# deep metric learning

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## pairwise similarity

- human cognitive process involves ability to detect similarities between objects
- objects can be images, text documents, sound, etc...
- use deep learning to estimate pairwise similarity / distance



Snowboarding is a recreational activity and Winter Olympic and Paralympic sport that involves descending a snow-covered slope while standing on a snowboard attached to a rider's feet. Skateboarding is an action sport that involves riding and performing tricks using a skateboard, as well as a recreational activity, an art form, an 

■ entertainment industry job, and a method of transportation.<sup>[1]</sup> Skateboarding has been shaped and influenced by many skateboarders throughout the years. A 2009 report found that the skateboarding market is worth an estimated \$4.8 billion in annual revenue, with 11.08 million active skateboarders in the world.<sup>[2]</sup> In 2016, it was announced that skateboarding will be represented at the 2020 Summer Olympics in Tokyo.<sup>[3]</sup>



- applications
  - information retrieval
  - k-nearest-neighbor classification
  - clustering
  - data visualization

## similarity / metric learning

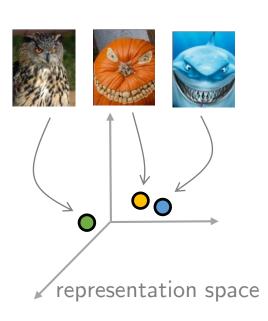
- definition of good similarity measure (metric) is task dependent
- different semantic notion of similarity per task
  - not well captured by hand-crafted representations and standard metrics

solution: learn it from the data

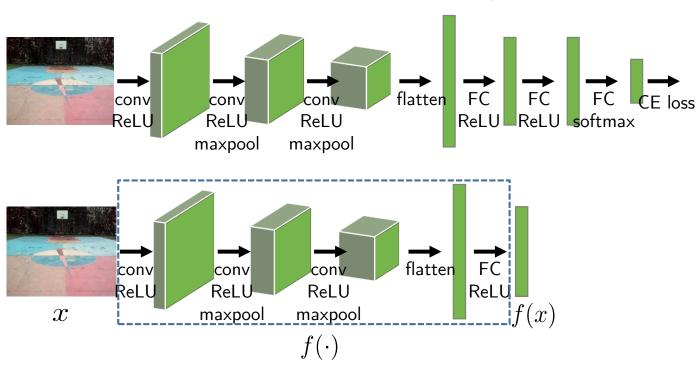


## representation and similarity learning

- lacktriangle space of input examples  ${\mathcal X}$
- learn the representation, use standard similarity measures / metrics
  - embed input examples to a representation (vector) space
  - embedding function  $f: \mathcal{X} \to \mathbb{R}^D$
  - $\mathbf{x} = f(x), x \in \mathcal{X}$
  - learn the representation conditioned on a standard metric
- directly learn the similarity function / metric
  - similarity function  $s: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$
  - involves learning the representation too



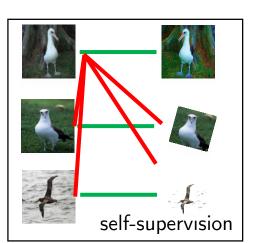
## transfer learning

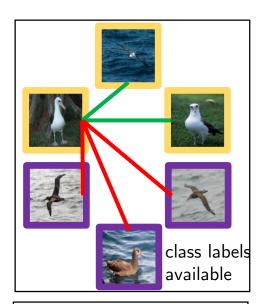


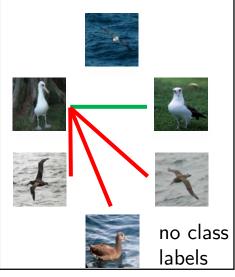
- pre-trained network is given, e.g. trained for classification with cross-entropy loss
- use internal activation vectors as representation
- use existing metrics to estimate pairwise similarity
  - Euclidean distance, cosine similarity, ...

