Interpretable Distribution Features with Maximum Testing Power

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NIPS 2016, Barcelona Spain

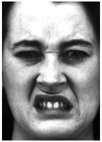
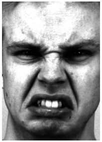
Overview

- **Have:** Two collections of samples X, Y from unknown distributions P and Q.

Positive emotions

$\mathsf{X} = \{$ , , , $\ldots\} \sim P$

Negative emotions

$\mathsf{Y} = \{$ , , , $\ldots\} \sim Q$

- **Goal:** Learn distinguishing features that indicate how P and Q differ.

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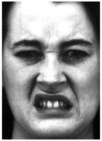
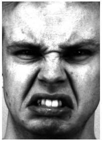
$\mathsf{Y} = \{$ , ,  $, \ldots \} \sim Q$

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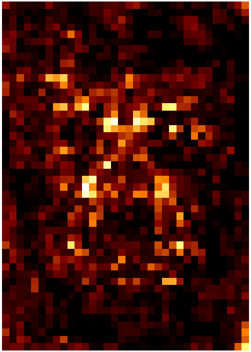

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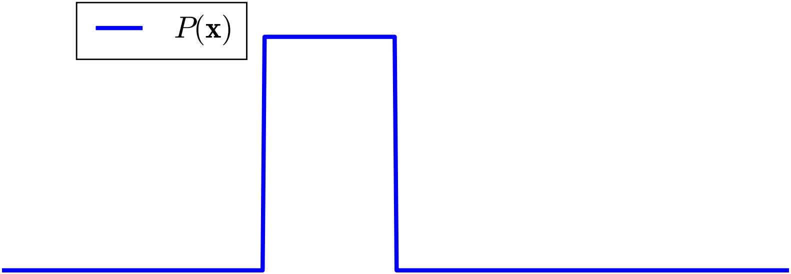
Distinguishing Feature(s)

Where is the best location to observe the difference of $P(\mathbf{x})$ and $Q(\mathbf{y})$?



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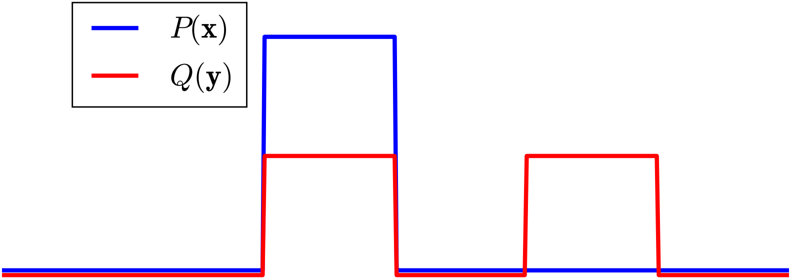

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- **Propose:** a linear-time algorithm to find such data-driven feature(s).

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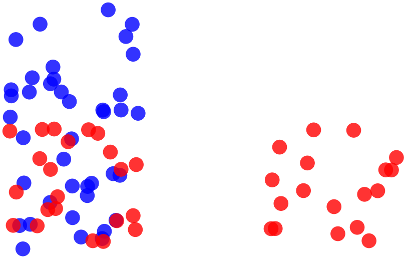

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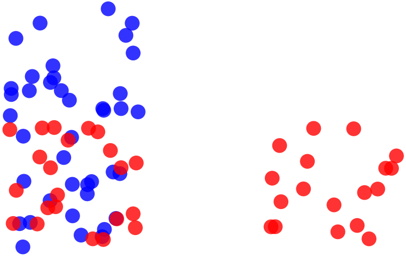

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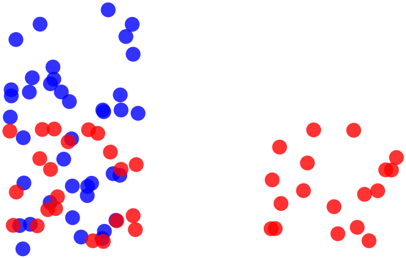

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Witness Function (Gretton et al., 2012)

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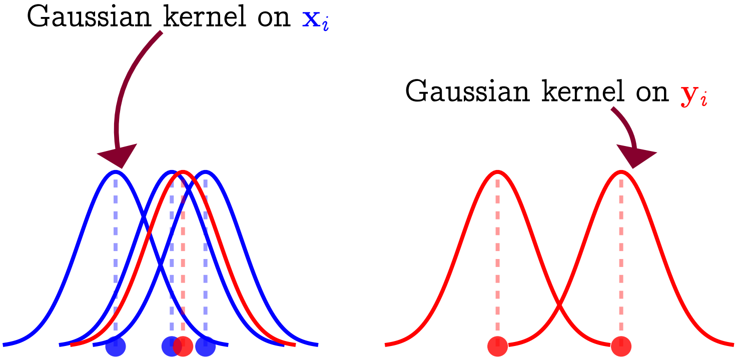
Observe $\mathsf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \sim P$

Observe $\mathsf{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_n\} \sim Q$

Witness Function (Gretton et al., 2012)



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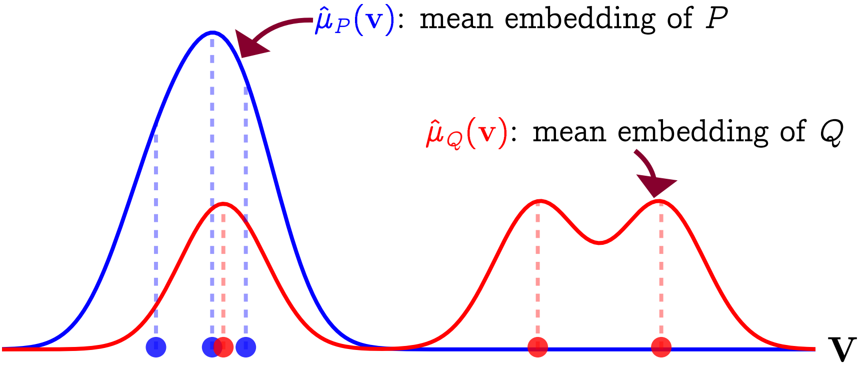

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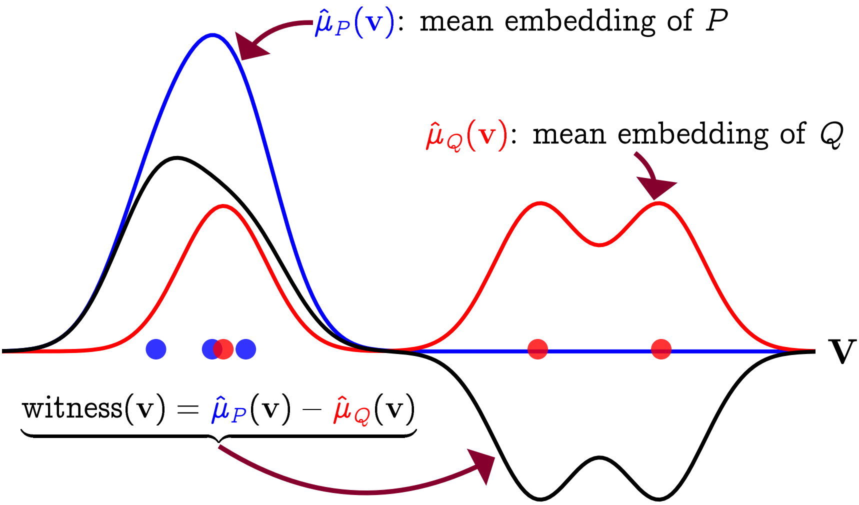

