Kernel Mean Embeddings

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Outline

RKHS

Kernel Mean Embeddings

Characteristic kernels

Two Sample Testing

- MMD
- Kernelised Stein Discrepancy

Kernel Bayes' Rule

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Kernels

A kernel k is a positive definite function $\mathcal{X} \times \mathcal{X} \rightarrow$, that is for all $a_1, \ldots, a_n \in$, $x_1, \ldots, x_n \in \mathcal{X}$,

$$\sum_{i,j=1}^{n} a_i a_j k(x_i, x_j) \geq 0$$

Intuitively a kernel is a measure of similarity between two elements of $\mathcal{X}$.

Kernels

Commonly used kernels:

- polynomial

$$(\langle x_1, x_2 \rangle + 1)^d$$

- Gaussian RBF

$$e^{-\frac{\|x-y\|^2}{2\sigma^2}}$$

- Laplace

$$e^{-\frac{\|x-y\|}{\sigma}}$$

RKHS

A reproducing kernel Hilbert space (RKHS) for a kernel k is one spanned by functions $k(x, \cdot)$ for all $x \in \mathcal{X}$ with the inner product defined by

$$\langle k(x_1, \cdot), k(x_2, \cdot) \rangle = k(x_1, x_2)$$

which is well-defined on all of $\mathcal{H}$ by linearity of the inner product.

The equation above is known as the kernel trick and lets us treat $\mathcal{H}$ as an implicit feature space, where we never have to explicitly evaluate the feature map.

RKHS

$\mathcal{H}$ has the reproducing property, that is for all $f \in \mathcal{H}$ and all $x \in \mathcal{X}$,

$$\langle f, k(x, \cdot) \rangle = f(x)$$

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- RKHS
- Kernel Mean Embeddings
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Expectations in RKHS

Goal: evaluating expected values of functions from an RKHS.

As with the kernel trick, it turns out that this is possible in terms of inner products, making the computation analytically tractable,

$$\mathop{\mathbb{E}}_{\mathrm{p}}[f(x)] = \int_{\mathcal{X}} \mathrm{p}(\mathrm{d}x) f(x) = \int_{\mathcal{X}} \mathrm{p}(\mathrm{d}x) \langle k(x,\cdot), f\rangle_{\mathcal{H}_k}$$
$$\stackrel{?}{=} \langle \int_{\mathcal{X}} \mathrm{p}(\mathrm{d}x) k(x,\cdot), f\rangle_{\mathcal{H}_k} =: \langle \mu_{\mathrm{p}}, f\rangle_{\mathcal{H}_k}$$

μ_{p} is so called *kernel mean embedding* (KME) of distribution p.

Note: $\mathcal{X}$ assumed measurable throughout the whole presentation.

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Existence of KME

Riesz representation theorem: For every *bounded linear functional* $\mathcal{T} : \mathcal{H} \to \mathbb{R}$ (resp. $\mathcal{T} : \mathcal{H} \to \mathbb{C}$), there exists a unique $g \in \mathcal{H}$ such that $\mathcal{T}(f) = \langle g, f \rangle_{\mathcal{H}}, \forall f \in \mathcal{H}$.

Expectation is a linear functional, and $\forall f \in \mathcal{H}$ we have,

$$\mathop{\mathbb{E}}_{\mathrm{p}} f(x) \leq \left| \mathop{\mathbb{E}}_{\mathrm{p}} f(x) \right| \leq \mathop{\mathbb{E}}_{\mathrm{p}} \left| f(x) \right| = \mathop{\mathbb{E}}_{\mathrm{p}} \left| \langle f, k(x, \cdot) \rangle_{\mathcal{H}} \right| \leq \|f\|_{\mathcal{H}} \mathop{\mathbb{E}}_{\mathrm{p}} \left\| k(x, \cdot) \right\|_{\mathcal{H}}$$

Thus if $\mathbb{E}_{\mathrm{p}} \sqrt{k(x, x)} < \infty$, then $\mu_{\mathrm{p}} \in \mathcal{H}$ exists, and $\mathbb{E}_{\mathrm{p}} f(x) = \langle \mu_{\mathrm{p}}, f \rangle_{\mathcal{H}}, \forall f \in \mathcal{H}$.

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Estimating KME

Because μ_{p} is generally unknown, it has to be estimated.

A natural (and minimax optimal) estimator is the sample mean,

$$\hat{\mu}_{\mathrm{p}} := \frac{1}{\mathrm{N}} \sum_{n=1}^{\mathrm{N}} k(x_n, \cdot)$$

and in particular,

$$\hat{\mu}_{\mathrm{p}}(x) = \langle \hat{\mu}_{\mathrm{p}}, k(x, \cdot) \rangle_{\mathcal{H}} = \frac{1}{\mathrm{N}} \sum_{n=1}^{\mathrm{N}} k(x_n, x) \xrightarrow{\mathrm{N} \to \infty} \mathop{\mathbb{E}}_{\mathrm{p}(x')} k(x', x)$$

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Representing Distributions via KME

A positive definite kernel is called *characteristic* if,

$$\begin{aligned} \mathcal{T} : \mathcal{M}_1^+(\mathcal{X}) &\to \mathcal{H} \\ \mathrm{p} &\mapsto \mu_{\mathrm{p}} \end{aligned}$$

is injective; $\mathcal{M}_1^+(\mathcal{X})$ is the set of probability measures on $\mathcal{X}$. [5, 6]

