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

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## Model Criticism



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## Model Criticism



Data $=$ robbery events in Chicago in 2016.

## Model Criticism



Is this a good model?

## Model Criticism

"All models are wrong."
G. Box (1976)

## Model comparison

- Have: two candidate models $P$ and $Q$, and samples $\left\{x_{i}\right\}_{i=1}^{n}$ 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

## Kernel Stein Discrepancy

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


## Integral probability metrics

Integral probability metric:
Find a "well behaved function" $f(x)$ to maximize

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



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## All of kernel methods

Functions are linear combinations of features:

## All of kernel methods

"The kernel trick"

$$
f(x)=\sum_{\ell=1}^{\infty} f_{\ell} \varphi_{\ell}(x)
$$



## All of kernel methods

"The kernel trick"

$$
\begin{aligned}
f(x) & =\sum_{\ell=1}^{\infty} f_{\ell} \varphi_{\ell}(x) \\
& =\sum_{i=1}^{m} \alpha_{i} \underbrace{k\left(x_{i}, x\right)}_{\left\langle\varphi\left(x_{i}\right), \varphi(x)\right\rangle_{\mathcal{F}}}
\end{aligned}
$$



Function of infinitely many features expressed using $m$ coefficients.

## MMD: an integral probability metric

Maximum mean discrepancy: smooth function for $P$ vs $Q$

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



## MMD: an integral probability metric

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

For characteristic RKHS $\mathcal{F}, \operatorname{MMD}(P, Q ; \mathcal{F})=0$ 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 $\mathrm{E}_{p} f$ in closed form.

$$
\operatorname{MMD}(P, Q)=\sup _{\|f\|_{\mathcal{F}} \leq 1}\left[\mathrm{E}_{q} f-\mathrm{E}_{p} f\right]
$$



## Stein idea

To get rid of $\mathrm{E}_{p} f$ in

$$
\sup _{\|f\|_{\mathcal{F} \leq 1}}\left[\mathrm{E}_{q} f-\mathrm{E}_{p} f\right]
$$

we use the (1-D) Langevin Stein operator

$$
\left[\mathcal{A}_{p} f\right](x)=\frac{1}{p(x)} \frac{d}{d x}(f(x) p(x))
$$

Then

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

subject to appropriate boundary conditions.

## Kernel Stein Discrepancy

Stein operator

$$
\mathcal{A}_{p} f=\frac{1}{p(x)} \frac{d}{d x}(f(x) p(x))
$$

Kernel Stein Discrepancy (KSD)

$$
\mathrm{KSD}_{p}(Q)=\sup _{\|g\|_{\mathcal{F}} \leq 1} \mathrm{E}_{q} \mathcal{A}_{p} g-\mathrm{E}_{p} \mathcal{A}_{p} g
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## Simple expression using kernels

Re-write stein operator as:

$$
\begin{aligned}
{\left[\mathcal{A}_{p} f\right](x) } & =\frac{1}{p(x)} \frac{d}{d x}(f(x) p(x)) \\
& =f(x) \frac{d}{d x} \log p(x)+\frac{d}{d x} f(x)
\end{aligned}
$$

Can we define "Stein features"?

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

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{\left[\mathcal{A}_{p} f\right](x) } & =\left(\frac{d}{d x} \log p(x)\right) f(x)+\frac{d}{d x} f(x) \\
& =:\langle f, \underbrace{\xi(x)}_{\text {stein features }}\rangle_{\mathcal{F}}
\end{aligned}
$$

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

## The kernel trick for derivatives

Reproducing property for the derivative: for differentiable $k\left(x, x^{\prime}\right)$,

$$
\frac{d}{d x} f(x)=\left\langle f, \frac{d}{d x} \varphi(x)\right\rangle_{\mathcal{F}} \quad \frac{d}{d x} k\left(x, x^{\prime}\right)=\left\langle\frac{d}{d x} \varphi(x), \varphi\left(x^{\prime}\right)\right\rangle_{\mathcal{F}}
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Using kernel derivative trick in (a),