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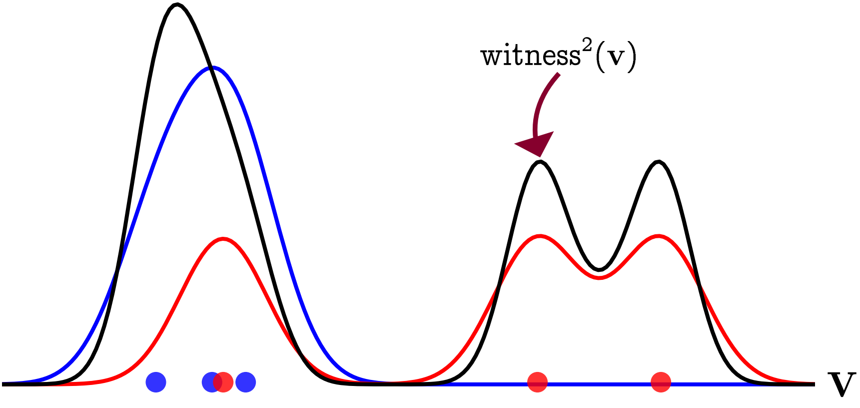

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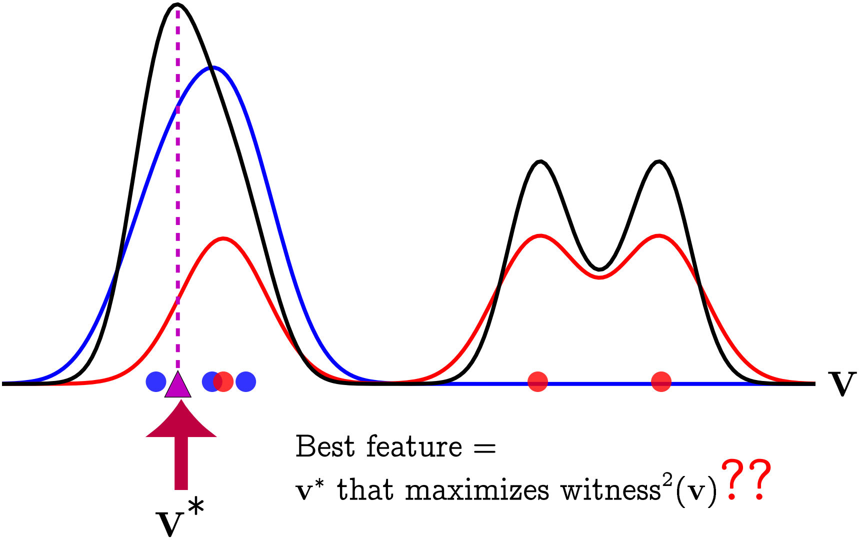
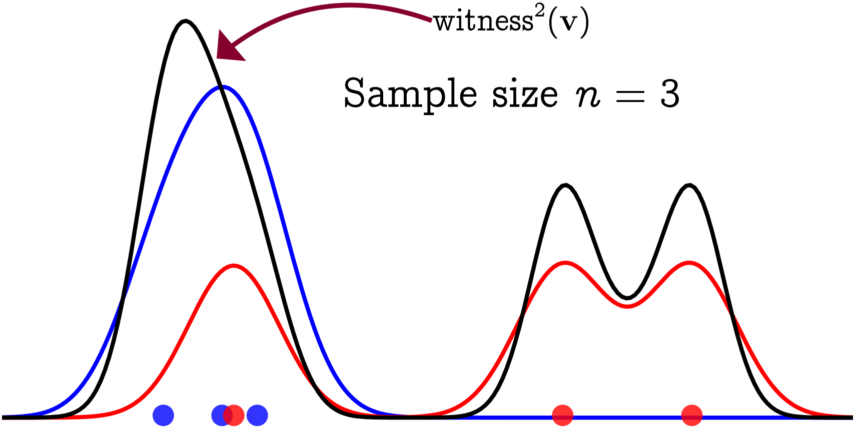


Best feature =
v^* that maximizes witness^2(v)??

Failure Mode of the Witness Function



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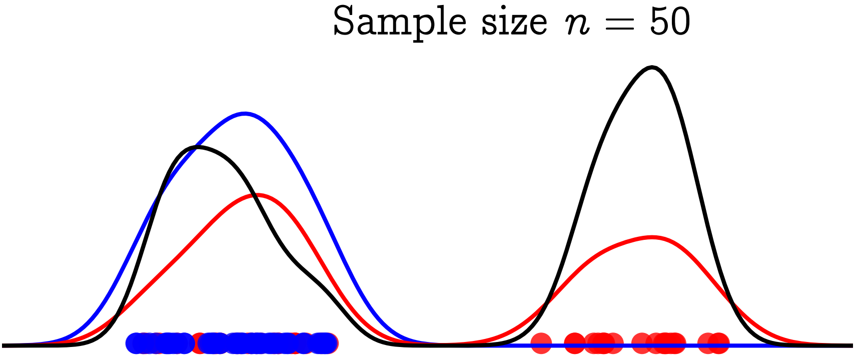
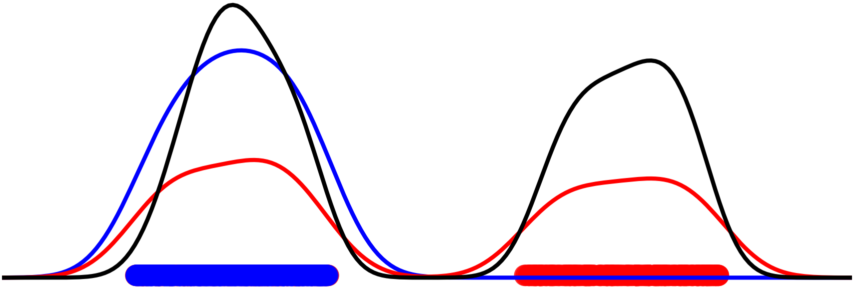


Failure Mode of the Witness Function

Sample size $n = 500$



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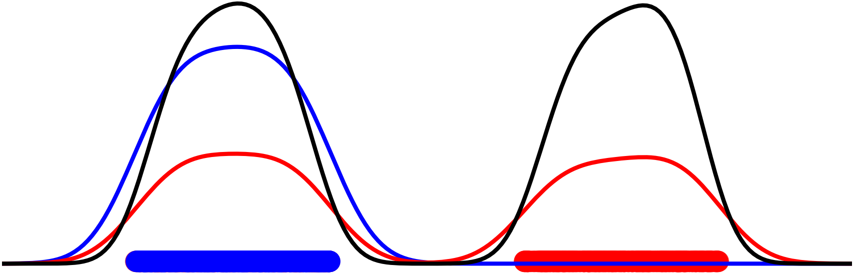
Sample size $n = 5000$