Characteristic kernels

Proving a kernel is characteristic is non-trivial in general, but sufficient conditions exist. Three well known examples:

- *Universality*: If k is continuous, $\mathcal{X}$ compact, and $\mathcal{H}_k$ dense in $\mathcal{C}(\mathcal{X})$ wrt L_∞, then k is characteristic. [6, 8]

- *Integral strict positive definiteness*: A bounded measurable kernel k is called *integrally strictly positive definite* if $\int_{\mathcal{X}} \int_{\mathcal{X}} k(x, y)\, \mu(\mathrm{d}x)\mu(\mathrm{d}y) > 0$ for all non–zero finite signed Borel measures μ on $\mathcal{X}$. [22]

- *Some stationary kernels*: For $\mathcal{X} = \mathbb{R}^d$, a stationary kernel k is characteristic **iff** $\operatorname{supp} \Lambda(\omega) = \mathbb{R}^d$, where $\Lambda(\omega)$ is the spectral density of k (cf. Bochner's theorem). [22]

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t-test

Have $\{x_1, \ldots, x_{\mathrm{N}}\} \overset{iid}{\sim} \mathcal{N}(\mu_1, \sigma_1^2)$, and $\{y_1, \ldots, y_{\mathrm{M}}\} \overset{iid}{\sim} \mathcal{N}(\mu_2, \sigma_2^2)$, where all parameters are unknown.

Declare $H_0 : \mu_1 = \mu_2; H_1 : \mu_1 \neq \mu_2$. Then for,

$$\hat{\mu}_1 := \frac{1}{\mathrm{N}} \sum_{n=1}^{\mathrm{N}} x_n \qquad \hat{\mu}_2 := \frac{1}{\mathrm{M}} \sum_{m=1}^{\mathrm{M}} y_m$$

$\hat{\mu}_i \sim \mathcal{N}(\mu_i, \frac{\sigma_i^2}{\mathrm{N}}), \forall i \in \{1, 2\}$, and $\hat{\mu}_1 - \hat{\mu}_2 \sim \mathcal{N}(\mu_1 - \mu_2, \frac{\sigma_1^2}{\mathrm{N}} + \frac{\sigma_2^2}{\mathrm{M}})$.

Hence $t \overset{H_0}{\sim} \mathrm{t}_{\,\nu}$, $\nu := \frac{(s_1^2/\mathrm{N} + s_2^2/\mathrm{M})^2}{\frac{(s_1^2/\mathrm{N})^2}{\mathrm{N}-1} + \frac{(s_2^2/\mathrm{M})^2}{\mathrm{M}-1}}$, where,

$$t := \frac{(\hat{\mu}_1 - \hat{\mu}_2) - 0}{\sqrt{\frac{s_1^2}{\mathrm{N}} + \frac{s_2^2}{\mathrm{M}}}}, \quad s_1^2 := \frac{\sum_{i=1}^{\mathrm{N}} (x_i - \hat{\mu}_1)^2}{\mathrm{N} - 1}, \quad s_2^2 := \frac{\sum_{i=1}^{\mathrm{M}} (y_i - \hat{\mu}_2)^2}{\mathrm{M} - 1}.$$

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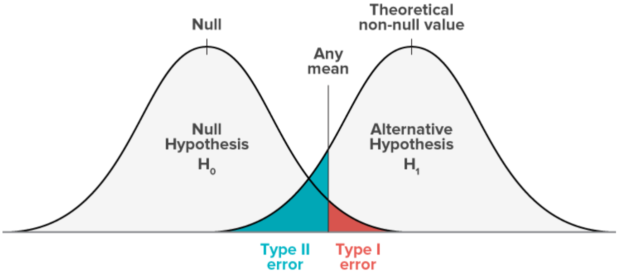
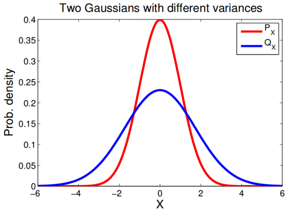
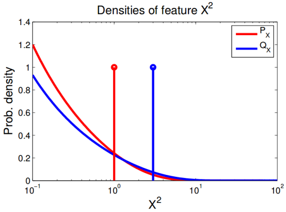


http://grasshopper.com/blog/the-errors-of-ab-testing-your-conclusions-can-make-things-worse/

More examples





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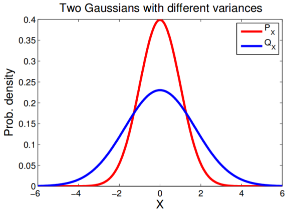

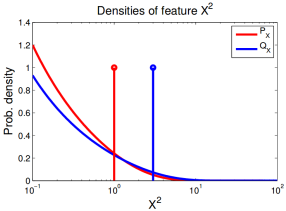

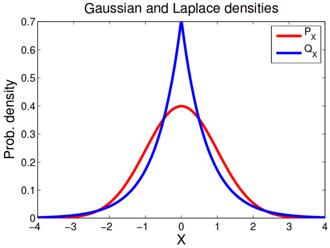

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Recap

Kernel mean embedding,

$$\mathbb{E}_{\mathrm{p}(\boldsymbol{x})}[f(\boldsymbol{x})] = \langle f, \mu_{\mathrm{p}} \rangle_{\mathcal{H}}, \forall f \in \mathcal{H}$$

For a characteristic kernel k and the corresponding RKHS $\mathcal{H}$,

$$\mu_{\mathrm{p}} = \mu_{\mathrm{q}} \text{ iff } \mathrm{p} = \mathrm{q}\,.$$

This means we might be able to distinguish distributions by comparing the corresponding kernel mean embeddings.