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

## Kernel stein discrepancy: derivation

Closed-form expression for KSD: given independent $x, x^{\prime} \sim Q$, then

$$
\operatorname{KSD}_{p}(Q)=\sup _{\|g\|_{\mathcal{F}} \leq 1} \mathrm{E}_{x \sim q}\left(\left[\mathcal{A}_{p} g\right](x)\right)
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& =\sup _{\|g\|_{\mathcal{F} \leq 1}} \mathrm{E}_{x \sim q}\left\langle g, \xi_{x}\right\rangle_{\mathcal{F}} \\
& =\sup _{(a)}\left\langle g \|_{\mathcal{F} \leq 1}\right.
\end{aligned}
$$

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

$$
\mathrm{E}_{x \sim q}\left(\frac{d}{d x} \log p(x)\right)^{2}<\infty
$$

## 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,

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

Then

$$
\frac{d}{d x} \log p(x)=-x
$$

## If $q$ is a Cauchy distribution, then the integral


is undefined.

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Then

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$$

If $q$ is a Cauchy distribution, then the integral

$$
\mathrm{E}_{x \sim q}\left(\frac{d}{d x} \log p(x)\right)^{2}=\int_{-\infty}^{\infty} x^{2} q(x) d x
$$

is undefined.

## Kernel stein discrepancy: population expression

Test statistic:

$$
\operatorname{KSD}_{p}^{2}(Q)=\left\|\mathrm{E}_{x \sim q} \xi_{x}\right\|_{\mathcal{F}}^{2}=\mathrm{E}_{x, x^{\prime} \sim Q} h_{p}\left(x, x^{\prime}\right)
$$

where

$$
\begin{array}{r}
h_{p}\left(x, x^{\prime}\right)=\mathrm{s}_{p}(x)^{\top} \mathrm{s}_{p}\left(x^{\prime}\right) k\left(x, x^{\prime}\right)+\mathrm{s}_{p}(x)^{\top} k_{2}\left(x, x^{\prime}\right) \\
+\mathrm{s}_{p}\left(x^{\prime}\right)^{\top} k_{1}\left(x, x^{\prime}\right)+\operatorname{tr}\left[k_{12}\left(x, x^{\prime}\right)\right]
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■ $\mathbf{s}_{p}(x) \in \mathbb{R}^{D}=\frac{\nabla p(x)}{p(x)}$

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- $\mathbf{s}_{p}(x) \in \mathbb{R}^{D}=\frac{\nabla p(x)}{p(x)}$

■ $k_{1}(a, b):=\left.\nabla_{x} k\left(x, x^{\prime}\right)\right|_{x=a, x^{\prime}=b} \in \mathbb{R}^{D}$,
$k_{2}(a, b):=\left.\nabla_{x^{\prime}} k\left(x, x^{\prime}\right)\right|_{x=a, x^{\prime}=b} \in \mathbb{R}^{D}$,
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- $\mathrm{s}_{p}(x) \in \mathbb{R}^{D}=\frac{\nabla p(x)}{p(x)}$
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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 $\mathrm{E}_{x \sim Q}\left\|\nabla\left(\log \frac{p(x)}{q(x)}\right)\right\|^{2}<\infty$, then $\operatorname{KSD}_{p}^{2}(Q)=0$ iff $P=Q$.

## KSD for discrete-valued variables

Discrete domains: $\mathcal{X}=\{1, \ldots, L\}^{D}$ with $L \in \mathbb{N}$.
The population KSD (discrete):

$$
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-\mathrm{s}_{p}\left(x^{\prime}\right)^{\top} k_{1}\left(x, x^{\prime}\right)+\operatorname{tr}\left[k_{12}\left(x, x^{\prime}\right)\right]
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$$

$k_{1}\left(x, x^{\prime}\right)=\Delta_{x}^{-1} k\left(x, x^{\prime}\right), \Delta_{x}^{-1}$ is difference on $x, \mathrm{~s}_{p}(x)=\frac{\Delta p(x)}{p(x)}$

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A discrete kernel: $k\left(x, x^{\prime}\right)=\exp \left(-d_{H}\left(x, x^{\prime}\right)\right)$, where $d_{H}\left(x, x^{\prime}\right)=D^{-1} \sum_{d=1}^{D} \mathbb{I}\left(x_{d} \neq x_{d}^{\prime}\right)$.

