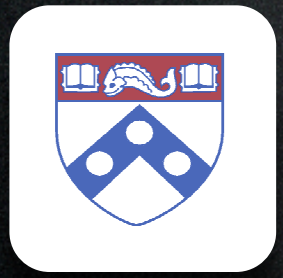
Distance Metric Learning for Large Margin Nearest Neighbor Classification



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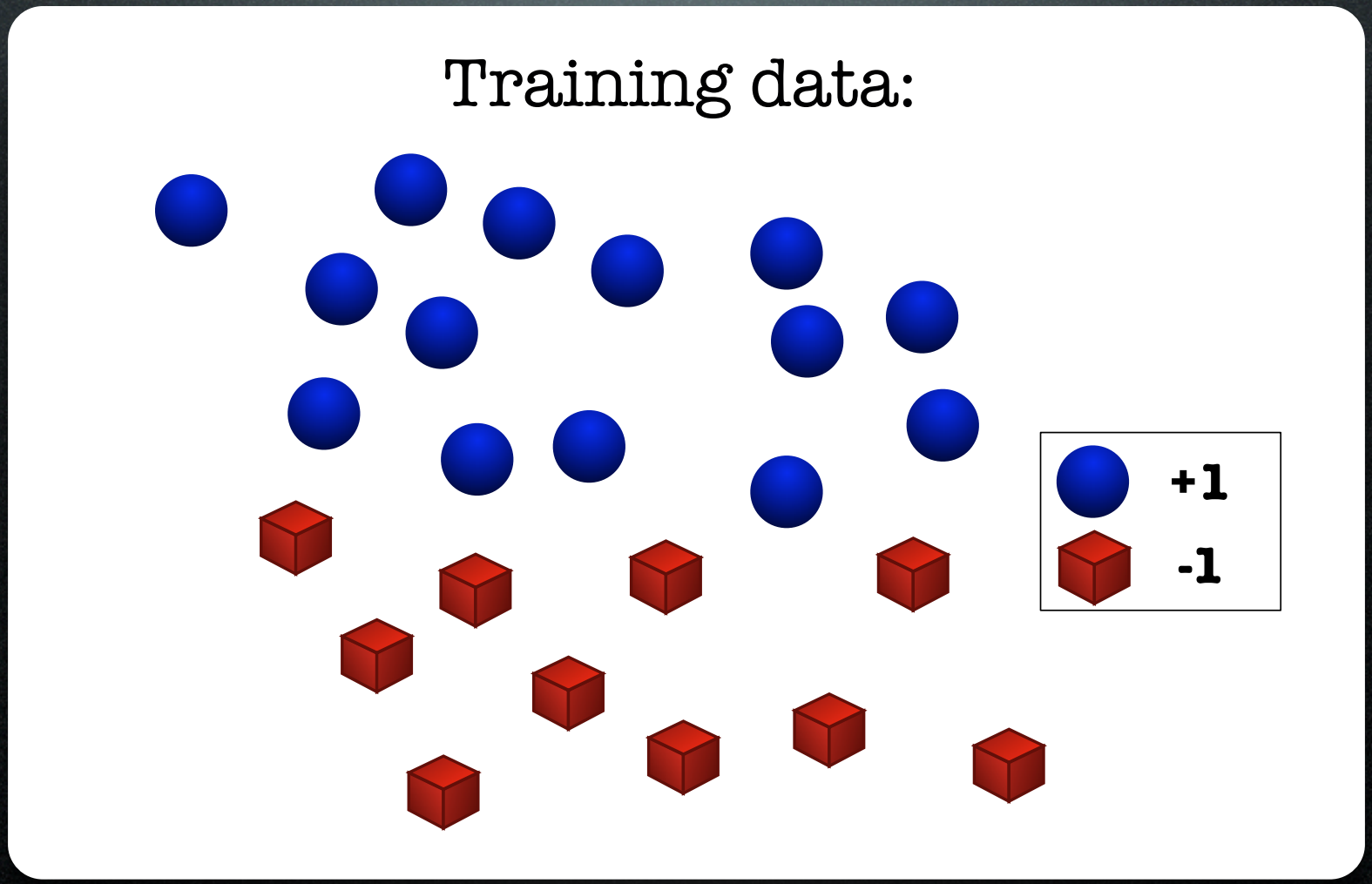
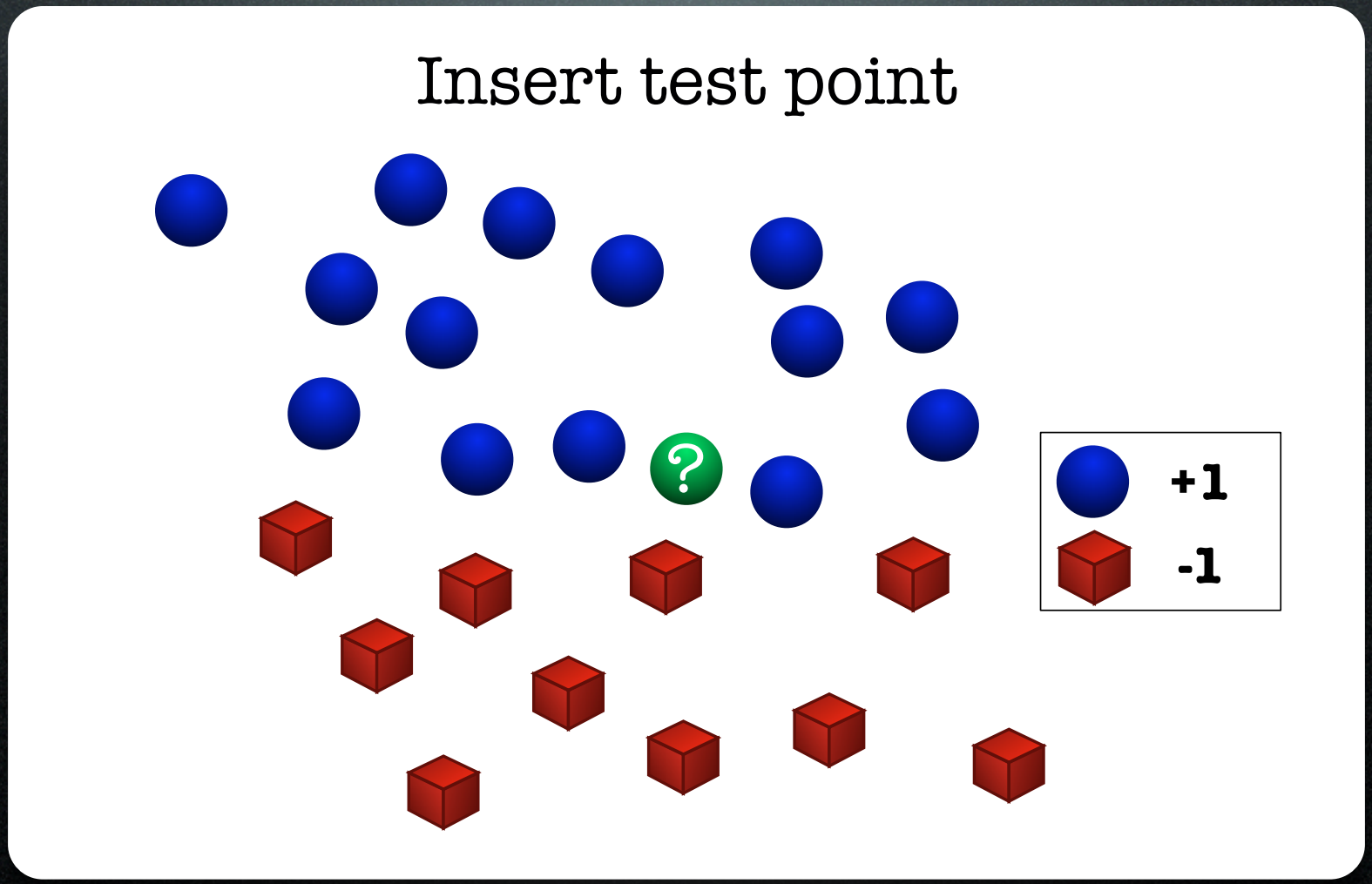
John C. Blitzer
Lawrence K. Saul

University of Pennsylvania
GRASP Laboratory

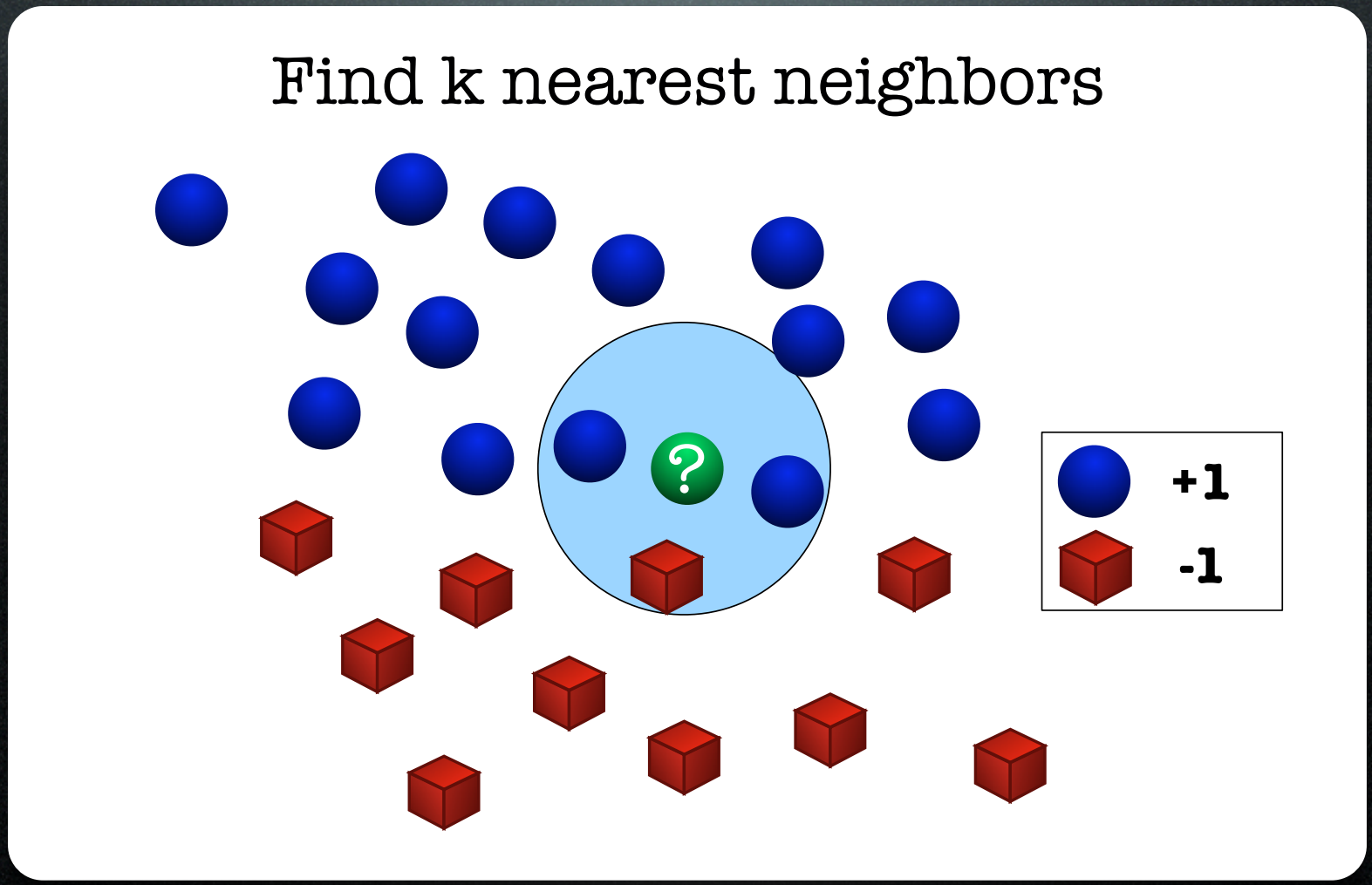
k-nearest neighbor classification



k-nearest neighbor classification

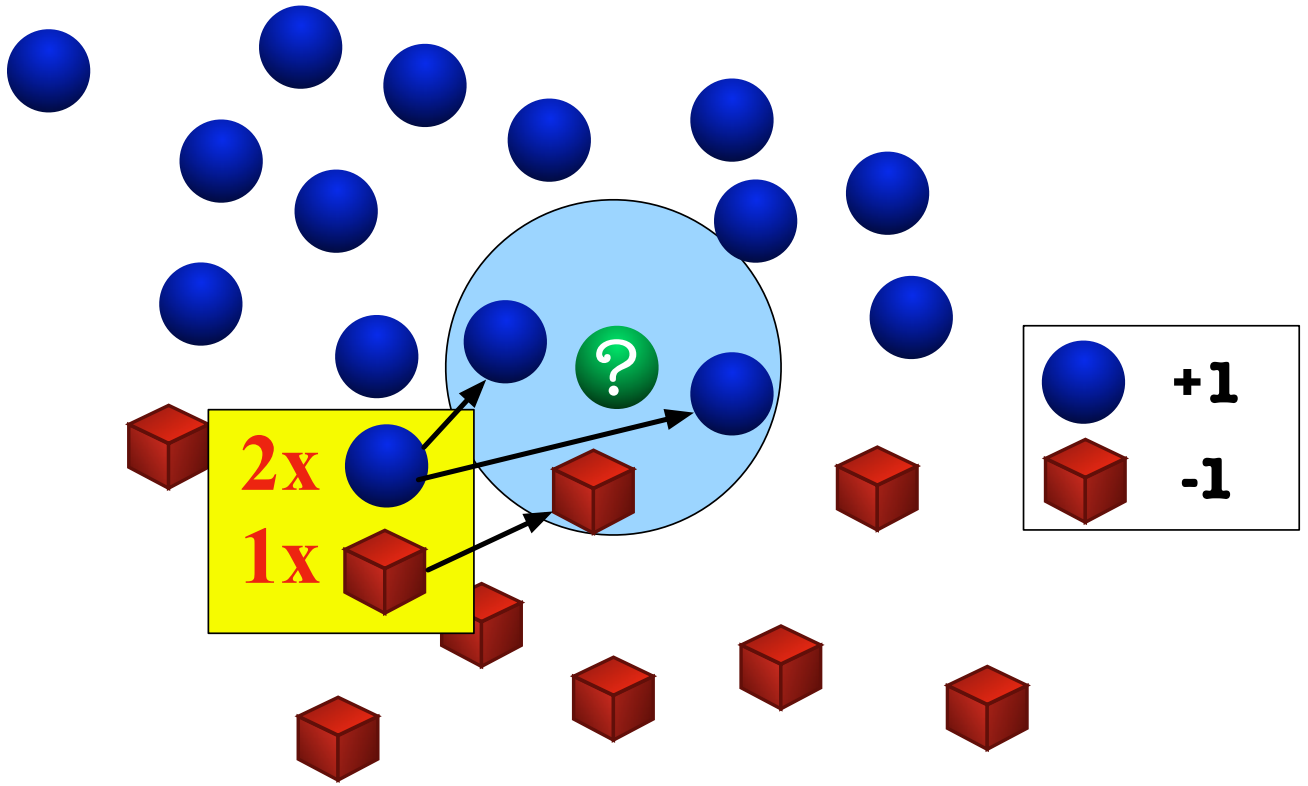


k-nearest neighbor classification



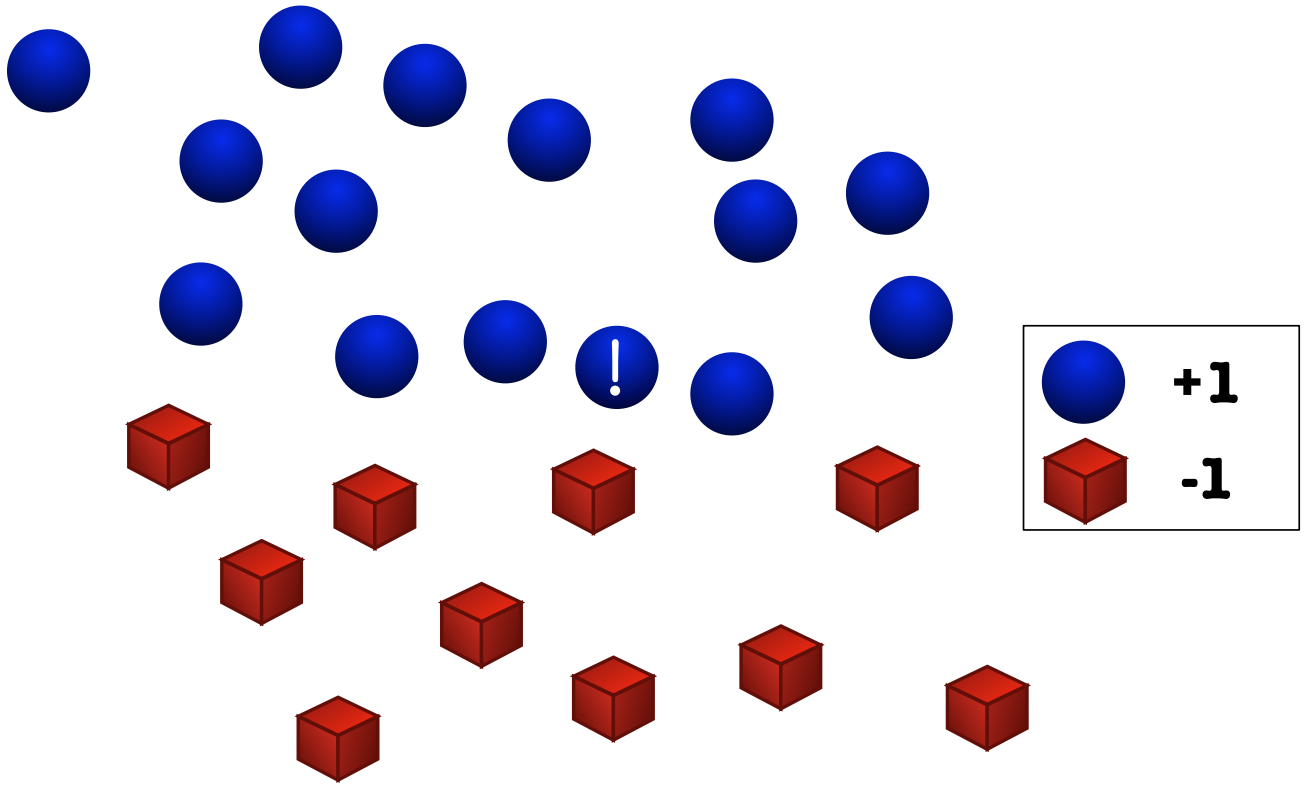
k-nearest neighbor classification

Let neighbors vote



k-nearest neighbor classification

Assign most common label



Strengths of k-NN classification

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- straightforward to implement