## training data - labels

- pairwise labels of training examples
  - relevant (positive, matching) pair
  - non-relevant (negative, non-matching) pair
- available image-level class labels
  - within (across) class pairs are positive (negative)
- manual annotation of pairs
  - typically very costly
- instance-discrimination
  - each image its own class
  - positives obtained by augmentations







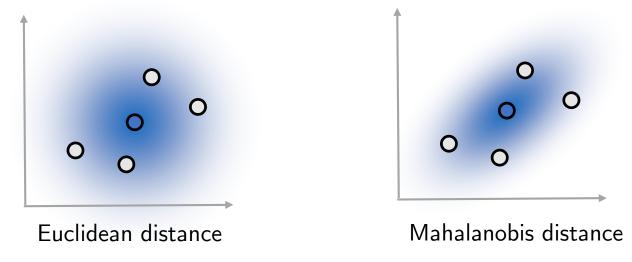
## metric learning: Mahalanobis distance

- learn a parametric distance function from the data
  - input examples are vectors
- example: Mahalanobis distance
  - M is a  $D \times D$  positive semi-definite matrix

• 
$$d_M(\mathbf{x}, \mathbf{z}) = \sqrt{(\mathbf{x} - \mathbf{z})^{\top} M(\mathbf{x} - \mathbf{z})}, \ \mathbf{x}, \mathbf{z} \in \mathbb{R}^D$$

• 
$$d_M(\mathbf{x}, \mathbf{z}) = \sqrt{(\mathbf{x} - \mathbf{z})^\top L^\top L(\mathbf{x} - \mathbf{z})} = \sqrt{(L(\mathbf{x} - \mathbf{z}))^\top L(\mathbf{x} - \mathbf{z})}$$
  
=  $\sqrt{(L\mathbf{x} - L\mathbf{z})^\top (L\mathbf{x} - L\mathbf{z})} = ||L\mathbf{x} - L\mathbf{z}||_2 = ||f(\mathbf{x}) - f(\mathbf{z})||_2$ 

- mapping function  $f(\mathbf{x}) = L\mathbf{x}$
- can be modeled by a single fully-connected layer



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  - mapping function  $f(\mathbf{x}) = L\mathbf{x}$
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- general cases:
  - $f: \mathbb{R}^D \to \mathbb{R}^{D'}$  is a feed-forward network
  - input examples are not vectors,  $f: \mathcal{X} \to \mathbb{R}^{D'}$

### contrastive loss

two branch network; 2 networks that share weights

$$(x_{i}, x_{j}) \in \mathcal{S}$$

$$y_{ij} = 1$$

$$x_{j} \longrightarrow f(\cdot) \longrightarrow f(\cdot)$$

$$\ell(x_i, x_j) = \frac{1}{2} y_{ij} ||\mathbf{x}_i - \mathbf{x}_j||_2^2 + \frac{1}{2} (1 - y_{ij}) [\tau - ||\mathbf{x}_i - \mathbf{x}_j||_2]_+^2$$

#### contrastive loss

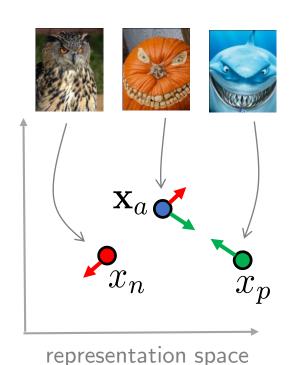
similar pair gradients

$$\frac{\partial \ell}{\partial \mathbf{x}_a} = \mathbf{x}_a - \mathbf{x}_p$$

$$\frac{\partial \ell}{\partial \mathbf{x}_p} = -\frac{\partial \ell}{\partial \mathbf{x}_a}$$

dissimilar pair gradients

$$\frac{\partial \ell}{\partial \mathbf{x}_a} = \frac{\tau - ||\mathbf{x}_a - \mathbf{x}_n||}{||\mathbf{x}_a - \mathbf{x}_n||} (\mathbf{x}_n - \mathbf{x}_a)$$
$$\frac{\partial \ell}{\partial \mathbf{x}_n} = -\frac{\partial \ell}{\partial \mathbf{x}_a}$$



$$\ell(x_i, x_j) = \frac{1}{2} y_{ij} ||\mathbf{x}_i - \mathbf{x}_j||_2^2 + \frac{1}{2} (1 - y_{ij}) [\tau - ||\mathbf{x}_i - \mathbf{x}_j||_2]_+^2$$

## triplet loss

three branch network; 3 networks that share weights

$$(x_{a}, x_{p}) \in \mathcal{S}$$

$$(x_{a}, x_{n}) \in \mathcal{D}$$

$$x_{p} \longrightarrow f(\cdot) \longrightarrow \longrightarrow \ell(x_{a}, x_{p}, x_{n})$$

$$x_{n} \longrightarrow f(\cdot) \longrightarrow \longrightarrow$$

$$\ell(x_a, x_p, x_n) = [||\mathbf{x}_a - \mathbf{x}_p||_2^2 - ||\mathbf{x}_a - \mathbf{x}_n||_2^2 + \alpha]_+$$

