Metric Learning for Graph-based Domain Adaptation

Paramveer S. Dhillon
Computer and Information Science, University of Pennsylvania, U.S.A
dhillon@cis.upenn.edu

Partha Pratim Talukdar
Machine Learning Department, Carnegie Mellon University, U.S.A
ppt@cs.cmu.edu

Koby Crammer
Department of Electrical Engineering, The Technion, Israel
koby@ee.technion.ac.il

Abstract

In many domain adaption formulations, it is assumed to have large amount of unlabeled data from the domain of interest (target domain), some portion of it may be labeled, and large amount of labeled data from other domains, also known as source domain(s). Motivated by the fact that labeled data is hard to obtain in any domain, we design algorithms for the settings in which there exists large amount of unlabeled data from all domains, small portion of which may be labeled.

We build on recent advances in graph-based semi-supervised learning and supervised metric learning. Given all instances, labeled and unlabeled, from all domains, we build a large similarity graph between them, where an edge exists between two instances if they are close according to some metric. Instead of using predefined metric, as commonly performed, we feed the labeled instances into metric-learning algorithms and (re)construct a data-dependent metric, which is used to construct the graph. We employ different types of edges depending on the domain-identity of the two vertices touching it, and learn the weights of each edge.

We provide extensive empirical evidence demonstrating that our approach leads to significant reduction in classification error across domains, and evaluate the contribution of each resource: labeled and unlabeled data of the various domains.

Keywords: Machine Learning, Domain Adaptation, Graph-based Semi-Supervised Learning, Sentiment Analysis.

1 Introduction

Domain adaptation is an important machine learning subtask where the goal is to perform well on a particular classification task on a *target domain*, especially when most of the resources are available from other different domains, called *source(s) domain(s)* (Pan and Yang, 2009), and only limited amount of supervision is available to the target domain. In the standard setting, most domain adaptation algorithms assume the availability of large amounts of labeled data for the source domain, with little or no labeled data from the target domain (Arnold et al., 2008; Dai et al., 2007; Wang et al., 2009). However, in many practical situations, obtaining labeled data from *any* domain is expensive and time consuming, while unlabeled data is easily available. This setting of domain

adaptation, where there is only limited amount of labeled data and large amounts of unlabeled data, both from all domains, is relatively unexplored.

To address the issue of labeled data sparsity even within a single domain, recent research has focused on Semi-Supervised Learning (SSL) algorithms, which learn from limited amounts of labeled data combined with widely available unlabeled data. Examples of a few graph-based SSL algorithms include Gaussian Random Fields (GRF) (Zhu et al., 2003), Quadratic Criteria (QR) (Bengio et al., 2006), and Modified Adsorption (MAD) (Talukdar and Crammer, 2009). Given a set of instances that contain small amount of labeled instances and a majority that is unlabeled, most graph based SSL algorithms first construct a graph where each node corresponds to an instance. Similar nodes are connected by an edge, with edge weight encoding the degree of similarity. Once the graph is constructed, the nodes corresponding to labeled instances are injected with the corresponding label. Using this initial label information along with the graph structure, graph based SSL algorithms assign labels to all unlabeled nodes in the graph. Most of the graph based SSL algorithms are iterative and also parallelizable, making them suitable for large scale SSL setting where vast amounts of unlabeled data is usually available.

Most of the graph based SSL algorithms mentioned above concentrate primarily on the label inference part, i.e., assigning labels to nodes *once the graph has already been constructed*, with very little emphasis on construction of the graph itself. Only recently, the issue of graph construction has begun to receive attention (Wang and Zhang, 2006; Jebara et al., 2009; Daitch et al., 2009; Talukdar, 2009). Most of these methods emphasize on constructing graphs which satisfy certain structural properties (e.g., degree constraints on each node). Since our focus is on SSL, a certain number of labeled instances are available at our disposal. However, the graph construction methods mentioned above are all unsupervised in nature, i.e., they do not utilize available label information during the graph construction process. As recently proposed by (Dhillon et al., 2010), the available label information can be used to *learn* a distance metric, which can then be used to set the edge weights in the constructed graph.

In this paper, we bring together these three lines of work: domain adaptation, graph-based SSL, and metric learning for graph construction, and make the following contributions:

1. We consider an important setting for domain adaptation: one where most of the data is unlabeled and only limited amount of instances are labeled. This holds across *all* domains. This setting is relatively unexplored.

