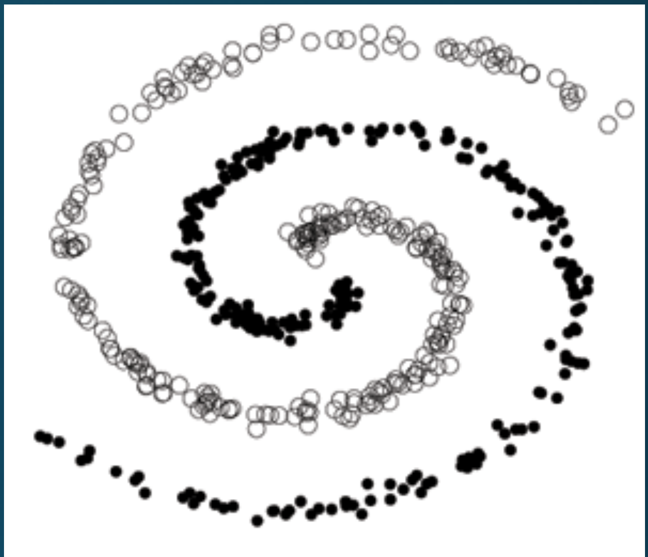
CSCI 4360/6360 Data Science II

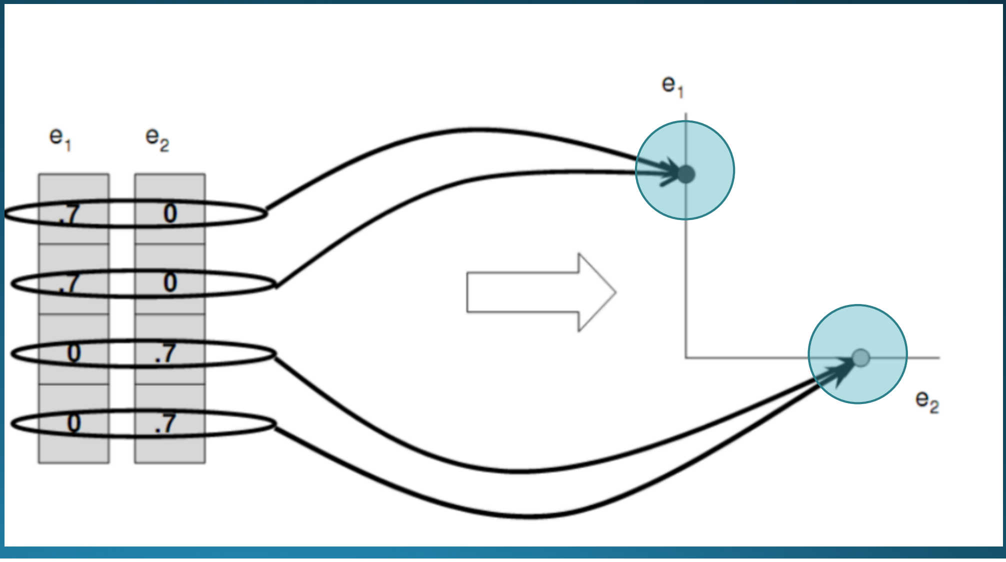
Metric Learning

Previously…

- Spectral clustering

1. Define graph (affinities -> Laplacian)
2. Compute eigenvectors (*embedding*)
3. Cluster embeddings trivially (K-means)



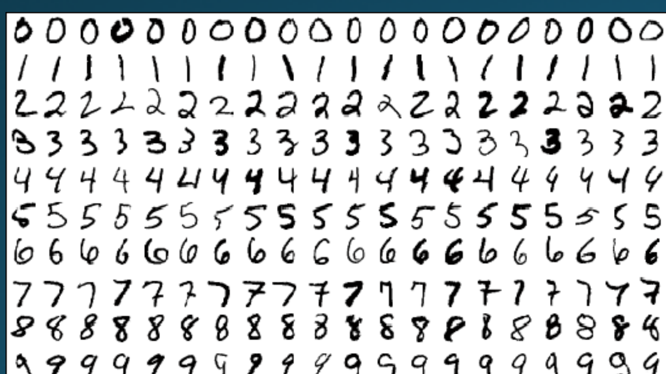


Embeddings

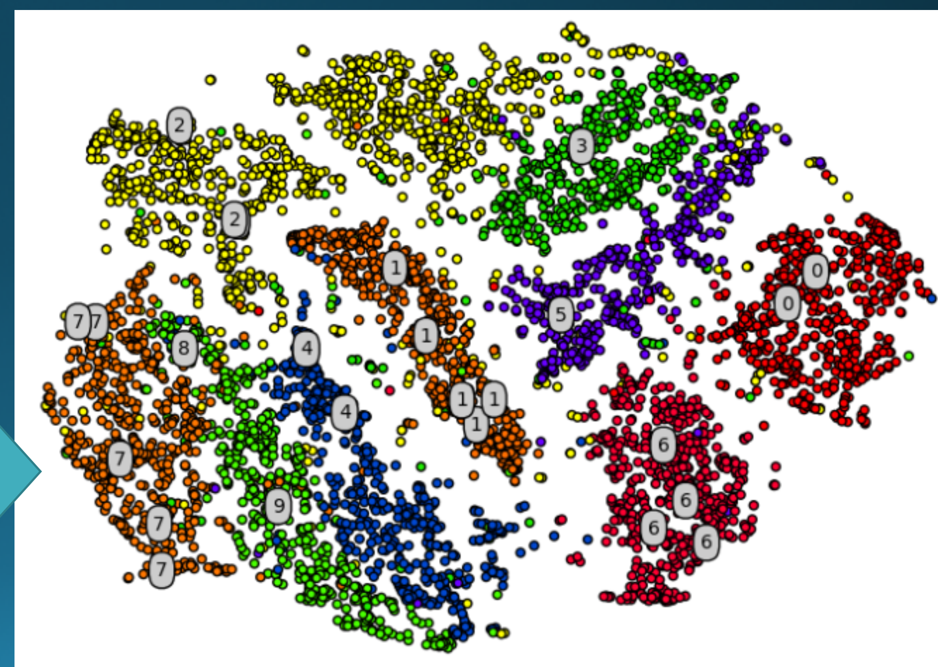
- What is an *embedding*?

