Relative Goodness-of-Fit Tests for Models with Latent Variables

Arthur Gretton



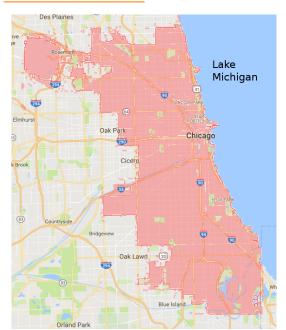


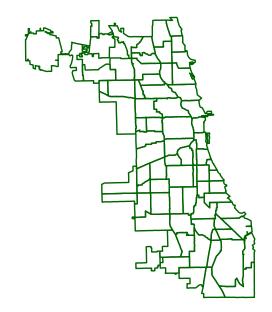


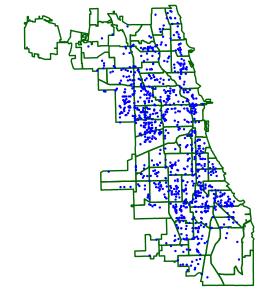


Gatsby Computational Neuroscience Unit, University College London

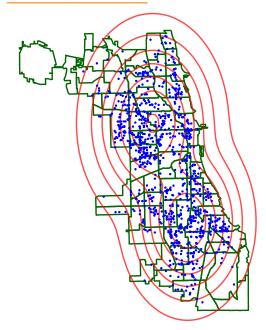
BIRS Stein Workshop, April, 2022







Data = robbery events in Chicago in 2016.



Is this a good model?

"All models are wrong."

G. Box (1976)

Model comparison

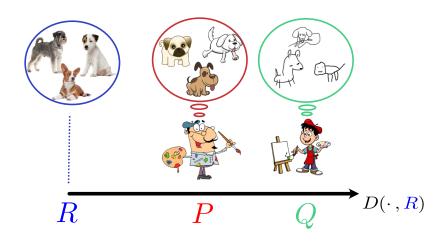
- Have: two candidate models P and Q, and samples $\{x_i\}_{i=1}^n$ from reference distribution R
- Goal: which of *P* and *Q* is better?



P: two components

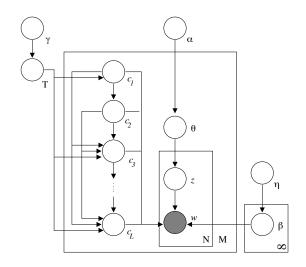
Q: ten components

A relative test of goodness-of-fit



Most interesting models have latent structure

Graphical model representation of hierarchical LDA with a nested CRP prior, Blei et al. (2003)

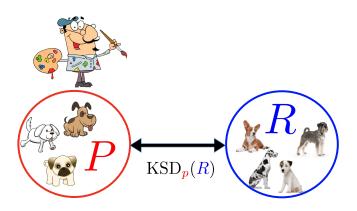


Outline

Relative goodness-of-fit tests for Models with Latent Variables

- The kernel Stein discrepancy
 - Comparing two models via samples: MMD and the witness function.
 - Comparing a sample and a model: Stein modification of the witness class
- Constructing a relative hypothesis test using the KSD
- Relative hypothesis tests with latent variables

- Model P, data $\{x_i\}_{i=1}^n \sim Q$.
- "All models are wrong" $(P \neq Q)$.

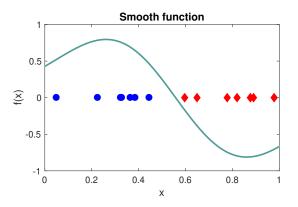


Integral probability metrics

Integral probability metric:

Find a "well behaved function" f(x) to maximize

$$\mathrm{E}_{Q}f(Y)-\mathrm{E}_{P}f(X)$$

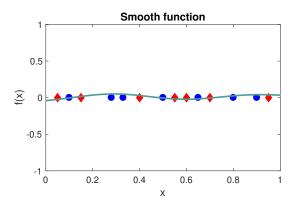


Integral probability metrics

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Find a "well behaved function" f(x) to maximize

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All of kernel methods

Functions are linear combinations of features:

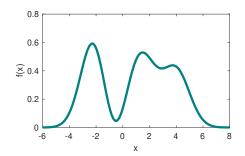
$$f(x) = \langle f, \varphi(x) \rangle_{\mathcal{F}} = \sum_{\ell=1}^{\infty} f_{\ell} \varphi_{\ell}(x) = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{bmatrix}^{\top} \begin{bmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \vdots \\ \varphi_3(x) \end{bmatrix}^{\top}$$

$$\|f\|_{\mathcal{F}}^2 := \sum_{\ell=1}^{\infty} f_{\ell}^2$$

All of kernel methods

"The kernel trick"

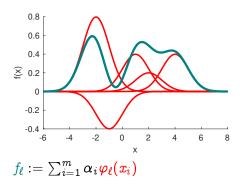
$$egin{aligned} f(oldsymbol{x}) &= \sum_{oldsymbol{\ell}=1}^{\infty} f_{oldsymbol{\ell}} arphi_{oldsymbol{\ell}}(oldsymbol{x}) \ &= \sum_{i=1}^{m} lpha_{i} \underbrace{oldsymbol{k}(oldsymbol{x}_{i}, oldsymbol{x})}_{\langle arphi(oldsymbol{x}_{i}), arphi(oldsymbol{x})
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All of kernel methods

"The kernel trick"

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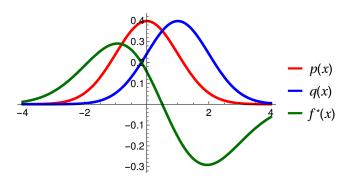


Function of infinitely many features expressed using m coefficients.

