Causal and Anti-causal Structure for Semi-supervised Learning

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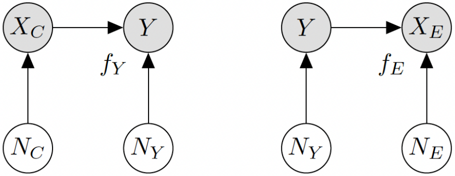
Causal Mechanisms

- Consider the input X and output Y
  - Causal learning: predict effect Y from cause X
  - Anticausal learning: predict cause Y from effect X



(a) Causal learning (b) Anticausal learning

- f is the deterministic mechanism
- N_C and N_Y (or N_E and N_Y) are independent noise variables

Causal learning:

$$X_C := N_C \tag{1}$$
$$Y := f_Y(X_C, N_Y) \tag{2}$$

Anticausal learning:

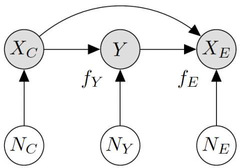
$$Y := N_Y \tag{3}$$
$$X_E := f_E(Y, N_E) \tag{4}$$

Causal Mechanism Effects on Semi-Supervised Learning (SSL)

- Training data:
  - Labeled sample: $(X^l, Y^l) = \{(x^i, y^i)\}_{i=1}^{n_l}$
  - Unlabeled sample: $X^u = \{x^i\}_{i=n_l+1}^{n_l+n_u}$
  - From same distribution P (MCAR)
- Goal: Estimate $P(Y|X)$
- SSL question: If those extra unlabeled $\{X^u\}$ can improve estimating $P(Y|X)$?
  - $\{X^u\}$ can improve the estimate of $P(X)$
  - Thus, $P(Y|X)$ can be improved if we have a link between $P(X)$ and $P(Y|X)$
  - Two common assumptions: cluster assumption; low-density separation
- Based on the Independent Causal Mechanisms (ICM) principle, $P(X_C)$ and $P(Y|X_C)$ are algorithmically independent, so intuitively:
  - Causal learning: SSL doesn't work since $P(X_C)$ contains no information about $P(Y|X_C)$
  - Anticausal learning: $P(X_E)$ may contain information about $P(Y|X_E)$

SSL with Cause and Effects Features

- Consider including both of the cause and effects features:
  - Labeled sample: $(X_C^l, Y^l, X_E^l) = \{(x_c^i, y^i, x_e^i)\}_{i=1}^{n_l}$
  - Unlabeled sample: $(X_C^u, X_E^u) = \{(x_c^i, x_e^i)\}_{i=n_l+1}^{n_l+n_u}$



$$X_C := N_C \tag{5}$$
$$Y := f_Y(X_C, N_Y) \tag{6}$$
$$X_E := f_E(Y, X_C, N_E) \tag{7}$$

- Goal: Estimate $P(Y|X_C, X_E)$ with additional information of $P(X_C, X_E)$ from unlabeled sample
- Subject to ICM, opposite to $P(X_C)$, $P(X_E|X_C)$ contains all relevant information about $P(Y|X_C, X_E)$ provided by the unlabeled sample
- Refined assumption: SSL should exploit links between two conditional distributions $P(X_E|X_C)$ and $P(Y|X_C, X_E)$ rather than the joint feature set $P(X_E, X_C)$ and $P(Y|X_C, X_E)$

SSL with Cause and Effects Features

- Assume binary classification:

$$Y := \mathbb{1}\{g(X_C) > U\} \tag{8}$$

$$X_E := Y f_1(X_C, N_E) + (1 - Y) f_0(X_C, N_E) \tag{9}$$

  - Allow arbitrary g, f_0, f_1 and N_E, without loss of generality
- Reformulate classical SSL assumptions:
  - Conditional cluster assumption: points in the same cluster of $p(X_E|X_C)$ share the same label Y
  - Low-conditional-density separation: class boundaries of $P(Y|X_C, X_E)$ should lie in regions where $P(X_E|X_C)$ is small

Algorithm 1: Semi-generative Model

- Only model the informative part of the generative process: $P(Y, X_E|X_C)$

$$argmax_{\theta} p(y^l, X_E^l|X_C^l;\theta) \sum_{y^u} p(y^u, X_E^u|X_C^u;\theta) \tag{10}$$

  where $\theta = (\theta_Y, \theta_E)$

- Minimize the negative log-likelihood (NLL) which for fixed labels decomposes into two separate terms optimized independently for θ_Y and θ_E

$$NLL(\theta|X_C, y, X_E) := -logp(y, X_E|X_C;\theta) \tag{11}$$

$$= -logp(y|X_C;\theta_Y) - logp(X_E|y, X_C;\theta_E) \tag{12}$$

Algorithm 1: Semi-generative Model

Algorithm 1: EM-like algorithm for fitting a semi-generative model by maximum likelihood