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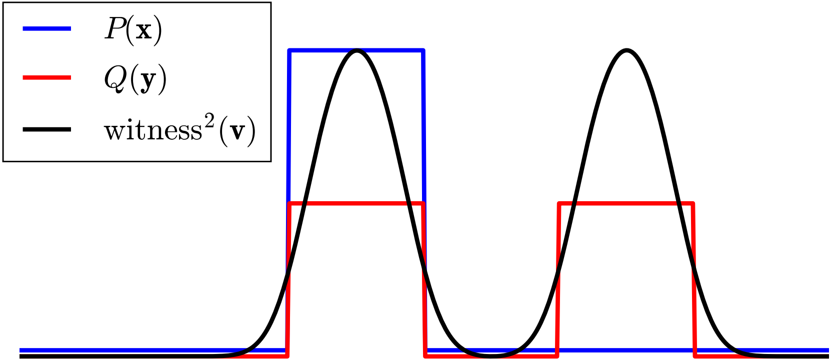

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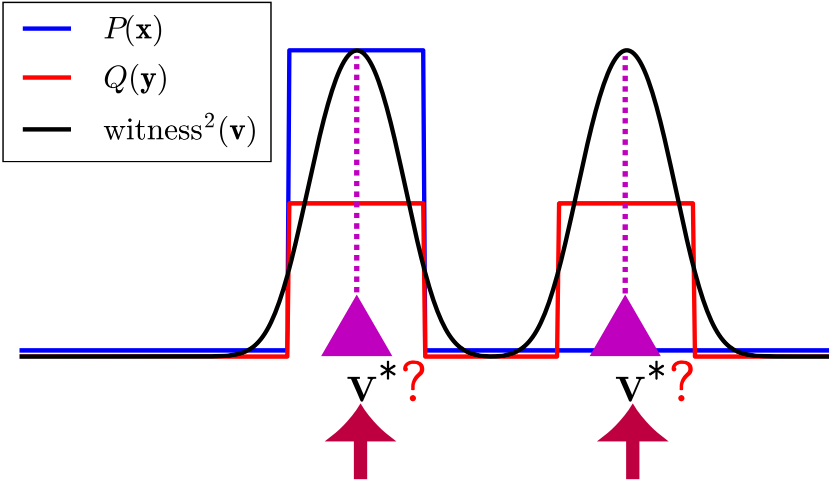

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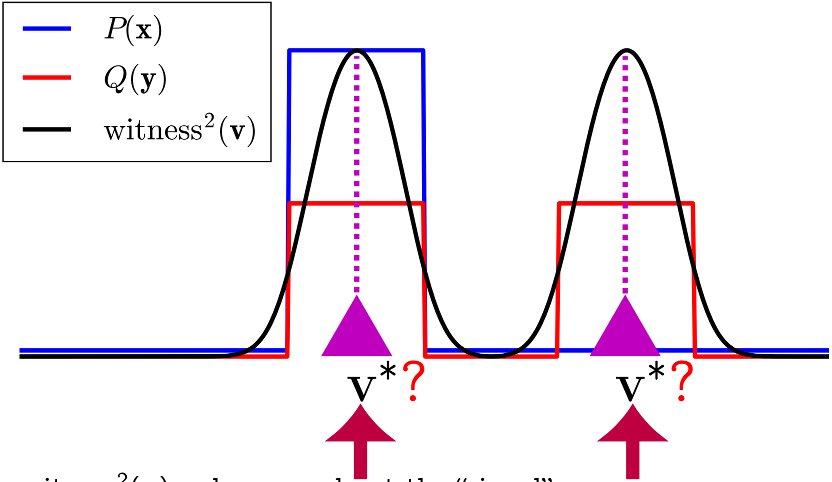

- $\text{witness}^2(\mathbf{v})$ only cares about the "signal".
- Not the "noise" (variability) at each feature.

The ME (Mean Embeddings) Statistic (Chwialkowski et al., 2015)

- **Variance of $\mathbf{v}$** = variance of $\mathbf{v}$ from X + variance of $\mathbf{v}$ from Y.
- ME Statistic: $\hat{\lambda}_n(\mathbf{v}) := n \frac{\text{witness}^2(\mathbf{v})}{\text{variance of } \mathbf{v}}$.

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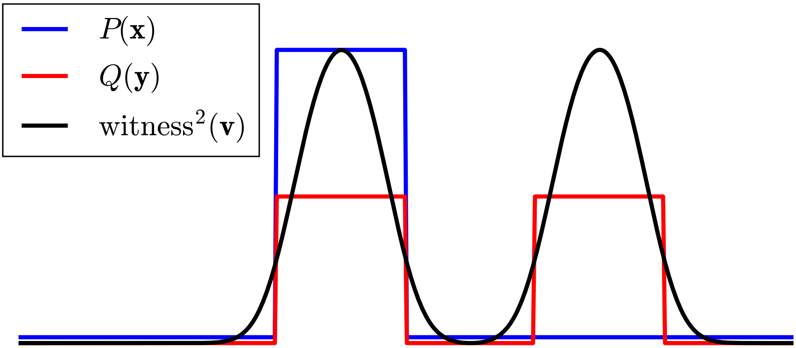

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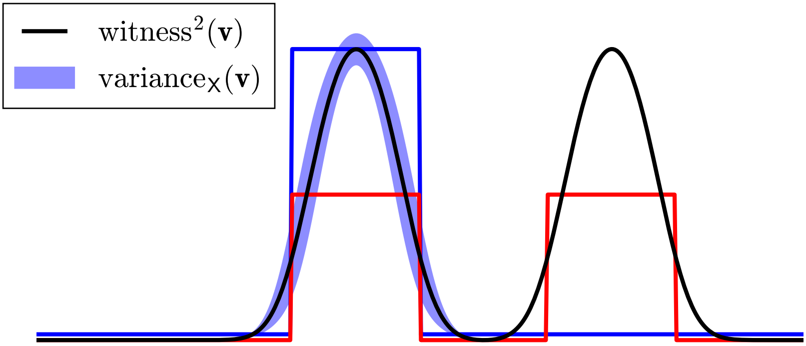

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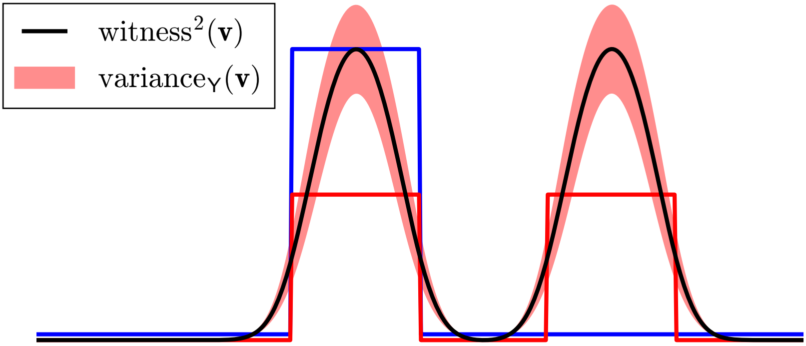

