Kernel tests of goodness-of-fit using Stein’s method

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Model Criticism
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Data = robbery events in Chicago in 2016.
Is this a good model?
Goals: Test if a (complicated) model fits the data.
Outline

- The kernel Stein discrepancy  
  Chwialkowski, Strathmann, G. ICML 2016
  - Comparing two models via samples: MMD and the witness function.
  - Comparing a sample and a model: Stein modification of the witness class

- A Linear-Time Kernel Goodness-of-Fit Test  
  Jitkrittum, Xu, Szabo, Fukumizu, G. NeurIPS 2017
  - Features learned to maximise (estimate of) test power
  - Better asymptotic relative efficiency vs a “naive” linear time test

- Relative hypothesis tests with latent variables  
  Kanagawa, Jitkrittum, Mackey, Fukumizu, G. 2019
Integral probability metrics

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

$$E_Q f(Y) - E_P f(X)$$
Integral probability metrics

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The MMD: an integral probability metric

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

\[
MMD(P, Q; \mathcal{F}) := \sup_{\|f\|_{\mathcal{F}} \leq 1} \left[ E_Q f(Y) - E_P f(X) \right]
\]
The MMD: an integral probability metric

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

$$MMD(P, Q; \mathcal{F}) := \sup_{\|f\|_\mathcal{F} \leq 1} [E_Q f(Y) - E_P f(X)]$$

Functions are linear combinations of features:

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

$$\|f\|_{\mathcal{F}}^2 := \sum_{i=1}^{\infty} f_i^2 \leq 1$$
The MMD: an integral probability metric

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

$$MMD(P, Q; \mathcal{F}) := \sup_{\|f\|_{\mathcal{F}} \leq 1} [E_Q f(Y) - E_P f(X)]$$

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

Other choices for witness function class:

- **Bounded continuous** [Dudley, 2002]
- **Bounded variation 1 (Kolmogorov metric)** [Müller, 1997]
- **Lipschitz (Wasserstein distances)** [Dudley, 2002]
The MMD: an integral probability metric

Maximum mean discrepancy: RKHS function for \( P \) vs \( Q \)

\[
    \text{MMD}(P, Q; \mathcal{F}) := \sup_{\|f\|_{\mathcal{F}} \leq 1} [E_Q f(Y) - E_P f(X)]
\]

Expectations of functions are linear combinations of expected features

\[
    E_P(f(X)) = E_P \langle f, \varphi(X) \rangle_{\mathcal{F}} = \langle f, E_P \varphi(X) \rangle_{\mathcal{F}} = \langle f, \mu_P \rangle_{\mathcal{F}}
\]

(if feature map \( \varphi \) Bochner integrable; always true if kernel is bounded)
Integral prob. metric vs feature mean difference

The MMD:

\[
\text{MMD}(P, Q; \mathcal{F}) = \sup_{\|f\| \leq 1} [\mathbb{E}_P f(X) - \mathbb{E}_Q f(Y)]
\]
Integral prob. metric vs feature mean difference

The MMD:

\[ MMD(P, Q; \mathcal{F}) = \sup_{\|f\| \leq 1} \left[ \mathbb{E}_P f(X) - \mathbb{E}_Q f(Y) \right] \]

use

\[ \mathbb{E}_P f(X) = \mathbb{E}_P \langle \varphi(X), f \rangle_{\mathcal{F}} = \langle \mu_P, f \rangle_{\mathcal{F}} \]

\[ = \sup_{\|f\| \leq 1} \langle f, \mu_P - \mu_Q \rangle_{\mathcal{F}} \]
Integral prob. metric vs feature mean difference

The MMD:

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\text{MMD}(P, Q; \mathcal{F}) = \sup_{\|f\| \leq 1} \left[ \mathbb{E}_P f(X) - \mathbb{E}_Q f(Y) \right]
\]

\[
= \sup_{\|f\| \leq 1} \left\langle f, \mu_P - \mu_Q \right\rangle_{\mathcal{F}}
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Integral prob. metric vs feature mean difference

The MMD:

\[ MMD(P, Q; \mathcal{F}) = \sup_{\|f\| \leq 1} [E_{P}f(X) - E_{Q}f(Y)] = \sup_{\|f\| \leq 1} \langle f, \mu_{P} - \mu_{Q} \rangle_{\mathcal{F}} \]

\[ f^{*} = \frac{\mu_{P} - \mu_{Q}}{\|\mu_{P} - \mu_{Q}\|} \]
Integral prob. metric vs feature mean difference

The MMD:

\[
MMD(P, Q; \mathcal{F}) = \sup_{\|f\| \leq 1} \left[ \mathbb{E}_P f(X) - \mathbb{E}_Q f(Y) \right]
\]

Consequently,

\[
f^*(v) = \langle f, \varphi(v) \rangle_{\mathcal{F}}
\]

\[
\propto \langle \mu_P - \mu_Q, \varphi(v) \rangle_{\mathcal{F}}
\]

\[
= \langle \mathbb{E}_P \varphi(X) - \mathbb{E}_Q \varphi(Y), \varphi(v) \rangle_{\mathcal{F}}
\]

\[
= \mathbb{E}_P k(X, v) - \mathbb{E}_Q k(Y, v)
\]
The maximum mean discrepancy

The **maximum mean discrepancy** in terms of **expected kernels**:

\[
MMD^2(P, Q; \mathcal{F}) = \|\mu_P - \mu_Q\|^2_{\mathcal{F}}
\]

\[
= \mathbb{E}_P k(x, x') + \mathbb{E}_Q k(y, y') - 2\mathbb{E}_{P,Q} k(x, y)
\]

(a) = within distrib. similarity, (b) = cross-distrib. similarity.
The maximum mean discrepancy

The maximum mean discrepancy in terms of expected kernels:

$$MMD^2(P, Q; \mathcal{F}) = \left\| \mu_P - \mu_Q \right\|^2_{\mathcal{F}}$$

$$= \underbrace{\mathbb{E}_P k(x, x')}_{(a)} + \underbrace{\mathbb{E}_Q k(y, y')}_{(a)} - 2\underbrace{\mathbb{E}_{P,Q} k(x, y)}_{(b)}$$

(a) = within distrib. similarity, (b) = cross-distrib. similarity.