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Maximum Mean Discrepancy (MMD)

Measure distance between mean embeddings by the worst case difference of expected values [9],

$$\begin{aligned}\mathrm{MMD}(\mathrm{p}, \mathrm{q}, \mathcal{H}) &:= \sup_{f \in \mathcal{H}, \|f\|_{\mathcal{H}} \leq 1} \left(\mathop{\mathbb{E}}_{\mathrm{p}(\boldsymbol{x})}[f(\boldsymbol{x})] - \mathop{\mathbb{E}}_{\mathrm{q}(\boldsymbol{y})}[f(\boldsymbol{y})] \right) \\ &= \sup_{f \in \mathcal{H}, \|f\|_{\mathcal{H}} \leq 1} \left(\langle \mu_{\mathrm{p}} - \mu_{\mathrm{q}}, f \rangle_{\mathcal{H}} \right)\end{aligned}$$

Notice that $\langle \mu_{\mathrm{p}} - \mu_{\mathrm{q}}, f \rangle_{\mathcal{H}} \leq \left\| \mu_{\mathrm{p}} - \mu_{\mathrm{q}} \right\|_{\mathcal{H}} \|f\|_{\mathcal{H}}$, with equality iff $f \propto \mu_{\mathrm{p}} - \mu_{\mathrm{q}}$. Hence,

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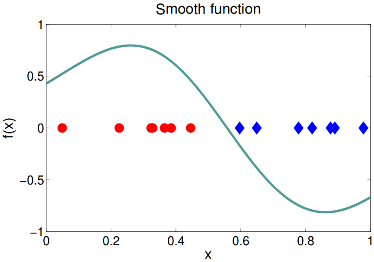
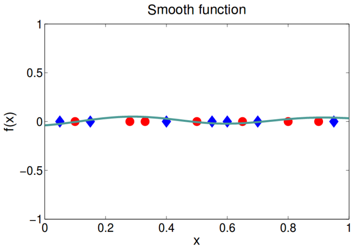
Witness function





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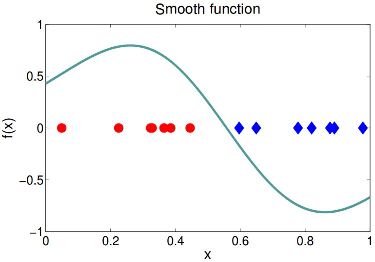

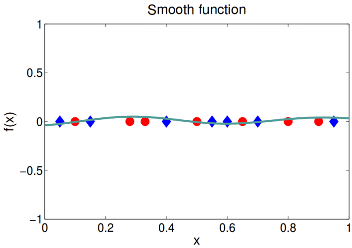

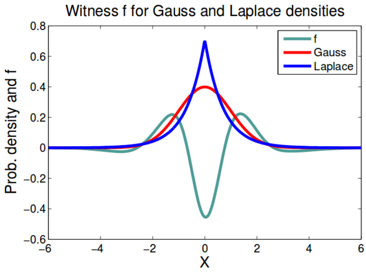

Estimation

Recall: empirical kernel mean embedding estimator,

$$\hat{\mu}_{\mathrm{p}} = \frac{1}{\mathrm{N}} \sum_{n=1}^{\mathrm{N}} k\left(x_n, \cdot\right)$$

We can estimate the square of MMD by substituting the empirical estimator. For $\{x_i\}_{i=1}^{\mathrm{N}} \overset{iid}{\sim} \mathrm{p}$ and $\{y_i\}_{i=1}^{\mathrm{N}} \overset{iid}{\sim} \mathrm{q}$,

$$\begin{aligned}\widehat{\mathrm{MMD}}^2 =& \frac{1}{\mathrm{N}(\mathrm{N}-1)} \sum_{i=1}^{\mathrm{N}} \sum_{j \neq i}^{\mathrm{N}} \left(k\left(x_i, x_j\right) + k\left(y_i, y_j\right)\right) \\ & - \frac{1}{\mathrm{N}^2} \sum_{i=1}^{\mathrm{N}} \sum_{j=1}^{\mathrm{N}} \left(k\left(x_i, y_j\right) + k\left(x_j, y_i\right)\right)\end{aligned}$$