MMD: an integral probability metric

Maximum mean discrepancy: smooth function for P vs Q

$$\mathrm{MMD}(\textcolor{red}{P}, \textcolor{blue}{Q}; \mathcal{F}) := \sup_{\|f\|_{\mathcal{F}} \leq 1} \left[\mathrm{E}_{\textcolor{blue}{P}} f(\textcolor{red}{\textbf{\textit{X}}}) - \mathrm{E}_{\textcolor{blue}{Q}} f(\textcolor{red}{\textbf{\textit{Y}}}) \right]$$



MMD: an integral probability metric

Maximum mean discrepancy: smooth function for P vs Q

$$\mathrm{MMD}(extcolor{P}, extcolor{Q}; \mathcal{F}) := \sup_{\|f\|_{\mathcal{F}} \leq 1} \left[\mathbb{E}_{ extcolor{P}} f(extcolor{X}) - \mathbb{E}_{ extcolor{Q}} f(extcolor{Y})
ight]$$

For characteristic RKHS
$$\mathcal{F}$$
, MMD(P , Q ; \mathcal{F}) = 0 iff $P = Q$

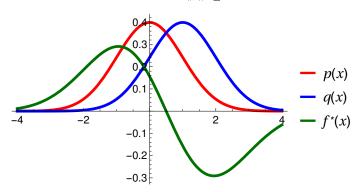
Other choices for witness function class:

- Bounded continuous [Dudley, 2002]
- Bounded variation 1 (Kolmogorov metric) [Müller, 1997]
- 1-Lipschitz (Wasserstein distances) [Dudley, 2002]

Statistical model criticism: toy example

Can we compute MMD with samples from Q and a model P? Problem: usualy can't compute $E_p f$ in closed form.

$$\mathrm{MMD}(extit{ extit{P}}, extit{ extit{Q}}) = \sup_{\|f\|_{\mathcal{F}} \leq 1} [\mathrm{E}_q f - \mathrm{E}_{ extit{ extit{p}}} f]$$



Stein idea

To get rid of $E_{p}f$ in

$$\sup_{\|f\|_{\mathcal{F}} \leq 1} [\mathbf{E}_q f - \mathbf{E}_{\textcolor{red}{p}} f]$$

we use the (1-D) Langevin Stein operator

$$\left[\mathcal{A}_{m{p}}f
ight](x)=rac{1}{m{p}(x)}\,rac{d}{dx}\left(f(x)m{p}(x)
ight)$$

Then

$$\mathbf{E}_{p} \mathcal{A}_{p} f = 0$$

subject to appropriate boundary conditions.

Stein operator

$$\mathcal{A}_{m p} f = rac{1}{m p(x)} \, rac{d}{dx} \left(f(x) m p(x)
ight)$$

$$\mathrm{KSD}_{m{p}}(m{Q}) = \sup_{\|g\|_{\mathcal{F}} \leq 1} \mathrm{E}_{m{q}} \mathcal{A}_{m{p}} g - \mathrm{E}_{m{p}} \mathcal{A}_{m{p}} g$$

Stein operator

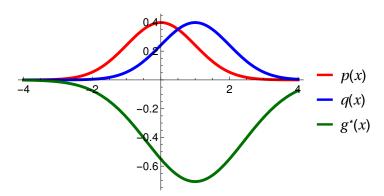
$$\mathcal{A}_{\mathbf{p}}f = rac{1}{\mathbf{p}(x)} \, rac{d}{dx} \left(f(x) \mathbf{p}(x)
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$$\mathrm{KSD}_{\pmb{p}}(Q) = \sup_{\|g\|_{\mathcal{F}} \leq 1} \mathrm{E}_{\pmb{q}} \mathcal{A}_{\pmb{p}} g - \operatorname{\underline{E}}_{\pmb{p}} \mathcal{A}_{\pmb{p}} g = \sup_{\|g\|_{\mathcal{F}} \leq 1} \mathrm{E}_{\pmb{q}} \mathcal{A}_{\pmb{p}} g$$

Stein operator

$$\mathcal{A}_{m p} f = rac{1}{m p(x)} \, rac{d}{dx} \left(f(x) m p(x)
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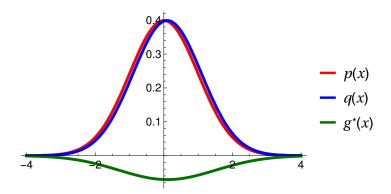
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Stein operator

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Simple expression using kernels

Re-write stein operator as:

$$egin{align} \left[\mathcal{A}_{m{p}}f
ight](x) &= rac{1}{m{p}(x)}\,rac{d}{dx}\left(f(x)m{p}(x)
ight) \ &= f(x)rac{d}{dx}\logm{p}(x) + rac{d}{dx}f(x) \end{split}$$

Can we define "Stein features"?

$$[\mathcal{A}_{p}f](x) = \left(\frac{d}{dx}\log p(x)\right)f(x) + \frac{d}{dx}f(x)$$

$$=: \langle f, \underbrace{\xi(x)}_{\text{stein features}} \rangle_{\mathcal{F}}$$

where $\mathrm{E}_{x\sim p}\xi(x)=0$.

