Learning with Approximate Kernel Embeddings

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Outline

1. Preliminaries on Kernel Embeddings

2. Testing and Learning on Distributions with Symmetric Noise Invariance

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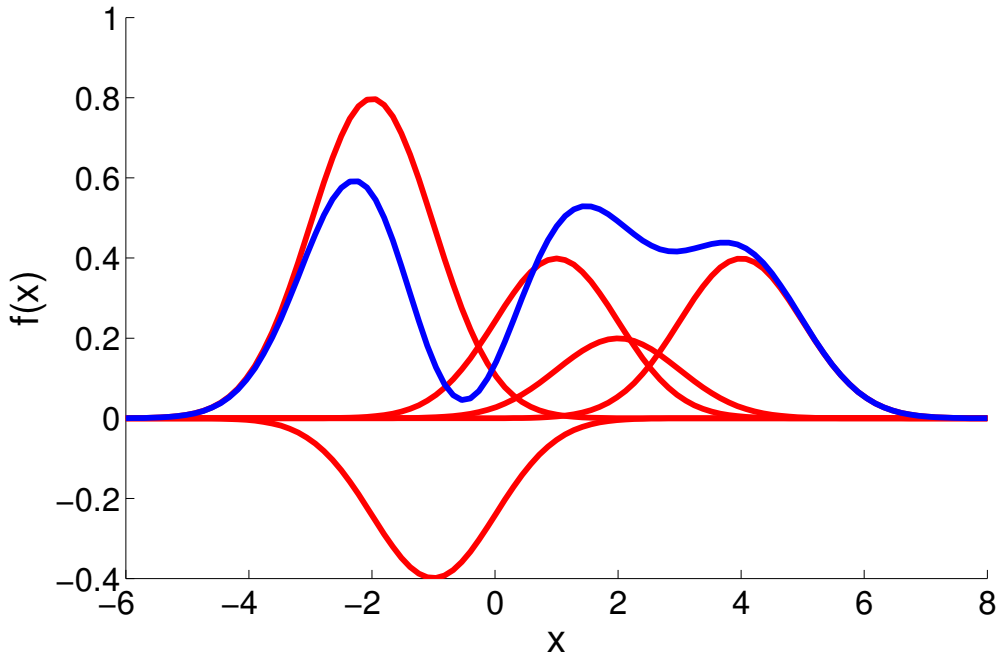
2. Testing and Learning on Distributions with Symmetric Noise Invariance

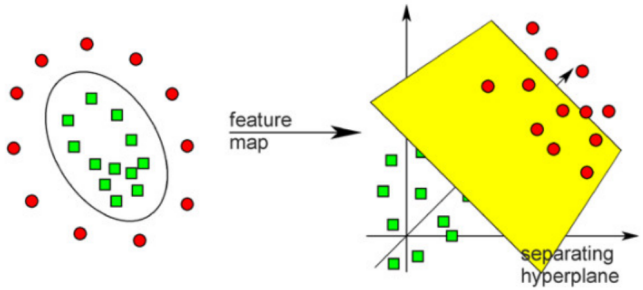
Reproducing Kernel Hilbert Spaces

- RKHS: a Hilbert space of functions on $\mathcal{X}$ with continuous evaluation $f \mapsto f(x)$, $\forall x \in \mathcal{X}$ (norm convergence implies pointwise convergence).
- Each RKHS corresponds to a positive definite kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, s.t.
  1. $\forall x \in \mathcal{X}, \quad k(\cdot, x) \in \mathcal{H}$, and
  2. $\forall x \in \mathcal{X}, \forall f \in \mathcal{H}, \quad \langle f, k(\cdot, x) \rangle_{\mathcal{H}} = f(x)$.
- RKHS can be constructed as $\mathcal{H}_k = \overline{span\left\{k(\cdot, x) \,|\, x \in \mathcal{X}\right\}}$ and includes functions $f(x) = \sum_{i=1}^{n} \alpha_i k(x, x_i)$ and their pointwise limits.



Kernel Trick and Kernel Mean Trick

- implicit feature map $x \mapsto k(\cdot, x) \in \mathcal{H}_k$
  replaces $x \mapsto [\phi_1(x), \ldots, \phi_s(x)] \in \mathbb{R}^s$
- $\langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}_k} = k(x, y)$
  inner products readily available
  - nonlinear decision boundaries, nonlinear regression functions, learning on non-Euclidean/structured data



[Cortes & Vapnik, 1995; Schölkopf & Smola, 2001]

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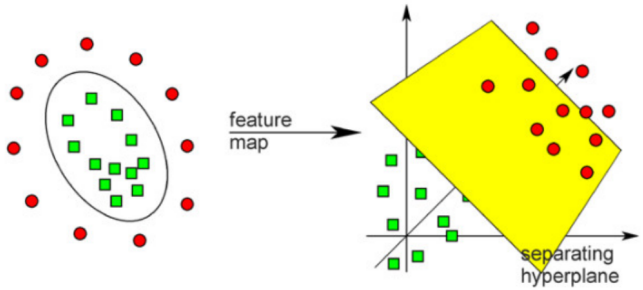
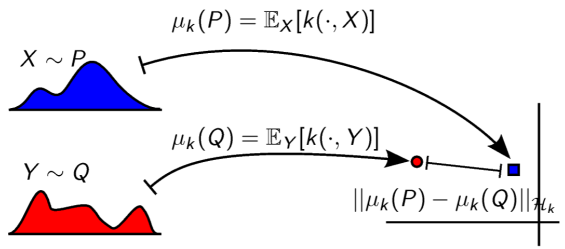


