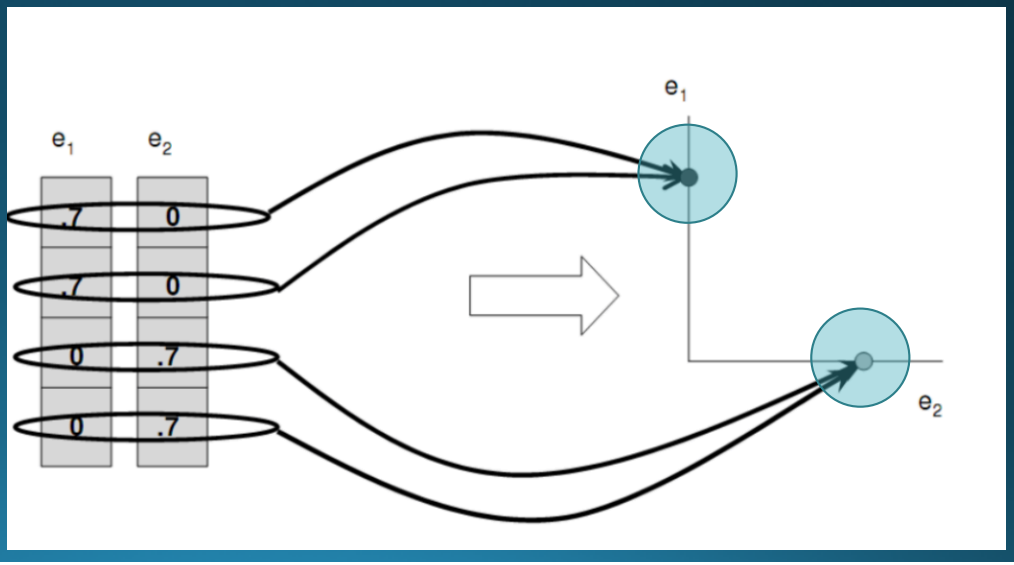
CSCI 4360/6360 Data Science II

Metric Learning

Previously…

- Spectral clustering

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

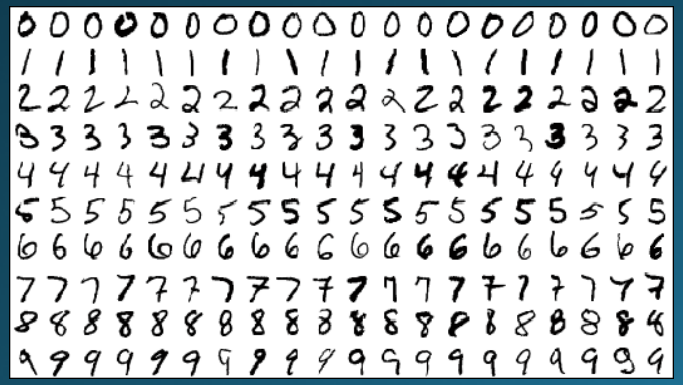


Embeddings

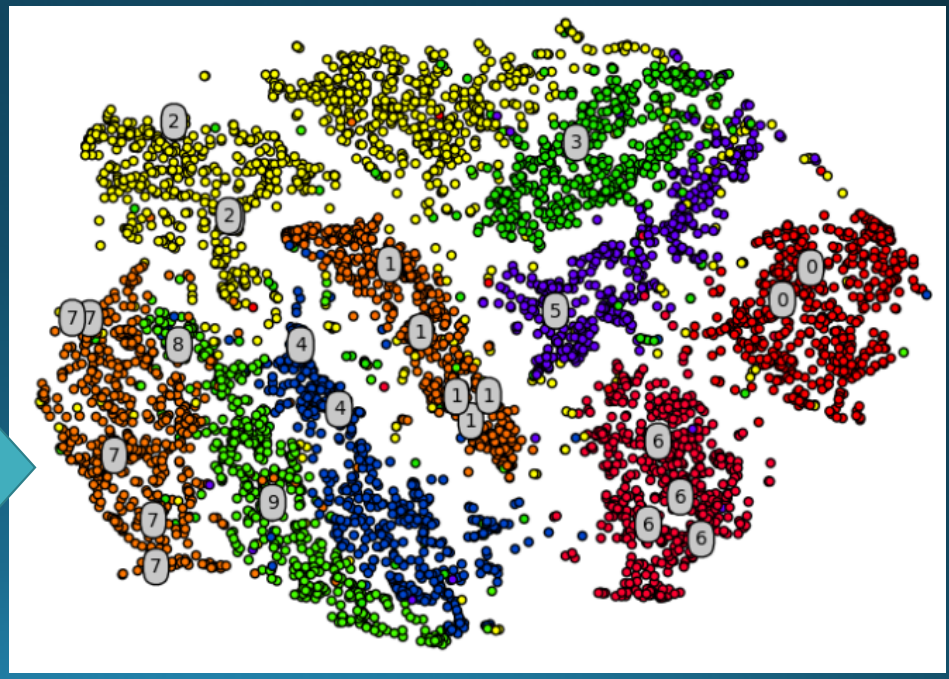
- What is an *embedding*?