Simple expression using kernels

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ight
angle_{\mathcal{F}} \end{aligned}$$

where $\mathbb{E}_{\boldsymbol{x}\sim p}\boldsymbol{\xi}(\boldsymbol{x})=0$.

The kernel trick for derivatives

Reproducing property for the derivative: for differentiable k(x, x'),

$$rac{d}{dx}f(x) = \left\langle f, rac{d}{dx}arphi(x)
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angle_{\mathcal{F}} \qquad rac{d}{dx}k(x,x') = \left\langle rac{d}{dx}arphi(x), arphi(x')
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ight
angle_{\mathcal{F}}$$

Using kernel derivative trick in (a),

$$\begin{aligned} \left[\mathcal{A}_{p} f \right](x) &= \left(\frac{d}{dx} \log p(x) \right) f(x) + \frac{d}{dx} f(x) \\ &= \left\langle f, \left(\frac{d}{dx} \log p(x) \right) \varphi(x) + \underbrace{\frac{d}{dx} \varphi(x)}_{(a)} \right\rangle_{\mathcal{F}} \\ &=: \left\langle f, \xi(x) \right\rangle_{\mathcal{T}}. \end{aligned}$$

Kernel stein discrepancy: derivation

Closed-form expression for KSD: given independent $x, x' \sim Q$, then

$$egin{aligned} \mathsf{KSD}_{m{p}}(m{Q}) &= \sup_{\|m{g}\|_{m{\mathcal{F}}} \leq 1} \mathrm{E}_{m{x} \sim m{q}}\left(\left[m{\mathcal{A}}_{m{p}}m{g}
ight](m{x})
ight) \ &= \sup_{\|m{g}\|_{m{\mathcal{F}}} \leq 1} \mathrm{E}_{m{x} \sim m{q}}\left\langle m{g}, m{\xi}_{m{x}}
ight
angle_{m{\mathcal{F}}} \ &= \sup_{m{a}} \left\langle m{g}, \mathrm{E}_{m{x} \sim m{q}}m{\xi}_{m{x}}
ight
angle_{m{\mathcal{F}}} = \|\mathrm{E}_{m{x} \sim m{q}}m{\xi}_{m{x}}\|_{m{\mathcal{F}}} \end{aligned}$$

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$$\begin{split} \text{KSD}_{\boldsymbol{p}}(Q) &= \sup_{\|g\|_{\mathcal{F}} \leq 1} \mathbb{E}_{\boldsymbol{x} \sim q} \left(\left[\mathcal{A}_{\boldsymbol{p}} g \right] (\boldsymbol{x}) \right) \\ &= \sup_{\|g\|_{\mathcal{F}} \leq 1} \mathbb{E}_{\boldsymbol{x} \sim q} \left\langle g, \boldsymbol{\xi}_{\boldsymbol{x}} \right\rangle_{\mathcal{F}} \\ &= \sup_{(a)} \left\langle g, \mathbb{E}_{\boldsymbol{x} \sim q} \boldsymbol{\xi}_{\boldsymbol{x}} \right\rangle_{\mathcal{F}} = \left\| \mathbb{E}_{\boldsymbol{x} \sim q} \boldsymbol{\xi}_{\boldsymbol{x}} \right\|_{\mathcal{F}} \end{split}$$

Kernel stein discrepancy: derivation

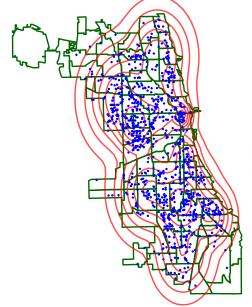
Closed-form expression for KSD: given independent $x, x' \sim Q$, then

$$\begin{split} \text{KSD}_{\pmb{p}}(\textit{Q}) &= \sup_{\|g\|_{\mathcal{F}} \leq 1} \mathbb{E}_{x \sim q} \left(\left[\mathcal{A}_{\pmb{p}} g \right] (x) \right) \\ &= \sup_{\|g\|_{\mathcal{F}} \leq 1} \mathbb{E}_{x \sim q} \left\langle g, \boldsymbol{\xi}_x \right\rangle_{\mathcal{F}} \\ &= \sup_{\substack{(a) \ \|g\|_{\mathcal{F}} \leq 1}} \left\langle g, \mathbb{E}_{x \sim q} \boldsymbol{\xi}_x \right\rangle_{\mathcal{F}} = \|\mathbb{E}_{x \sim q} \boldsymbol{\xi}_x \|_{\mathcal{F}} \end{split}$$

Caution: (a) requires a condition for the Riesz theorem to hold,

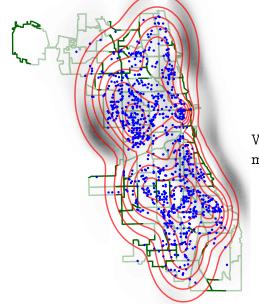
$$\mathrm{E}_{x \sim q} \left(rac{d}{dx} \log p(x)
ight)^2 < \infty.$$

The witness function: Chicago Crime



Model p = 10-component Gaussian mixture.