2. To the best of our knowledge, we are the first to employ graph-based non-parametric methods for domain adaptation.

3. We provide extensive experimental results on real-world datasets, to both demonstrate the effectiveness of metric learning for graph construction for domain adaptation.

2 Related Work

Several methods for domain adaptation have recently been proposed (Arnold et al., 2008; Blitzer et al., 2006; Dai et al., 2007; Pan and Yang, 2009; Eaton et al., 2008; Wang et al., 2009). In (Arnold et al., 2008), the labeled data comes entirely from the source domain, while certain amount of unlabeled target data is also used during transduction. Similar setting is also explored in (Dai et al., 2007; Wang et al., 2009). In contrast to these methods, we assume that limited amount of labeled

data and large amounts of unlabeled data from both source and target domains are available. This is motivated by the fact that obtaining large amount of labeled data from any domain is expensive to prepare. The method presented by (Blitzer et al., 2006) also explores a similar setting, but our method is easier to implement and it does not make use of the high domain specific prior knowledge (i.e., for pivot selection) performed by (Blitzer et al., 2006).

All previously proposed methods mentioned above are parametric in nature. The graph-based adaptation method presented in this paper is non-parametric. To the best of our knowledge, it is novel in the context of domain adaptation.The method of (Wang et al., 2009) is similar in spirit as both employ graphs, yet they use a hybrid graph structure involving both instances and features for transfer learning, while we focus on domain adaptation and use homogeneous graph consisting of instance nodes only. Another important difference is that the graphs their algorithms build do *not* take available label information into account, while our algorithms do take such information into account. We will see below in Section 8, that this leads to significant improvement in performance. Another work similar in spirit to ours is of (Eaton et al., 2008). They build a graph over tasks (i.e., a node in such a graph is a task) to decide on the transferability among different tasks for transfer learning. In contrast, we focus on domain adaptation and build a graph over data instances, i.e., a node in our graph corresponds to a data instance.

3 Notation

We denote by n_l^s and n_u^s, the number of labeled and unlabeled instances (respectively) from the source domain. Similarly, n_l^t and n_u^t are the number of labeled and unlabeled instances from the target domain. Denote by n the total number of instances. Let X be the $d \times n$ matrix of n d-dimensional column instances (from source and target domains combined). We define the $n \times n$ diagonal label-indicator matrix S to be $S_{ii} = 1$ iff instance x_i is labeled, and zero otherwise. We denote by $\mathscr{L}$ the set of all possible labels of size $m = |\mathscr{L}|$. We define the $n \times m$ instance-label matrix by Y, where $Y_{i,j} = 1$ iff the ith instance is labeled by the jth label. Note, that the ith column of Y is undefined if $S_{i,i} = 0$, i.e., the data instance is not labeled. Similarly, we denote by $\hat{Y}$ the $n \times m$ matrix of estimated label information, i.e., output of a inference algorithm (e.g., see Section 5). Such algorithms assign a labeling score to all instances, including labeled and unlabeled.

4 Domain Adaptation

Formally, we consider the following problem. Given, a total of $n_l^s + n_l^t$ labeled instances from the source(s) and target domains combined, and in addition $n_u^s + n_u^t$ unlabeled instances from the same domains. Our goal is to label these n_u^t unlabeled instances from the target domain (domain of interest). The task is challenging and non-trivial since we assume that $n_l^s \ll n_u^s$, and similarly $n_l^t \ll n_u^t$. Our setting is different from previous approaches in two ways: First, we assume small amount of labeled data from all domains, as opposed to most previous work in domain adaption which have focused in the "asymmetric" case where there is large amount of labeled source instances, and only very few, if any, labeled target instances. Second, we compensate, this lack in labeled data by considering unlabeled data from all domains, source and target, as opposed to previous settings which assumed unlabeled data only from the target domain. We believe that our "symmetric" setting is very realistic, since labeled data is expensive in any domain.

In Section 8, we report the results of experiments using a sentiment dataset, which contains reviews on products from a few categories. We assume that only a few instances are hand-labeled with the correct sentiment for every category, and our goal is to exploit the labeled and *unlabeled* instances from all domains to perform well on a single pre-defined *target* domain. Our task is harder, since we

have only few labeled examples from each domain, however, we exploit additional cheap resource, namely unlabeled data from all the domains.