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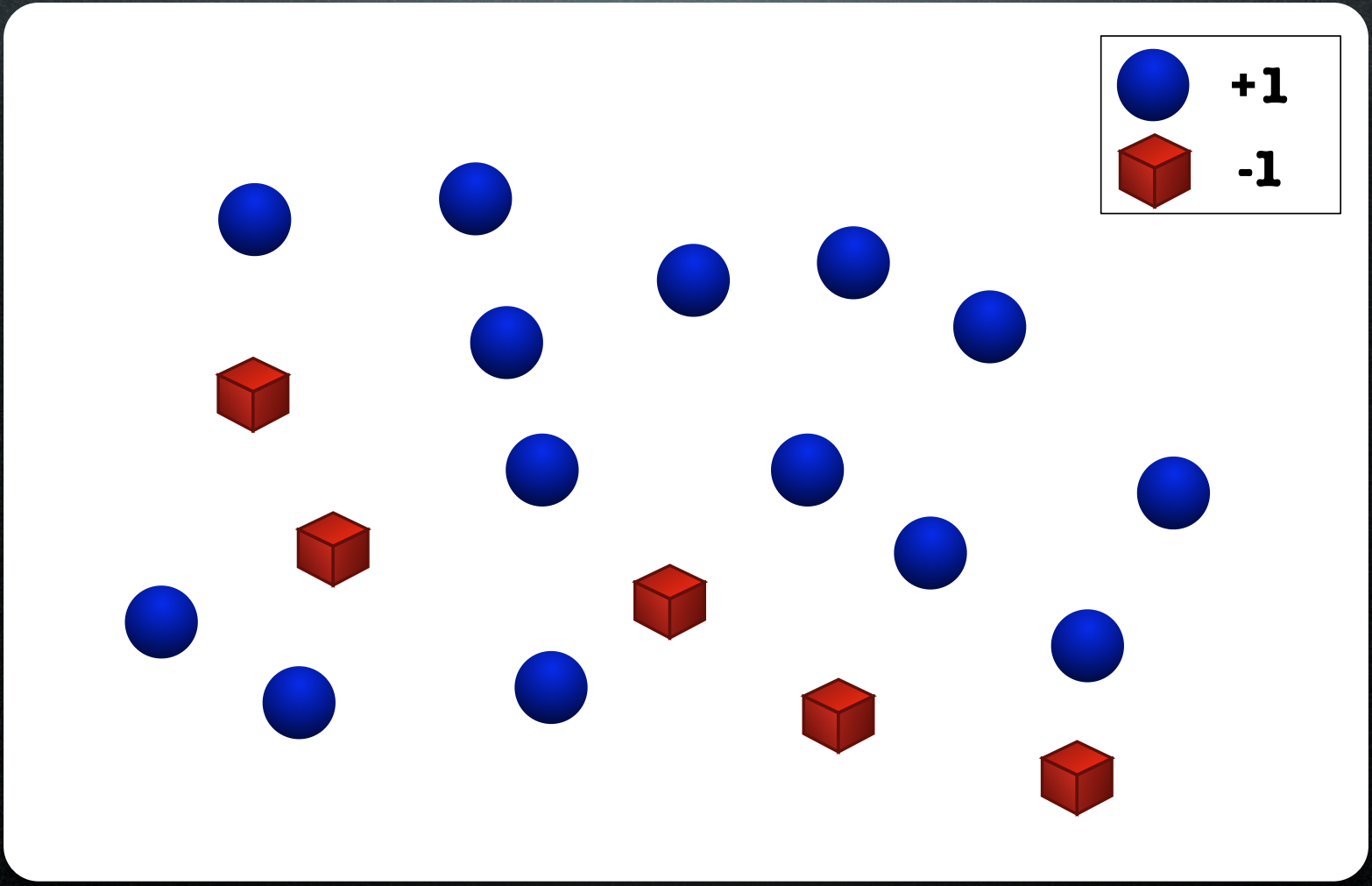
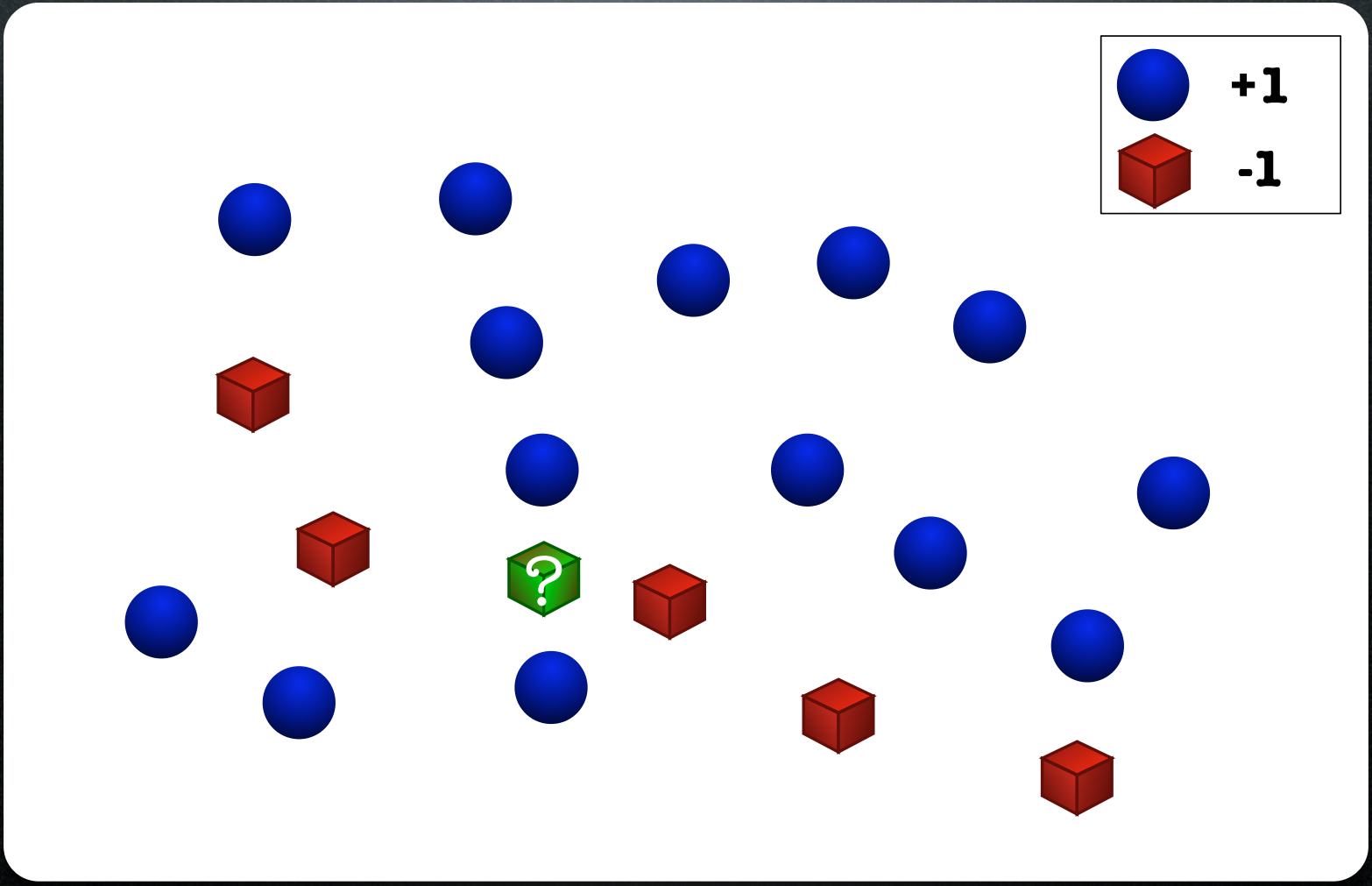
- straightforward to implement
- nonlinear decision boundaries
- complexity independent of # of classes
- asymptotic guarantees

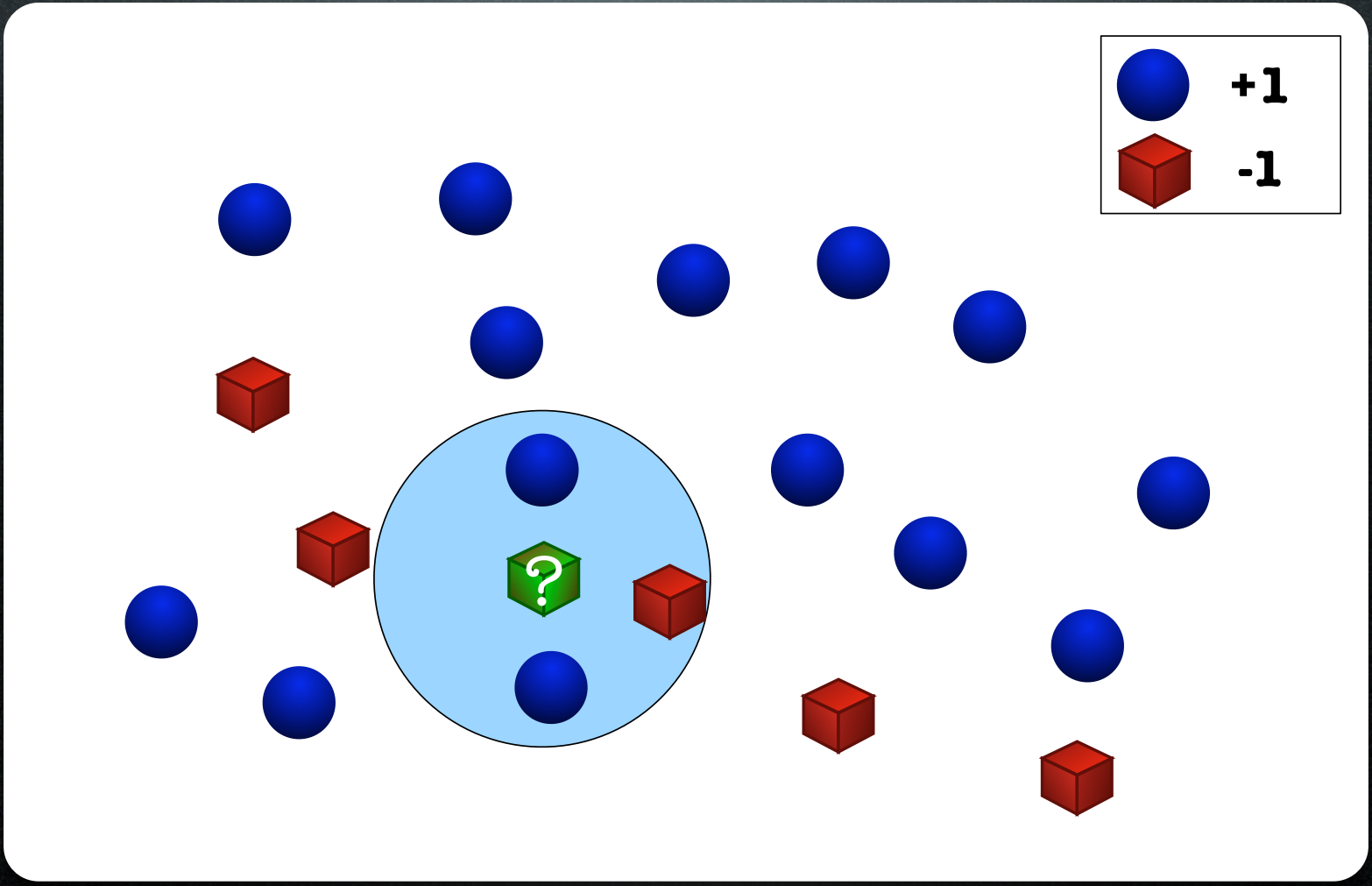
Problem with k-NN



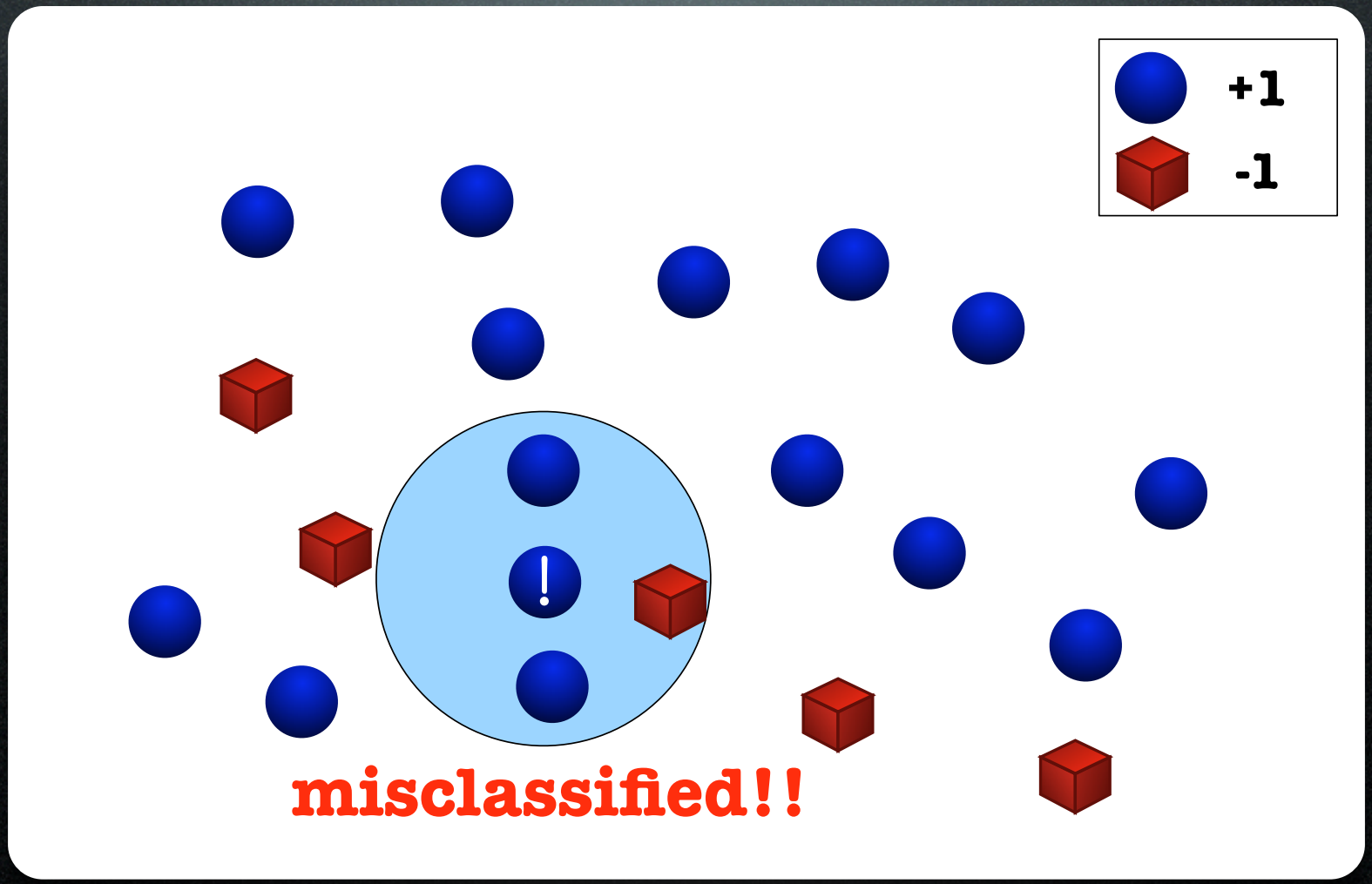
Problem with k-NN



Problem with k-NN



Problem with k-NN

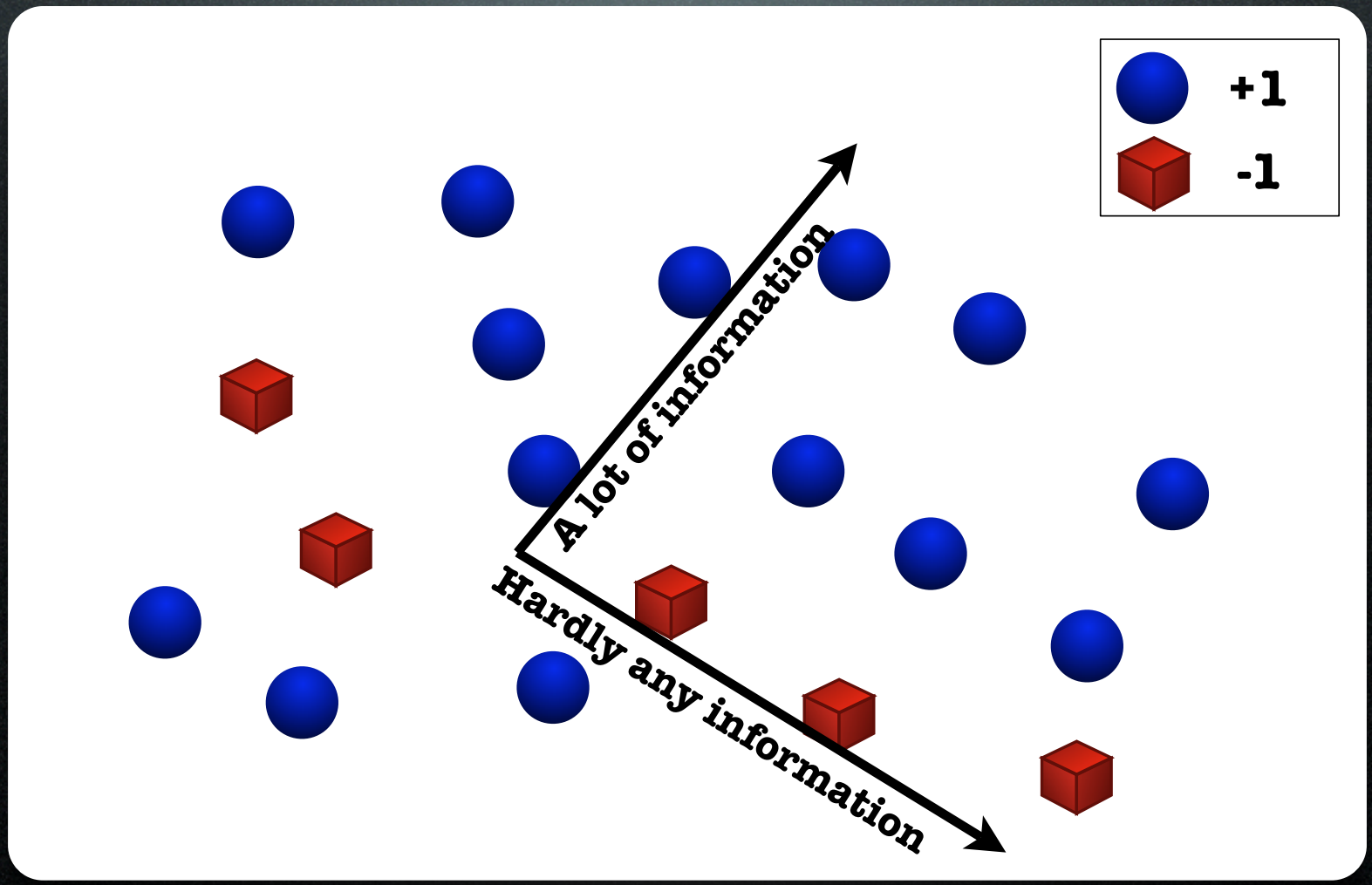


Problem with k-NN

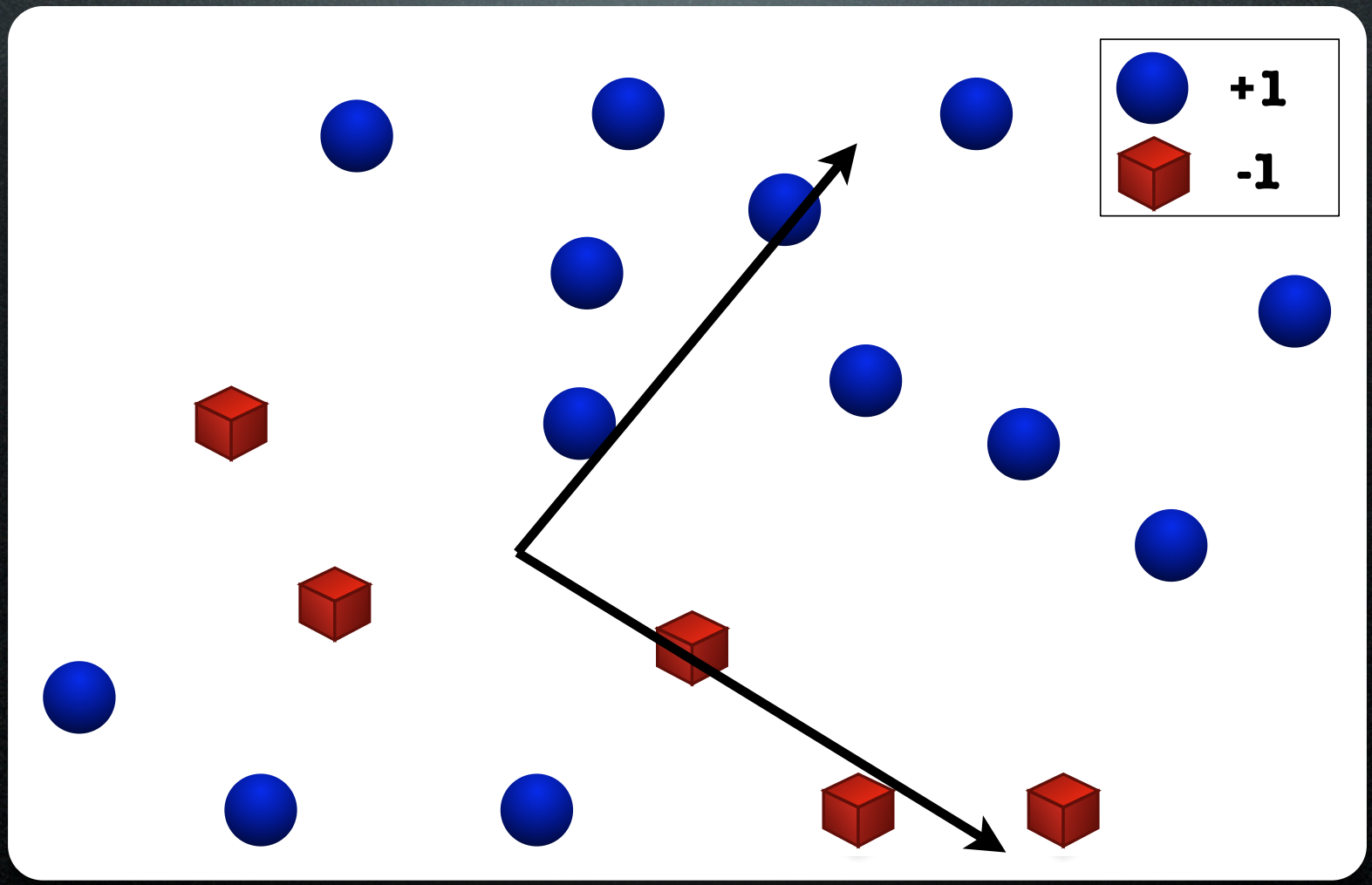
The problem:

Euclidean distances

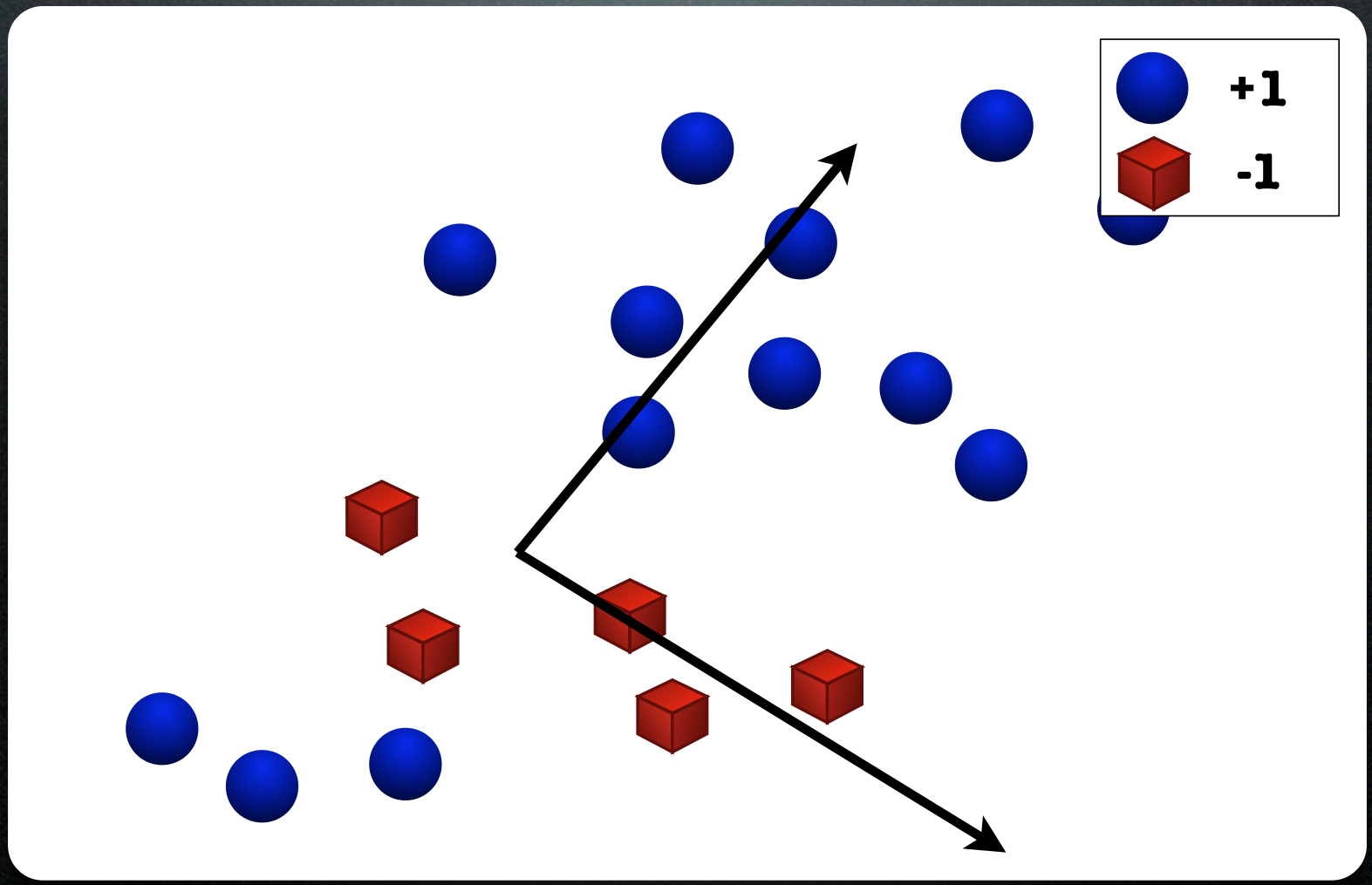
Problem with k-NN



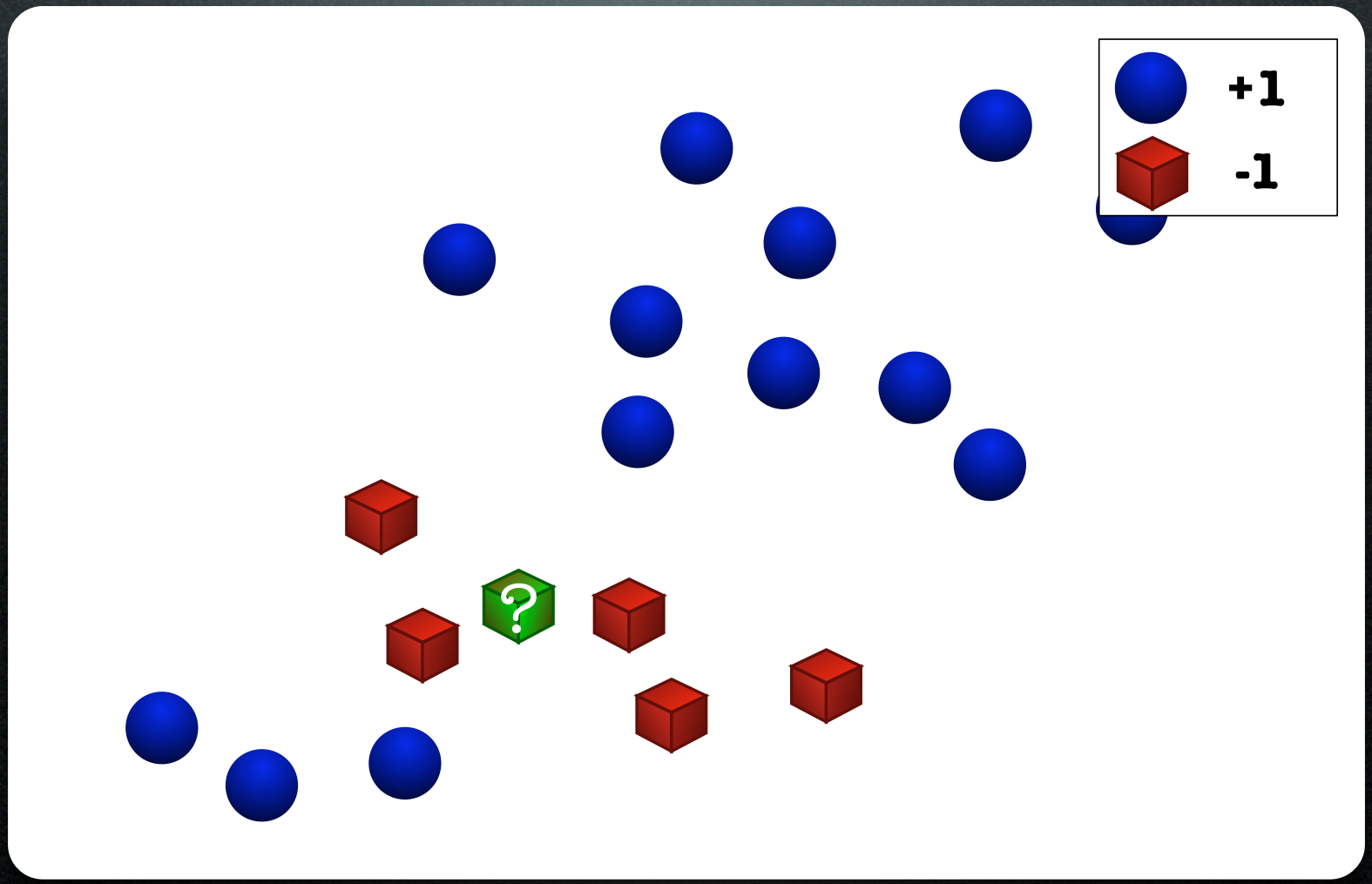
Amplify informative directions



Dampen non-informative directions



Finally!!



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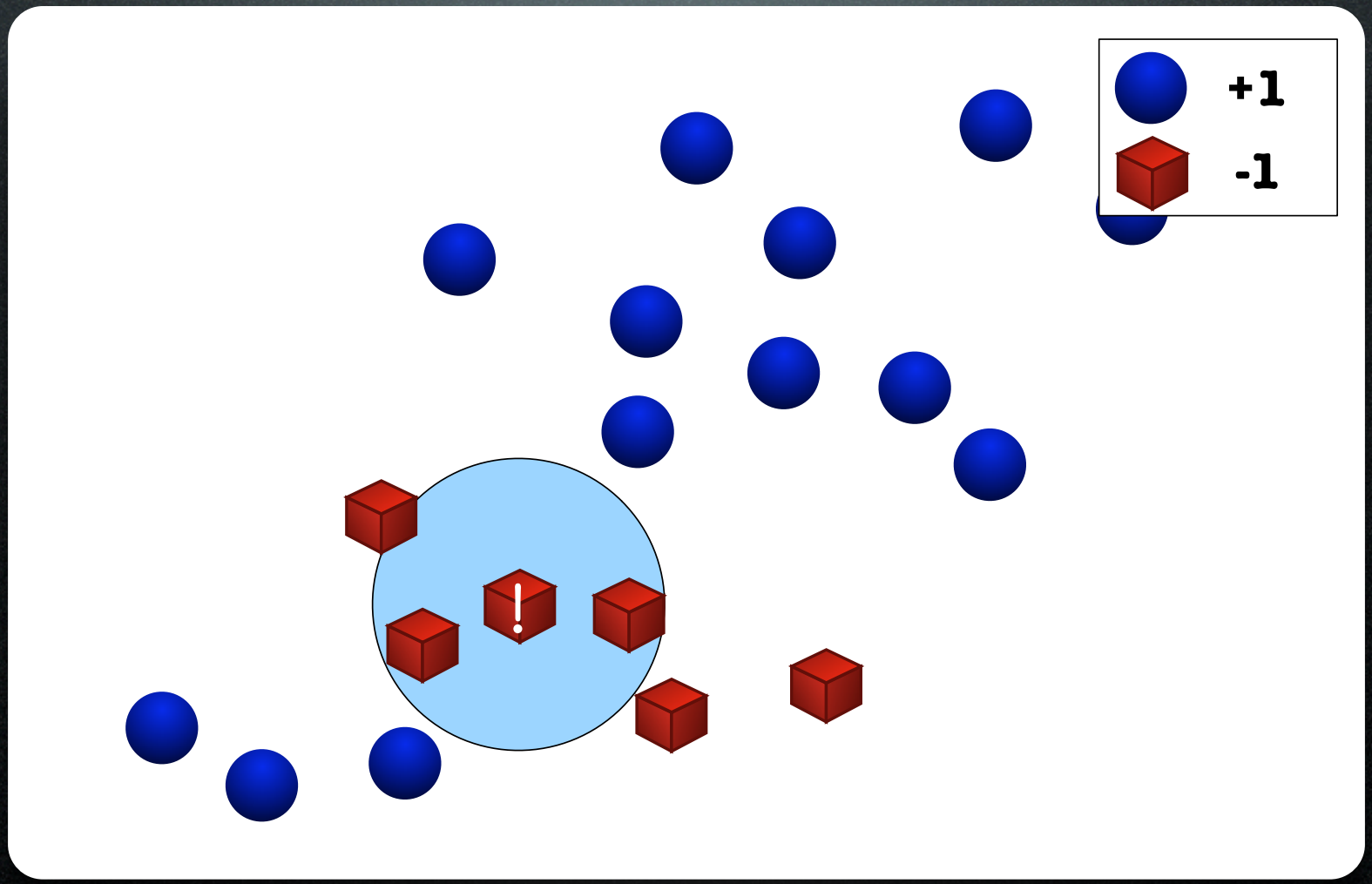
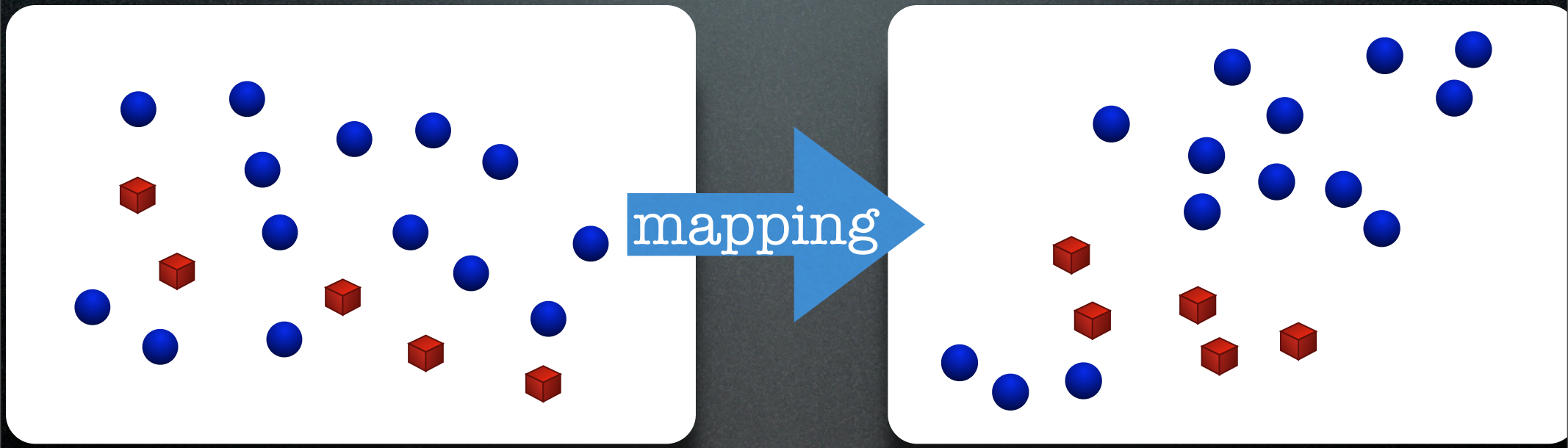


Our goal: Learn the transformation



Input space

Feature space
(meaningful distances)

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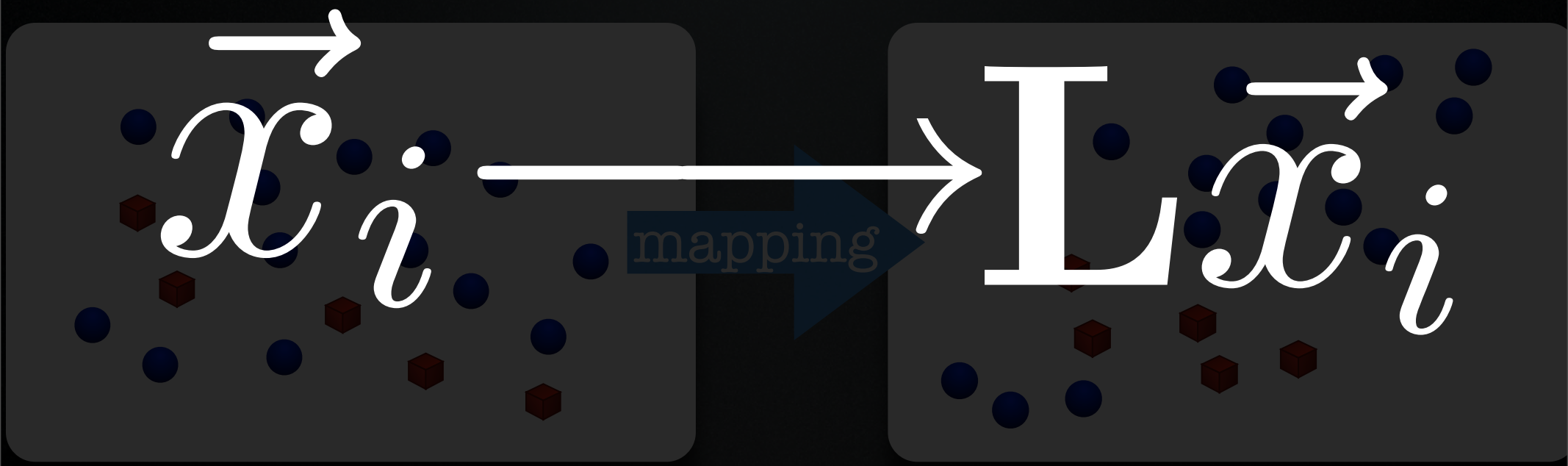

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Feature space
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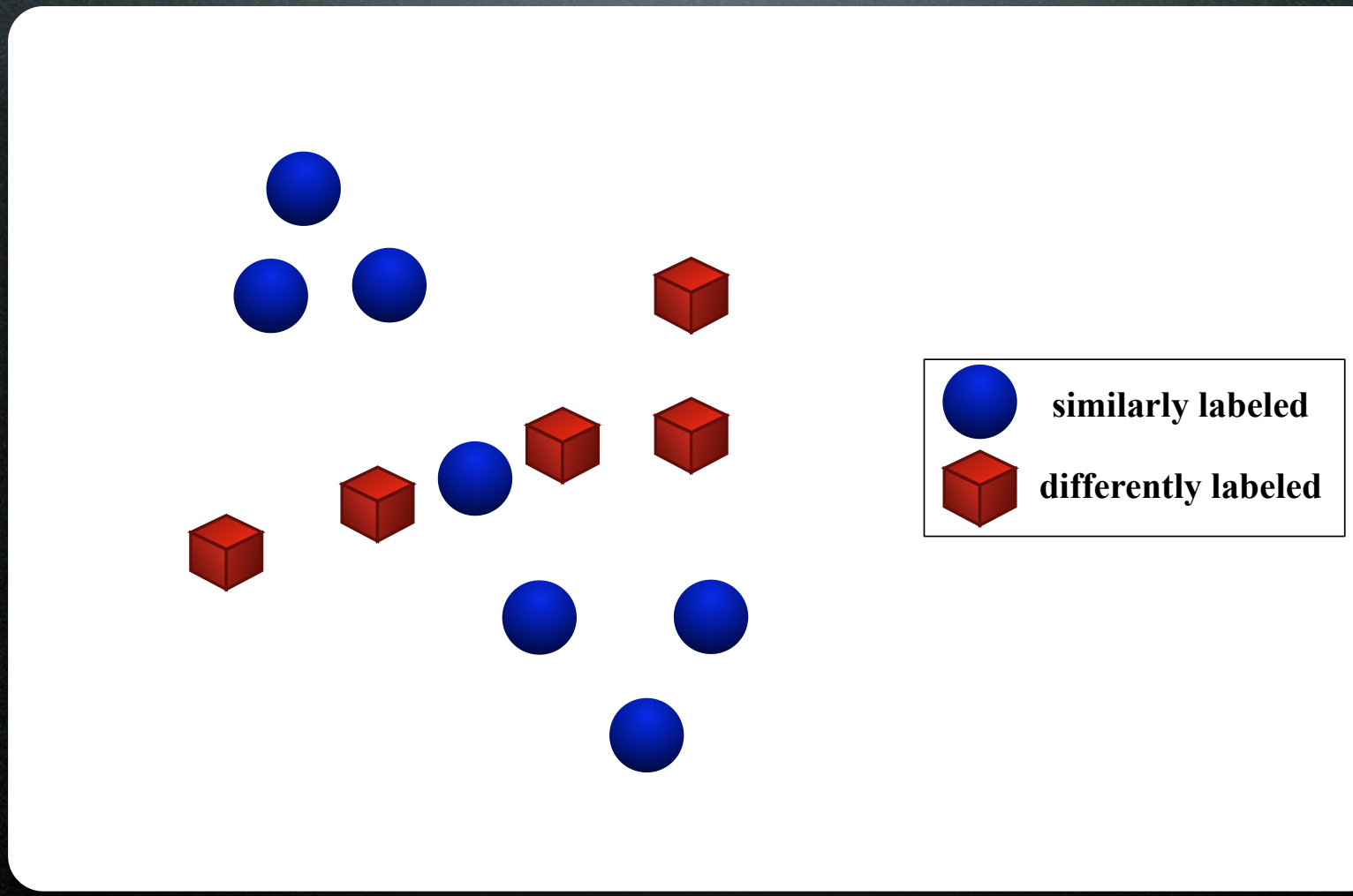
Intuition