The witness function: Chicago Crime



Witness function g shows mismatch

Does the Riesz condition matter?

Consider the standard normal,

$$p(x) = rac{1}{\sqrt{2\pi}} \exp\left(-x^2/2
ight).$$

Then

$$rac{d}{dx}\log p(x) = -x.$$

If q is a Cauchy distribution, then the integral

$$\mathbb{E}_{x \sim q} \left(rac{d}{dx} \log p(x)
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is undefined

Does the Riesz condition matter?

Consider the standard normal,

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Kernel stein discrepancy: population expression

Test statistic:

$$ext{KSD}^2_{m p}(Q) = \left\| \operatorname{E}_{x \sim q} m{\xi}_x
ight\|_{\mathcal{F}}^2 = \operatorname{E}_{x,x' \sim Q} h_{m p}(x,x')$$

where

$$egin{aligned} h_{m p}(x,x') &= \mathrm{s}_{m p}(x)^{ op} \mathrm{s}_{m p}(x') k(x,x') + \mathrm{s}_{m p}(x)^{ op} k_2(x,x') \ &+ \mathrm{s}_{m p}(x')^{ op} k_1(x,x') + \mathrm{tr}\left[k_{12}(x,x')
ight] \end{aligned}$$

- lacksquare $\mathbf{s}_{p}(x) \in \mathbb{R}^{D} = rac{
 abla_{p}(x)}{p(x)}$
- $egin{aligned} oldsymbol{\mathbb{R}} k_1(a,b) &:=
 abla_x k(x,x')|_{x=a,x'=b} \in \mathbb{R}^D, \ k_2(a,b) &:=
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Kernel stein discrepancy: population expression

Test statistic:

$$\mathsf{KSD}^2_{\textcolor{red}{p}}(\textcolor{blue}{Q}) = \left\| \mathbb{E}_{x \sim \textcolor{blue}{q}} \textcolor{blue}{\xi_x} \right\|_{\mathcal{F}}^2 = \mathbb{E}_{x, x' \sim \textcolor{blue}{Q}} h_{\textcolor{blue}{p}}(x, x')$$

where

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Kernel stein discrepancy: population expression

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Do not need to normalize p, or sample from it.

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If kernel is C_0 -universal and Q satisfies $\mathbb{E}_{x \sim Q} \left\| \nabla \left(\log \frac{p(x)}{q(x)} \right) \right\|^2 < \infty$, then $KSD_p^2(Q) = 0$ iff P = Q.

KSD for discrete-valued variables

Discrete domains: $\mathcal{X} = \{1, \dots, L\}^D$ with $L \in \mathbb{N}$.

The population KSD (discrete):

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$$k_1(x,x')=\Delta_x^{-1}k(x,x'),\ \Delta_x^{-1}$$
 is difference on $x,\,\mathrm{s}_p(x)=rac{\Delta_p(x)}{p(x)}$

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A discrete kernel:
$$k(x,x')=\exp{(-d_H(x,x'))}$$
, where $d_H(x,x')=D^{-1}\sum_{d=1}^D\mathbb{I}(x_d\neq x_d')$.

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A discrete kernel: $k(x, x') = \exp(-d_H(x, x'))$, where $d_H(x, x') = D^{-1} \sum_{d=1}^{D} \mathbb{I}(x_d \neq x'_d)$.

$$KSD_p^2(Q) = 0 \text{ iff } P = Q \text{ if}$$

- Gram matrix over all the configurations in \mathcal{X} is strictly positive definite,
- \blacksquare P > 0 and Q > 0.

Empirical statistic, asymptotic normality for $P \neq Q$

The empirical statistic:

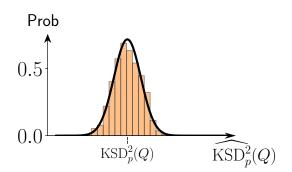
$$\widehat{ ext{KSD}_p^2}(Q) \coloneqq rac{1}{n(n-1)} \sum_{i
eq j} h_p(x_i, x_j).$$

Empirical statistic, asymptotic normality for $P \neq Q$

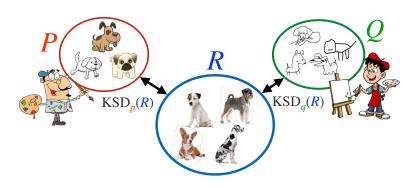
The empirical statistic:

$$\widehat{\mathrm{KSD}^2_p}(Q) := \frac{1}{n(n-1)} \sum_{i \neq j} h_p(x_i, x_j).$$
 Asymptotic distribution when $P \neq Q$:

$$\sqrt{n}\left(\widehat{ ext{KSD}_p^2}(Q) - ext{KSD}_p(Q)
ight) \stackrel{d}{ o} \mathcal{N}(0,\sigma_{h_p}^2) \qquad \sigma_{h_p}^2 = 4 ext{Var}[\mathbb{E}_{x'}[h_p(x,x')]].$$



