# Skada and Skada-Bench: Benchmarking Unsupervised Domain Adaptation Methods with Realistic Validation

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# Table of contents

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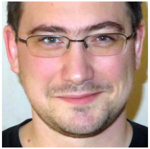

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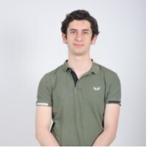

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# 1. Introduction to **Domain Adaptation** (DA)

# Supervised learning

**Independent** and **identically** distributed data:

$$\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \sim \mathbb{P}(X, Y)$$

$\boldsymbol{x}_i \in \mathbb{R}^d$, $y_i \in \mathcal{Y}$, e.g. $\{-1, 1\}$ for binary classification.

**Goal** : find a predictor $f : \mathbb{R}^d \to \mathcal{Y}$ by empirical risk minimization

$$\min_{f \in \mathcal{F}} \left\{ R(f) = \frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i, f(\boldsymbol{x}_i)\right) \right\}$$

with $\ell$ a loss function.

- Hyper-parameters tuning with a grid search cross-validation.
- Generalization performance estimation with a cross-validation.
- Easy to implement with Scikit-Learn.

# Domain Adaptation Problem

**Source** domain ($\mathcal{S}$) and **Target** domain ($\mathcal{T}$) with

$$\mathbb{P}_{\mathcal{S}}(X, Y) \neq \mathbb{P}_{\mathcal{T}}(X, Y)$$

Source domain ($\mathcal{S}$): MNIST

Target domain ($\mathcal{T}$): SVHN

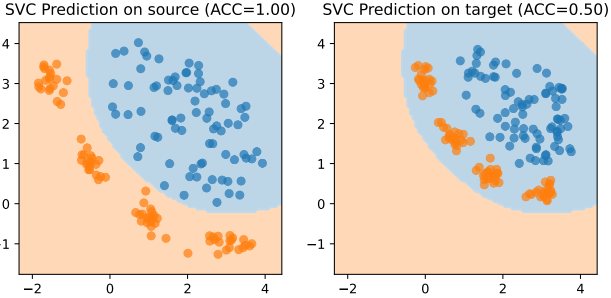
Domain adaptation: MNIST $\rightarrow$ SVHN

# Domain Adaptation Problem

**Source** domain ($\mathcal{S}$) and **Target** domain ($\mathcal{T}$) with

$$\mathbb{P}_{\mathcal{S}}(X, Y) \neq \mathbb{P}_{\mathcal{T}}(X, Y)$$

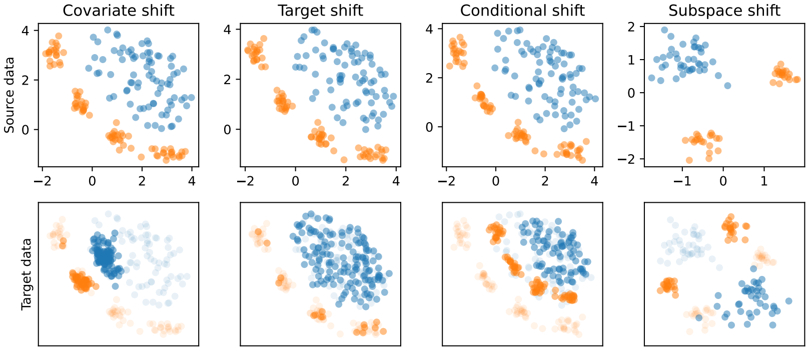
Training on the source domain (classical empirical risk minimization):



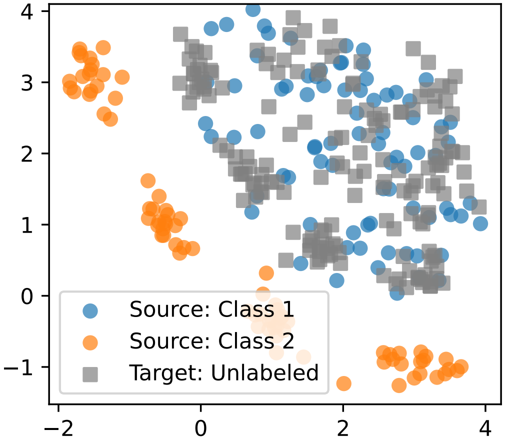

Simple shifts can lead to very bad classifications on the target domain.