[Cortes & Vapnik, 1995; Schölkopf & Smola, 2001]

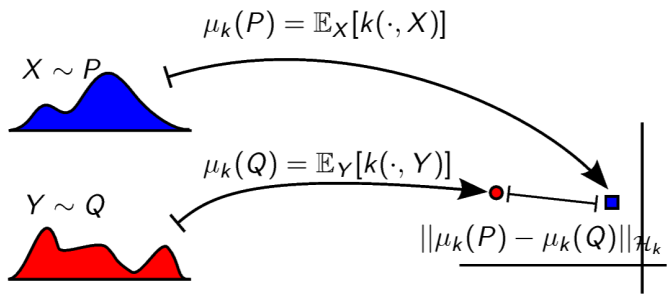
- **RKHS embedding**: implicit feature mean
  [Smola et al, 2007; Sriperumbudur et al, 2010]
  $P \mapsto \mu_k(P) = \mathbb{E}_{X \sim P} k(\cdot, X) \in \mathcal{H}_k$
  replaces $P \mapsto [\mathbb{E}\phi_1(X), \ldots, \mathbb{E}\phi_s(X)] \in \mathbb{R}^s$
- $\langle \mu_k(P), \mu_k(Q) \rangle_{\mathcal{H}_k} = \mathbb{E}_{X \sim P, Y \sim Q} k(X, Y)$
  inner products easy to estimate
  - nonparametric two-sample, independence, conditional independence, interaction testing, learning on distributions

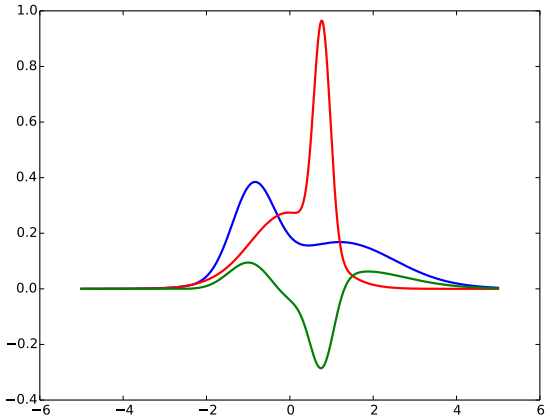


[Gretton et al, 2005; Gretton et al, 2006; Fukumizu et al, 2007; DS et al, 2013; Muandet et al, 2012; Szabo et al, 2015]

Maximum Mean Discrepancy

- **Maximum Mean Discrepancy (MMD)** [Borgwardt et al, 2006; Gretton et al, 2007] between P and Q:





$$\mathrm{MMD}_k(P, Q) = \|\mu_k(P) - \mu_k(Q)\|_{\mathcal{H}_k} = \sup_{f \in \mathcal{H}_k : \|f\|_{\mathcal{H}_k} \leq 1} |\mathbb{E}f(X) - \mathbb{E}f(Y)|$$

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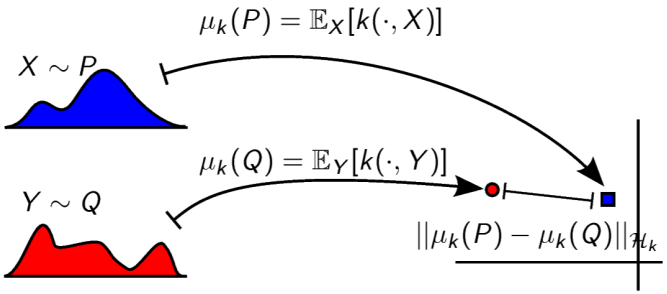

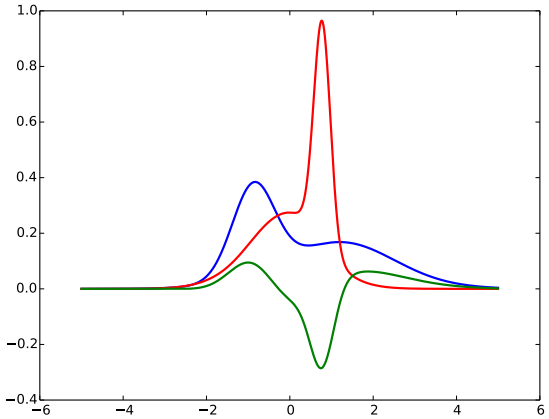

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- **Characteristic** kernels: $\mathrm{MMD}_k(P, Q) = 0$ iff $P = Q$.
  - Gaussian RBF $\exp(-\frac{1}{2\sigma^2}\|x - x'\|_2^2)$, Matérn family, inverse multiquadrics.
- For characteristic kernels on LCH $\mathcal{X}$, MMD metrizes weak* topology on probability measures [Sriperumbudur,2010],