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Estimation

Proof sketch:

$$\mathrm{MMD}^2(\mathrm{p}, \mathrm{q}, \mathcal{H}) = \left\|\mu_{\mathrm{p}} - \mu_{\mathrm{q}}\right\|_{\mathcal{H}}^2 = \left\|\mu_{\mathrm{p}}\right\|_{\mathcal{H}}^2 + \left\|\mu_{\mathrm{q}}\right\|_{\mathcal{H}}^2 - 2\langle \mu_{\mathrm{p}}, \mu_{\mathrm{q}} \rangle_{\mathcal{H}}$$

where,

$$\begin{aligned}\left\|\mu_{\mathrm{p}}\right\|_{\mathcal{H}}^2 = \langle \mu_{\mathrm{p}}, \mu_{\mathrm{p}} \rangle_{\mathcal{H}} = \mathop{\mathbb{E}}_{x\sim \mathrm{p}} \mu_{\mathrm{p}}(x) = \mathop{\mathbb{E}}_{x\sim \mathrm{p}} \langle \mu_{\mathrm{p}}, k(x, \cdot) \rangle_{\mathcal{H}} \\ = \mathop{\mathbb{E}}_{x\sim \mathrm{p}} \mathop{\mathbb{E}}_{\tilde{x}\sim \mathrm{p}} k(x, \tilde{x}) \approx \frac{1}{\mathrm{N}(\mathrm{N}-1)} \sum_{i=1}^{\mathrm{N}} \sum_{j\neq i}^{\mathrm{N}} k(x_i, x_j)\end{aligned}$$

Similarly for the other terms.

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$$\mathrm{MMD}^2(\mathrm{p}, \mathrm{q}, \mathcal{H}) = \left\|\mu_\mathrm{p} - \mu_\mathrm{q}\right\|_\mathcal{H}^2 = \left\|\mu_\mathrm{p}\right\|_\mathcal{H}^2 + \left\|\mu_\mathrm{q}\right\|_\mathcal{H}^2 - 2\langle\mu_\mathrm{p}, \mu_\mathrm{q}\rangle_\mathcal{H}$$

where,

$$\begin{aligned}\left\|\mu_\mathrm{p}\right\|_\mathcal{H}^2 &= \langle\mu_\mathrm{p}, \mu_\mathrm{p}\rangle_\mathcal{H} = \underset{x\sim\mathrm{p}}{\mathbb{E}}\, \mu_\mathrm{p}(x) = \underset{x\sim\mathrm{p}}{\mathbb{E}} \langle\mu_\mathrm{p}, k(x,\cdot)\rangle_\mathcal{H} \\ &= \underset{x\sim\mathrm{p}}{\mathbb{E}}\ \underset{\tilde{x}\sim\mathrm{p}}{\mathbb{E}}\, k(x,\tilde{x}) \approx \frac{1}{\mathrm{N}(\mathrm{N}-1)} \sum_{i=1}^{\mathrm{N}} \sum_{j\neq i}^{\mathrm{N}} k(x_i, x_j)\end{aligned}$$

Similarly for the other terms.

Estimation

Proof sketch:

$$\mathsf{MMD}^2(\mathrm{p}, \mathrm{q}, \mathcal{H}) = \left\|\mu_{\mathrm{p}} - \mu_{\mathrm{q}}\right\|_{\mathcal{H}}^2 = \left\|\mu_{\mathrm{p}}\right\|_{\mathcal{H}}^2 + \left\|\mu_{\mathrm{q}}\right\|_{\mathcal{H}}^2 - 2\langle \mu_{\mathrm{p}}, \mu_{\mathrm{q}} \rangle_{\mathcal{H}}$$

where,

$$\begin{aligned}\left\|\mu_{\mathrm{p}}\right\|_{\mathcal{H}}^2 = \langle \mu_{\mathrm{p}}, \mu_{\mathrm{p}} \rangle_{\mathcal{H}} &= \mathop{\mathbb{E}}_{x\sim \mathrm{p}} \mu_{\mathrm{p}}(x) = \mathop{\mathbb{E}}_{x\sim \mathrm{p}} \langle \mu_{\mathrm{p}}, k(x, \cdot) \rangle_{\mathcal{H}} \\ &= \mathop{\mathbb{E}}_{x\sim \mathrm{p}} \mathop{\mathbb{E}}_{\tilde{x}\sim \mathrm{p}} k(x, \tilde{x}) \approx \frac{1}{\mathrm{N}(\mathrm{N}-1)} \sum_{i=1}^{\mathrm{N}} \sum_{j\neq i}^{\mathrm{N}} k(x_i, x_j)\end{aligned}$$

Similarly for the other terms.

Considerations

- The distribution of $\widehat{\mathrm{MMD}}^2$ under H_0 assymptotically approaches an infinite sum of shifted chi-squared random variables multiplied by eigenvalues of the RKHS.
  - Approximations to the sampling distribution [1, 10, 11, 12].
- Calculation of the naive $\widehat{\mathrm{MMD}}^2$ estimator is $\mathcal{O}(\mathrm{N}^2)$.
  - Linear time approximations [2, 26].
- Performance is dependent on choice of the kernel. There is no universally best performing kernel.
  - Previously heuristical, recently replaced by hyperparameter optimisation based on test power, or Bayesian evidence [4, 24].
- Empirical kernel mean estimator might be suboptimal.
  - Better estimators exist [4, 16, 17].