Proof:

$$\left\| \mu_P - \mu_Q \right\|^2_{\mathcal{F}} = \langle \mu_P - \mu_Q, \mu_P - \mu_Q \rangle_{\mathcal{F}}$$

$$= \langle \mu_P, \mu_P \rangle_{\mathcal{F}} + \langle \mu_Q, \mu_Q \rangle_{\mathcal{F}} - 2 \langle \mu_P, \mu_Q \rangle_{\mathcal{F}}$$.
Model criticism

\[
\text{MMD}(P, Q; \mathcal{F}) = \sup_{\|f\|_{\mathcal{F}} \leq 1} \left[ \mathbb{E}_q f - \mathbb{E}_p f \right]
\]

Can we compute MMD with samples from \(Q\) and a model \(P\)?

**Problem:** usually can’t compute \(\mathbb{E}_p f\) in closed form.
Stein idea

To get rid of $E_p f$ in

$$\sup_{\|f\|_\infty \leq 1} [E_q f - E_p f]$$

we define the (1-D) **Stein operator**

$$[T_p f] (x) = \frac{1}{p(x)} \frac{d}{dx} (f(x)p(x))$$

Then

$$E_p T_p f = 0$$

subject to appropriate boundary conditions.

**Proof:**

$$E_p [T_p f]$$

$$\int \left[ \frac{d}{dx} (f(x)p(x)) \right] dx$$

$$= [f(x)p(x)]_{-\infty}^{\infty} = 0$$
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Proof:

$$E_p [T_p f] = \int \left[ \frac{1}{p(x)} \frac{d}{dx} \left( f(x)p(x) \right) \right] p(x) \, dx$$

$$\int \left[ \frac{d}{dx} (f(x)p(x)) \right] \, dx$$

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Stein idea

To get rid of $\mathbb{E}_p f$ in

$$\sup_{\|f\|_F \leq 1} \left[ \mathbb{E}_q f - \mathbb{E}_p f \right]$$

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Kernel Stein Discrepancy

Stein operator

\[ T_pf = \frac{1}{p(x)} \frac{d}{dx} (f(x)p(x)) \]

Kernel Stein Discrepancy (KSD)

\[ \text{KSD}_p(Q) = \sup_{\|g\|_F \leq 1} E_q T_pg - E_p T_pg \]
Kernel Stein Discrepancy

Stein operator

\[ T_p f = \frac{1}{p(x)} \frac{d}{dx} (f(x)p(x)) \]

Kernel Stein Discrepancy (KSD)

\[ \text{KSD}_p(Q) = \sup_{\|g\|_{\mathcal{F}} \leq 1} E_q T_p g - E_p T_p g = \sup_{\|g\|_{\mathcal{F}} \leq 1} E_q T_p g \]
The witness function: Chicago Crime

Model $p = 10$-component Gaussian mixture.
The witness function: Chicago Crime

Witness function $g$ shows mismatch
Simple expression using kernels

Re-write stein operator as:

\[
[T_pf](x) = \frac{1}{p(x)} \frac{d}{dx} (f(x)p(x)) = f(x) \frac{d}{dx} \log p(x) + \frac{d}{dx} f(x)
\]

Can we define “Stein features” in \(\mathcal{F}\)?

\[
[T_pf](x) = \left( \frac{d}{dx} \log p(x) \right) f(x) + \frac{d}{dx} f(x)
\]

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

where \(\mathbb{E}_{x \sim p} \xi(x) = 0\).
Simple expression using kernels

Re-write stein operator as:

\[
[T_pf](x) = \frac{1}{p(x)} \frac{d}{dx} (f(x)p(x)) \\
= f(x) \frac{d}{dx} \log p(x) + \frac{d}{dx} f(x)
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Can we define “Stein features” in \( \mathcal{F} \)?

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

where \( \mathbb{E}_{x \sim p} \xi(x) = 0 \).
The kernel trick for derivatives

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

\[
\frac{d}{dx} f(x) = \left\langle f, \frac{d}{dx} \varphi(x) \right\rangle_F
\]
The kernel trick for derivatives

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

$$\frac{d}{dx} f(x) = \left\langle f, \frac{d}{dx} \varphi(x) \right\rangle_F$$

Using kernel derivative trick in (a),

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

$$= \left\langle f, \left( \frac{d}{dx} \log p(x) \right) \varphi(x) + \frac{d}{dx} \varphi(x) \right\rangle_F$$

$$=: \langle f, \xi(x) \rangle_F.$$
Kernel stein discrepancy: derivation

Closed-form expression for KSD:

\[
\text{KSD}_p(Q) = \sup_{\|g\|_\mathcal{F} \leq 1} \mathbb{E}_{x \sim q} \left( [T_p g](x) \right)
\]

\[
= \sup_{\|g\|_\mathcal{F} \leq 1} \mathbb{E}_{x \sim q} \langle g, \xi_x \rangle_{\mathcal{F}}
\]

\[
= \sup_{\|g\|_\mathcal{F} \leq 1} \langle g, \mathbb{E}_{x \sim q} \xi_x \rangle_{\mathcal{F}} = \| \mathbb{E}_{x \sim q} \xi_x \|_{\mathcal{F}}
\]