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

Some uses of MMD

within-sample average similarity

–

between-sample average similarity

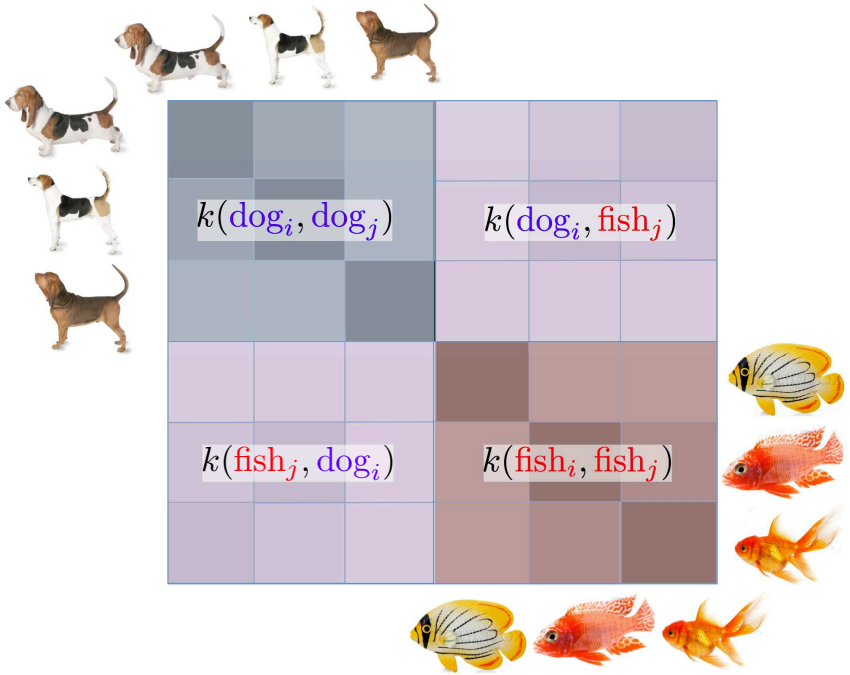


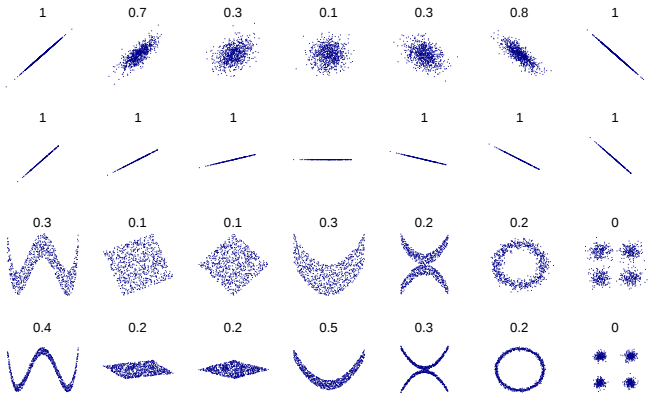
Figure by Arthur Gretton

MMD has been applied to:

- two-sample tests and independence tests [Gretton et al, 2009, Gretton et al, 2012]
- model criticism and interpretability [Lloyd & Ghahramani, 2015; Kim, Khanna & Koyejo, 2016]
- analysis of Bayesian quadrature [Briol et al, 2015+]
- ABC summary statistics [Park, Jitkrittum & DS, 2015]
- summarising streaming data [Paige, DS & Wood, 2016]
- traversal of manifolds learned by convolutional nets [Gardner et al, 2015]
- training deep generative models [Dziugaite, Roy & Ghahramani, 2015; Sutherland et al, 2017]

$$\text{MMD}_k^2(P, Q) = \mathbb{E}_{X,X' \overset{i.i.d.}{\sim} P} k(X, X') + \mathbb{E}_{Y,Y' \overset{i.i.d.}{\sim} Q} k(Y, Y') - 2\mathbb{E}_{X \sim P, Y \sim Q} k(X, Y).$$

Kernel dependence measures



cor vs. dcor

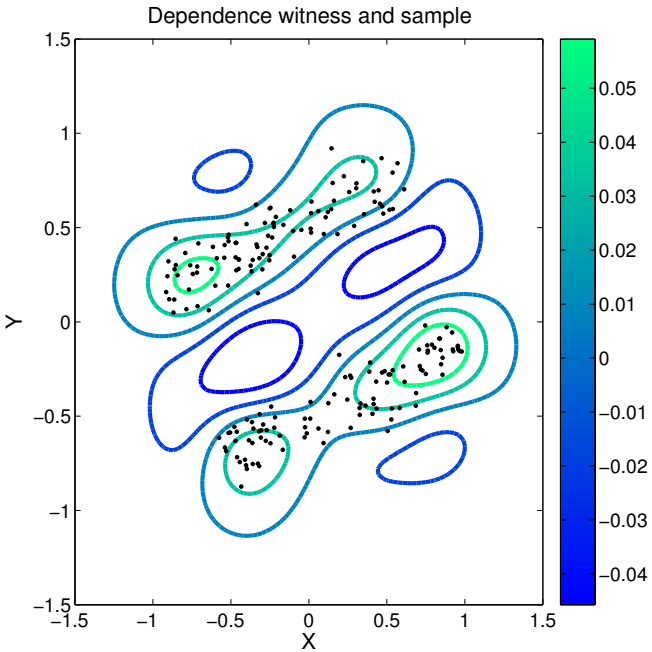


Figure by Arthur Gretton

$$HSIC^2(X, Y; \kappa) = \|\mu_\kappa(P_{XY}) - \mu_\kappa(P_X P_Y)\|^2_{\mathcal{H}_\kappa}$$

- Hilbert-Schmidt norm of the feature-space cross-covariance [Gretton et al, 2009]
- dependence witness is a smooth function in the RKHS $\mathcal{H}_\kappa$ of functions on $\mathcal{X} \times \mathcal{Y}$

$$k(\boxed{1}, \boxed{2}) \quad l(\boxed{1}, \boxed{2})$$

$$\kappa(\boxed{1}\boxed{1}, \boxed{2}\boxed{2}) = k(\boxed{1}, \boxed{2}) \times l(\boxed{1}, \boxed{2})$$

- Independence testing framework that generalises Distance Correlation (dcor) of [Szekely et al, 2007]: HSIC with Brownian motion covariance kernels [DS et al, 2013]

Distribution Regression

- supervised learning where labels are available at the group, rather than at the individual level.

