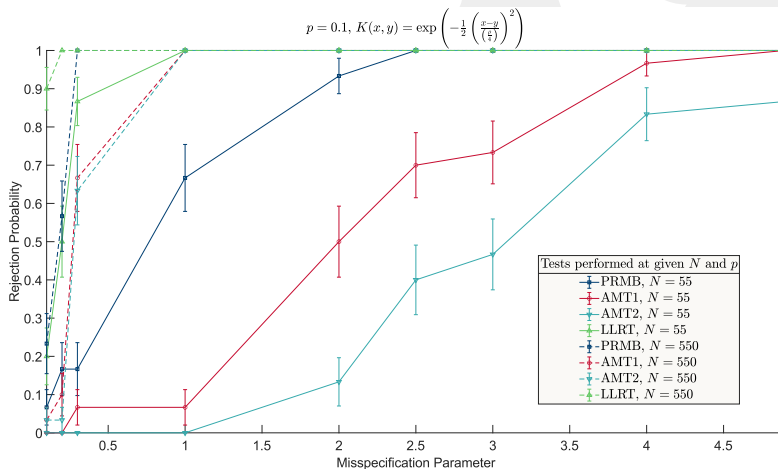
▶ Concentration Inequality Configuration, based off [12].

- ▶ Calculate $\exp \left(-1 - \frac{\max\{\frac{T_N}{k}, 2\}}{2} + \sqrt{2 \max\left(\left\{\frac{T_N}{k}, 2\right\}\right)} \right)$

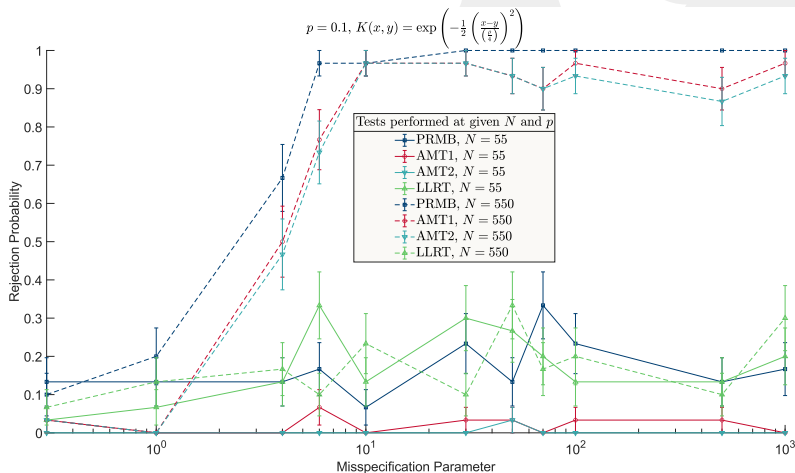
Experiment 1



Experiment 2



Experiment 3



Poisson Gaussian KMEs

For $\lambda, \mu \geq 0$, $\rho > 0$, P_λ distributing $\mathbb{R}$ according to $\text{Po}(\lambda)$ and $K(x, y) = \exp\left(-\frac{1}{2}\left(\frac{x-y}{\rho}\right)^2\right)$, the following holds:

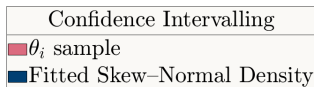
1. $\int K(x, y) dP_\lambda(y)$ is equal to:

$$\frac{\int_{-\infty}^{\infty} \frac{\exp\left(-\frac{1}{2}t^2\right)}{\sqrt{2\pi}} \left(\exp\left(\lambda \exp\left(\frac{x}{\rho^2}\right) \cos\left(\frac{t}{\rho}\right)\right) \cos\left(\lambda \exp\left(\frac{x}{\rho^2}\right) \sin\left(\frac{t}{\rho}\right)\right) \right) dt}{\exp\left(\lambda + \frac{x^2}{2\rho^2}\right)} \quad \forall x.$$

2. $\iint K(x, y) dP_\lambda(x) dP_\mu(y)$ is equal to:

$$\frac{\int_{-\infty}^{\infty} \frac{\exp\left(-\frac{1}{2}t^2\right)}{\sqrt{2\pi}} \left(\exp\left((\lambda + \mu) \cos\left(\frac{t}{\rho}\right)\right) \cos\left((\lambda - \mu) \sin\left(\frac{t}{\rho}\right)\right) \right) dt}{\exp(\lambda + \mu)}.$$

A use case!



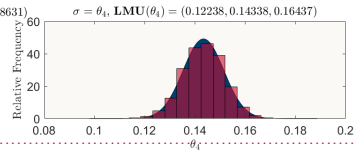
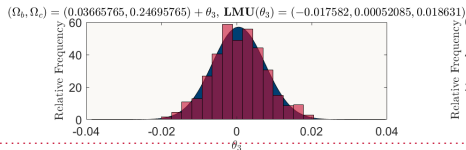
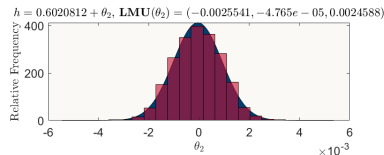
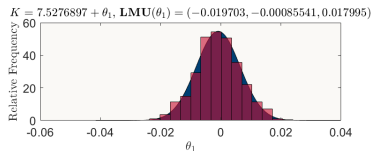
$$K = 7.5268^{+0.01885}_{-0.018847}$$

$$h = 0.60203^{+0.0025064}_{-0.0025064}$$

$$\Omega_b = 0.037178^{+0.01811}_{-0.018103}$$

$$\Omega_c = 0.24748^{+0.01811}_{-0.018103}$$

$$\sigma = 0.14338^{+0.020989}_{-0.021}$$



The END

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