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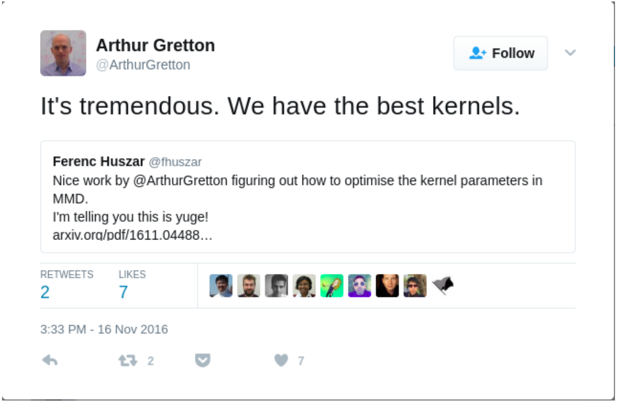
Optimised MMD and model criticism



Arthur Gretton's twitter.

Optimised MMD and model criticism

MMD tends to lose test power with increasing dimensionality. [18]

Pick the kernel such that the test power is maximised, [24]

$$\mathrm{p}_{H_1}\left(\frac{\widehat{\mathrm{MMD}}^2 - \mathrm{MMD}^2}{\sqrt{V_m}} > \frac{\hat{c}_\alpha/m - \mathrm{MMD}^2}{\sqrt{V_m}}\right)$$

$$\xrightarrow{m\to\infty} 1 - \Phi\left(\frac{c_\alpha}{m\sqrt{V_m}} - \frac{\mathrm{MMD}^2}{\sqrt{V_m}}\right)$$

where $\hat{c}_\alpha$ is an estimator of the theoretical rejection threshold c_α.

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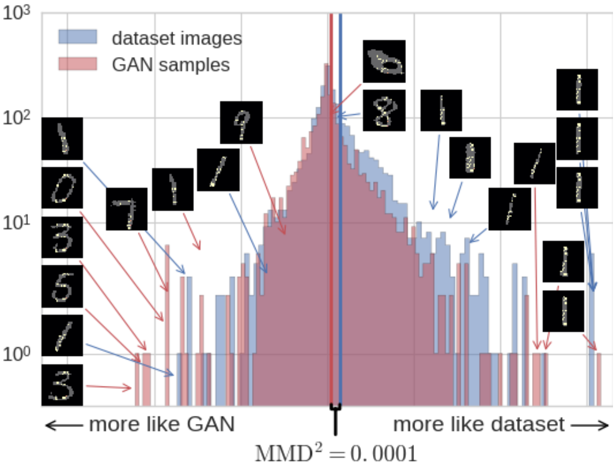

Witness function evaluated on a test set, ARD weights highlighted [24].

Outline

RKHS

Kernel Mean Embeddings

Characteristic kernels

Two Sample Testing

- MMD
- Kernelised Stein Discrepancy

Kernel Bayes' Rule

Integral Probability metrics

Have two probability measure p, and q. Integral Probability Metric (IPM) defines a discrepancy measure,

$$d_{\mathcal{H}}(\mathrm{p}, \mathrm{q}) := \sup_{f \in \mathcal{H}} \left| \mathop{\mathbb{E}}_{\mathrm{p}(\boldsymbol{x})} \big(f(\boldsymbol{x})\big) - \mathop{\mathbb{E}}_{\mathrm{q}(\boldsymbol{y})} \big(f(\boldsymbol{y})\big) \right|$$

where the space of functions $\mathcal{H}$ must be rich enough such that $d_{\mathcal{H}}(\mathrm{p}, \mathrm{q}) = 0$ iff $\mathrm{p} = \mathrm{q}$.

$f^* := \mathrm{argmax}_{f \in \mathcal{H}} \left| \mathbb{E}_{\mathrm{p}}(f(\boldsymbol{x})) - \mathbb{E}_{\mathrm{q}}(f(\boldsymbol{y})) \right|$ is the *witness function*.

MMD is an IPM where $\mathcal{H}$ is the unit ball in characteristic RKHS.

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Stein Discrepancy

Construct $\mathcal{H}$ such that $\mathbb{E}_{\mathrm{q}}(f(\boldsymbol{y})) = 0, \forall f \in \mathcal{H}$.

$$d_{\mathcal{H}}(\mathrm{p}, \mathrm{q}) = S_{\mathrm{q}}(\mathrm{p}, \mathcal{T}, \mathcal{H}) := \sup_{f \in \mathcal{H}} \left| \mathop{\mathbb{E}}_{\mathrm{p}(\boldsymbol{x})} \left[(\mathcal{T} f)(\boldsymbol{x}) \right] \right|$$

where $\mathcal{T}$ is a real–valued operator and $\mathbb{E}_{\mathrm{q}}[(\mathcal{T} f)(\boldsymbol{y})] = 0, \forall f \in \mathcal{H}$.

A standard choice of $\mathcal{T}$ when $\boldsymbol{x} = x \in \mathbb{R}$ is the *Stein's operator*,

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Kernelised Stein Discrepancy (KSD)

Assume that $\mathrm{p}(\boldsymbol{x})$, and $\mathrm{q}(\boldsymbol{y})$ are differentiable continuous density functions; q might be unnormalised [3, 15].