$$f : X \to Y$$

- **Mapping**
- **Transformation**
- **Reveals / preserves “structure”**



Embedding



Embeddings

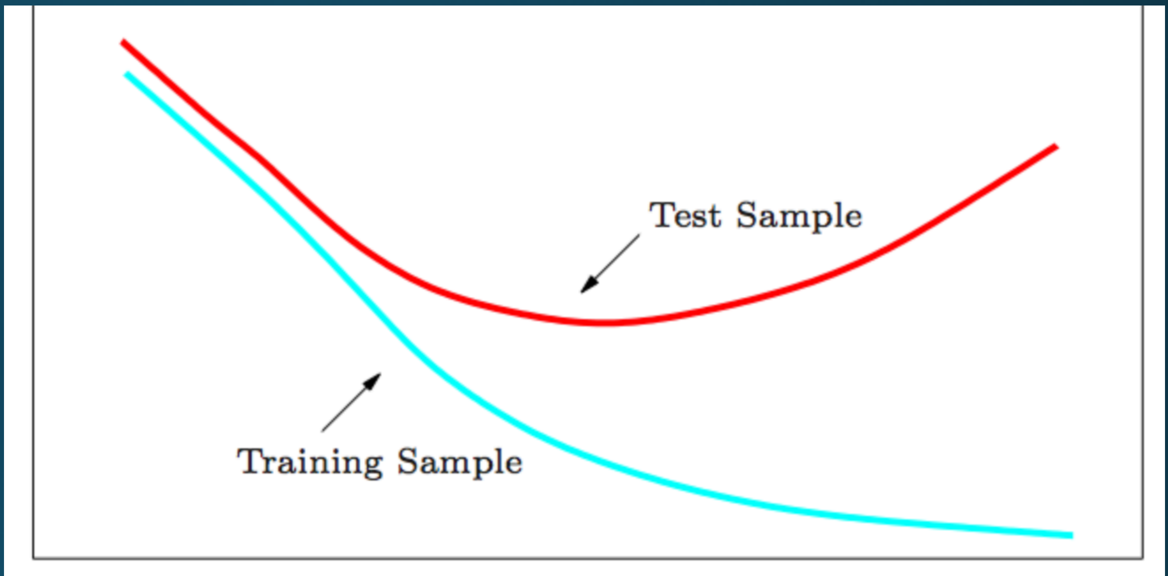
- Principal Components Analysis (PCA)
  - **Sparse & Kernel PCA (Thursday!)**
- Independent Components Analysis (ICA)
- Non-negative Matrix Factorization (NMF)
- Locally-linear Embeddings (LLE)
- **Dictionary Learning (next Thursday!)**

Million Dollar Question:

How do you know the embedding is **right?**

Embeddings

- If you're performing **classification**, it's pretty easy to know if your embedding is "right"



- Error decreases?
- Error increases?

- What about **unsupervised learning?**

Assumptions

- Choice of embedding -> Assumptions about the data
- **What if we knew something about the data?**
- **“Side information”:** we don’t know what classes/clusters the data belong to, but we do have some notion of similarity

Side Information

- Define a set *S*
  - for every pair x_i and x_j that are similar, we put this pair in *S*
- "Similar" is user-defined; can mean anything
- Likewise have a set *D*
  - for every pair x_i and x_j that are **dis**similar, we put this pair in *D*
  - can consist of every pair not in *S*, or specific pairs if information is available

- We have this similarity information; what can we do with it?

Distance Metrics

- Goal: use side-information to **learn a new distance metric**
- Encode our side-information in a "metric" *A*
- Generalization of Euclidean distance
  - Note when $A = I$, this is regular Euclidean distance
  - When *A* is diagonal, this is a "weighted" Euclidean distance
  - When data are put through nonlinear basis functions ϕ, nonlinear metrics can be learned

$$d(\vec{x}, \vec{y}) = d_A(\vec{x}, \vec{y})$$

$$= ||\vec{x} - \vec{y}||_A$$

$$= \sqrt{(\vec{x} - \vec{y})^T A (\vec{x} - \vec{y})}$$

$$= \sqrt{(\phi(\vec{x}) - \phi(\vec{y}))^T A (\phi(\vec{x}) - \phi(\vec{y}))}$$

Distance Metrics

- Quick Review: **What constitutes a *valid distance metric?***

1: Non-negativity $d(\vec{x}, \vec{y}) \geq 0$

2: Symmetry $d(\vec{x}, \vec{y}) = d(\vec{y}, \vec{x})$

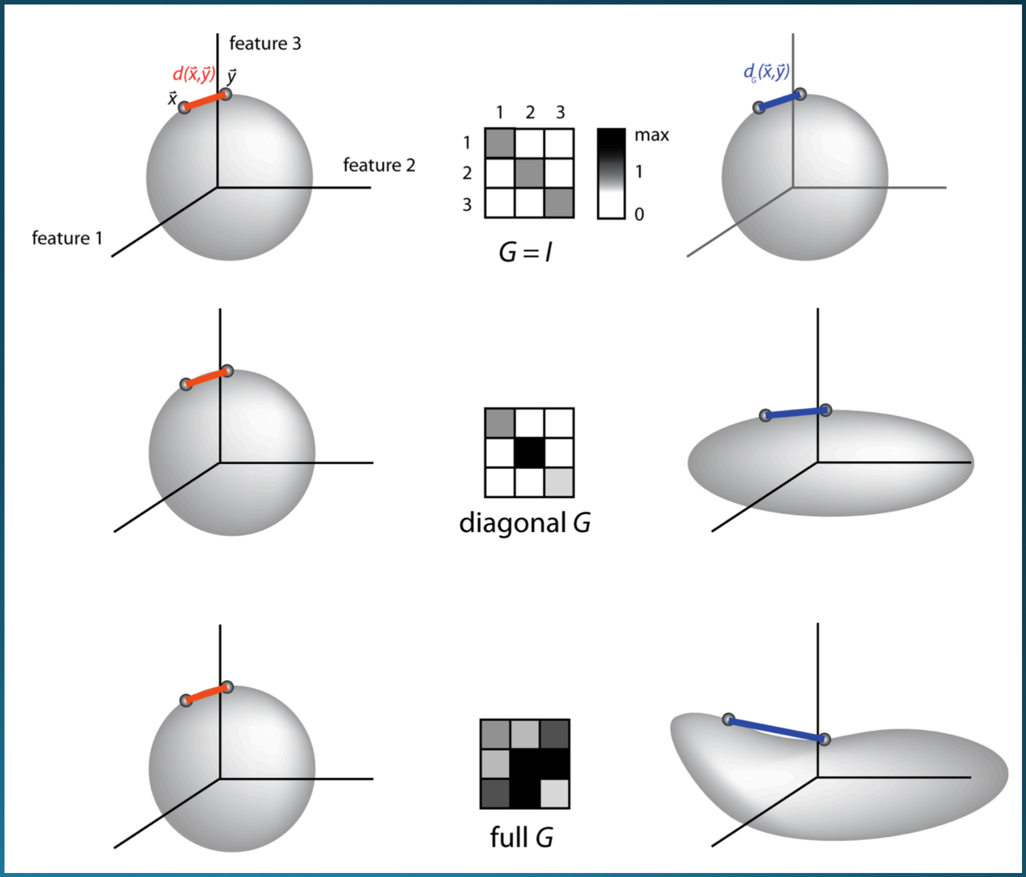
3: Triangle Inequality $d(\vec{x}, \vec{z}) \leq d(\vec{x}, \vec{y}) + d(\vec{y}, \vec{z})$