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

\[
\frac{d}{dx} \log p(x)^2 < 1
\]

Chwialkowski, Strathmann, G., (ICML 2016) Liu, Lee, Jordan (ICML 2016)
Kernel stein discrepancy: derivation

Closed-form expression for KSD:

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Kernelstein discrepancy: derivation

Closed-form expression for KSD:

\[
\text{KSD}_p(Q) = \sup_{\|g\|_\mathcal{F} \leq 1} \mathbb{E}_{x \sim q} \left( \mathbb{E}_{T_p g} (x) \right)
= \sup_{\|g\|_\mathcal{F} \leq 1} \mathbb{E}_{x \sim q} \left( g, \xi_x \right)_{\mathcal{F}}
= \sup_{\|g\|_\mathcal{F} \leq 1} \langle g, \mathbb{E}_{x \sim q} \xi_x \rangle_{\mathcal{F}} = \|\mathbb{E}_{x \sim q} \xi_x\|_{\mathcal{F}}
\]

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

\[
\mathbb{E}_{x \sim q} \left( \frac{d}{dx} \log p(x) \right)^2 < \infty.
\]

Chwialkowski, Strathmann, G., (ICML 2016) Liu, Lee, Jordan (ICML 2016)
Does the Riesz condition matter?

Consider the standard normal, 

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

Then

\[ \frac{d}{dx} \log p(x) = -x. \]

If \( q \) is a Cauchy distribution, then the integral

\[ E_{x \sim q} \left( \frac{d}{dx} \log p(x) \right)^2 = \int_{-\infty}^{\infty} x^2 q(x) \, dx \]

is undefined.
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is undefined.
Kernel stein discrepancy: population expression

Test statistic when $x \in \mathbb{R}^d$, given independent $x, x' \sim q$,

$$
KSD_p^2(Q) = \| \mathbb{E}_{x \sim q} \xi \|_F^2 = \mathbb{E}_{x, x' \sim q} h_p(x, x')
$$

where

$$
h_p(x, x') = s_p(x)^\top s_p(x') k(x, x') + s_p(x)^\top k_2(x, x')
\quad + s_p(x')^\top k_1(x, x') + \text{tr} [k_{12}(x, x')]
$$

- $s_p(x) \in \mathbb{R}^d = \frac{\nabla p(x)}{p(x)}$
- $k_1(a, b) := \nabla_x k(x, x')|_{x=a, x'=b} \in \mathbb{R}^d$,
- $k_2(a, b) := \nabla_{x'} k(x, x')|_{x=a, x'=b} \in \mathbb{R}^d$,
- $k_{12}(a, b) := \nabla_x \nabla_{x'} k(x, x')|_{x=a, x'=b} \in \mathbb{R}^{d \times d}$
Kernel stein discrepancy: population expression

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\text{KSD}^2_p(Q) = \| E_{x \sim q} \xi_x \|^2_F = E_{x, x' \sim q} h_p(x, x')
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h_p(x, x') = s_p(x)^\top s_p(x')k(x, x') + s_p(x)^\top k_2(x, x') \\
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Do not need to normalize \( p \), or sample from it.
Kernel stein discrepancy: population expression

Test statistic when \( x \in \mathbb{R}^d \), given independent \( x, x' \sim q \),

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\text{KSD}_p^2(Q) = \|E_{x \sim q} \xi x\|^2 = E_{x, x' \sim q} h_p(x, x')
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where

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 h_p(x, x') = s_p(x)^\top s_p(x') k(x, x') + s_p(x)^\top k_2(x, x')
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+ s_p(x')^\top k_1(x, x') + \text{tr} \left[ k_{12}(x, x') \right]
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- \( k_{12}(a, b) := \nabla x \nabla x' k(x, x') |_{x=a, x'=b} \in \mathbb{R}^{d \times d} \)

If kernel is \( C_0 \)-universal and \( Q \) satisfies \( E_{x \sim q} \left\| \nabla \left( \log \frac{p(x)}{q(x)} \right) \right\|^2 < \infty \), then

\[
\text{KSD}_p^2(Q) = 0 \iff P = Q.
\]
KSD for discrete-valued variables

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

The population KSD (discrete):

\[
\text{KSD}^2_p(Q) = \mathbb{E}_{x,x' \sim q} h_p(x, x')
\]

where

\[
h_p(x, x') = s_p(x) \top s_p(x') k(x, x') - s_p(x) \top k_2(x, x') - s_p(x') \top k_1(x, x') + \text{tr} [k_{12}(x, x')]
\]

\[
k_1(x, x') = \Delta_x^{-1} k(x, x'), \quad \Delta_x^{-1} \text{ is cyclic backwards difference on } x,
\]

\[
s_p(x) = \frac{\Delta p(x)}{p(x)}
\]

Ranganath et al. (NeurIPS 2016), Yang et al. (ICML 2018)
KSD for discrete-valued variables

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

The population KSD (discrete):

$$KSD^2_p(Q) = E_{x,x' \sim q} h_p(x, x')$$

where

$$h_p(x, x') = s_p(x)^\top s_p(x') k(x, x') - s_p(x)^\top k_2(x, x')$$

$$- s_p(x')^\top k_1(x, x') + \text{tr} [k_{12}(x, x')]$$

$$k_1(x, x') = \Delta_x^{-1} k(x, x'), \quad \Delta_x^{-1} \text{ is cyclic backwards difference on x},$$

$$s_p(x) = \frac{\Delta p(x)}{p(x)}$$

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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where