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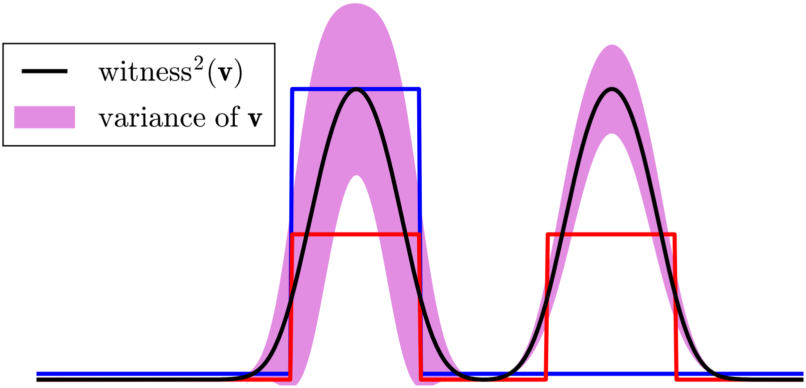

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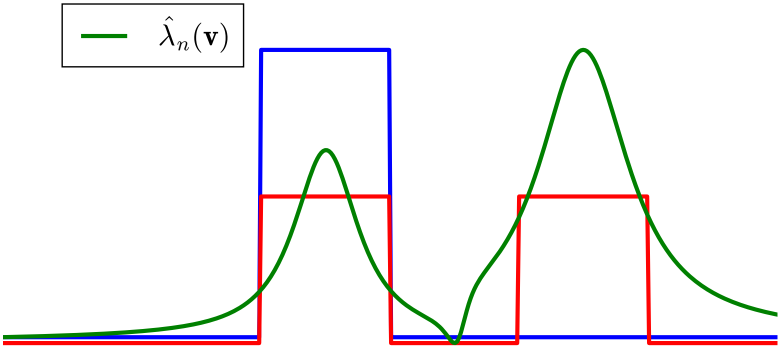

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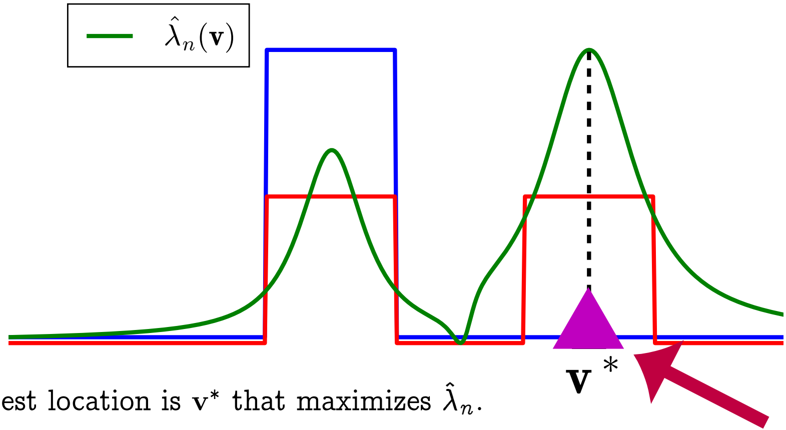

- Best location is $\mathbf{v}^*$ that maximizes $\hat{\lambda}_n$.

Properties of the ME Statistic

- Can construct a two-sample test using J features.
  - $H_0 : P = Q$ vs. $H_1 : P \neq Q$.
- Choosing the best J features increases a lower bound on the test power.
  - Test power $= \mathbb{P}(\text{reject } H_0 \mid H_1 \text{ is true})$.
- **Runtime:** $\mathcal{O}(n)$. Fast.

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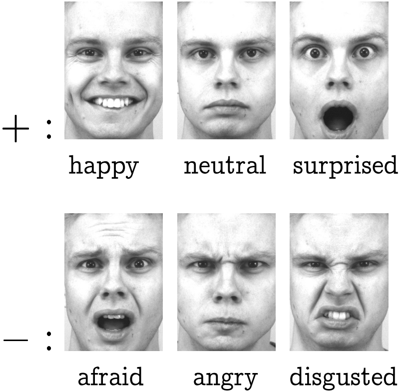
Distinguishing Positive/Negative Emotions



- 35 females and 35 males (Lundqvist et al., 1998).
- $48 \times 34 = 1632$ dimensions. Pixel features.
- $n = 201$.

- Test power comparable to the state-of-the-art MMD test.
- Informative features: differences at the nose, and smile lines.

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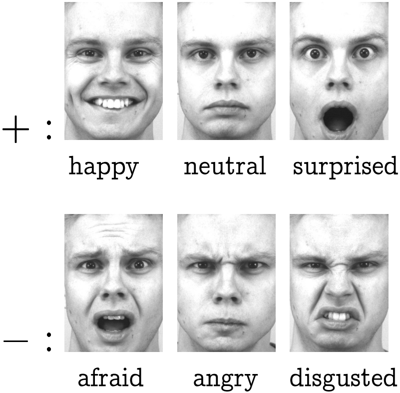

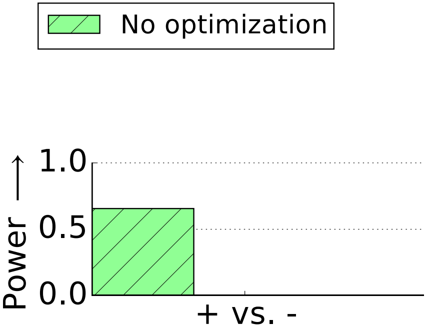

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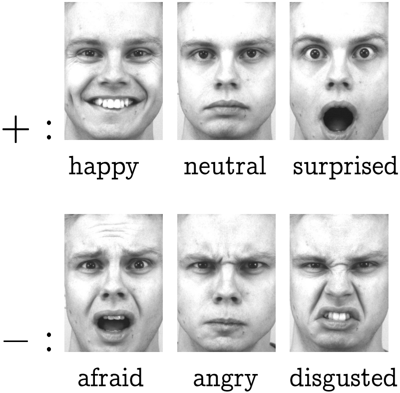

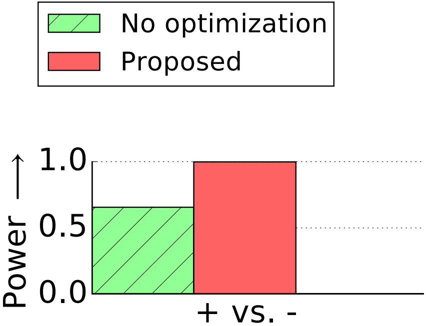

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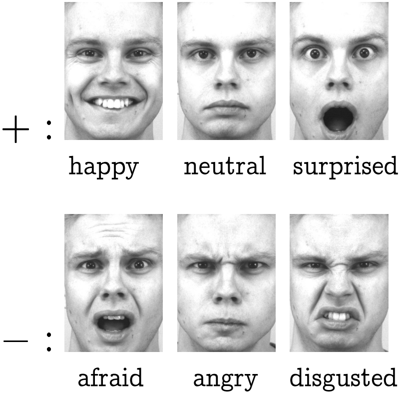