~~4: Identity of indiscernibles~~ $\cancel{d(\vec{x}, \vec{y}) = 0 \Leftrightarrow x = y}$

"Pseudometric"

Form of a Metric

- Learning metric *A* (*G* in figure) also equivalent to replacing each point *x* with $A^{1/2}x$ and using standard Euclidean distance
- **It's an embedding!**
- Learning a **space** inhabited by your data
  - Bonus: easy to incorporate new data! (unlike LLE or others)



Learning a Metric (1)

- Goal: Define a metric *A* that respects constraint sets *S* and *D*
- Simple enough: constrain all pairs in *S* to have small distances
- Is that all?
- **Nope – trivially solved with *A* = *0***

$$\min_{A} \sum_{\vec{x},\vec{y} \in S} ||\vec{x} - \vec{y}||_A^2$$

Learning a Metric (2)

- Additional constraint: use pairs in *D* to guarantee non-zero distances
- (choice of 1 is arbitrary; any other constant *c* would have the effect of replacing *A* with c^2A)
- Is that all?

- **Nope – need to ensure *A* is positive semi-definite (why?)**

$$\sum_{\vec{x},\vec{y}\in D} ||\vec{x}-\vec{y}||_A \geq 1$$

Aside!

- We used squared Euclidean distance in the first constraint

$$\min_A \sum_{\vec{x},\vec{y} \in S} ||\vec{x} - \vec{y}||_A^2$$

- But not in the second! Why?

$$\sum_{\vec{x},\vec{y} \in D} ||\vec{x} - \vec{y}||_A \geq 1$$

- Squared distance in 2^{nd} constraint would always result in **rank-1 *A***, i.e. the data would always be projected on a line
- (proof left as an exercise!)

Learning a Metric (3)

- A third constraint: keep *A* positive semi-definite
  - (this means the diagonal is always ≥ 0)
- If *A* is PSD, its eigenvectors and eigenvalues exist and are real
- Set any negative eigenvalues to 0
- Compute A'

$$A \succeq 0$$

$$A = X \Lambda X^T$$

$$\Lambda' = \mathrm{diag}(\max\{0, \lambda_1\}, ..., \{0, \lambda_n\})$$
$$A' = X \Lambda' X^T$$

Learning a Metric

- We have our constraints!
- How do we learn *A*?
- *(Hint)* Linear in parameters of *A*
- *(HINT)* First two constraints are verifiably convex

$$\min_{A} \sum_{\vec{x},\vec{y} \in S} ||\vec{x} - \vec{y}||_A^2$$

$$\sum_{\vec{x},\vec{y} \in D} ||\vec{x} - \vec{y}||_A \geq 1$$

$$A \succeq 0$$

Convex Optimization

- For diagonal *A*, this is easy

$$g(A) = g(A_{11}, \ldots, A_{nn}) = \sum_{(x_i, x_j) \in \mathcal{S}} ||x_i - x_j||_A^2 - \log \left(\sum_{(x_i, x_j) \in \mathcal{D}} ||x_i - x_j||_A \right)$$

- (just a fancy reformulation of the original constraints)
- Minimizing *g* is equivalent to solving original problem, up to multiplication of *A* by a positive constant

- **Gradient descent!** (step-size intrinsically enforces PSD of *A*)

Convex Optimization

- Trickier for full *A*
- Gradient ascent + iterative projections
- For this to work, constraints needed to be reversed

Iterate

  Iterate

    $A := \arg\min_{A'} \{||A' - A||_F : A' \in C_1\}$

    $A := \arg\min_{A'} \{||A' - A||_F : A' \in C_2\}$

  until A converges

  $A := A + \alpha(\nabla_A g(A))_{\perp \nabla_A f}$

until convergence

Constraint Reformulation

Previous

Current

$$\min_{A} \sum_{\vec{x},\vec{y}\in S} ||\vec{x}-\vec{y}||_A^2 \Rightarrow \sum_{\vec{x},\vec{y}\in S} ||\vec{x}-\vec{y}||_A^2 \leq 1$$

C_1

$$\sum_{\vec{x},\vec{y}\in D} ||\vec{x}-\vec{y}||_A \geq 1 \Rightarrow \max_{A} \sum_{\vec{x},\vec{y}\in D} ||\vec{x}-\vec{y}||_A$$