Use the Stein's operator in the unit ball of the product RKHS $\mathcal{F}^{\mathrm{D}}$,

$$
\begin{aligned}
S_{\mathrm{q}}(\mathrm{p}, \mathcal{A}_{\mathrm{q}}, \mathcal{F}^{\mathrm{D}}) &:= \sup_{f \in \mathcal{F}^{\mathrm{D}}, \|f\|_{\mathcal{F}^{\mathrm{D}}} \leq 1} \left| \mathop{\mathbb{E}}_{\mathrm{p}(\boldsymbol{x})} \left[\mathrm{Tr}\left(\mathcal{A}_{\mathrm{q}} f(\boldsymbol{x}) \right) \right] \right| \\
&= \sup_{f \in \mathcal{F}^{\mathrm{D}}, \|f\|_{\mathcal{F}^{\mathrm{D}}} \leq 1} \left| \mathop{\mathbb{E}}_{\mathrm{p}(\boldsymbol{x})} \left[\mathrm{Tr}\left(f(\boldsymbol{x}) s_{\mathrm{q}}(\boldsymbol{x})^{\mathrm{T}} + \nabla^2 f(\boldsymbol{x}) \right) \right] \right| \\
&= \sup_{f \in \mathcal{F}^{\mathrm{D}}, \|f\|_{\mathcal{F}^{\mathrm{D}}} \leq 1} \left| \sum_{d=1}^{\mathrm{D}} \mathop{\mathbb{E}}_{\mathrm{p}(\boldsymbol{x})} \left[f_d(\boldsymbol{x}) s_{\mathrm{q},d}(\boldsymbol{x}) + \frac{\partial f_d(\boldsymbol{x})}{\partial \boldsymbol{x}_d} \right] \right| \\
&= \sup_{f \in \mathcal{F}^{\mathrm{D}}, \|f\|_{\mathcal{F}^{\mathrm{D}}} \leq 1} \left| \langle f, \boldsymbol{\beta}_{\mathrm{q}} \rangle_{\mathcal{F}^{\mathrm{D}}} \right| = \left\| \boldsymbol{\beta}_{\mathrm{q}} \right\|_{\mathcal{F}^{\mathrm{D}}} \ (\text{s.t. } \boldsymbol{\beta}_{\mathrm{q}} \in \mathcal{F}^{\mathrm{D}})
\end{aligned}
$$

$\langle f, g \rangle_{\mathcal{F}^{\mathrm{D}}} := \sum_{d=1}^{\mathrm{D}} \langle f_d, g_d \rangle_{\mathcal{F}}$, $\boldsymbol{\beta}_{\mathrm{q}} := \mathbb{E}_{\mathrm{p}}[k(\boldsymbol{x}, \cdot) u_{\mathrm{q}}(\boldsymbol{x}) + \nabla_{\boldsymbol{x}} k(\boldsymbol{x}, \cdot)]$.

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KSD vs. alternative GoF tests

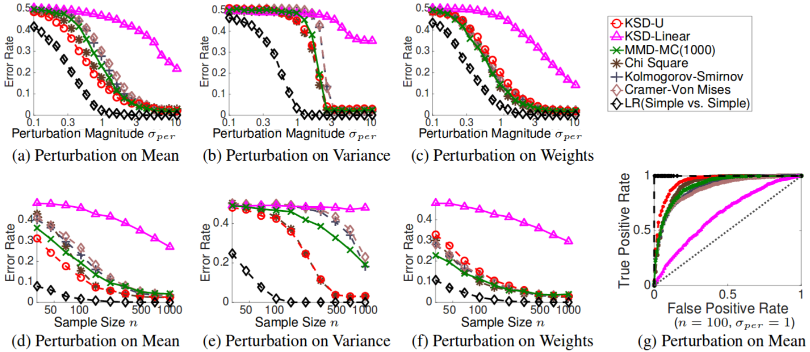

Figure 1. Results on 1D Gaussian mixture. (a)-(c) The error rates of different methods vs. the perturbation magnitude σ_{per} when perturbing the mean, variance and mixture weights, respectively; we use a fixed sample size of $n = 100$. (d)-(f) the error rates vs. the sample size n, with fixed perturbation magnitude $\sigma_{per} = 1$. We find that the type I errors of all the methods are well controlled under 0.05, and hence the reported error rates are essentially type II errors. (g) The ROC curve with mean perturbation, $n = 100$, $\sigma_{per} = 1$.

Variational Inference using KSD

Natural idea: minimise KSD between the true and an approximate posterior distribution $\rightarrow$ a particular case of *Operator Variational Inference*. [19]

Quick detour: For the true posterior $\mathrm{p}(\boldsymbol{x}) = \widetilde{\mathrm{p}}(\boldsymbol{x})/Z_{\mathrm{p}}$ and an approximation $\mathrm{q}(\boldsymbol{x}) = \widetilde{\mathrm{q}}(\boldsymbol{x})/Z_{\mathrm{q}}$,

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S(\mathrm{p}, \mathrm{q}) &= \sup_{f \in \mathcal{F}^{\mathrm{D}}, \|f\|_{\mathcal{F}^{\mathrm{D}}} \leq 1} \left| \mathop{\mathbb{E}}_{\mathrm{q}(\boldsymbol{x})} \left[\mathrm{Tr}\left(\mathcal{A}_{\mathrm{p}} f(\boldsymbol{x}) \right) \right] \right| \\
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$\rightarrow \mathrm{q}(\boldsymbol{x}) =\propto \mathrm{q}(\boldsymbol{x}, \epsilon)$, e.g. $\mathrm{q}(\boldsymbol{x}, \epsilon) = \mathcal{N}(\boldsymbol{x} \mid \mathcal{T}_{\boldsymbol{\theta}}(\epsilon), \sigma^2 \boldsymbol{I})\, \mathcal{N}(\epsilon \mid \boldsymbol{0}, \boldsymbol{I})$