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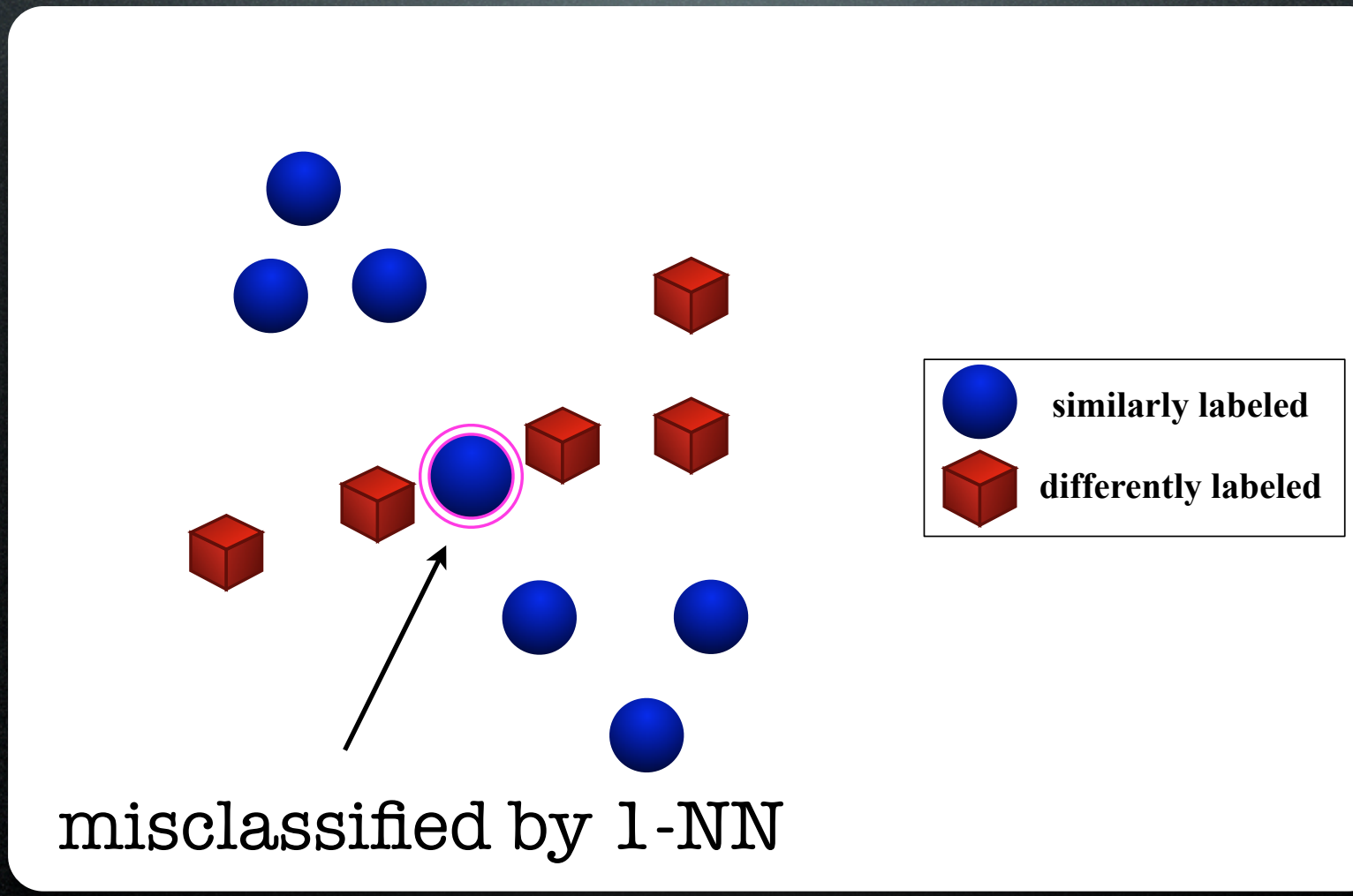
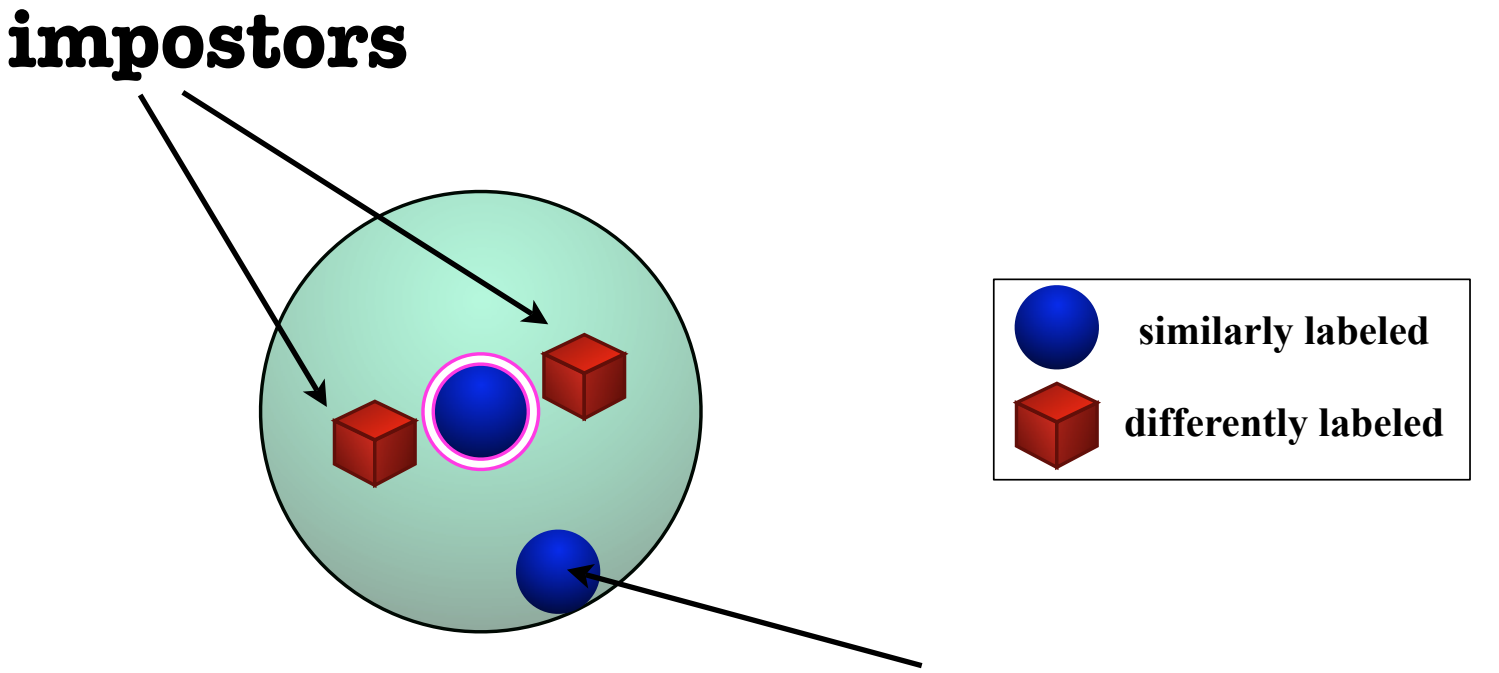
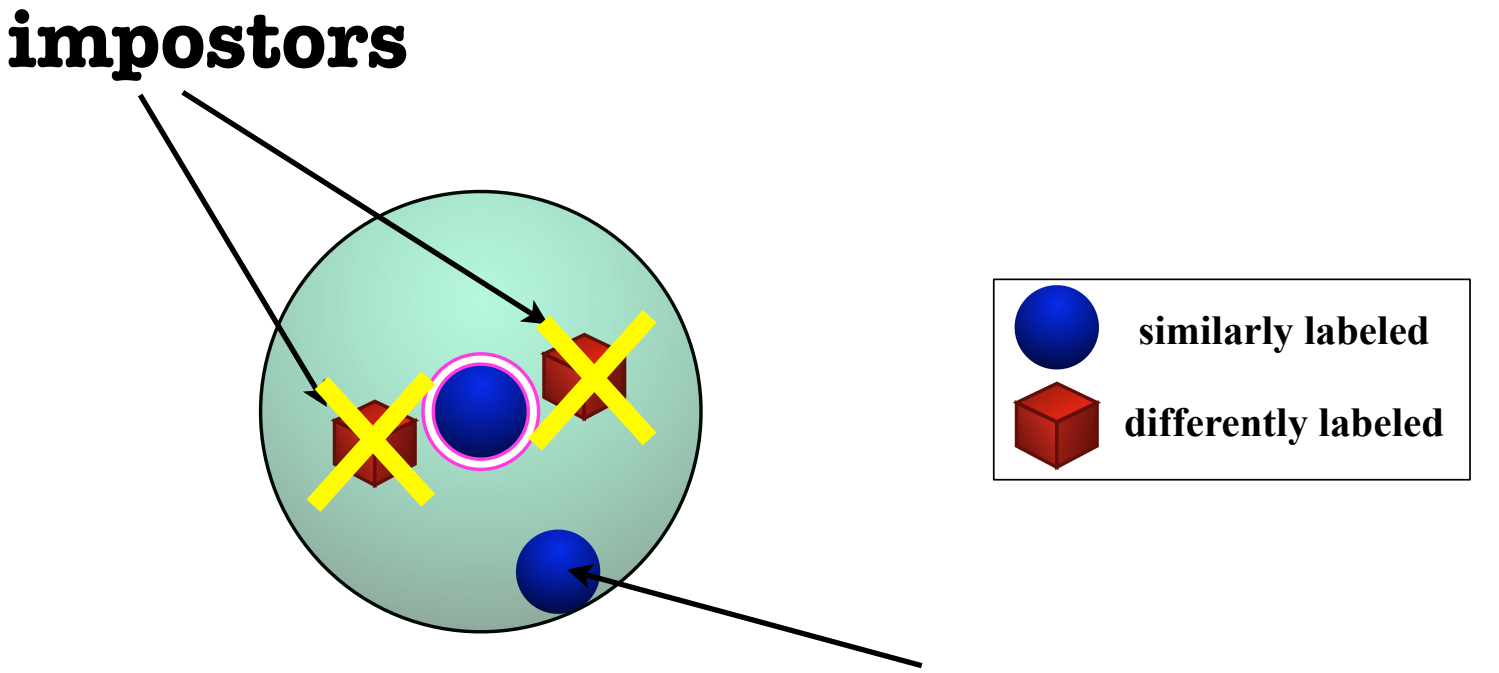

similarly labeled
differently labeled
misclassified by 1-NN

Intuition



closest **similarly** labeled point
("target neighbor")

Intuition



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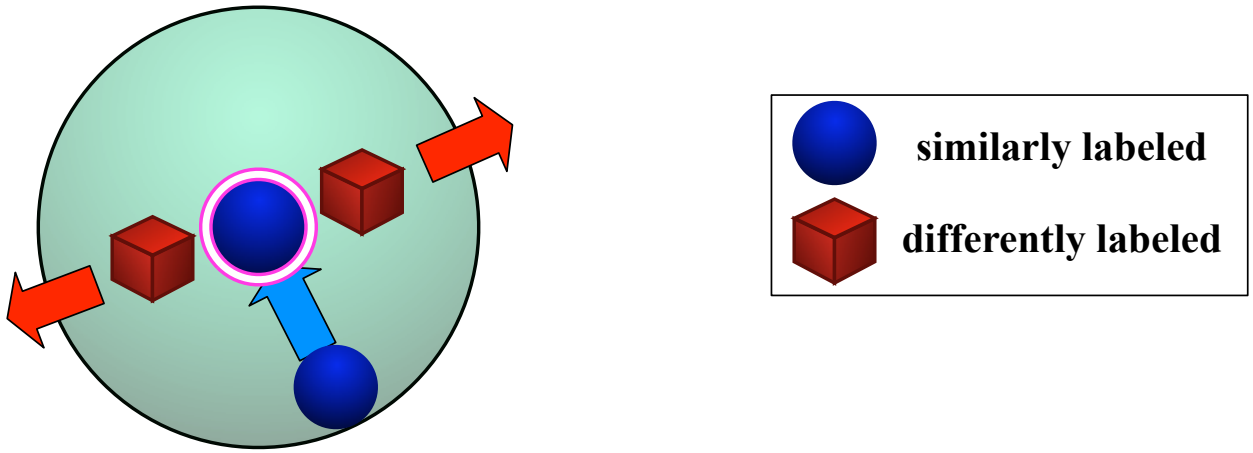
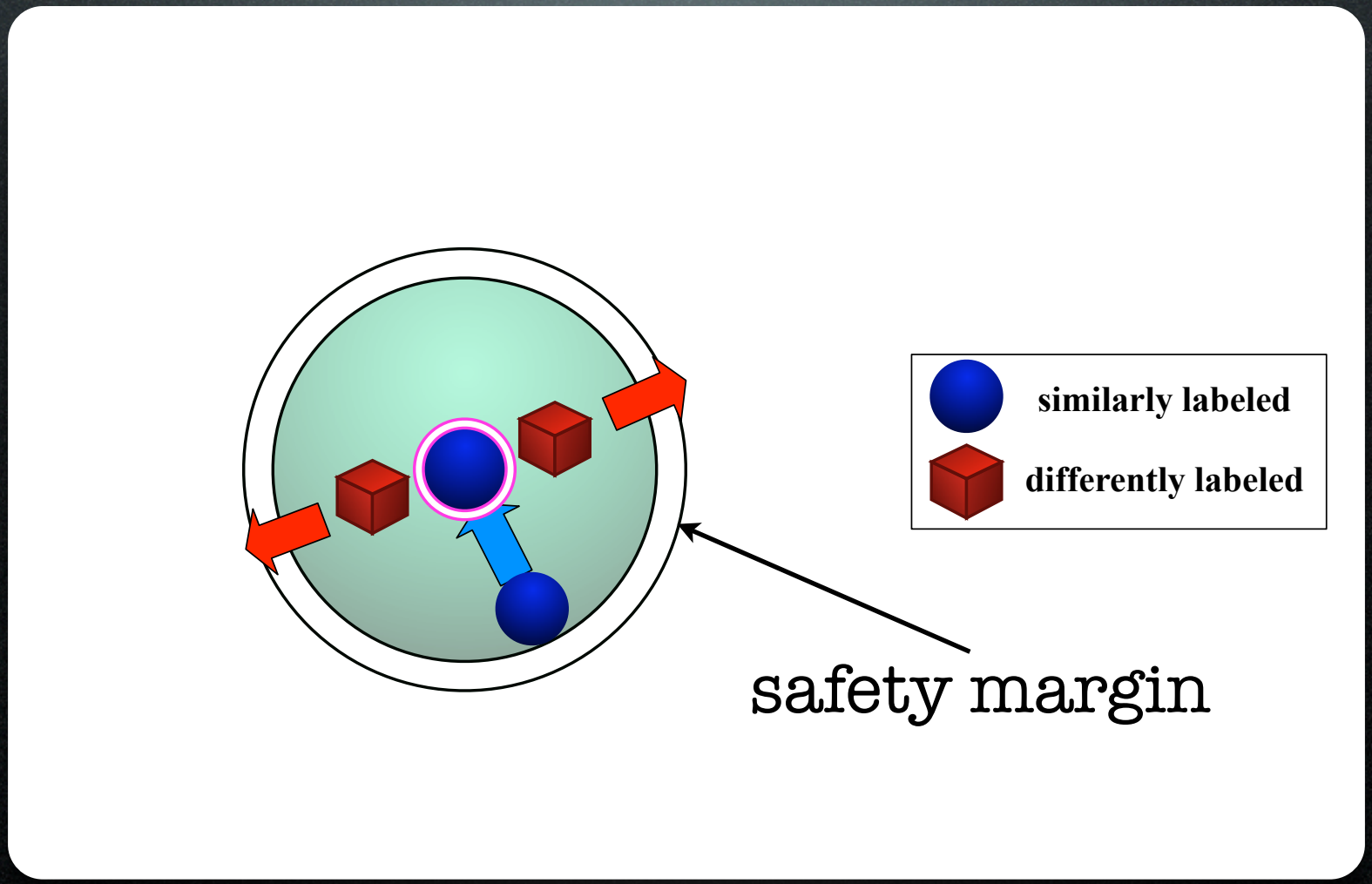
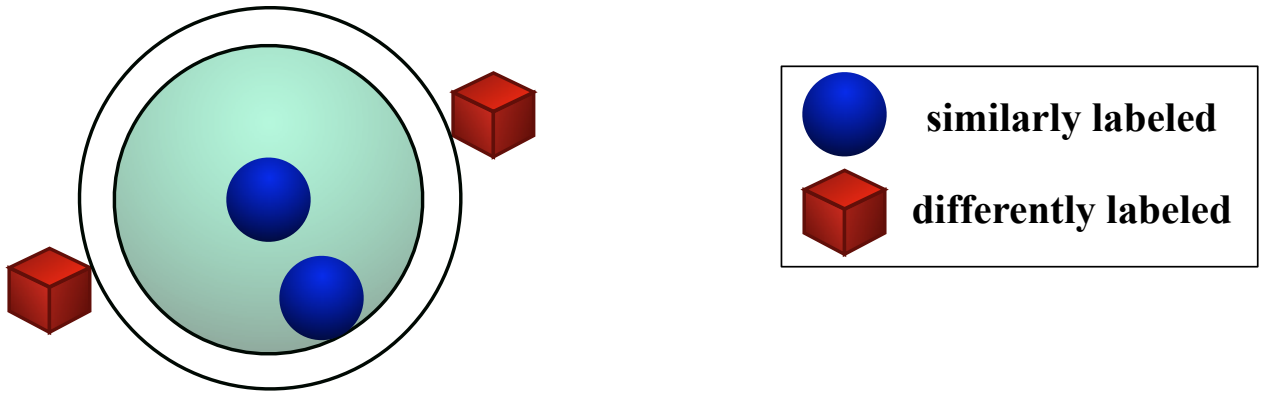


1. pull target neighbors closer
2. push impostors away

Intuition



Clean neighborhood!