Relative goodness-of-fit testing



- Two latent variable models P and Q, data $\{x_i\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} R$.
- Distinct models $p \neq q$

Hypotheses:

$$H_0: \mathrm{KSD}_p(R) \leq \mathrm{KSD}_q(R) \text{ vs. } H_1: \mathrm{KSD}_p(R) > \mathrm{KSD}_q(R)$$

($H_0: {}^{\bullet}P$ is as good as Q , or better' vs. $H_1: {}^{\bullet}Q$ is better')

Relative GOF testing: joint asymptotic normality

Joint asymptotic normality when $P \neq R$ and $Q \neq R$

$$\sqrt{n}\left[\begin{array}{c} \widehat{\mathrm{KSD}}_{m{p}}^2(R) - \mathrm{KSD}_{m{p}}(R) \\ \widehat{\mathrm{KSD}}_{m{q}}^2(R) - \mathrm{KSD}_{m{q}}(R) \end{array}
ight] \stackrel{d}{ o} \mathcal{N}\left(\left[egin{array}{c} 0 \ 0 \end{array}
ight], \left[egin{array}{c} \sigma_{h_{m{p}}}^2 & \sigma_{h_{m{p}}h_{m{q}}} \\ \sigma_{h_{m{p}}h_{m{q}}} & \sigma_{h_{m{q}}}^2 \end{array}
ight]
ight)$$

$$\operatorname{KSD}_q^2(R)$$
 $\operatorname{KSD}_q^2(R)$
 $\operatorname{KSD}_p^2(R)$
 $\operatorname{KSD}_p^2(R)$

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Relative GOF testing: joint asymptotic normality

Joint asymptotic normality when $P \neq R$ and $Q \neq R$

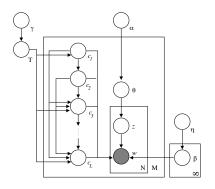
$$\sqrt{n} \left[\begin{array}{c} \widehat{\mathrm{KSD}}_{\pmb{p}}^2(R) - \mathrm{KSD}_{\pmb{p}}(R) \\ \widehat{\mathrm{KSD}}_{\pmb{q}}^2(R) - \mathrm{KSD}_{\pmb{q}}(R) \end{array} \right] \overset{d}{\to} \mathcal{N} \left(\left[\begin{array}{c} 0 \\ 0 \end{array} \right], \left[\begin{array}{cc} \sigma_{h_p}^2 & \sigma_{h_p h_q} \\ \sigma_{h_p h_q} & \sigma_{h_q}^2 \end{array} \right] \right)$$

Difference in statistics is asymptotically normal:

$$egin{split} \sqrt{n} \left[\widehat{ ext{KSD}_{m{p}}^2}(R) - \widehat{ ext{KSD}_q^2}(R) - (ext{KSD}_{m{p}}(R) - ext{KSD}_q(R))
ight] \ & \stackrel{d}{ o} \mathcal{N} \left(0, \sigma_{h_{m{p}}}^2 + \sigma_{h_q}^2 - 2 \sigma_{h_{m{p}} h_q}
ight) \end{split}$$

 \implies a statistical test with null hypothesis $KSD_p(R) - KSD_q(R) \le 0$ is straightforward.

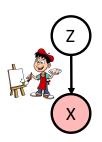
Latent variable models

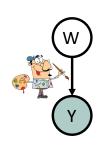


Latent variable models

Can we compare latent variable models with KSD?

$$egin{aligned} oldsymbol{p}(x) &= \int oldsymbol{p}(x|z) p(z) dz \ &q(y) &= \int q(y|w) p(w) dw \end{aligned}$$





Recall multi-dimensional Stein operator:

$$\left[\left.T_{p}f
ight](x)=f(x)rac{\overline{igtriangledown}(x)}{\underline{p(x)}}+\left\langle
abla,f(x)
ight
angle .$$

Expression (a) requires marginal p(x), often intractable...

What not to do

Approximate the integral using $\{z_j\}_{j=1}^m \sim p(z)$:

$$egin{aligned} oldsymbol{p}(x) &= \int oldsymbol{p}(x) oldsymbol{p}(z) oldsymbol{p}(z) dz \ &pprox oldsymbol{p}_{m}(x) &= rac{1}{m} \sum_{j=1}^{m} oldsymbol{p}(x|z_{j}) \end{aligned}$$

Estimate KSD with approxiomate density:

$$\widehat{\mathrm{KSD}^2_p}(R) \approx \widehat{\mathrm{KSD}^2_{p_m}}(R)$$

What not to do

Approximate the integral using $\{z_j\}_{j=1}^m \sim p(z)$:

$$egin{aligned} oldsymbol{p}(x) &= \int oldsymbol{p}(x|z)oldsymbol{p}(z)dz \ &pprox oldsymbol{p}_m(x) &= rac{1}{m}\sum_{j=1}^m oldsymbol{p}(x|z_j) \end{aligned}$$

Estimate KSD with approxiomate density:

$$\widehat{\mathrm{KSD}^2_p}(R) pprox \widehat{\mathrm{KSD}^2_{p_m}}(R)$$

Problem: $\frac{\nabla p_m(x)}{p_m(x)}$ very numerically unstable. Thus $\widehat{\text{KSD}}_{p_m}^2(R)$ has high variance.