$$f : X \rightarrow Y$$

- **Mapping**
- **Transformation**
- **Reveals / preserves "structure"**



Embedding



Embeddings

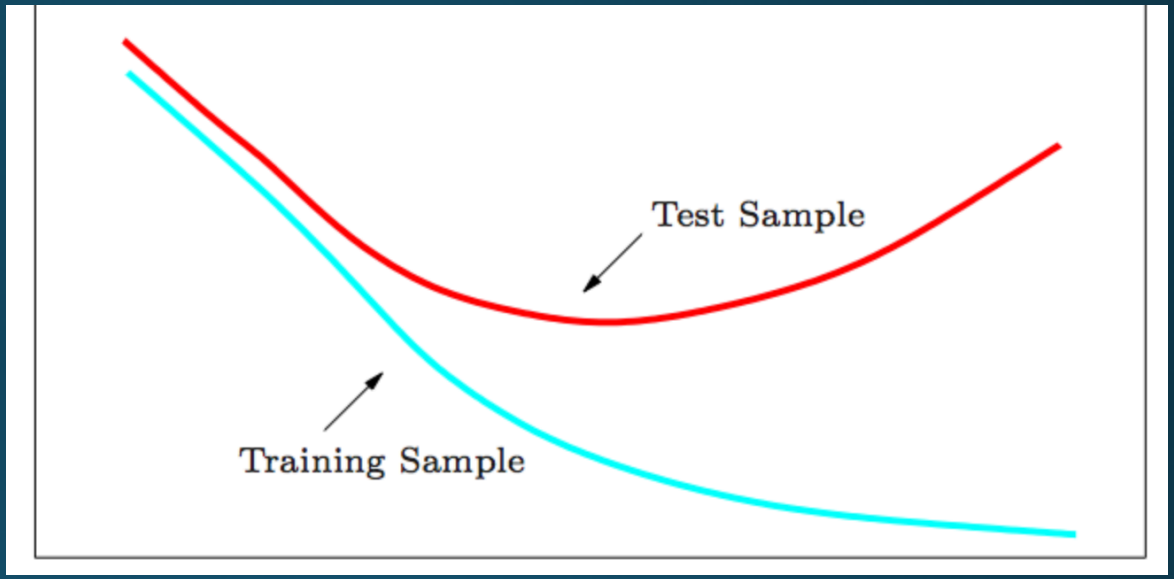
- Principal Components Analysis (PCA)
  - **Sparse & Kernel PCA (Thursday!)**
- Independent Components Analysis (ICA)
- Non-negative Matrix Factorization (NMF)
- Locally-linear Embeddings (LLE)
- **Dictionary Learning (SOON!)**

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

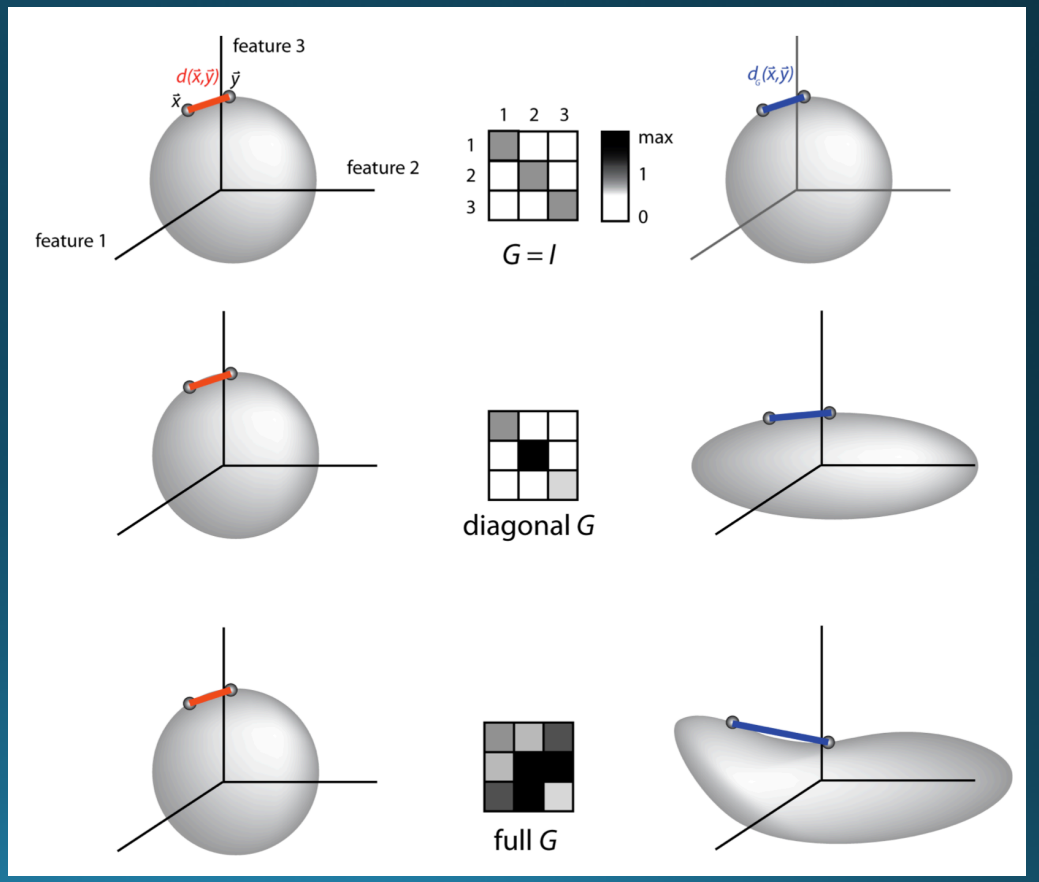
3: Triangle Inequality $d(\vec{x}, \vec{z}) \leq d(\vec{x}, \vec{y}) + d(\vec{y}, \vec{z})$

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

"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?