# Unsupervised Domain Adaptation problem

- Source domain is **labeled** : $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n_\mathcal{S}} \sim \mathbb{P}_\mathcal{S}(X, Y)$
- Target domain is **unlabeled** : $\{(\boldsymbol{x}_i, .\ )\}_{i=1}^{n_\mathcal{T}} \sim \mathbb{P}_\mathcal{T}(X, Y)$
- Assumptions on the shift between $\mathbb{P}_\mathcal{S}(X, Y)$ and $\mathbb{P}_\mathcal{T}(X, Y)$:

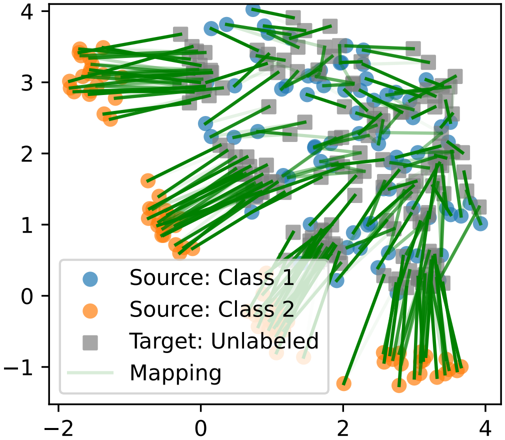


# Toy example of Unsupervised DA



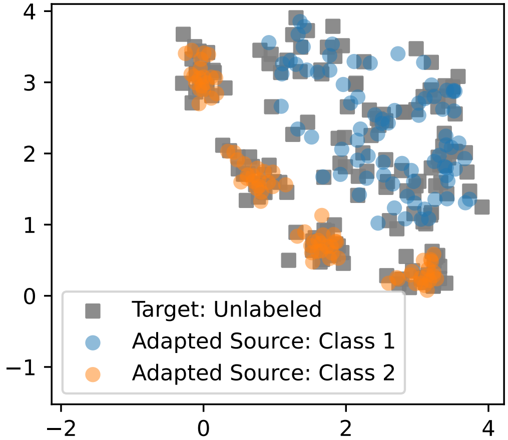

Problem setting

# Toy example of Unsupervised DA



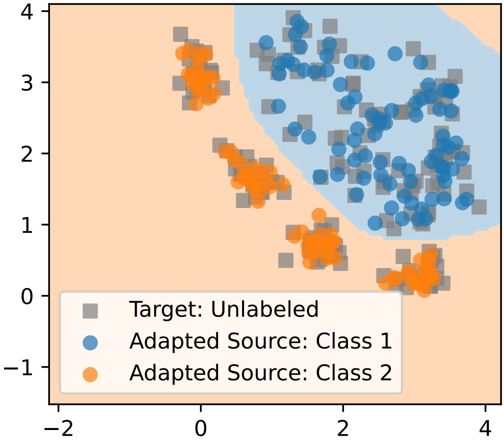

Step 1: Minimize a discrepancy between source and target domains

# Toy example of Unsupervised DA




Step 2: Adapt source distribution to target distribution

# Toy example of Unsupervised DA




Step 3: Train on adapted source and predict on target (ACC=1.00)

# DA methods

## Mapping

- Learn a mapping function $m$ to align source and target domains.
- The domain-adapted predictor becomes:

$$f_{\mathrm{DA}} = f \circ m$$

## Reweighting

$$f_{\mathrm{DA}} \in \arg\min_{f \in \mathcal{F}} \frac{1}{n_{\mathcal{S}}} \sum_{i=1}^{n_{\mathcal{S}}} w_i \, \ell(f(\mathbf{x}_i), y_i)$$

where $w_i$ are importance weights depending on source and target domains.

## End-to-End Deep Learning

- Jointly learn feature representations and a classifier using deep networks.
- Train with adversarial or discrepancy-based objectives to align source and target distributions.

# DA scorers

**Huge variety of DA methods** : mapping, subspace, reweighting, ...
with many different hyper-parameters to tune.
$\hookrightarrow$ **DA scorers** to validate hyper-parameters without using target label.

$$\mathrm{DA\_scorer}(\underbrace{f_{\mathrm{DA}}}_{\text{Predictive model}}, \underbrace{\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n_{\mathcal{S}}}}_{\text{Source data}}, \underbrace{\{\boldsymbol{x}_i\}_{i=1}^{n_{\mathcal{T}}}}_{\text{Target data}}) \in \mathbb{R}$$

Rely on **proxys** of the target accuracy.