MCMC approximation of score function

Result we use:

$$\mathbf{s}_{\textcolor{red}{p}}(x) = \mathbb{E}_{z|x}[\mathbf{s}_{\textcolor{red}{p}}(x|z)]$$

Proof:

$$egin{aligned} \mathbf{s}_{m{p}}(x) &= rac{
abla_{m{p}}(x)}{m{p}(x)} = rac{1}{m{p}(x)} \int
abla_{m{p}}(x|z) \mathrm{d}p(z) \ &= \int rac{
abla_{m{p}}(x|z)}{m{p}(x|z)} \cdot rac{m{p}(x|z) dp(z)}{m{p}(x)} = \mathbb{E}_{z|x}[\mathbf{s}_{m{p}}(x|z)], \end{aligned}$$

Friel, N., Mira, A. and Oates, C. J. (2016) Exploiting multi-core architectures for reduced-variance estimation with intractable likelihoods. Bayesian Analysis, 11, 215–245.

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Approximate intractable posterior $\mathbb{E}_{z|x_i}[\mathbf{s}_p(x_i|z)]$

$$ar{\mathbf{s}}_{oldsymbol{p}}(x_i; z_i^{(t)}) \coloneqq rac{1}{m} \sum_{j=1}^m \mathbf{s}_{oldsymbol{p}}(x_i|z_{i,j}^{(t)}) pprox \mathbf{s}_{oldsymbol{p}}(x_i)$$

with $z_i^{(t)} = (z_{i,1}^{(t)}, \dots, z_{i,m}^{(t)})$ via MCMC (after t burn-in steps)

Friel, N., Mira, A. and Oates, C. J. (2016) Exploiting multi-core architectures for reduced-variance estimation with intractable likelihoods. Bayesian Analysis, 11, 215–245.

KSD for latent variable models

Recall earlier KSD estimate:

$$U_n(extstyle{P}) = rac{1}{n(n-1)} \sum_{i
eq j} h_{ extstyle{p}}(x_i, x_j) \; (pprox ext{KSD}^2_{ extstyle{p}}(R))$$

KSD for latent variable models

Recall earlier KSD estimate:

$$U_n(extstyle{p\over p}) = rac{1}{n(n-1)} \sum_{i
eq j} h_p(x_i,x_j) \; (pprox ext{KSD}^2_{ extstyle{p}}(R))$$

KSD estimate for latent variable models:

$$U_n^{(t)}(extstyle{P}) \coloneqq rac{1}{n(n-1)} \sum_{i
eq j} ar{H}_{m{p}}[(x_i, z_i^{(t)}), (x_j, z_j^{(t)})] \; (pprox \operatorname{KSD}_{m{p}}^2(R))$$

where \bar{H}_p is the Stein kernel h_p with $s_p(x_i)$ replaced with $\bar{s}_p(x_i; z_i^{(t)})$.

Return to relative GOF test, latent variable models

Hypotheses:

```
H_0: \mathrm{KSD}_p(R) \leq \mathrm{KSD}_q(R) \text{ vs. } H_1: \mathrm{KSD}_p(R) > \mathrm{KSD}_q(R)
(H_0: {}^{\prime}P is as good as Q, or better' vs. H_1: {}^{\prime}Q is better')
```

Return to relative GOF test, latent variable models

Hypotheses:

$$H_0: \mathrm{KSD}_{p}(R) \leq \mathrm{KSD}_{q}(R) \text{ vs. } H_1: \mathrm{KSD}_{p}(R) > \mathrm{KSD}_{q}(R)$$

($H_0: {}^{\circ}P$ is as good as Q , or better' vs. $H_1: {}^{\circ}Q$ is better')

Strategy:

■ Estimate the difference $KSD_p^2(R) - KSD_q^2(R)$ by

$$D_n^{(t)}(P,Q) = U_n^{(t)}(P) - U_n^{(t)}(Q).$$

- If $D_n^{(t)}(P,Q)$ is sufficiently large, reject H_0 .
 - "Sufficient": control type-I error (falsely rejecting H_0)
 - Requires the (asymptotic) behaviour of $D_n^{(t)}(P,Q)$

Asymptotic distribution for relative KSD test

Asymptotic distribution of approximate KSD estimate $n, t \to \infty$:

$$\sqrt{n}\left[D_n^{(t)}(extbf{P},Q)-\mu_{ extbf{P}Q}
ight] \stackrel{d}{ o} \mathcal{N}(0,\sigma_{ extbf{P}Q}^2)$$

where

$$\mu_{PQ} = \mathrm{KSD}_p^2(R) - \mathrm{KSD}_q^2(R),$$
 $\sigma_{PQ}^2 = \lim_{n,t \to \infty} n \cdot \mathrm{Var}\left[D_n^{(t)}(P,Q)\right].$

Fine print:

■ The double limit requires fast bias decay $\sqrt{n} [\mathbb{E} \{D_n^{(t)}(P,Q)\} - \mu_{PQ}] \to 0 \ (t \to \infty).$

$$\nabla^{n} = (D_{n} (1, \mathbb{Q})) \quad \mu_{p} = (0, 1, \dots, 1)$$

■ The fourth moment of $\bar{H}_{p}^{(t)} - \bar{H}_{q}^{(t)}$ has finite limit sup. $(t \to \infty)$.