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

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

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 2nd 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′*

$$A \succeq 0$$

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

$$\Lambda' = \text{diag}(\max\{0, \lambda_1\}, ..., \{0, \lambda_n\})$$

$$A' = X \Lambda' X^T$$

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"

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

- (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

- Less "easy" 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

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

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

$$A \succeq 0$$

Current

$$\sum_{\vec{x},\vec{y}\in S} ||\vec{x}-\vec{y}||_A^2 \leq 1 \quad C_1$$

$$\max_A \sum_{\vec{x},\vec{y}\in D} ||\vec{x}-\vec{y}||_A \quad g(A)$$

$$A \succeq 0 \quad C_2$$

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

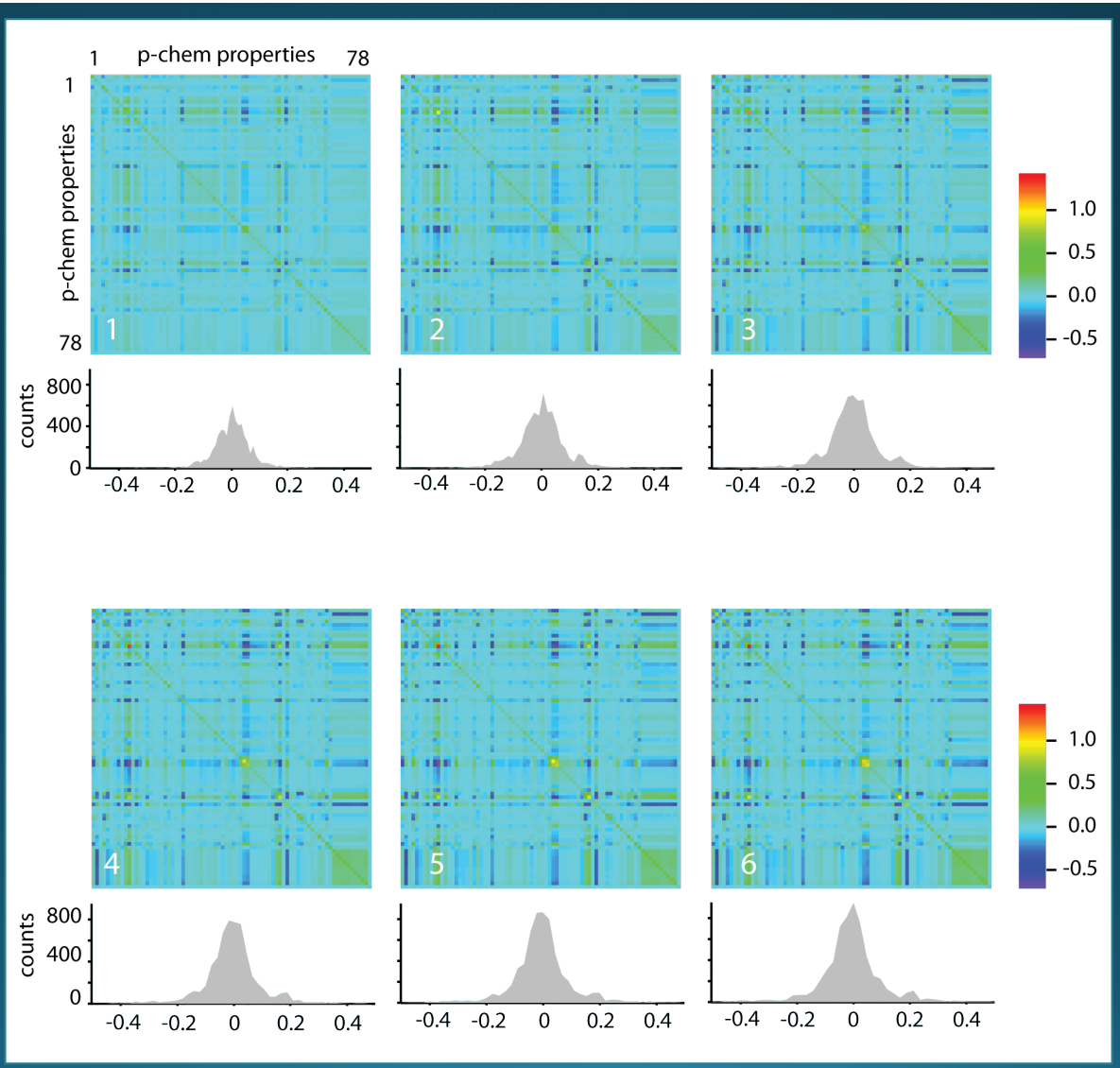
$$\sum_{\vec{x},\vec{y} \in S} ||\vec{x} - \vec{y}||_A^2 \leq 1$$  $$A \succeq 0$$

