Big Hypothesis Testing with Kernel Embeddings

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9 January 2015
UCL Workshop on the Theory of Big Data

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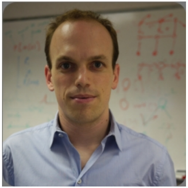
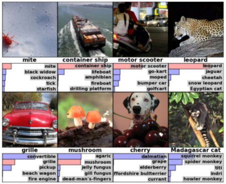
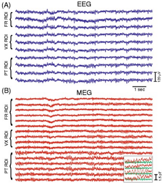


Wojciech Zaremba Matthew Blaschko Arthur Gretton

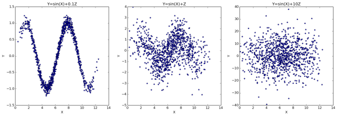
Making Hard Inference Possible

- many dimensions



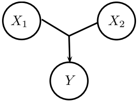


- low signal-to-noise ratio



- highly non-linear assocations

- higher-order interactions



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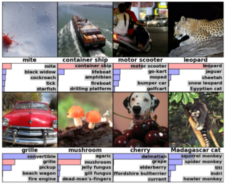

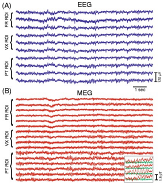

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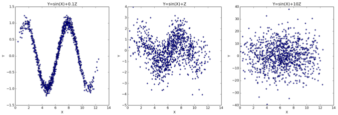

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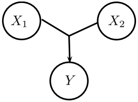

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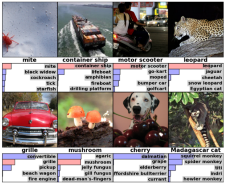

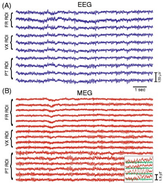

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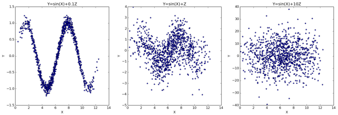

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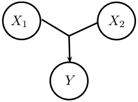

need an expressive model **and** a very large number of observations

cannot use batch algorithms

Overview

1. Kernel Embeddings and MMD
2. Scaling up Kernel Tests
3. Experiments

Outline

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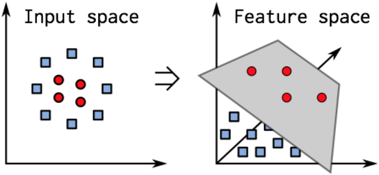
2. Scaling up Kernel Tests
3. Experiments

Kernel Embedding

- **feature map**: $x \mapsto k(\cdot, x) \in \mathcal{H}_k$ instead of $x \mapsto (\varphi_1(x), \ldots, \varphi_s(x)) \in \mathbb{R}^s$
- $\langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}_k} = k(x, y)$ inner products easily **computed**



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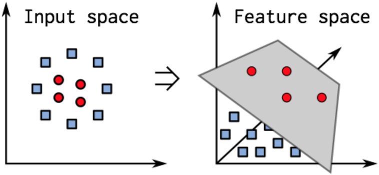
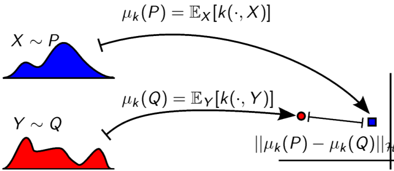


- **embedding**: $P \mapsto \mu_k(P) = \mathbb{E}_{X\sim P} k(\cdot, X) \in \mathcal{H}_k$ instead of $P \mapsto (\mathbb{E}\varphi_1(X), \ldots, \mathbb{E}\varphi_s(X)) \in \mathbb{R}^s$
- $\langle \mu_k(P), \mu_k(Q)\rangle_{\mathcal{H}_k} = \mathbb{E}_{X,Y} k(X, Y)$ inner products easily **estimated**

