

# A Linear-Time Kernel Goodness-of-Fit Test

Wittawat Jitkrittum<sup>1,\*</sup>

Wenkai Xu<sup>1</sup>

Zoltán Szabó<sup>2</sup>

NIPS 2017  
Best paper!

Kenji Fukumizu<sup>3</sup>

Arthur Gretton<sup>1</sup>



wittawatj@gmail.com

<sup>1</sup>Gatsby Unit, University College London

<sup>\*</sup>(Now at Max Planck Institute for Intelligent Systems)

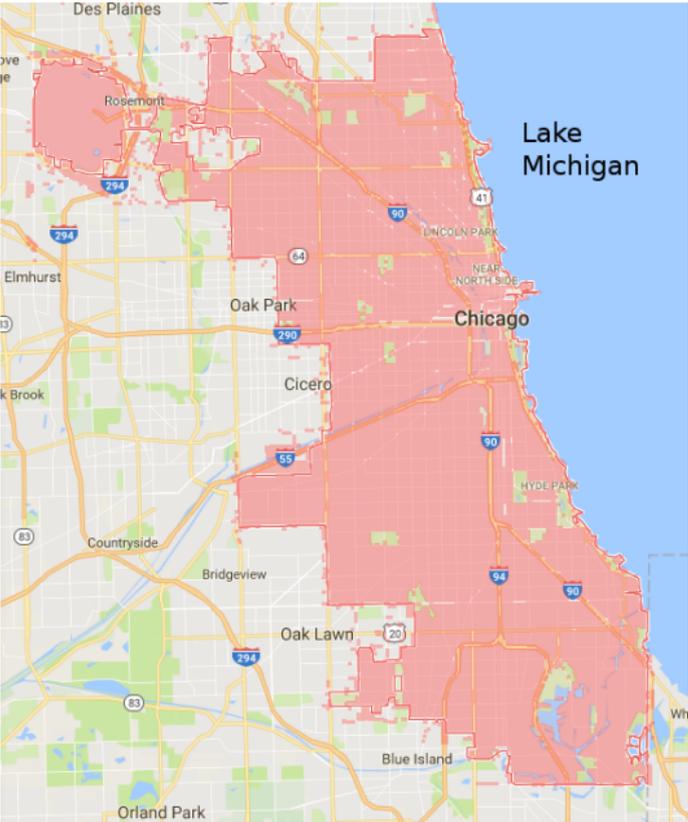
<sup>2</sup>CMAP, École Polytechnique

<sup>3</sup>The Institute of Statistical Mathematics, Tokyo

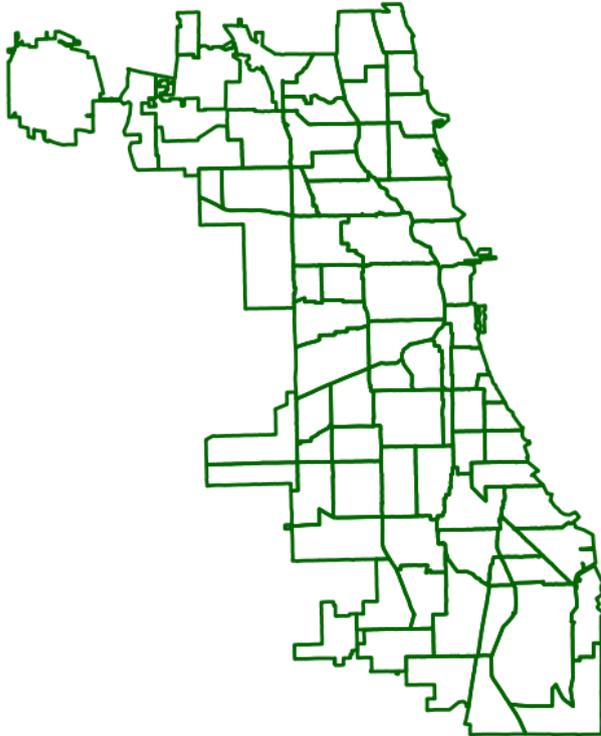
Workshop on Functional Inference and Machine Intelligence, Tokyo

20 February 2018

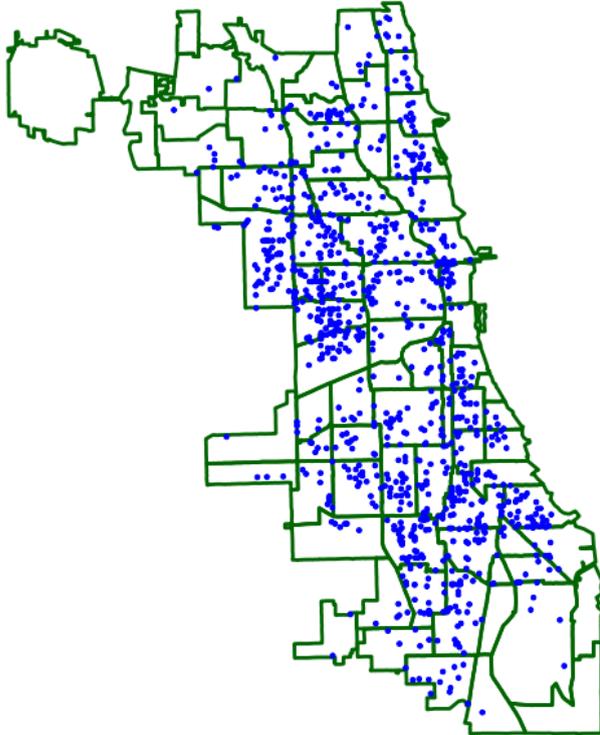
# Model Criticism



# Model Criticism

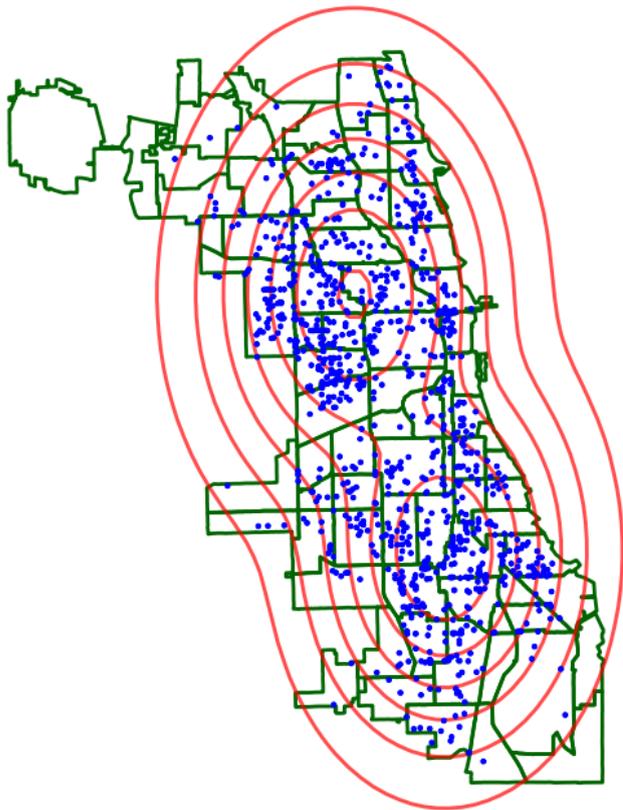


## Model Criticism



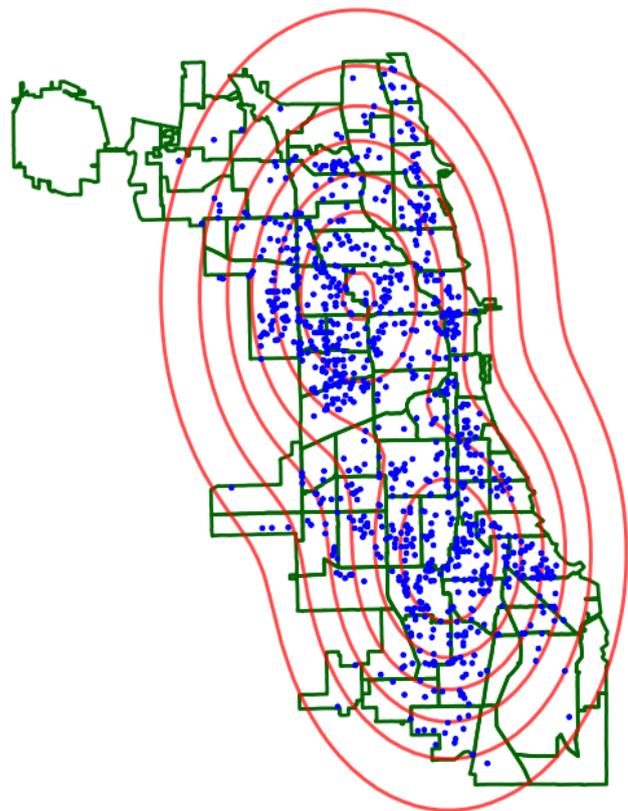
Data = robbery events in  
Chicago in 2016.

## Model Criticism



Is this a good **model**?

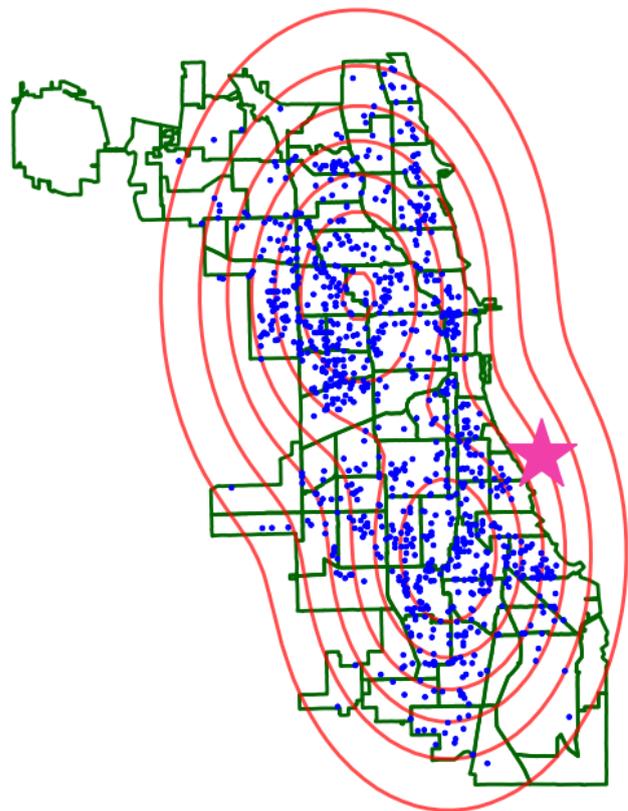
## Model Criticism



### Goals:

- 1 Test if a (complicated) **model** fits the **data**.
- 2 If it does not, show **a location** where it fails.

## Model Criticism



### Goals:

- 1 Test if a (complicated) **model** fits the **data**.
- 2 If it does not, show **a location** where it fails.

# Goodness-of-fit Testing

Given:

- 1 Sample  $\{\mathbf{x}_i\}_{i=1}^n \stackrel{i.i.d.}{\sim} q$  (unknown) on  $\mathbb{R}^d$ ,
- 2 Unnormalized density  $p$  (known model).

$$H_0: p = q$$

$$H_1: p \neq q$$

Want a test ...

- 1 Nonparametric.
- 2 Linear-time. Runtime is  $\mathcal{O}(n)$ . Fast.
- 3 Interpretable. Model criticism by finding .

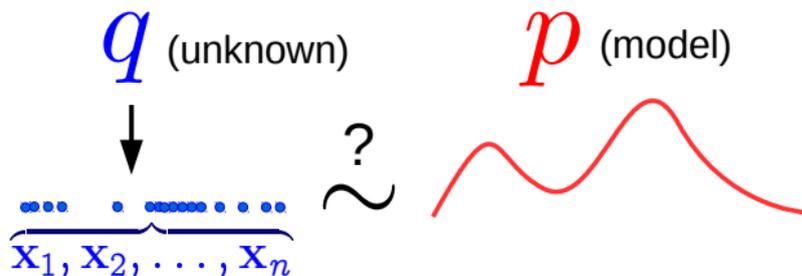
# Goodness-of-fit Testing

Given:

- 1 Sample  $\{\mathbf{x}_i\}_{i=1}^n \stackrel{i.i.d.}{\sim} q$  (unknown) on  $\mathbb{R}^d$ ,
- 2 Unnormalized density  $p$  (known model).

$$H_0: p = q$$

$$H_1: p \neq q$$



Want a test ...

- 1 Nonparametric.
- 2 Linear-time. Runtime is  $\mathcal{O}(n)$ . Fast.
- 3 Interpretable. Model criticism by finding .

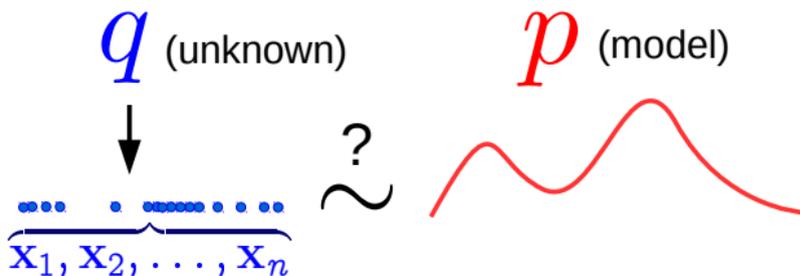
# Goodness-of-fit Testing

Given:

- 1 Sample  $\{\mathbf{x}_i\}_{i=1}^n \stackrel{i.i.d.}{\sim} q$  (unknown) on  $\mathbb{R}^d$ ,
- 2 Unnormalized density  $p$  (known model).

$$H_0: p = q$$

$$H_1: p \neq q$$



Want a test ...

- 1 **Nonparametric.**
- 2 **Linear-time.** Runtime is  $\mathcal{O}(n)$ . Fast.
- 3 **Interpretable.** Model criticism by finding .

## Maximum Mean Discrepancy (MMD) Witness Function (Gretton et al., 2012)

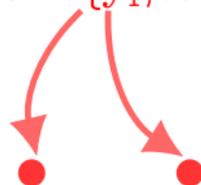


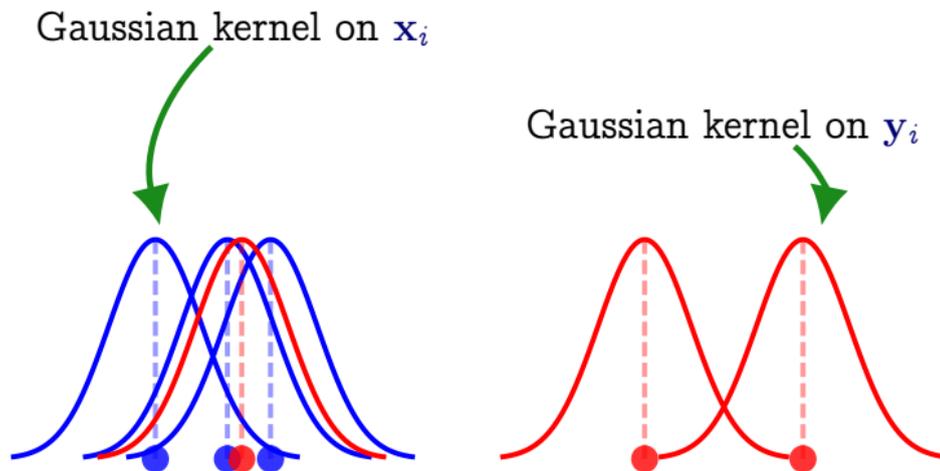
## Maximum Mean Discrepancy (MMD) Witness Function (Gretton et al., 2012)

Observe  $X = \{x_1, \dots, x_n\} \sim q$

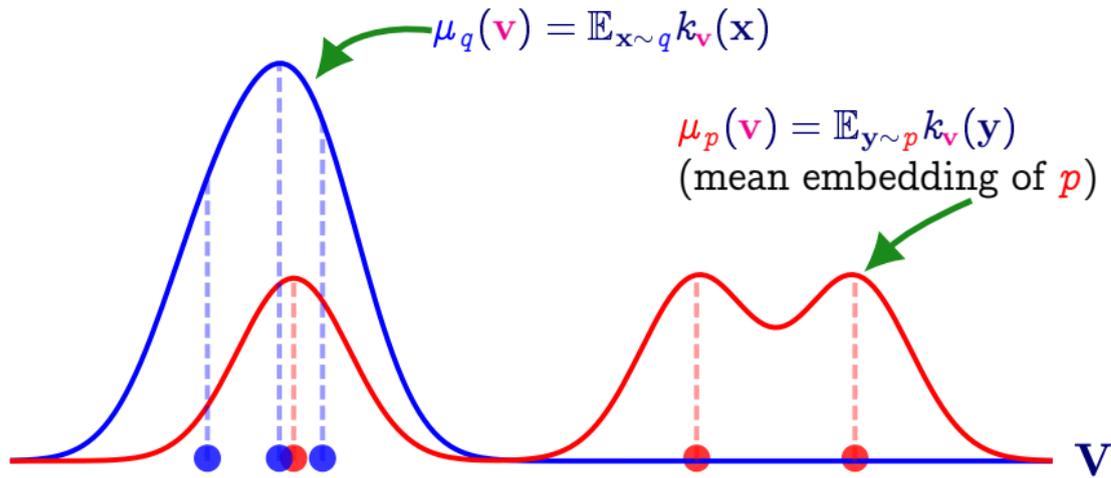


Observe  $Y = \{y_1, \dots, y_n\} \sim p$

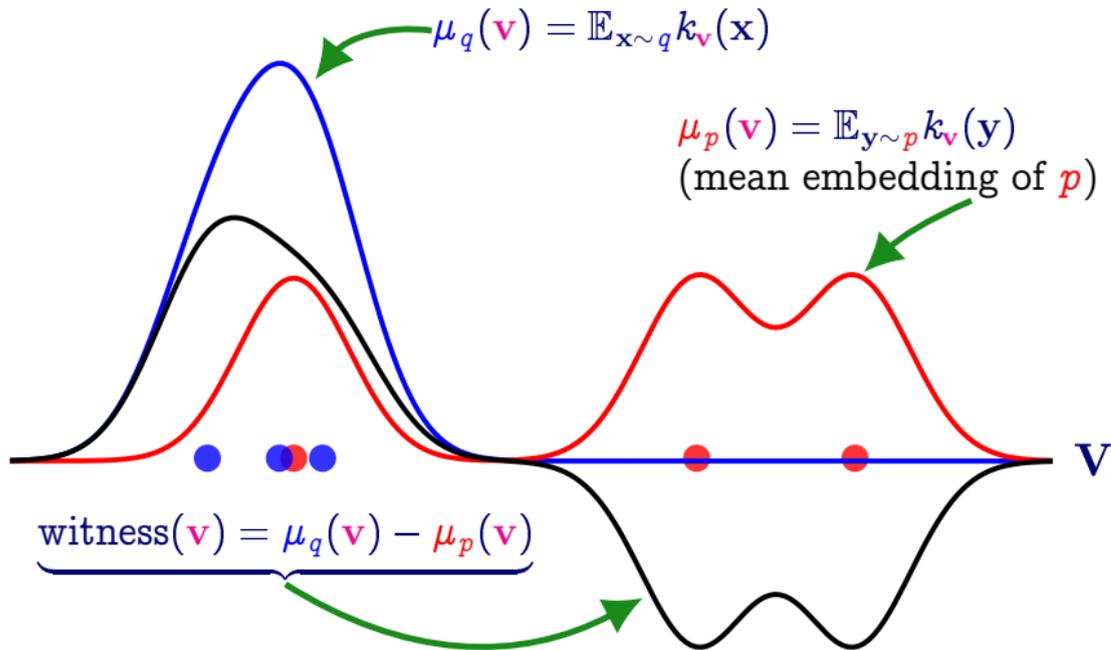




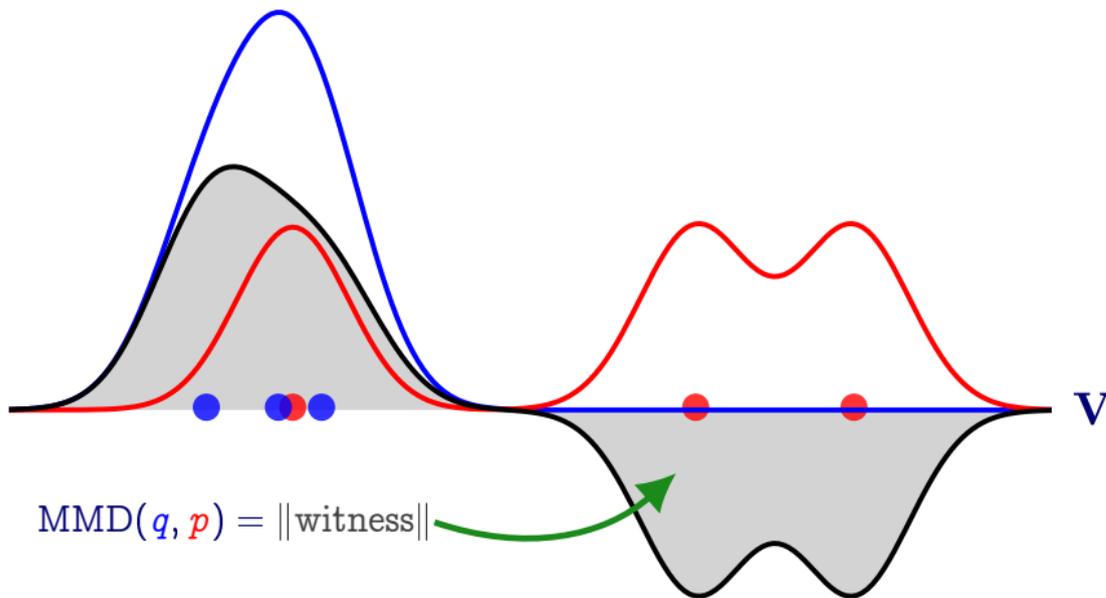
## Maximum Mean Discrepancy (MMD) Witness Function (Gretton et al., 2012)