  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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p-chem properties
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6
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-0.5
counts
800
400
0
-0.4
-0.2
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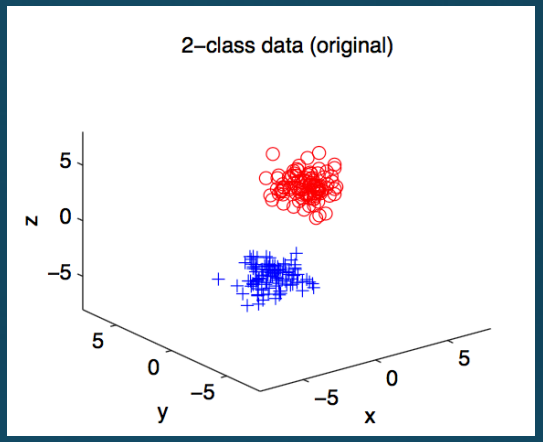
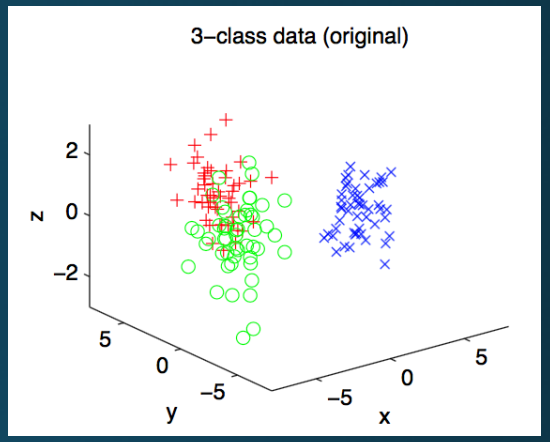
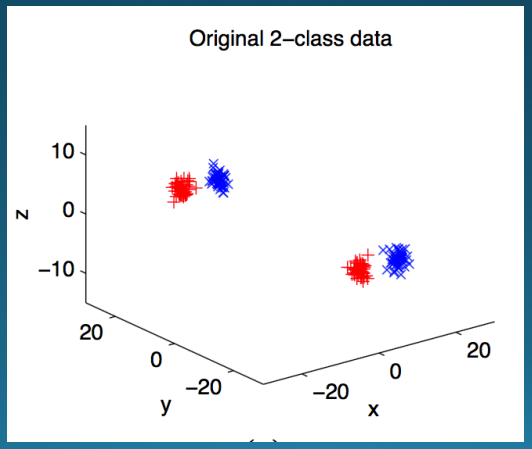
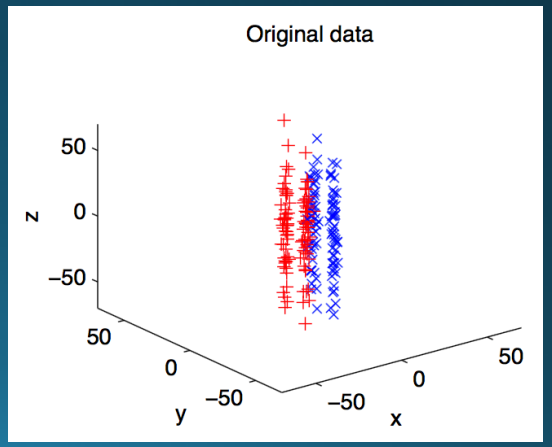
Experiments