$g(A)$

$$A \succeq 0 \Rightarrow A \succeq 0$$

C_2

GA + IP

Iterate

Iterate

$A := \arg\min_{A'}\{||A' - A||_F : A' \in C_1\}$

$A := \arg\min_{A'}\{||A' - A||_F : A' \in C_2\}$

until A converges

$A := A + \alpha(\nabla_A g(A))_{\perp \nabla_A f}$

until convergence

Iterate

Iterate

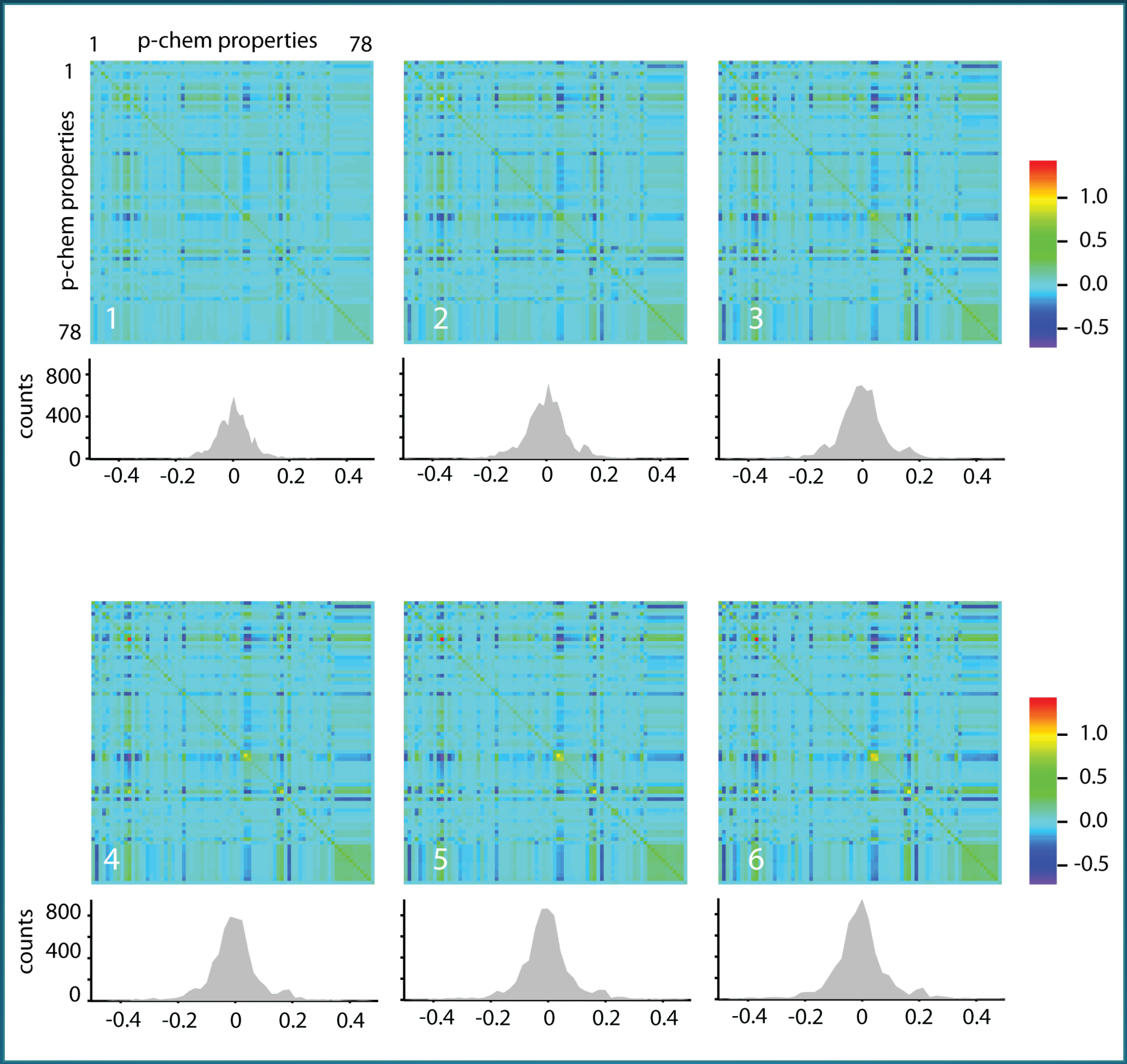
$$\sum_{\vec{x},\vec{y} \in S} ||\vec{x} - \vec{y}||_A^2 \leq 1 \quad + \quad A \succeq 0$$

until A converges

$$A := A + \alpha \nabla \max_A \sum_{\vec{x},\vec{y} \in D} ||\vec{x} - \vec{y}||_A$$

until convergence

GA + IP



1
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p-chem properties
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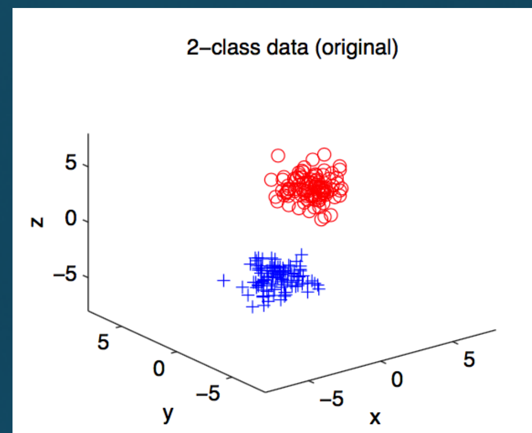
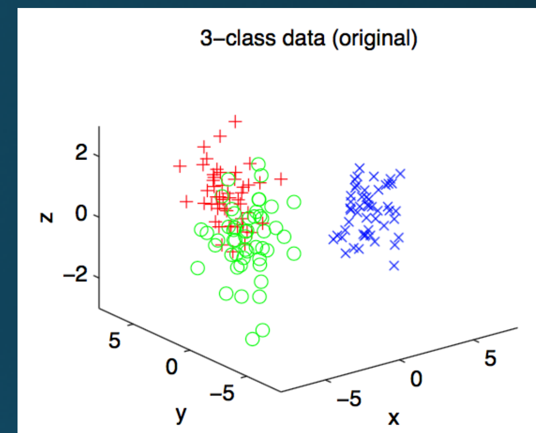
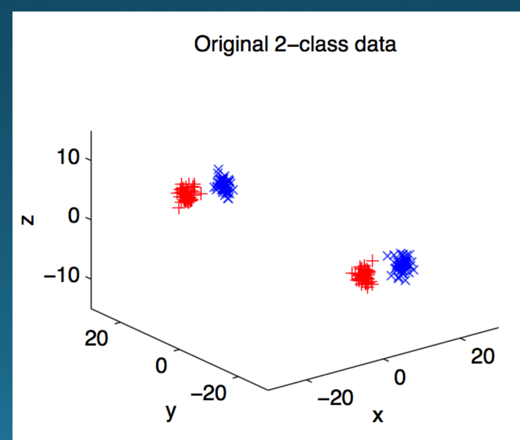
-0.4
-0.2
0
0.2
0.4
1.0
0.5
0.0
-0.5

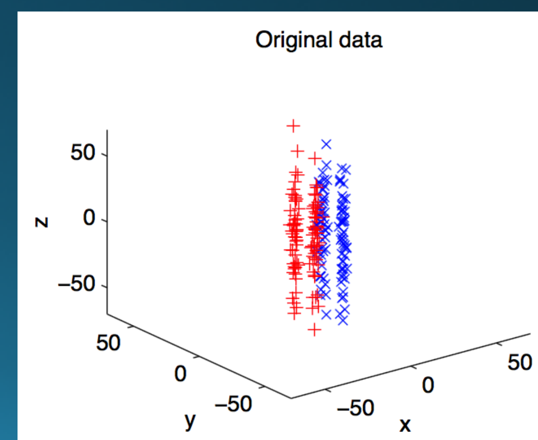
Experiments

- Generated artificial 3D data
  - 2 class
  - 3 class
  - Separated by y-axis
  - Separated by z-axis