Notation

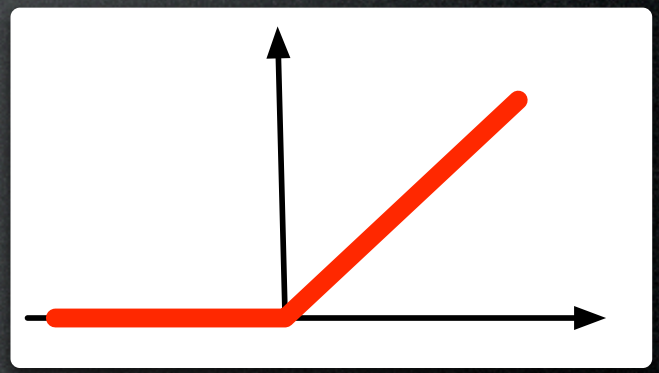
$\vec{x}_i$ input vectors

y_{ij} $\begin{cases} 1 \text{ if } \vec{x}_i \text{ and } \vec{x}_j\text{'s labels match} \\ 0 \text{ otherwise} \end{cases}$

η_{ij} $\begin{cases} 1 \text{ if } \vec{x}_j \text{ is ``target neighbor'' of } \vec{x}_i \\ 0 \text{ otherwise} \end{cases}$

$[a]_+ = \max(a, 0)$

(hinge loss)



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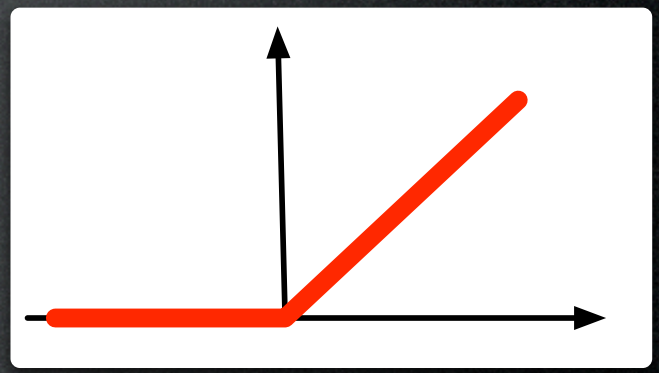

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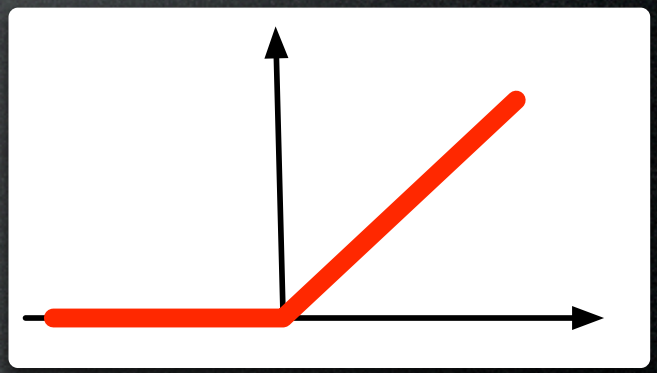

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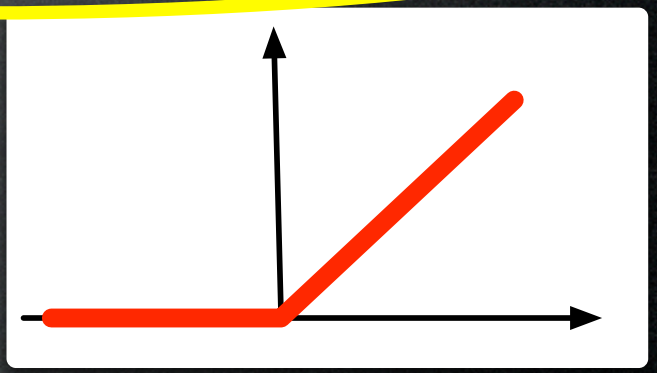

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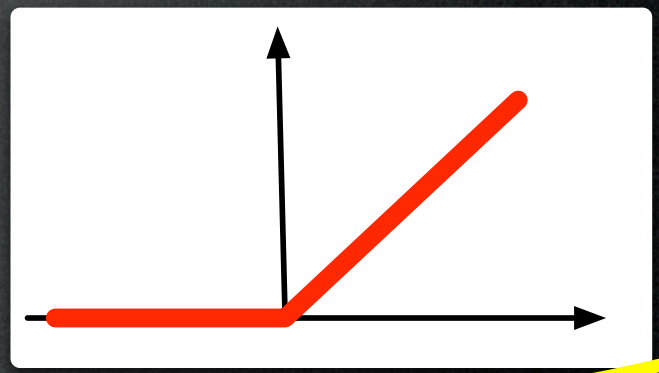
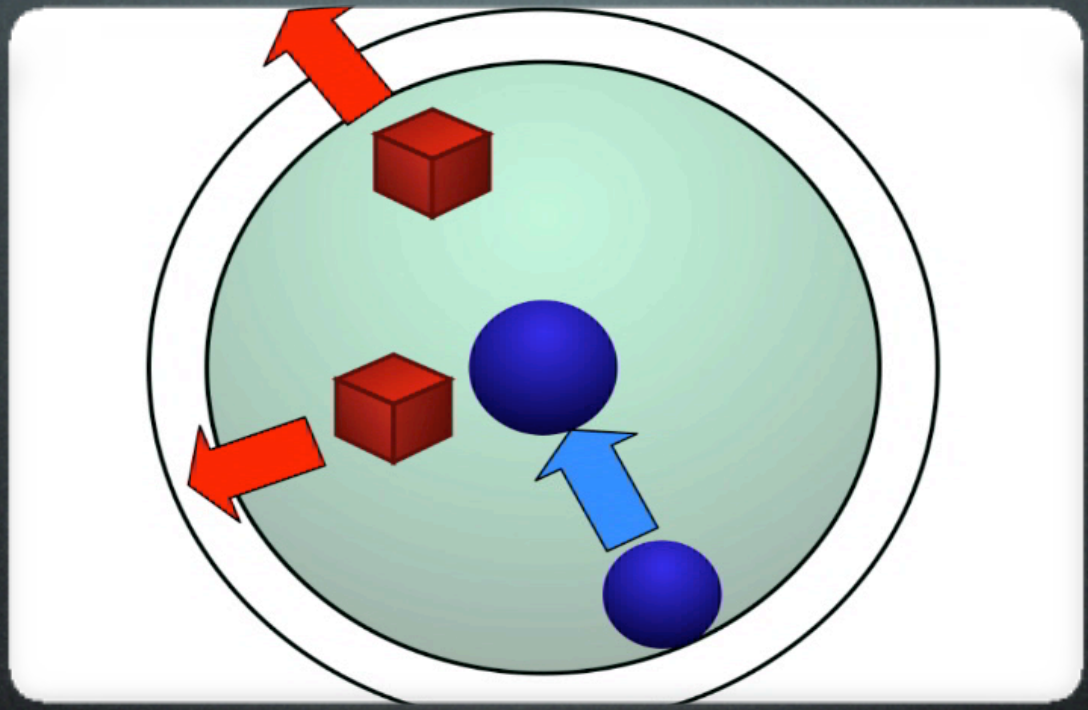
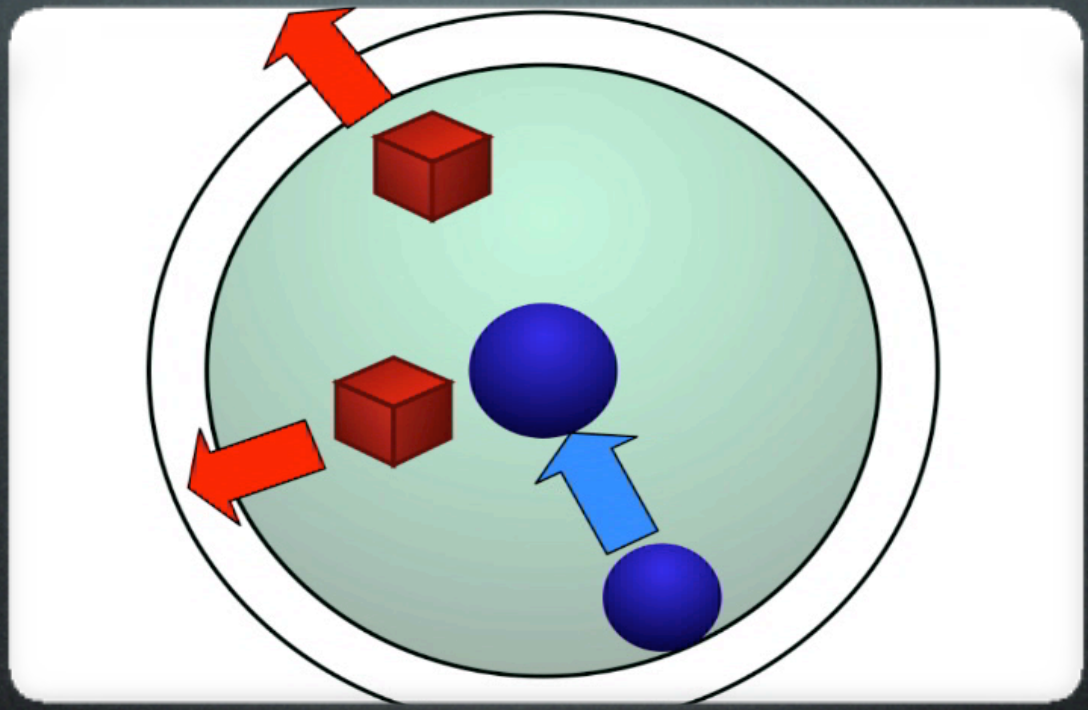




minimize: $\varepsilon(\mathbf{L}) = \varepsilon_{\text{pull}}(\mathbf{L}) + \varepsilon_{\text{push}}(\mathbf{L})$



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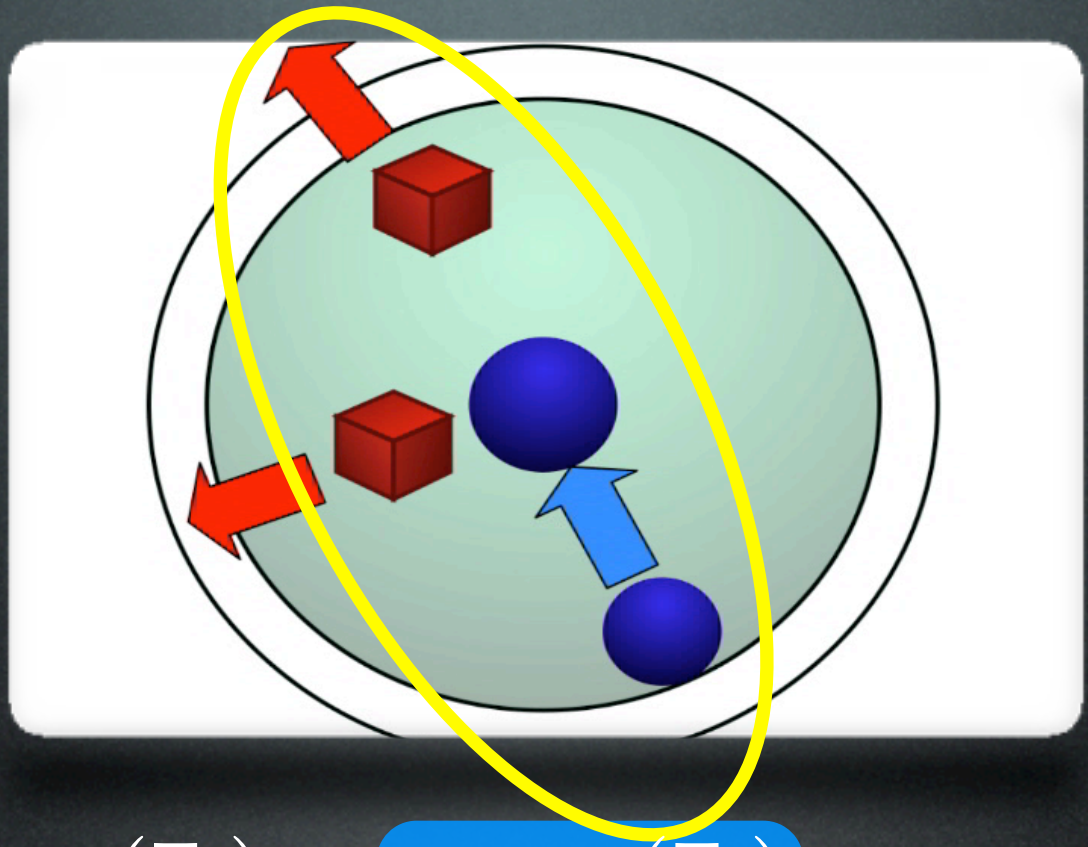

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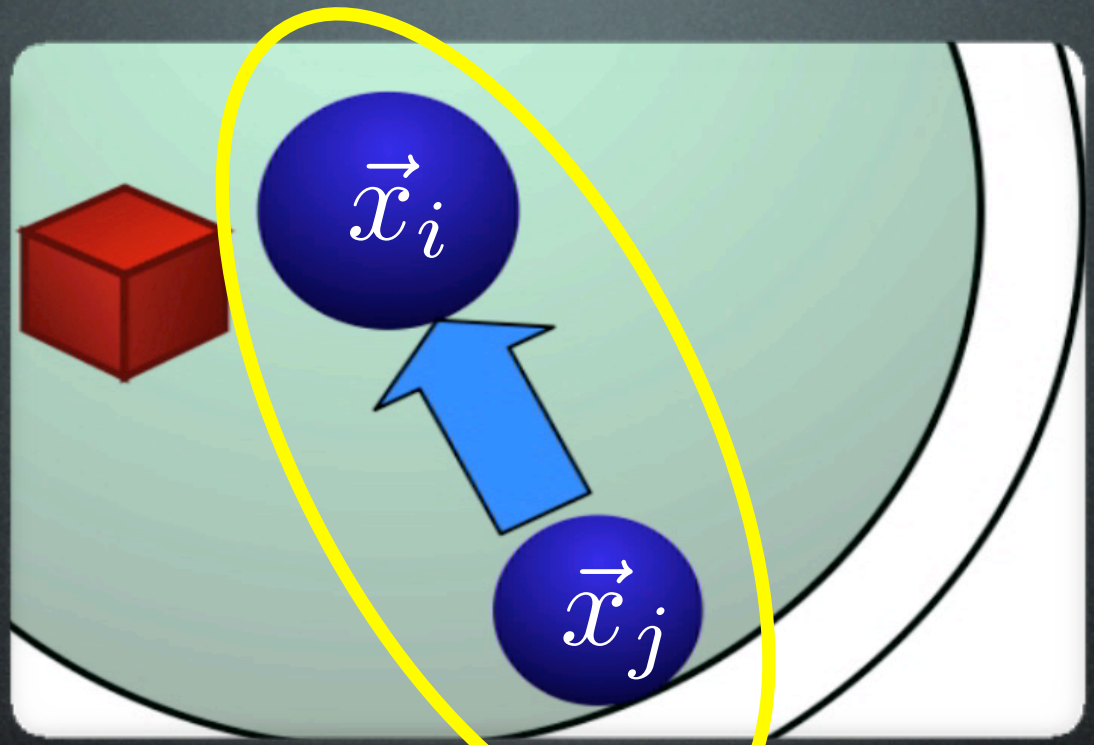

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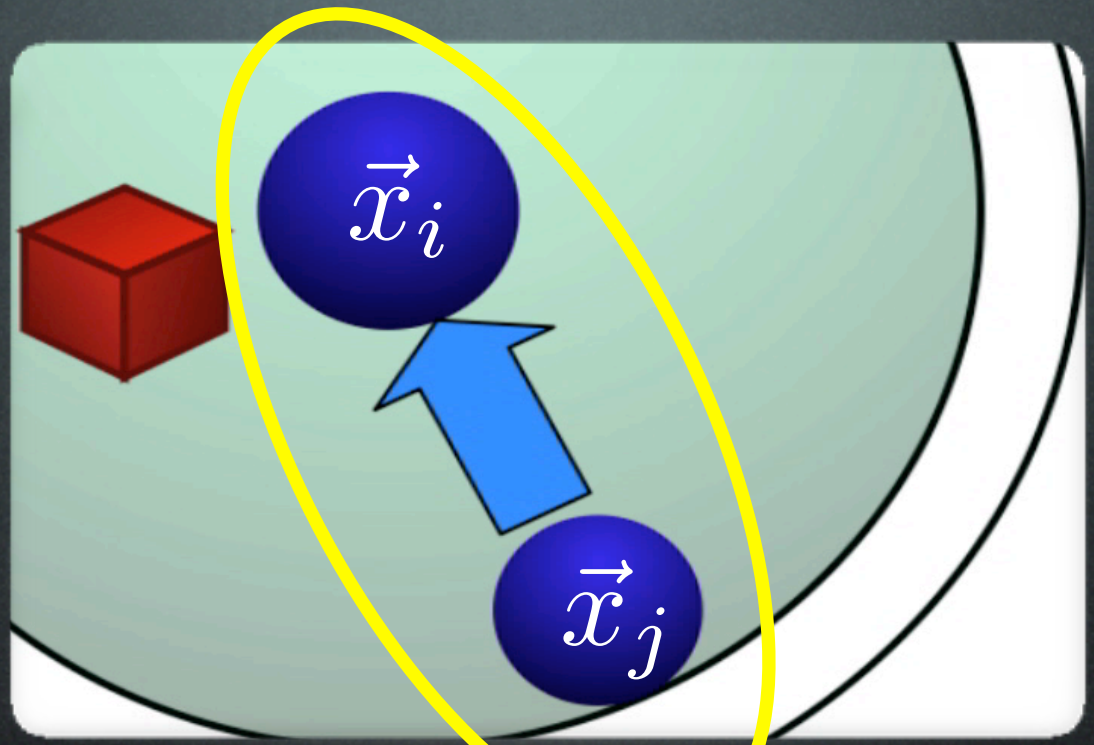
Neighborhood indicator



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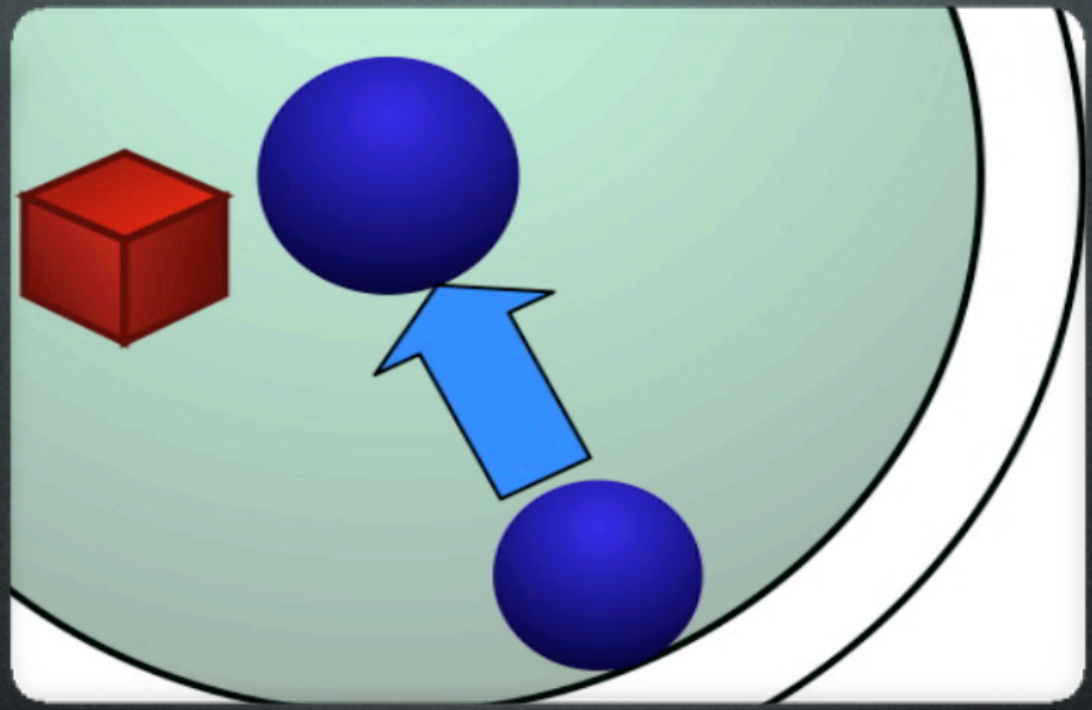
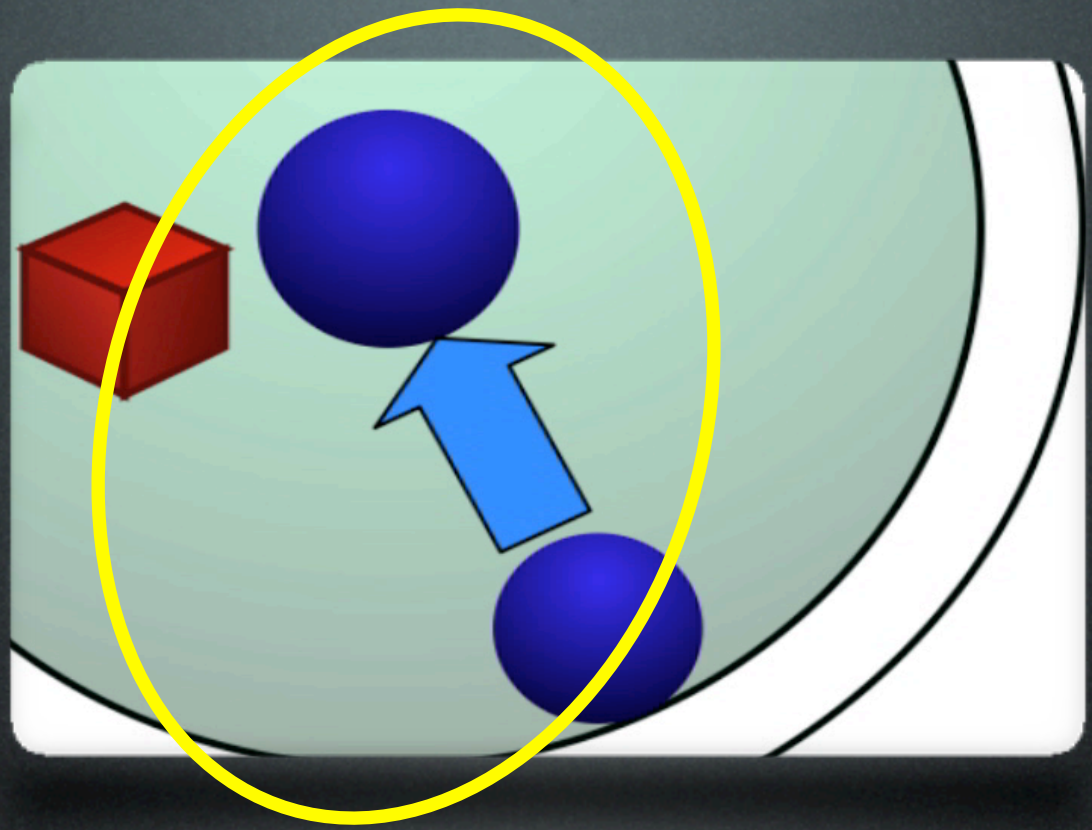
Distance to target neighbor



minimize: $\varepsilon(\mathbf{L}) = \varepsilon_{\text{pull}}(\mathbf{L}) + \varepsilon_{\text{push}}(\mathbf{L})$

$$\varepsilon_{\text{push}}(\mathbf{L}) = \sum_{ijl} \eta_{ij}(1-y_{il}) \left[1 + \|\mathbf{L}(\vec{x}_i - \vec{x}_j)\|^2 - \|\mathbf{L}(\vec{x}_i - \vec{x}_l)\|^2\right]_+$$



