## 1 Proposal scratch notes

- $\mathcal{D}$ ,  $\mathcal{I}$ : (unknown) disjoint sets of indices that describe the groups of transformations that are relevant and irrelevant to the output, respectively.  $\mathcal{D} \cup \mathcal{I} = \{1, \dots, m\}$ .
- $U_Y$ ,  $U_{\mathcal{I}}$ ,  $U_{\mathcal{D}}$ ,  $\widetilde{U}_{\mathcal{I}}$ : independent latent variables that influence the value of the variable(s) that they point to.
- $X^{\text{(hid)}}$ : some unknown canonical form of the observed input X. It is assumed that given  $U_{\mathcal{D}}$  and  $U_{\mathcal{I}}$ , X was obtained from an ordered sequence of transformations on the canonical form, i.e.,

$$X = T_{U_{\mathcal{D}}, U_{\mathcal{I}}} \circ X^{\text{(hid)}}$$

where transformations

$$T_{U_{\mathcal{D}},U_{\mathcal{I}}} = T_{\mathcal{I}}^{(1)} \circ T_{\mathcal{D}}^{(1)} \circ T_{\mathcal{I}}^{(2)} \circ \dots$$

make up the overgroup  $\mathcal{G}_{\mathcal{D}\cup\mathcal{I}}$ ,  $T_{\mathcal{D}}^{(j)}$  is a transformation in group  $\mathcal{G}_j$  from the overgroup  $\mathcal{G}_{\mathcal{D}} = \langle \cup_{j\in\mathcal{D}} \mathcal{G}_j \rangle$ , and  $T_{\mathcal{I}}^{(i)} \in \mathcal{G}_i \subset \mathcal{G}_{\mathcal{I}} = \langle \cup_{i\in\mathcal{I}} \mathcal{G}_i \rangle$ . Note that  $\mathcal{G}_{\mathcal{I}}$  is also assumed to be a normal subgroup of  $\mathcal{G}_{\mathcal{D}\cup\mathcal{I}}$ .

• Y: observed output assumed to be generated by

$$Y = h(X^{\text{(hid)}}, U_{\mathcal{D}}, U_{Y})$$

where h is a deterministic function.

•  $X_{U_{\mathcal{I}} \leftarrow \widetilde{U}_{\mathcal{I}}}$ : counterfactual variable to X where  $U_{\mathcal{I}}$  has been replaced by  $\widetilde{U}_{\mathcal{I}}$ , i.e.,

$$X_{U_{\mathcal{I}} \leftarrow \widetilde{U}_{\mathcal{I}}} = T_{U_{\mathcal{D}}, \widetilde{U}_{\mathcal{I}}} \circ X^{(\mathrm{hid})}$$

• Want CG-invariant representation

$$\Gamma(X) = \Gamma(T_{U_{\mathcal{D}},U_{\mathcal{I}}} \circ X^{(\mathrm{hid})}) = \Gamma(T_{U_{\mathcal{D}},\widetilde{U}_{\mathcal{I}}} \circ X^{(\mathrm{hid})}) = \Gamma(X_{U_{\mathcal{I}} \leftarrow \widetilde{U}_{\mathcal{I}}})$$

When  $\mathcal{G}_{\mathcal{I}}$  is a normal subgroup of  $\mathcal{G}_{\mathcal{D}\cup\mathcal{I}}$ , G-invariant representation

$$\Gamma(X) = \Gamma(T_{\mathcal{I}} \circ X)$$

for all  $T_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}$  is sufficient.

• Because groups are finite linear automorphisms, each transformation T is just a linear function and so Reynolds operator can be applied directly to the group actions

$$\bar{T} = \frac{1}{|\mathcal{G}|} \sum_{T \in \mathcal{G}} T$$

For continuous linear groups, orbit-average over a Haar measure  $\lambda$ 

$$\bar{T} = \int_{\mathcal{G}} T\lambda(T)$$

TODO: need to estimate the operator. Assume uniform Haar and sample?

## 2 Kernel hypothesis test notes

• Let X be a r.v. on domain  $\mathcal{X}$ . A kernel  $k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$  induces a RHKS  $\mathcal{H}$  of functions  $f: \mathcal{X} \to \mathbb{R}$  where for  $f \in \mathcal{H}$  and  $x \in \mathcal{X}$ ,

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

(reproducing property).  $k(x,\cdot) = \phi_x$  can also be considered an implicit feature map  $(\phi_x : \mathcal{X} \to \mathbb{R})$  where

$$\langle \phi_x, \phi_{x'} \rangle = k(x, x')$$

is a measure of similarity.

- Kernel methods work on inner products of feature maps of observations in the RKHS associated with kernel. Inner products may be computed without explicitly computing the high-dimensional feature map ("kernel trick").
- Main challenge of designing kernel-based hypothesis tests is deriving large-sample distribution of test statistic under null.
- Gram matrix should be positive semidefinite. Satisfised if kernel is symmetric and positive semidefinite.
- Let X be a r.v. with distribution  $\mathbb{P}$ . Mean element

$$\mu_{\mathbb{P}} = \mathbb{E}_{\mathbb{P}}[\phi_X]$$

associated with X is unique element of RKHS  $\mathcal{H}$  s.t. for all  $f \in \mathcal{H}$ ,

$$\langle \mu_{\mathbb{P}}, f \rangle = \mathbb{E}_{\mathbb{P}}[f(X)]$$

Covariance operator  $\Sigma_{\mathbb{P}}: \mathcal{H} \times \mathcal{H} \to \mathbb{R}$  associated with X is unique operator s.t. for all  $f, g \in \mathcal{H}$ ,

$$\langle f, \Sigma_{\mathbb{P}} g \rangle = \operatorname{Cov}(f(X), g(X)) = \mathbb{E}_{\mathbb{P}}[f(X), g(X)] - \langle \mu_{\mathbb{P}}, f \rangle \langle \mu_{\mathbb{P}}, g \rangle$$

Empirical estimates of inner products that lead to estimates of element/operator are available.

- Kernel is characteristic if mean embedding  $\mu : \mathbb{P} \to \mathcal{H}$  is injective. Each distribution can be uniquely represented in the RKHS and all statistica features of distributions are preserved (TODO) by a characteristic kernel.
- If  $\dim(\mathcal{H}) = \infty$ ,  $\mu_{\mathbb{P}}$  has more significance than in classical statistics.
- Detecting (conditional?) invariances in single training environment via hypothesis testing. Explicitly testing for invariances? Invariant testing