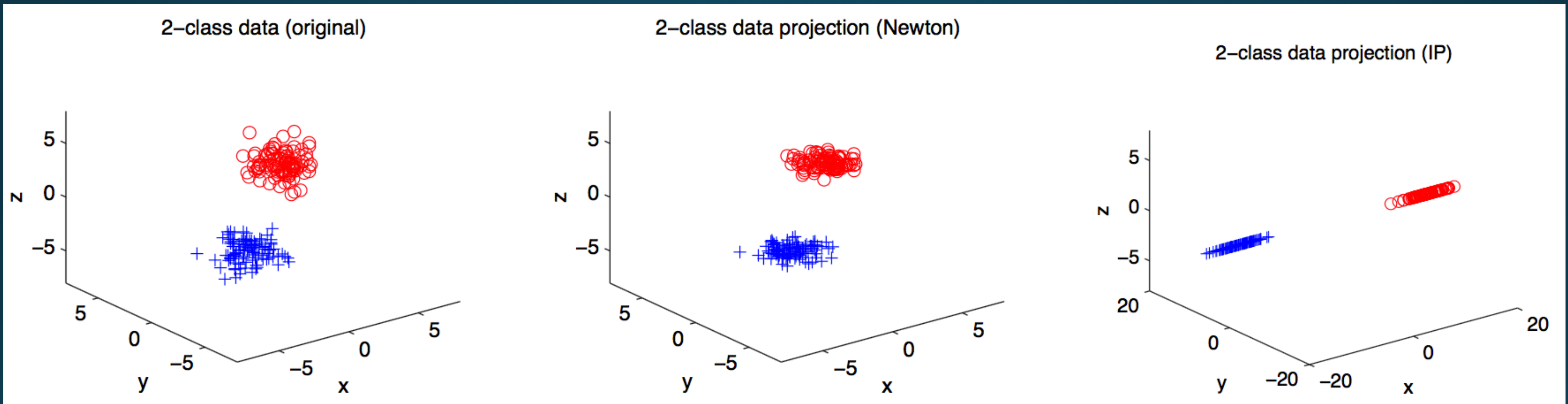




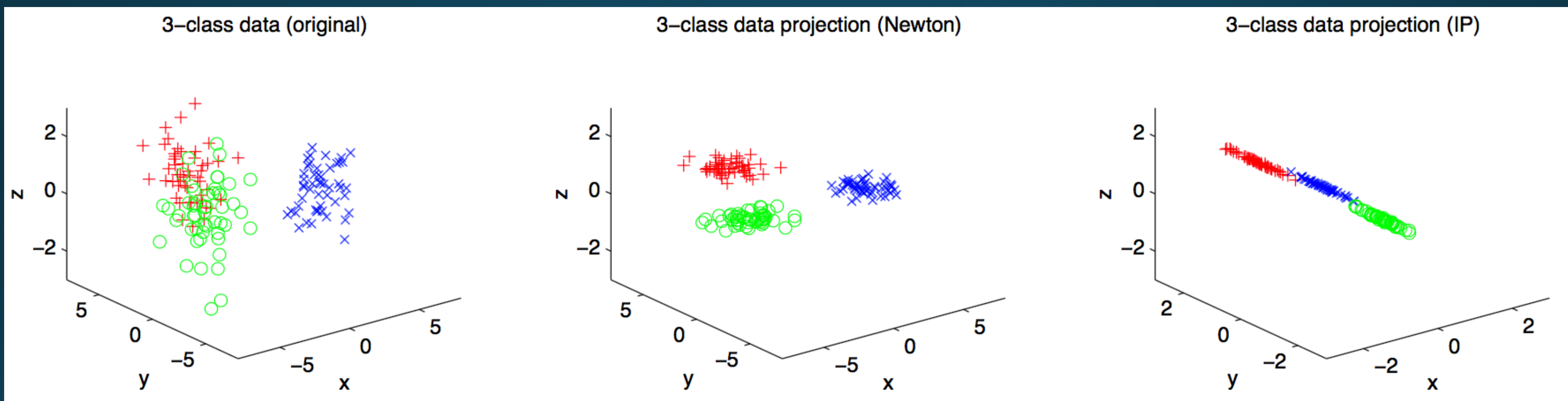




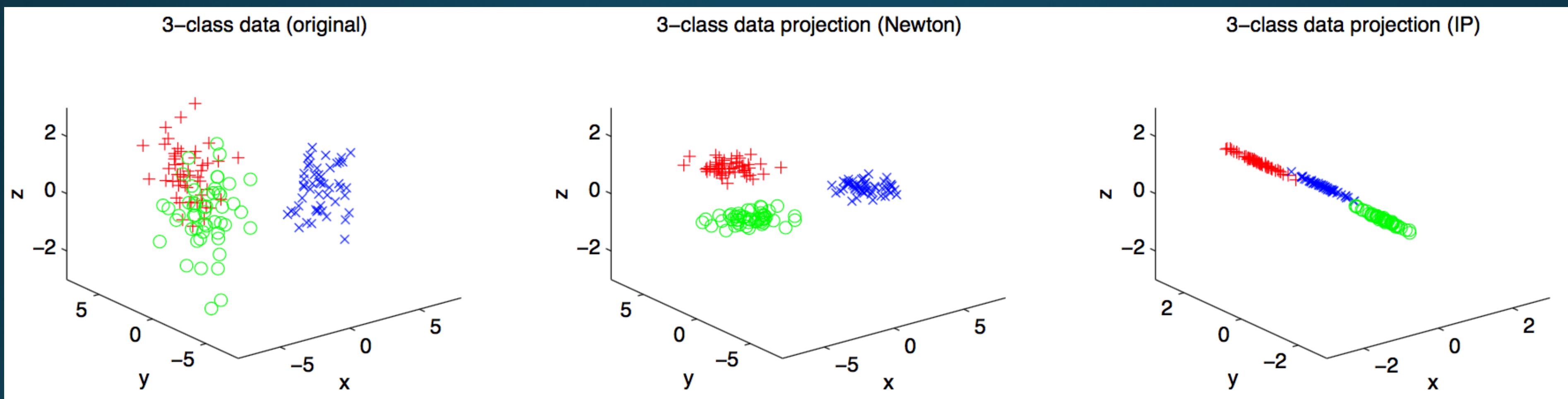
Experiments



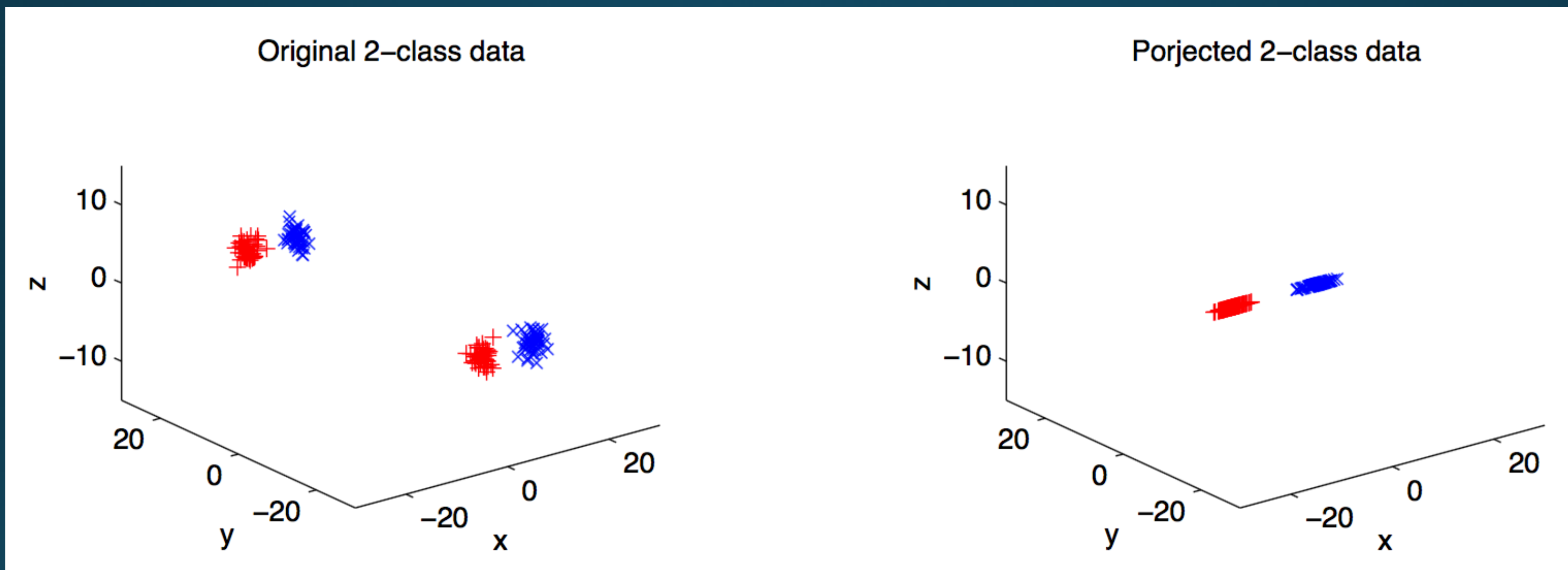
Experiments



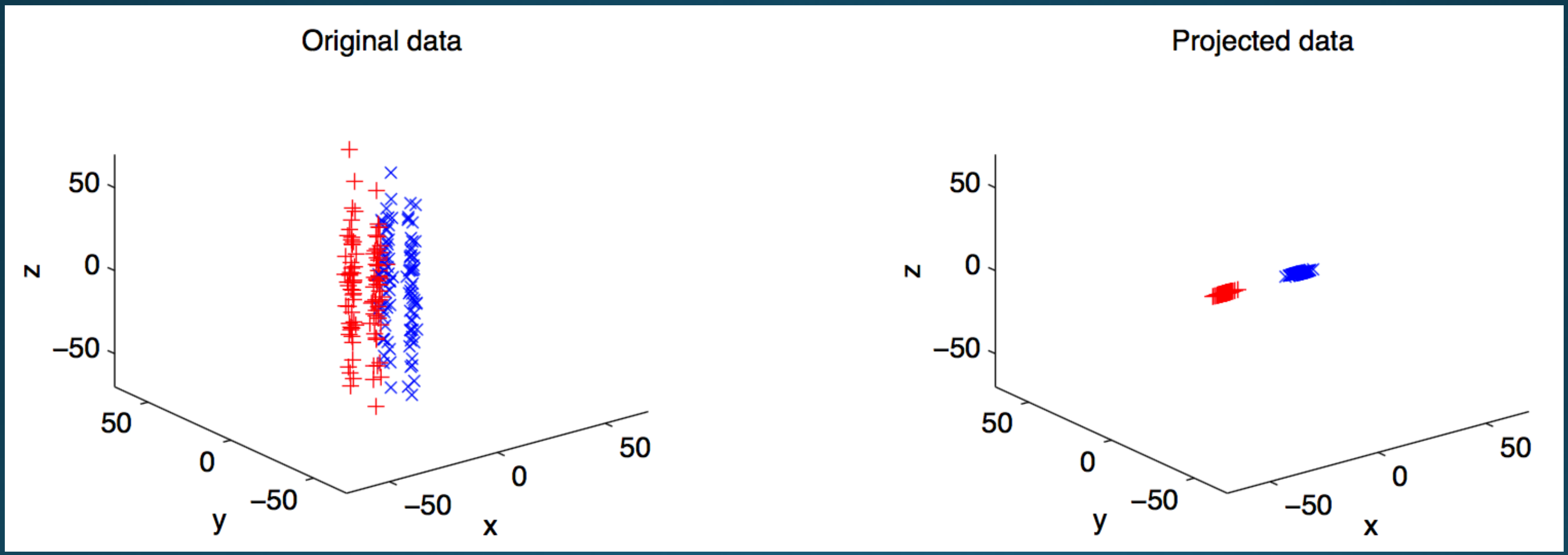
Experiments



Experiments