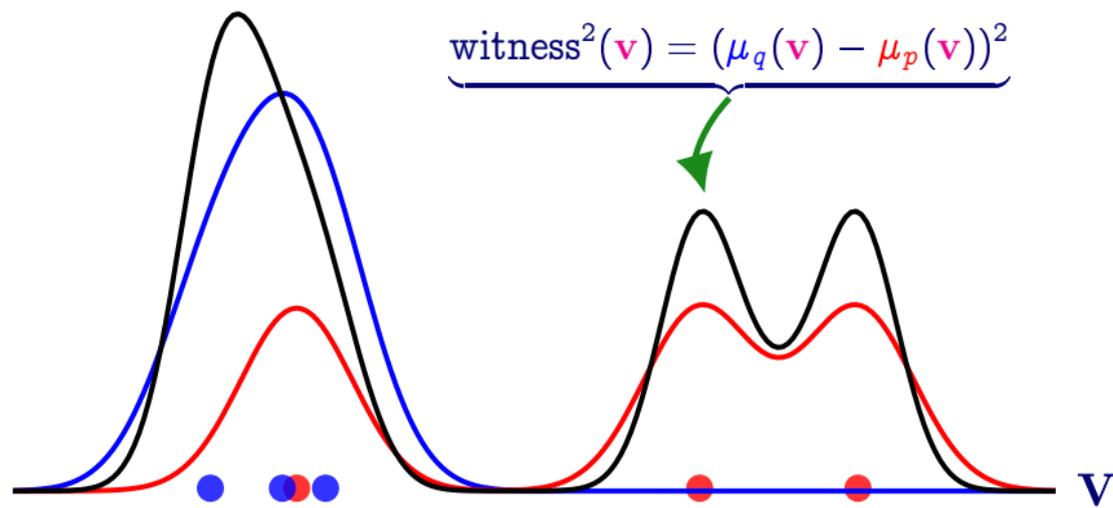
## Maximum Mean Discrepancy (MMD) Witness Function (Gretton et al., 2012)

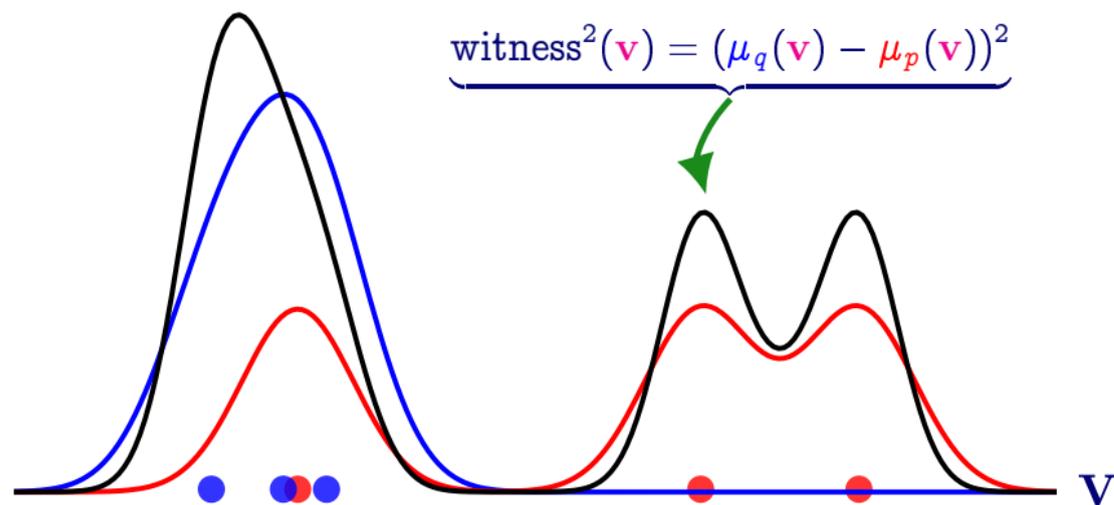


## Maximum Mean Discrepancy (MMD) Witness Function (Gretton et al., 2012)



## Maximum Mean Discrepancy (MMD) Witness Function (Gretton et al., 2012)





■  $\text{witness}^2(\mathbf{v})$  can be used to find a good test location  $\mathbf{v}^* = \star$ .

## Model Criticism by the MMD Witness

- Find a location  $\mathbf{v}$  at which  $q$  and  $p$  differ most (ME test)  
[Jitkrittum et al., 2016].

## Model Criticism by the MMD Witness

- Find a location  $\mathbf{v}$  at which  $q$  and  $p$  differ most (ME test)  
[Jitkrittum et al., 2016].

$$\text{witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q} [ k_{\mathbf{v}}(\mathbf{x}) ] - \mathbb{E}_{\mathbf{y} \sim p} [ k_{\mathbf{v}}(\mathbf{y}) ]$$

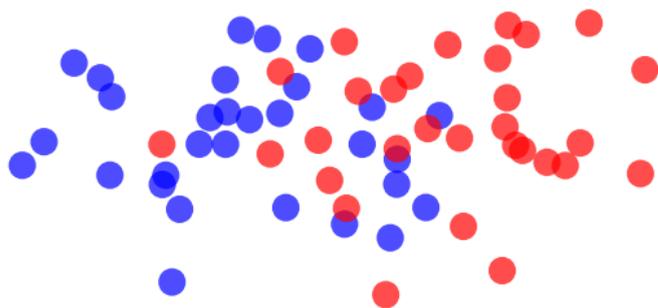
## Model Criticism by the MMD Witness

- Find a location  $\mathbf{v}$  at which  $q$  and  $p$  differ most (ME test)  
[Jitkrittum et al., 2016].

$$\begin{aligned} \text{witness}(\mathbf{v}) &= \mathbb{E}_{\mathbf{x} \sim q} [k_{\mathbf{v}}(\mathbf{x})] - \mathbb{E}_{\mathbf{y} \sim p} [k_{\mathbf{v}}(\mathbf{y})] \\ \text{score}(\mathbf{v}) &= \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})} = \frac{\text{witness}^2(\mathbf{v})}{\sqrt{\mathbb{V}_{\mathbf{x} \sim q} [k_{\mathbf{v}}(\mathbf{x})] + \mathbb{V}_{\mathbf{y} \sim p} [k_{\mathbf{v}}(\mathbf{y})]}}. \end{aligned}$$

## Model Criticism by the MMD Witness

- Find a location  $\mathbf{v}$  at which  $q$  and  $p$  differ most (ME test)  
[Jitkrittum et al., 2016].

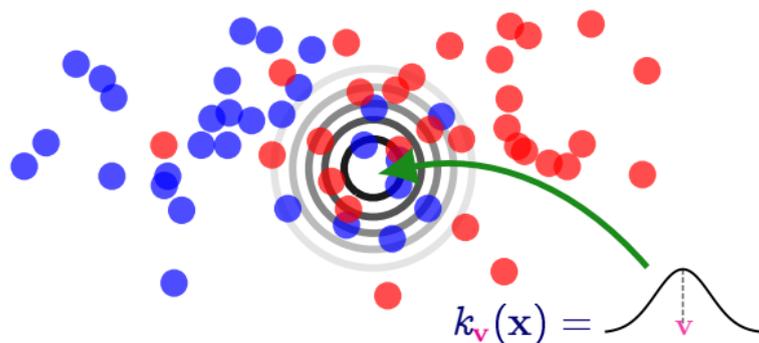


$$\begin{aligned} \text{witness}(\mathbf{v}) &= \mathbb{E}_{\mathbf{x} \sim q} [k_{\mathbf{v}}(\mathbf{x})] - \mathbb{E}_{\mathbf{y} \sim p} [k_{\mathbf{v}}(\mathbf{y})] \\ \text{score}(\mathbf{v}) &= \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})} = \frac{\text{witness}^2(\mathbf{v})}{\sqrt{\mathbb{V}_{\mathbf{x} \sim q} [k_{\mathbf{v}}(\mathbf{x})] + \mathbb{V}_{\mathbf{y} \sim p} [k_{\mathbf{v}}(\mathbf{y})]}}. \end{aligned}$$

## Model Criticism by the MMD Witness

- Find a location  $\mathbf{v}$  at which  $q$  and  $p$  differ most (ME test)  
[Jitkrittum et al., 2016].

score: 0.008

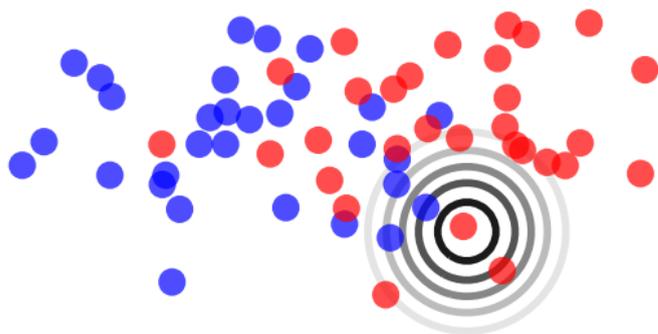


$$\begin{aligned} \text{witness}(\mathbf{v}) &= \mathbb{E}_{\mathbf{x} \sim q} [ k_{\mathbf{v}}(\mathbf{x}) ] - \mathbb{E}_{\mathbf{y} \sim p} [ k_{\mathbf{v}}(\mathbf{y}) ] \\ \text{score}(\mathbf{v}) &= \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})} = \frac{\text{witness}^2(\mathbf{v})}{\sqrt{\mathbb{V}_{\mathbf{x} \sim q} [ k_{\mathbf{v}}(\mathbf{x}) ] + \mathbb{V}_{\mathbf{y} \sim p} [ k_{\mathbf{v}}(\mathbf{y}) ]}}. \end{aligned}$$

## Model Criticism by the MMD Witness

- Find a location  $\mathbf{v}$  at which  $q$  and  $p$  differ most (ME test)  
[Jitkrittum et al., 2016].

score: 1.6

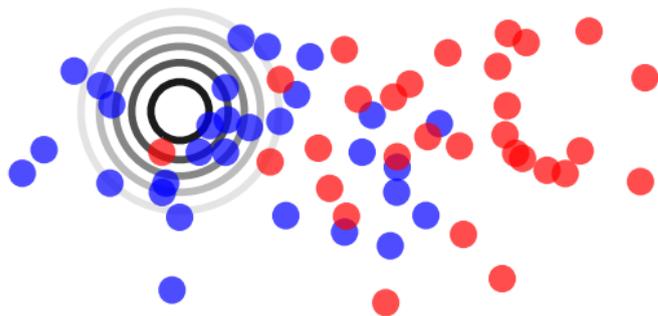


$$\begin{aligned} \text{witness}(\mathbf{v}) &= \mathbb{E}_{\mathbf{x} \sim q} [k_{\mathbf{v}}(\mathbf{x})] - \mathbb{E}_{\mathbf{y} \sim p} [k_{\mathbf{v}}(\mathbf{y})] \\ \text{score}(\mathbf{v}) &= \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})} = \frac{\text{witness}^2(\mathbf{v})}{\sqrt{\mathbb{V}_{\mathbf{x} \sim q} [k_{\mathbf{v}}(\mathbf{x})] + \mathbb{V}_{\mathbf{y} \sim p} [k_{\mathbf{v}}(\mathbf{y})]}}. \end{aligned}$$

## Model Criticism by the MMD Witness

- Find a location  $\mathbf{v}$  at which  $q$  and  $p$  differ most (ME test)  
[Jitkrittum et al., 2016].

score: 13

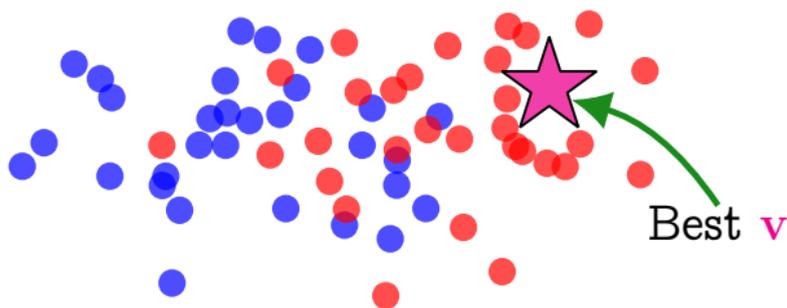


$$\begin{aligned} \text{witness}(\mathbf{v}) &= \mathbb{E}_{\mathbf{x} \sim q} [k_{\mathbf{v}}(\mathbf{x})] - \mathbb{E}_{\mathbf{y} \sim p} [k_{\mathbf{v}}(\mathbf{y})] \\ \text{score}(\mathbf{v}) &= \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})} = \frac{\text{witness}^2(\mathbf{v})}{\sqrt{\mathbb{V}_{\mathbf{x} \sim q} [k_{\mathbf{v}}(\mathbf{x})] + \mathbb{V}_{\mathbf{y} \sim p} [k_{\mathbf{v}}(\mathbf{y})]}}. \end{aligned}$$

## Model Criticism by the MMD Witness

- Find a location  $\mathbf{v}$  at which  $q$  and  $p$  differ most (ME test)  
[Jitkrittum et al., 2016].

score: 25

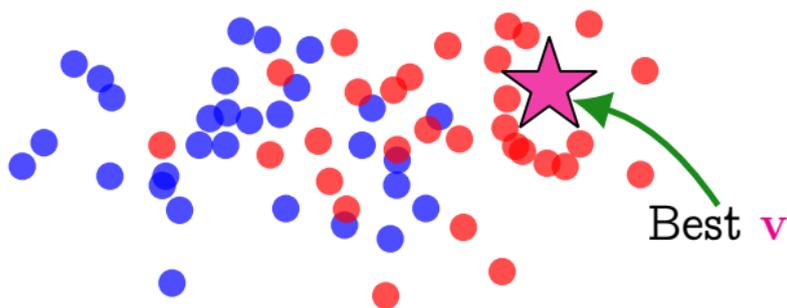


$$\begin{aligned} \text{witness}(\mathbf{v}) &= \mathbb{E}_{\mathbf{x} \sim q} [k_{\mathbf{v}}(\mathbf{x})] - \mathbb{E}_{\mathbf{y} \sim p} [k_{\mathbf{v}}(\mathbf{y})] \\ \text{score}(\mathbf{v}) &= \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})} = \frac{\text{witness}^2(\mathbf{v})}{\sqrt{\mathbb{V}_{\mathbf{x} \sim q} [k_{\mathbf{v}}(\mathbf{x})] + \mathbb{V}_{\mathbf{y} \sim p} [k_{\mathbf{v}}(\mathbf{y})]}}. \end{aligned}$$

## Model Criticism by the MMD Witness

- Find a location  $\mathbf{v}$  at which  $q$  and  $p$  differ most (ME test)  
[Jitkrittum et al., 2016].

score: 25



$$\begin{aligned} \text{witness}(\mathbf{v}) &= \mathbb{E}_{\mathbf{x} \sim q} [k_{\mathbf{v}}(\mathbf{x})] - \mathbb{E}_{\mathbf{y} \sim p} [k_{\mathbf{v}}(\mathbf{y})] \\ \text{score}(\mathbf{v}) &= \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})} = \end{aligned}$$

No sample from  $p$ .  
Difficult to generate.

## The Stein Witness Function [Liu et al., 2016, Chwialkowski et al., 2016]

**Problem:** No sample from  $p$ . Cannot estimate  $\mathbb{E}_{\mathbf{y} \sim p}[k_{\mathbf{v}}(\mathbf{y})]$ .

## The Stein Witness Function [Liu et al., 2016, Chwialkowski et al., 2016]

**Problem:** No sample from  $p$ . Cannot estimate  $\mathbb{E}_{\mathbf{y} \sim p}[k_{\mathbf{v}}(\mathbf{y})]$ .

$$\text{(Stein) witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q} [ T_p k_{\mathbf{v}}(\mathbf{x}) ] - \mathbb{E}_{\mathbf{y} \sim p} [ T_p k_{\mathbf{v}}(\mathbf{y}) ]$$

## The Stein Witness Function [Liu et al., 2016, Chwialkowski et al., 2016]

**Problem:** No sample from  $p$ . Cannot estimate  $\mathbb{E}_{\mathbf{y} \sim p}[k_{\mathbf{v}}(\mathbf{y})]$ .

$$\text{(Stein) witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q} [T_p \text{ --- } \mathbf{v}] - \mathbb{E}_{\mathbf{y} \sim p} [T_p \text{ --- } \mathbf{v}]$$

## The Stein Witness Function [Liu et al., 2016, Chwialkowski et al., 2016]

**Problem:** No sample from  $p$ . Cannot estimate  $\mathbb{E}_{\mathbf{y} \sim p}[k_{\mathbf{v}}(\mathbf{y})]$ .

$$\text{(Stein) witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q} \left[ \text{graph of } k_{\mathbf{v}}(\mathbf{x}) \right] - \mathbb{E}_{\mathbf{y} \sim p} \left[ \text{graph of } k_{\mathbf{v}}(\mathbf{y}) \right]$$

## The Stein Witness Function [Liu et al., 2016, Chwialkowski et al., 2016]

**Problem:** No sample from  $p$ . Cannot estimate  $\mathbb{E}_{\mathbf{y} \sim p}[k_{\mathbf{v}}(\mathbf{y})]$ .

(Stein) witness( $\mathbf{v}$ ) =  $\mathbb{E}_{\mathbf{x} \sim q}$  [  ] -  ~~$\mathbb{E}_{\mathbf{y} \sim p}$  [  ]~~

**Idea:** Define  $T_p$  such that  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_{\mathbf{v}})(\mathbf{y}) = 0$ , for any  $\mathbf{v}$ .

## The Stein Witness Function [Liu et al., 2016, Chwialkowski et al., 2016]

**Problem:** No sample from  $p$ . Cannot estimate  $\mathbb{E}_{\mathbf{y} \sim p}[k_{\mathbf{v}}(\mathbf{y})]$ .

$$\text{(Stein) witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q} [ \text{---} ]$$


**Idea:** Define  $T_p$  such that  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_{\mathbf{v}})(\mathbf{y}) = 0$ , for any  $\mathbf{v}$ .

## The Stein Witness Function [Liu et al., 2016, Chwialkowski et al., 2016]

**Problem:** No sample from  $p$ . Cannot estimate  $\mathbb{E}_{\mathbf{y} \sim p}[k_{\mathbf{v}}(\mathbf{y})]$ .

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

**Idea:** Define  $T_p$  such that  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_{\mathbf{v}})(\mathbf{y}) = 0$ , for any  $\mathbf{v}$ .

## The Stein Witness Function [Liu et al., 2016, Chwialkowski et al., 2016]

**Problem:** No sample from  $p$ . Cannot estimate  $\mathbb{E}_{\mathbf{y} \sim p}[k_{\mathbf{v}}(\mathbf{y})]$ .

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

**Idea:** Define  $T_p$  such that  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_{\mathbf{v}})(\mathbf{y}) = 0$ , for any  $\mathbf{v}$ .

**Proposal:** Good  $\mathbf{v}$  should have high

$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## The Stein Witness Function [Liu et al., 2016, Chwialkowski et al., 2016]

**Problem:** No sample from  $p$ . Cannot estimate  $\mathbb{E}_{\mathbf{y} \sim p}[k_{\mathbf{v}}(\mathbf{y})]$ .

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

**Idea:** Define  $T_p$  such that  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_{\mathbf{v}})(\mathbf{y}) = 0$ , for any  $\mathbf{v}$ .

**Proposal:** Good  $\mathbf{v}$  should have high

$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

signal-to-noise  
ratio



## The Stein Witness Function [Liu et al., 2016, Chwialkowski et al., 2016]

**Problem:** No sample from  $p$ . Cannot estimate  $\mathbb{E}_{\mathbf{y} \sim p}[k_{\mathbf{v}}(\mathbf{y})]$ .

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

**Idea:** Define  $T_p$  such that  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_{\mathbf{v}})(\mathbf{y}) = 0$ , for any  $\mathbf{v}$ .

**Proposal:** Good  $\mathbf{v}$  should have high

$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

signal-to-noise  
ratio



- $\text{score}(\mathbf{v})$  can be estimated in linear-time.

## The Stein Witness Function [Liu et al., 2016, Chwialkowski et al., 2016]

**Problem:** No sample from  $p$ . Cannot estimate  $\mathbb{E}_{\mathbf{y} \sim p}[k_{\mathbf{v}}(\mathbf{y})]$ .

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

**Idea:** Define  $T_p$  such that  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_{\mathbf{v}})(\mathbf{y}) = 0$ , for any  $\mathbf{v}$ .

**Proposal:** Good  $\mathbf{v}$  should have high

$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

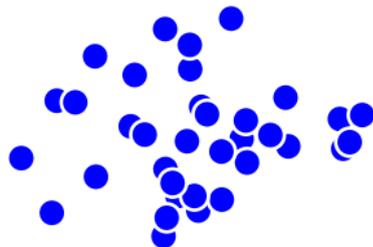
signal-to-noise  
ratio

■  $\text{score}(\mathbf{v})$  can be estimated in linear-time.

**Goodness-of-fit test:**

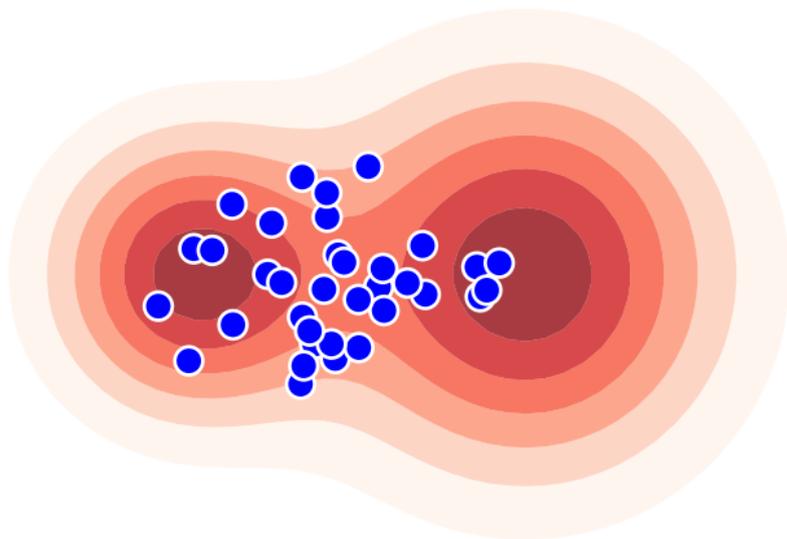
- 1 Find  $\mathbf{v}^* = \arg \max_{\mathbf{v}} \text{score}(\mathbf{v})$ .
- 2 Reject  $H_0$  if  $\text{witness}^2(\mathbf{v}^*) > \text{threshold}$ .