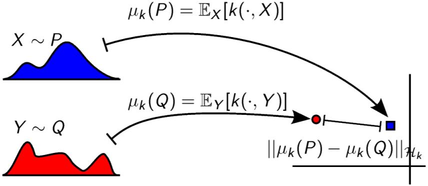


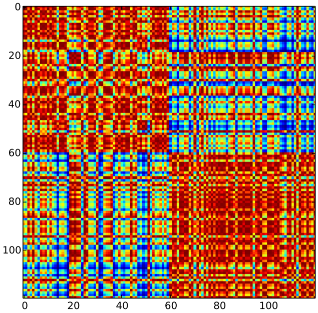
Kernel MMD (1)

Definition

Kernel metric (MMD) between P and Q:

$$\begin{aligned}\mathrm{MMD}_k^2(P,Q) &= \|\mathbb{E}k(\cdot,X)-\mathbb{E}k(\cdot,Y)\|_{\mathcal{H}_k}^2 \\ &= \mathbb{E}_{XX'}k(X,X')+\mathbb{E}_{YY'}k(Y,Y')-2\mathbb{E}_{XY}k(X,Y)\end{aligned}$$





Kernel MMD (2)

- A polynomial kernel $k(z,z') = \left(1 + z^\top z'\right)^s$ captures the difference in first s moments only
- For a certain family of kernels (**characteristic**): $\mathrm{MMD}_k(P,Q) = 0$ if and only if $P = Q$: Gaussian $\exp(-\frac{1}{2\sigma^2}\|z - z'\|_2^2)$, Laplacian, inverse multiquadratics, B_{2n+1}- splines...
- Under mild assumptions, k-MMD metrizes weak* topology on probability measures (Sriperumbudur, 2010):

$$\mathrm{MMD}_k(P_n, P) \to 0 \Leftrightarrow P_n \rightsquigarrow P$$

Nonparametric two-sample tests

- Testing $\mathbf{H_0}$: $\mathbf{P} = \mathbf{Q}$ vs. $\mathbf{H_A}$: $\mathbf{P} \neq \mathbf{Q}$
  based on samples $\{x_i\}_{i=1}^{n_x} \sim \mathbf{P}$, $\{y_i\}_{i=1}^{n_y} \sim \mathbf{Q}$.
- Test statistic is an estimate of
  $\mathrm{MMD}_k^2(P, Q) = \mathbb{E}_{XX'} k(X, X') + \mathbb{E}_{YY'} k(Y, Y') - 2\mathbb{E}_{XY} k(X, Y)$:

$$
\begin{aligned}
\widehat{\mathrm{MMD}} &= \frac{1}{n_x(n_x-1)} \sum_{i \neq j} k(x_i, x_j) + \frac{1}{n_y(n_y-1)} \sum_{i \neq j} k(y_i, y_j) \\
&\quad - \frac{2}{n_x n_y} \sum_{i,j} k(x_i, y_j).
\end{aligned}
$$

- $O(n^2)$ to compute ($n = n_x + n_y$)
- Degenerate U-statistic: $\frac{1}{\sqrt{n}}$-convergence to MMD under $\mathbf{H_A}$, $\frac{1}{n}$-convergence to 0 under $\mathbf{H_0}$.

Gretton et al (2009, 2012)

Nonparametric independence tests

- $\mathbf{H_0}$: $X \perp\!\!\!\perp Y$
- $\mathbf{H_A}$: $X \not\perp\!\!\!\perp Y$

Nonparametric independence tests

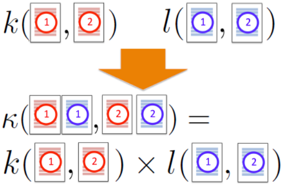
- $\mathbf{H_0}: X \perp\!\!\!\perp Y \Leftrightarrow \mathbf{P}_{XY} = \mathbf{P}_X \mathbf{P}_Y$
- $\mathbf{H_A}: X \not\perp\!\!\!\perp Y \Leftrightarrow \mathbf{P}_{XY} \neq \mathbf{P}_X \mathbf{P}_Y$