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h_p(x, x') = s_p(x)^\top s_p(x') k(x, x') - s_p(x)^\top k_2(x, x') - s_p(x')^\top k_1(x, x') + \text{tr} [k_{12}(x, x')]
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k_1(x, x') = \Delta^{-1}_x k(x, x'), \quad \Delta^{-1}_x \text{ is cyclic backwards difference on } x,
\]

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s_p(x) = \frac{\Delta p(x)}{p(x)}
\]

A discrete kernel: \( k(x, x') = \exp(-d_H(x, x')) \), where

\[
d_H(x, x') = D^{-1} \sum_{d=1}^D \mathbb{I}(x_d \neq x'_d).
\]

\[
\text{KSD}_p^2(Q) = 0 \text{ iff } P = Q \text{ if}
\]

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

Ranganath et al. (NeurIPS 2016), Yang et al. (ICML 2018)
Empirical statistic and asymptotics

The empirical statistic:

\[ \overline{\text{KSD}}_p^2(Q) := \frac{1}{n(n-1)} \sum_{i \neq j} h_p(x_i, x_j). \]
Empirical statistic and asymptotics

The empirical statistic:

\[
\hat{\text{KSD}}_p^2(Q) := \frac{1}{n(n - 1)} \sum_{i \neq j} h_p(x_i, x_j).
\]

Asymptotic distribution when \( P \neq Q \):

\[
\sqrt{n} \left( \hat{\text{KSD}}_p^2(Q) - \text{KSD}_p^2(Q) \right) \overset{d}{\rightarrow} \mathcal{N}(0, \sigma_{h_p}^2) \quad \sigma_{h_p}^2 = 4 \text{Var}_x[E_{x'}[h_p(x, x')]].
\]
Empirical statistic and asymptotics

The empirical statistic:

\[ \hat{\text{KSD}}_p^2(Q) := \frac{1}{n(n-1)} \sum_{i \neq j} h_p(x_i, x_j). \]

Asymptotic distribution when \( P = Q \):

\[ n\hat{\text{KSD}}_p^2(Q) \sim \sum_{\ell=1}^{\infty} \lambda_{\ell} Z_{\ell}^2 \]

\[ \lambda_{\ell} \psi_{\ell}(x') = \int_{\mathcal{X}} h_p(x, x') \psi_{\ell}(x) d\mu(x) \]

\[ Z_{\ell} \sim \mathcal{N}(0,1) \text{ i.i.d.} \]

Test threshold via wild bootstrap.
A naive linear time statistic

A running average:

\[ \overline{LKS}^2_p(Q) := \frac{2}{n} \sum_{i=1}^{n/2} h_p(x_{2i-1}, x_{2i}). \]

Asymptotically normal when \( P \neq Q \) and when \( P = Q \).
A naive linear time statistic

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Asymptotically normal when $P \neq Q$ and when $P = Q$.

Can we do better? Wishlist:

1. still linear-time
2. adaptive (parameters automatically tuned)
3. more interpretable
Linear-time, interpretable
Goodness-of-fit Test
Stein Witness Function at a Single Location

Idea:

\[
(\text{Stein}) \ \text{witness}(v) = \mathbb{E}_{x \sim q}[T_p k_v(x)] - \mathbb{E}_{y \sim p}[T_p k_v(y)]
\]
Stein Witness Function at a Single Location

Idea:

\[(\text{Stein}) \text{ witness}(v) = \mathbb{E}_{x \sim q}[T_p] - \mathbb{E}_{y \sim p}[T_p] \]
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$$(\text{Stein) witness}(v) = E_{x \sim q}[v] - E_{y \sim p}[v]$$
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Stein Witness Function at a Single Location

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Stein Witness Function at a Single Location

Idea:

\[
(\text{Stein}) \; \text{witness}(v) = E_{x \sim q}[T_p k_v(x)]
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Stein Witness Function at a Single Location

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\[(\text{Stein}) \ \text{witness}(v) = \mathbb{E}_{x \sim q}[T_p k_v(x)]\]

Proposal: Good \(v\) should have high

\[
\text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}.
\]
Stein Witness Function at a Single Location

Idea:

\[(\text{Stein}) \text{ witness}(v) = E_{x \sim q} [ T_p k_v(x) ]\]

Proposal: Good \(v\) should have high

\[\text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}.\]

- \(\text{witness}(v)\) and \(\text{standard deviation}(v)\) can be estimated in **linear** time.
Proposal: Model Criticism with the Stein Witness

$$\text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}.$$
Proposal: Model Criticism with the Stein Witness

\[
\text{score}(\mathbf{v}) = \frac{|\text{witness}(\mathbf{v})|}{\text{standard deviation}(\mathbf{v})}.
\]
Proposal: Model Criticism with the Stein Witness

\[ (T_p k_v)(x) = v \]

\[
\text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}.
\]
Proposal: Model Criticism with the Stein Witness

\[ \text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}. \]
score: 0.17

\[
\text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}.
\]
Proposal: Model Criticism with the Stein Witness

score: 0.26

\[
\text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}.
\]
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score: 0.33

score(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}.
Proposal: Model Criticism with the Stein Witness

score: 0.37

\[ \text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}. \]
Proposal: Model Criticism with the Stein Witness

\[ \text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}. \]
Proposal: Model Criticism with the Stein Witness

score: 0.45

\[ \text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}. \]
Proposal: Model Criticism with the Stein Witness

score: 0.44

\[
\text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}.
\]
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score: 0.39

\[ \text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}. \]
Proposal: Model Criticism with the Stein Witness

score: 0.31

\[
\text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}.
\]
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score: 0.32

\[
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\]
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Proposal: Model Criticism with the Stein Witness

score: 0.37

\[ \text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}. \]
Proposal: Model Criticism with the Stein Witness

score: 0.48

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Proposal: Model Criticism with the Stein Witness

score: 0.49

\[
score(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}.
\]
Proposal: Model Criticism with the Stein Witness

score: 0.47

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\[ \text{score}(v) = \frac{|\text{witness}(v)|}{\text{standard deviation}(v)}. \]
FSSD is a Discrepancy Measure

Theorem 1.