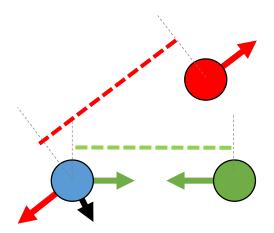
### triplet loss

#### gradients

$$\frac{\partial \ell}{\partial \mathbf{x}_p} = 2(\mathbf{x}_p - \mathbf{x}_a)$$

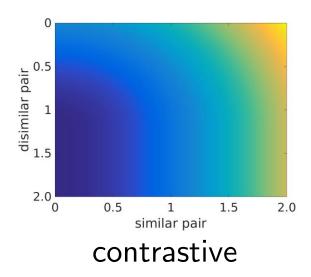
$$\frac{\partial \ell}{\partial \mathbf{x}_n} = 2(\mathbf{x}_a - \mathbf{x}_n)$$

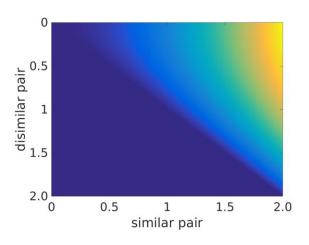
$$\frac{\partial \ell}{\partial \mathbf{x}_a} = 2(\mathbf{x}_a - \mathbf{x}_p) - 2(\mathbf{x}_a - \mathbf{x}_n) = 2(\mathbf{x}_n - \mathbf{x}_p)$$



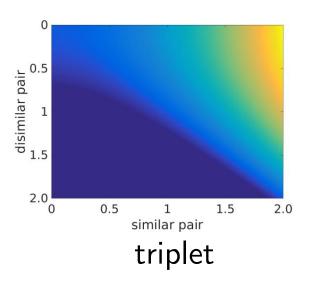
$$\ell(x_a, x_p, x_n) = [||\mathbf{x}_a - \mathbf{x}_p||_2^2 - ||\mathbf{x}_a - \mathbf{x}_n||_2^2 + \alpha]_+$$

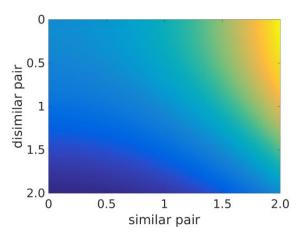
### pairwise losses





 $[\mathbf{x}_a^{\top}\mathbf{x}_n - \mathbf{x}_a^{\top}\mathbf{x}_p]_+$ 





$$\log(1 + e^{\mathbf{x}_a^{\top}\mathbf{x}_n - \mathbf{x}_a^{\top}\mathbf{x}_p}) \text{ [Sohn 2016]}$$

## mini-batches & hard negatives

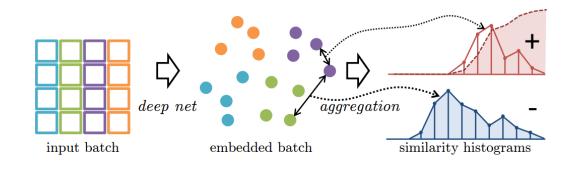
- mini-batch construction [Roth et al., 2020]
  - randomly sample n classes and b/n examples per class
  - greedy approach to maximize covered space
    - next example maximizes the distances to already included examples
  - match training dataset statistics (distribution of pairwise distances)
    - set of random mini-batches: pick to minimize distribution distance
- sampling of negatives matters
  - random sampling: zero loss for most pairs/triplets
  - hard negatives: negative pair, but nearby in the representation space
- online sampling
  - within batch single hardest, semi-hard mining [Schroff et al. 2015], distance-weighted sampling [Wu et al. 2017]
- offline sampling
  - nearest-neighbor search: guaranteed hard negatives in the batch
  - hardness changes: repeat the process during training

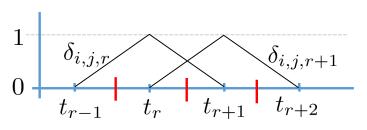
### histogram OSS [Ustinova & Lempitsky, 2016]

minimize probability that similarity of a random negative pair is higher than the similarity of a random positive pair