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$\operatorname{KSD}_{p}^{2}(Q)=0$ iff $P=Q$ if

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

Empirical statistic, asymptotic normality for $P \neq Q$
The empirical statistic:

$$
\widehat{\mathrm{KSD}_{p}^{2}}(Q):=\frac{1}{n(n-1)} \sum_{i \neq j} h_{p}\left(x_{i}, x_{j}\right)
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## Empirical statistic, asymptotic normality for $P \neq Q$

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$$

Asymptotic distribution when $P \neq Q$ :
$\sqrt{n}\left(\widehat{\mathrm{KSD}_{p}^{2}}(Q)-\mathrm{KSD}_{p}(Q)\right) \xrightarrow{d} \mathcal{N}\left(0, \sigma_{h_{p}}^{2}\right) \quad \sigma_{h_{p}}^{2}=4 \operatorname{Var}\left[\mathbb{E}_{x^{\prime}}\left[h_{p}\left(x, x^{\prime}\right)\right]\right]$.


## Relative goodness-of-fit testing



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

Hypotheses:

$$
\begin{aligned}
& H_{0}: \operatorname{KSD}_{p}(R) \leq \mathrm{KSD}_{q}(R) \text { vs. } H_{1}: \mathrm{KSD}_{p}(R)>\operatorname{KSD}_{q}(R) \\
& \left(H_{0}: ' P \text { is as good as } Q, \text { or better' vs. } H_{1}: \text { ' } Q \text { is better' }\right)
\end{aligned}
$$

## Relative GOF testing: joint asymptotic normality

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


## Relative GOF testing: joint asymptotic normality

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

$$
\sqrt{n}\left[\frac{\mathrm{KSD}_{p}^{2}}{}(R)-\mathrm{KSD}_{p}(R)\right] \stackrel{d}{\mathrm{KSD}_{q}^{2}}(R)-\mathrm{KSD}_{q}(R) ~\left(\left[\begin{array}{l}
0 \\
0
\end{array}\right],\left[\begin{array}{cc}
\sigma_{h_{p}}^{2} & \sigma_{h_{p} h_{q}} \\
\sigma_{h_{p} h_{q}} & \sigma_{h_{q}}^{2}
\end{array}\right]\right)
$$

Difference in statistics is asymptotically normal:

$$
\begin{aligned}
& \sqrt{n}\left[\widehat{\mathrm{KSD}_{p}^{2}}(R)-\widehat{\mathrm{KSD}_{q}^{2}}(R)-\left(\mathrm{KSD}_{p}(R)-\mathrm{KSD}_{q}(R)\right)\right] \\
& \xrightarrow{d} \mathcal{N}\left(0, \sigma_{h_{p}}^{2}+\sigma_{h_{q}}^{2}-2 \sigma_{h_{p} h_{q}}\right)
\end{aligned}
$$

$\Longrightarrow$ a statistical test with null hypothesis $\operatorname{KSD}_{p}(R)-\operatorname{KSD}_{q}(R) \leq 0$ is straightforward.

## Latent variable models



## Latent variable models

Can we compare latent variable models with KSD?

$$
\begin{aligned}
& p(x)=\int p(x \mid z) p(z) d z \\
& q(y)=\int q(y \mid w) p(w) d w
\end{aligned}
$$



Recall multi-dimensional Stein operator:

$$
\left[T_{p} f\right](x)=f(x) \underbrace{\frac{\nabla p(x)}{p(x)}}_{(a)}+\langle\nabla, f(x)\rangle .
$$

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

## What not to do

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

$$
\begin{aligned}
& p(x)=\int p(x \mid z) p(z) d z \\
& \approx p_{m}(x)=\frac{1}{m} \sum_{j=1}^{m} p\left(x \mid z_{j}\right)
\end{aligned}
$$

Estimate KSD with approxiomate density:

$$
\widehat{\mathrm{KSD}_{p}^{2}}(R) \approx \widehat{\mathrm{KSD}_{p_{m}}^{2}}(R)
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Estimate KSD with approxiomate density:

$$
\widehat{\mathrm{KSD}_{p}^{2}}(R) \approx \widehat{\mathrm{KSD}_{p_{m}}^{2}}(R)
$$