Input: labelled data $(\mathbf{X}_C^l, \mathbf{y}^l, \mathbf{X}_E^l)$; unlabelled data $(\mathbf{X}_C^u, \mathbf{X}_E^u)$; parametric models $p(y|\mathbf{x}_C; \boldsymbol{\theta}_Y)$ and $p(\mathbf{x}_E|\mathbf{x}_C, y; \boldsymbol{\theta}_E)$

Output: fitted labels $\mathbf{y}^u$; estimates $\hat{\boldsymbol{\theta}}_Y, \hat{\boldsymbol{\theta}}_E$

$t \leftarrow 0$

$\hat{\boldsymbol{\theta}}_Y^{(0)} \leftarrow \arg\min \mathrm{NLL}(\boldsymbol{\theta}_Y|\mathbf{y}^l)$

$\hat{\boldsymbol{\theta}}_E^{(0)} \leftarrow \arg\min \mathrm{NLL}(\boldsymbol{\theta}_E|\mathbf{y}^l)$

while *not converged* **do**

- $\mathbf{y}^{(t)} \leftarrow \mathbb{I}\{p(\mathbf{y}|\mathbf{X}_C^u, \mathbf{X}_E^u; \boldsymbol{\theta}_Y^{(t)}, \boldsymbol{\theta}_E^{(t)}) > 0.5\}$
- $\hat{\boldsymbol{\theta}}_Y^{(t+1)} \leftarrow \arg\min \mathrm{NLL}(\boldsymbol{\theta}_Y|\mathbf{y}^l, \mathbf{y}^{(t)})$
- $\hat{\boldsymbol{\theta}}_E^{(t+1)} \leftarrow \arg\min \mathrm{NLL}(\boldsymbol{\theta}_E|\mathbf{y}^l, \mathbf{y}^{(t)})$
- $t \leftarrow t + 1$

end

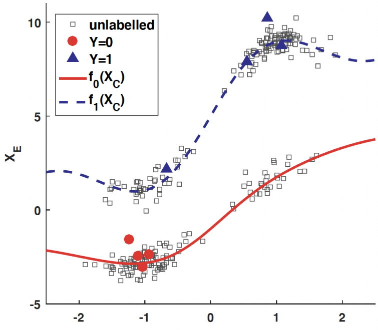
return $\mathbf{y}^{(t-1)}, \boldsymbol{\theta}_Y^{(t)}, \boldsymbol{\theta}_E^{(t)}$

Algorithm 2: Conditional Self-learning

- Extract information from $P(X_E|X_C)$ instead of propagating labels based on similarities between points in the joint feature space (X_C, X_E).
- Assume an additive noise model:

$$f_i(X_C, N_E) = f_i(X_C) + N_{E,i}, i = 0, 1 \tag{13}$$

- Assumption for the noise: mean zero and unimodal. Ensure the one-to-one function from X_C to X_E for each label.
- Learn functions $\hat{f}_0$ and $\hat{f}_1$.



Algorithm 2: Conditional Self-learning

Algorithm 2: Conditional self-learning

Input: labelled data $(\mathbf{X}_C^l, \mathbf{y}^l, \mathbf{X}_E^l)$; unlabelled data;
$(\mathbf{X}_C^u, \mathbf{X}_E^u)$; `regress()` method

Output: fitted labels $\mathbf{y}^u$; functions $\hat{f}_0, \hat{f}_1$

$t \leftarrow 0$
while *unlabelled data left* **do**
  for $i = 0, 1$ **do**
    $\hat{f}_i^{(t)} \leftarrow \texttt{regress}(\mathbf{X}_{E,i}^l, \mathbf{X}_{C,i}^l)$
    $\mathbf{r}_i \leftarrow ||\mathbf{X}_E^u - \hat{f}_i^{(t)}(\mathbf{X}_C^u)||^2$
  end
  $(i, j) \leftarrow \arg\min\{\mathbf{r}_{i,j} : i = 0, 1; j = 1, ..., n_u\}$
  $y^{n_l+j} \leftarrow i$
  $\mathbf{X}_{E,i}^l, \mathbf{X}_{C,i}^l \leftarrow \texttt{append}(\mathbf{x}_E^{n_l+j}, \mathbf{x}_C^{n_l+j})$
  $t \leftarrow t + 1$
end
return $\mathbf{y}^u, \hat{f}_0^{(t-1)}, \hat{f}_1^{(t-1)}$