5 Graph Construction & Inference

Given a set X of n instances, both from the source and target domains, we construct a graph where each instance is associated with a node. We add an edge between two nodes if the two nodes are similar and the edge's weight represents the degree of similarity between the corresponding instances. Denote the resulting graph by $G = (V, E, W)$ be this graph, where $V = V_l^s \cup V_u^s \cup V_l^t \cup V_u^t$ is the set of vertices with $|V| = n$, $|V_l^s| = n_l^s$, $|V_u^s| = n_u^s$, $|V_l^t| = n_l^t$, $|V_u^t| = n_u^t$; E is the set of edges, and W is the symmetric $n \times n$ matrix of edge weights. W_{ij} is the weight of edge (i, j) which is monotonic in the similarity between instances x_i and x_j. Additionally, $V^s = V_l^s \cup V_u^s$, and $V^t = V_l^t \cup V_u^t$ are the set of vertices associated with sources and target domain instances, respectively. Gaussian kernel (Zhu et al., 2003) is a widely used measure of similarity between data instances, which can be used to compute edge weights as shown in Eq. (1).

$$W_{ij} = \alpha_{ij} \times \exp\left(-d_A(x_i, x_j)/(2\sigma^2)\right) \tag{1}$$

where $d_A(x_i, x_j)$ is the distance measure between instances x_i and x_j and A is a positive definite matrix of size $d \times d$, which parameterizes the (squared) Mahalanobis distance (Eq. (3)). Furthermore, σ is the kernel bandwidth parameter, and $\alpha_{ij} = \alpha$ $(0 \leq \alpha \leq 1)$ if the edge connects instances from two different domains, and $\alpha_{ij} = 1$, otherwise. In other words, the hyperparameter, α, controls the importance of cross domain edges. Setting edge weights directly using Eq. (1) results in a complete graph, where *any* two pair of nodes are connected, since the Gaussian kernel always attains strictly positive values by definition. This is undesirable as the graph is dense (and in fact complete) and thus all computation times are at least quadratic in the number of instances, which may be very large. We thus generate a sparse graph by retaining only edges to k nearest neighbors of each node, and dropping all other edges (i.e., setting corresponding edge weights to 0), a commonly used graph sparsification strategy. The number of edges in the resulting graph is linear in the number of instances.

With the graph $G = (V, E, W)$ constructed, we perform inference over this graph to assign labels to all n_u unlabeled nodes. This is done by propagating the label information from the labeled nodes to the unlabeled nodes. Any of the several graph based SSL algorithms mentioned in Section 1 may be used for this task. For the experiments in this paper, we use the GRF algorithm (Zhu et al., 2003) which minimizes the optimization problem shown in (2).

$$\min_{\hat{Y}} \sum_{i,j} \sum_{l \in \mathcal{L}} W_{i,j} (\hat{Y}_{il} - \hat{Y}_{jl})^2, \text{ s.t. } SY = S\hat{Y} \tag{2}$$

As outlined in (Zhu et al., 2003), this optimization can be efficiently and exactly solved to obtain $\hat{Y}$. The result, is a labeling of all instances, including the n_u^t unlabeled instances from the target domain.

In most previous graph-based SSL methods (e.g., (Zhu et al., 2003)), the matrix A is predefined to the identity $A = I$, in Eq. (1), resulting in the standard Euclidean distance in input space. This method of unsupervised graph construction is *not* task dependent. Instead, we also learn the matrix A using the (small) set of labeled instances using metric learning algorithms. We add more detail below in Section 7. In a nutshell, we construct a similarity metric tailored to the current specific adaptation task.