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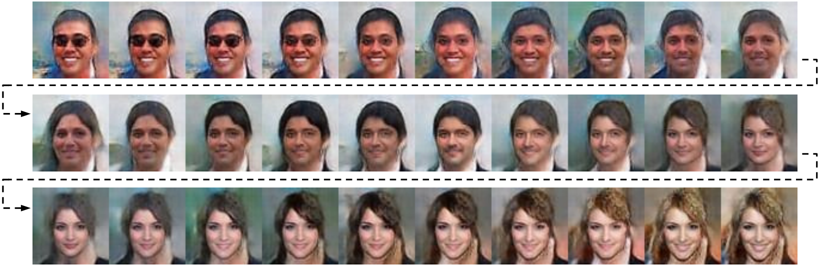
Learning to Sample using KSD

Two papers [15, 25] on optimising a set of particles, resp. a set of samples from a model (amortisation), repeatedly using KL-optimal perturbations $\boldsymbol{x}_t = \boldsymbol{x}_{t-1} + \varepsilon_t f(\boldsymbol{x})$.

Read Yingzhen's blog post [13] and a recent paper [14]!



Random walk through the latent space of a GAN trained with KSD adversary. [25]

Outline

RKHS

Kernel Mean Embeddings

Characteristic kernels

Two Sample Testing

- MMD
- Kernelised Stein Discrepancy

Kernel Bayes' Rule

Tensor product

If $\mathcal{H}$ and $\mathcal{K}$ are Hilbert spaces then so is $\mathcal{H} \otimes \mathcal{K}$.

If $\{a_i\}_{i=1}^{\infty}$ spans $\mathcal{H}$ and $\{b_j\}_{j=1}^{\infty}$ spans $\mathcal{K}$ then $\{a_i \otimes b_j\}_{i,j=0}^{\infty}$ spans $\mathcal{H} \otimes \mathcal{K}$.

For any $f, f' \in \mathcal{H}$ and $g, g' \in \mathcal{K}$ we have

$$\langle f \otimes g, f' \otimes g' \rangle = \langle f, f' \rangle \langle g, g' \rangle$$

$\mathcal{H} \otimes \mathcal{K}$ is isomporphic to a space of bounded linear operators $\mathcal{K} \to \mathcal{H}$

$$(f \otimes g)g' = f \langle g, g' \rangle$$

Covariance operators

Covariance operators $C_{XY} : \mathcal{K} \to \mathcal{H}$ are defined as

$$C_{XY} = \mathbb{E}[k_X(X, \cdot) \otimes k_Y(Y, \cdot)]$$
$$C_{XX} = \mathbb{E}[k_X(X, \cdot) \otimes k_X(X, \cdot)]$$

For any $f \in \mathcal{H}$ and $g \in \mathcal{K}$

$$\langle f, C_{XY} g \rangle = \langle C_{YX} f, g \rangle = \mathbb{E}[f(X)g(Y)]$$

Empirical estimators

$$(X_i, Y_i) \sim_{i.i.d.} P(X, Y)$$
$$\hat{C}_{XY} = \frac{1}{N} \sum_{i=1}^{N} k_X(X_i, \cdot) \otimes k_Y(Y_i, \cdot)$$
$$\hat{C}_{XX} = \frac{1}{N} \sum_{i=1}^{N} k_X(X_i, \cdot) \otimes k_X(X_i, \cdot)$$

Conditional embeddings

Let

$$\mu_{X|Y=y} = \mathbb{E}[k_X(X,\cdot)|Y=y]$$

We seek an operator $\mathcal{U}_{X|Y}$ such that for all y

$$\mu_{X|Y=y} = \mathcal{U}_{X|Y} k_Y(y,\cdot)$$

which we call the conditional mean embedding.

Conditional embeddings

Lemma ([21])

For any $f \in \mathcal{H}$ *let* $h(y) = \mathbb{E}[f(X)|Y = y]$ *and assume that* $h \in \mathcal{K}$. *Then*

$$C_{YY}h = C_{YX}f$$

Proof.

Take any $g \in \mathcal{K}$.

$$\langle g, C_{YY}h\rangle = \mathop{\mathbb{E}}_{Y\sim P(Y)}[g(Y)h(Y)] =$$
$$\mathop{\mathbb{E}}_{Y\sim P(Y)}[g(Y)\mathop{\mathbb{E}}_{X\sim P(X|Y)}[f(X)|Y]] = \mathop{\mathbb{E}}_{Y\sim P(Y)}[\mathop{\mathbb{E}}_{X\sim P(X|Y)}[g(Y)f(X)|Y]]$$
$$\mathop{\mathbb{E}}_{X,Y\sim P(X,Y)}[g(Y)f(X)] = \langle g, C_{YX}f\rangle$$

$\square$

Conditional embeddings

Whenever C_{YY} is invertible we have

$$\mathcal{U}_{X|Y} = C_{XY} C_{YY}^{-1}$$

in practice we use a regularized version

$$\mathcal{U}_{X|Y}^{\epsilon} = C_{XY}(C_{YY} + \epsilon I)^{-1}$$

which can be estimated by

$$\hat{\mathcal{U}}_{X|Y}^{\epsilon} = \hat{C}_{XY}(\hat{C}_{YY} + \epsilon I)^{-1}$$

Kernel Bayes' rule

We could compute posterior embedding by

$$\mu_{X|Y=y} = \mathcal{U}_{X|Y} k_Y(y, \cdot)$$

but we may want a different prior.