Let $V = \{\mathbf{v}_1, \ldots, \mathbf{v}_J\} \subset \mathbb{R}^d$ be drawn i.i.d. from a distribution $\eta$ which has a density. Let $\mathcal{X}$ be a connected open set in $\mathbb{R}^d$. Assume

1. (Nice RKHS) Kernel $k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is $C_0$-universal, and real analytic.
2. (Riesz condition holds) $\|g\|_F^2 < \infty$.
3. (Finite Fisher divergence) $\mathbb{E}_{x \sim q} \| \nabla_x \log \frac{p(x)}{q(x)} \|^2 < \infty$.
4. (Vanishing boundary condition) $\lim_{\|x\| \to \infty} p(x)g(x) = 0$.

Then, $\eta$-almost surely

$$FSSD^2 = 0 \text{ if and only if } p = q, \text{ for any } J \geq 1.$$ 

- Gaussian kernel $k(x, v) = \exp \left( -\frac{\|x-v\|^2}{2\sigma_k^2} \right)$ works.
- In practice, $J = 1$ or $J = 5$. 

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When $d > 1$, the Stein witness $g$ has $d$ outputs.

Define

$$\xi(x, v) := \frac{1}{p(x)} \nabla_x [p(x)k(x, v)] \in \mathbb{R}^d.$$

$d$-output Stein witness

$$g(v) = \mathbb{E}_{x \sim q} \xi(x, v) \in \mathbb{R}^d.$$

General form:

$$\text{FSSD}^2 = \frac{1}{dJ} \sum_{j=1}^{J} ||g(v_j)||_2^2,$$

where unbiased estimator $\widehat{\text{FSSD}}^2$ computable in $\mathcal{O}(d^2 Jn)$. 

Asymptotic Distributions of $\overset{\text{FSSD}}{2}$

- $\tau(x) := \text{vertically stack } \xi(x, v_1), \ldots \xi(x, v_J) \in \mathbb{R}^{dJ}$. Feature vector of $x$.
- Mean feature: $\mu := \mathbb{E}_{x \sim q}[\tau(x)]$.
- Equivalently, $\text{FSSD}^2 = \frac{1}{dJ} \|\mu\|^2_2$ (mean feature).
- $\Sigma_r := \text{cov}_{x \sim r}[\tau(x)] \in \mathbb{R}^{dJ \times dJ}$ for $r \in \{p, q\}$

Proposition 1 (Asymptotic distributions).

Let $Z_1, \ldots, Z_{dJ} \overset{i.i.d.}{\sim} \mathcal{N}(0, 1)$, and $\{\omega_i\}_{i=1}^{dJ}$ be the eigenvalues of $\Sigma_p$.

1. Under $H_0 : p = q$, asymptotically $n\text{FSSD}^2 \xrightarrow{d} \sum_{i=1}^{dJ} (Z_i^2 - 1)\omega_i$.
   - Easy to simulate to get $p$-value.
   - Simulation cost independent of $n$.

2. Under $H_1 : p \neq q$, we have $\sqrt{n}(\text{FSSD}^2 - \text{FSSD}^2) \xrightarrow{d} \mathcal{N}(0, \sigma_{H_1}^2)$ where $\sigma_{H_1}^2 := 4\mu^\top \Sigma_q \mu$. Implies $\mathbb{P}(\text{reject } H_0) \to 1$ as $n \to \infty$.

But, how to estimate $\Sigma_p$? No sample from $p$!

- Theorem: Using $\hat{\Sigma}_q$ (computed with $\{x_i\}_{i=1}^n \sim q$) still leads to asymptotically consistent test.
Asymptotic Distributions of $\text{FSSD}^2$

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Parameter Tuning

- Jointly optimise locations $V = \{v_1, \ldots, v_J\}$ for more test power

**Proposition 2 (Approx. power for large $n$).**

*Under $H_1$, for large $n$ and fixed threshold $r$, the test power*

$$P(\text{reject } H_0 \mid H_1 \text{ true})$$

$$P_{H_1}(n \overline{\text{FSSD}}^2 > r) \approx 1 - \Phi \left( \frac{r}{\sqrt{n} \sigma_{H_1}} - \sqrt{n} \frac{\overline{\text{FSSD}}^2}{\sigma_{H_1}} \right),$$

*where $\Phi = CDF$ of $\mathcal{N}(0, 1)$.*

- For large $n$, second term dominates. So

$$\arg \max_{V, \sigma_k^2} \text{(power)} \approx \arg \max_{V, \sigma_k^2} \frac{\overline{\text{FSSD}}^2}{\sigma_{H_1}}.$$  

- Split $\{x_i\}_{i=1}^n$ into independent training/test sets. Optimize $V$ on tr. Test on te.
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$$

$$
P_{H_1}(n \frac{\text{FSSD}^2}{\sigma^2} > r) \approx 1 - \Phi \left( \frac{r}{\sqrt{n} \sigma_{H_1}} - \sqrt{n} \frac{\text{FSSD}^2}{\sigma_{H_1}} \right),
$$

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Interpretable Features: Chicago Crime

Model $p = 2$-component Gaussian mixture.
Interpretable Features: Chicago Crime

Score surface
Interpretable Features: Chicago Crime

= optimized $v$. 