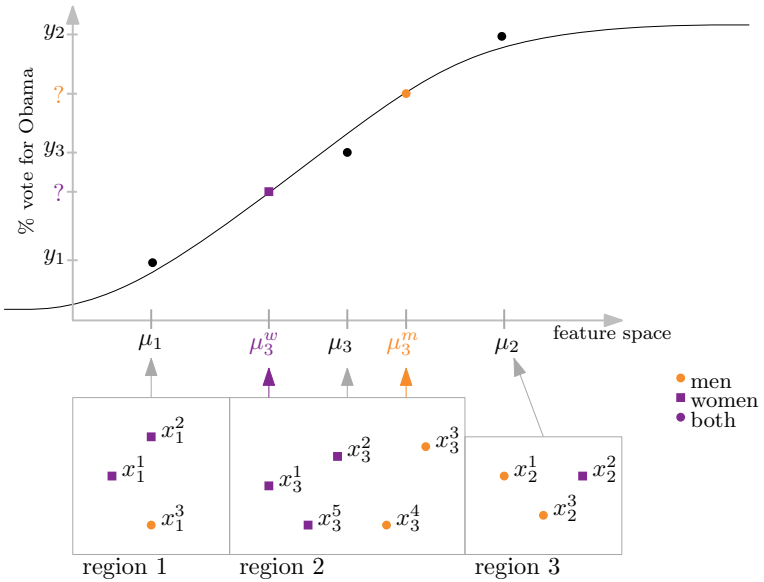


Figure from Flaxman et al, 2015

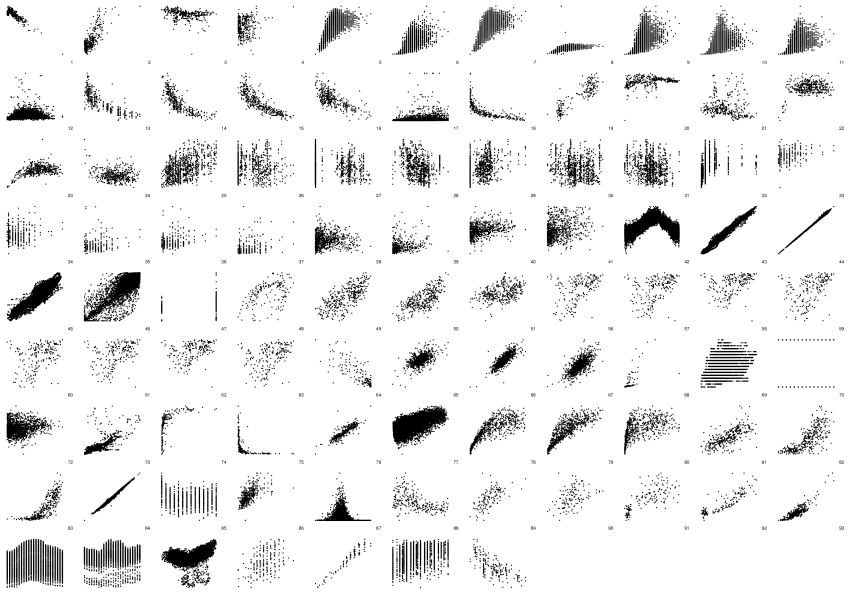


Figure from Mooij et al, 2014

- classifying text based on word features [Yoshikawa et al, 2014; Kusner et al, 2015]
- aggregate voting behaviour of demographic groups [Flaxman et al, 2015; 2016]
- image labels based on a distribution of small patches [Szabo et al, 2016]
- "traditional" parametric statistical inference by learning a function from sets of samples to parameters: ABC [Mitrovic et al, 2016], EP [Jitkrittum et al, 2015]
- identify the cause-effect direction between a pair of variables from a joint sample [Lopez-Paz et al,2015]

- Possible (distributional) covariate shift?

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2 Testing and Learning on Distributions with Symmetric Noise Invariance

All possible differences between generating processes?

- differences discovered by an MMD two-sample test can be due to different types of measurement noise or data collection artefacts
  - With a large sample-size, uncovers potentially irrelevant sources of variability: slightly different calibration of the data collecting equipment, different numerical precision, different conventions of dealing with edge-cases
- Learning on distributions: each label y_i in supervised learning is associated to a whole bag of observations $B_i = \{X_{ij}\}_{j=1}^{N_i}$ – assumed to come from a probability distribution P_i
  - Each bag of observations could be impaired by a different measurement noise process. Distributional covariate shift: different measurement noise on test bags?
- Both problems require encoding the distribution with a representation invariant to symmetric noise.