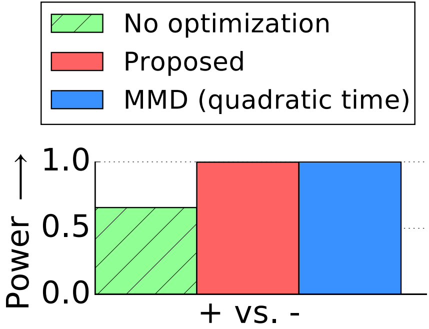

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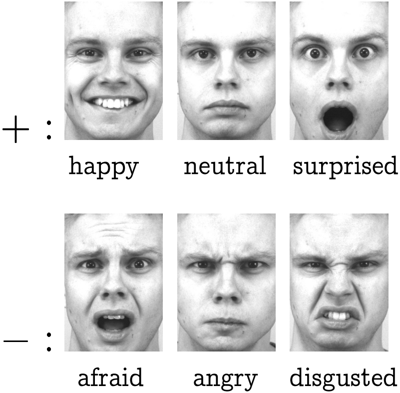

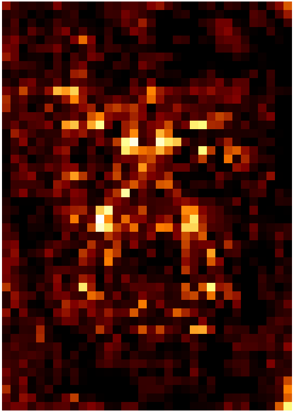

Learned feature

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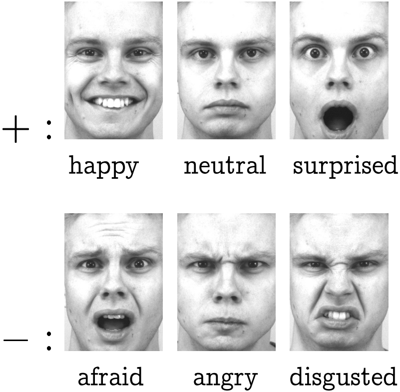

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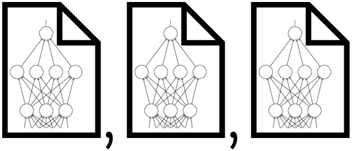
Bayesian Inference Vs. Deep Learning Papers

Papers on Bayesian inference

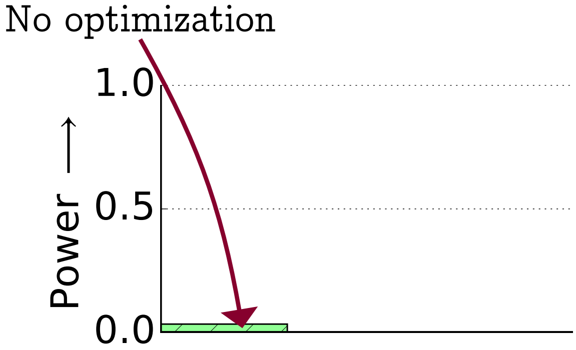
$X = \{$  $, \ldots\} \sim P$

Papers on deep learning

$Y = \{$  $, \ldots\} \sim Q$

- NIPS papers (1988-2015)
- Sample size $n = 216$.
- Random 2000 nouns (dimensions). TF-IDF representation.

Bayesian Inference Vs. Deep Learning Papers



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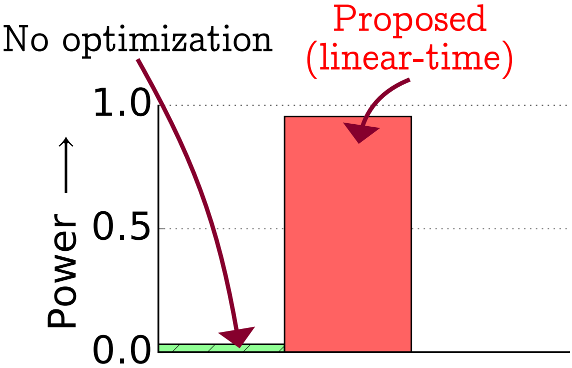

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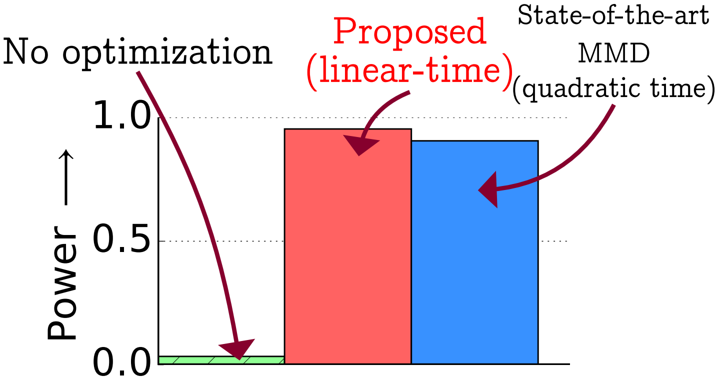

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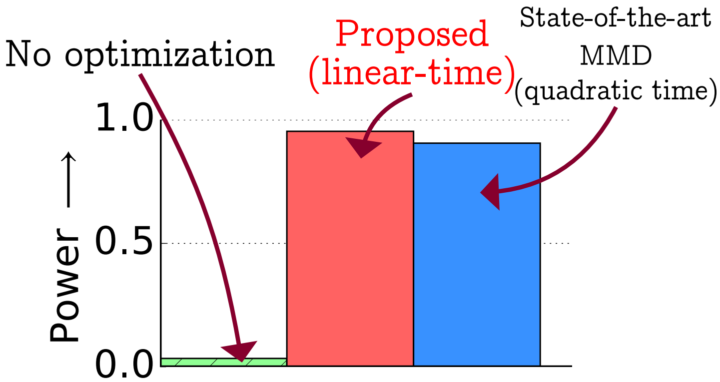


Learned informative feature (a new document):

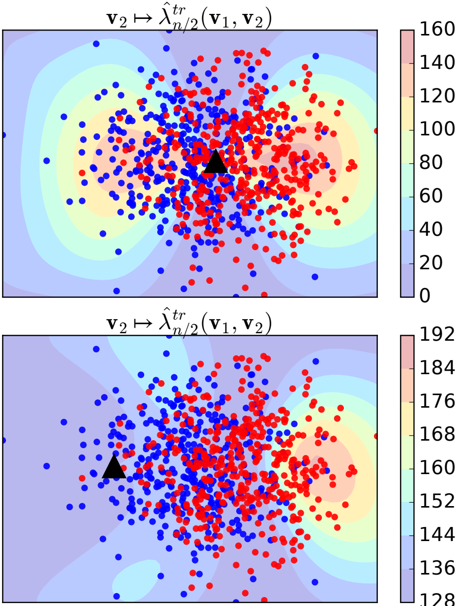
infer, Bayes, Monte Carlo, adaptor, motif,
haplotype, ECG, covariance, Boltzmann