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ightarrow}\mathcal{N}(0,\sigma_{ extbf{P}Q}^2)$$

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$$egin{aligned} \mu_{PQ} &= \mathrm{KSD}_p^2(R) - \mathrm{KSD}_q^2(R), \ \sigma_{PQ}^2 &= \lim_{n,t o \infty} n \cdot \mathrm{Var}\left[D_n^{(t)}(P,Q)
ight]. \end{aligned}$$

Level- α test:

Reject
$$H_0$$
 if $D_n^{(t)}(P,Q) \geq \frac{\hat{\sigma}_{PQ}}{\sqrt{n}}c_{1-\alpha}$

- $c_{1-\alpha}$ is $(1-\alpha)$ -quantile of $\mathcal{N}(0,1)$.
- $\hat{\sigma}_{PQ}$ estimated via jackknife

Experiments

Experiment 1: sensitivity to model difference

■ Data R: Probabilistic Principal Component Analysis PPCA(A):

$$x_i \in \mathbb{R}^{100} \sim \mathcal{N}(Az_i, I), \,\, z_i \in \mathbb{R}^{10} \sim \mathcal{N}(0, I_z)$$

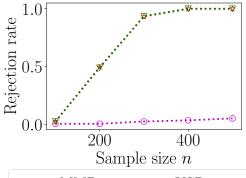
■ Generate P, Q: perturb (1,1)-entry: $A_{\delta} = A + \delta E_{1,1}$

Experiment 1: sensitivity to model difference

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■ Generate P, Q: perturb (1,1)-entry : $A_{\delta} = A + \delta E_{1,1}$



- Alt. H_1 (Q is better):
 - P's perturbation $\delta_P = 2$
 - Q's perturbation $\delta_Q = 1$
- IMQ kernel: $k(x, x') = (1 + ||x x'||_2^2 / \sigma_{\text{med}}^2)^{-1/2}$
- NUTS-HMC with sample size m = 500 (after t = 200 steps).

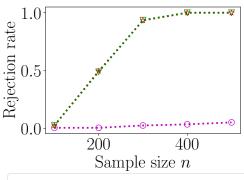
 $\cdots \circ \cdots \quad \text{MMD} \qquad \cdots \star \cdots \quad \text{KSD} \qquad \cdots \overline{} \cdots \overline{} \quad \text{LKSD}$

Experiment 1: sensitivity to model difference

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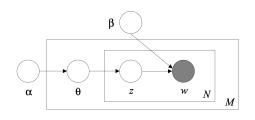
KSD = higher power

- Sample-wise difference in models = subtle (MMD fails)
- Model's information is exploited

···•··· MMD ···•··· KSD ····▼··· LKSD

Experiment 2: topic models for arXiv articles

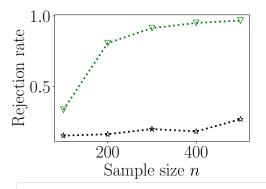
- Data R: arXiv articles from category stat.TH (stat theory):
- Models P, Q: LDAs trained on articles from different categories
 - P: math.PR (math probability theory)
 - Q: stat.ME (stat methodology)



Graphical model of LDA

Experiment 2: topic models for arXiv articles

- Data R: arXiv articles from category stat.TH (stat theory):
- Models P, Q: LDAs trained on articles from different categories (100 topics)
 - P: math.PR (math probability theory)
 - Q: stat.ME (stat methodology)

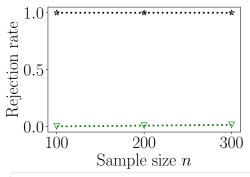


- $\mathcal{X} = \{1, \dots, L\}^D, D = 100,$ L = 126, 190.
- IMQ kernel in BoW rep.: $k(x, x') = (1 + \|B(x) B(x')\|_2^2)^{-1/2}$
- MCMC size m = 5000 (after t = 500 steps).

···*··· MMD (IMQBoW) ····▽··· LKSD (IMQ BoW)

A failure mode

- Data R: arXiv articles from category stat.TH (stat theory):
- Models P, Q: LDAs trained on articles from different categories (100 topics)
 - P: cs.LG (CS machine learning)
 - Q: stat.ME (stat methodology)



- $\mathcal{X} = \{1, \dots, L\}^D, D = 100,$ L = 208, 671.
- IMQ kernel in BoW rep.: $k(x, x') = (1 + \|B(x) B(x')\|_2^2)^{-1/2}$
- MCMC size m = 5000 (after t = 500 steps).

 $\cdots * \cdots \quad \text{MMD (IMQBoW)} \qquad \cdots \\ \overline{} \cdots \qquad \text{LKSD (IMQ BoW)}$

What went wrong?