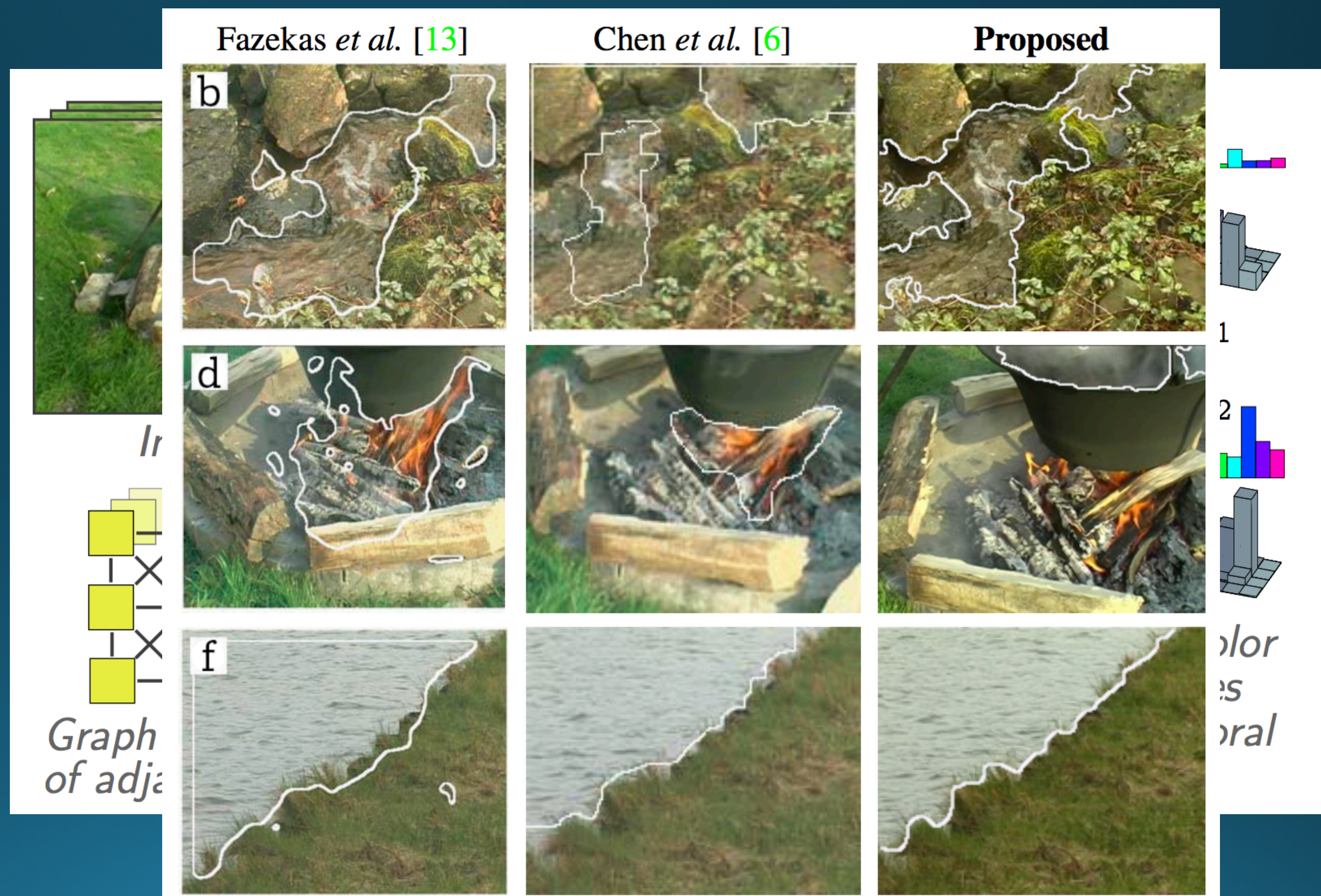


Experiments



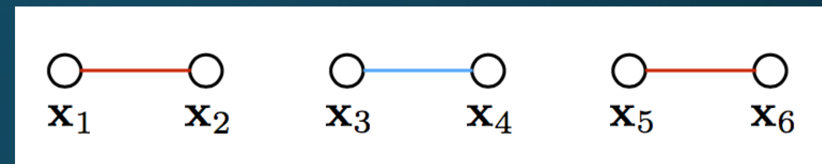
Other Applications

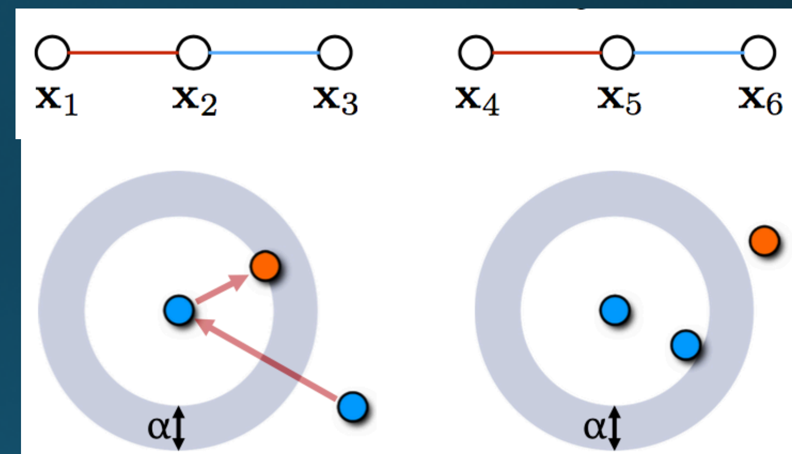
- Video scene segmentation
- Identifying dynamic textures in videos



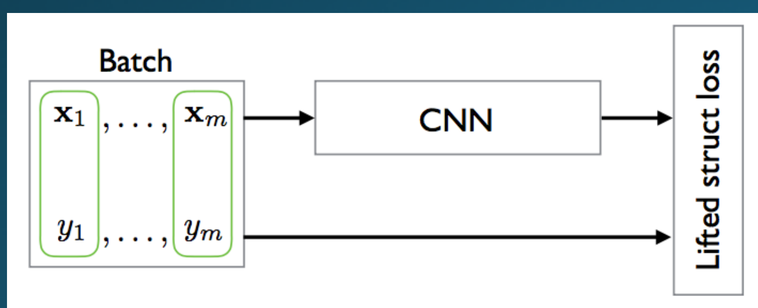