Illustration: Two Informative Features

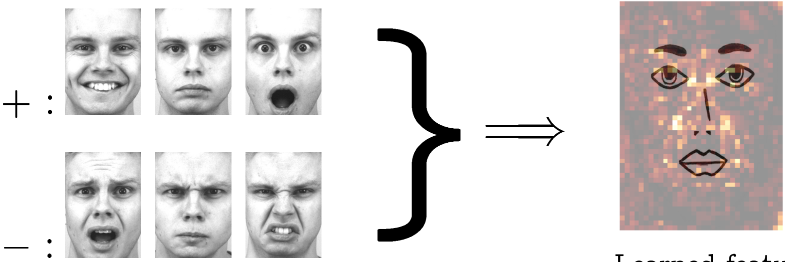
- 2D problem.

$$P : \mathcal{N}([0,0], I)$$
$$Q : \mathcal{N}([1,0], I)$$

- $J = 2$ features.
- Fix $\mathbf{v}_1$ to ▲.
- Contour plot of $\mathbf{v}_2 \mapsto \hat{\lambda}_n(\{\mathbf{v}_1, \mathbf{v}_2\})$.
- $\{\mathbf{v}_1, \mathbf{v}_2\}$ chosen to reveal the difference of P and Q.



Summary



Learned feature

Fast method to extract features
for distinguishing two distributions

- Python code available: http://wittawat.com

Questions?

Thank you

Full ME Test Statistic

- Let $\mathcal{V} = \{\mathbf{v}_1, \ldots, \mathbf{v}_J\}$ be the J test locations.
- Let $\bar{\mathbf{z}}_n := \begin{pmatrix} \hat{\mu}_P(\mathbf{v}_1) - \hat{\mu}_Q(\mathbf{v}_1) \\ \vdots \\ \hat{\mu}_P(\mathbf{v}_J) - \hat{\mu}_Q(\mathbf{v}_J) \end{pmatrix} \in \mathbb{R}^J$.
- Let $(\mathbf{S}_n)_{ij} := \widehat{\text{cov}}_{\mathbf{x}}[k(\mathbf{x}, \mathbf{v}_i), k(\mathbf{x}, \mathbf{v}_j)] + \widehat{\text{cov}}_{\mathbf{y}}[k(\mathbf{y}, \mathbf{v}_i), k(\mathbf{y}, \mathbf{v}_j)] \in \mathbb{R}^{J \times J}$.
- Then, the statistic

$$\hat{\lambda}_n := n \bar{\mathbf{z}}_n^\top (\mathbf{S}_n + \gamma_n I)^{-1} \bar{\mathbf{z}}_n,$$

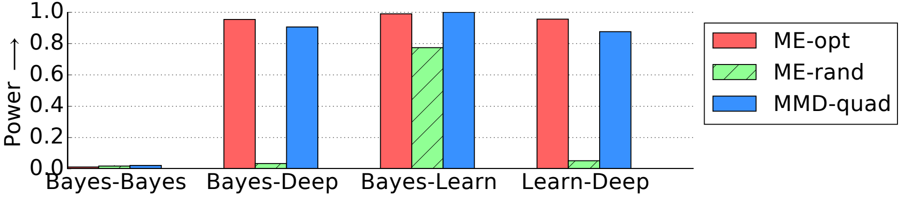
  where $\gamma_n > 0$ is a regularization parameter.
- When $J = 1$,

$$\hat{\lambda}_n = n \frac{[\hat{\mu}_P(\mathbf{v}) - \hat{\mu}_Q(\mathbf{v})]^2}{\gamma_\text{n} + \text{var}_{\mathbf{x}}[k(\mathbf{x}, \mathbf{v})] + \text{var}_{\mathbf{y}}[k(\mathbf{y}, \mathbf{v})]}.$$

- Computing $\hat{\lambda}_n$: $\mathcal{O}(J^3 + J^2 n + Jdn)$.
- Optimization of $\mathcal{V}$: $\mathcal{O}(J^3 + J^2 dn)$.

Distinguishing NIPS Articles

- Bayesian inference, Deep learning, Learning theory
- Random 2000 nouns (dimensions). TF-IDF representation.



Learned informative features (bags of words):

Bayes-Deep: infer, Bayes, Monte Carlo, adaptor, motif, haplotype, ECG

Bayes-Learn: infer, Markov, graphic, segment, bandit, boundary, favor

Learn-Deep: deep, forward, delay, subgroup, bandit, receptor, invariance

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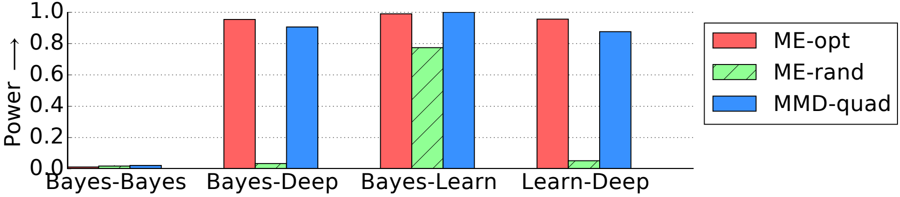
- Bayesian inference, Deep learning, Learning theory
- Random 2000 nouns (dimensions). TF-IDF representation.



Learned informative features (bags of words):

Bayes-Deep: infer, Bayes, Monte Carlo, adaptor, motif, haplotype, ECG
Bayes-Learn: infer, Markov, graphic, segment, bandit, boundary, favor
Learn-Deep: deep, forward, delay, subgroup, bandit, receptor, invariance

Preprocessing of NIPS articles

- Remove stop words, and stem.
- A paper belongs to a group if it has at least one keyword.

1. **Bayesian inference** (Bayes): graphical model, bayesian, inference, mcmc, monte carlo, posterior, prior, variational, markov, latent, probabilistic, exponential family.
2. **Deep learning** (Deep): deep, drop out, auto-encod, convolutional, neural net, belief net, boltzmann.
3. **Learning theory** (Learn): learning theory, consistency, theoretical guarantee, complexity, pac-bayes, pac-learning, generalization, uniform converg, bound, deviation, inequality, risk min, minimax, structural risk, VC, rademacher, asymptotic.
4. **Neuroscience** (Neuro): motor control, neural, neuron, spiking, spike, cortex, plasticity, neural decod, neural encod, brain imag, biolog, perception, cognitive, emotion, synap, neural population, cortical, firing rate, firing-rate, sensor.

Lower Bound on Test Power

- Let $\mathcal{K}$ be a kernel class such that $\sup_{k\in\mathcal{K}} \sup_{(\mathbf{x},\mathbf{y})\in\mathcal{X}^2} |k(\mathbf{x},\mathbf{y})| \le B$.
- Let $\mathbb{V}$ be a collection in which each element is a set of J test locations.
- Assume $\tilde{c} := \sup_{\mathcal{V}\in\mathbb{V}, k\in\mathcal{K}} \|\Sigma^{-1}\|_F < \infty$.