## Proposal: Model Criticism with the Stein Witness



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

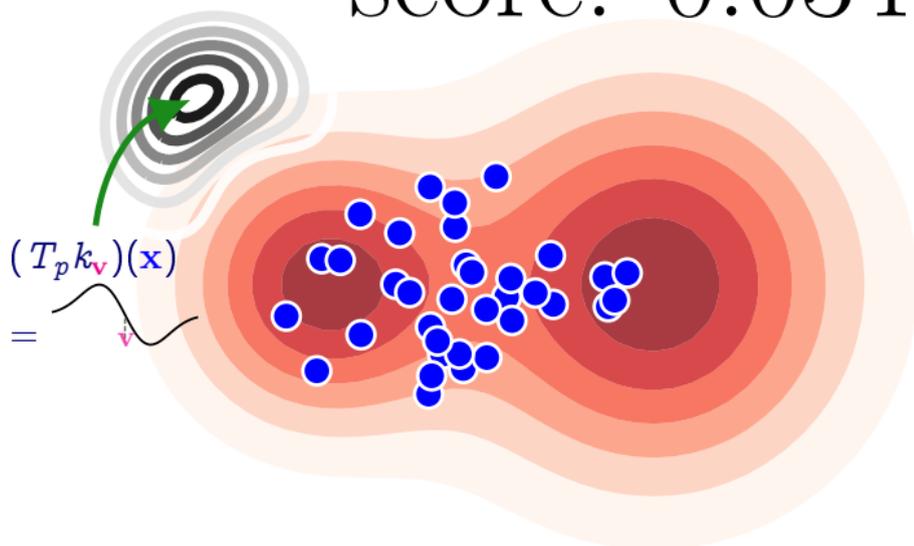
## Proposal: Model Criticism with the Stein Witness