Other Formulations

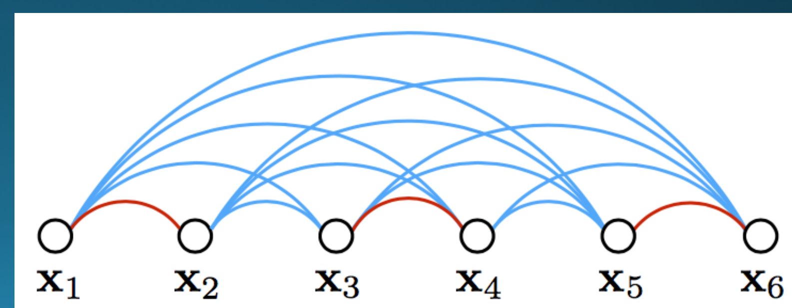
- Deep metric learning
- Differentiates different metric constraints
  - Contrastive
  - Triplet
  - Lifted structure





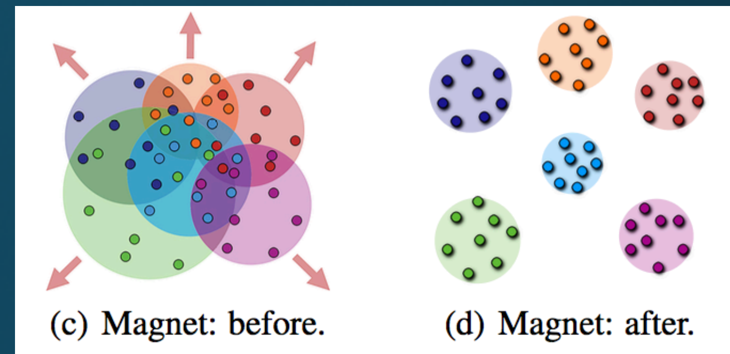
(a) Triplet: before. (b) Triplet: after.