# Many extensions

- Multi-source DA
- DA for regression problems
- Deep DA: deep learning models for DA
- Semi-supervised DA: few labeled target data
- Test-time DA: adapt to a new target domain with forgotten source data
- Heterogeneous DA: different feature spaces
- ...

# 2. **Skada** : a Scikit-Learn compatible library for shallow and deep DA

# Scikit-Adaptation: Skada

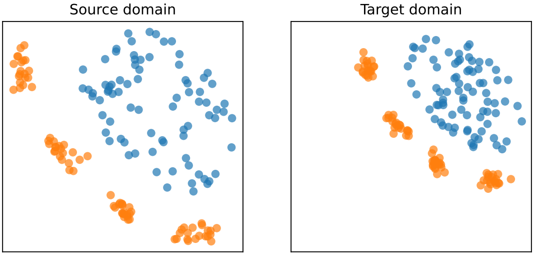
Implementation of Python library for domain adaptation, including:

- Homogeneous API for all DA methods: **Shallow and Deep learning** .
- **Sklearn-like API** with estimator class (.fit, .predict, ...), pipeline, grid search ...
- **DA scorer** to validate hyper-parameters without using target label.

# Example of conditional shift

```
from skada.datasets import make_shifted_datasets

dataset = make_shifted_datasets(
    n_samples_source=20,
    n_samples_target=20,
    shift="concept_drift",
    return_dataset=True
)
```



# Training OT Mapping model

```python
from skada import OTMapping

X, y, sample_domain = dataset.pack_train(as_sources=["s"], as_targets=["t"])
model = OTMapping()
model.fit(X, y, sample_domain=sample_domain)

X_target, y_target, sample_domain = dataset.pack_test(as_targets=["t"])
model.score(X_target, y_target)
```

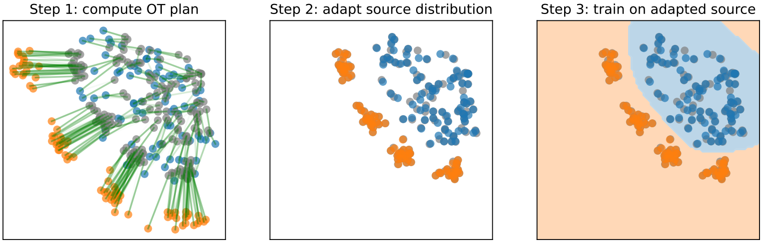
```
y = [ 0  0  0  0  0  0  0  0  1  1  1  1  1  1  1  1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1]
sample_domain = [ 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 -2 -2 -2 -2 -2 -2 -2 -2
 -2 -2 -2 -2 -2 -2 -2 -2]
```

# What are Skada model: Sklearn pipeline

```python
from sklearn.svm import SVC

from skada import make_da_pipeline
from skada import OTMappingAdapter

model = make_da_pipeline(
    OTMappingAdapter(),
    SVC(),
)
```

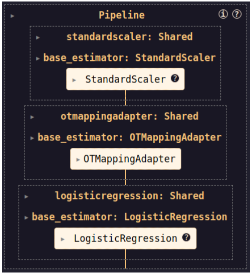


# What are Skada model: Sklearn pipeline

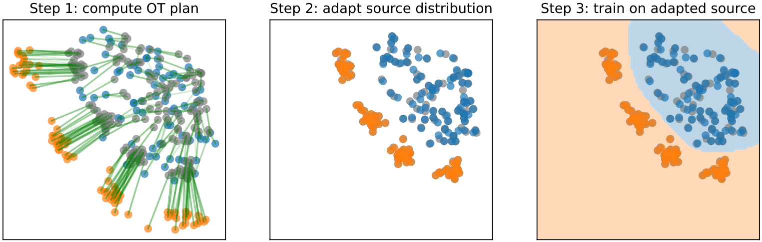
```python
from sklearn.linear_model import LogisticRegression
from sklearn.preprocessing import StandardScaler

from skada import make_da_pipeline
from skada import OTMappingAdapter

model = make_da_pipeline(
    StandardScaler(),
    OTMappingAdapter(),
    LogisticRegression(),
)
```