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

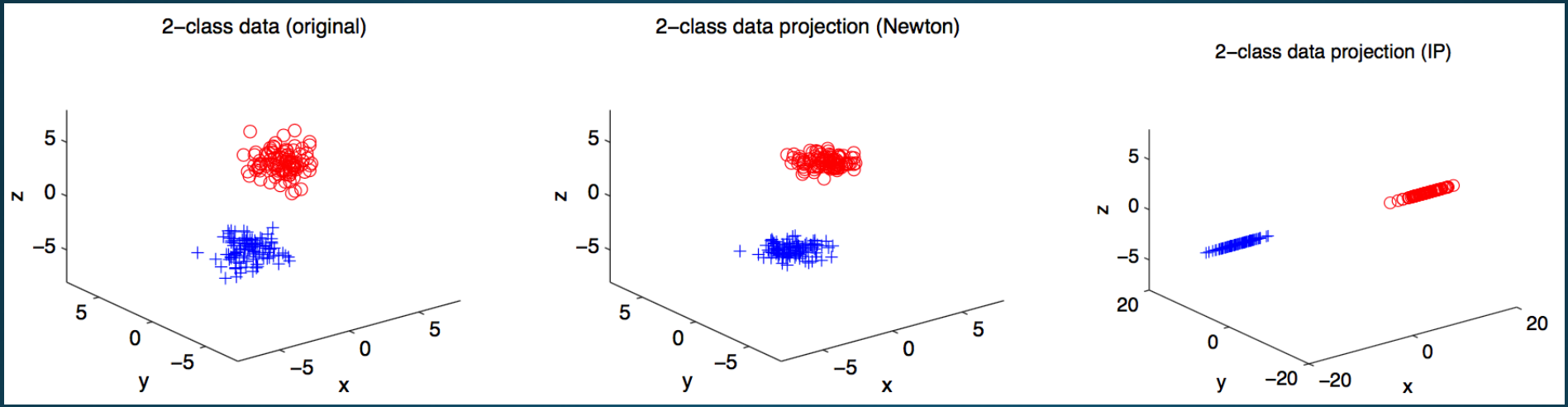




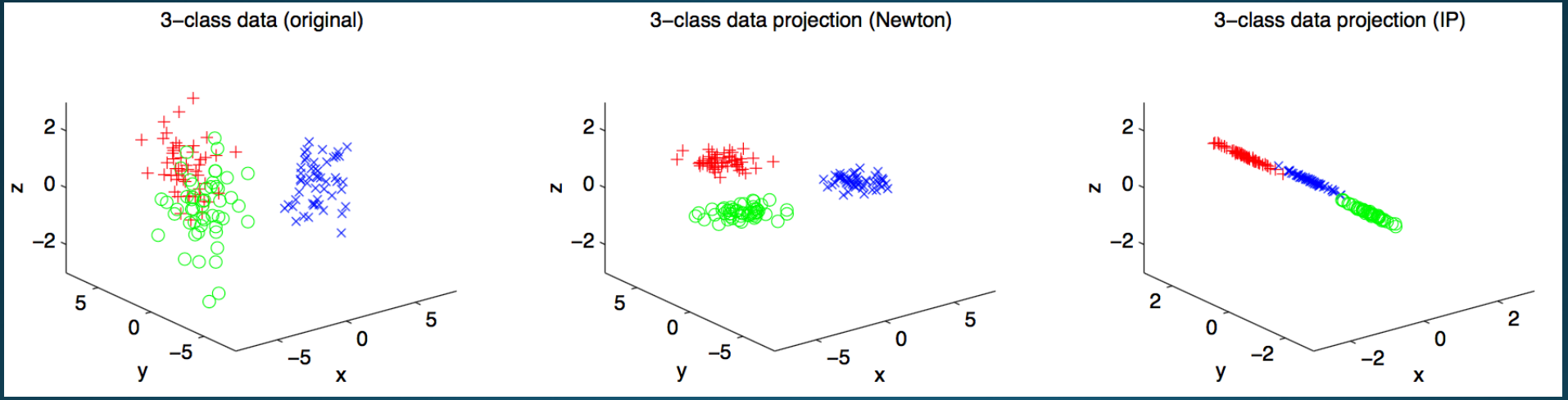