- Test statistic:

  $$\mathrm{HSIC}(X, Y) = \left\| \mu_\kappa(\hat{P}_{XY}) - \mu_\kappa(\hat{P}_X \hat{P}_Y) \right\|^2_{\mathcal{H}_\kappa},$$

  with $\kappa = k \otimes l$

  Gretton et al (2005, 2008); Smola et al (2007)



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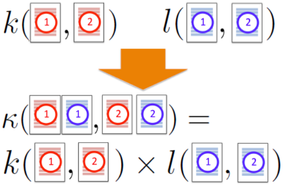
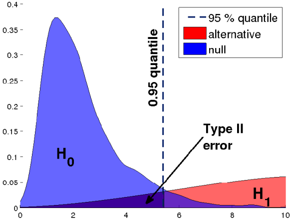


Extensions: conditional independence testing (Fukumizu, Gretton, Sun and Schölkopf, 2008; Zhang, Peters, Janzing and Schölkopf, 2011), three-variable interaction (DS, Gretton and Bergsma, 2013)

Outline

Test threshold

- under $\mathbf{H_0}$: $\mathbf{P} = \mathbf{Q}$:
$$\frac{n_x n_y}{n_x + n_y} \widehat{\mathrm{MMD}}_k \rightsquigarrow \sum_{r=1}^{\infty} \lambda_r \left(Z_r^2 - 1\right), \quad \{Z_r\} \overset{i.i.d.}{\sim} \mathcal{N}(0,1)$$
  - $\{\lambda_r\}$ depend on both k and $\mathbf{P}$.
- expensive threshold computation:
  - Estimate leading λ_r's (requires eigendecomposition of the kernel matrix): $O(n^3)$
  - Permutation test: #shuffles $\times$ $O(n^2)$



Limited data, unlimited time

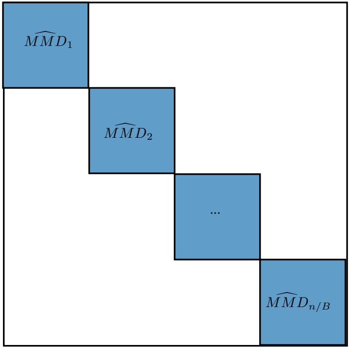
$$\mathrm{MMD}_k^2(P,Q) = \mathbb{E}_{XX'}k(X,X') + \mathbb{E}_{YY'}k(Y,Y') - 2\mathbb{E}_{XY}k(X,Y)$$

- Estimate with

$$\widehat{\mathrm{MMD}} = \frac{1}{n_x(n_x-1)}\sum_{i\neq j}k(x_i,x_j) + \frac{1}{n_y(n_y-1)}\sum_{i\neq j}k(y_i,y_j) - \frac{2}{n_x n_y}\sum_{i,j}k(x_i,y_j).$$

- Complexity: $O\left(n^2\right)$.

Limited time, unlimited data



- Process mini-batches of size B at a time: $\hat{\eta}_k = \frac{B}{n} \sum_{b=1}^{n/B} \widehat{MMD}_{k,b}$
- Complexity: $O(nB)$.
- Provided $B/n \to 0$: $\frac{1}{\sqrt{n}}$-convergence to MMD if MMD $\neq 0$, $\frac{1}{\sqrt{nB}}$-convergence to 0 under $\mathbf{H_0}$.

- A.Gretton, B.Sriperumbudur, DS, H.Strathmann, S.Balakrishnan, M.Pontil and K.Fukumizu, **Optimal kernel choice for large-scale two-sample tests**, *NIPS* 2012.
- W.Zaremba, A.Gretton, M.Blaschko, **B-test: A Non-Parametric, Low Variance Kernel Two-Sample Test**, *NIPS* 2013.