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

## MCMC approximation of score function

Result we use:

$$
\mathrm{s}_{p}(x)=\mathbb{E}_{z \mid x}\left[\mathrm{~s}_{p}(x \mid z)\right]
$$

Proof:

$$
\begin{aligned}
\mathrm{s}_{p}(x)=\frac{\nabla p(x)}{p(x)} & =\frac{1}{p(x)} \int \nabla p(x \mid z) \mathrm{d} p(z) \\
& =\int \frac{\nabla p(x \mid z)}{p(x \mid z)} \cdot \frac{p(x \mid z) d p(z)}{p(x)}=\mathbb{E}_{z \mid x}\left[\mathrm{~s}_{p}(x \mid z)\right]
\end{aligned}
$$

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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\begin{aligned}
\mathrm{s}_{p}(x)=\frac{\nabla p(x)}{p(x)} & =\frac{1}{p(x)} \int \nabla p(x \mid z) \mathrm{d} p(z) \\
& =\int \frac{\nabla p(x \mid z)}{p(x \mid z)} \cdot \frac{p(x \mid z) d p(z)}{p(x)}=\mathbb{E}_{z \mid x}\left[\mathrm{~s}_{p}(x \mid z)\right]
\end{aligned}
$$

Approximate intractable posterior $\mathbb{E}_{z \mid x_{i}}\left[\mathrm{~s}_{p}\left(x_{i} \mid z\right)\right]$

$$
\overline{\mathrm{s}}_{p}\left(x_{i} ; z_{i}^{(t)}\right):=\frac{1}{m} \sum_{j=1}^{m} \mathrm{~s}_{p}\left(x_{i} \mid z_{i, j}^{(t)}\right) \approx \mathrm{s}_{p}\left(x_{i}\right)
$$

with $z_{i}^{(t)}=\left(z_{i, 1}^{(t)}, \ldots, z_{i, m}^{(t)}\right)$ 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}(P)=\frac{1}{n(n-1)} \sum_{i \neq j} h_{p}\left(x_{i}, x_{j}\right)\left(\approx \mathrm{KSD}_{p}^{2}(R)\right)
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KSD estimate for latent variable models:

$$
U_{n}^{(t)}(P):=\frac{1}{n(n-1)} \sum_{i \neq j} \bar{H}_{p}\left[\left(x_{i}, z_{i}^{(t)}\right),\left(x_{j}, z_{j}^{(t)}\right)\right]\left(\approx \operatorname{KSD}_{p}^{2}(R)\right)
$$

where $\bar{H}_{p}$ is the Stein kernel $h_{p}$ with $\mathbf{s}_{p}\left(x_{i}\right)$ replaced with $\overline{\mathbf{s}}_{p}\left(x_{i} ; z_{i}^{(t)}\right)$.

## Return to relative GOF test, latent variable models

Hypotheses:
$H_{0}: \operatorname{KSD}_{p}(R) \leq \operatorname{KSD}_{q}(R)$ vs. $H_{1}: \operatorname{KSD}_{p}(R)>\operatorname{KSD}_{q}(R)$
( $H_{0}$ : ' $P$ is as good as $Q$, or better' vs. $H_{1}$ : ' $Q$ is better')

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\end{aligned}
$$

## Strategy:

■ Estimate the difference $\operatorname{KSD}_{p}^{2}(R)-\operatorname{KSD}_{q}^{2}(R)$ 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 $n, t \rightarrow \infty$ :

$$
\sqrt{n}\left[D_{n}^{(t)}(P, Q)-\mu_{P Q}\right] \xrightarrow{d} \mathcal{N}\left(0, \sigma_{P Q}^{2}\right)
$$

where

$$
\begin{aligned}
\mu_{P Q} & =\operatorname{KSD}_{p}^{2}(R)-\operatorname{KSD}_{q}^{2}(R) \\
\sigma_{P Q}^{2} & =\lim _{n, t \rightarrow \infty} n \cdot \operatorname{Var}\left[D_{n}^{(t)}(P, Q)\right]
\end{aligned}
$$

Fine print:
■ The double limit requires fast bias decay
$\sqrt{n}\left[\mathbb{E}\left\{D_{n}^{(t)}(P, Q)\right\}-\mu_{P Q}\right] \rightarrow 0(t \rightarrow \infty)$.