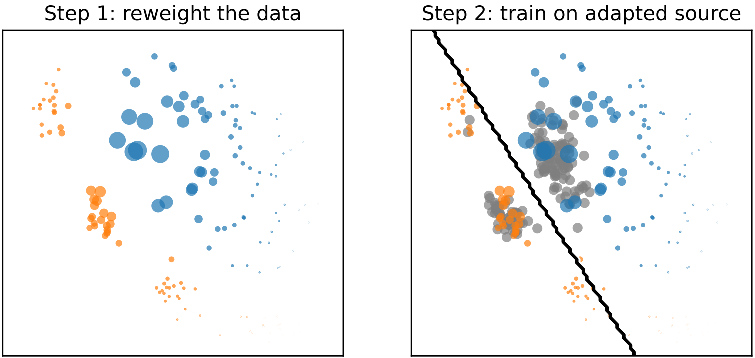


# Mapping methods



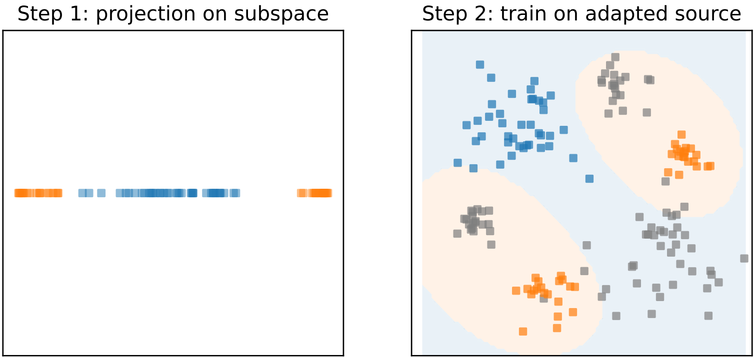

**6** available mapping methods in `Skada` : `CORAL`, `OTMapping`, `EntropicOTMapping`, `ClassRegularizerOTMapping`, `LinearOTMapping`, `MMDLSConSMapping`

# Reweighting methods




**6** available reweighting methods in `Skada` : `GaussianReweight`, `KLIEPReweight`, `KMMReweight`, `DiscriminatorReweight`, `NearestNeighborReweight`, `MMDTarSReweight`

# Subspace methods

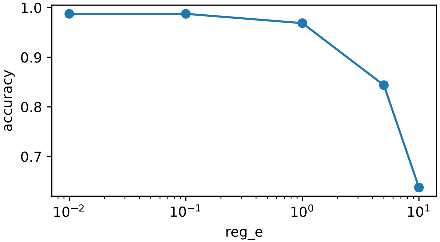



**4** available subspace methods in **Skada** : `SubspaceAlignment`, `TransferComponentAnalysis`, `TransferJointMatching`, `TransferSubspaceLearning`

# How to validate parameters in DA?

```python
from skada import EntropicOTMapping

model = EntropicOTMapping(reg_e=1e-1, base_estimator=SVC(probability=True))
```




How to validate the parameter `reg_e` ?

- Gridsearch on **source** $\rightarrow$ **Bad parameter**
- Gridsearch on **target** $\rightarrow$ **Cheating!** (no label available)

$\hookrightarrow$ Use specific **DA scorers** !

# Validation with DA scorers

```python
from sklearn.model_selection import GridSearchCV, ShuffleSplit

from skada import EntropicOTMapping
from skada.metrics import PredictionEntropyScorer

model = EntropicOTMapping(base_estimator=SVC(probability=True))

cv = ShuffleSplit(n_splits=5, test_size=0.3, random_state=42)
reg_e = [0.01, 0.03, 0.05, 0.08, 0.1]

grid_search = GridSearchCV(
    model,
    {"entropicotmappingadapter__reg_e": reg_e},
    cv=cv,
    scoring=PredictionEntropyScorer(),
)
grid_search.fit(X, y, sample_domain=sample_domain)
```

# Validation with DA scorers

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from sklearn.model_selection import GridSearchCV, ShuffleSplit