Full statistic vs. mini-batch statistic

	U-statistic	mini-batch
time	$O(n^2)$	$O(nB)$
storage	$O(n^2)$	$O(B^2)$
null distribution	infinite sum of chi-squares	**normal**
computing p-value	$O(n^3)$ or #shuffles $\times$ $O(n^2)$	$O(nB)$
convergence rate	$1/n$	$1/\sqrt{nB}$

- $\frac{n_x n_y}{(n_x+n_y)^{3/2}}\sqrt{B}\hat{\eta}_k \rightsquigarrow \mathcal{N}\left(0,\sigma_k^2\right)$ under $\mathbf{H_0}$
- σ_k^2 (depends on k and **P**) can be unbiasedly estimated on each block in $O(B^2)$ time

Asymptotic efficiency criterion

- A. Gretton, B. Sriperumbudur, DS, H. Strathmann, S. Balakrishnan, M. Pontil and K. Fukumizu, **Optimal kernel choice for large-scale two-sample tests**, *NIPS* 2012.

Proposition

For given P and Q. Let $\eta_k = MMD_k^2(P, Q)$, *and let* σ_k^2 *be the asymptotic variance of the linear-time statistic* $\hat{\eta}_k$. *Then*

$$k_* = \arg\max_{k \in \mathcal{K}} \eta_k / \sigma_k$$

minimizes the asymptotic Type II error probability on $\mathcal{K}$.

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- We only have estimates of η_k and σ_k !
- Will the kernel optimization using plug-in esimates be consistent?
- Over what families of kernels can we perform such optimization *efficiently*?

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- We only have estimates of η_k and σ_k !
- Will the kernel optimization using plug-in esimates be consistent? yes!
- Over what families of kernels can we perform such optimization *efficiently*? linear combinations (MKL)

Outline

Hard-to-detect differences: Gaussian blobs

Difficult problems: lengthscale of the *difference* in distributions not the same as that of the distributions.

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We distinguish grids of Gaussian blobs with different covariances.

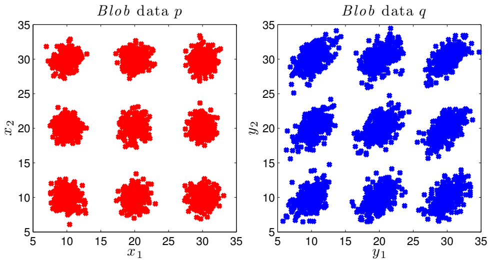

Figure : 3×3 blobs, ratio $\varepsilon = 3.2$ of largest-to-smallest eigenvalues of blobs in Q.

Gaussian blobs (2)

12×12 blobs with $\varepsilon = 1.4$. Linear time statistic vs. Quadratic time statistic. Fixed kernel.

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	m **per trial**	**Type II error**	**Trials**
Quadratic	5,000	$[0.7996, 0.8516]$	820
	10,000	$[0.5161, 0.6175]$	367
	$> 10,000$	Buy more RAM!	

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Linear	$\sim 100,000,000$	$[0.2250, 0.3049]$	468
	$\sim 200,000,000$	$[0.1873, 0.2829]$	302
	$\vdots$	$\vdots$	$\vdots$
	$\sim 500,000,000$	$\mathbf{0.0270} \pm \mathbf{0.0302}$	111

Gaussian blobs (3)

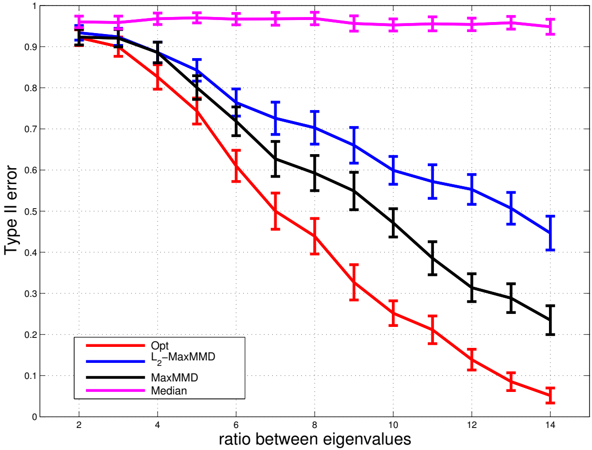

Figure : $m = 10,000$; family generated by gaussian kernels with bandwiths $\{2^{-5}, \ldots, 2^{15}\}$.