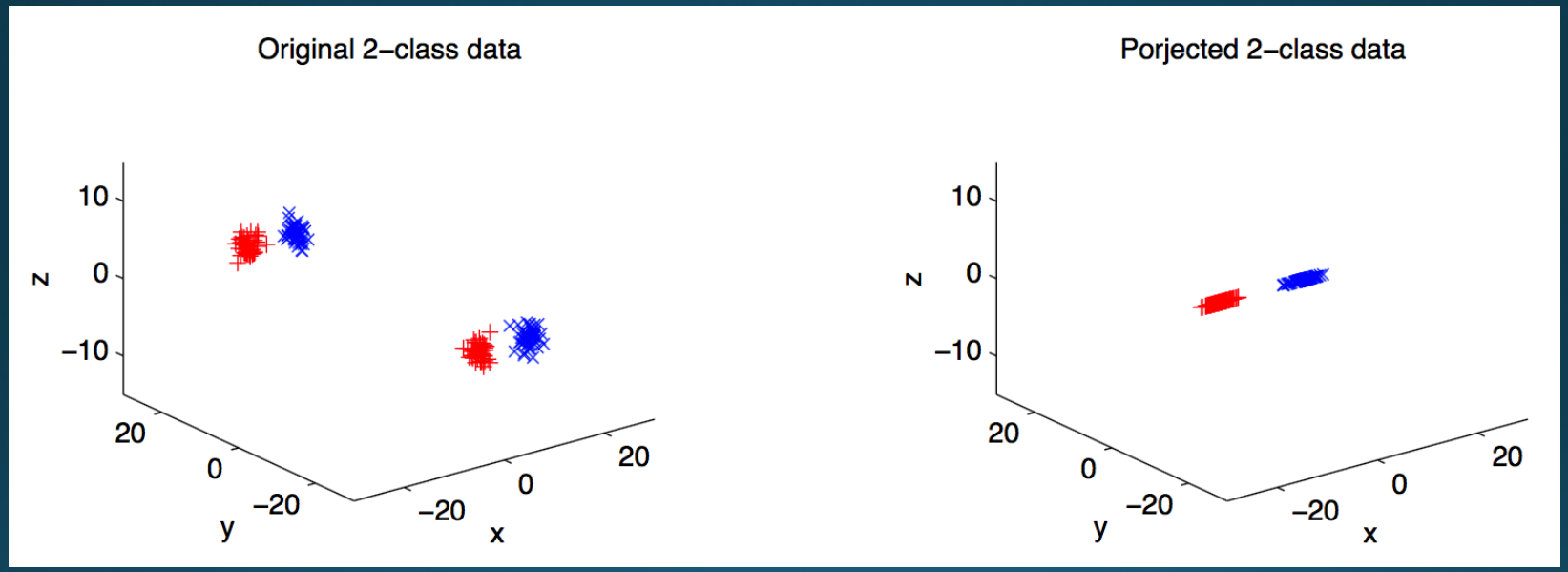
Experiments



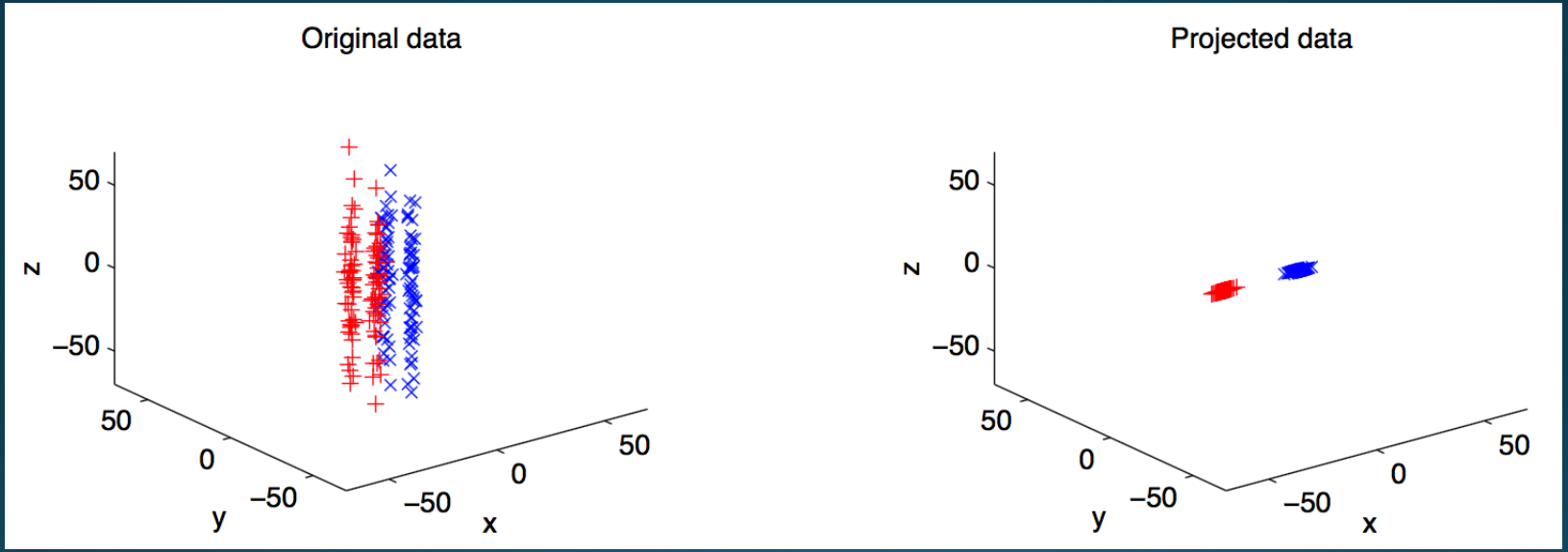
Experiments



Experiments

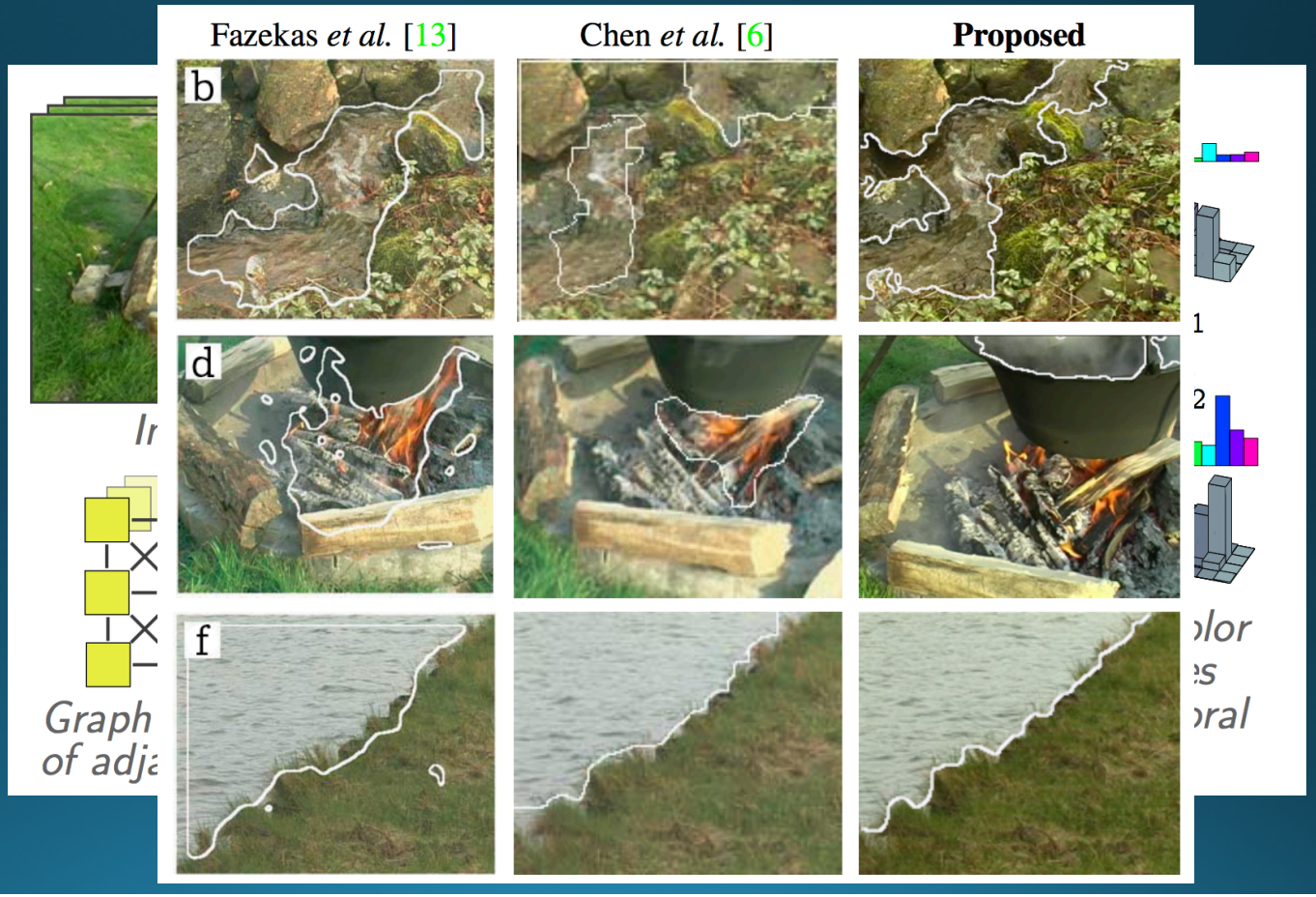


Experiments



Other Applications

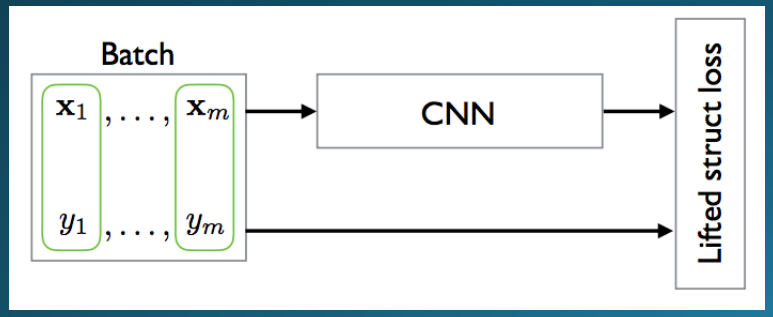
- Video scene segmentation
- Identifying dynamic textures in videos