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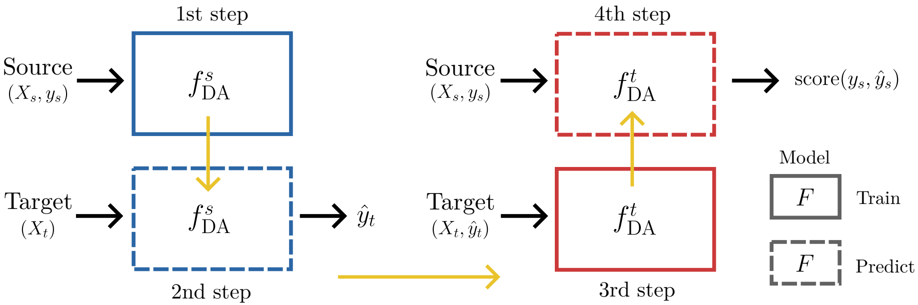
)
grid_search.fit(X, y, sample_domain=sample_domain)
```

$\hookrightarrow$ **6** DA scorer available in `Skada`

# Circular validation [BM10]

- Train a model on **source** domain and predict on **target** domain.
- Train a model on **target** domain with **predicted label**.
- Predict on **source** domain and compute **accuracy**.



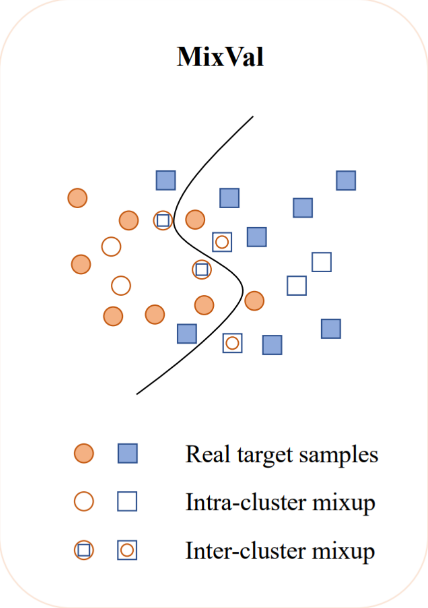
# Mixval scorer [HLL+23]

- Create **mixed sample** from source

$$\tilde{X} = \lambda X_i^s + (1-\lambda) X_j^s$$

$$\tilde{y} = \begin{cases} y_i^s & \text{if } \lambda \geq 0.5 \\ y_j^s & \text{otherwise} \end{cases}$$

- Distinguish between samples mixed from **same classes** and **different classes** .
- Validate on mixed samples.



# Other DA scorers

- Validate on **source** domain with **weighted samples** : `ImportanceWeightedScorer`, `DeepEmbeddedValidation`.
- Compute the **entropy** of the **target** predictions: `PredictionEntropyScorer`, `SoftNeighborhoodDensity`.

# Deep DA methods

Deep DA methods $\rightarrow$ Reduce **divergence** between source and target domains in the **embedding space** .

$$\ell = \sum_{i=1}^{n_{\mathcal{S}}} \overbrace{\ell_{\mathrm{CE}}}^{\text{Cross-entropy loss}} (f(g(\boldsymbol{x}_i^s)), y_i^s) + \underbrace{\mathrm{reg}}_{\text{Regularization term}} \sum_{i=1}^{n_{\mathcal{S}}} \sum_{j=1}^{n_{\mathcal{T}}} \underbrace{\ell_{\mathrm{DA}}}_{\text{DA loss}} (g(\boldsymbol{x}_i^s), g(\boldsymbol{x}_j^t), y_i^s)$$

- $f$ is the classifier, $g$ is the feature extractor.
- $\ell_{\mathrm{DA}}$ can compute **OT distance** , **MMD distance** , **adversarial loss** , ...

# Deep DA methods

- Wrapper of **Skorch**
- Param `layer_name` to know which **feature space** to consider
- Parameter `reg` is the **threshold** between classical and DA loss
- All the rest work the same as before: learning rate, batch size ...

```python
from skada.deep import DeepCoral
from skada.deep.modules import ToyCNN

model = DeepCoral(
    ToyCNN(),
    layer_name="feature_extractor",
    batch_size=128,
    max_epochs=5,
    reg=1,
    lr=1e-2,
)