★ = optimized $v$. 

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Interpretable Features: Chicago Crime

★ = optimized v.
No robbery in Lake Michigan.
Interpretable Features: Chicago Crime

Model $p = 10$-component Gaussian mixture.
Interpretable Features: Chicago Crime

Capture the right tail better.
Still, does not capture the left tail.
Interpretable Features: Chicago Crime

Still, does not capture the left tail.

Learned test locations are interpretable.
Experiment: Restricted Boltzmann Machine (RBM)

Model $p =$

40 hidden units

50 visible units
Experiment: Restricted Boltzmann Machine (RBM)

40 hidden units

50 visible units

Model $p =$

Perturb one weight

Sample from

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Experiment: Restricted Boltzmann Machine (RBM)

Model $p = \cdots \cdot \cdots \cdot \cdot \cdots$

40 hidden units
50 visible units

Perturb one weight
Sample from

Better

$P(\text{detect difference})$

Sample size $n$

0.75
0.50
0.25
0.00

MMD test (quadratic-time)

[Gretton et al., 2012]
Experiment: Restricted Boltzmann Machine (RBM)

Model $p =$

40 hidden units

50 visible units

Perturb one weight

Sample from

Better

$P(detect\ difference) = \begin{cases} 0.00 & n = 2000 \\ 0.25 & n = 2500 \\ 0.50 & n = 3000 \\ 0.75 & n = 4000 \end{cases}$

MMD test (quadratic-time) [Gretton et al., 2012]

Proposed (linear-time)
"All models are wrong."

G. Box (1976)
**Relative 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?

Samples from GAN, Goodfellow et al. (2014)

Samples from LSGAN, Mao et al. (2017)

Which model is better?
Most interesting models have latent structure

Graphical model representation of hierarchical LDA with a nested CRP prior, Blei et al. (2003)
Relative goodness-of-fit testing

- Two generative models $P$ and $Q$, data $\{x_i\}_{i=1}^n \sim R$.
- Neither model gives a perfect fit ($P \neq R$ and $Q \neq R$).
Joint asymptotic normality

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

$$\sqrt{n} \left[ \frac{\hat{\text{KSD}}_p^2(R) - \text{KSD}_p^2(R)}{\text{KSD}_q^2(R) - \text{KSD}_q^2(R)} \right] \xrightarrow{d} \mathcal{N} \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma_{hp}^2 & \sigma_{hpq} \\ \sigma_{hpq} & \sigma_{hq}^2 \end{bmatrix} \right)$$
Joint asymptotic normality

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

$$\sqrt{n} \left[ \frac{\text{KSD}^2_p(R) - \text{KSD}^2_p(R)}{\text{KSD}^2_q(R) - \text{KSD}^2_q(R)} \right] \xrightarrow{d} \mathcal{N} \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma^2_{hp} & \sigma_{hp\,hq} \\ \sigma_{hp\,hq} & \sigma^2_{hq} \end{bmatrix} \right)$$

Difference in statistics is asymptotically normal:

$$\sqrt{n} \left[ \frac{\text{KSD}^2_p(R)}{\text{KSD}^2_q(R)} - \left( \text{KSD}^2_p(R) - \text{KSD}^2_q(R) \right) \right] \xrightarrow{d} \mathcal{N} \left( 0, \sigma^2_{hp} + \sigma^2_{hq} - 2\sigma_{hp\,hq} \right)$$

$\implies$ a statistical test with null hypothesis $\text{KSD}^2_p(R) - \text{KSD}^2_q(R) \leq 0$ is straightforward.
Latent variable models

Can we compare latent variable models with KSD?

\[ p(x) = \int p(x|z)p(z)\,dz \]
\[ q(y) = \int q(y|w)p(w)\,dw \]

Recall multi-dimensional Stein operator:

\[ [T_p f](x) = \left\langle \frac{\nabla p(x)}{p(x)}, f(x) \right\rangle + \langle \nabla, f(x) \rangle . \]

Expression \((a)\) requires marginal \(p(x)\), often intractable…
Latent variable models

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\]

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

...but sampling can be straightforward!
Monte Carlo approximation

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

\[
p(x) = \int p(x|z)p(z)dz
\]

\[
\approx p_m(x) = \frac{1}{m} \sum_{j=1}^m p(x|z_j)
\]

Estimate KSDs with approxiomatic densities:

\[
\overline{\text{KSD}}^2_p(R) - \overline{\text{KSD}}^2_q(R) \approx \overline{\text{KSD}}^2_{p_m}(R) - \overline{\text{KSD}}^2_{q_m}(R)
\]
Monte Carlo approximation

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

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Estimate KSDs with approximate densities:

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\widehat{\text{KSD}_p^2}(R) - \widehat{\text{KSD}_q^2}(R) \approx \widehat{\text{KSD}_p^2}(R) - \widehat{\text{KSD}_q^2}(R)
\]

Recall

\[
\sqrt{n} \left[ \widehat{\text{KSD}_p^2}(R) - \widehat{\text{KSD}_q^2}(R) - \left( \text{KSD}_p^2(R) - \text{KSD}_q^2(R) \right) \right]
\]

\[
\xrightarrow{d} \mathcal{N} \left( 0, \sigma_{h_p}^2 + \sigma_{h_q}^2 - 2\sigma_{h_p h_q} \right)
\]

\rightarrow \text{if } m \text{ is large, can we simply substitute } p_m \text{ and } q_m \text{?}
Simple proof of concept

Check $\widehat{\text{KSD}}_p^2(R) \approx \widehat{\text{KSD}}_{p_m}^2(R)$ with a toy model:

- **Model:** Beta-Binomial $\text{BetaBinom}(\alpha, \beta)$

  $$p(x|z) = \binom{N}{x} z^x (1 - z)^{n-x}, \quad p(z) = \text{Beta}(a, b)$$

- Latent $z \in (0, 1)$: success probability for binomial likelihood
- Marginal $p(x)$: tractable (given by the beta function)

- **Generate** $\sqrt{n}\widehat{\text{KSD}}_p^2(R)$ and $\sqrt{n}\widehat{\text{KSD}}_{p_m}^2(R)$

  $\rightarrow$ what do their distribution look like?
Effect of sampling the latents (Beta-binomial)
Effect of sampling the latents (Beta-binomial)
Effect of sampling the latents (Beta-binomial)
Why this happens

$P(KSD^2_{pm})$

$KSD^2_p (R)$ is normally distributed around $KSD^2_p (R)$
(approximation error)
Why this happens

Approximation $p_m$ gives a random draw $\text{KSD}_{p_m}^2(R)$
Why this happens

\[ KSD^2_{p_m}(R) \text{ is normally distributed around } KSD^2_{p_m}(R) \]
Why this happens

Distribution of $KSD_{pm}^2(R)$ is averaged over random draws of $KSD_{pm}^2(R)$
Distribution of $\overline{\text{KSD}}^2_{pm}(R)$ is averaged over random draws of $\text{KSD}^2_{pm}(R)$.
Why this happens

\[ \text{KSD}_p^2 (R) \] has a higher variance than \[ \text{KSD}_p^2 (R) \]
Correction for this effect

- BetaBinomial models with $p = q_m$ vs $q$
  - numerical vs closed-form marginalisation.
- With correction for increased $\text{KSD}^2_{q_m}(R)$ variance, null accepted w.p. $1 - \alpha$.

\[
Q = \text{BetaBinom}(5 + a, 1 + b)
\]

\[
P = q_m
\]

\[
R = \text{BetaBinom}(a, b)
\]

\[
k(x, x') = \exp(-\mathbb{I}(x \neq x'))
\]

\[
\alpha = 0.05
\]
Correction for this effect

- BetaBinomial models with $p = q_m$ vs $q$
  $\rightarrow$ numerical vs closed-form marginalisation.
- With correction for increased $\text{KSD}^2_{q_m}(R)$ variance,
  null accepted w.p. $1 - \alpha$.

Naive Rel-KSD test has incorrect type-I error

Naive KSD: $p = q_m \neq q$
$\Rightarrow$ rejection rate $\to 1$ as $n \to \infty$
Asymptotics for approximate KSD

We have asymptotic normality for $\text{KSD}_{p_m}(R)$,

$$\sqrt{m}(\text{KSD}_{p_m}(R) - \text{KSD}_p(R)) \overset{d}{\to} \mathcal{N}(0, \gamma_p^2)$$

The fine print:

- $\inf_x p(x) > 0$
- $\sup_x \left| \frac{d p(x)}{dx} \right| < \infty$
- (Uniform CLT) Likelihoods $\{p(x|\cdot)| x \in \mathcal{X}\}$ and derivatives $\{\frac{d}{dx} p(x|\cdot)| x \in \mathcal{X}\}$ are $p(z)$ - Donsker class
Asymptotic distribution for relative KSD test

Asymptotic distribution of approximate KSD estimate

\((n, m) \to \infty, \frac{n}{m} \to r \in [0, \infty)\):

\[
\sqrt{n} \left[ \left( \hat{\text{KSD}}^2_{pm}(R) - \hat{\text{KSD}}^2_{qm}(R) \right) - \left( \text{KSD}^2_p(R) - \text{KSD}^2_q(R) \right) \right] \xrightarrow{d} \mathcal{N}(0, c^2)
\]

where

- \(c = \sigma_{pq} \sqrt{1 + r(\gamma_{pq}/\sigma_{pq})^2}\)
- \(\gamma_{pq}^2 = \lim_{m \to \infty} m \cdot \text{Var} \left[ E_{x,x'} h_{pm}(x, x') - E_{x,x'} h_{qm}(x, x') \right]\)
- \(\sigma_{pq}^2 = \lim_{n \to \infty} n \cdot \text{Var} \left[ \hat{\text{KSD}}^2_p(R) - \hat{\text{KSD}}^2_q(R) \right]\)

Fine print:

- \(h_p(x, x') - h_q(x, x')\) has a finite third moment
- Additional technical conditions
Relative test, further detail

Theorem (Asymptotic distribution of random kernel U-statistic).

Let

- \( U_{n,m} \) : a U-statistic defined by a random U-statistic kernel \( H_m \)
- \( U_n \) : a U-statistic defined by a fixed U-statistic kernel \( h \)

Assume that

- \( \sigma_{H_m}^2 \to \sigma_h^2 \) in probability
- \( \nu_3(H_m) \to \nu_3(h) < \infty \) in probability
  
  where \( \nu_3(H_m) = \mathbb{E}_{x,x'} |H_m(x, x') - \mathbb{E}_{x,x'} H_m(x, x')|^3 \)
- \( Y_m := \sqrt{m} \left( \mathbb{E}_n[U_{n,m}|H_m] - \mathbb{E}_n[U_n] \right) \xrightarrow{d} Y \)

Then, with \( n/m \to r \in [0, \infty) \),

\[
\lim_{n,m \to \infty} \Pr \left[ \sqrt{n} \left( U_{n,m} - \mathbb{E}_n U_n \right) < t \right] = \mathbb{E}_Y \left[ \Phi \left( \frac{t - \sqrt{r} Y}{\sigma_h} \right) \right]
\]
Experiment: sensitivity to model difference