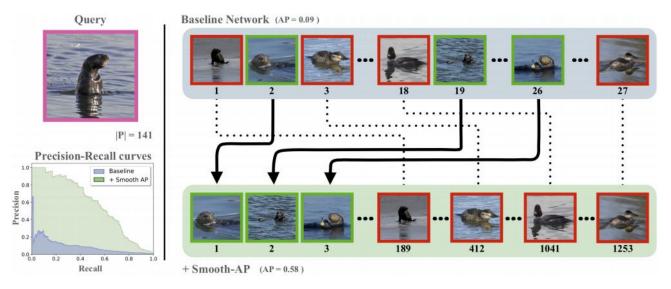
$$\mathbb{E}_{u \sim p^{-}} [\Phi^{+}(u)] = \int_{-1}^{1} p^{-}(u) \Phi^{+}(u) \, \mathrm{d}u = \int_{-1}^{1} p^{-}(u) \left[ \int_{-1}^{u} p^{+}(v) \, \mathrm{d}v \right] \, \mathrm{d}u$$

- approximated by  $\sum_{r=1}^{R} \left( h_r^- \sum_{q=1}^{r} h_q^+ \right) = \sum_{r=1}^{R} \left( h_r^- \phi_q^+ \right)$
- histogram for positive pairs:  $h_r^+ = \frac{1}{|\mathcal{P}^+|}$  $(i,j):(x_i,x_j)\in\mathcal{P}^+$
- equivalently for the negative pairs





### smooth AP loss



Average-Precision (AP) is a common retrieval metric

$$\begin{split} \mathsf{AP}_q &= \frac{1}{|\mathcal{S}_P|} \sum_{i \in \mathcal{S}_P} \mathsf{precision@ranking}_i \\ &= \frac{1}{|\mathcal{S}_P|} \sum_{i \in \mathcal{S}_P} \frac{\# \mathsf{positives-up-to-ranking}_i}{\mathsf{ranking}_i} \\ &= \frac{1}{|\mathcal{S}_P|} \sum_{i \in \mathcal{S}_P} \frac{\mathcal{R}(i, \mathcal{S}_P)}{\mathcal{R}(i, \mathcal{S}_\Omega)} \end{split}$$

- AP is not differentiable
- optimize a smooth approximation instead [Brown et al. 2020]

### smooth AP loss

rewrite AP as

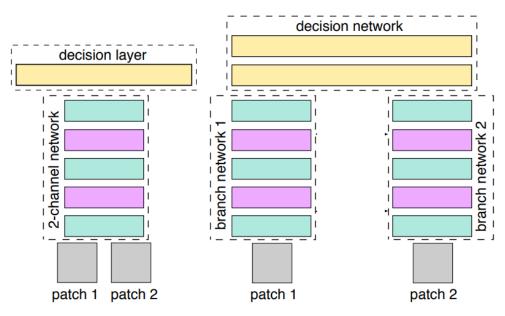
$$AP_{q} = \frac{1}{|\mathcal{S}_{P}|} \sum_{i \in \mathcal{S}_{P}} \frac{1 + \sum_{j \in \mathcal{S}_{P}, j \neq i} \mathbb{1}\{D_{ij} > 0\}}{1 + \sum_{j \in \mathcal{S}_{P}, j \neq i} \mathbb{1}\{D_{ij} > 0\} + \sum_{j \in \mathcal{S}_{N}, j \neq i} \mathbb{1}\{D_{ij} > 0\}}$$

replace the indicator function with sigmoid

$$AP_{q} = \frac{1}{|\mathcal{S}_{P}|} \sum_{i \in \mathcal{S}_{P}} \frac{1}{1 + \sum_{j \in \mathcal{S}_{P}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{P}, j \neq i} G(D_{ij}) + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_{j \in \mathcal{S}_{N}, j \neq i} G(D_{ij})} \frac{1}{1 + \sum_$$

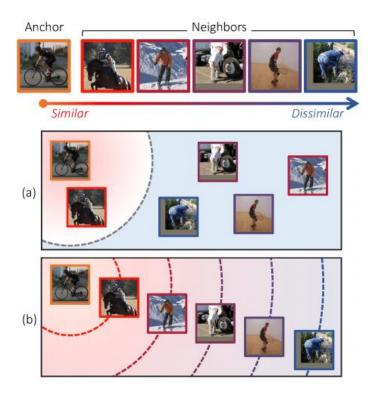
## similarity function learning

- learn similarity function  $s: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$
- input is an example pair
- higher cost for inference