Recall (one-dimension, informally)

$$\mathrm{s}_p(x) = rac{p(x+1)}{p(x)} - 1$$

Numerical instability arises when

- \blacksquare Observed word x has low probability
- \blacksquare Word next to x in vocabulary has non-negiligible probability

LDA's score = concatenation of 1d-score functions (by conditional independence)

$$egin{aligned} \mathbf{s}_p(x) &= (\mathbf{s}_{p,1}(x), \ldots, \mathbf{s}_{p,d}(x), \ldots, \mathbf{s}_{p,\mathcal{D}}(x)) \ \end{aligned}$$
 where $\mathbf{s}_{p,d}(x) = \mathbb{E}_{z^d|x}[\mathbf{s}_p(x^d|z^d)] = \mathbb{E}_{z^d|x}\left[rac{p(x^d+1|z^d,oldsymbol{eta})}{p(x^d|z^d,oldsymbol{eta})}
ight] - 1$

 \Rightarrow Higher chance of instability

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ight] - 1$$

 \Rightarrow Higher chance of instability

Observations on the sampler

Requirements on n and t

The KSD difference estimate $D_n^{(t)}(P,Q)$ is biased for finite t:

$$\mathbb{E}[D_n^{(t)}(P,Q)] \neq \mu_{P,Q} \coloneqq \mathrm{KSD}_p^2(R) - \mathrm{KSD}_q^2(R)$$

If the bias decay is slower than \sqrt{n} , i.e.,

$$\sqrt{n}\underbrace{\left(\mathbb{E}[D_n^{(t)}(\textcolor{red}{P},\textcolor{blue}{Q})]-\mu_{\textcolor{blue}{P},\textcolor{blue}{Q}}\right)}_{\text{bias}(t)\downarrow 0} \nrightarrow 0,$$

then, the asymptotic normality around $\mu_{P,Q}$ does not hold:

$$\sqrt{n}\left[D_n^{(t)}(\red{P}, \red{Q}) - \mu_{\red{P} \red{Q}}
ight] \overset{d}{
ightarrow} \mathcal{N}(0, \sigma_{\red{P} \red{Q}}^2).$$

How important is the quality of $\frac{1}{m} \sum_{j=1}^{m} \mathbf{s}_{p}(x|z_{j}^{(t)})$? Experiment with PPCA:

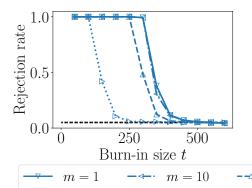
- P: MALA with a bad step size (poor sampler)
- Q: NUTS-HMC (good sampler)

Expectation:

If poor, the test would reject even if P and Q are equally good

How important is the quality of $\frac{1}{m} \sum_{j=1}^{m} s_{p}(x|z_{j}^{(t)})$? Experiment with PPCA:

- \blacksquare P: MALA with a bad step size (poor sampler)
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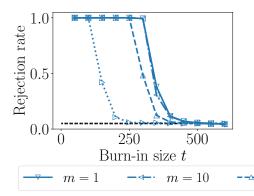
- Null H_0 (should not reject)
- Significance level $\alpha = 0.05$
- Sample size n = 100

m = 100

m = 1000

How important is the quality of $\frac{1}{m} \sum_{j=1}^{m} s_p(x|z_j^{(t)})$? Experiment with PPCA:

- P: MALA with a bad step size (poor sampler)
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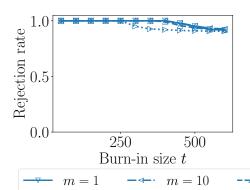
Sufficient burn-in

→ correct type-I error

$$m = 1000$$

How important is the quality of $\frac{1}{m} \sum_{j=1}^{m} s_p(x|z_j^{(t)})$? Experiment with PPCA:

- P: MALA with a bad step size (poor sampler)
- Q: NUTS-HMC (good sampler)



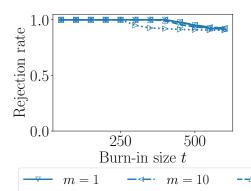
- Null H_0 (should not reject)
- Significance level $\alpha = 0.05$
- Sample size n = 300

m = 100

m = 1000

How important is the quality of $\frac{1}{m} \sum_{j=1}^{m} s_p(x|z_j^{(t)})$? Experiment with PPCA:

- \blacksquare P: MALA with a bad step size (poor sampler)
- Q: NUTS-HMC (good sampler)



- Null H_0 (should not reject)
- Significance level $\alpha = 0.05$
- Sample size n = 300

m = 100

 $\left\{ egin{array}{ll} {
m Larger} \ n \implies {
m more} \ {
m sensitive to mismatch} \end{array}
ight.$

... p ... m = 1000

References

A Kernel Test of Goodness of Fit Kacper Chwialkowski, Heiko Strathmann, Arthur Gretton https://arxiv.org/abs/1602.02964

A Kernel Stein Test for Comparing Latent Variable Models Heishiro Kanagawa, Wittawat Jitkrittum, Lester Mackey, Kenji Fukumizu, Arthur Gretton

https://arxiv.org/abs/1907.00586

Questions?