Proposition

The test power $\mathbb{P}_{H_1}\left(\hat{\lambda}_n \ge T_\alpha\right)$ of the ME test satisfies $\mathbb{P}_{H_1}\left(\hat{\lambda}_n \ge T_\alpha\right) \ge L(\lambda_n)$ where

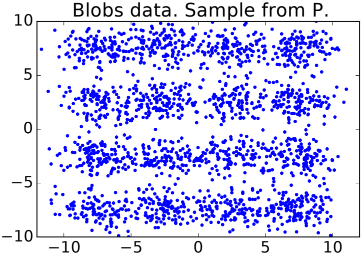
$$L(\lambda_n) := 1 - 2e^{-\xi_1(\lambda_n - T_\alpha)^2/n} - 2e^{-\frac{[\gamma_n(\lambda_n - T_\alpha)(n-1) - \xi_2 n]^2}{\xi_3 n(2n-1)^2}} - 2e^{-[(\lambda_n - T_\alpha)/3 - \bar{c}_3 n\gamma_n]^2 \gamma_n^2/\xi_4},$$

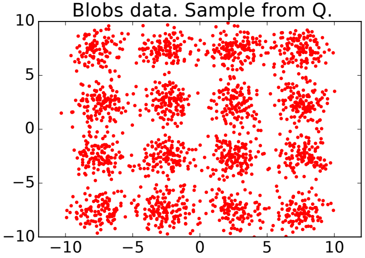
and $\bar{c}_3, \xi_1, \ldots \xi_4$ are positive constants depending on only B, J and $\tilde{c}$. For large n, $L(\lambda_n)$ is increasing in λ_n.

- $\lambda_n := n\mu^\top\Sigma^{-1}\mu$ is the population counterpart of $\hat{\lambda}_n$.
- $\mu = \mathbb{E}_{\mathbf{xy}}[\mathbf{z}_1]$ and $\Sigma = \mathbb{E}_{\mathbf{xy}}[(\mathbf{z}_1 - \mu)(\mathbf{z}_1 - \mu)^\top]$.

Four Toy Problems

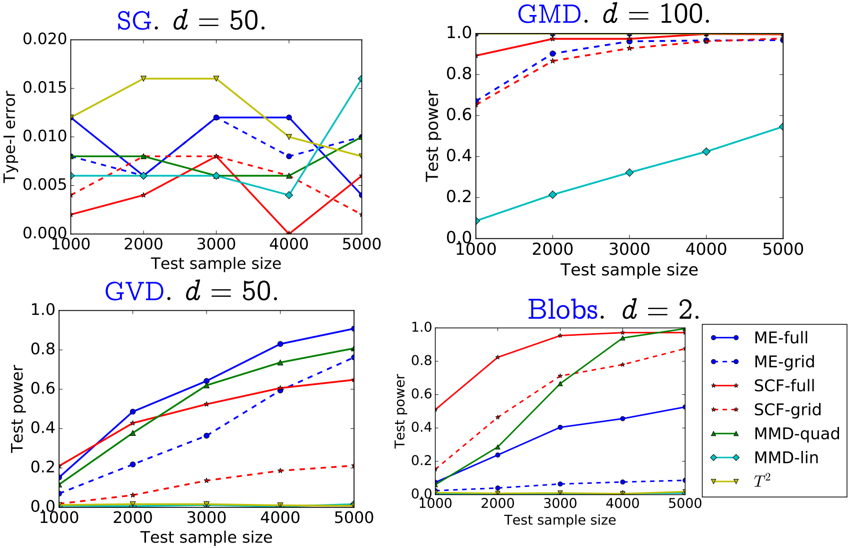
Data	P	Q
1. Same Gaussian (**SG**)	$\mathcal{N}(0_d, I_d)$	$\mathcal{N}(0_d, I_d)$
2. Gauss. mean difference (**GMD**)	$\mathcal{N}(0_d, I_d)$	$\mathcal{N}((1, 0, \ldots, 0)^\top, I_d)$
3. Gauss. variance difference (**GVD**)	$\mathcal{N}(0_d, I_d)$	$\mathcal{N}(0_d, \mathrm{diag}(2, 1, \ldots, 1))$
4. **Blobs** (4×4 grid of Gaussian blobs)		

P : 

Q : 

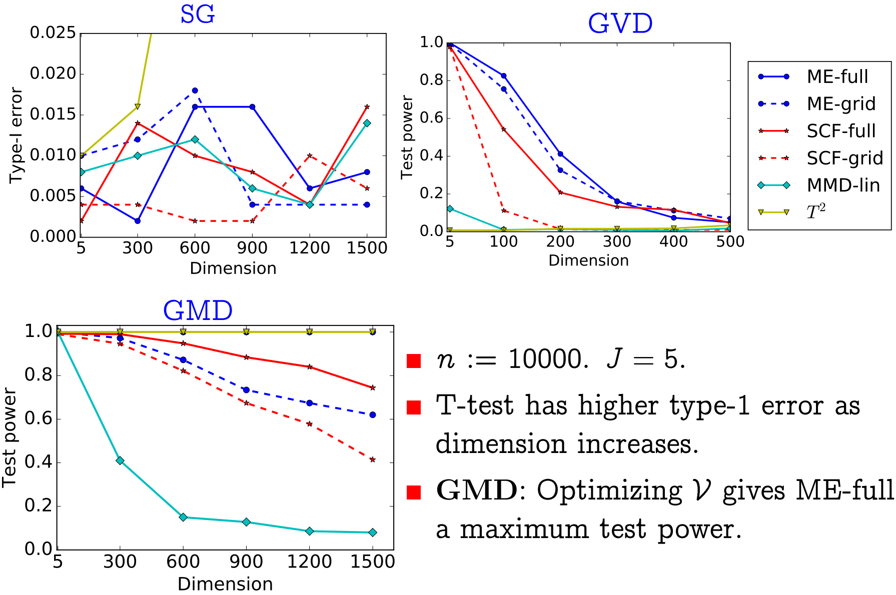
- H_0 is true in SG.
- H_1 is true in others.

Rejection Rate vs. Sample Size



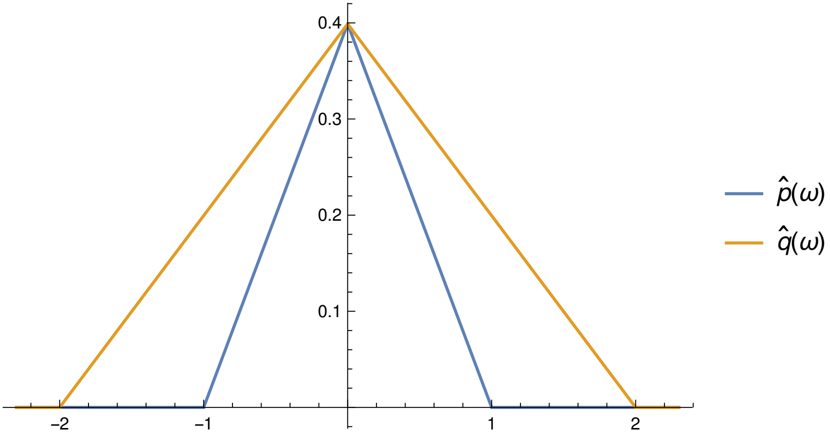
- $J = 5$. Gaussian kernel.
- Right level of type-1 error. Optimizing $\mathcal{V}, \sigma^2$ helps.