Testing and Learning on Distributions with Symmetric Noise Invariance.
Ho Chung Leon Law, Christopher Yau, DS.
http://arxiv.org/abs/1703.07596

Random Fourier features: Inverse Kernel Trick

Bochner's representation: Assume that k is a positive definite **translation-invariant** kernel on $\mathbb{R}^p$. Then k can be written as

$$\begin{aligned} k(x,y) &= \int_{\mathbb{R}^p} \exp\left(i\omega^\top (x-y)\right) d\Lambda(\omega) \\ &= 2\int_{\mathbb{R}^p} \left\{\cos\left(\omega^\top x\right)\cos\left(\omega^\top y\right) + \sin\left(\omega^\top x\right)\sin\left(\omega^\top y\right)\right\} d\Lambda(\omega) \end{aligned}$$

for some positive measure (w.l.o.g. a probability distribution) Λ.

- Sample m frequencies $\Omega = \{\omega_j\}_{j=1}^m \sim \Lambda$ and use a Monte Carlo estimator of the kernel function instead [Rahimi & Recht, 2007]:

$$\begin{aligned} \hat{k}(x,y) &= \frac{2}{m}\sum_{j=1}^{m} \left\{\cos\left(\omega_j^\top x\right)\cos\left(\omega_j^\top y\right) + \sin\left(\omega_j^\top x\right)\sin\left(\omega_j^\top y\right)\right\} \\ &= \langle \xi_\Omega(x), \xi_\Omega(y)\rangle_{\mathbb{R}^{2m}}, \end{aligned}$$

  with an explicit set of features $\xi_\Omega : x \mapsto \sqrt{\frac{2}{m}}\left[\cos\left(\omega_1^\top x\right), \sin\left(\omega_1^\top x\right), \ldots\right]^\top$.
- How fast does m need to grow with n? Can be sublinear for regression [Bach, 2015].

Approximate Mean Embeddings and Characteristic Functions

If k is translation-invariant, MMD becomes the weighted L_2-distance between the characteristic functions of P and Q [Sriperumbudur, 2010].

$$\|\mu_P - \mu_Q\|^2_{\mathcal{H}_k} = \int_{\mathbb{R}^d} |\varphi_P(\omega) - \varphi_Q(\omega)|^2 \, d\Lambda(\omega),$$

Approximate mean embedding using random Fourier features is simply the evaluation (real and complex part stacked together) of the characteristic function at the frequencies $\{\omega_j\}_{j=1}^m \sim \Lambda$:

$$\begin{aligned}\Phi(P) &= \mathbb{E}_{X\sim P}\xi_\Omega(X) \\ &= \sqrt{\frac{2}{m}}\mathbb{E}_{X\sim P}\left[\cos\left(\omega_1^\top x\right), \sin\left(\omega_1^\top x\right), \ldots, \cos\left(\omega_m^\top x\right), \sin\left(\omega_m^\top x\right)\right]^\top\end{aligned}$$

Used for distribution regression [Sutherland et al, 2015] and for sketching / compressive learning [Keriven et al, 2016].

The Noise and the Signal

Adopting similar ides from nonparametric deconvolution of [Delaigle and Hall, 2016].

- define a *symmetric positive definite (SPD) noise component* to be any random vector E on $\mathbb{R}^d$ with a positive characteristic function, $\varphi_E(\omega) = \mathbb{E}_{X \sim E}\left[\exp(i\omega^\top E)\right] > 0$, $\forall \omega \in \mathbb{R}^d$ (but E is not a.s. 0)
  - symmetric about zero, i.e. E and $-E$ have the same distribution
  - if E has a density, it must be a positive definite function
  - spherical zero-mean Gaussian distribution, as well as multivariate Laplace, Cauchy or Student's t (but not uniform).
- define an (SPD-)*decomposable* random vector X if its characteristic function can be written as $\varphi_X = \varphi_{X_0}\varphi_E$, with E SPD noise component.
- Assume that only the indecomposable components of distributions are of interest.

Phase Discrepancy and Phase Features

[Delaigle and Hall, 2016] construct density estimators for nonparametric deconvolution, i.e. estimate density f_0 of X_0 with observations $X_i \sim X_0 + E$. E has unknown SPD distribution. Matching phase functions:

$$\rho_X(\omega) = \frac{\varphi_X(\omega)}{|\varphi_X(\omega)|} = \exp(i\tau_X(\omega))$$

Phase function is *invariant to SPD noise* as it only changes the amplitude of the characteristic function.

We are not interested in density estimation but in measuring differences up to SPD noise. In analogy to MMD, define **phase discrepancy**:

$$\mathrm{PhD}(X, Y) = \int_{\mathbb{R}^d} |\rho_X(\omega) - \rho_Y(\omega)|^2 \, d\Lambda(\omega)$$

for some spectral measure Λ.

Construct distribution features by simply normalising approximate mean embeddings:

$$\Psi(P_X) = \sqrt{\frac{1}{m}} \left[\frac{\mathbb{E}\xi_{\omega_1}(X)}{\|\mathbb{E}\xi_{\omega_1}(X)\|}, \ldots, \frac{\mathbb{E}\xi_{\omega_m}(X)}{\|\mathbb{E}\xi_{\omega_m}(X)\|} \right]^\top$$

where $\xi_{\omega_j}(x) = \left[\cos\left(\omega_j^\top x\right), \sin\left(\omega_j^\top x\right)\right]$.