model.fit(X, y, sample_domain=sample_domain)
model.score(X_target, y_target)
```

**5** available deep DA methods in `Skada` : `DeepCORAL`, `DANN`, `CDAN`, `DAN`, `DeepJDOT`.

# 3. **Skada-Bench** : Benchmarking Unsupervised DA Methods with Realistic Validation

# Question in DA field

3 main questions emerge after implementing **Skada** :

- Does the DA methods have been compared properly?
- How the different **DA methods** **perform** on **diverse datasets** (other than Computer Vision)?
- Is there a **best DA scorers** for all methods? for each specific type of method?

# Question in DA field

3 main questions emerge after implementing **Skada** :

- Does the DA methods have been compared properly?
- How the different **DA methods perform** on **diverse datasets** (other than Computer Vision)?
- Is there a **best DA scorers** for all methods? for each specific type of method?

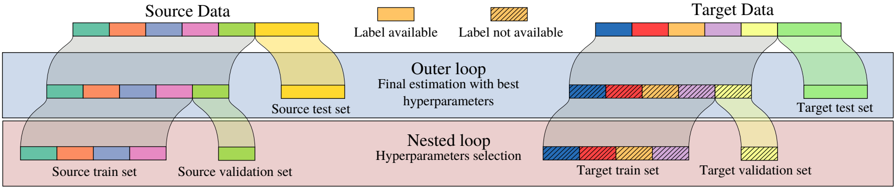
$\hookrightarrow$ **Benchmark** !

# Validation in the litterature

| | Method | Validation Procedure | Comment |
|---|---|---|---|
| Reweighting | Density Reweight [SM05] | None | Bandwidth fixed by Silverman method |
| | Discriminative Reweight [Shi00] | NA | No hyperparameters |
| | Gaussian Reweight [Shi00] | None | Not specified in [Shi00] |
| | KLIEP [SNK$^+$07] | Integrated CV | Likelihood CV [SNK$^+$07] on target |
| | KMM [HGB$^+$06] | None | Fixed data-dependent hyperparameters |
| | NN Reweight [Loo12] | None | Number of neighbors fixed to one |
| | MMDTarS [ZSMW13] | CV | Not specified if done on source or target |
| Mapping | Coral [SFS17] | NA | No hyperparameters |
| | OT mapping [CFTR17] | CV target/CircCV | Unclear in the text |
| | Lin. OT mapping [FLF20] | NA | No hyperparameters |
| | MMD-LS [ZSMW13] | CV | Not specified if done on source or target |
| Subsp. | SA [FHST13] | 2-fold CV on source | - |
| | TCA [PTKY11] | Validation on target | Target subset used to tune parameters |
| | TSL [STG10] | None | Not specified in [STG10] |
| Other | JDOT [CFHR17] | Reverse CV [ZFY$^+$10] | - |
| | OT label prop [SRGB14] | NA | No hyperparameters |
| | DASVM [BM10] | Circular Validation [BM10] | - |

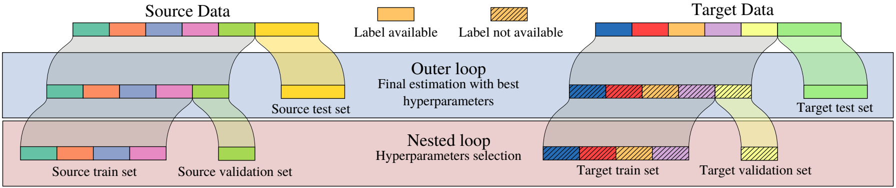
$\hookrightarrow$ **few realistic validation** procedure in the **literature** .

# Performance evaluation and Hyper-parameters selection




Nested cross-validation on source and target domains

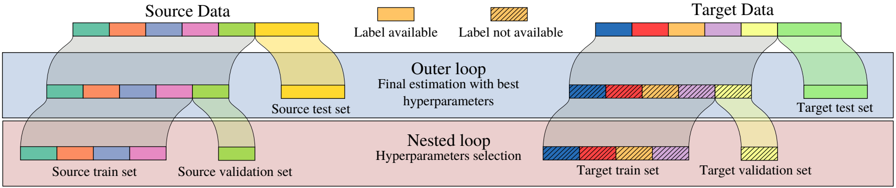