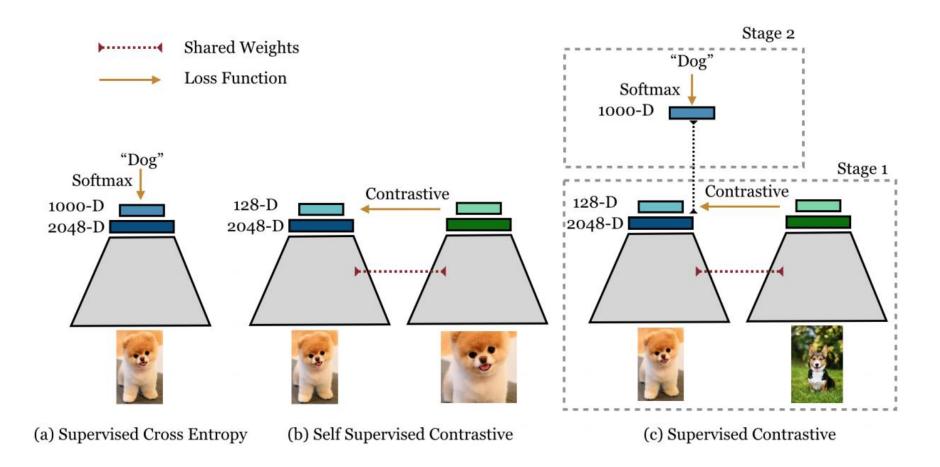
[Zagoruyko & Komodakis, 2015]

## beyond binary supervision



$$\ell(x_a,x_i,x_j,y_a,y_i,y_j) = \left(\log\frac{||\mathbf{x}_a-\mathbf{x}_i||_2}{||\mathbf{x}_a-\mathbf{x}_j||_2} - \log\frac{D(y_a,y_i)}{D(y_a,y_j)}\right)^2$$
 distance ratio distance ratio representation space label space

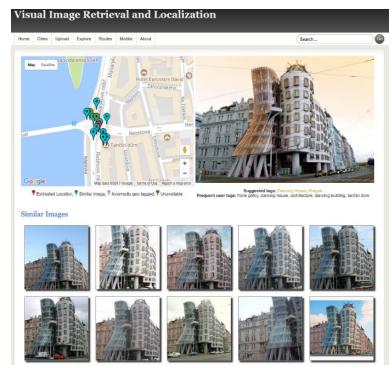
## self-supervised representation learning



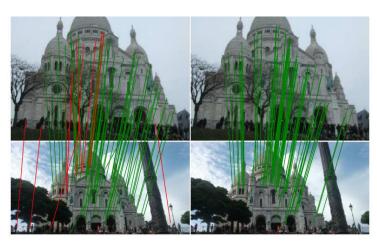
## applications



visual search



visual localization

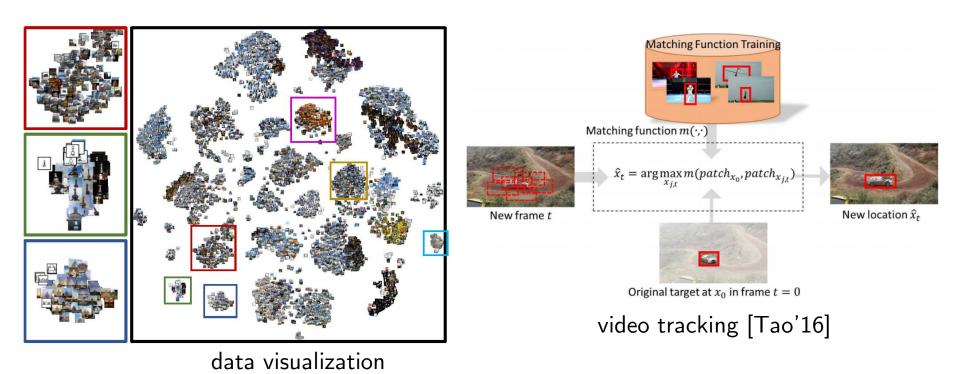


local descriptors [Mishkin'16]



image classification [Song'16]

## applications





data exploration [Johnson et al.'17]