Hard-to-detect differences: UCI HIGGS

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- benchmark dataset for distinguishing a signature of Higgs boson vs. background
- joint distributions of the azimuthal angular momenta φ for four particle jets: low-signal, low-level features
- Do *joint* angular momenta carry any discriminating information?

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sample size:	1e4	5e4	1e5	5e5	1e6
p-value (gauss-med):	.757	.217	.475	.391	.074

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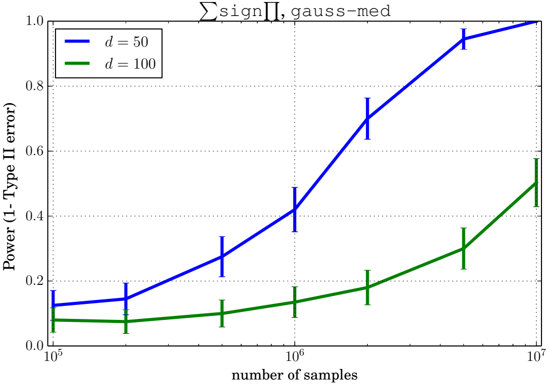
sample size:	1e4	5e4	1e5	5e5	1e6
p-value (gauss-med):	.757	.217	.475	.391	.074

train/test size:	2e3/8e3	1e4/4e4	2e4/8e4	1e5/4e5	2e5/8e5
p-value (gauss-opt):	.139	.476	.035	**6.12e-5**	**1.02e-18**

Experiment: Independence Test ($\sum \texttt{sign} \prod$)

- $X \sim \mathcal{N}(0, I_d)$,
  $Y = \sqrt{\frac{2}{d}} \sum_{j=1}^{d/2} \text{sign}\left(X_{2j-1}X_{2j}\right)|Z_j| + Z_{\frac{d}{2}+1}$, where $Z \sim \mathcal{N}\left(0, I_{\frac{d}{2}+1}\right)$



Experiment: Independence Test (`sine` $\sum$)

- $X_1, X_2 \overset{i.i.d.}{\sim} \mathrm{Unif}[0, 2\pi]$,
  $Y = \sin(X_1 + X_2) + 10Z$, with $Z \sim \mathcal{N}(0, 1)$.

`sine` $\sum$, $B = 100$	brown: $q = 1$	brown: opt	gauss: med	gauss: opt
$N = 5e5$, 1-Type II	$.277 \pm .059$	$\mathbf{.675 \pm .065}$	$.190 \pm .054$	$\mathbf{.740 \pm .061}$
Type I	$.035 \pm .025$	$.025 \pm .022$	$.085 \pm .039$	$.040 \pm .027$
$N = 1e6$, 1-Type II	$.460 \pm .069$	$\mathbf{.915 \pm .039}$	$.325 \pm .065$	$\mathbf{.905 \pm .041}$
Type I	$.055 \pm .032$	$.050 \pm .030$	$.025 \pm .022$	$.060 \pm .033$

Shogun

- Written in C++ with interfaces to Python, Matlab, Java, R.
- Google Summer of Code (2012, 2014).

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- A simple mini-batch procedure allows us to run the tests on large-scale problems and on streaming data.
- Can select kernel parameters on-the-fly in order to explicitly maximise test power.
- Both kernel selection and testing in $O(n)$ time and $O(1)$ storage (if $B = \text{const}$).