Phase and Indecomposability

Is phase discrepancy a metric on indecomposable random variables?

Phase and Indecomposability

Is phase discrepancy a metric on indecomposable random variables? No

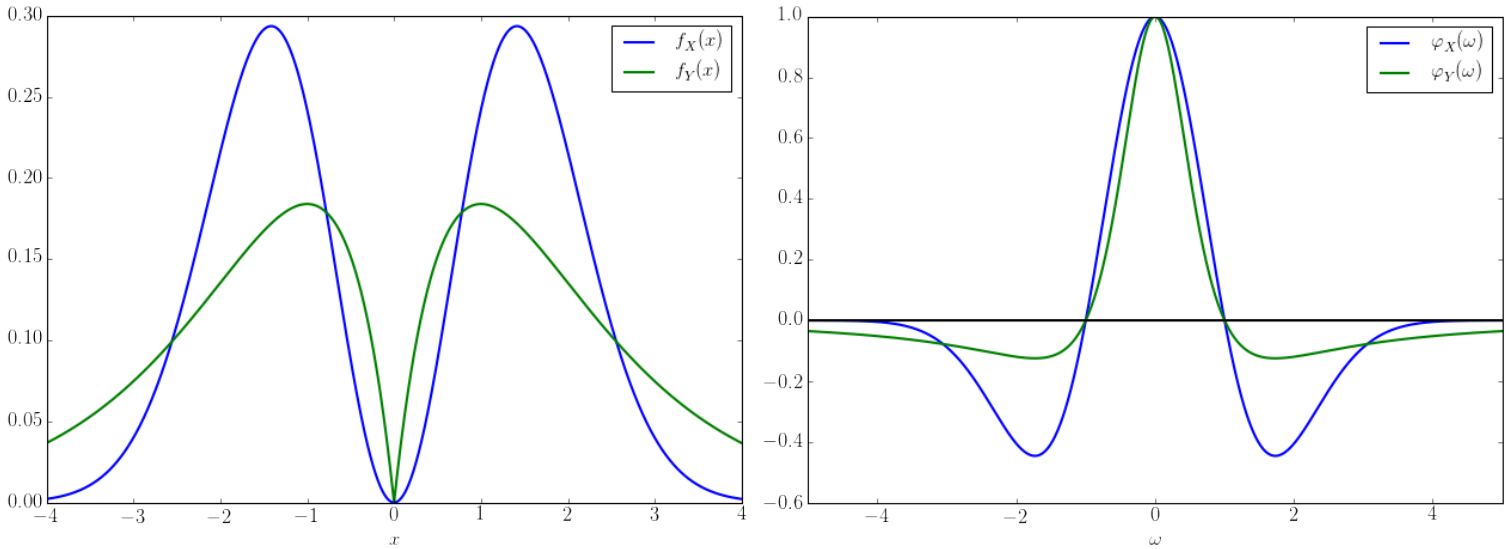
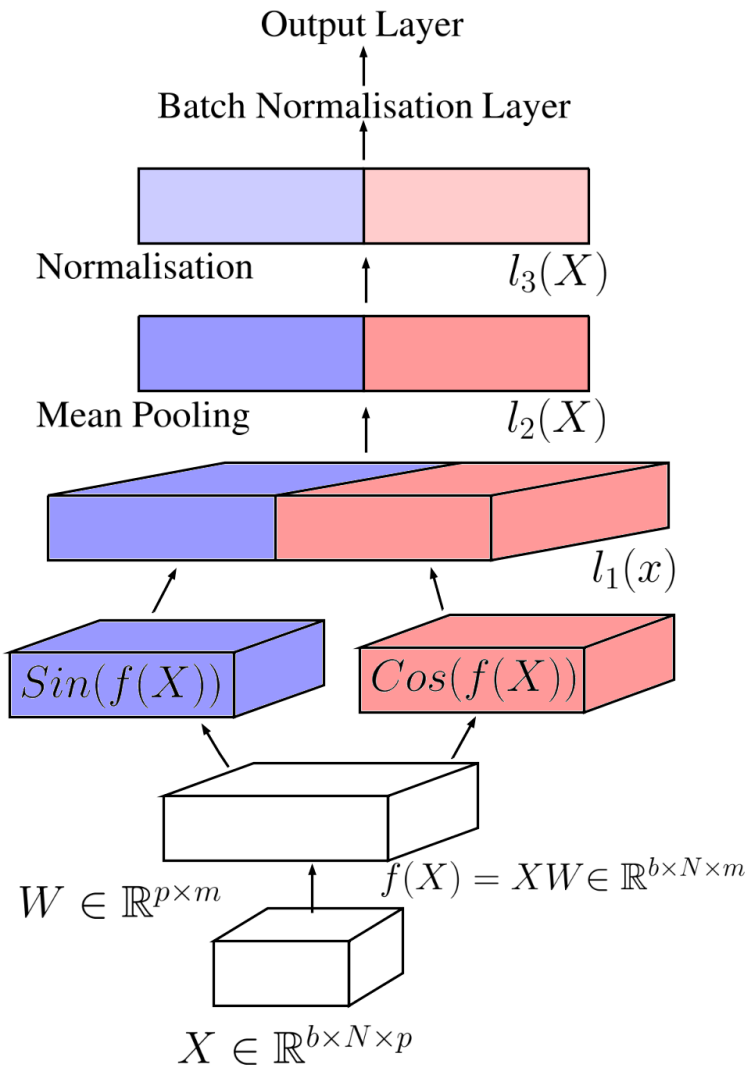