Algorithm 1 Supervised Graph Construction (SGC) **Input**: instances X, training labels Y, training instance indicator S, neighborhood size k **Output**: Graph edge weight matrix, W

$A \leftarrow \text{MetricLearner}(X, S, Y)$
$W \leftarrow \text{ConstructKnnGraph}(X, A, k)$
return W

Algorithm 2 Iterative Graph Construction (IGC) **Input**: instances X, training labels Y, training instance indicator S, label entropy threshold β, neighborhood size k **Output**: Graph edge weight matrix, W

$\hat{Y} \leftarrow Y, \hat{S} \leftarrow S$
repeat
  $W \leftarrow \text{SGC}(X, \hat{Y}, k)$
  $\hat{Y}' \leftarrow \text{GraphLabelInference}(W, \hat{S}, \hat{Y})$
  $U \leftarrow \text{SelectLowEntInstances}(\hat{Y}', \hat{S}, \beta)$
  $\hat{Y} \leftarrow \hat{Y} + U\hat{Y}'$
  $\hat{S} \leftarrow \hat{S} + U$
until convergence (i.e., $U_{ii} = 0,\ \forall i$)
return W

6 Metric Learning Review

We now review a recently proposed *supervised* method for learning Mahalanobis distance between instance pairs. We shall concentrate on learning the PSD matrix $A \succeq 0$ which parametrizes the distance, $d_A(x_i, x_j)$, between instances x_i and x_j.

$$d_A(x_i, x_j) = (x_i - x_j)^\top A (x_i - x_j) \tag{3}$$

This is equivalent to finding a linear transformation P of the input space, and then applying Euclidean distance on the transformed instances Px_i.

Information-Theoretic Metric Learning (ITML) (Davis et al., 2007) assumes the availability of prior knowledge about inter-instance distances. In this scheme, similar instances should have low Mahalanobis distance between them, i.e., $d_A(x_i, x_j) \leq u$, for some non-trivial upper bound u. Similarly, dissimilar instances should have a large distance between them, that is, $d_A(x_i, x_j) \geq l$ for some l. Given a set of similar instances S and dissimilar instances D, the ITML algorithm chooses the matrix A that minimizes the following optimization problem:

$$\begin{aligned} \min_{A \succeq 0, \xi} \quad & D_{\text{ld}}(A, A_0) + \gamma \cdot D_{\text{ld}}(\xi, \xi_0) \\ \text{s.t.} \quad & \text{tr}\{A(x_i - x_j)(x_i - x_j)^\top\} \leq \xi_{c(i,j)},\ \forall (i,j) \in S \\ & \text{tr}\{A(x_i - x_j)(x_i - x_j)^\top\} \geq \xi_{c(i,j)},\ \forall (i,j) \in D \end{aligned} \tag{4}$$

where γ is a hyperparameter which determines the importance of violated constraints and A_0 is a Mahalanobis matrix provided using prior knowledge. To solve the optimization problem in (4), an algorithm involving repeated Bregman projections is presented in (Davis et al., 2007), which we use for the experiments reported in this paper.

7 Using Labeled Data for Graph Construction

We now describe how to incorporate labeled and unlabeled data during graph construction. We start with a review of a new graph construction framework (Dhillon et al., 2010) which combines existing *supervised* metric learning algorithms (such as ITML) with *transductive* graph-based label inference to learn a new distance metric from labeled as well as unlabeled data combined. In self-training styled iterations, IGC alternates between graph construction and label inference; with output of label inference used during next round of graph construction, and so on.

7.1 Iterative Graph Construction (IGC)

IGC builds on the assumption that supervised (metric) learning improves with more labeled data. Since we are focusing on the SSL setting with n_l labeled and n_u unlabeled instances, the algorithm automatically labels the unlabeled instances using some existing graph based SSL algorithm, and then includes a subset of the labeled instances in the training set for the next round of metric learning. Naturally, only examples with low assigned label entropy (i.e., high confidence label assignments) are used. Specifically, we use a threshold parameter $\beta > 0$ to determine which examples will be used for the next round. (In practice we set $\beta = 0.05$ and observed that indeed most of the low entropy instances which are selected for inclusion in next iteration of metric learning, are classified correctly.) This iterative process continues until no new instances are set of labeled instances. This occurs when either all the instances are already exhausted, or when none of the remaining unlabeled instances can be assigned labels with high confidence.