# Performance evaluation and Hyper-parameters selection




Nested cross-validation on source and target domains

- **Outer loop** : estimate generalization performance with unlabeled train target set but labeled test target set.

# Performance evaluation and Hyper-parameters selection




Nested cross-validation on source and target domains

- **Outer loop** : estimate generalization performance with unlabeled train target set but labeled test target set.
- **Nested loop** : select hyper-parameters with the unlabeled train target domain and a DA scorer.

# Dataset description

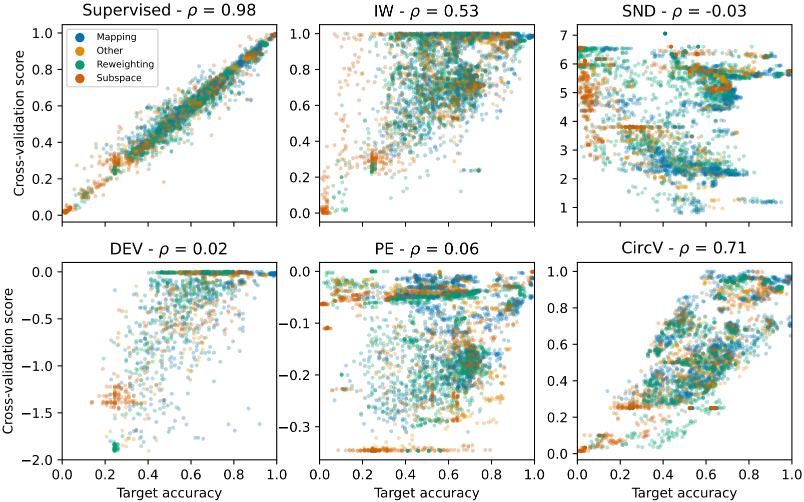
| Dataset | Modality | Preprocessing | # adapt | # classes | # samples | # features |
|---|---|---|---|---|---|---|
| `Office 31` [KTP17] | CV | Decaff [DJV+14] + PCA | 6 | 31 | $470 \pm 350$ | 100 |
| `Office Home` [VECP17] | CV | ResNet [HZRS16] + PCA | 12 | 65 | $3897 \pm 850$ | 100 |
| `MNIST/USPS` [LC15] | CV | Vect + PCA | 2 | 10 | 3000 / 10000 | 50 |
| `20 Newsgroup` [Lan95] | NLP | LLM [RG19, XLZM23] + PCA | 6 | 2 | $3728 \pm 174$ | 50 |
| `Amazon Review` [ML13, MTSvdH15] | NLP | LLM [RG19, XLZM23] + PCA | 12 | 4 | 2000 | 50 |
| `Mushrooms` [DYXY07] | Tabular | One Hot Encoding | 2 | 2 | $4062 \pm 546$ | 117 |
| `Phishing` [MTM12] | Tabular | NA | 2 | 2 | $5527 \pm 1734$ | 30 |
| `BCI` [TMA+12] | Biosignals | Cov+TS [BBCJ12] | 9 | 4 | 288 | 253 |

$\hookrightarrow$ **8** datasets from different modalities: Computer Vision, NLP, Tabular, Biosignals.

# Table results

| | | Cov. shift | Tar. shift | Cond. shift | Sub. shift | Office31 | OfficeHome | MNIST/USPS | 20NewsGroups | AmazonReview | Mushrooms | Phishing | BCI | Selected Scorer | Rank |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Train Src | 0.88 | 0.85 | 0.66 | 0.19 | 0.59 | 0.56 | 0.54 | 0.59 | 0.7 | 0.72 | 0.91 | 0.55 | | 9.75 |
| | Train Tgt | 0.92 | 0.93 | 0.82 | 0.98 | 0.88 | 0.8 | 0.96 | 1.0 | 0.73 | 1.0 | 0.97 | 0.64 | | 1.06 |
| Reweighting | Dens. RW [SM05] | 0.88 | 0.86 | 0.66 | 0.18 | 0.57 | 0.55 | 0.54 | 0.58 | 0.7 | 0.71 | 0.91 | 0.55 | IW | 10.76 |
| | Disc. RW [Shi00] | 0.85 | 0.83 | 0.71 | 0.18 | 0.58 | 0.53 | 0.5 | 0.6 | 0.68 | 0.75 | 0.91 | 0.56 | CircV | 11.12 |
| | Gauss. RW [Shi00] | 0.89 | 0.86 | 0.65 | 0.21 | 0.2 | 0.44 | 0.11 | 0.54 | 0.6 | 0.51 | 0.46 | 0.25 | CircV | 19.42 |
| | KLIEP [SNK+07] | 0.88 | 0.86 | 0.66 | 0.19 | 0.59 | 0.56 | 0.54 | 0.6 | 0.69 | 0.72 | 0.91 | 0.55 | CircV | 10.36 |