Figure: Example of two indecomposable distributions which have the same phase function. **Left**: densities. **Right**: characteristic functions.

$$f_X(x) = \frac{1}{\sqrt{2\pi}} x^2 \exp(-x^2/2), \quad f_Y(x) = \frac{1}{2}|x| \exp(-|x|).$$

Learning Phase Features



- Random Phase features have a large variance, due to empirical normalisation.
- Given a supervised signal, we can optimise a set of frequencies $\{w_i\}_{i=1}^m$ that will give us a useful discriminative representation. In other words, we are no longer focusing on a specific translation-invariant kernel k (specific Λ), but are learning Fourier/phase features.
- A neural network with coupled cos/sin activation functions, mean pooling and normalisation.
- Straightforward implementation in `Tensorflow` (code: `https://github.com/hcllaw/Fourier-Phase-Neural-Network`)

Synthetic Example

$$
\begin{aligned}
\theta &\sim \Gamma(\alpha, \beta), \\
Z &\sim U[0, \sigma], \\
\epsilon|Z &\sim \mathcal{N}(0, Z), \\
\{X_i\}|\theta, \epsilon &\overset{i.i.d.}{\sim} \frac{\Gamma\left(\theta/2, 1/2\right)}{\sqrt{2\theta}} + \epsilon,
\end{aligned}
$$

- Goal: Learn a mapping $\{X_i\} \mapsto \theta$
- Can be used for semi-automatic ABC [Fearnhead & Prangle, 2012] with kernel distribution regression for summary statistics [Mitrovic, DS & Teh, 2016].

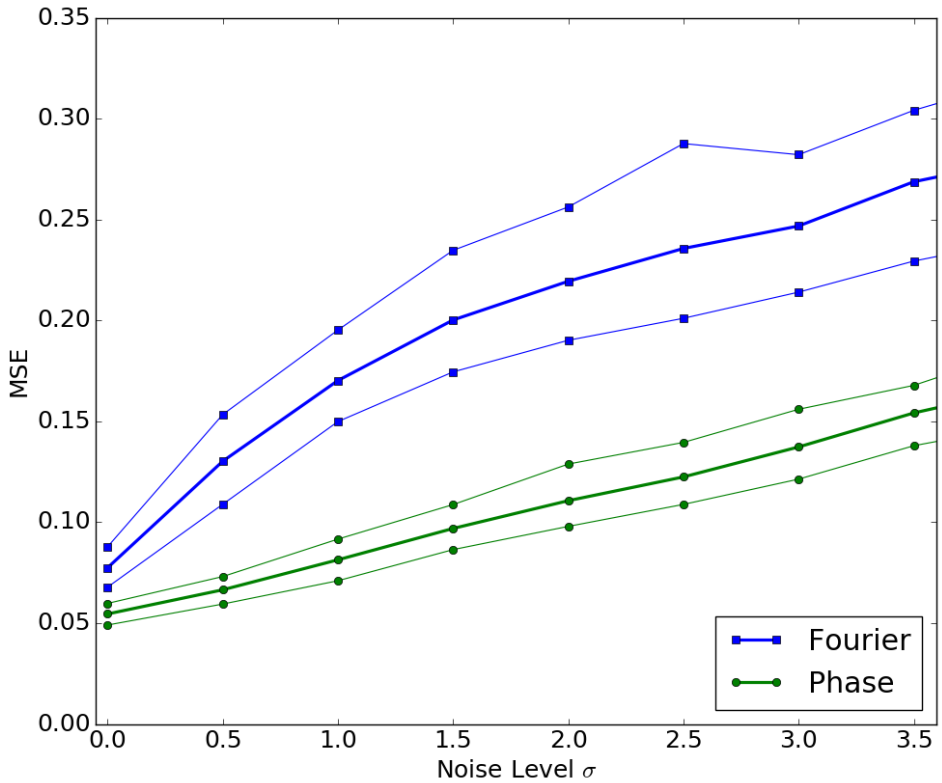


Figure: MSE of θ, using the Fourier and phase neural network averaged over 100 runs. Here noise σ is varied between 0 and 3.5, and the 5^{th} and the 95^{th} percentile is shown.

Aerosol MISR1 Dataset [Wang et al, 2012] with Covariate Shift

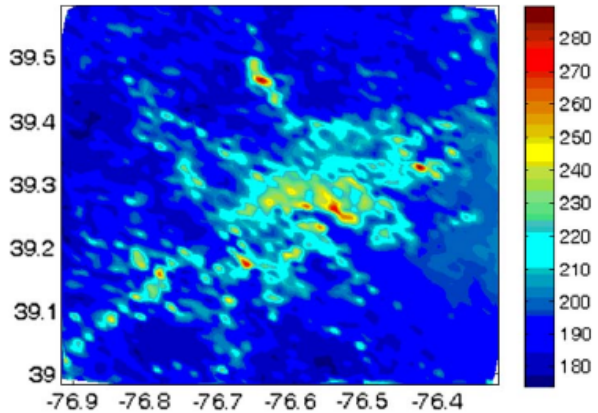


figure from Wang et al, 2012

- Aerosol Optical Depth (AOD) multiple-instance learning problem with 800 bags, each containing 100 randomly selected 16-dim multispectral pixels (satellite imaging) within 20km radius of AOD sensor.
- Image variability due to surface properties – small spatial variability of AOD.
- The label y_i provided by the ground AOD sensors.