The IGC framework is presented in Algorithm 2. The algorithm iterates between the two main steps as follows. In Line 1, any supervised metric learner, such as ITML, may be used as the MetricLearner. Using the distance metric learned in Line 1, a new k-NN graph is constructed in Line 2, whose edge weight matrix is stored in W. In Line 4, GraphLabelInference optimizes over the newly constructed graph the GRF objective (Zhu et al., 2003) shown in Eq. (5).

$$\min_{\hat{Y}'} \ \mathrm{tr}\{\hat{Y}'^{\top} L \hat{Y}'\}, \ \text{s.t.} \ \hat{S}\hat{Y} = \hat{S}\hat{Y}' \tag{5}$$

where $L = D - W$ is the (unnormalized) Laplacian, and D is a diagonal matrix with $D_{ii} = \sum_j W_{ij}$. The constraint, $\hat{S}\hat{Y} = \hat{S}\hat{Y}'$, in (5) makes sure that labels on training instances are not changed during inference. In Line 5, a currently unlabeled instance x_i (i.e., $\hat{S}_{ii} = 0$) is considered a new labeled training instance, i.e., $U_{ii} = 1$, for next round of metric learning if the instance has been assigned labels with high confidence in the current iteration, i.e., if its label distribution has low entropy (i.e., $\text{Entropy}(\hat{Y}'_{i:}) \leq \beta$). Finally in Line 6, training instance label information is updated. This iterative process is continued till no new labeled instance can be added, i.e., when $U_{ii} = 0 \ \forall i$. IGC returns the learned matrix A which can be used to compute Mahalanobis distance using Eq. (3). The number of parameters estimated by IGC (i.e., dimensions of W) increases as the number data instances increase. Hence, we note that that IGC is non-parametric, just as other graph-based methods.

8 Experiments

Data: We use data from 12 domain pairs obtained from (Crammer et al., 2009), and preprocessed to keep only those features which occurred more than 20 times. The classification task is the following: given a product review, predict user's sentiment, i.e., whether it is positive or negative. Hence, this is a binary classification problem with number of classes $m = 2$. A total of $1,500$ instances from each domain were sampled, i.e., $n = 3000$. We note that the goal is to label

Domain Pairs	SVM	PCA	IGC
Electronics-DVDs	43.1 ± 0.3	41.4 ± 0.2	$\mathbf{38.3 \pm 0.3}$
DVDs-Electronics	37.1 ± 0.2	36.5 ± 0.3	$\mathbf{27.9 \pm 0.3}$
DVDs-Books	41.0 ± 0.3	40.3 ± 0.4	$\mathbf{31.9 \pm 0.4}$
Books-DVDs	43.9 ± 0.2	43.1 ± 0.3	$\mathbf{40.3 \pm 0.2}$
Music-Books	41.0 ± 0.3	39.9 ± 0.3	$\mathbf{30.1 \pm 0.3}$
Books-Music	36.7 ± 0.3	36.4 ± 0.2	$\mathbf{31.8 \pm 0.5}$
Video-Electronics	35.9 ± 0.2	35.5 ± 0.3	$\mathbf{28.4 \pm 0.3}$
Electronics-Video	37.4 ± 0.3	36.6 ± 0.4	$\mathbf{32.9 \pm 0.4}$
Video-DVDs	43.0 ± 0.2	42.0 ± 0.3	$\mathbf{40.1 \pm 0.3}$
DVDs-Video	38.1 ± 0.3	36.8 ± 0.2	$\mathbf{33.0 \pm 0.2}$
Kitchen-Apparel	35.0 ± 0.2	33.8 ± 0.3	$\mathbf{32.9 \pm 0.5}$
Apparel-Kitchen	38.2 ± 0.3	37.0 ± 0.4	$\mathbf{27.5 \pm 0.4}$

Table 1: Classification errors (lower is better, lowest marked in bold) comparing SVM, GRF (see Section 5) in PCA space, and GRF in IGC space. Total $n = 3000$ instances, with total 300 labeled instances ($n_l^s = 200$ and $n_l^t = 100$). The reported errors are on $n_u^t = 1400$ instances, with results averaged over 4 trials.

unlabeled target data (n_u^t), so in all experiments reported below we have at least $1,300$ instances to be labeled.

Experimental Setup: We used cosine similarity[1] (using appropriate A) to set edge weights, followed by k-NN graph sparsification, as described in Section 5. The hyperparameters $k \in \{2, 5, 10, 50, 100, 200, 500, 1000\}$ and the Gaussian kernel bandwidth multiplier[2], $\rho \in \{1, 2, 5, 10, 50, 100\}$, are tuned on a separate development set. The hyperparameter, α (see Eq. (1)) was tuned over the range $[0.1, 1]$, with step size 0.1. The α value which gave the best GRF objective (Eq. (2)) was selected. Please note that this is an automatic parameter selection mechanism requiring no additional held out data. For all graph-based experiments, GRF (see Section 5) is used as the inference algorithm.