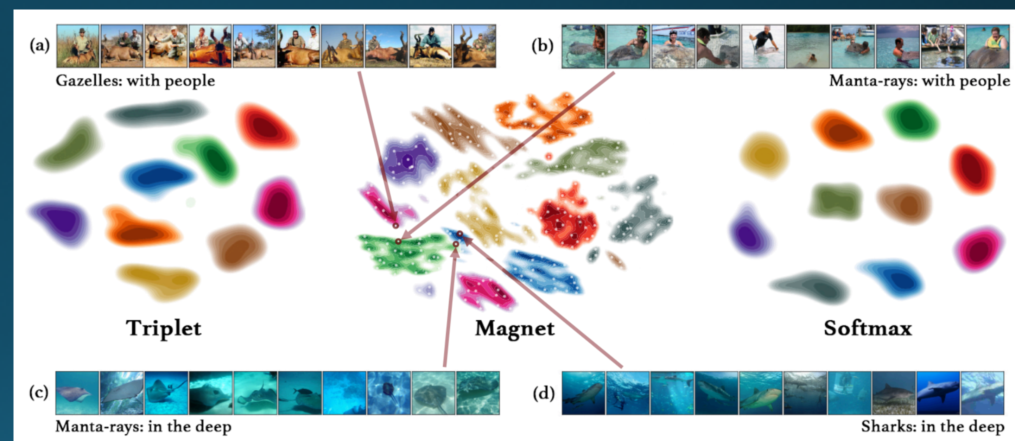


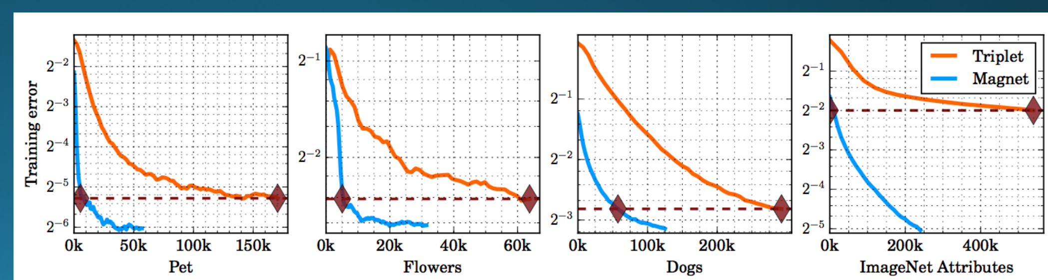


Other Formulations

- Adaptive densities
- Introduces “magnet loss” *(how does it work?)*
  - Optimizes over entire neighborhoods simultaneously
  - Reduces distribution overlap, rather than just pairs or triplets
- Requires ground-truth labels







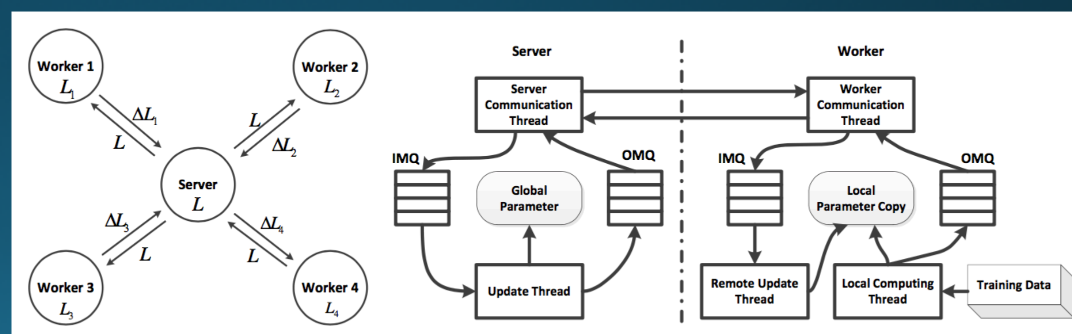
Other Formulations

$$
\begin{aligned}
\min_L \quad & \sum_{(x,y)\in\mathcal{S}} \|L(x-y)\|^2 \\
s.t. \quad & \|L(x-y)\|^2 \geq 1, \forall (x,y) \in \mathcal{D}
\end{aligned}
$$

$$
\begin{aligned}
\min_L \quad & \sum_{(x,y)\in\mathcal{S}} \|L(x-y)\|^2 + \lambda \sum_{(x,y)\in\mathcal{D}} \xi_{x,y} \\
s.t. \quad & \|L(x-y)\|^2 \geq 1 - \xi_{x,y}, \xi_{x,y} \geq 0, \forall (x,y) \in \mathcal{D}
\end{aligned}
$$

$$
\min_L \sum_{(x,y)\in\mathcal{S}} \|L(x-y)\|^2 + \lambda \sum_{(x,y)\in\mathcal{D}} \max(0, 1 - \|L(x-y)\|^2)
$$

- Large-scale metric learning
  - If feature space is extremely large, iterative eigen-decompositions are a deal-breaker
  - Nested convex optimization is a deal-breaker
- Represent metric $A = L^T L$
  - Learn L directly, instead of A
- Use hinge loss to induce unconstrained optimization
- Parameter server for SGD-based metric updates



Questions?

Updates

- Assignment 2 is being examined
  - Some grade changes already made (re: effects of regularization by imposing Gaussian prior on weights); check eLC
- Final project proposals due **Thursday**
  - 1-2 pages, **max**
  - Clear, cogent, concise: tell me **exactly** what you're planning to do, and **exactly** how you'll measure success/failure
  - Students in 6360: Make sure you're also identifying potential submission venues
- How is Assignment 4 going?

References

- Xing, Eric P., Michael I. Jordan, Stuart J. Russell, and Andrew Y. Ng. "Distance metric learning with application to clustering with side-information" http://papers.nips.cc/paper/2164-distance-metric-learning-with-application-to-clustering-with-side-information.pdf
- Teney, Damien, Matthew Brown, Dmitry Kit, and Peter Hall. "Learning similarity metrics for dynamic scene segmentation" http://www.cv-foundation.org/openaccess/content_cvpr_2015/papers/Teney_Learning_Similarity_Metrics_2015_CVPR_paper.pdf
- Oh Song, Hyun, Yu Xiang, Stefanie Jegelka, and Silvio Savarese. "Deep metric learning via lifted structured feature embedding" http://www.cv-foundation.org/openaccess/content_cvpr_2016/papers/Song_Deep_Metric_Learning_CVPR_2016_paper.pdf