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


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\end{aligned}
$$

Level $\alpha$ test:

$$
\text { Reject } H_{0} \text { if } D_{n}^{(t)}(P, Q) \geq \frac{\hat{\sigma}_{P Q}}{\sqrt{n}} c_{1-\alpha}
$$

- $c_{1-\alpha}$ is $(1-\alpha)$-quantile of $\mathcal{N}(0,1)$.

■ $\hat{\sigma}_{P Q}$ estimated via jackknife

## Experiments

## Experiment 1: sensitivity to model difference

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

$$
x_{i} \in \mathbb{R}^{100} \sim \mathcal{N}\left(A z_{i}, I\right), z_{i} \in \mathbb{R}^{10} \sim \mathcal{N}\left(0, I_{z}\right)
$$

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

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Sample size $n$

- Alt. $H_{1}$ ( $Q$ is better):
- $P$ 's perturbation $\delta_{P}=2$
- $Q$ 's perturbation $\delta_{Q}=1$

■ IMQ kernel: $k\left(x, x^{\prime}\right)=$ $\left(1+\left\|x-x^{\prime}\right\|_{2}^{2} / \sigma_{\text {med }}^{2}\right)^{-1 / 2}$
■ NUTS-HMC with sample size $m=500$ (after $t=200$ steps).
…… MMD ...ж... KSD ...ж... LKSD

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


$$
\mathrm{KSD}=\text { higher power }
$$

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

$$
\cdots \text { … } \operatorname{MMD} \quad \cdots \cdots \quad \text { KSD } \cdots \neq \cdots \quad \text { LKSD }
$$

## 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

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■ Data $R$ : arXiv articles from category stat.TH (stat theory) :
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## 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)



## What went wrong?

Recall (one-dimension, informally)

$$
\mathrm{s}_{p}(x)=\frac{p(x+1)}{p(x)}-1
$$

Numerical instability arises when

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

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

$$
\mathrm{s}_{p}(x)=\left(\mathrm{s}_{p, 1}(x), \ldots, \mathrm{s}_{p, d}(x), \ldots, \mathrm{s}_{p, D}(x)\right)
$$

$$
\text { where } \mathrm{s}_{p, d}(x)=\mathbb{E}_{z^{d} \mid x}\left[\mathrm{~s}_{p}\left(x^{d} \mid z^{d}\right)\right]=\mathbb{E}_{z^{d} \mid x}\left[\frac{p\left(x^{d}+1 \mid z^{d}, \beta\right)}{p\left(x^{d} \mid z^{d}, \beta\right)}\right]
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\end{aligned}
$$

$\Rightarrow$ 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 $t$ :

$$
\mathbb{E}\left[D_{n}^{(t)}(P, Q)\right] \neq \mu_{P, Q}:=\operatorname{KSD}_{p}^{2}(R)-\operatorname{KSD}_{q}^{2}(R)
$$

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

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

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

$$
\sqrt{n}\left[D_{n}^{(t)}(P, Q)-\mu_{P Q}\right] \stackrel{d}{\rightarrow} \mathcal{N}\left(0, \sigma_{P Q}^{2}\right) .
$$

## Poor MCMC hurts the test

How important is the quality of $\frac{1}{m} \sum_{j=1}^{m} \mathrm{~s}_{p}\left(x \mid z_{j}^{(t)}\right)$ ?
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

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$$
\longrightarrow m=1 \quad-\leftrightarrow m=10 \quad-\leadsto-m=100 \quad \cdots \triangleright \cdots \quad m=1000
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■ Null $H_{0}$ (should not reject)
■ Significance level $\alpha=0.05$
■ Sample size $n=100$

## Sufficient burn-in

$\rightarrow$ correct type-I error

$$
\multimap m=1 \quad-\leftrightarrow m=10 \quad-\sim-\quad m=100 \quad \cdots>\cdots \quad m=1000
$$

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■ Significance level $\alpha=0.05$

- Sample size $n=300$

$$
\sqcap m=1 \quad-\varangle \sim m=10 \quad-\Perp-m=100 \quad \cdots \triangleright \cdots \quad m=1000
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$$
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$$

## References

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

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https://arxiv.org/abs/1907. 00586

## Questions?