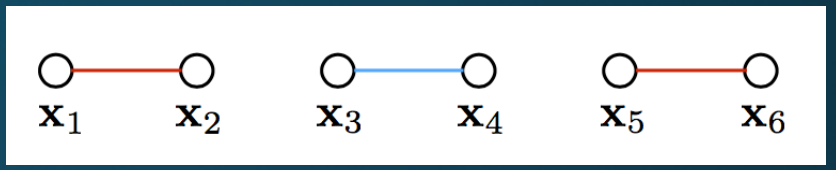


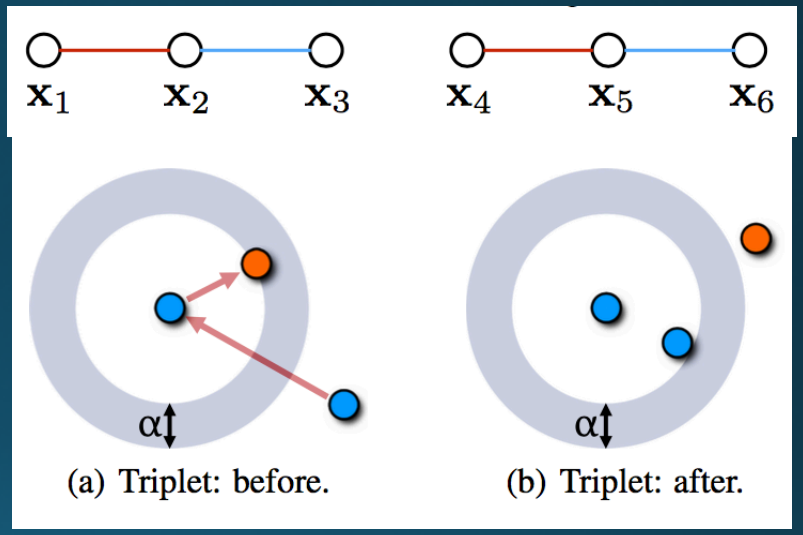
Other Formulations

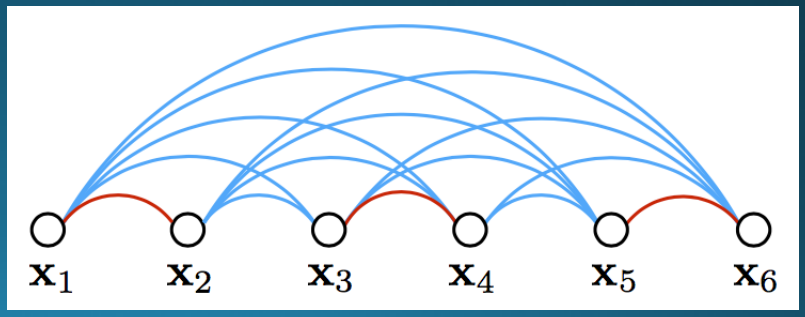
- Deep metric learning

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





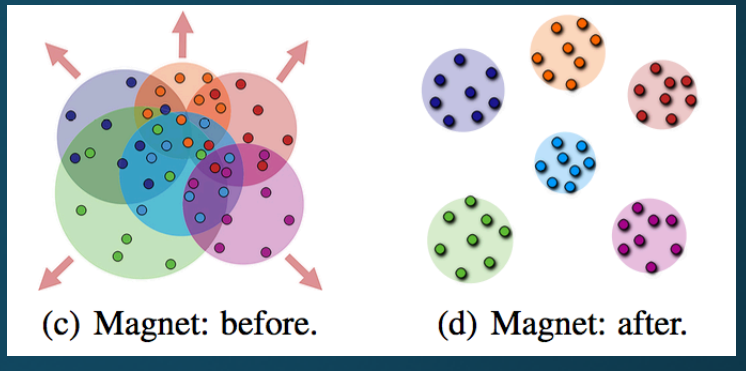


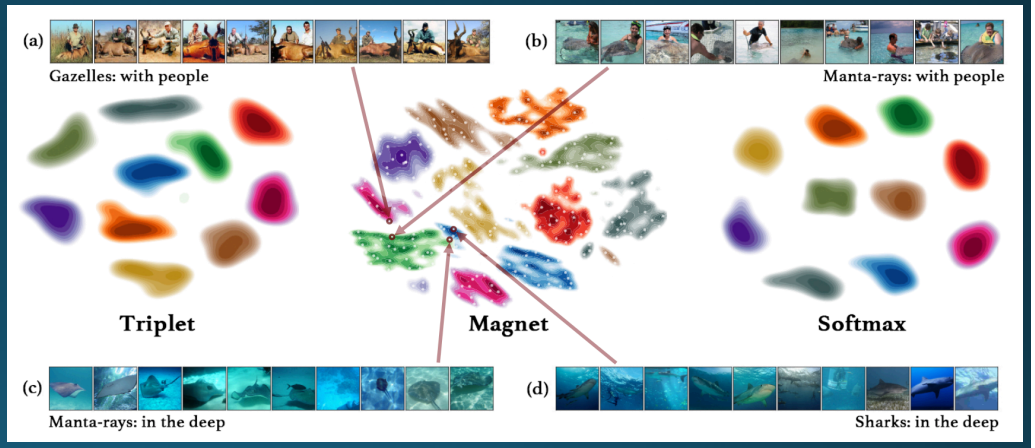


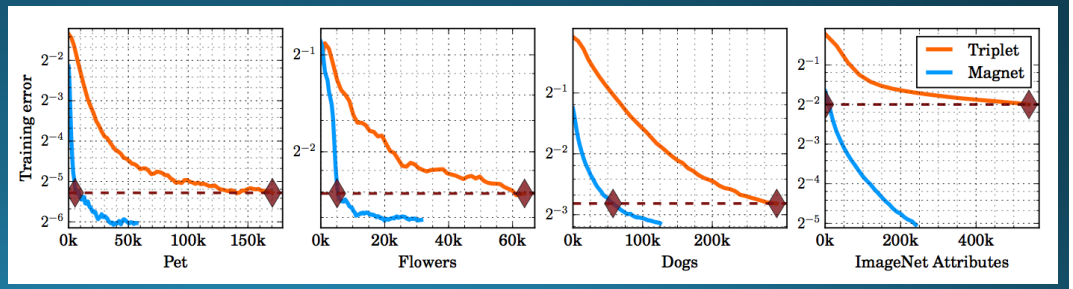
Other Formulations

- 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







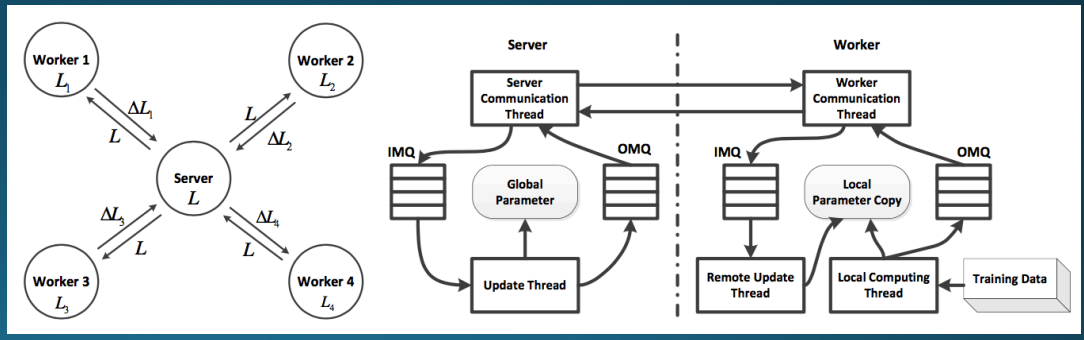
Other Formulations

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

- 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

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

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



Questions?

Updates

References

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