The test data is impaired by additive SPD noise components.

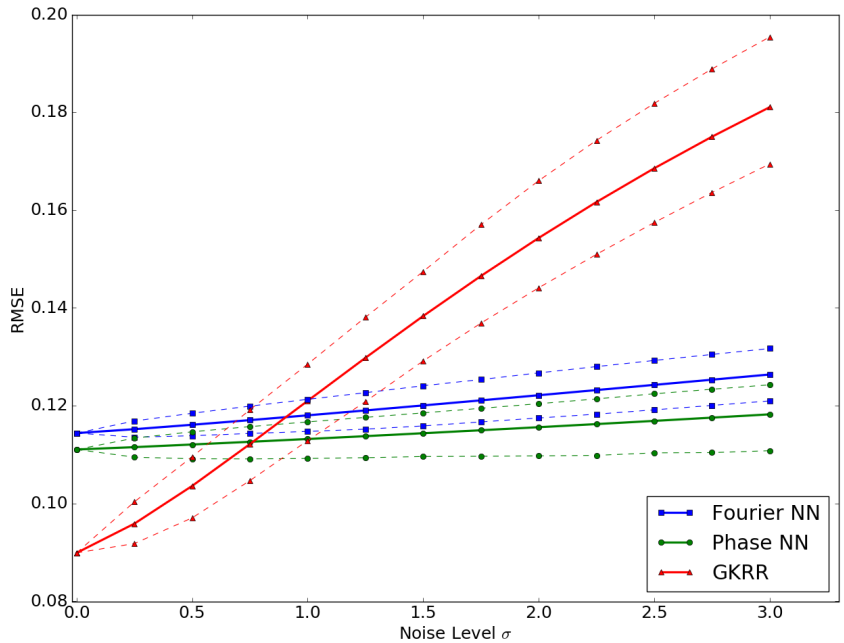


Figure: RMSE on the test set, corrupted by various levels of noise, using the Fourier and phase neural network and GKKR averaged over 100 runs. Here noise-to-signal ratio σ is varied between 0 and 3.0, and the 5^{th} and the 95^{th} percentile is shown.

Can Fourier features learn invariance?

- Discriminative frequencies learned on the "noiseless" training data correspond to *Fourier features* that are nearly normalised (i.e. they are close to unit norm).
- This means that the Fourier NN has *learned to be approximately invariant* based on training data, indicating that Aerosol data potentially has irrelevant SPD noise components ("cloudy pixels")

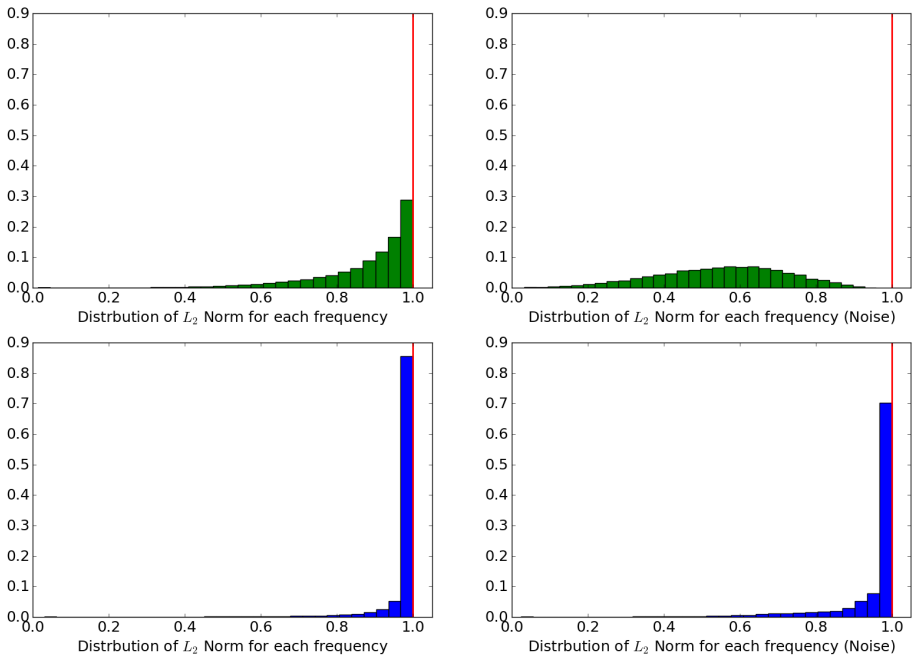


Figure: Histograms for the distribution of the modulus of Fourier features over each frequency w for the Aerosol data (test set); **Green:** Random Fourier Features (with the kernel bandwidth optimised on training data)
Bottom Blue: Learned Fourier features; **Left:** Original test set; **Right:** Test set with (additional) noise.

Summary

- When measuring nonparametric distances between distributions, can we disentangle the differences in noise from the differences in the signal?
- We considered two different ways to encode invariances to symmetric noise:
  - MMD for asymmetry (not discussed in the talk) in paired sample differences, $MMD(X-Y, Y-X)$, which can be used to construct a two-sample test up to symmetric noise.
  - weighted distance between the empirical phase functions for learning algorithms on distribution inputs which are robust to measurement noise and covariate shift.