Simulation Study

- Compare the semi-generative model and conditional self-learning with the baseline methods:
  - Supervised Logistic Regression (SLR): only use the labeled data and ignore the causal structure.
  - Transductive Support Vector Machine (T-SVM) with linear and RBF kernels: conventional SSL methods.
- Simulate the data in the following three different cases: Draw $X_C \in \mathbb{R}^{d_C}$ from a mixture of m d_C-dimensional Gaussian.

$$Y := \mathbb{1}\{\sigma(a'X_C + b) > N_Y\} \tag{14}$$

$$X_E := \{f_i(X_C) + D_i N_E\}\mathbb{1}\{Y = i\} \tag{15}$$

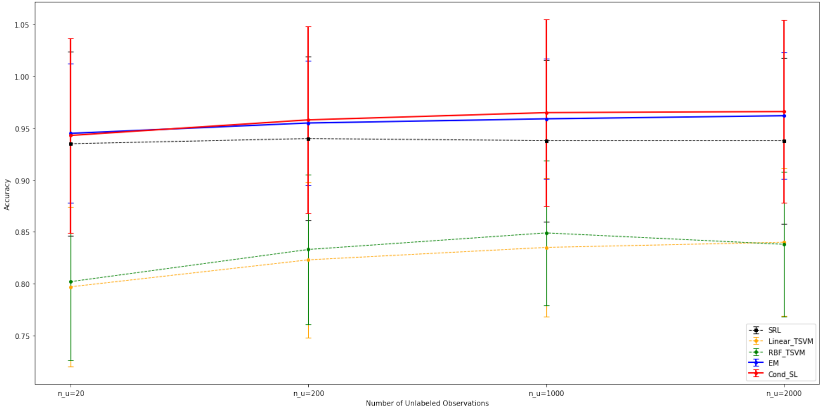
  with $N_Y \sim U[0,1]$, $N_E \sim N_{d_E}(0, I)$, $a \in \mathbb{R}^{d_C}$, $D_i \in \mathbb{R}^{d_E \times d_E}$, $\sigma(x)$ is the sigmoid function, $i = 0, 1$.
  - Case I: Linear additive noise model with one-dimensional feature dimensions
  - Case II: Linear additive noise model with high dimensional feature dimensions
  - Case III: Non-linear additive noise model with high dimensional feature dimensions
- Generate the data in each case with 10 labeled data and 20, 200, 1000 and 2000 unlabeled data (with the increase of missing proportions).

Case I

$$f_i(X_C) = {A_i}' X_C + b_i \tag{16}$$

- feature dimensions: $d_C = d_E = 1$
- $X_C \sim \sum_{m=1}^{3} \omega_m N(\mu_{C_m}, \sigma^2_{C_m})$: $\omega = [0.3, 0.4, 0.3]$, $\mu_C = [-5, 0, 5]$, $\sigma_C = [0.5, 0.5, 0.5]$
- Y: $a = 0.5$, $b = 0$
- X_E: $A_0 = -A_1 = 1$, $b_0 = -b_1 = 2$, $D_0 = D_1 = 0.25$
- Use the linear regression for $P(X_E|X_C, y; \theta_E)$ in the semi-generative model and $P(X_E^l|X_C^l)$ in the conditional self-learning.

Case I



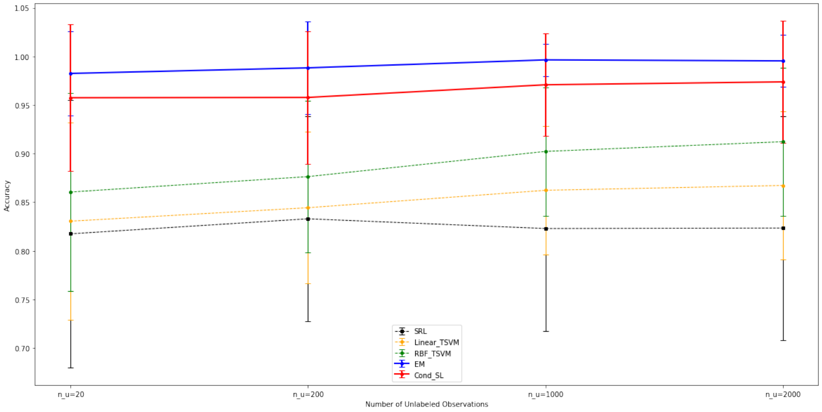
- Causally-motivated methods outperform the other three and have no significant difference.
- Two T-SVM methods provide similar results and perform even worse than the supervised logistic regression.