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

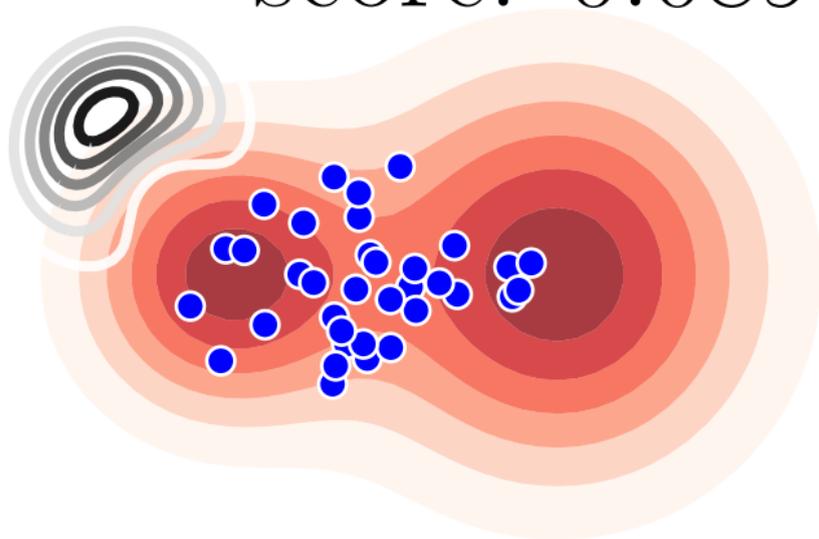
score: 0.034



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

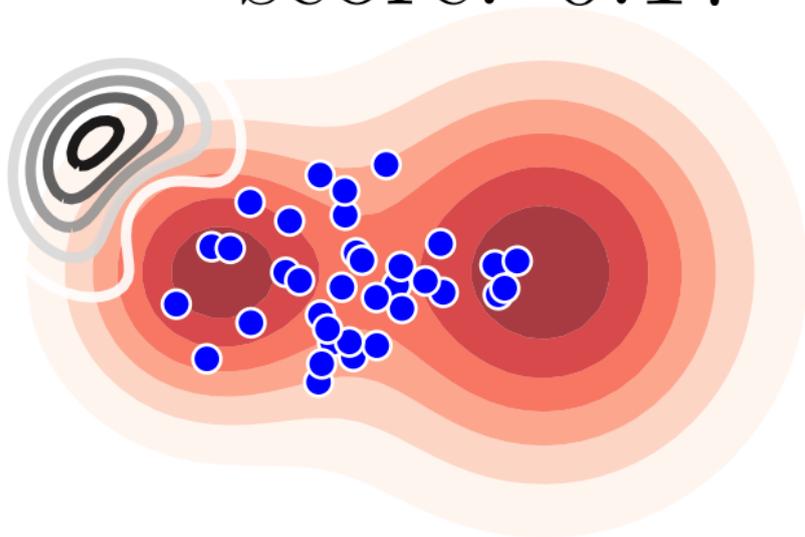
score: 0.089



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

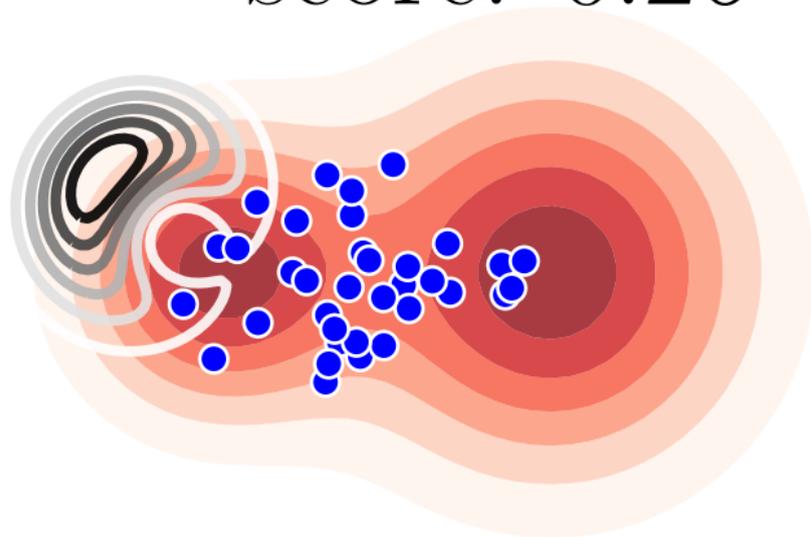
score: 0.17



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

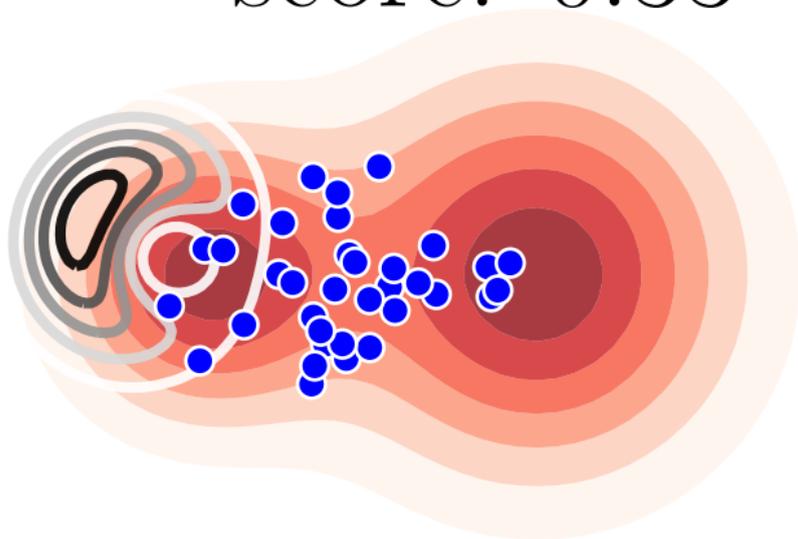
score: 0.26



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

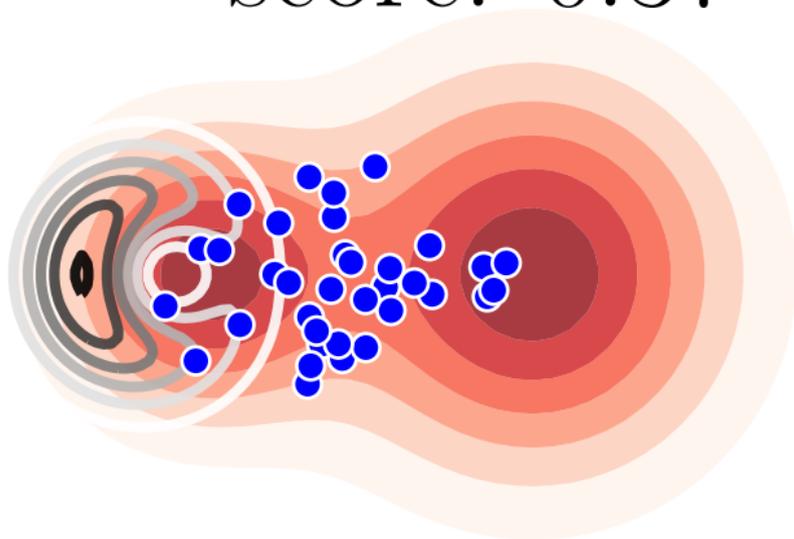
score: 0.33



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

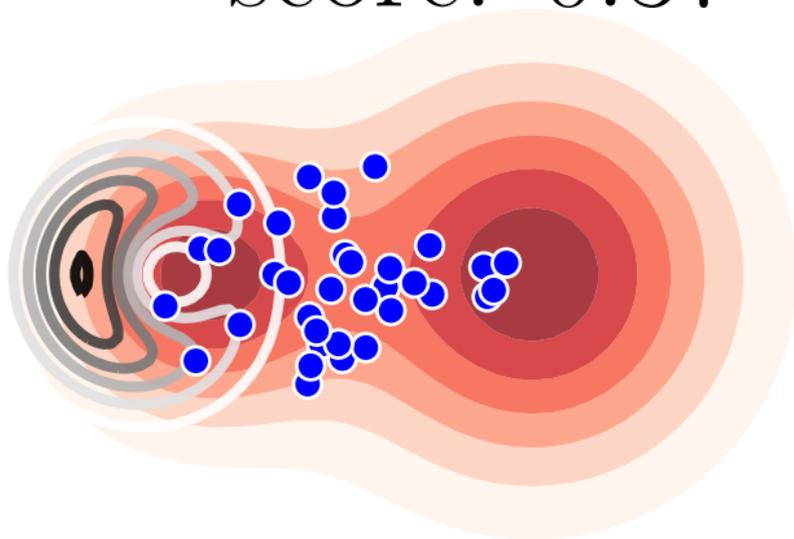
score: 0.37



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

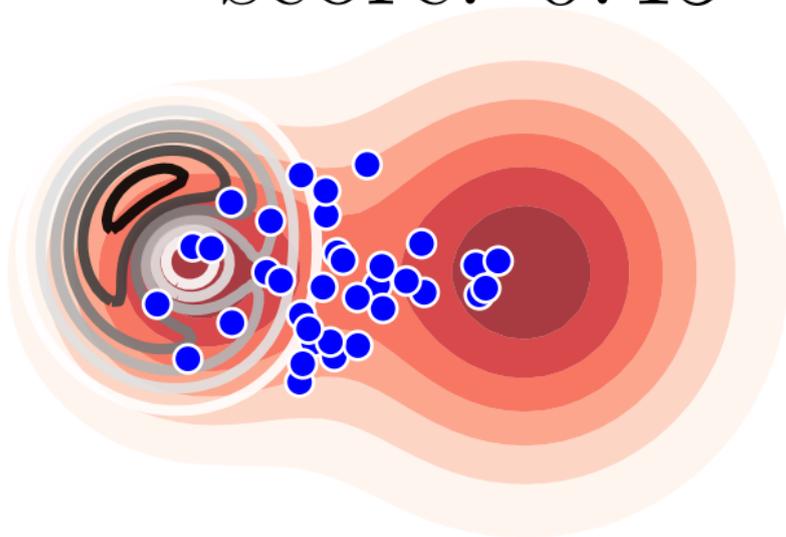
score: 0.37



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

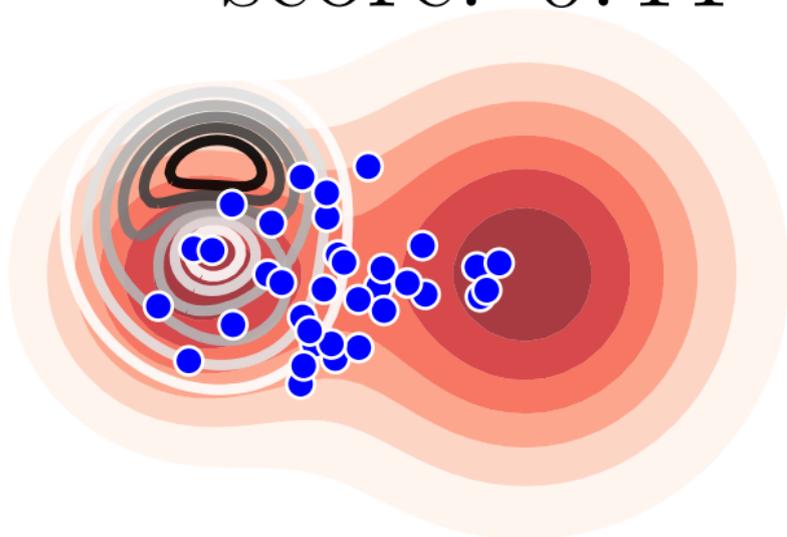
score: 0.45



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

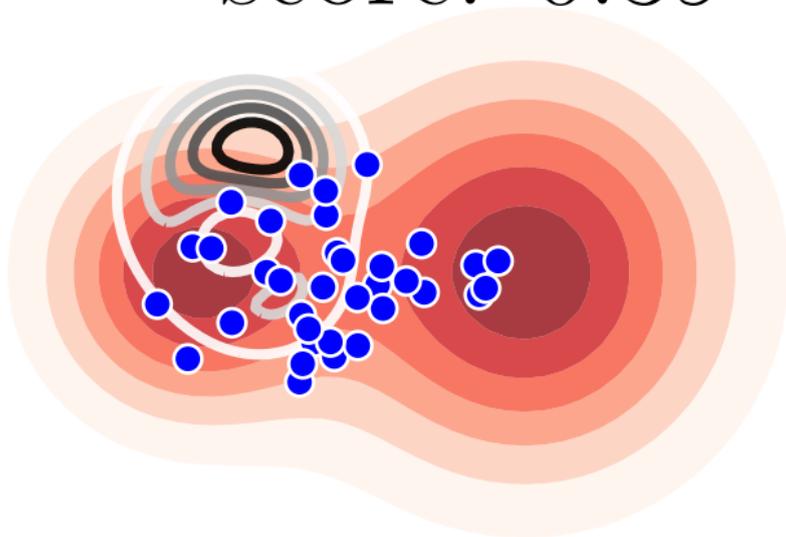
score: 0.44



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

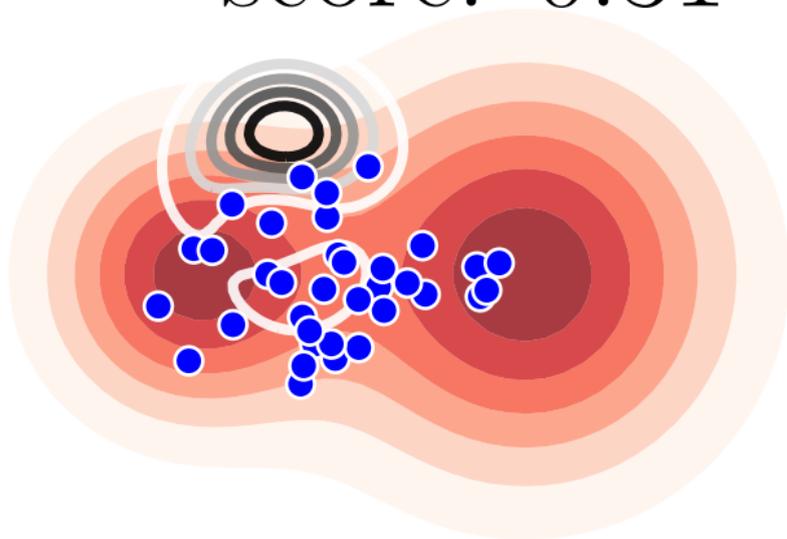
score: 0.39



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

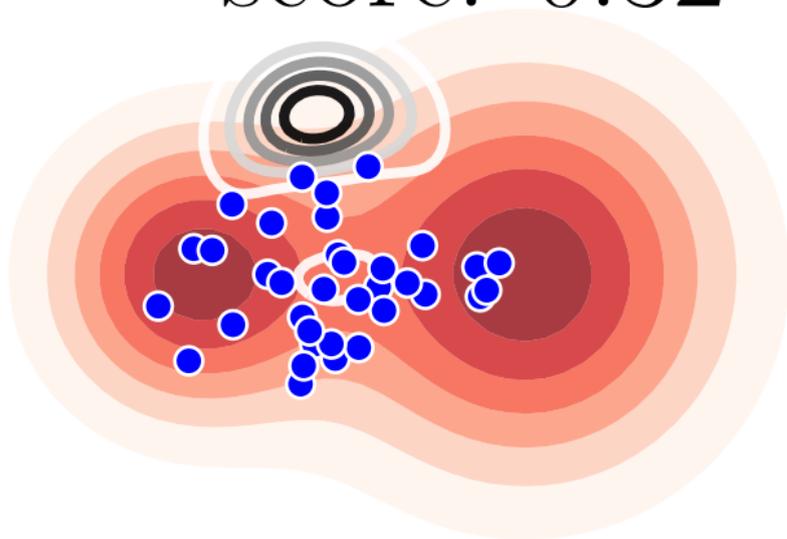
score: 0.31



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

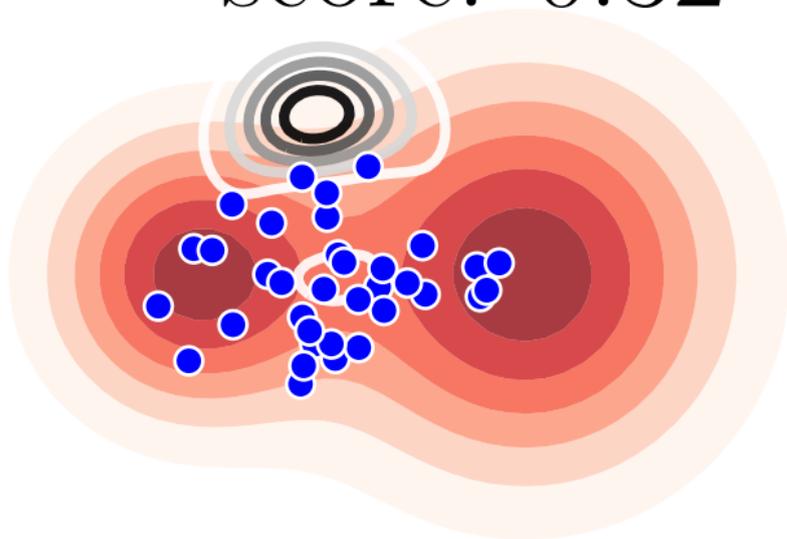
score: 0.32



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

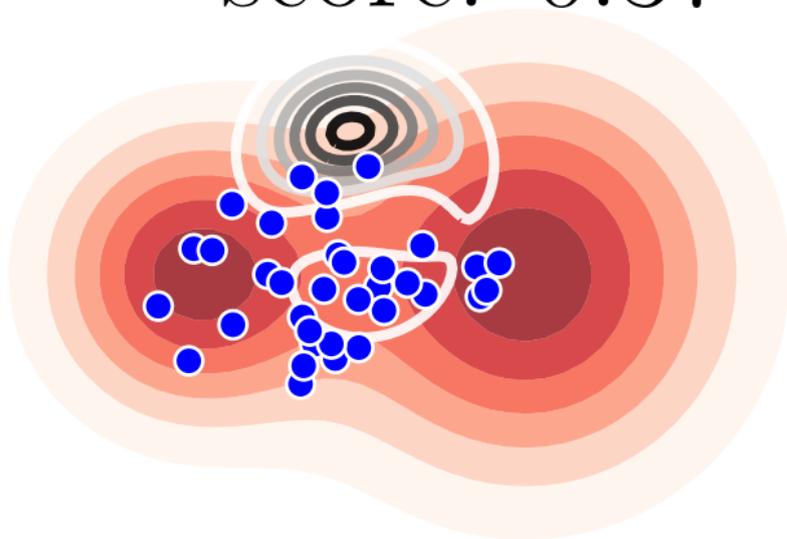
score: 0.32



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

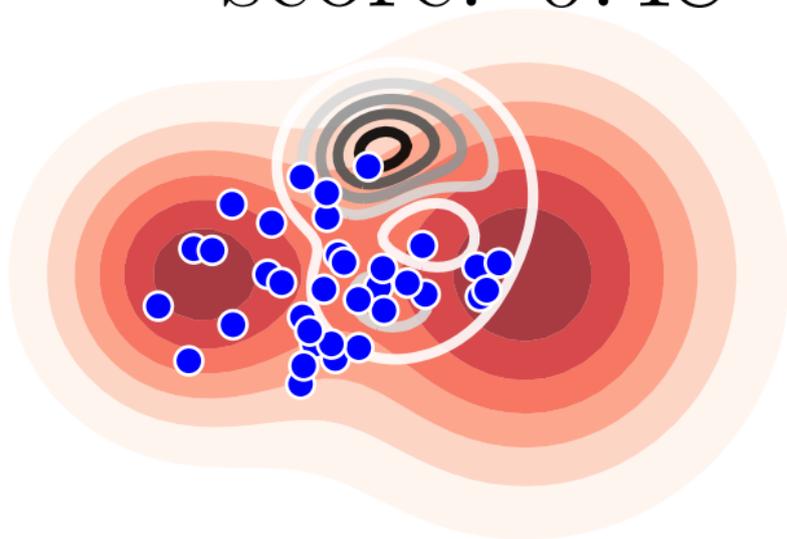
score: 0.37



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

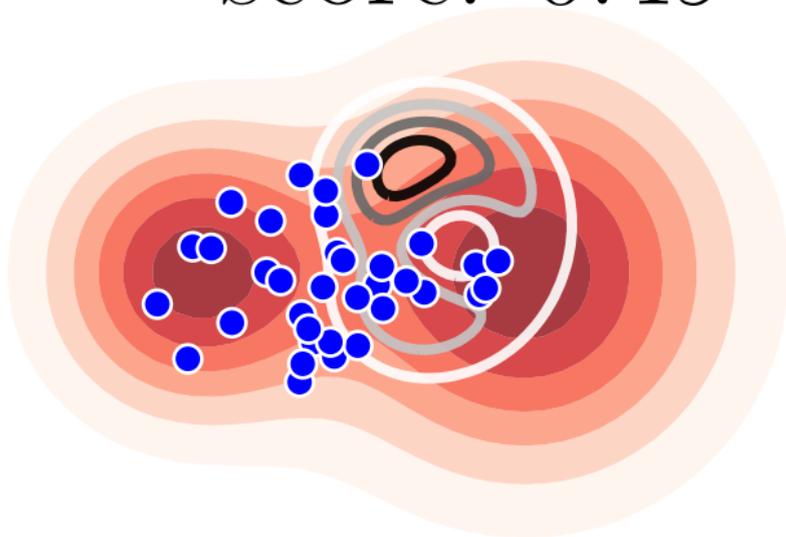
score: 0.48



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

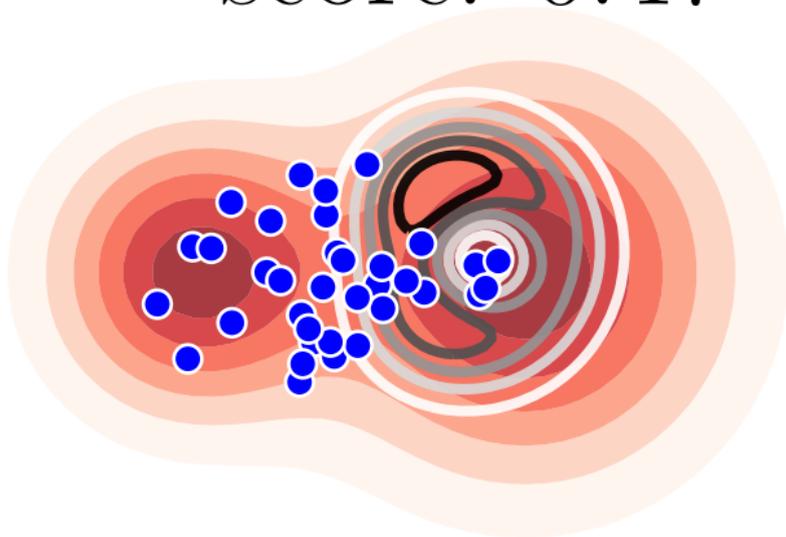
score: 0.49



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

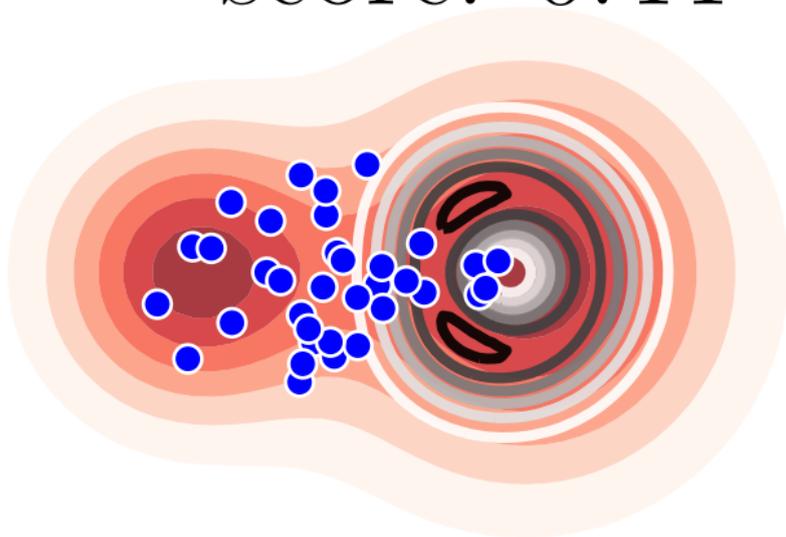
score: 0.47



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

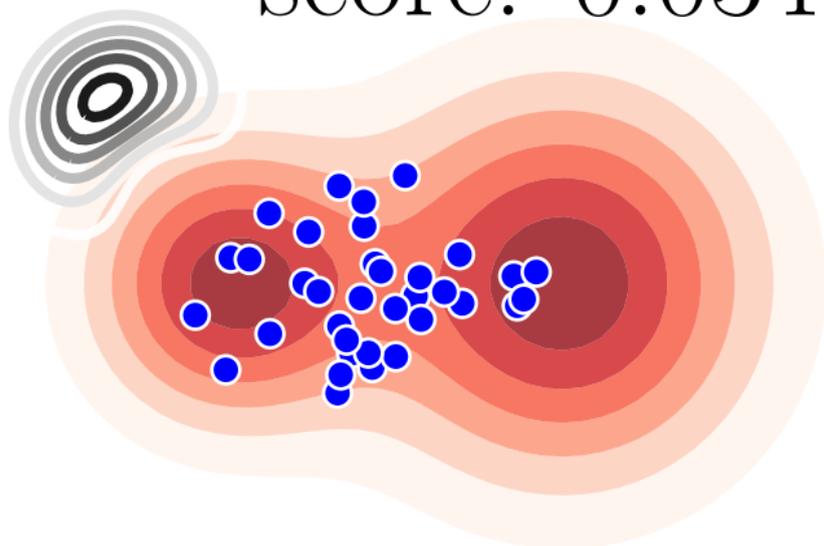
score: 0.44



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

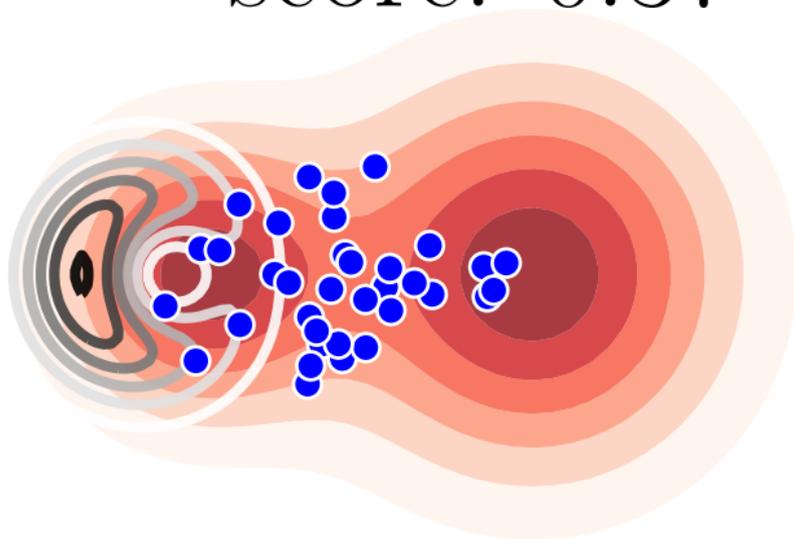
score: 0.034



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

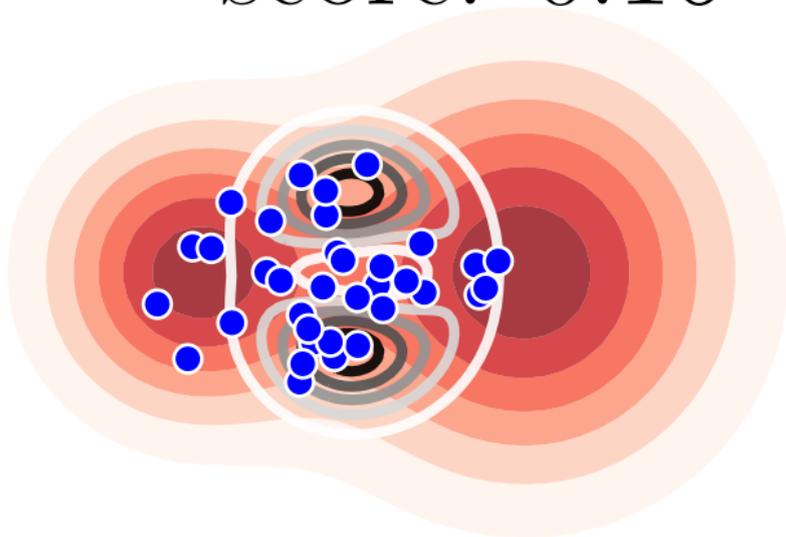
score: 0.37



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

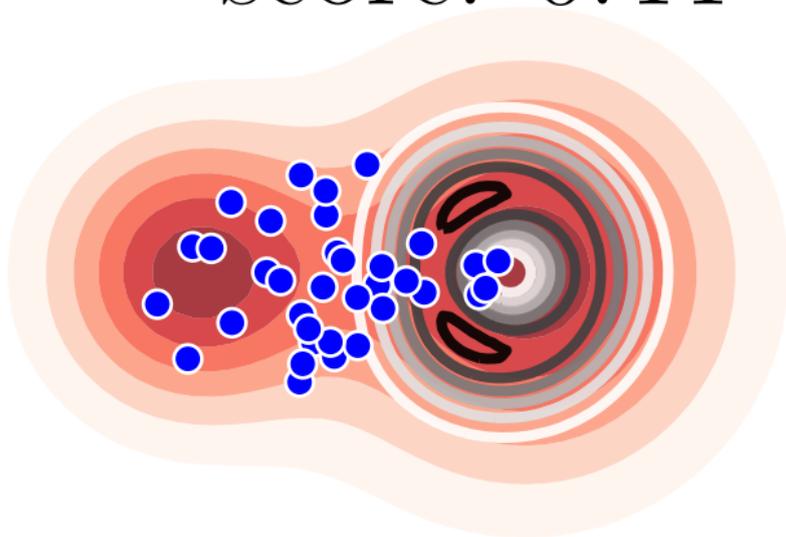
score: 0.16



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

## Proposal: Model Criticism with the Stein Witness

score: 0.44



$$\text{score}(\mathbf{v}) = \frac{\text{witness}^2(\mathbf{v})}{\text{noise}(\mathbf{v})}.$$

# Theory

- 1 What is  $T_p k_v$ ?
- 2 Test statistic
- 3 Distributions of the test statistic, test threshold.
- 4 What does  $\mathbf{v}^* = \arg \max_{\mathbf{v}} \text{score}(\mathbf{v})$  do theoretically?

# (1) What is $T_p k_v$ ?

Recall  $\text{witness}(v) = \mathbb{E}_{x \sim q}(T_p k_v)(x) - \mathbb{E}_{y \sim p}(T_p k_v)(y)$

## (1) What is $T_p k_v$ ?

Recall  $\text{witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q}(T_p k_v)(\mathbf{x}) - \mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y})$

$$(T_p k_v)(\mathbf{y}) = \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})].$$

Then,  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y}) = 0$ .

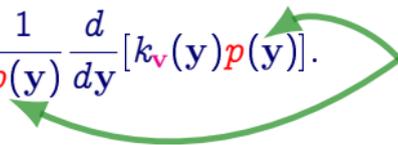
[Liu et al., 2016, Chwialkowski et al., 2016]

## (1) What is $T_p k_v$ ?

Recall  $\text{witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q}(T_p k_v)(\mathbf{x}) - \mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y})$

$$(T_p k_v)(\mathbf{y}) = \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y}) p(\mathbf{y})].$$

Normalizer  
cancels



Then,  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y}) = 0$ .

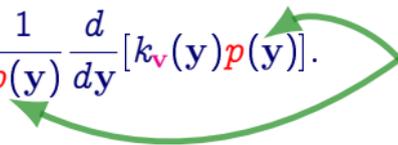
[Liu et al., 2016, Chwialkowski et al., 2016]

## (1) What is $T_p k_v$ ?

Recall  $\text{witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q}(T_p k_v)(\mathbf{x}) - \mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y})$

$$(T_p k_v)(\mathbf{y}) = \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y}) p(\mathbf{y})].$$

Normalizer  
cancels



Then,  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y}) = 0$ .

[Liu et al., 2016, Chwialkowski et al., 2016]

**Proof:**

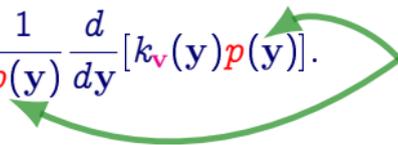
$$\mathbb{E}_{\mathbf{y} \sim p} [(T_p k_v)(\mathbf{y})]$$

# (1) What is $T_p k_v$ ?

Recall  $\text{witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q}(T_p k_v)(\mathbf{x}) - \mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y})$

$$(T_p k_v)(\mathbf{y}) = \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y}) p(\mathbf{y})].$$

Normalizer cancels



Then,  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y}) = 0$ .

[Liu et al., 2016, Chwialkowski et al., 2016]

**Proof:**

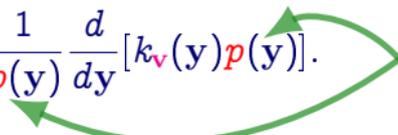
$$\mathbb{E}_{\mathbf{y} \sim p} [(T_p k_v)(\mathbf{y})] = \int_{-\infty}^{\infty} [(T_p k_v)(\mathbf{y})] p(\mathbf{y}) d\mathbf{y}$$

## (1) What is $T_p k_v$ ?

Recall  $\text{witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q}(T_p k_v)(\mathbf{x}) - \mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y})$

$$(T_p k_v)(\mathbf{y}) = \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})].$$

Normalizer  
cancels



Then,  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y}) = 0$ .

[Liu et al., 2016, Chwialkowski et al., 2016]

**Proof:**

$$\mathbb{E}_{\mathbf{y} \sim p} [(T_p k_v)(\mathbf{y})] = \int_{-\infty}^{\infty} \left[ \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})] \right] p(\mathbf{y}) d\mathbf{y}$$

# (1) What is $T_p k_v$ ?

Recall  $\text{witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q}(T_p k_v)(\mathbf{x}) - \mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y})$

$$(T_p k_v)(\mathbf{y}) = \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y}) p(\mathbf{y})].$$

Normalizer  
cancels

Then,  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y}) = 0$ .

[Liu et al., 2016, Chwialkowski et al., 2016]

**Proof:**

$$\mathbb{E}_{\mathbf{y} \sim p} [(T_p k_v)(\mathbf{y})] = \int_{-\infty}^{\infty} \left[ \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y}) p(\mathbf{y})] \right] p(\mathbf{y}) d\mathbf{y}$$

# (1) What is $T_p k_v$ ?

Recall  $\text{witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q}(T_p k_v)(\mathbf{x}) - \mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y})$

$$(T_p k_v)(\mathbf{y}) = \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})].$$

Normalizer  
cancels

Then,  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y}) = 0$ .

[Liu et al., 2016, Chwialkowski et al., 2016]

**Proof:**

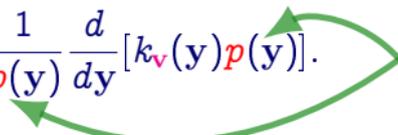
$$\begin{aligned} \mathbb{E}_{\mathbf{y} \sim p} [(T_p k_v)(\mathbf{y})] &= \int_{-\infty}^{\infty} \left[ \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})] \right] p(\mathbf{y}) d\mathbf{y} \\ &= \int_{-\infty}^{\infty} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})] d\mathbf{y} \end{aligned}$$

# (1) What is $T_p k_v$ ?

Recall  $\text{witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q}(T_p k_v)(\mathbf{x}) - \mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y})$

$$(T_p k_v)(\mathbf{y}) = \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})].$$

Normalizer cancels



Then,  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y}) = 0$ .

[Liu et al., 2016, Chwialkowski et al., 2016]

**Proof:**

$$\begin{aligned} \mathbb{E}_{\mathbf{y} \sim p} [(T_p k_v)(\mathbf{y})] &= \int_{-\infty}^{\infty} \left[ \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})] \right] p(\mathbf{y}) d\mathbf{y} \\ &= \int_{-\infty}^{\infty} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})] d\mathbf{y} \\ &= [k_v(\mathbf{y})p(\mathbf{y})]_{\mathbf{y}=-\infty}^{\mathbf{y}=\infty} \end{aligned}$$

# (1) What is $T_p k_v$ ?

Recall  $\text{witness}(\mathbf{v}) = \mathbb{E}_{\mathbf{x} \sim q}(T_p k_v)(\mathbf{x}) - \mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y})$

$$(T_p k_v)(\mathbf{y}) = \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})].$$

Normalizer  
cancels

Then,  $\mathbb{E}_{\mathbf{y} \sim p}(T_p k_v)(\mathbf{y}) = 0$ .

[Liu et al., 2016, Chwialkowski et al., 2016]

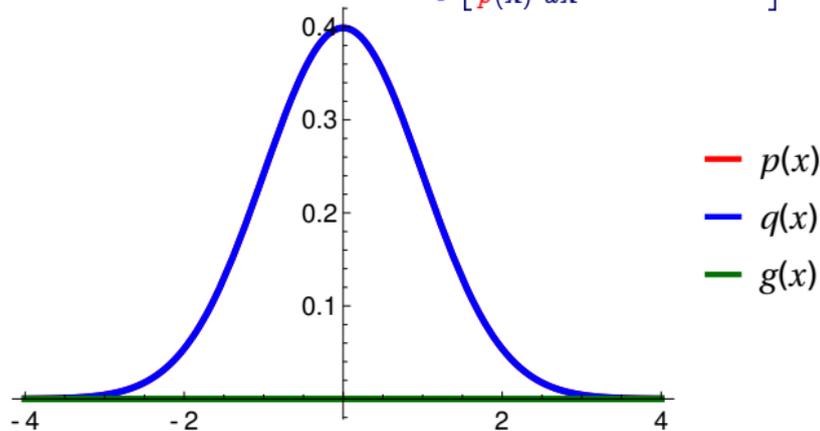
**Proof:**

$$\begin{aligned} \mathbb{E}_{\mathbf{y} \sim p} [(T_p k_v)(\mathbf{y})] &= \int_{-\infty}^{\infty} \left[ \frac{1}{p(\mathbf{y})} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})] \right] p(\mathbf{y}) d\mathbf{y} \\ &= \int_{-\infty}^{\infty} \frac{d}{d\mathbf{y}} [k_v(\mathbf{y})p(\mathbf{y})] d\mathbf{y} \\ &= [k_v(\mathbf{y})p(\mathbf{y})]_{\mathbf{y}=-\infty}^{\mathbf{y}=\infty} \\ &= 0 \end{aligned}$$

(assume  $\lim_{|\mathbf{y}| \rightarrow \infty} k_v(\mathbf{y})p(\mathbf{y})$ )

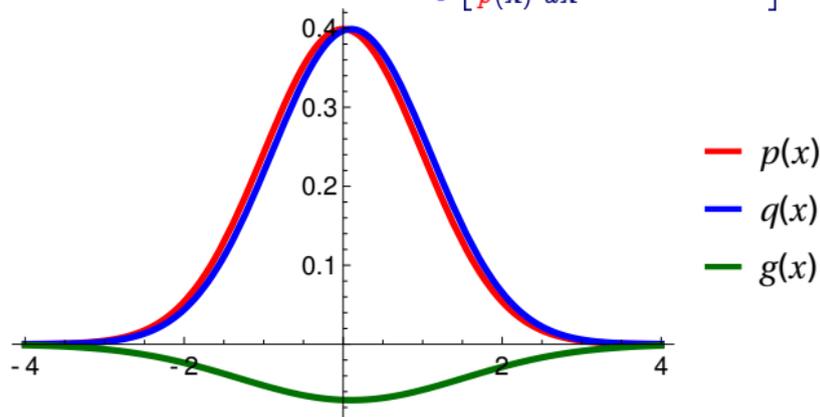
## (2) Proposal: The Finite Set Stein Discrepancy (FSSD)

- Recall Stein witness:  $g(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right]$ .



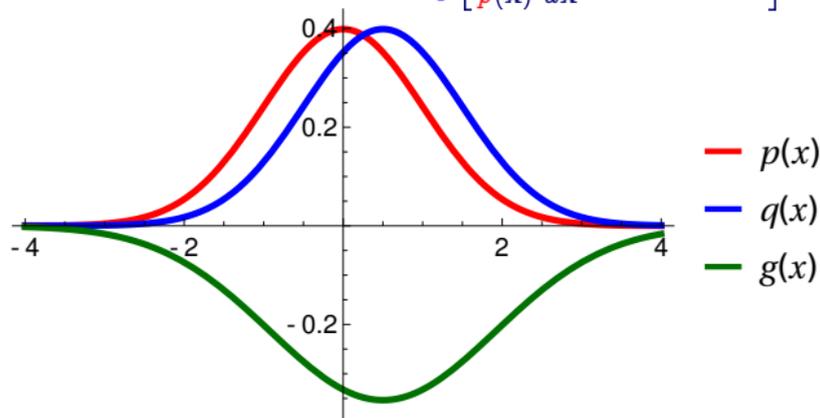
## (2) Proposal: The Finite Set Stein Discrepancy (FSSD)

- Recall Stein witness:  $g(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right]$ .