Setting:

- let $P(X, Y)$ be the joint distribution of the model
- let $Q(X, Y)$ be a different distribution such that $P(Y|X = x) = Q(Y|X = x)$ for all x
- we have a sample $(X_i, Y_i) \sim Q$ and $\tilde{X}_j \sim P(X)$
- we want to estimate the posterior embedding $\mathbb{E}_{X \sim P(X|Y=y)}[k_X(X, \cdot)]$ for some particular y

Kernel sum rule

Sum rule

$$P(X) = \sum_{Y} P(X, Y)$$

Kernel sum rule

$$\mu_X = \mathcal{U}_{X|Y} \mu_Y$$

Corollary

$$C_{XX} = \mathcal{U}_{XX|Y} \mu_Y$$

Kernel product rule

Product rule

$$P(X, Y) = P(X|Y)P(Y)$$

Kernel product rule

$$C_{XY} = \mathcal{U}_{XY} C_{YY}$$

Kernel Bayes' rule

Observe that

$$
\begin{aligned}
C_{XY} &= \mathcal{U}_{Y|X} C_{XX} \\
C_{YY} &= \mathcal{U}_{YY|X} \mu_X
\end{aligned}
$$

and so

$$\mathcal{U}_{X|Y} = C_{XY} C_{YY}^{-1} = (\mathcal{U}_{Y|X} C_{XX})(\mathcal{U}_{YY|X} \mu_X)^{-1}$$

lets us express $\mathcal{U}_{X|Y}$ in terms of $\mathcal{U}_{Y|X}$.

Reminder

Setting:

- let $P(X, Y)$ be the joint distribution of the model
- let $Q(X, Y)$ be a different distribution such that $P(Y|X = x) = Q(Y|X = x)$ for all x
- we have a sample $(X_i, Y_i) \sim Q$ and $\tilde{X}_j \sim P(X)$
- we want to estimate the posterior embedding $\mathbb{E}_{X \sim P(X|Y=y)}[k_X(X, \cdot)]$ for some particular y

Kernel Bayes' rule

We have

$$\mathcal{U}^P_{Y|X} = \mathcal{U}^Q_{Y|X}$$
$$\mathcal{U}^P_{X|Y} \neq \mathcal{U}^Q_{X|Y}$$

but

$$\begin{aligned}\mathcal{U}^P_{X|Y} &= (\mathcal{U}^P_{Y|X} C^P_{XX})(\mathcal{U}^P_{YY|X} \mu^P_X)^{-1} \\ &= (\mathcal{U}^Q_{Y|X} C^P_{XX})(\mathcal{U}^Q_{YY|X} \mu^P_X)^{-1}\end{aligned}$$

so

$$\mu^P_{X|Y=y} = (\mathcal{U}^Q_{Y|X} C^P_{XX})(\mathcal{U}^Q_{YY|X} \mu^P_X)^{-1} k_Y(y, \cdot)$$

Kernel Bayes' rule

In practice we use the following estimator

$$\hat{\mu}_{X|Y=y} = (\hat{\mathcal{U}}^{Q}_{Y|X}\hat{C}^{P}_{XX})((\hat{\mathcal{U}}^{Q}_{YY|X}\hat{\mu}^{P}_{X})^2 + \epsilon I)^{-1}(\hat{\mathcal{U}}^{Q}_{YY|X}\hat{\mu}^{P}_{X})k_Y(y,\cdot)$$

which can be written as

$$\hat{\mu}_{X|Y=y} = A(B^2 + \delta I)^{-1}Bk_Y(y,\cdot)$$
$$A = \hat{\mathcal{U}}^{Q}_{Y|X}\hat{C}^{P}_{XX} = \hat{C}^{Q}_{YX}(\hat{C}^{Q}_{XX} + \epsilon I)^{-1}\hat{C}^{P}_{XX}$$
$$B = \hat{\mathcal{U}}^{Q}_{YY|X}\hat{\mu}^{P}_{X} = \hat{C}^{Q}_{YYX}(\hat{C}^{Q}_{XX} + \epsilon I)^{-1}\hat{\mu}^{P}_{X}$$

For $\epsilon = N^{-\frac{1}{3}}$ and $\delta = N^{-\frac{4}{27}}$ it can be shown [7] that

$$\left\|\mu_{X|Y=y} - \hat{\mu}_{X|Y=y}\right\| = O_p(N^{-\frac{4}{27}})$$

Kernel Bayes' rule

When is Kernel Bayes' Rule useful?

- when densities aren't tractable (ABC)
- when you don't know how to write a model but you know how to pick a kernel
- perhaps it can perform better than alternatives even if the above aren't satisfied

Other topics

Other topics combining KMEs with Bayesian inference

- adaptive Metropolis-Hastings using KME [20]
- Hamiltonian Monte Carlo without gradients [23]
- Bayesian estimation of KMEs [4]

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