- Data $R = \text{Sigmoid Belief Network } \text{SBN}(W)$:

  $$R(x|z) = \text{sigmoid}(Wz), \quad R(z) = \mathcal{N}(0, I), \quad W \in \mathbb{R}^{30 \times 10}$$

- Models: $P = \text{SBN}(W + \epsilon[1, 0, \ldots, 0]), \quad Q = \text{SBN}(W + [1, 0, \ldots, 0])$

- Only the first column of weight $W$ is perturbed by $\epsilon$
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Two scenarios:
- Null: $\epsilon \leq 1$
  \quad \left(\alpha = 0.05\right)
- Alternative: $\epsilon > 1$
  \quad \left(\text{the higher the better}\right)

- Hamming kernel
- Sample size $n = 300$
Experiment: sensitivity to model difference

- Data $R = \text{Sigmoid Belief Network } SBN(W)$:
  
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- Models: $P = SBN(W + \epsilon[1, 0, \ldots, 0]), \quad Q = SBN(W + [1, 0, \ldots, 0])$

- Only the first column of weight $W$ is perturbed by $\epsilon$

KSD has higher power ($\epsilon > 1$)

- Sample-wise difference in models = subtle (MMD fails)
- Model’s information is better utilised

<table>
<thead>
<tr>
<th>Perturbation $\epsilon$</th>
<th>Rejection rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>MMD</td>
</tr>
<tr>
<td>2</td>
<td>LKSD (KSD for Latent Models) m=100</td>
</tr>
<tr>
<td>4</td>
<td>LKSD m=1000</td>
</tr>
</tbody>
</table>
Papers referenced

A Linear-Time Kernel Goodness-of-Fit Test.
Wittawat Jitkrittum, Wenkai Xu, Zoltán Szabó, Kenji Fukumizu, Arthur Gretton
https://arxiv.org/abs/1705.07673

- Python code: https://github.com/wittawatj/kernel-gof

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?
Efficiency comparison, linear-time tests
Bahadur Slope and Bahadur Efficiency

- Bahadur slope \( \approx \) rate of p-value \( \to 0 \) under \( H_1 \) as \( n \to \infty \).
- Measure a test’s sensitivity to the departure from \( H_0 \).

\[
H_0 : \theta = 0,
\]
\[
H_1 : \theta \neq 0.
\]

- Typically \( \text{pval}_n \approx \exp\left( -\frac{1}{2} c(\theta)n \right) \) where \( c(\theta) > 0 \) under \( H_1 \), and \( c(0) = 0 \). [?].
- \( c(\theta) \) higher \( \implies \) more sensitive. Good.

Bahadur slope

\[
c(\theta) := -2 \lim_{n \to \infty} \frac{\log (1 - F(T_n))}{n},
\]

where \( F(t) = \text{CDF of } T_n \) under \( H_0 \).

- Bahadur efficiency = ratio of slopes of two tests.
Bahadur Slope and Bahadur Efficiency

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- Bahadur efficiency = ratio of slopes of two tests.
Theorem 2. 

The Bahadur slope of $n \overset{FSSD}{=}^2$ is

$$c^{(\text{FSSD})} := \frac{\text{FSSD}^2}{\omega_1},$$

where $\omega_1$ is the maximum eigenvalue of $\Sigma_p := \text{cov}_{x \sim p}[\tau(x)].$

Theorem 3. 

The Bahadur slope of the linear-time kernel Stein (LKS) statistic $\sqrt{n \hat{S}^2}$ is

$$c^{(\text{LKS})} = \frac{1}{2} \frac{\mathbb{E}_q h_p(x, x')^2}{\mathbb{E}_p \left[ h_p^2(x, x') \right]},$$

where $h_p$ is the U-statistic kernel of the KSD statistic.

Let’s consider a specific case ...
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Let’s consider a specific case...
Gaussian Mean Shift Problem

Consider $p = \mathcal{N}(0, 1)$ and $q = \mathcal{N}(\mu_q, 1)$.

- Assume $J = 1$ feature for $\text{FSSD}^2$. Gaussian kernel (bandwidth $= \sigma_k^2$)

$$
c^{(\text{FSSD})}(\mu_q, \nu, \sigma_k^2) = \frac{\sigma_k^2 (\sigma_k^2 + 2)^3 \mu_q^2 e^{\frac{\nu^2}{\sigma_k^2 + 2}} - (\nu - \mu_q)^2}{\sqrt{\frac{2}{\sigma_k^2} + 1 (\sigma_k^2 + 1) (\sigma_k^6 + 4\sigma_k^4 + (\nu^2 + 5) \sigma_k^2 + 2)}}.
$$

- For LKS, Gaussian kernel (bandwidth $= \kappa^2$).

$$
c^{(\text{LKS})}(\mu_q, \kappa^2) = \frac{(\kappa^2)^{5/2} (\kappa^2 + 4)^{5/2} \mu_q^4}{2 (\kappa^2 + 2) (\kappa^8 + 8\kappa^6 + 21\kappa^4 + 20\kappa^2 + 12)}.
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\]
Theorem 4 (FSSD is at least two times more efficient).

Fix $\sigma_k^2 = 1$ for $nFSSD^2$.

Then, $\forall \mu_q \neq 0$, $\exists \nu \in \mathbb{R}$, $\forall \kappa^2 > 0$, we have Bahadur efficiency

$$\frac{c^{(FSSD)}(\mu_q, \nu, \sigma_k^2)}{c^{(LKS)}(\mu_q, \kappa^2)} > 2.$$