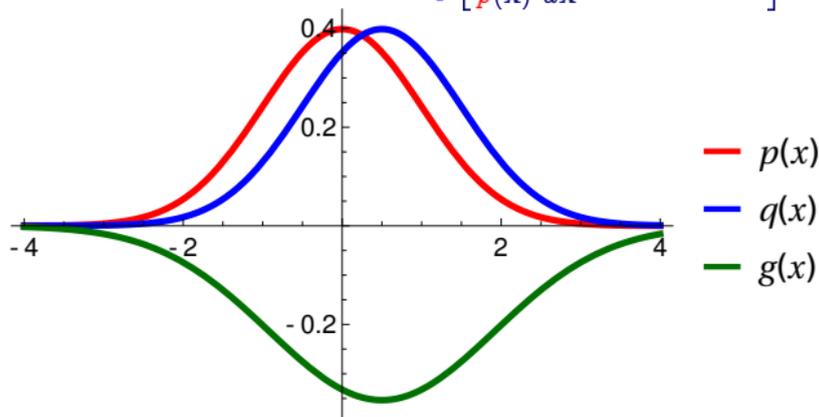
## (2) Proposal: The Finite Set Stein Discrepancy (FSSD)

- Recall Stein witness:  $g(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right]$ .



## (2) Proposal: The Finite Set Stein Discrepancy (FSSD)

- Recall Stein witness:  $\mathbf{g}(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right]$ .



- FSSD statistic: Evaluate  $g^2$  at  $J$  test locations  $V = \{\mathbf{v}_1, \dots, \mathbf{v}_J\}$ .
- Population FSSD

$$\text{FSSD}^2 = \frac{1}{dJ} \sum_{j=1}^J \|\mathbf{g}(\mathbf{v}_j)\|_2^2.$$

- Unbiased estimator  $\widehat{\text{FSSD}}^2$  computable in  $\mathcal{O}(d^2 Jn)$  time. ( $d$  = input dimension)

## (2) FSSD is a Discrepancy Measure

$$\blacksquare \text{FSSD}^2 = \frac{1}{dJ} \sum_{j=1}^J \|\mathbf{g}(\mathbf{v}_j)\|_2^2.$$

**Theorem 1 (FSSD is a discrepancy measure).**

*Main conditions:*

- 1 (*Nice kernel*) Kernel  $k$  is  $C_0$ -universal, and *real analytic* e.g., Gaussian kernel.
- 2 (*Vanishing boundary*)  $\lim_{\|\mathbf{x}\| \rightarrow \infty} p(\mathbf{x})k_{\mathbf{v}}(\mathbf{x}) = 0$ .
- 3 (*Avoid "blind spots"*) Locations  $\mathbf{v}_1, \dots, \mathbf{v}_J \sim \eta$  which has a density.

Then, for any  $J \geq 1$ ,  $\eta$ -almost surely,

$$\text{FSSD}^2 = 0 \iff p = q.$$

**Summary:** Evaluating the witness at random locations is sufficient to detect the discrepancy between  $p, q$ .

## (2) What Are “Blind Spots”?

$$\text{Recall } g(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right].$$

Consider  $p = \mathcal{N}(0, 1)$  and  $q = \mathcal{N}(0, \sigma_q^2)$ . Use unit-width Gaussian kernel.

$$g(v) = \frac{v \exp\left(-\frac{v^2}{2+2\sigma_q^2}\right) (\sigma_q^2 - 1)}{(1 + \sigma_q^2)^{3/2}}$$

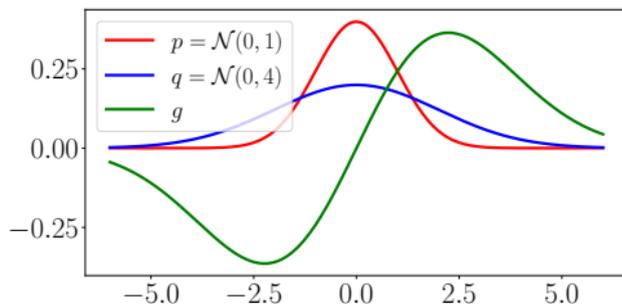
- If  $v = 0$ , then  $\text{FSSD}^2 = g^2(v) = 0$  regardless of  $\sigma_q^2$ .
- If  $g \neq 0$ , and  $k$  is real analytic,  $R = \{v \mid g(v) = 0\}$  (blind spots) has 0 Lebesgue measure.
- So, if  $v \sim$  a distribution with a density, then  $v \notin R$ .

## (2) What Are “Blind Spots”?

$$\text{Recall } g(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right].$$

Consider  $p = \mathcal{N}(0, 1)$  and  $q = \mathcal{N}(0, \sigma_q^2)$ . Use unit-width Gaussian kernel.

$$g(v) = \frac{v \exp\left(-\frac{v^2}{2+2\sigma_q^2}\right) (\sigma_q^2 - 1)}{(1 + \sigma_q^2)^{3/2}}$$



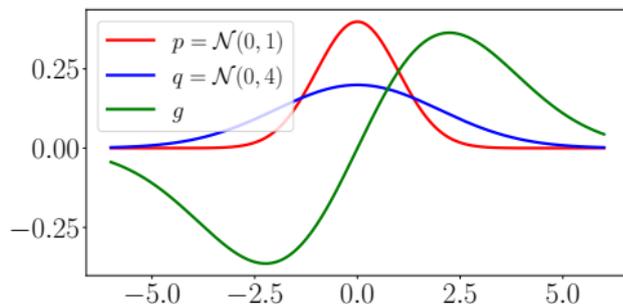
- If  $v = 0$ , then  $\text{FSSD}^2 = g^2(v) = 0$  regardless of  $\sigma_q^2$ .
- If  $g \neq 0$ , and  $k$  is real analytic,  $R = \{v \mid g(v) = 0\}$  (blind spots) has 0 Lebesgue measure.
- So, if  $v \sim$  a distribution with a density, then  $v \notin R$ .

## (2) What Are “Blind Spots”?

$$\text{Recall } g(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right].$$

Consider  $p = \mathcal{N}(0, 1)$  and  $q = \mathcal{N}(0, \sigma_q^2)$ . Use unit-width Gaussian kernel.

$$g(v) = \frac{v \exp\left(-\frac{v^2}{2+2\sigma_q^2}\right) (\sigma_q^2 - 1)}{(1 + \sigma_q^2)^{3/2}}$$



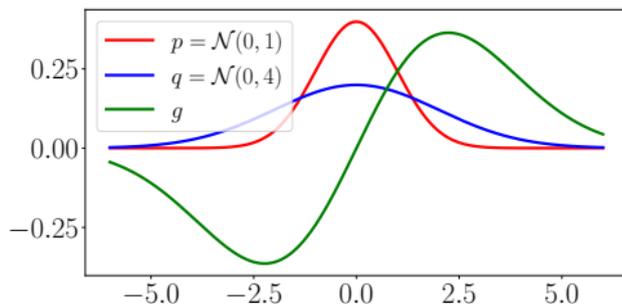
- If  $v = 0$ , then  $\text{FSSD}^2 = g^2(v) = 0$  regardless of  $\sigma_q^2$ .
- If  $g \neq 0$ , and  $k$  is real analytic,  $R = \{v \mid g(v) = 0\}$  (blind spots) has 0 Lebesgue measure.
- So, if  $v \sim$  a distribution with a density, then  $v \notin R$ .

## (2) What Are “Blind Spots”?

$$\text{Recall } g(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right].$$

Consider  $p = \mathcal{N}(0, 1)$  and  $q = \mathcal{N}(0, \sigma_q^2)$ . Use unit-width Gaussian kernel.

$$g(v) = \frac{v \exp\left(-\frac{v^2}{2+2\sigma_q^2}\right) (\sigma_q^2 - 1)}{(1 + \sigma_q^2)^{3/2}}$$



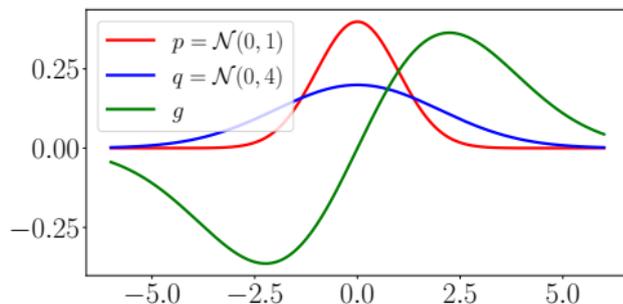
- If  $v = 0$ , then  $\text{FSSD}^2 = g^2(v) = 0$  regardless of  $\sigma_q^2$ .
- If  $g \neq 0$ , and  $k$  is real analytic,  $R = \{v \mid g(v) = 0\}$  (blind spots) has 0 Lebesgue measure.
- So, if  $v \sim$  a distribution with a density, then  $v \notin R$ .

## (2) What Are “Blind Spots”?

$$\text{Recall } g(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right].$$

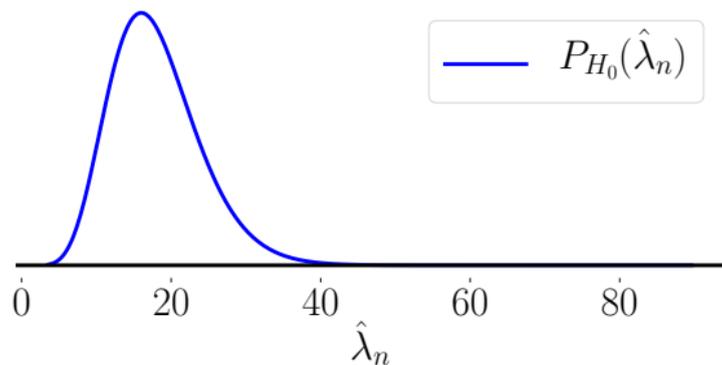
Consider  $p = \mathcal{N}(0, 1)$  and  $q = \mathcal{N}(0, \sigma_q^2)$ . Use unit-width Gaussian kernel.

$$g(v) = \frac{v \exp\left(-\frac{v^2}{2+2\sigma_q^2}\right) (\sigma_q^2 - 1)}{(1 + \sigma_q^2)^{3/2}}$$

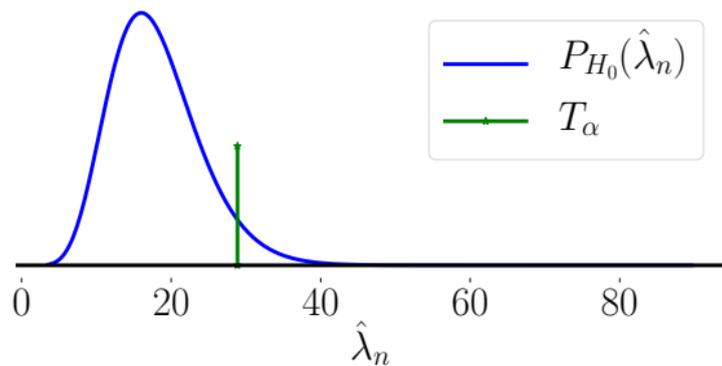


- If  $v = 0$ , then  $\text{FSSD}^2 = g^2(v) = 0$  regardless of  $\sigma_q^2$ .
- If  $g \neq 0$ , and  $k$  is real analytic,  $R = \{v \mid g(v) = 0\}$  (blind spots) has 0 Lebesgue measure.
- So, if  $v \sim$  a distribution with a density, then  $v \notin R$ .

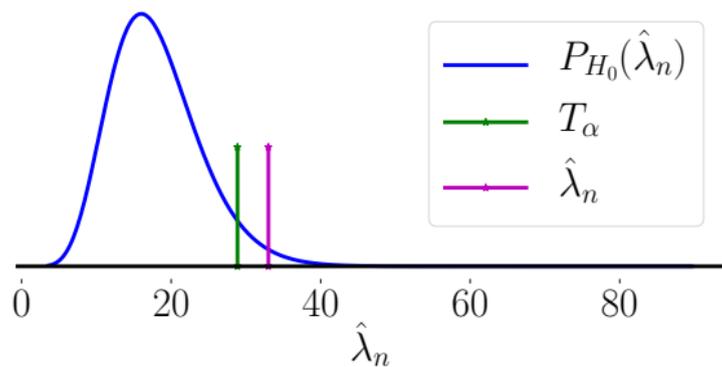
(3) Asymptotic Distributions of  $\hat{\lambda}_n := n\widehat{\text{FSSD}}^2$



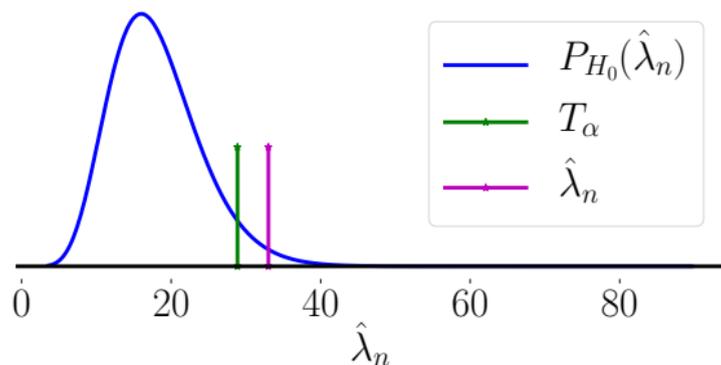
(3) Asymptotic Distributions of  $\hat{\lambda}_n := n\widehat{\text{FSSD}}^2$



### (3) Asymptotic Distributions of $\hat{\lambda}_n := n\widehat{\text{FSSD}}^2$



### (3) Asymptotic Distributions of $\hat{\lambda}_n := n\widehat{\text{FSSD}}^2$

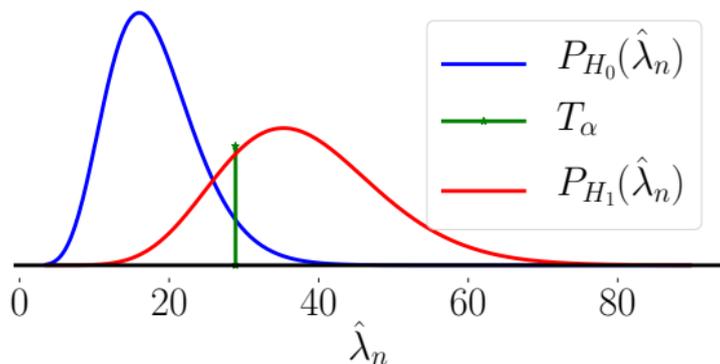


- Under  $H_0 : p = q$ , asymptotically

$$\hat{\lambda}_n := n\widehat{\text{FSSD}}^2 \xrightarrow{d} \sum_{i=1}^{dJ} (Z_i^2 - 1)\omega_i,$$

- $\{\omega_i\}_{i=1}^{dJ}$  are non-negative, computable quantities.  
 $Z_1, \dots, Z_{dJ} \stackrel{i.i.d.}{\sim} \mathcal{N}(0, 1)$

### (3) Asymptotic Distributions of $\hat{\lambda}_n := n\widehat{\text{FSSD}}^2$



- Under  $H_0 : p = q$ , asymptotically

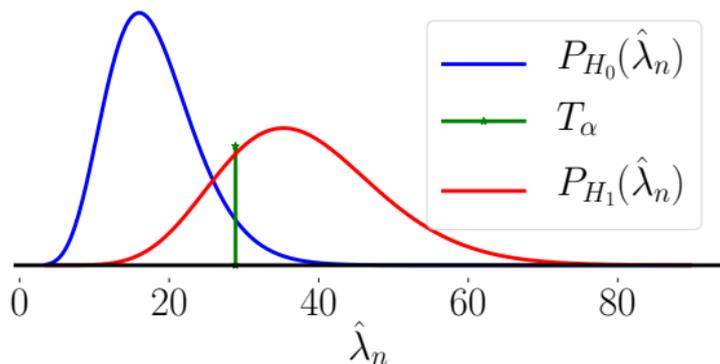
$$\hat{\lambda}_n := n\widehat{\text{FSSD}}^2 \xrightarrow{d} \sum_{i=1}^{dJ} (Z_i^2 - 1)\omega_i,$$

- $\{\omega_i\}_{i=1}^{dJ}$  are non-negative, computable quantities.

$$Z_1, \dots, Z_{dJ} \stackrel{i.i.d.}{\sim} \mathcal{N}(0, 1)$$

- Under  $H_1 : p \neq q$ , asymptotically  $\sqrt{n}(\widehat{\text{FSSD}}^2 - \text{FSSD}^2) \xrightarrow{d} \mathcal{N}(0, \sigma_{H_1}^2)$ .

### (3) Asymptotic Distributions of $\hat{\lambda}_n := n\widehat{\text{FSSD}}^2$



- Under  $H_0 : p = q$ , asymptotically

$$\hat{\lambda}_n := n\widehat{\text{FSSD}}^2 \xrightarrow{d} \sum_{i=1}^{dJ} (Z_i^2 - 1)\omega_i,$$

- $\{\omega_i\}_{i=1}^{dJ}$  are non-negative, computable quantities.

$$Z_1, \dots, Z_{dJ} \stackrel{i.i.d.}{\sim} \mathcal{N}(0, 1)$$

- Under  $H_1 : p \neq q$ , asymptotically  $\sqrt{n}(\widehat{\text{FSSD}}^2 - \text{FSSD}^2) \xrightarrow{d} \mathcal{N}(0, \sigma_{H_1}^2)$ .

witness<sup>2</sup>(V)

noise(V)

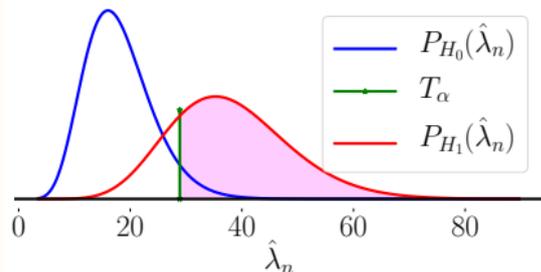
#### (4) What Does $\arg \max_{\mathbf{v}} \text{score}(\mathbf{v})$ Do?

##### Proposition 1 (Asymptotic test power).

For large  $n$ , the test power  $\mathbb{P}(\text{reject } H_0 \mid H_1 \text{ true}) =$

$$\begin{aligned} & \mathbb{P}_{H_1}(n\widehat{\text{FSSD}}^2 > T_\alpha) \\ & \approx \Phi\left(\sqrt{n}\frac{\text{FSSD}^2}{\sigma_{H_1}} - \frac{T_\alpha}{\sqrt{n}\sigma_{H_1}}\right), \end{aligned}$$

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



- For large  $n$ , the 2<sup>nd</sup> term dominates.

$$\arg \max_{V, \sigma_k^2} \mathbb{P}_{H_1}(n\widehat{\text{FSSD}}^2 > T_\alpha) \approx \arg \max_{V, \sigma_k^2} \left[ \frac{\widehat{\text{FSSD}}^2}{\widehat{\sigma}_{H_1}} = \text{score}(V, \sigma_k^2) \right].$$

Maximize  $\text{score}(V, \sigma_k^2) \iff$  Maximize test power

- In practice, split  $\{\mathbf{x}_i\}_{i=1}^n$  into independent training/test sets. Optimize on **tr**. Goodness-of-fit test on **te**.

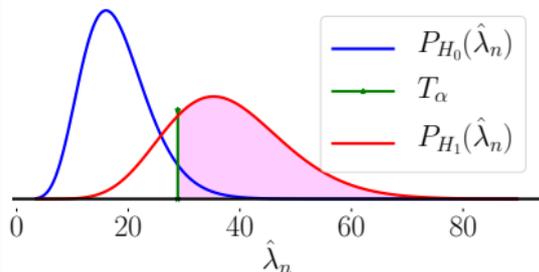
#### (4) What Does $\arg \max_v \text{score}(v)$ Do?

##### Proposition 1 (Asymptotic test power).

For large  $n$ , the test power  $\mathbb{P}(\text{reject } H_0 \mid H_1 \text{ true}) =$

$$\begin{aligned} & \mathbb{P}_{H_1}(n\widehat{\text{FSSD}}^2 > T_\alpha) \\ & \approx \Phi\left(\sqrt{n}\frac{\widehat{\text{FSSD}}}{\widehat{\sigma}_{H_1}} - \frac{T_\alpha}{\sqrt{n}\sigma_{H_1}}\right), \end{aligned}$$

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



- For large  $n$ , the  $2^{\text{nd}}$  term dominates.

$$\arg \max_{V, \sigma_k^2} \mathbb{P}_{H_1}(n\widehat{\text{FSSD}}^2 > T_\alpha) \approx \arg \max_{V, \sigma_k^2} \left[ \frac{\widehat{\text{FSSD}}^2}{\widehat{\sigma}_{H_1}} = \text{score}(V, \sigma_k^2) \right].$$

Maximize  $\text{score}(V, \sigma_k^2) \iff$  Maximize test power

- In practice, split  $\{\mathbf{x}_i\}_{i=1}^n$  into independent training/test sets. Optimize on *tr*. Goodness-of-fit test on *te*.

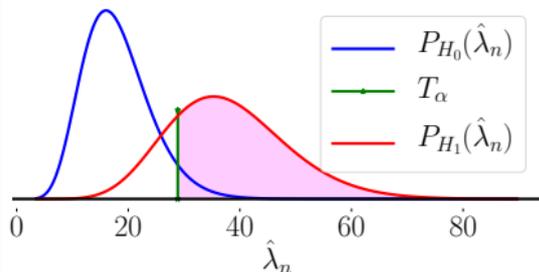
#### (4) What Does $\arg \max_v \text{score}(v)$ Do?