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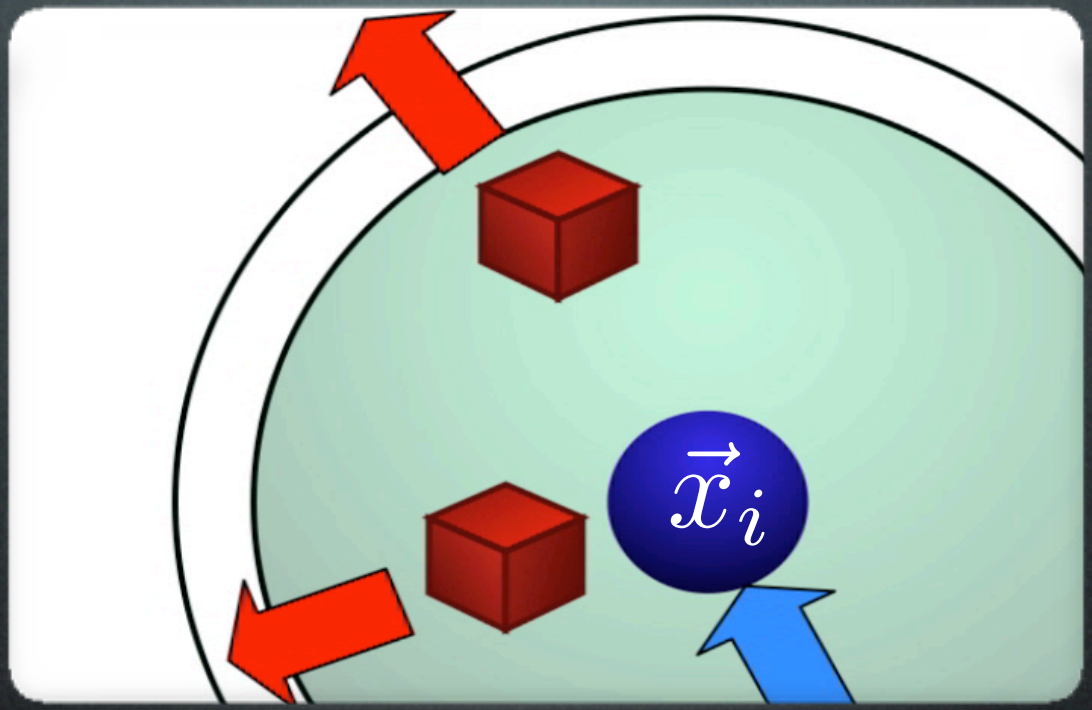

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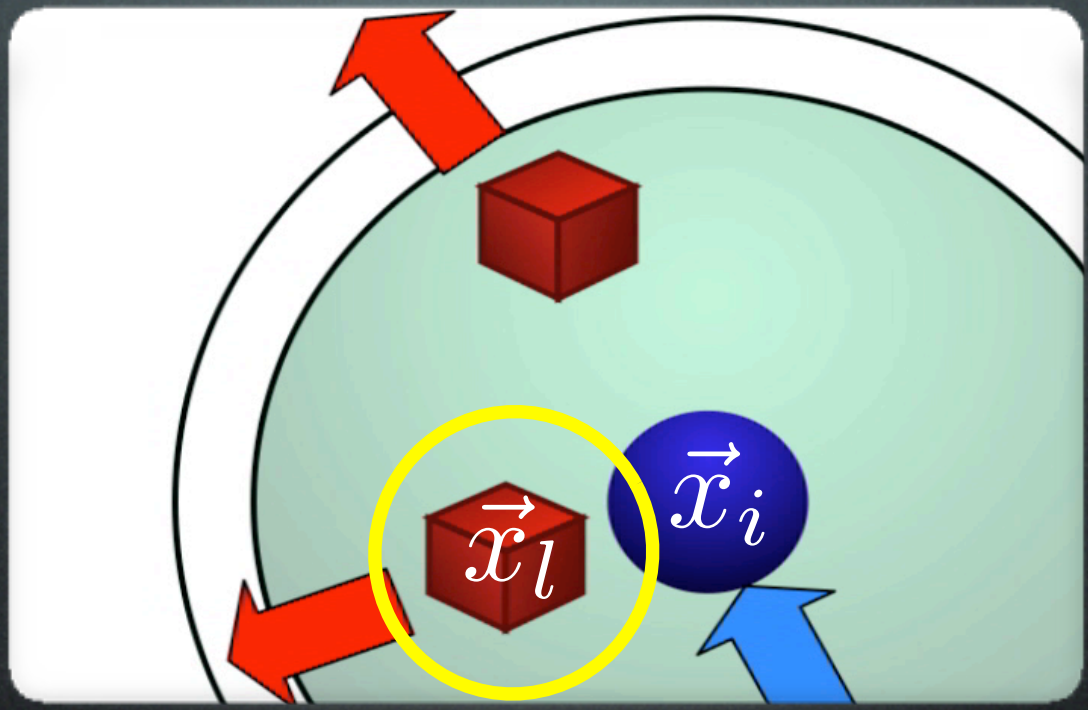
neighborhood indicator



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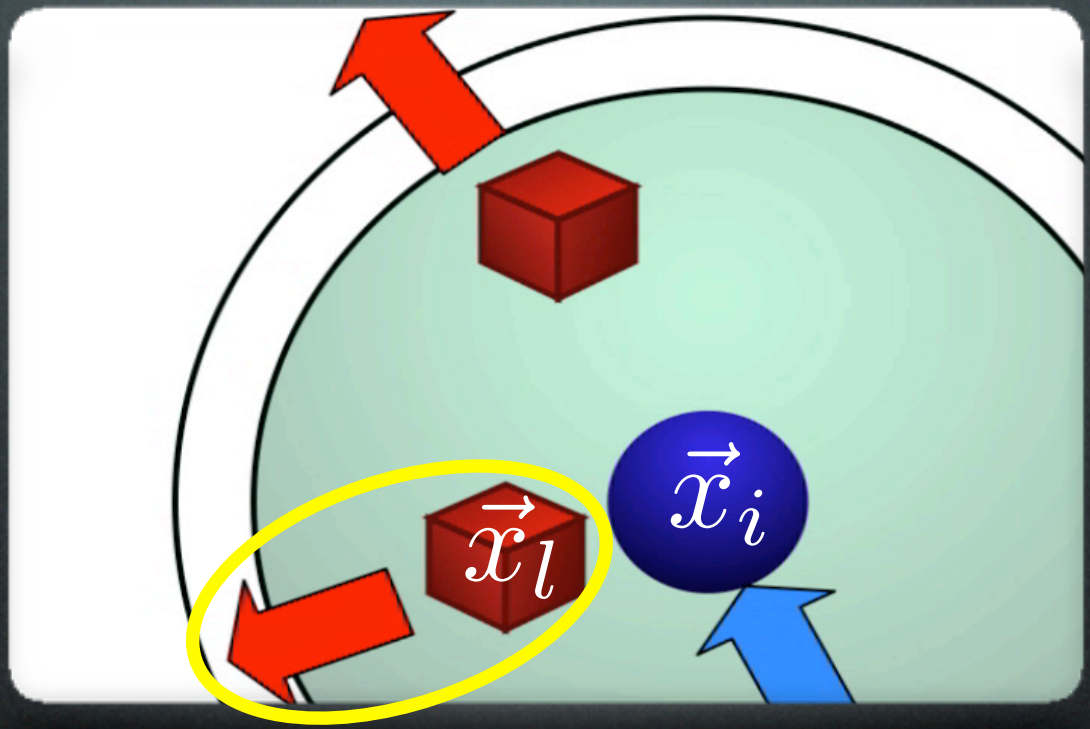
impostor



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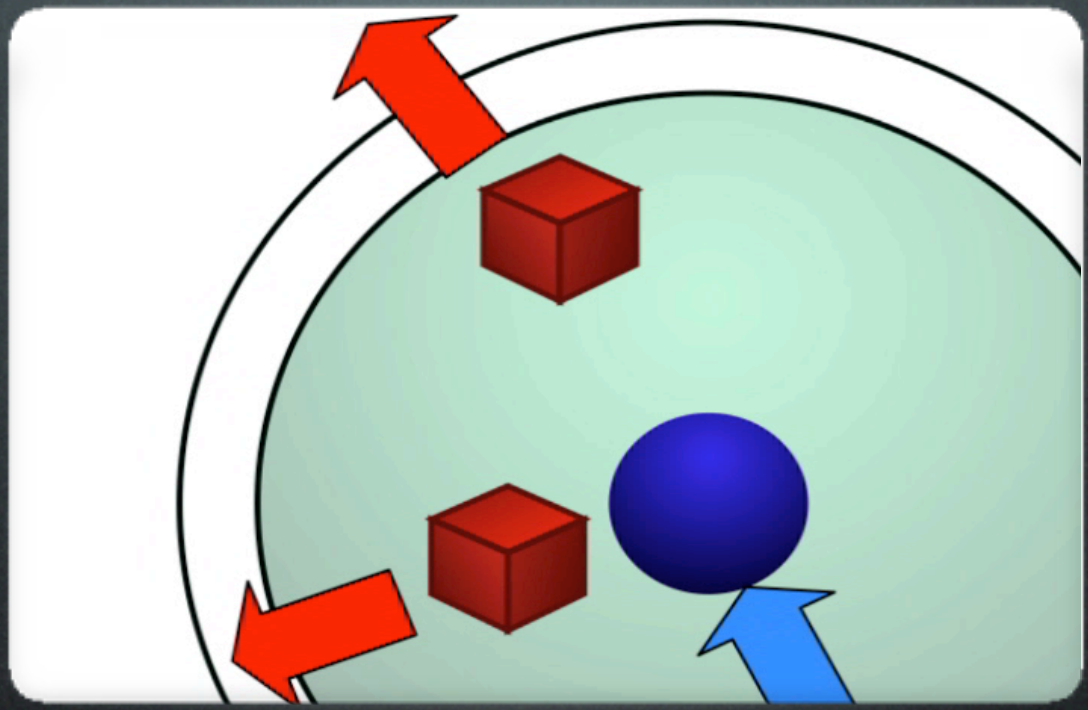
hinge loss



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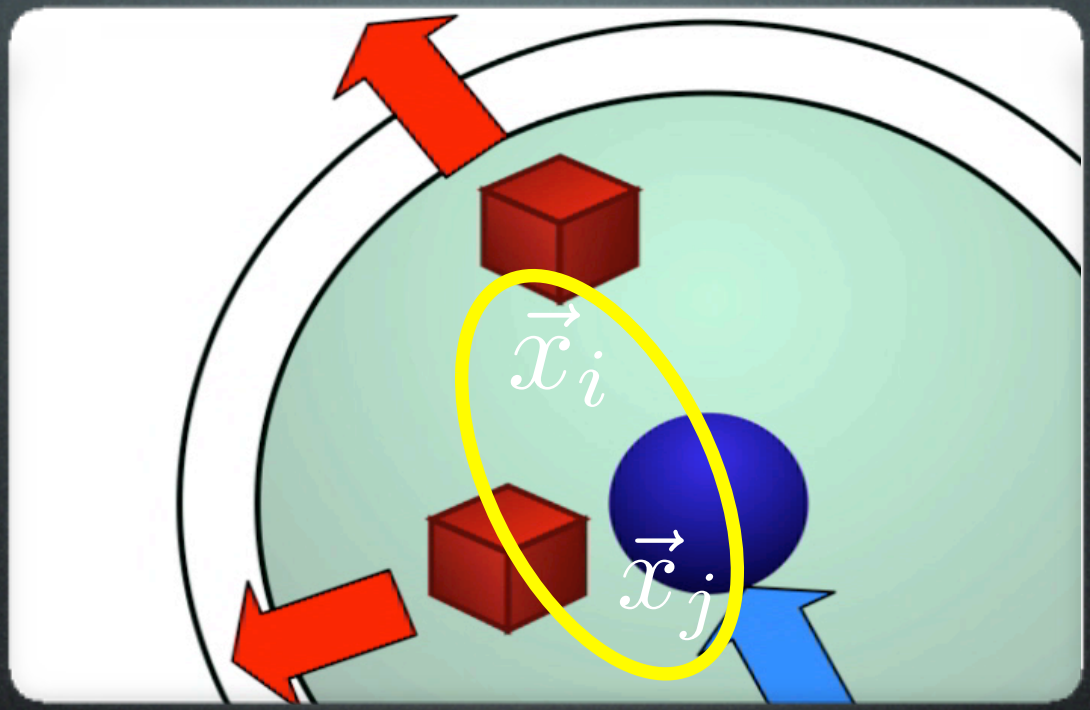
neighborhood radius



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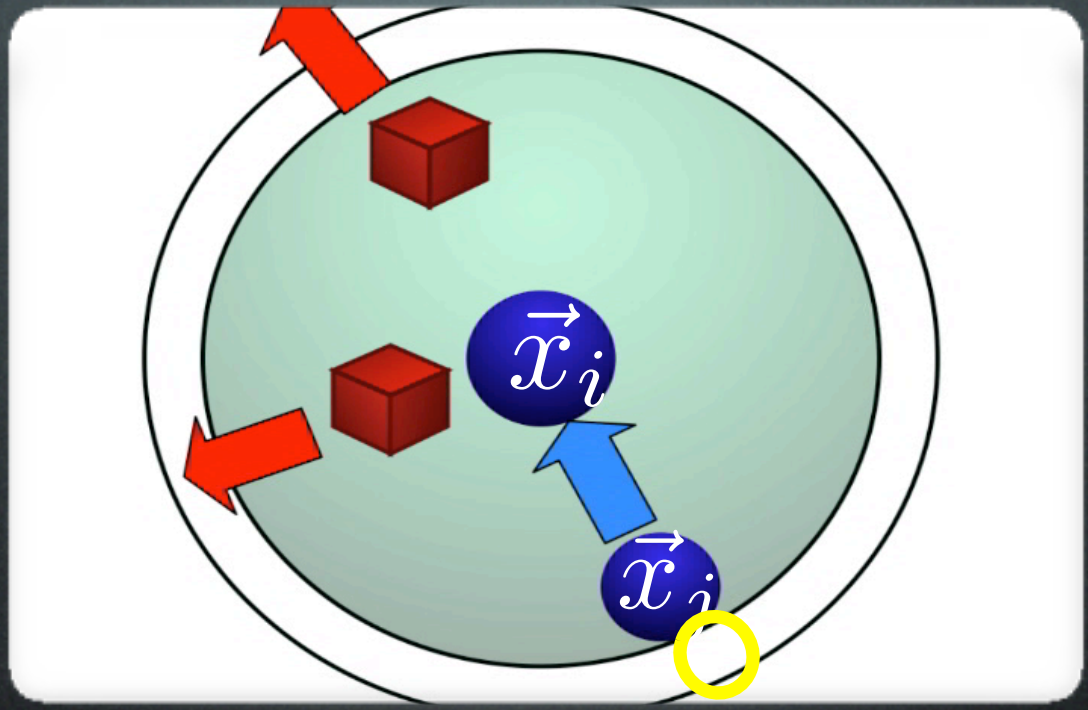

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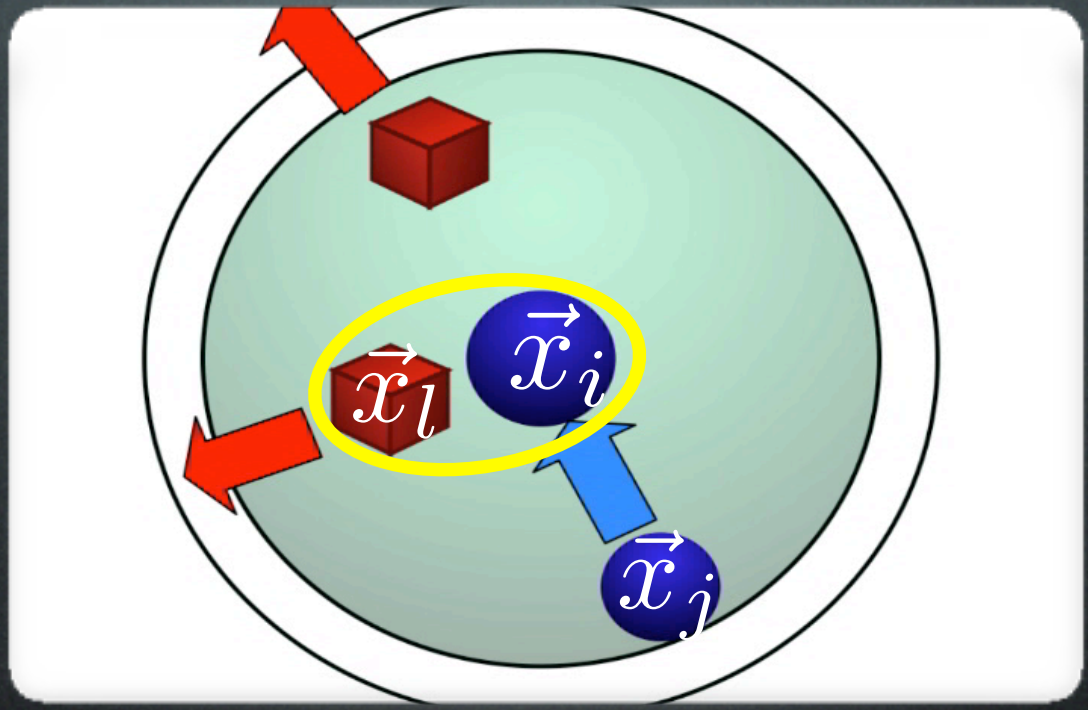
safety margin