Case II

$$f_i(X_C) = A_i{}' X_C + b_i \tag{17}$$

- feature dimensions: $d_C = d_E = 10$
- $X_C \sim \sum_{m=1}^{2} \omega_m MVN_{d_C}(\mu_{C_m}, \Sigma_{C_m})$: $\omega = [0.5, 0.5]$, $\mu_{C_1} = [-\frac{1}{2}, -\frac{2}{2}, ..., -\frac{d_C}{2}]$, $\mu_{C_2} = [\frac{1}{2}, \frac{2}{2}, ..., \frac{d_C}{2}]$, $\Sigma_{C_1} = \Sigma_{C_2} = diag_{d_C}(0.5)$
- Y: $a = 0.5$, $b = 0$
- X_E: $A_0 = -A_1 = 0.5J_{10}$, $b_0 = b_1 = 0$, $D_0 = D_1 = diag_{d_E}(0.25)$
- Use the ridge regression with penalty $\lambda = 1$ for $P(X_E|X_C, y; \theta_E)$ in the semi-generative model and $P(X_E^l|X_C^l)$ in the conditional self-learning.

Case II



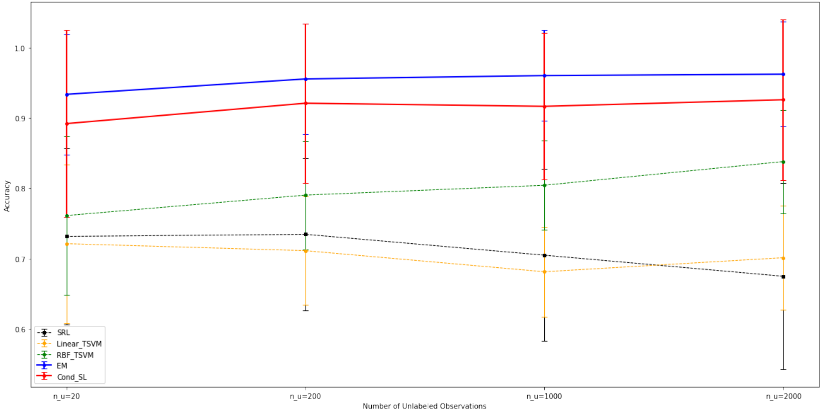
- Causally-motivated methods still outperform the other three.
- Most of the SSL methods perform better than the low-dimensional Case I, and overwhelm the supervised logistic regression.

Case III

$$f_0(X_C) = A_0{}'X_C + sin(X_C) + b_0 \tag{18}$$
$$f_1(X_C) = A_1{}'X_C + cos(X_C) + b_1 \tag{19}$$

- feature dimensions: $d_C = d_E = 10$
- $X_C \sim \sum_{m=1}^{2} \omega_m MVN_{d_C}(\mu_{C_m}, \Sigma_{C_m})$: $\omega = [0.5, 0.5]$, $\mu_{C_1} = [-\frac{1}{2}, -\frac{2}{2}, ..., -\frac{d_C}{2}]$, $\mu_{C_2} = [\frac{1}{2}, \frac{2}{2}, ..., \frac{d_C}{2}]$, $\Sigma_{C_1} = \Sigma_{C_2} = diag_{d_C}(0.5)$
- Y: $a = 0.5$, $b = 0$
- X_E: $A_0 = -A_1 = 0.5J_{10}$, $b_0 = b_1 = 0$, $D_0 = D_1 = diag_{d_E}(0.25)$
- Use the ridge regression with penalty $\lambda = 1$ for $P(X_E|X_C, y; \theta_E)$ in the semi-generative model and the kernel ridge regression with penalty $\lambda = 1$ for $P(X_E^l|X_C^l)$ in the conditional self-learning.

Case III



- All the methods perform worse compared with Case II.
- EM-like approach still provides stable performance.
- T-SVM with RBF kernel can work better compared with linear T-SVM and supervised logistic regression.

Conclusions

- Exploration of the conditional distribution $X_E|X_C$ instead of the joint distribution of (X_E, X_C) can help improve the classification performance.
- The increase of unlabeled data can slightly contribute to higher accuracy for SSL methods (T-SVM and proposed methods) with both cause and effect features, but also increase the standard deviations.
- Connections to domain adaptation: the proposed approaches are robust to changes in $P(X_C)$. $P(Y|X_C)$ and $P(X_E, Y|X_C)$ remain stable.
- Model flexibility: for structured data such as natural images or text, we can use GANs or VAEs to model the additive noise functions.

Reference

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