### Returning the Favour: When Regression Benefits from Probabilistic Causal Knowledge



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• Colliders provide additional information on  $\mathbb{P}(Y|X)$  which is unused





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Squared-loss regression problem

$$\arg\min_{f\in\mathcal{F}}\frac{1}{n}\sum_{i=1}^{n}\left(y_{i}-f(x_{1i},x_{2i})\right)^{2}+\lambda\Omega(f)$$





 $(Y) \rightarrow (X_1) \leftarrow (X_2) \qquad 6$ 

Optimal regressor:  $f^*(x_1, x_2) = \mathbb{E}[Y|X_1 = x_1, X_2 = x_2]$ 

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=  $\mathbb{E}[Y]$  ( $Y \perp X_2$ )  
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Objective

Find a regressor  $\hat{f} : \mathcal{X} \to \mathcal{Y}$  in hypothesis space  $\mathcal{F}$  that satisfies

$$\hat{f} \in \{f \in \mathcal{F} \mid \mathbb{E}[f(X_1, X_2) \mid X_2] = 0\}.$$



## Constraining the hypothesis space $\mathcal{F}$



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# $\{f \in \mathcal{F} \mid \mathbb{E}[f(X_1, X_2) \mid X_2] = 0\} = \operatorname{Range}(P)$

Collider regression in 
$$\mathcal{F} = L^2(X)$$





Take  $P: L^2(X) \to L^2(X)$ ,

$$Pf(x_1, x_2) = f(x_1, x_2) - \mathbb{E}[f(X_1, X_2) | X_2 = x_2].$$

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#### Proposition

Let  $h \in L^2(X)$ , then we have

$$\Delta(h, Ph) = \mathbb{E}[(Y - h(X))^2] - \mathbb{E}[(Y - Ph(X))^2] = \|(\mathrm{Id} - P)h\|_{L^2(X)}^2.$$



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▶ Reproducing kernel Hilbert space with kernel k(x, x')



assumptions



#### Theorem

assumptions

Assume  $M = \sup_{x \in \mathcal{X}} k(x, x) < \infty$  and  $\operatorname{Var}(Y|X) \ge \eta > 0$ . Then, the generalisation gap between  $\hat{f}$  and  $P\hat{f}$  satisfies

$$\mathbb{E}[\Delta(\hat{f}, P\hat{f})] \ge \frac{\eta \mathbb{E}\left[\|\mu_{X|X_2}(X)\|_{L^2(X)}^2\right]}{\left(\sqrt{n}M + \lambda/\sqrt{n}\right)^2} \tag{1}$$

where  $\mu_{X|X_2} = \mathbb{E}[k(X, \cdot)|X_2]$  is a RKHS representation of  $\mathbb{P}(X|X_2)$ .



 $\mathcal{F} = \mathcal{H}$  with kernel  $k(x, x') = \langle k(x, \cdot), k(x', \cdot) \rangle$ 



 $\mathcal{F} = \mathcal{H}_P$  with kernel  $k_P(x, x') = \langle P^*k(x, \cdot), P^*k(x', \cdot) \rangle$ 



(a) : Test MSEs for the simulation experiment ; dataset is generated using  $d_1 = 3$ ,  $d_2 = 3$ , n = 50 and 100 semi-supervised samples ; experiments is run for 100 datasets generated with different seeds ; statistical significance is confirmed via Wilcoxon signed-rank ; (b, c, d) : Ablation study on the number of training samples, number of semi-supervised samples and dimensionality of  $X_2$ .

Table 1: MSE, signal-to-noise ratio (SNR) and correlation on test data for the aerosol radiative forcing experiment; n = 50 and 200 semi-supervised samples; statistical significance is confirmed via Wilcoxon signed-rank; experiments are run for 100 datasets generated by FaIR with different seeds;  $\uparrow/\downarrow$  indicates higher/lower is better; we report 1 standard deviation;  $\dagger$  indicates our proposed methods.

	$\mathrm{MSE}\downarrow$	$\mathrm{SNR}\uparrow$	Correlation $\uparrow$
$\mathbf{RF}$	$0.90{\pm}0.04$	$0.44 {\pm} 0.19$	$0.32{\pm}0.08$
$P\text{-}\mathrm{RF}^{\dagger}$	$0.89{\scriptstyle \pm 0.03}$	$0.49{\scriptstyle \pm 0.15}$	$0.34{\scriptstyle \pm 0.07}$
$\mathbf{KRR}$	$0.88{\pm}0.04$	$0.56{\scriptstyle\pm0.21}$	$0.37{\pm}0.05$
P-KRR <sup>†</sup>	$0.86{\scriptstyle \pm 0.03}$	$0.65{\scriptstyle \pm 0.14}$	$0.40{\scriptstyle \pm 0.02}$
${\cal H}_P$ -KRR <sup>†</sup>	$0.86{\scriptstyle \pm 0.03}$	$0.64{\scriptstyle \pm 0.14}$	$0.39{\pm}0.03$

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- Similar reasoning can be applied to other forms of inference about  $\mathbb{P}(Y|X)$ , e.g. classification or quantile regression