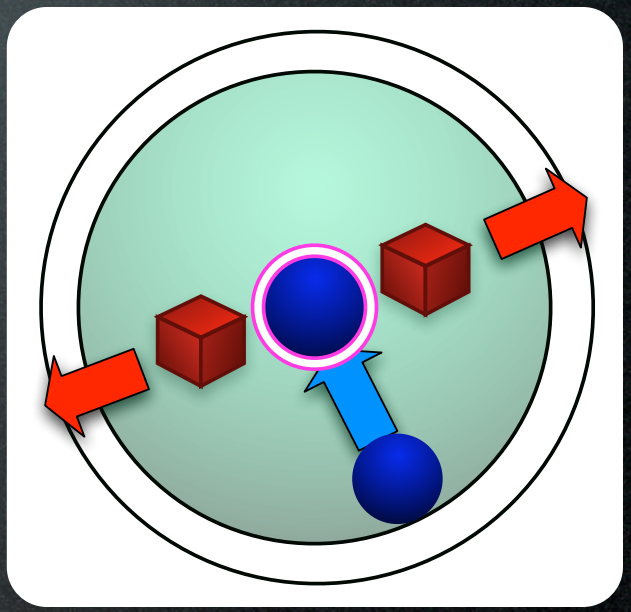
minimize: $\varepsilon(\mathbf{L}) = \varepsilon_{\text{pull}}(\mathbf{L}) + \varepsilon_{\text{push}}(\mathbf{L})$

$$\varepsilon_{\text{push}}(\mathbf{L}) = \sum_{ijl} \eta_{ij}(1-y_{il}) \left[1 + \|\mathbf{L}(\vec{x}_i - \vec{x}_j)\|^2 - \|\mathbf{L}(\vec{x}_i - \vec{x}_l)\|^2\right]_+$$

distance to impostor

Loss function

1. pull target neighbors closer
2. push impostors away



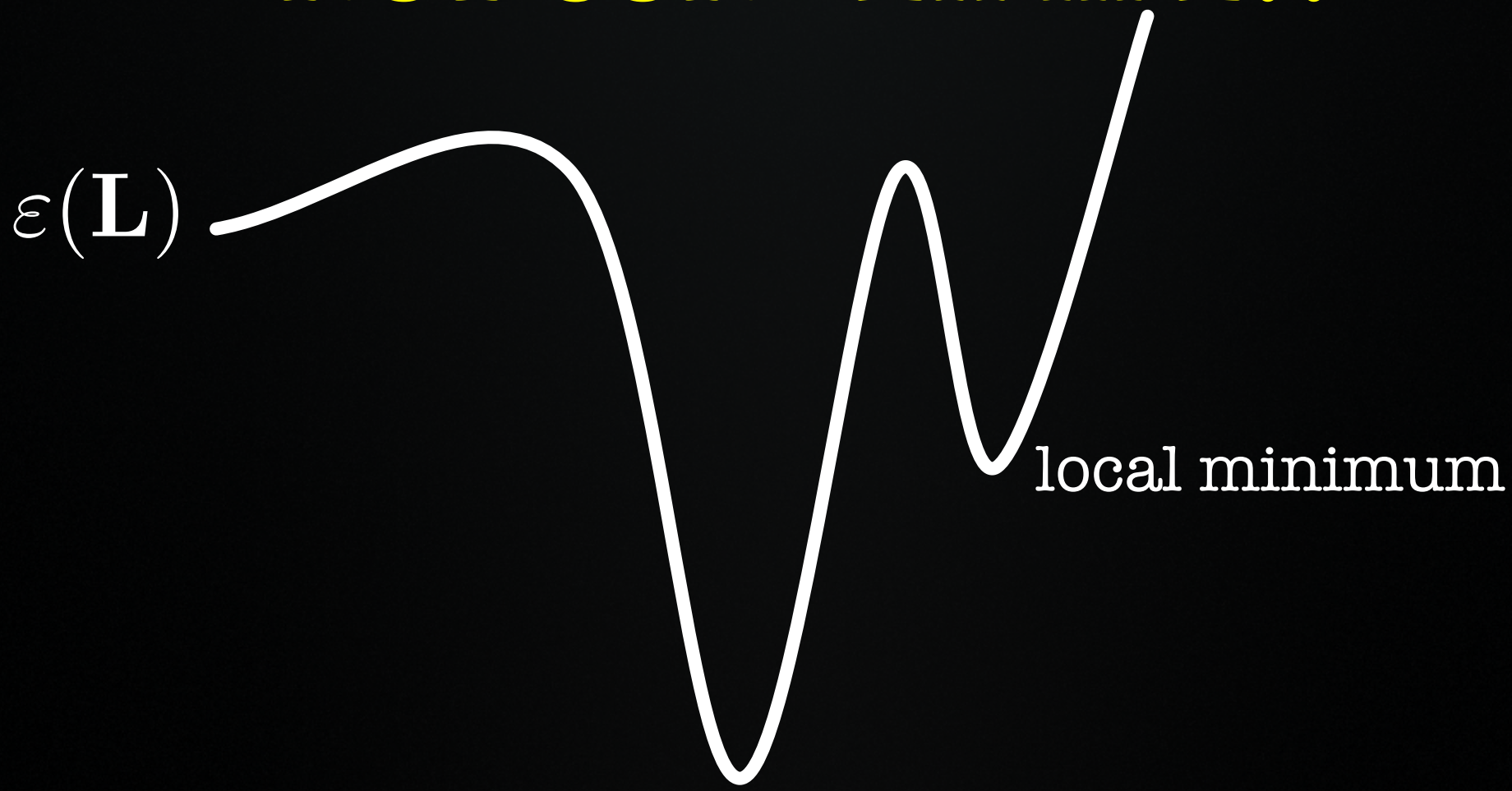
$$\varepsilon(\mathbf{L}) = \varepsilon_{\text{pull}}(\mathbf{L}) + \varepsilon_{\text{push}}(\mathbf{L})$$

$$\varepsilon_{\text{pull}}(\mathbf{L}) = \sum_{ij} \eta_{ij} \|\mathbf{L}(\vec{x}_i - \vec{x}_j)\|^2$$

$$\varepsilon_{\text{push}}(\mathbf{L}) = \sum_{ijl} \eta_{ij}(1 - y_{il}) \left[1 + \|\mathbf{L}(\vec{x}_i - \vec{x}_j)\|^2 - \|\mathbf{L}(\vec{x}_i - \vec{x}_l)\|^2\right]_+$$

(unit margin)

NOT CONVEX in L!!



Change of variable

Instead of learning $\mathbf{L}$ we learn $\mathbf{M} = \mathbf{L}^\top \mathbf{L}$.

with $\mathbf{M} \succeq 0$

$$\begin{aligned}\|\mathbf{L}(\vec{x}_i - \vec{x}_j)\|^2 &= (\vec{x}_i - \vec{x}_j)^\top \mathbf{L}^\top \mathbf{L}(\vec{x}_i - \vec{x}_j) \\ &= (\vec{x}_i - \vec{x}_j)^\top \mathbf{M}(\vec{x}_i - \vec{x}_j) \\ &= \|\vec{x}_i - \vec{x}_j\|^2_{\mathbf{M}}\end{aligned}$$

M defines Mahalanobis distance

Loss function is convex in M!

Convex optimization

minimize:

$$\underset{\mathrm{M}}{\text{minimize}}: \quad \varepsilon(\mathrm{M}) = \varepsilon_{\mathrm{pull}}(\mathrm{M}) + \varepsilon_{\mathrm{push}}(\mathrm{M})$$

subject to:

$$\mathrm{M} \succeq 0$$

Semidefinite Programming Problem

minimize:
M

$$\varepsilon(\mathrm{M}) = \varepsilon_{\mathrm{pull}}(\mathrm{M}) + \varepsilon_{\mathrm{push}}(\mathrm{M})$$

subject to:

$$\mathrm{M} \succeq 0$$

Linear programming problem with positive-semidefinite constraint.

Semidefinite Programming Problem

minimize:
M

$$\varepsilon(\mathrm{M}) = \varepsilon_{\mathrm{pull}}(\mathrm{M}) + \varepsilon_{\mathrm{push}}(\mathrm{M})$$

subject to:

$$\mathrm{M} \succeq 0$$

Linear programming problem with positive-semidefinite constraint.

Semidefinite Programmin[illegible]m

Can be solved efficiently with alternating projection or cutting plane algorithm.

$$\succeq 0$$

Line[illegible]rogramming problem with positive-semidefinite constraint.

Two ways of classification

k-NN using Mahalanobis distance

1. Learn M that minimizes $\varepsilon(\mathrm{M})$
2. Use k-NN with Mahalanobis distance

Two ways of classification

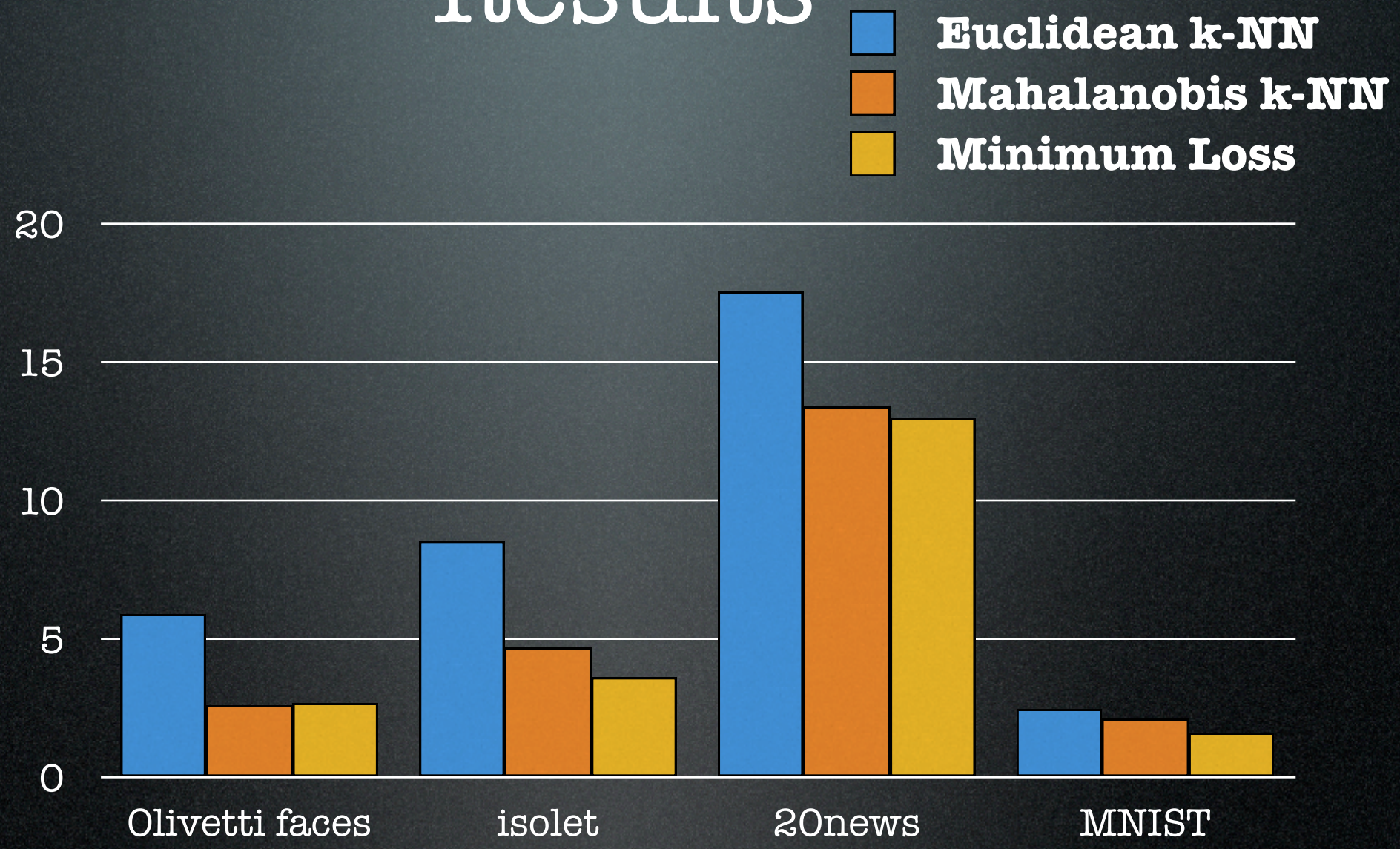
k-NN using Mahalanobis distance

1. Learn $\mathbf{M}$ that minimizes $\varepsilon(\mathbf{M})$
2. Use k-NN with Mahalanobis distance

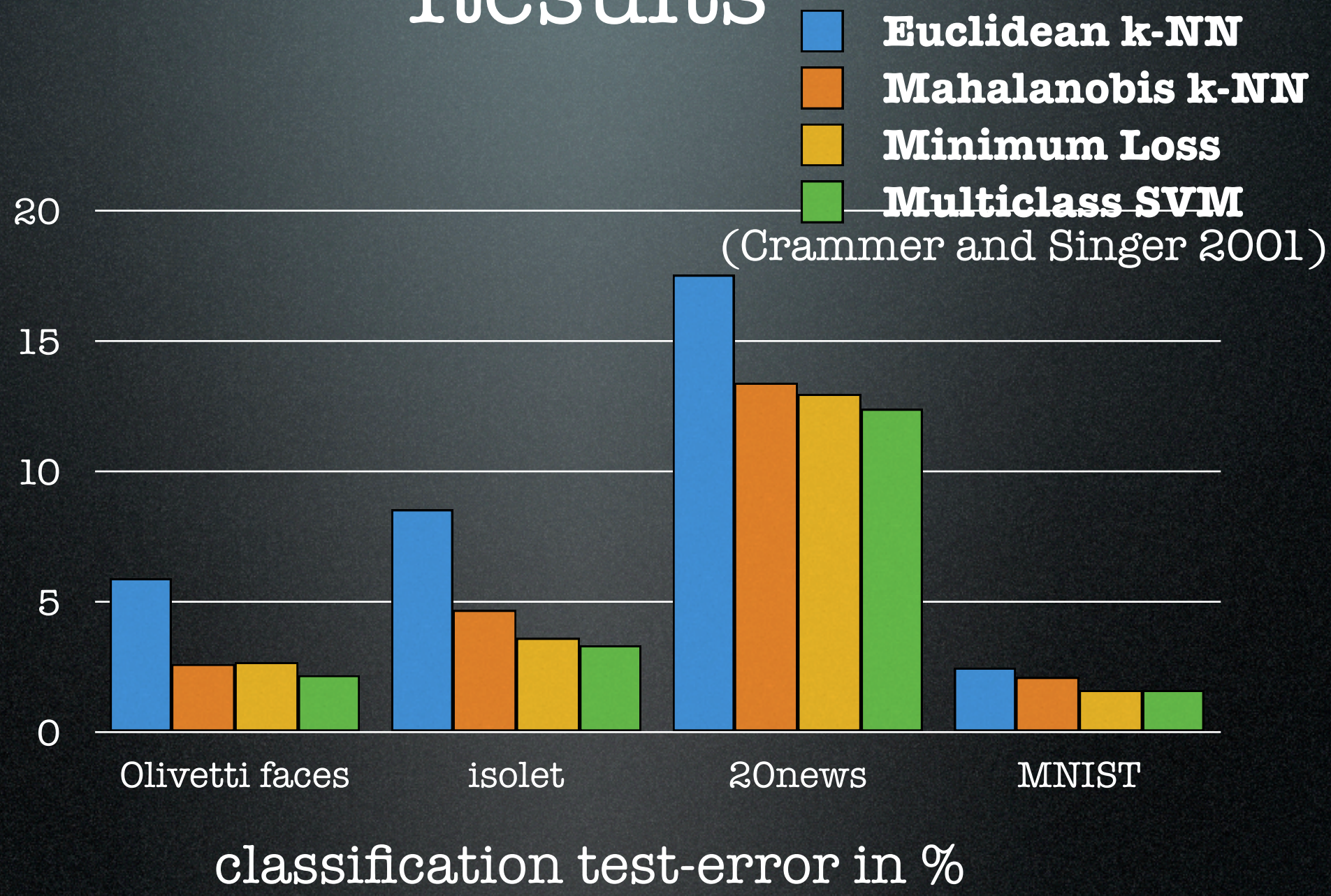
Minimum loss classification

1. Learn $\mathbf{M}$ that minimizes $\varepsilon(\mathbf{M})$
2. For each test point choose label that minimizes the loss function

Results


Euclidean k-NN
Mahalanobis k-NN
Minimum Loss
20
15
10
5
0
Olivetti faces
isolet
20news
MNIST
classification test error in %

Results


Euclidean k-NN
Mahalanobis k-NN
Minimum Loss
Multiclass SVM
(Crammer and Singer 2001)
20
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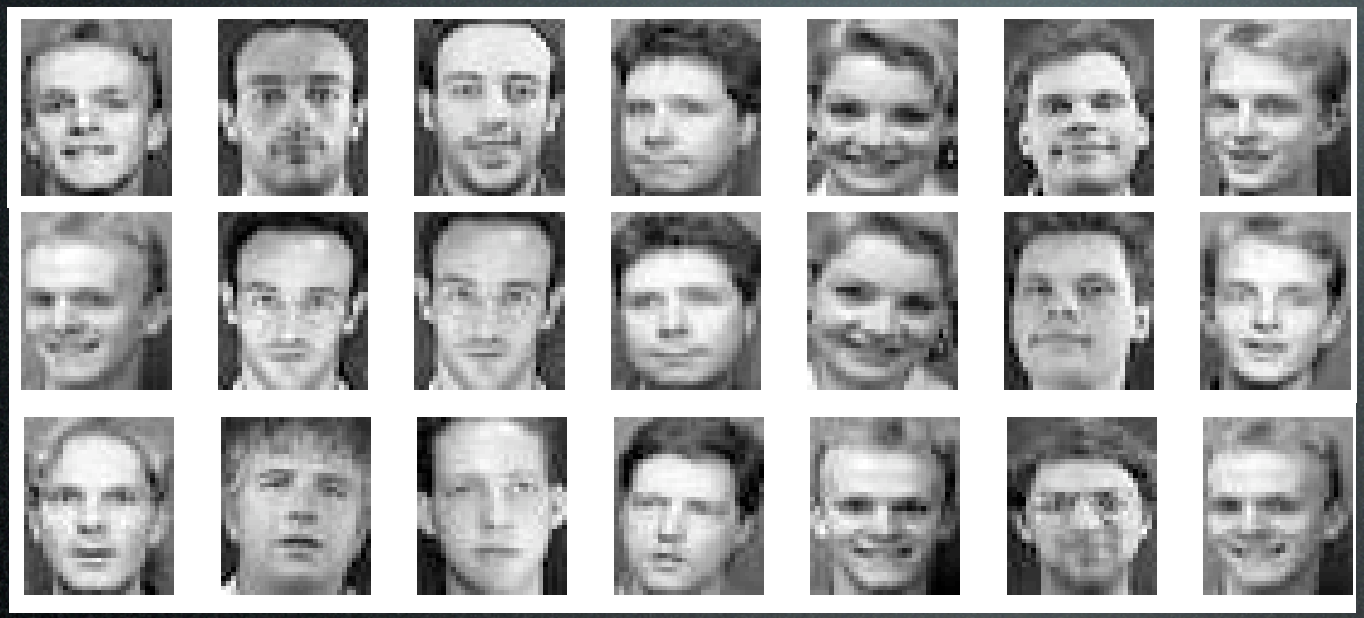
20news
MNIST
classification test-error in %

Olivetti Faces



test image

Mahalanobis NN

Euclidean NN

Train / Test images	**= 280/120**
Total constraints	**= 76 440**
Active constraints	**= 2 680**
Training time	**= 2 mins**