| | KMM [HGB+06] | 0.89 | 0.87 | 0.64 | 0.15 | 0.58 | 0.55 | 0.52 | 0.7 | 0.57 | 0.74 | 0.91 | 0.52 | CircV | 12.11 |
| | NN RW [Loo12] | 0.89 | 0.86 | 0.67 | 0.15 | 0.58 | 0.55 | 0.54 | 0.59 | 0.66 | 0.71 | 0.91 | 0.54 | CircV | 11.91 |
| | MMDTarS [ZSMW13] | 0.88 | 0.86 | 0.64 | 0.2 | 0.56 | 0.55 | 0.54 | 0.59 | 0.7 | 0.74 | 0.91 | 0.55 | IW | 9.51 |
| Mapping | CORAL [SFS17] | 0.66 | 0.84 | 0.66 | 0.19 | 0.59 | 0.57 | 0.62 | 0.73 | 0.69 | 0.72 | 0.92 | 0.62 | CircV | 7.10 |
| | MapOT [CFTR17] | 0.72 | 0.57 | 0.82 | 0.02 | 0.55 | 0.51 | 0.61 | 0.76 | 0.67 | 0.63 | 0.84 | 0.47 | PE | 10.98 |
| | EntOT [CFTR17] | 0.71 | 0.6 | 0.82 | 0.12 | 0.58 | 0.58 | 0.6 | 0.83 | 0.62 | 0.75 | 0.86 | 0.54 | CircV | 9.75 |
| | ClassRegOT [CFTR17] | 0.74 | 0.58 | 0.81 | 0.11 | 0.61 | 0.53 | 0.62 | 0.96 | 0.68 | 0.82 | 0.88 | 0.52 | IW | 8.71 |
| | LinOT [FLF20] | 0.73 | 0.73 | 0.76 | 0.18 | 0.59 | 0.57 | 0.64 | 0.82 | 0.7 | 0.76 | 0.91 | 0.61 | CircV | 5.33 |
| | MMD-LS [ZSMW13] | 0.65 | 0.68 | 0.81 | 0.52 | 0.55 | 0.54 | 0.52 | 0.97 | 0.68 | 0.86 | 0.88 | 0.56 | IW | 9.66 |
| Subspace | JPCA | 0.88 | 0.85 | 0.66 | 0.15 | 0.55 | 0.47 | 0.51 | 0.77 | 0.69 | 0.78 | 0.9 | 0.54 | PE | 8.77 |
| | SA [FHST13] | 0.74 | 0.68 | 0.8 | 0.11 | 0.59 | 0.57 | 0.56 | 0.88 | 0.66 | 0.88 | 0.89 | 0.53 | CircV | 8.53 |
| | TCA [PTKY11] | 0.46 | 0.48 | 0.55 | 0.56 | 0.04 | NA | 0.11 | 0.57 | 0.6 | 0.45 | NA | 0.27 | CircV | 19.57 |
| | TSL [STG10] | 0.88 | 0.85 | 0.66 | 0.19 | 0.59 | 0.2 | 0.25 | 0.68 | 0.7 | 0.56 | 0.86 | 0.25 | IW | 14.65 |
| Other | JDOT [CFHR17] | 0.72 | 0.57 | 0.82 | 0.14 | 0.6 | 0.51 | 0.63 | 0.77 | 0.67 | 0.63 | 0.8 | 0.46 | DEV | 10.12 |
| | OTLabelProp [SRGB14] | 0.72 | 0.59 | 0.81 | 0.05 | 0.61 | 0.56 | 0.62 | 0.86 | 0.67 | 0.64 | 0.86 | 0.5 | CircV | 10.49 |
| | DASVM [BM10] | 0.89 | 0.86 | 0.65 | 0.14 | NA | NA | NA | 0.68 | NA | 0.78 | 0.88 | NA | CircV | 11.00 |

# Results



Supervised - $\rho$ = 0.98
IW - $\rho$ = 0.53
SND - $\rho$ = -0.03
DEV - $\rho$ = 0.02
PE - $\rho$ = 0.06
CircV - $\rho$ = 0.71
Mapping
Other
Reweighting
Subspace
Cross-validation score
Target accuracy

# Conclusion

**`Skada`**

- First release few month ago
- Still a lot of work: examples, documentation of `skada.deep` ...

**`Skada-bench`**

- Benchmark only on **shallow** DA methods
- Currently adding **deep** DA methods

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