Setting The Mahalanobis Matrix A: We consider two methods to set the value of the matrix A. First, instances are projected into a lower dimensional space using Principal Components Analysis (PCA). For all experiments, dimensionality of the projected space was set at 250. We set $A = P^\top P$, where P is the projection matrix generated by PCA. We found the baseline algorithms to perform better in this space than the input d-dimensional space, and hence this is used as the original space. Second, the matrix A is learned by applying IGC (Algorithm 2) (see Section 7) on the PCA projected space (above); with ITML used as MetricLearner in IGC. We use standard implementations of ITML and IGC made available by respective authors.

8.1 Domain Adaptation Results

We experimented with a variety of settings in which we varied the amount of source and target labeled and unlabeled data (ranging from 0 labeled instances to 200 labeled instances). Due to paucity of space we can not describe the details of those experiments here; the interested reader

[1] We experimented with both Gaussian kernels and cosine similarity, and cosine similarity lead to better performance, and we use it in all experiments.

[2] $\sigma = \rho\ \sigma_0$, where ρ is the tuned multiplier, and σ_0 is set to average distance.

is encouraged to refer to the longer version of this paper (Dhillon et al., 2012). The setting that performed the best was the one which used source unlabeled data, 200 source labeled instances, and 100 target labeled instances. So, for this setting, we compared the performance of GRF in IGC space to GRF in PCA space and a Support Vector Machine (SVM) classifier trained over the 300 training instances (200 from the source domain, and 100 from the target domain) using a polynomial kernel whose degree is tuned on a development set.

The results are summarized in Table 1. Clearly, for all domain pairs, GRF in PCA space is either comparable or better than SVM. This may not be surprising since SVM did not use the additional $1,300$ source unlabeled data. Also, as already seen above, GRF in IGC space outperforms both SVM baseline and GRF in PCA space. This demonstrates the benefit of using a learned metric (in this case using IGC) during graph construction for graph-based domain adaptation.

8.2 Comparison with Other Methods

Domain Pairs	TSVM	EasyAdapt	IGC
Electronics-DVDS	40.1 ± 0.2	41.0 ± 0.4	$\mathbf{38.3 \pm 0.3}$
Books-Music	32.7 ± 0.3	33.4 ± 0.3	$\mathbf{31.8 \pm 0.5}$
DVDs-Videos	33.8 ± 0.4	34.9 ± 0.4	$\mathbf{33.0 \pm 0.2}$
Videos-Electronics	29.7 ± 0.2	30.1 ± 0.4	$\mathbf{28.4 \pm 0.3}$
Kitchen-Apparel	33.9 ± 0.3	33.7 ± 0.1	$\mathbf{32.9 \pm 0.5}$

Table 2: Classification errors for IGC comparison with TSVM and EasyAdapt. In all cases, we use $n_l^s = 200$ and $n_l^t = 100$ labeled instances. The reported errors are on $n_u^t = 1400$ instances, results averaged over four trials. Lowest errors are marked in bold.

In previous sections, we have shown the superior performance of IGC over projections learnt using PCA and standard SVM (a state-of-the-art baseline which is also the top performing algorithm in the seminal sentiment classification work of (Pang et al., 2002)). However, a comparison with state-of-the-art semi-supervised learning and domain adaptation approaches was pending. So, in this section we compare the performance of IGC with TSVM (Transductive SVM) – a widely used large margin transductive model which has shown state-of-the-art performance on many text classification tasks (Joachims, 1999) and EasyAdapt (Daume III, 2007) which is a state-of-the-art domain adaptation algorithm. The results are shown in Table 2, where we observe that IGC outperforms TSVM and EasyAdapt.

9 Conclusion

We brought together three active directions of research: domain adaptation, graph-based learning, and metric learning, and made the following contributions: (1) investigated usage of unlabeled data from all domains and limited labeled data from all domains; and (2) employed graph-based non-parametric methods for domain adaptation. We plan to further investigate improved usage of graph-based techniques to adaptation. Here, we considered only two domains at once. We plan to extend these methods for multiple source domains.

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