Rejection Rate vs. Data Dimension



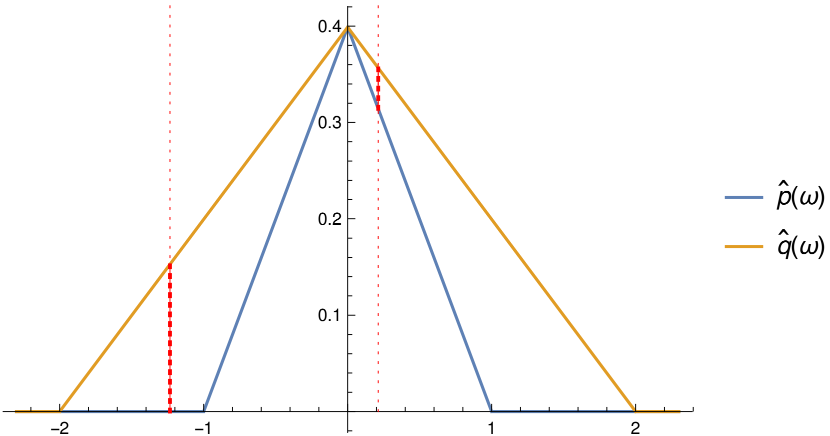
- $n := 10000$. $J = 5$.
- T-test has higher type-1 error as dimension increases.
- **GMD**: Optimizing $\mathcal{V}$ gives ME-full a maximum test power.

Test with smooth characteristic functions (Chwialkowski e



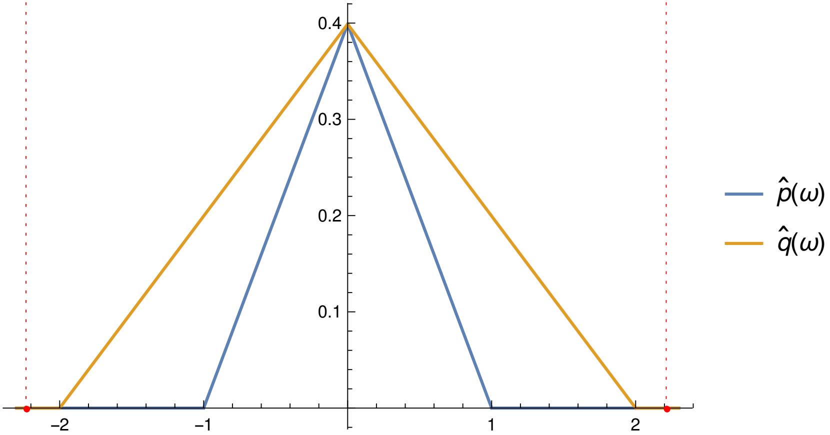
- $\hat{p}(\omega)$, $\hat{q}(\omega)$ are characteristic functions of P, Q.

Illustration: SCF test



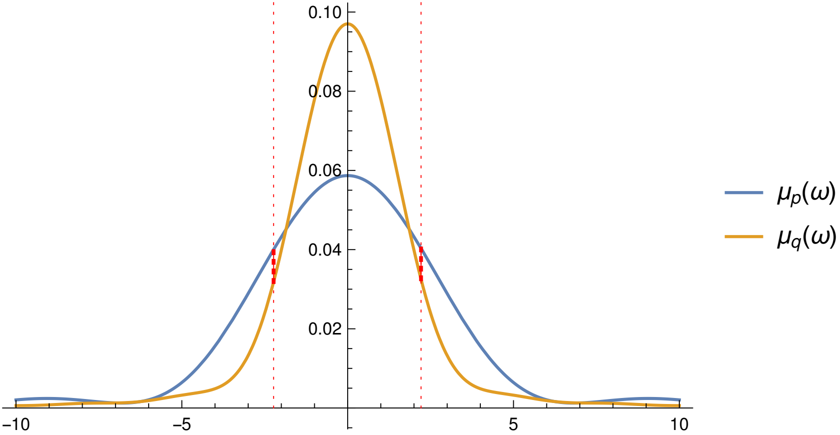
- Checking the difference at finite locations may work.

Illustration: SCF test



- It may also fail if locations are poorly chosen.

Illustration: SCF test



- Smooth the characteristic functions.
- Theoretically, any locations will reveal the difference.

SCF test (Chwialkowski et al., 2015)

- Test based on smooth characteristic functions (SCF) ϕ_P.
- Characteristic function of P is $\hat{p}(\mathbf{w}) := \mathbb{E}_{\mathbf{x}\sim P} \exp(i\mathbf{w}^\top \mathbf{x})$.
- Convolve with an analytic smoothing kernel $l(a) = \exp\left(-\frac{\|a\|^2}{2\sigma^2}\right)$

$$\phi_P(\mathbf{w}) = \int_{\mathbb{R}^d} \hat{p}(\mathbf{w}) l(\mathbf{v}-\mathbf{w})\,\mathrm{d}\mathbf{w} \overset{\text{(algebra)}}{=} \int_{\mathbb{R}^d} \exp(i\mathbf{v}^\top \mathbf{x})\hat{l}(\mathbf{x})\,\mathrm{d}P(\mathbf{x}),$$

  where $\hat{l}$ = inverse Fourier transform of l.
- Test statistic: $d^2_{\phi,J}(P,Q) = \frac{1}{J}\sum_{j=1}^J \left(\phi_P(\mathbf{v}_j) - \phi_Q(\mathbf{v}_j)\right)^2$.
- $\hat{d}^2_{\phi,J}$ uses
  $\hat{\phi}_P(\mathbf{v}) = \frac{1}{n}\sum_{i=1}^n \exp\left(i\mathbf{v}^\top \mathbf{x}_i\right)\hat{l}(\mathbf{x}_i)$.
- $\mathbf{z}_i :=$

$$\begin{pmatrix} \vdots \\ \hat{l}(\mathbf{x}_i)\sin(\mathbf{x}_i^\top \mathbf{v}_j) - \hat{l}(\mathbf{y}_i)\sin(\mathbf{y}_i^\top \mathbf{v}_j) \\ \hat{l}(\mathbf{x}_i)\cos(\mathbf{x}_i^\top \mathbf{v}_j) - \hat{l}(\mathbf{y}_i)\cos(\mathbf{y}_i^\top \mathbf{v}_j) \\ \vdots \end{pmatrix}.$$

Statistic $\hat{\lambda}_n = n\bar{\mathbf{z}}_n (\mathbf{S}+\gamma_n)^{-1}\bar{\mathbf{z}}_n$

References I