##### Proposition 1 (Asymptotic test power).

For large  $n$ , the test power  $\mathbb{P}(\text{reject } H_0 \mid H_1 \text{ true}) =$

$$\begin{aligned} & \mathbb{P}_{H_1}(n\widehat{\text{FSSD}}^2 > T_\alpha) \\ & \approx \Phi\left(\sqrt{n} \frac{\text{FSSD}^2}{\sigma_{H_1}} - \frac{T_\alpha}{\sqrt{n}\sigma_{H_1}}\right), \end{aligned}$$

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



- For large  $n$ , the  $2^{\text{nd}}$  term dominates.

$$\arg \max_{V, \sigma_k^2} \mathbb{P}_{H_1}(n\widehat{\text{FSSD}}^2 > T_\alpha) \approx \arg \max_{V, \sigma_k^2} \left[ \frac{\widehat{\text{FSSD}}^2}{\widehat{\sigma}_{H_1}} = \text{score}(V, \sigma_k^2) \right].$$

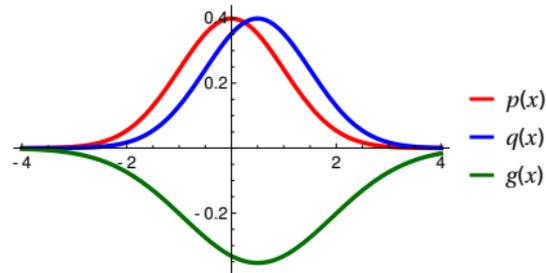
Maximize  $\text{score}(V, \sigma_k^2) \iff$  Maximize test power

- In practice, split  $\{\mathbf{x}_i\}_{i=1}^n$  into independent training/test sets. Optimize on **tr**. Goodness-of-fit test on **te**.

# Related Works

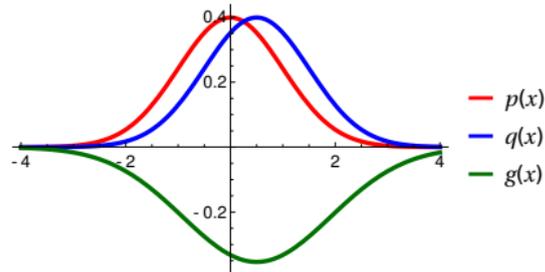
- Recall Stein witness:

$$\mathbf{g}(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right].$$

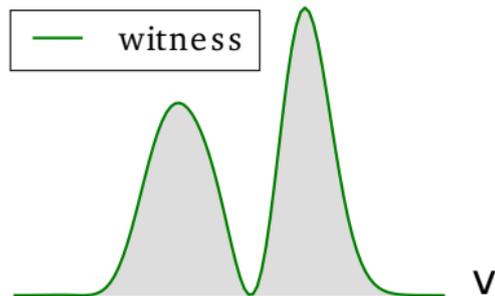


- Recall Stein witness:

$$\mathbf{g}(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right].$$



KSD



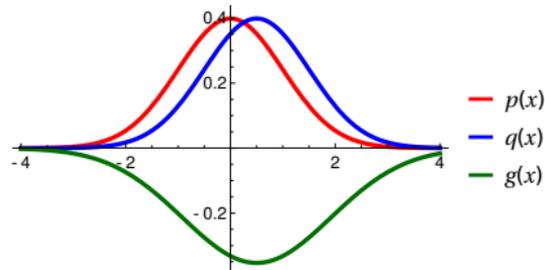
$$\text{KSD}^2 = \|\mathbf{g}\|_{\text{RKHS}}^2 \text{ (RKHS norm).}$$

Good when the difference between

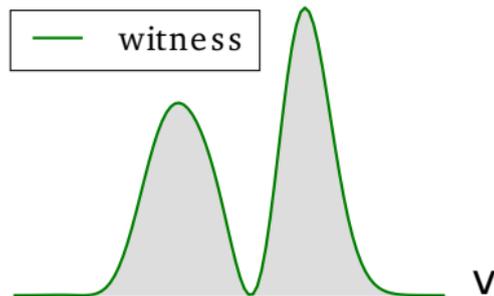
$p, q$  is spatially diffuse.

■ Recall Stein witness:

$$\mathbf{g}(\mathbf{v}) := \mathbb{E}_{\mathbf{x} \sim q} \left[ \frac{1}{p(\mathbf{x})} \frac{d}{d\mathbf{x}} [k_{\mathbf{v}}(\mathbf{x}) p(\mathbf{x})] \right].$$



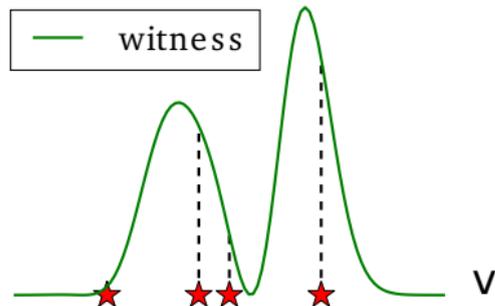
**KSD**



$$\text{KSD}^2 = \|\mathbf{g}\|_{\text{RKHS}}^2 \text{ (RKHS norm).}$$

Good when the difference between  $p, q$  is spatially diffuse.

**Proposed FSSD**



$$\text{FSSD}^2 = \frac{1}{dJ} \sum_{j=1}^J \|\mathbf{g}(\mathbf{v}_j)\|_2^2.$$

Good when the difference between  $p, q$  is local.

## Kernel Stein Discrepancy (KSD)

Closed-form expression for KSD: [Liu et al., 2016, Chwialkowski et al., 2016]

$$\text{KSD}^2 = \|\mathbf{g}\|_{\text{RKHS}}^2 = \overbrace{\mathbb{E}_{\mathbf{x} \sim q} \mathbb{E}_{\mathbf{y} \sim q}}^{\text{double sums}} h_p(\mathbf{x}, \mathbf{y})$$

where

$$\begin{aligned} h_p(\mathbf{x}, \mathbf{y}) := & [\partial_{\mathbf{x}} \log p(\mathbf{x})] k(\mathbf{x}, \mathbf{y}) [\partial_{\mathbf{y}} \log p(\mathbf{y})] \\ & + [\partial_{\mathbf{y}} \log p(\mathbf{y})] \partial_{\mathbf{x}} k(\mathbf{x}, \mathbf{y}) \\ & + [\partial_{\mathbf{x}} \log p(\mathbf{x})] \partial_{\mathbf{y}} k(\mathbf{x}, \mathbf{y}) \\ & + \partial_{\mathbf{x}} \partial_{\mathbf{y}} k(\mathbf{x}, \mathbf{y}) \end{aligned}$$

and  $k$  is a kernel.

- ✗ The “double sums” make it  $\mathcal{O}(d^2 n^2)$ . Slow.

## Kernel Stein Discrepancy (KSD)

Closed-form expression for KSD: [Liu et al., 2016, Chwialkowski et al., 2016]

$$\text{KSD}^2 = \|\mathbf{g}\|_{\text{RKHS}}^2 = \overbrace{\mathbb{E}_{\mathbf{x} \sim q} \mathbb{E}_{\mathbf{y} \sim q}}^{\text{double sums}} h_p(\mathbf{x}, \mathbf{y})$$

where

$$\begin{aligned} h_p(\mathbf{x}, \mathbf{y}) := & [\partial_{\mathbf{x}} \log p(\mathbf{x})] k(\mathbf{x}, \mathbf{y}) [\partial_{\mathbf{y}} \log p(\mathbf{y})] \\ & + [\partial_{\mathbf{y}} \log p(\mathbf{y})] \partial_{\mathbf{x}} k(\mathbf{x}, \mathbf{y}) \\ & + [\partial_{\mathbf{x}} \log p(\mathbf{x})] \partial_{\mathbf{y}} k(\mathbf{x}, \mathbf{y}) \\ & + \partial_{\mathbf{x}} \partial_{\mathbf{y}} k(\mathbf{x}, \mathbf{y}) \end{aligned}$$

and  $k$  is a kernel.

- ✗ The “double sums” make it  $\mathcal{O}(d^2 n^2)$ . Slow.

## Linear-Time Kernel Stein Discrepancy (LKS)

- [Liu et al., 2016] also proposed a linear version of KSD.
- For  $\{\mathbf{x}_i\}_{i=1}^n \sim q$ , KSD test statistic is

$$\frac{2}{n(n-1)} \sum_{i < j} h_p(\mathbf{x}_i, \mathbf{x}_j).$$

	1	2	3	4	5	6	7	8
1	gray							
2	green	gray						
3	green	green	gray					
4	green	green	green	gray				
5	green	green	green	green	gray			
6	green	green	green	green	green	gray		
7	green	green	green	green	green	green	gray	
8	green	gray						

- LKS test statistic is a “running average”

$$\frac{2}{n} \sum_{i=1}^{n/2} h_p(\mathbf{x}_{2i-1}, \mathbf{x}_{2i}).$$

	1	2	3	4	5	6	7	8
1	gray							
2	green	gray						
3			gray					
4			green	gray				
5					gray			
6					green	gray		
7							gray	
8							green	gray

- Both unbiased. LKS has  $\mathcal{O}(d^2 n)$  runtime. Same as proposed FSSD.
- ~~X~~ LKS has high variance. Poor test power.

## Simulation Settings

- Gaussian kernel  $k(\mathbf{x}, \mathbf{v}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{v}\|_2^2}{2\sigma_k^2}\right)$

	Method	Description
1	<b>FSSD-opt</b>	Proposed. With optimization. $J = 5$ .
2	<b>FSSD-rand</b>	Proposed. Random test locations.
3	<b>KSD</b>	Quadratic-time kernel Stein discrepancy [Liu et al., 2016, Chwialkowski et al., 2016]
4	<b>LKS</b>	Linear-time running average version of KSD.
5	<b>MMD-opt</b>	MMD two-sample test [Gretton et al., 2012]. With optimization.
6	<b>ME-test</b>	<u>M</u> ean <u>E</u> mbeddings two-sample test [Jitkrittum et al., 2016]. With optimization.

- Two-sample tests need to draw sample from  $p$ .
- Tests with optimization use 20% of the data.
- Significance level  $\alpha = 0.05$ .

## Simulation Settings

- Gaussian kernel  $k(\mathbf{x}, \mathbf{v}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{v}\|_2^2}{2\sigma_k^2}\right)$

	Method	Description
1	<b>FSSD-opt</b>	Proposed. With optimization. $J = 5$ .
2	<b>FSSD-rand</b>	Proposed. Random test locations.
3	<b>KSD</b>	Quadratic-time kernel Stein discrepancy [Liu et al., 2016, Chwialkowski et al., 2016]
4	<b>LKS</b>	Linear-time running average version of KSD.
5	MMD-opt	MMD two-sample test [Gretton et al., 2012]. With optimization.
6	ME-test	Mean Embeddings two-sample test [Jitkrittum et al., 2016]. With optimization.

- Two-sample tests need to draw sample from  $p$ .
- Tests with optimization use 20% of the data.
- Significance level  $\alpha = 0.05$ .

## Simulation Settings

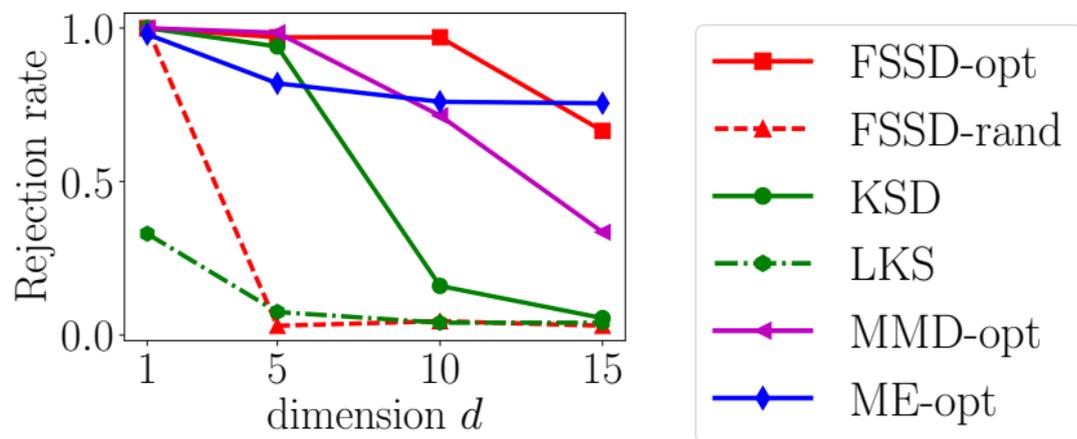
- Gaussian kernel  $k(\mathbf{x}, \mathbf{v}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{v}\|_2^2}{2\sigma_k^2}\right)$

	Method	Description
1	<b>FSSD-opt</b>	Proposed. With optimization. $J = 5$ .
2	<b>FSSD-rand</b>	Proposed. Random test locations.
3	<b>KSD</b>	Quadratic-time kernel Stein discrepancy [Liu et al., 2016, Chwialkowski et al., 2016]
4	<b>LKS</b>	Linear-time running average version of KSD.
5	<b>MMD-opt</b>	MMD two-sample test [Gretton et al., 2012]. With optimization.
6	<b>ME-test</b>	<u>M</u> ean <u>E</u> MBEDDINGS two-sample test [Jitkrittum et al., 2016]. With optimization.

- Two-sample tests need to draw sample from  $p$ .
- Tests with optimization use 20% of the data.
- Significance level  $\alpha = 0.05$ .

## Gaussian Vs. Laplace

- $p = \text{Gaussian}$ .  $q = \text{Laplace}$ . Same mean and variance. High-order moments differ.
- Sample size  $n = 1000$ .



- Optimization increases the power.
- Two-sample tests can perform well in this case ( $p, q$  clearly differ).

## Gaussian-Bernoulli Restricted Boltzmann Machine (RBM)

- $p(\mathbf{x})$  is the marginal of

$$p(\mathbf{x}, \mathbf{h}) = \frac{1}{Z} \exp \left( \mathbf{x}^\top \mathbf{B} \mathbf{h} + \mathbf{b}^\top \mathbf{x} + \mathbf{c}^\top \mathbf{x} - \frac{1}{2} \|\mathbf{x}\|^2 \right),$$

where  $\mathbf{x} \in \mathbb{R}^{50}$ ,  $\mathbf{h} \in \{\pm 1\}^{40}$  is latent. Randomly pick  $\mathbf{B}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ .

- $q(\mathbf{x}) = p(\mathbf{x})$  with i.i.d.  $\mathcal{N}(0, \sigma_{per})$  noise added to all entries of  $\mathbf{B}$ .
- Sample size  $n = 1000$ .

## Gaussian-Bernoulli Restricted Boltzmann Machine (RBM)

- $p(\mathbf{x})$  is the marginal of

$$p(\mathbf{x}, \mathbf{h}) = \frac{1}{Z} \exp \left( \mathbf{x}^\top \mathbf{B} \mathbf{h} + \mathbf{b}^\top \mathbf{x} + \mathbf{c}^\top \mathbf{x} - \frac{1}{2} \|\mathbf{x}\|^2 \right),$$

where  $\mathbf{x} \in \mathbb{R}^{50}$ ,  $\mathbf{h} \in \{\pm 1\}^{40}$  is latent. Randomly pick  $\mathbf{B}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ .

- $q(\mathbf{x}) = p(\mathbf{x})$  with i.i.d.  $\mathcal{N}(0, \sigma_{per})$  noise added to all entries of  $\mathbf{B}$ .
- Sample size  $n = 1000$ .

## Gaussian-Bernoulli Restricted Boltzmann Machine (RBM)

- $p(\mathbf{x})$  is the marginal of

$$p(\mathbf{x}, \mathbf{h}) = \frac{1}{Z} \exp \left( \mathbf{x}^\top \mathbf{B} \mathbf{h} + \mathbf{b}^\top \mathbf{x} + \mathbf{c}^\top \mathbf{x} - \frac{1}{2} \|\mathbf{x}\|^2 \right),$$

where  $\mathbf{x} \in \mathbb{R}^{50}$ ,  $\mathbf{h} \in \{\pm 1\}^{40}$  is latent. Randomly pick  $\mathbf{B}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ .

- $q(\mathbf{x}) = p(\mathbf{x})$  with i.i.d.  $\mathcal{N}(0, \sigma_{per})$  noise added to all entries of  $\mathbf{B}$ .
- Sample size  $n = 1000$ .

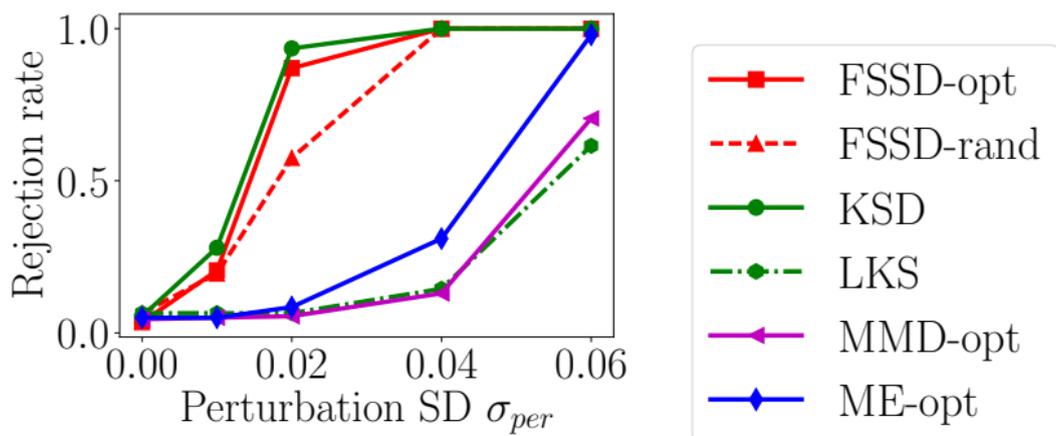
# Gaussian-Bernoulli Restricted Boltzmann Machine (RBM)

- $p(\mathbf{x})$  is the marginal of

$$p(\mathbf{x}, \mathbf{h}) = \frac{1}{Z} \exp \left( \mathbf{x}^\top \mathbf{B} \mathbf{h} + \mathbf{b}^\top \mathbf{x} + \mathbf{c}^\top \mathbf{x} - \frac{1}{2} \|\mathbf{x}\|^2 \right),$$

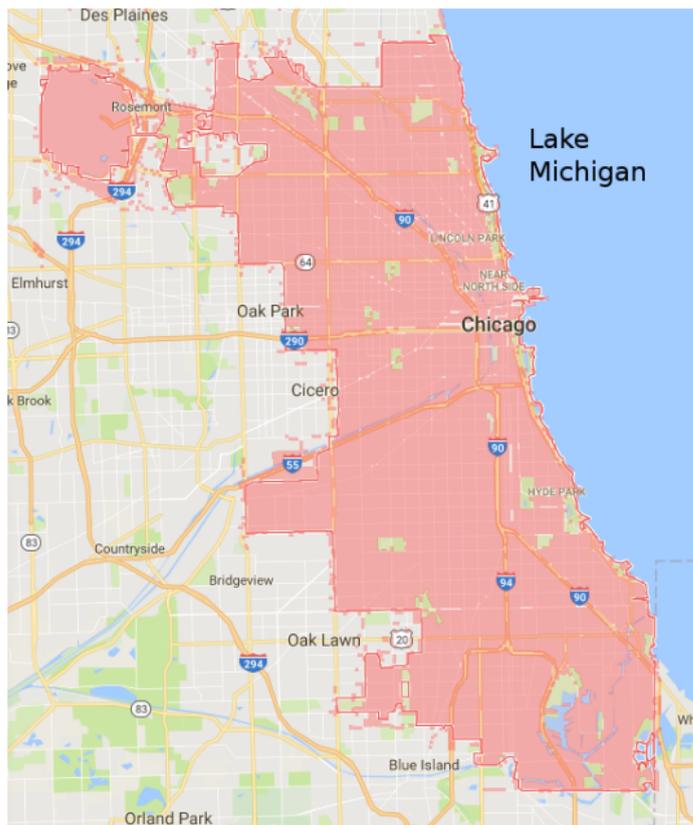
where  $\mathbf{x} \in \mathbb{R}^{50}$ ,  $\mathbf{h} \in \{\pm 1\}^{40}$  is latent. Randomly pick  $\mathbf{B}, \mathbf{b}, \mathbf{c}$ .

- $q(\mathbf{x}) = p(\mathbf{x})$  with i.i.d.  $\mathcal{N}(0, \sigma_{per})$  noise added to all entries of  $\mathbf{B}$ .
- Sample size  $n = 1000$ .

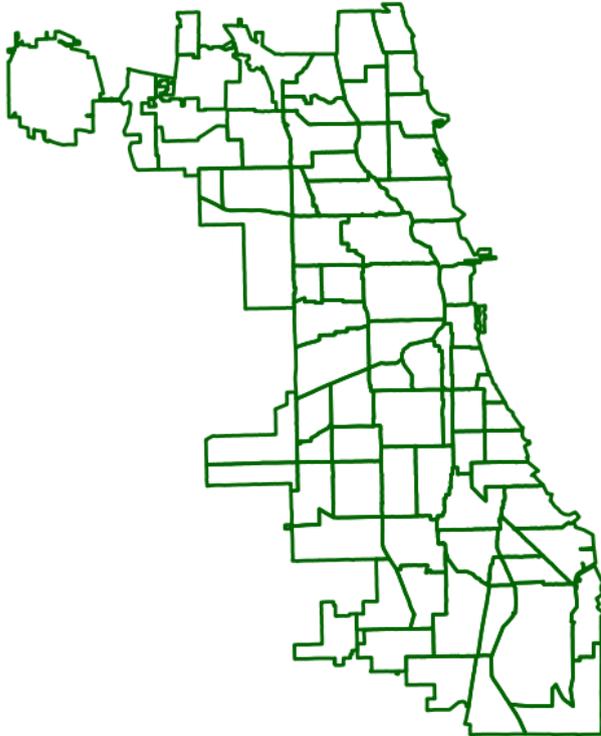


KSD ( $\mathcal{O}(n^2)$ ), FSSD-opt ( $\mathcal{O}(n)$ ) comparable. LKS has low power. 21/25

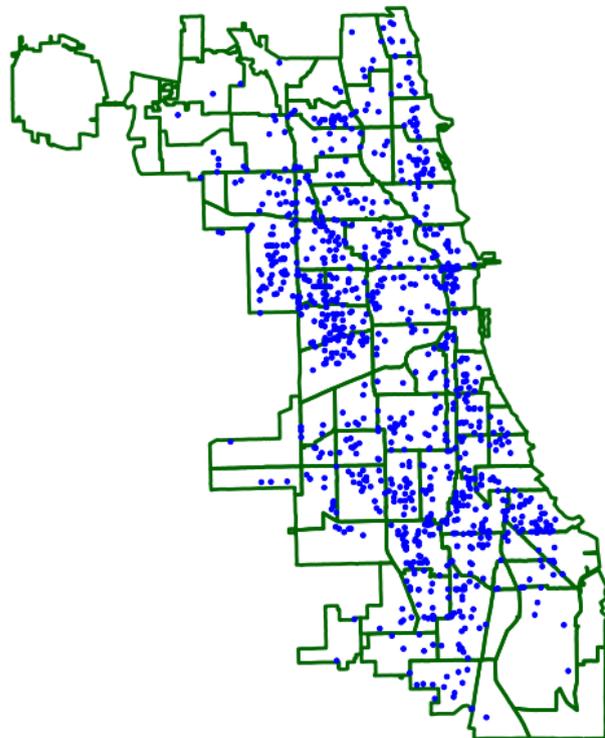
# Interpretable Test Locations: Chicago Crime



## Interpretable Test Locations: Chicago Crime

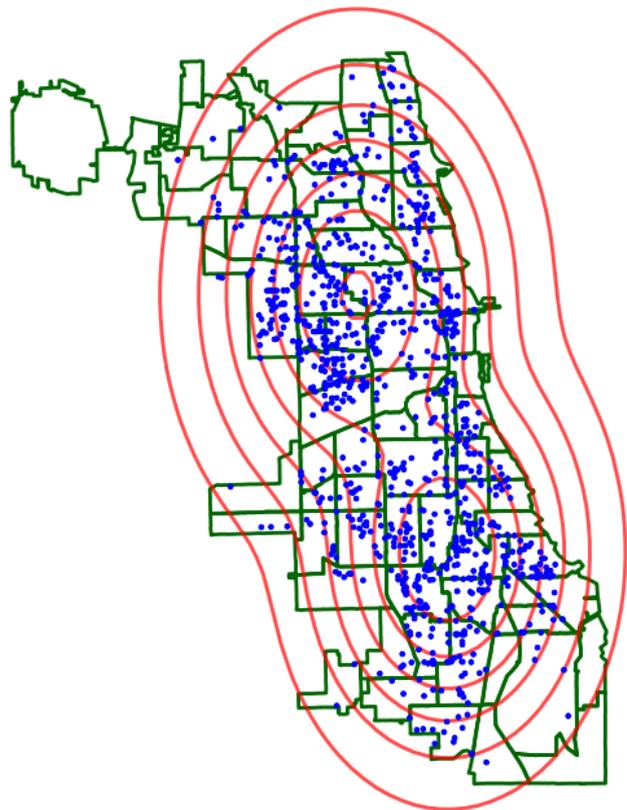


## Interpretable Test Locations: Chicago Crime



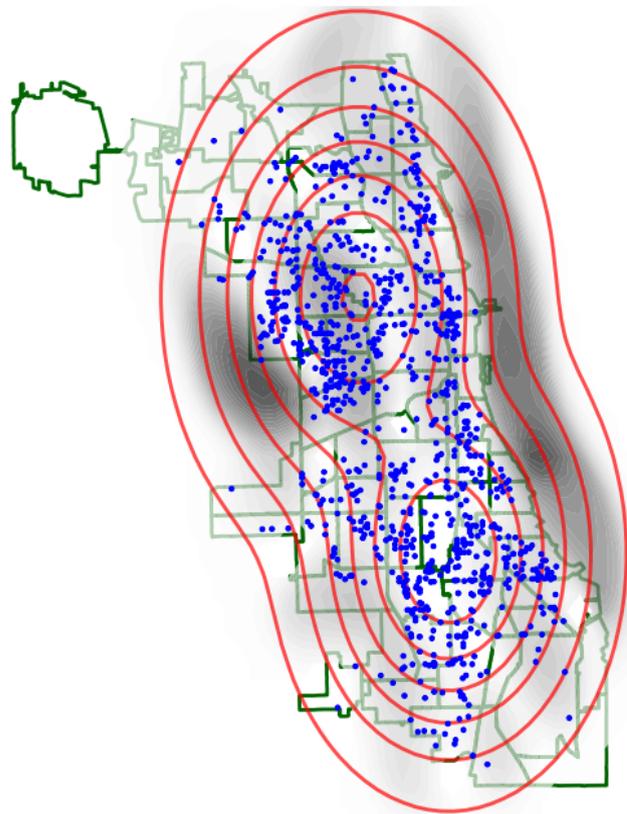
- $n = 11957$  robbery events in Chicago in 2016.
  - lat/long coordinates = sample from  $q$ .
- Model spatial density with Gaussian mixtures.

## Interpretable Test Locations: Chicago Crime



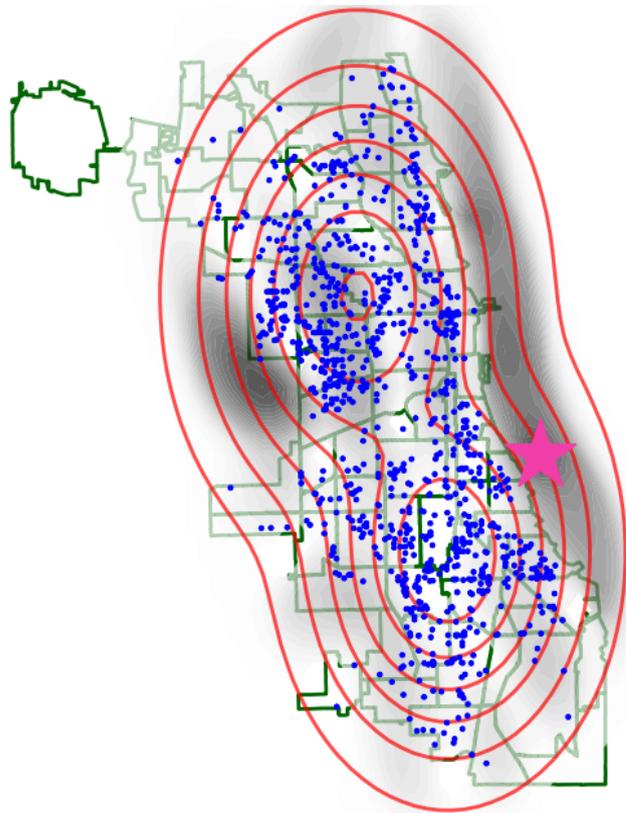
Model  $p = 2$ -component Gaussian mixture.

## Interpretable Test Locations: Chicago Crime



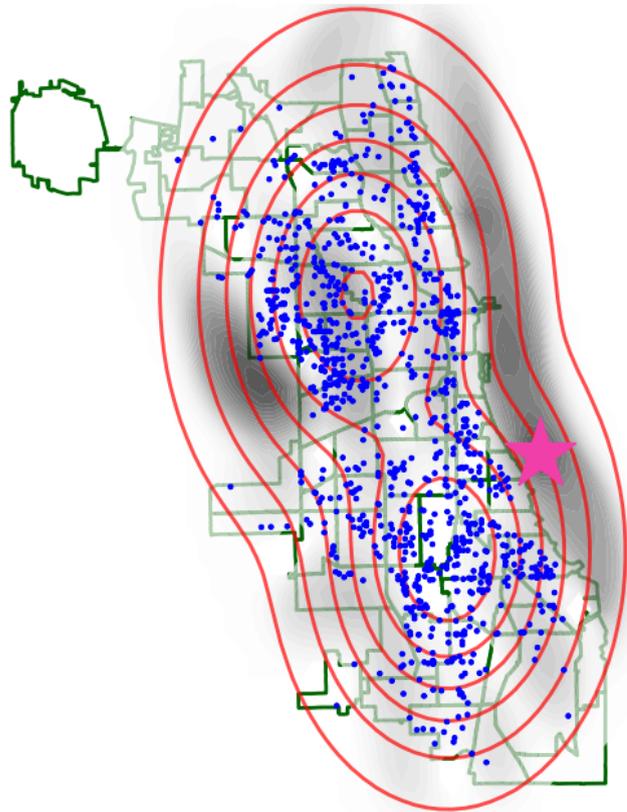
Score surface

## Interpretable Test Locations: Chicago Crime



★ = optimized  $v$ .

## Interpretable Test Locations: Chicago Crime

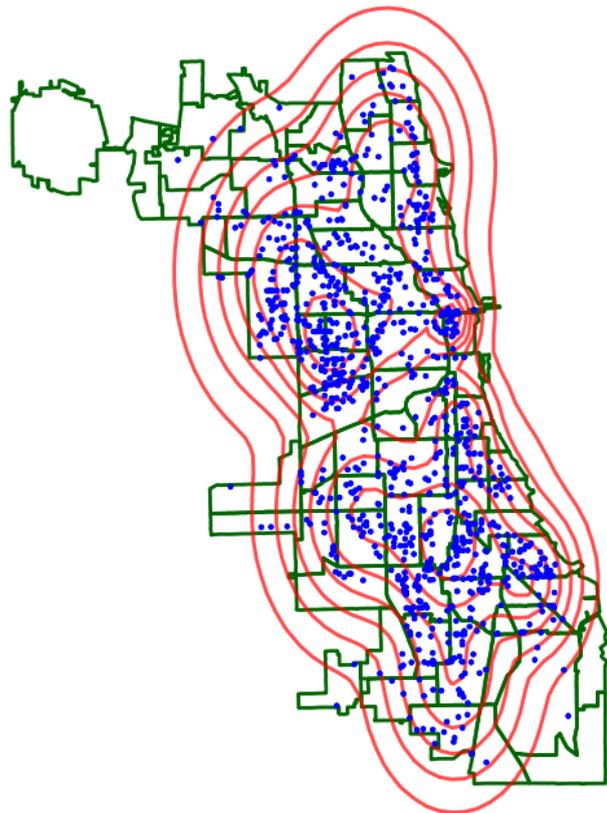


★ = optimized v.

No robbery in Lake Michigan.

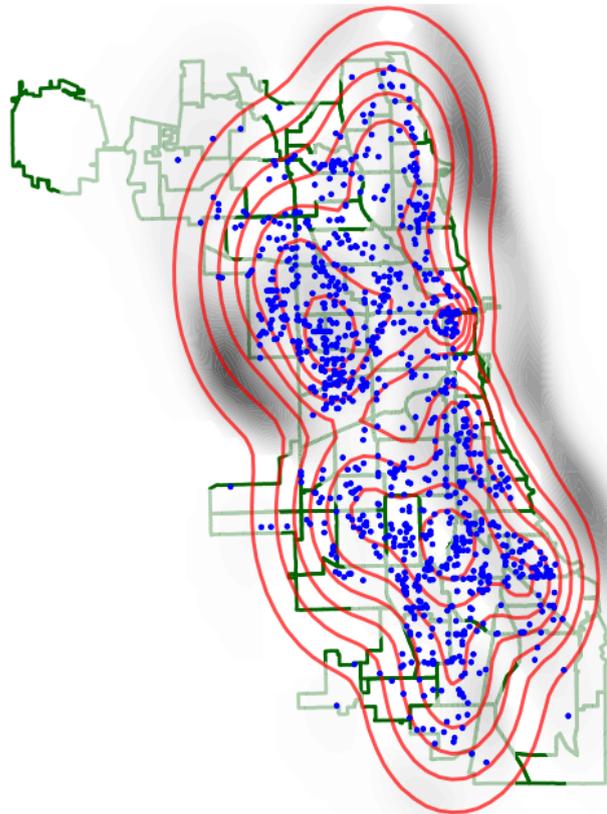


## Interpretable Test Locations: Chicago Crime



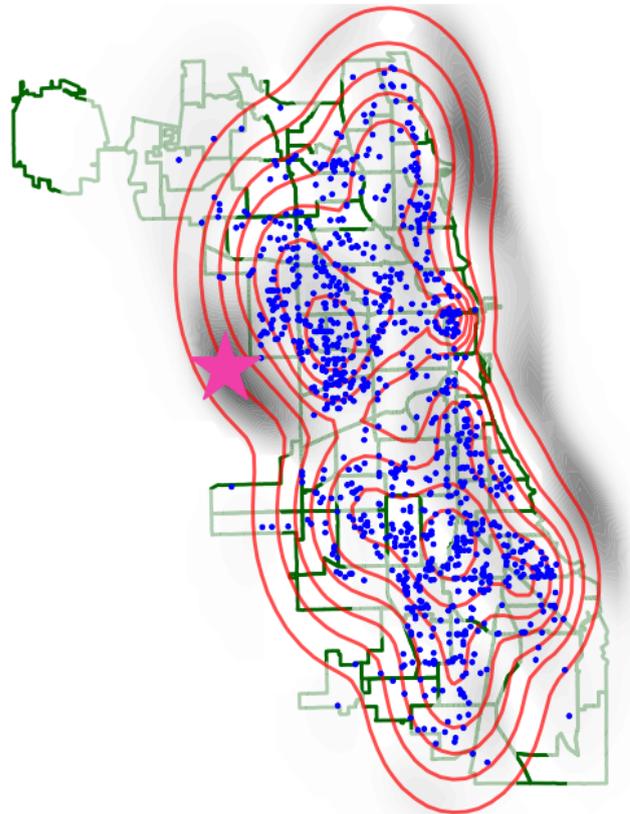
Model  $p = 10$ -component Gaussian mixture.

## Interpretable Test Locations: Chicago Crime



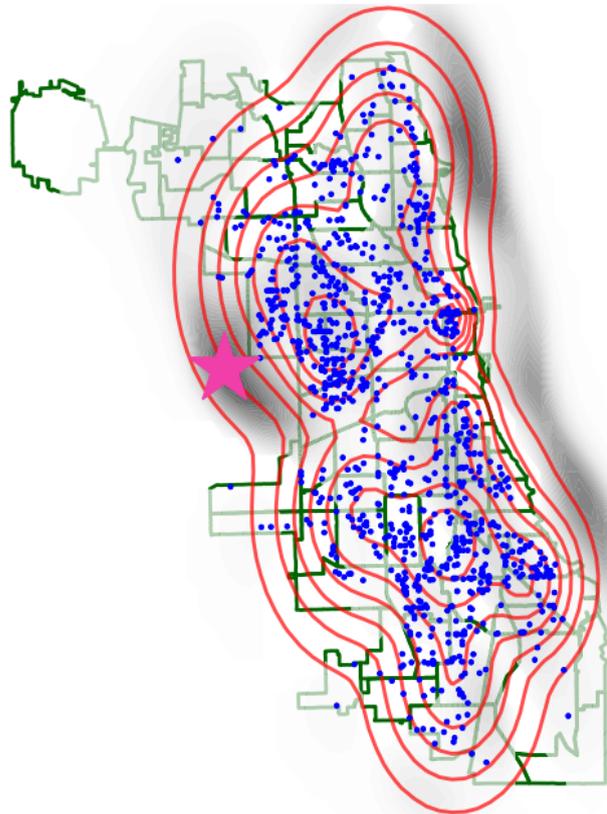
Capture the right tail better.

## Interpretable Test Locations: Chicago Crime



Still, does not capture the left tail.

## Interpretable Test Locations: Chicago Crime



Still, does not capture the left tail.

**Learned test locations are interpretable.**

## Bahadur Slope and Bahadur Efficiency

- Bahadur slope  $\cong$  rate of p-value  $\rightarrow 0$  under  $H_1$  as  $n \rightarrow \infty$ .
- 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  $c(0) = 0$  [Bahadur, 1960].
- $c(\theta)$  higher  $\implies$  more sensitive. Good.

### Bahadur slope

$$c(\theta) := -2 \text{plim}_{n \rightarrow \infty} \frac{\log(1 - F(T_n))}{n},$$

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

- Bahadur efficiency = ratio of slopes of two tests.

## Bahadur Slope and Bahadur Efficiency

- Bahadur slope  $\cong$  rate of p-value  $\rightarrow 0$  under  $H_1$  as  $n \rightarrow \infty$ .
- Measure a test's sensitivity to the departure from  $H_0$ .

$$H_0: \theta = \mathbf{0},$$

$$H_1: \theta \neq \mathbf{0}.$$

- Typically  $\text{pval}_n \approx \exp\left(-\frac{1}{2}c(\theta)n\right)$  where  $c(\theta) > 0$  under  $H_1$ , and  $c(\mathbf{0}) = 0$  [Bahadur, 1960].
- $c(\theta)$  higher  $\implies$  more sensitive. Good.

### Bahadur slope

$$c(\theta) := -2 \text{plim}_{n \rightarrow \infty} \frac{\log(1 - F(T_n))}{n},$$

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

- Bahadur efficiency = ratio of slopes of two tests.

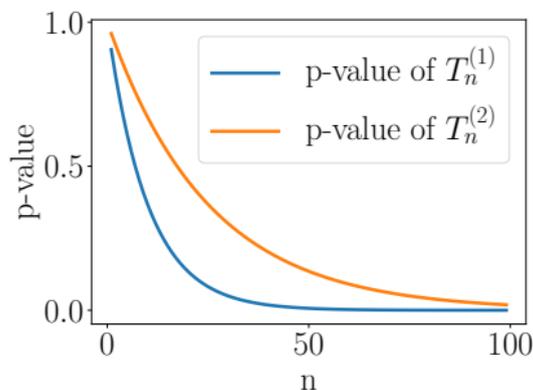
## Bahadur Slope and Bahadur Efficiency

- Bahadur slope  $\approx$  rate of p-value  $\rightarrow 0$  under  $H_1$  as  $n \rightarrow \infty$ .
- 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  $c(0) = 0$  [Bahadur, 1960].
- $c(\theta)$  higher  $\implies$  more sensitive. Good.



Bahadur slope

$$c(\theta) := -2 \operatorname{plim}_{n \rightarrow \infty} \frac{\log(1 - F(T_n))}{n},$$

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

- Bahadur efficiency = ratio of slopes of two tests.

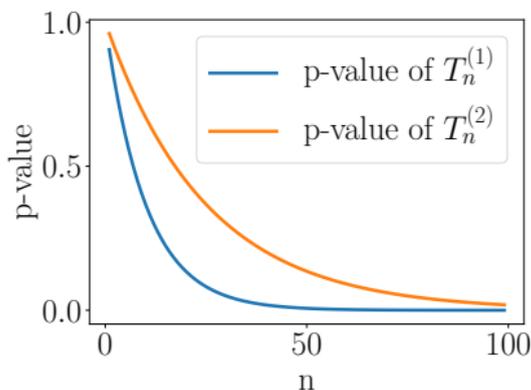
## Bahadur Slope and Bahadur Efficiency

- Bahadur slope  $\approx$  rate of p-value  $\rightarrow 0$  under  $H_1$  as  $n \rightarrow \infty$ .
- 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  $c(0) = 0$  [Bahadur, 1960].
- $c(\theta)$  higher  $\implies$  more sensitive. Good.



Bahadur slope

$$c(\theta) := -2 \text{plim}_{n \rightarrow \infty} \frac{\log(1 - F(T_n))}{n},$$

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

- Bahadur efficiency = ratio of slopes of two tests.

## Gaussian Mean Shift Problem

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

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

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

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

$$c^{(\text{LKS})}(\mu_q, \kappa^2) = \frac{(\kappa^2)^{5/2} (\kappa^2 + 4)^{5/2} \mu_q^4}{2(\kappa^2 + 2)(\kappa^8 + 8\kappa^6 + 21\kappa^4 + 20\kappa^2 + 12)}.$$

**Theorem 2 (FSSD is at least two times more efficient).**

Fix  $\sigma_k^2 = 1$  for  $\widehat{n\text{FSSD}}^2$ . Then,  $\forall \mu_q \neq 0, \exists v \in \mathbb{R}, \forall \kappa^2 > 0$ , we have Bahadur efficiency

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

## Gaussian Mean Shift Problem

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

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

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

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

$$c^{(\text{LKS})}(\mu_q, \kappa^2) = \frac{(\kappa^2)^{5/2} (\kappa^2 + 4)^{5/2} \mu_q^4}{2(\kappa^2 + 2)(\kappa^8 + 8\kappa^6 + 21\kappa^4 + 20\kappa^2 + 12)}.$$

**Theorem 2** (FSSD is at least two times more efficient).

Fix  $\sigma_k^2 = 1$  for  $\widehat{n\text{FSSD}}^2$ . Then,  $\forall \mu_q \neq 0, \exists v \in \mathbb{R}, \forall \kappa^2 > 0$ , we have Bahadur efficiency

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

## Gaussian Mean Shift Problem

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

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

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

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

$$c^{(\text{LKS})}(\mu_q, \kappa^2) = \frac{(\kappa^2)^{5/2} (\kappa^2 + 4)^{5/2} \mu_q^4}{2 (\kappa^2 + 2) (\kappa^8 + 8\kappa^6 + 21\kappa^4 + 20\kappa^2 + 12)}.$$

Theorem 2 (FSSD is at least two times more efficient).

Fix  $\sigma_k^2 = 1$  for  $\widehat{n\text{FSSD}}^2$ . Then,  $\forall \mu_q \neq 0, \exists v \in \mathbb{R}, \forall \kappa^2 > 0$ , we have Bahadur efficiency

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

## Gaussian Mean Shift Problem

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

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

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

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

$$c^{(\text{LKS})}(\mu_q, \kappa^2) = \frac{(\kappa^2)^{5/2} (\kappa^2 + 4)^{5/2} \mu_q^4}{2(\kappa^2 + 2)(\kappa^8 + 8\kappa^6 + 21\kappa^4 + 20\kappa^2 + 12)}.$$

**Theorem 2 (FSSD is at least two times more efficient).**

Fix  $\sigma_k^2 = 1$  for  $\widehat{n\text{FSSD}}^2$ . Then,  $\forall \mu_q \neq 0, \exists v \in \mathbb{R}, \forall \kappa^2 > 0$ , we have Bahadur efficiency

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

## Conclusion

- Proposed **The Finite Set Stein Discrepancy (FSSD)**.
- Goodness-of-fit test based on FSSD is
  - 1 nonparametric,
  - 2 linear-time,
  - 3 tunable (parameters automatically tuned).
  - 4 interpretable.

### **A Linear-Time Kernel Goodness-of-Fit Test**

Wittawat Jitkrittum, Wenkai Xu, Zoltán Szabó, Kenji Fukumizu, Arthur Gretton  
NIPS 2017 (best paper award)

Python code: <https://github.com/wittawatj/kgof>

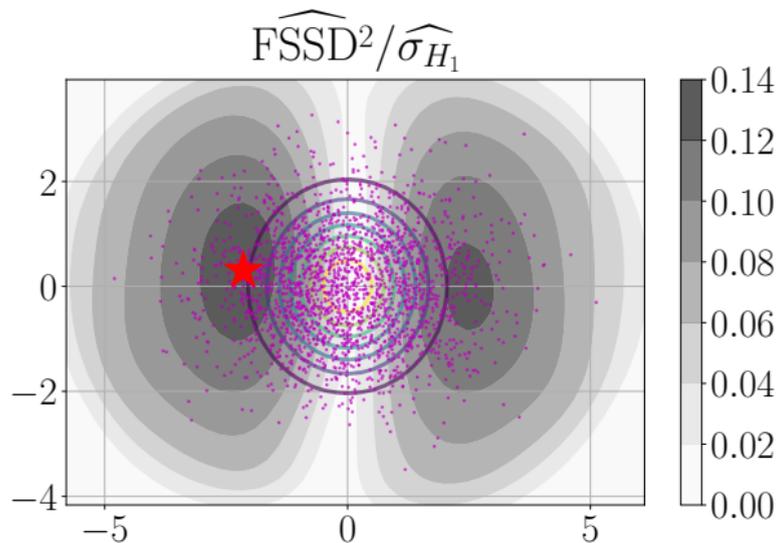
Questions?

Thank you

## Illustration: Score Surface

- Consider  $J = 1$  location.
- $\text{score}(\mathbf{v}) = \frac{\widehat{\text{FSSD}}^2(\mathbf{v})}{\widehat{\sigma}_{H_1}(\mathbf{v})}$  (gray),  $p$  in wireframe,  $\{\mathbf{x}_i\}_{i=1}^n \sim q$  in purple, ★ = best  $\mathbf{v}$ .

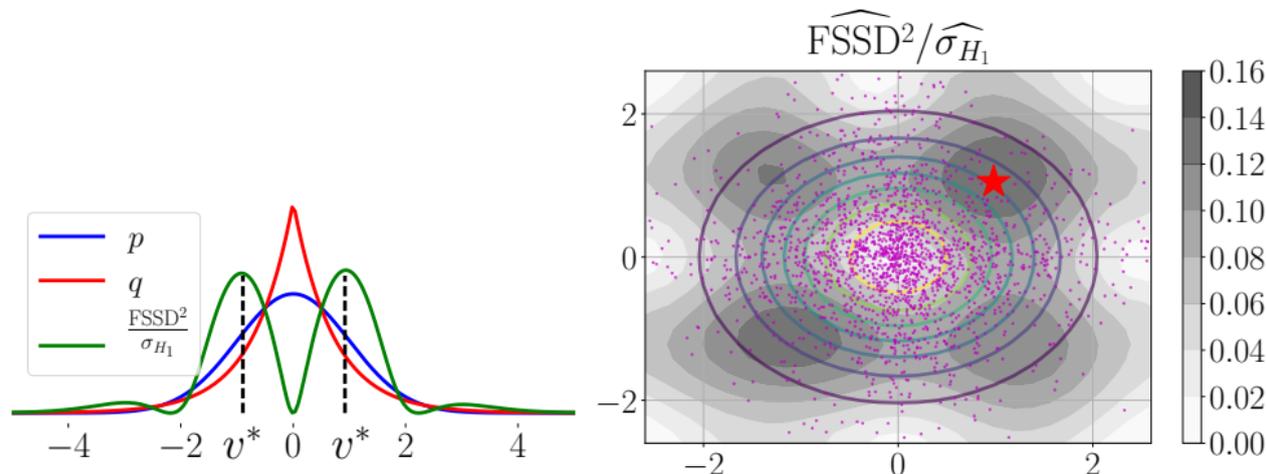
$$p = \mathcal{N}\left(\mathbf{0}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right) \text{ vs. } q = \mathcal{N}\left(\mathbf{0}, \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}\right).$$



## Illustration: Score Surface

- Consider  $J \equiv 1$  location.
- $\text{score}(\mathbf{v}) = \frac{\widehat{\text{FSSD}}^2(\mathbf{v})}{\widehat{\sigma}_{H_1}(\mathbf{v})}$  (gray),  $p$  in wireframe,  $\{\mathbf{x}_i\}_{i=1}^n \sim q$  in purple, ★ = best  $\mathbf{v}$ .

$p = \mathcal{N}(\mathbf{0}, \mathbf{I})$  vs.  $q = \text{Laplace}$  with same mean & variance.



## FSSD and KSD in 1D Gaussian Case

Consider  $p = \mathcal{N}(0, 1)$  and  $q = \mathcal{N}(\mu_q, \sigma_q^2)$ .

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

$$\text{FSSD}^2 = \frac{\sigma_k^2 e^{-\frac{(v-\mu_q)^2}{\sigma_k^2 + \sigma_q^2}} \left( (\sigma_k^2 + 1) \mu_q + v (\sigma_q^2 - 1) \right)^2}{(\sigma_k^2 + \sigma_q^2)^3}.$$

- If  $\mu_q \neq 0$ ,  $\sigma_q^2 \neq 1$ , and  $v = -\frac{(\sigma_k^2 + 1)\mu_q}{(\sigma_q^2 - 1)}$ , then  $\text{FSSD}^2 = 0$ !
  - This is why  $v$  should be drawn from a distribution with a density.
- For KSD, Gaussian kernel (bandwidth =  $\kappa^2$ ).

$$S^2 = \frac{\mu_q^2 (\kappa^2 + 2\sigma_q^2) + (\sigma_q^2 - 1)^2}{(\kappa^2 + 2\sigma_q^2) \sqrt{\frac{2\sigma_q^2}{\kappa^2} + 1}}.$$

## FSSD and KSD in 1D Gaussian Case

Consider  $p = \mathcal{N}(0, 1)$  and  $q = \mathcal{N}(\mu_q, \sigma_q^2)$ .

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

$$\text{FSSD}^2 = \frac{\sigma_k^2 e^{-\frac{(v-\mu_q)^2}{\sigma_k^2 + \sigma_q^2}} \left( (\sigma_k^2 + 1) \mu_q + v (\sigma_q^2 - 1) \right)^2}{(\sigma_k^2 + \sigma_q^2)^3}.$$

- If  $\mu_q \neq 0$ ,  $\sigma_q^2 \neq 1$ , and  $v = -\frac{(\sigma_k^2 + 1)\mu_q}{(\sigma_q^2 - 1)}$ , then  $\text{FSSD}^2 = 0$ !
  - This is why  $v$  should be drawn from a distribution with a density.
- For KSD, Gaussian kernel (bandwidth =  $\kappa^2$ ).

$$S^2 = \frac{\mu_q^2 (\kappa^2 + 2\sigma_q^2) + (\sigma_q^2 - 1)^2}{(\kappa^2 + 2\sigma_q^2) \sqrt{\frac{2\sigma_q^2}{\kappa^2} + 1}}.$$

## FSSD is a Discrepancy Measure

### Theorem 3.

Let  $V = \{\mathbf{v}_1, \dots, \mathbf{v}_J\} \subset \mathbb{R}^d$  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  $k: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  is  $C_0$ -universal, and real analytic.
- 2 (Stein witness not too rough)  $\|g\|_{\mathcal{F}}^2 < \infty$ .
- 3 (Finite Fisher divergence)  $\mathbb{E}_{\mathbf{x} \sim q} \|\nabla_{\mathbf{x}} \log \frac{p(\mathbf{x})}{q(\mathbf{x})}\|^2 < \infty$ .
- 4 (Vanishing boundary)  $\lim_{\|\mathbf{x}\| \rightarrow \infty} p(\mathbf{x})g(\mathbf{x}) = 0$ .

Then, for any  $J \geq 1$ ,  $\eta$ -almost surely

$$\text{FSSD}^2 = 0 \text{ if and only if } p = q.$$

- Gaussian kernel  $k(\mathbf{x}, \mathbf{v}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{v}\|_2^2}{2\sigma_k^2}\right)$  works.
- In practice,  $J = 1$  or  $J = 5$ .

## Asymptotic Distributions of $\widehat{\text{FSSD}}^2$

- Recall  $\xi(\mathbf{x}, \mathbf{v}) := \frac{1}{p(\mathbf{x})} \partial_{\mathbf{x}} [k(\mathbf{x}, \mathbf{v}) p(\mathbf{x})] \in \mathbb{R}^d$ .
- $\tau(\mathbf{x}) :=$  vertically stack  $\xi(\mathbf{x}, \mathbf{v}_1), \dots, \xi(\mathbf{x}, \mathbf{v}_J) \in \mathbb{R}^{dJ}$ . Feature vector of  $\mathbf{x}$ .
- Mean feature:  $\mu := \mathbb{E}_{\mathbf{x} \sim q} [\tau(\mathbf{x})]$ .
- $\Sigma_r := \text{cov}_{\mathbf{x} \sim r} [\tau(\mathbf{x})] \in \mathbb{R}^{dJ \times dJ}$  for  $r \in \{p, q\}$

### Proposition 2 (Asymptotic distributions).

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

- 1 Under  $H_0 : p = q$ , asymptotically  $n \widehat{\text{FSSD}}^2 \xrightarrow{d} \sum_{i=1}^{dJ} (Z_i^2 - 1) w_i$ .
  - Easy to simulate to get p-value.
  - Simulation cost independent of  $n$ .
- 2 Under  $H_1 : p \neq q$ , we have  $\sqrt{n}(\widehat{\text{FSSD}}^2 - \text{FSSD}^2) \xrightarrow{d} \mathcal{N}(0, \sigma_{H_1}^2)$  where  $\sigma_{H_1}^2 := 4\mu^\top \Sigma_q \mu$ . Implies  $\mathbb{P}(\text{reject } H_0) \rightarrow 1$  as  $n \rightarrow \infty$ .

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

- Theorem: Using  $\hat{\Sigma}_q$  (computed with  $\{\mathbf{x}_i\}_{i=1}^n \sim q$ ) still leads to a consistent test.

## Asymptotic Distributions of $\widehat{\text{FSSD}}^2$

- Recall  $\xi(\mathbf{x}, \mathbf{v}) := \frac{1}{p(\mathbf{x})} \partial_{\mathbf{x}} [k(\mathbf{x}, \mathbf{v}) p(\mathbf{x})] \in \mathbb{R}^d$ .
- $\tau(\mathbf{x}) :=$  vertically stack  $\xi(\mathbf{x}, \mathbf{v}_1), \dots, \xi(\mathbf{x}, \mathbf{v}_J) \in \mathbb{R}^{dJ}$ . Feature vector of  $\mathbf{x}$ .
- Mean feature:  $\mu := \mathbb{E}_{\mathbf{x} \sim q} [\tau(\mathbf{x})]$ .
- $\Sigma_r := \text{cov}_{\mathbf{x} \sim r} [\tau(\mathbf{x})] \in \mathbb{R}^{dJ \times dJ}$  for  $r \in \{p, q\}$

### Proposition 2 (Asymptotic distributions).

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

- 1 Under  $H_0 : p = q$ , asymptotically  $n \widehat{\text{FSSD}}^2 \xrightarrow{d} \sum_{i=1}^{dJ} (Z_i^2 - 1) \omega_i$ .
  - Easy to simulate to get p-value.
  - Simulation cost independent of  $n$ .
- 2 Under  $H_1 : p \neq q$ , we have  $\sqrt{n}(\widehat{\text{FSSD}}^2 - \text{FSSD}^2) \xrightarrow{d} \mathcal{N}(0, \sigma_{H_1}^2)$  where  $\sigma_{H_1}^2 := 4\mu^\top \Sigma_q \mu$ . Implies  $\mathbb{P}(\text{reject } H_0) \rightarrow 1$  as  $n \rightarrow \infty$ .

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

- Theorem: Using  $\hat{\Sigma}_q$  (computed with  $\{\mathbf{x}_i\}_{i=1}^n \sim q$ ) still leads to a consistent test.

## Asymptotic Distributions of $\widehat{\text{FSSD}}^2$

- Recall  $\xi(\mathbf{x}, \mathbf{v}) := \frac{1}{p(\mathbf{x})} \partial_{\mathbf{x}} [k(\mathbf{x}, \mathbf{v}) p(\mathbf{x})] \in \mathbb{R}^d$ .
- $\tau(\mathbf{x}) :=$  vertically stack  $\xi(\mathbf{x}, \mathbf{v}_1), \dots, \xi(\mathbf{x}, \mathbf{v}_J) \in \mathbb{R}^{dJ}$ . Feature vector of  $\mathbf{x}$ .
- Mean feature:  $\mu := \mathbb{E}_{\mathbf{x} \sim q} [\tau(\mathbf{x})]$ .
- $\Sigma_r := \text{cov}_{\mathbf{x} \sim r} [\tau(\mathbf{x})] \in \mathbb{R}^{dJ \times dJ}$  for  $r \in \{p, q\}$

### Proposition 2 (Asymptotic distributions).

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

- 1 Under  $H_0 : p = q$ , asymptotically  $n \widehat{\text{FSSD}}^2 \xrightarrow{d} \sum_{i=1}^{dJ} (Z_i^2 - 1) \omega_i$ .
  - Easy to simulate to get p-value.
  - Simulation cost independent of  $n$ .
- 2 Under  $H_1 : p \neq q$ , we have  $\sqrt{n}(\widehat{\text{FSSD}}^2 - \text{FSSD}^2) \xrightarrow{d} \mathcal{N}(0, \sigma_{H_1}^2)$  where  $\sigma_{H_1}^2 := 4\mu^\top \Sigma_q \mu$ . Implies  $\mathbb{P}(\text{reject } H_0) \rightarrow 1$  as  $n \rightarrow \infty$ .

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

- Theorem: Using  $\hat{\Sigma}_q$  (computed with  $\{\mathbf{x}_i\}_{i=1}^n \sim q$ ) still leads to a consistent test.

## Asymptotic Distributions of $\widehat{\text{FSSD}}^2$

- Recall  $\xi(\mathbf{x}, \mathbf{v}) := \frac{1}{p(\mathbf{x})} \partial_{\mathbf{x}} [k(\mathbf{x}, \mathbf{v}) p(\mathbf{x})] \in \mathbb{R}^d$ .
- $\tau(\mathbf{x}) :=$  vertically stack  $\xi(\mathbf{x}, \mathbf{v}_1), \dots, \xi(\mathbf{x}, \mathbf{v}_J) \in \mathbb{R}^{dJ}$ . Feature vector of  $\mathbf{x}$ .
- Mean feature:  $\mu := \mathbb{E}_{\mathbf{x} \sim q} [\tau(\mathbf{x})]$ .
- $\Sigma_r := \text{cov}_{\mathbf{x} \sim r} [\tau(\mathbf{x})] \in \mathbb{R}^{dJ \times dJ}$  for  $r \in \{p, q\}$

### Proposition 2 (Asymptotic distributions).

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

- 1 Under  $H_0 : p = q$ , asymptotically  $n \widehat{\text{FSSD}}^2 \xrightarrow{d} \sum_{i=1}^{dJ} (Z_i^2 - 1) w_i$ .
  - Easy to simulate to get p-value.
  - Simulation cost independent of  $n$ .
- 2 Under  $H_1 : p \neq q$ , we have  $\sqrt{n}(\widehat{\text{FSSD}}^2 - \text{FSSD}^2) \xrightarrow{d} \mathcal{N}(0, \sigma_{H_1}^2)$  where  $\sigma_{H_1}^2 := 4\mu^\top \Sigma_q \mu$ . Implies  $\mathbb{P}(\text{reject } H_0) \rightarrow 1$  as  $n \rightarrow \infty$ .

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

- **Theorem:** Using  $\widehat{\Sigma}_q$  (computed with  $\{\mathbf{x}_i\}_{i=1}^n \sim q$ ) still leads to a consistent test.

## Bahadur Slopes of FSSD and LKS

### Theorem 4.

The Bahadur slope of  $n\widehat{\text{FSSD}}^2$  is

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

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

### Theorem 5.

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

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

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

## Bahadur Slopes of FSSD and LKS

### Theorem 4.

The Bahadur slope of  $n\widehat{\text{FSSD}}^2$  is

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

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

### Theorem 5.

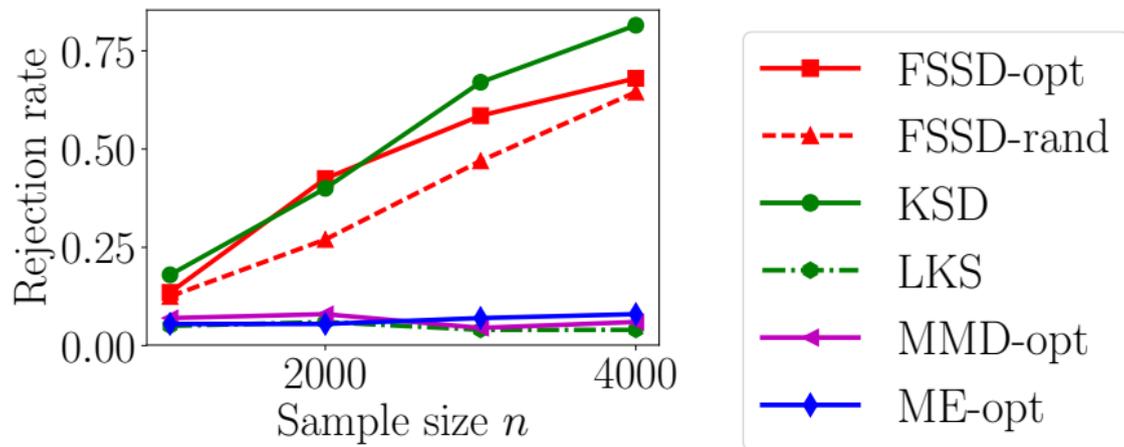
The Bahadur slope of the linear-time kernel Stein (LKS) statistic  $\sqrt{n}\widehat{S}_l^2$  is

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

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

## Harder RBM Problem

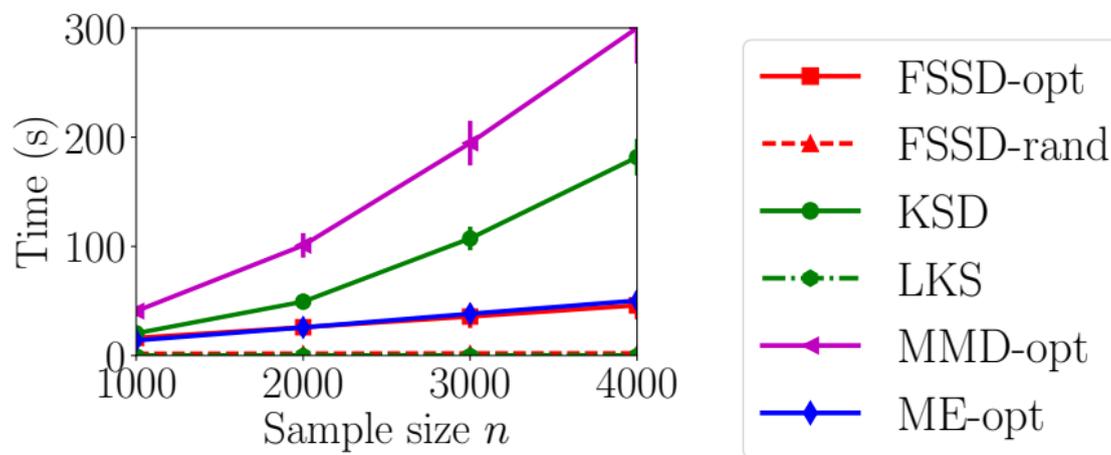
- Perturb only one entry of  $\mathbf{B} \in \mathbb{R}^{50 \times 40}$  (in the RBM).
- $B_{1,1} \leftarrow B_{1,1} + \mathcal{N}(0, \sigma_{per}^2 = 0.1^2)$ .



- Two-sample tests fail. Samples from  $p, q$  look roughly the same.
- FSSD-opt is comparable to KSD at low  $n$ . One order of magnitude faster.

## Harder RBM Problem

- Perturb only one entry of  $\mathbf{B} \in \mathbb{R}^{50 \times 40}$  (in the RBM).
- $B_{1,1} \leftarrow B_{1,1} + \mathcal{N}(0, \sigma_{per}^2 = 0.1^2)$ .



- Two-sample tests fail. Samples from  $p, q$  look roughly the same.
- FSSD-opt is comparable to KSD at low  $n$ . One order of magnitude faster.

## References I

-  Bahadur, R. R. (1960).  
Stochastic comparison of tests.  
*The Annals of Mathematical Statistics*, 31(2):276–295.
-  Chwialkowski, K., Strathmann, H., and Gretton, A. (2016).  
A kernel test of goodness of fit.  
In *ICML*, pages 2606–2615.
-  Gretton, A., Borgwardt, K. M., Rasch, M. J., Schölkopf, B., and Smola, A. (2012).  
A Kernel Two-Sample Test.  
*JMLR*, 13:723–773.
-  Jitkrittum, W., Szabó, Z., Chwialkowski, K. P., and Gretton, A. (2016).  
Interpretable Distribution Features with Maximum Testing Power.  
In *NIPS*, pages 181–189.

## References II

-  Liu, Q., Lee, J., and Jordan, M. (2016).  
A Kernelized Stein Discrepancy for Goodness-of-fit Tests.  
In *ICML*, pages 276–284.