MNIST

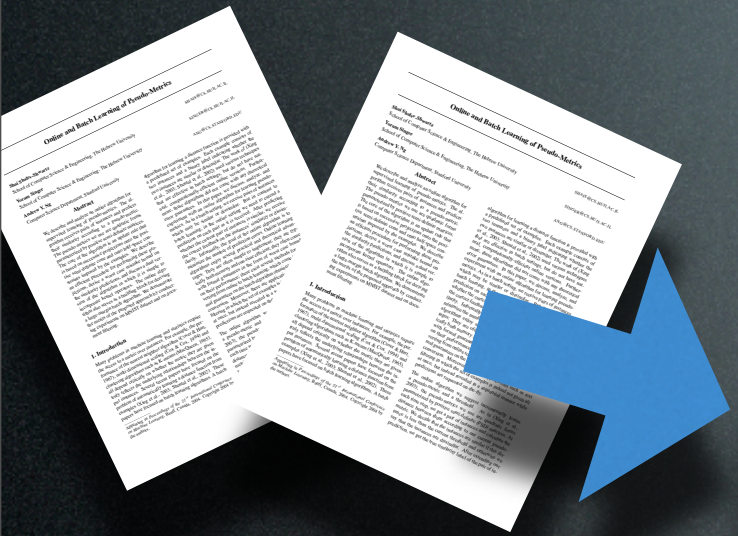
test digit

Mahalanobis NN

Euclidean NN

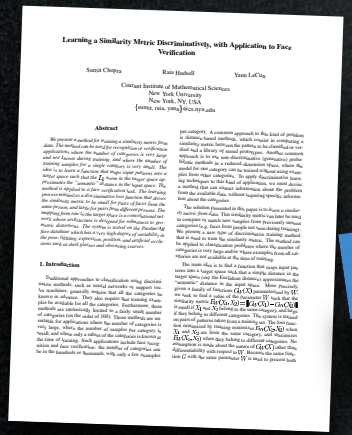
Train / Test images	=	60k/10k
Total constraints	=	3.3 Billion
Active constraints	=	243 596
Training time	=	3 hours

Connection to previous work



Xing et al, NIPS 2003

Shalev-Shwartz et al, ICML 2004



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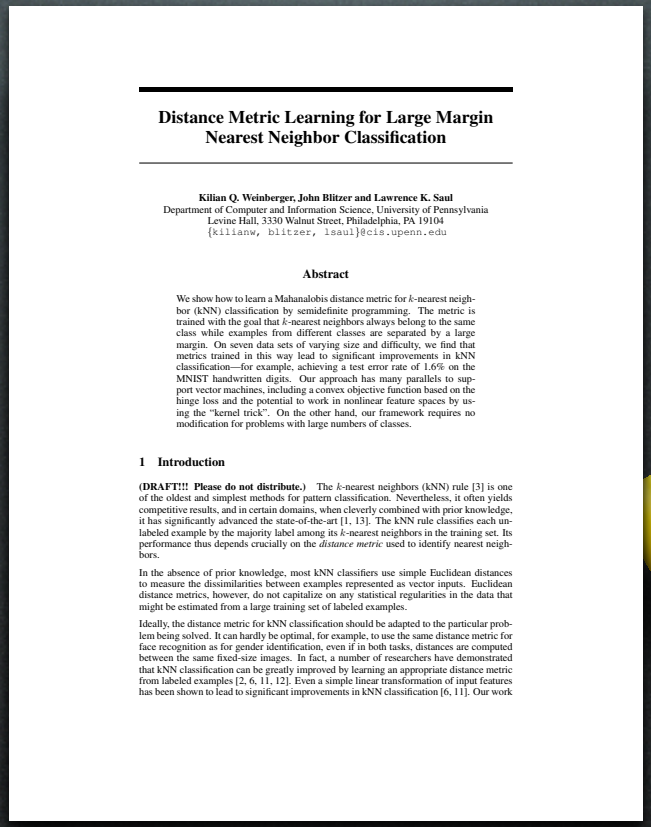

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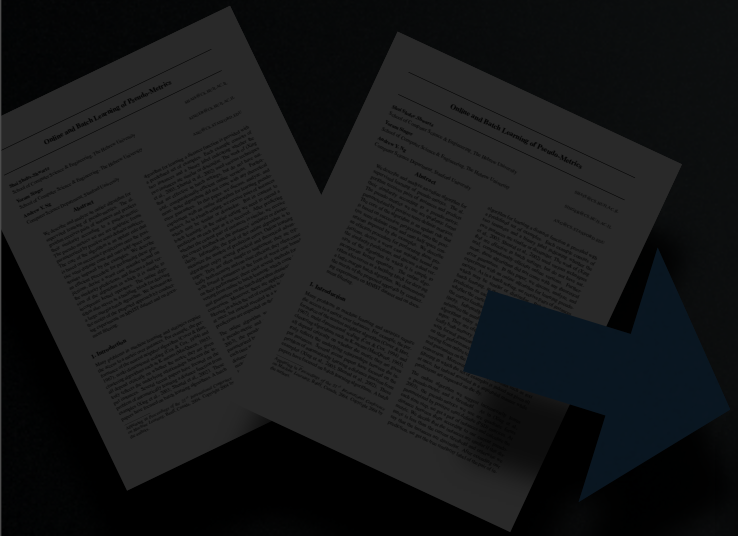

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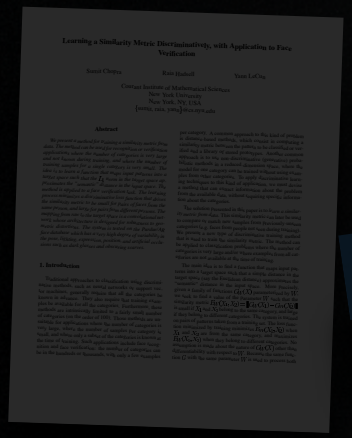

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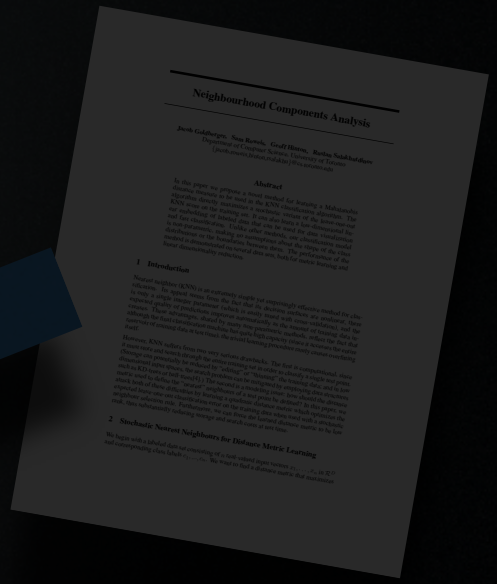

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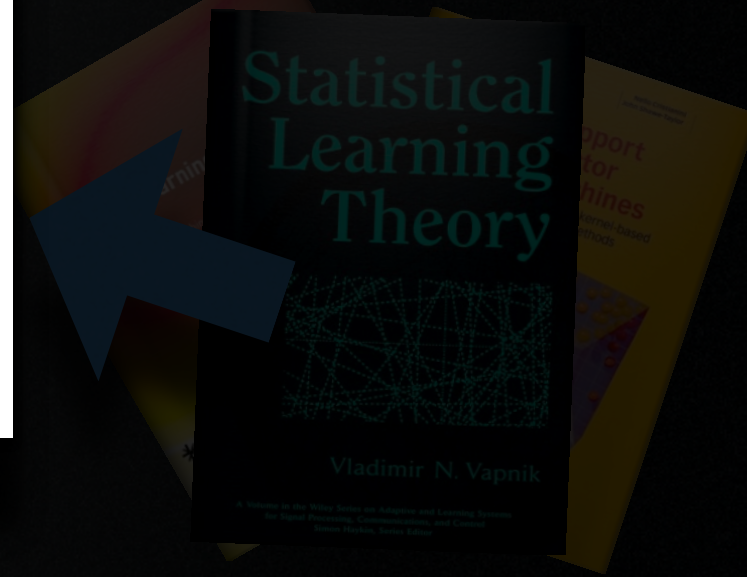

Vapnik 1998

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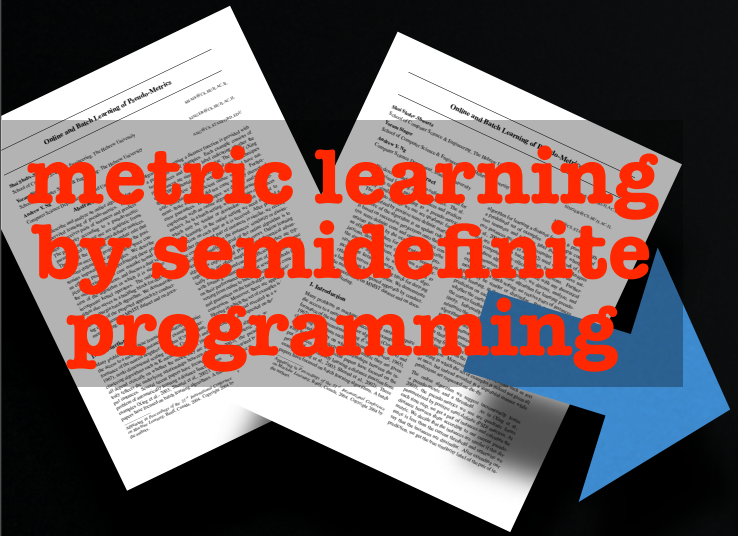

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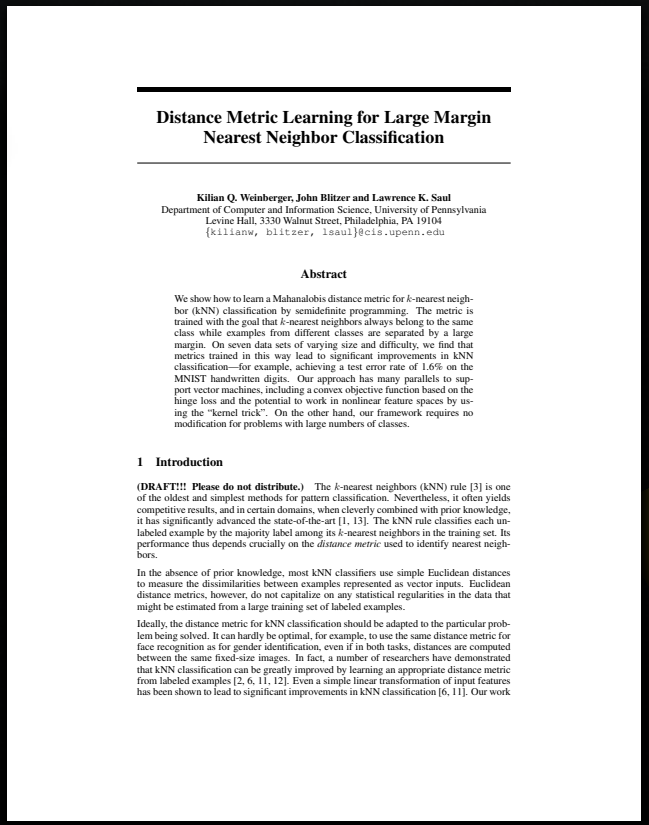

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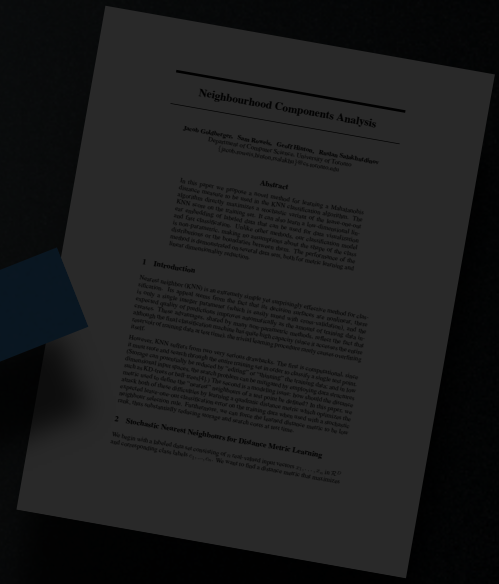

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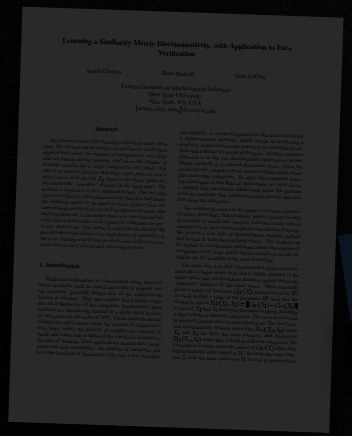

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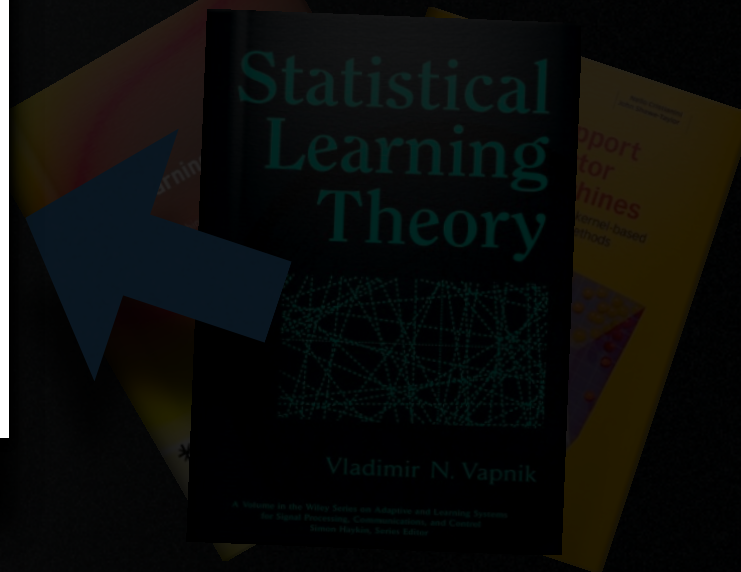

Vapnik 1998

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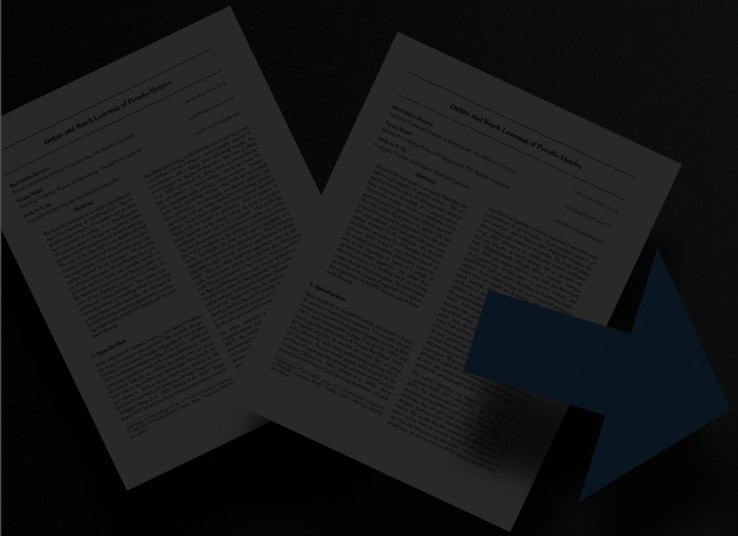

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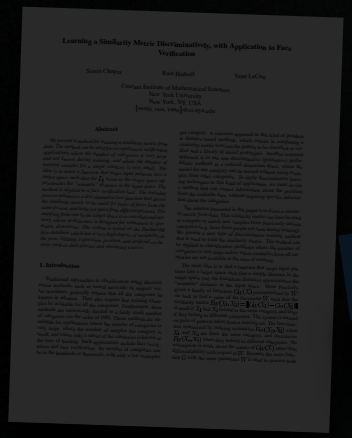

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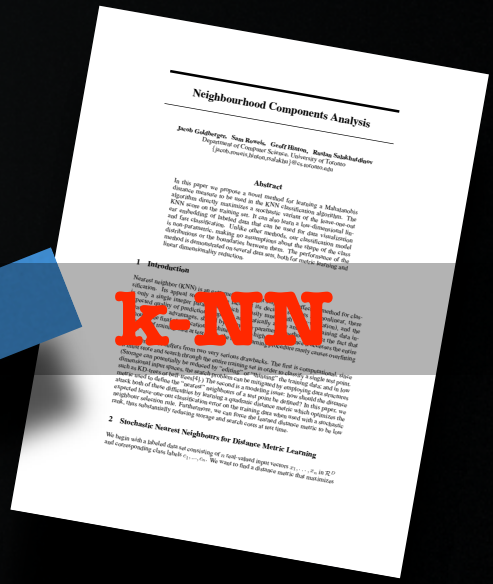

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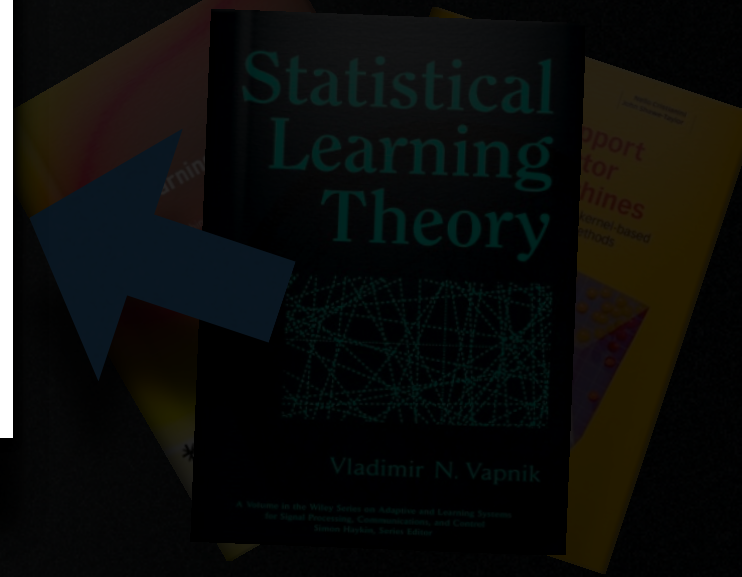

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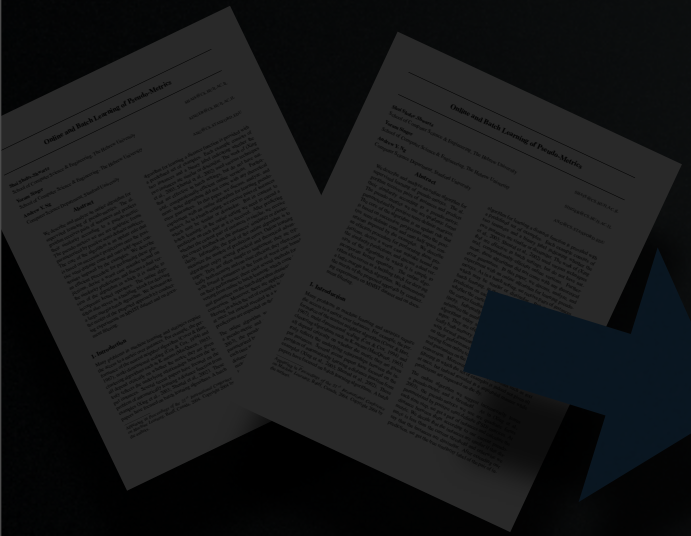

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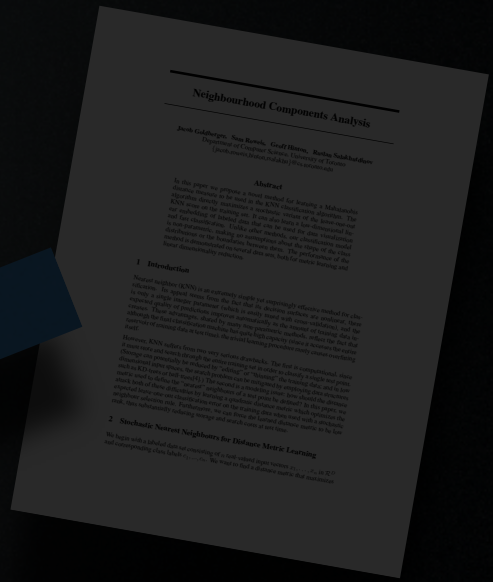

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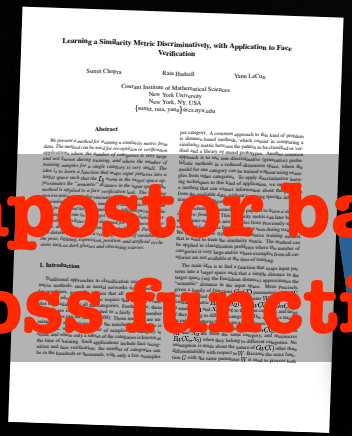
impostor based loss function



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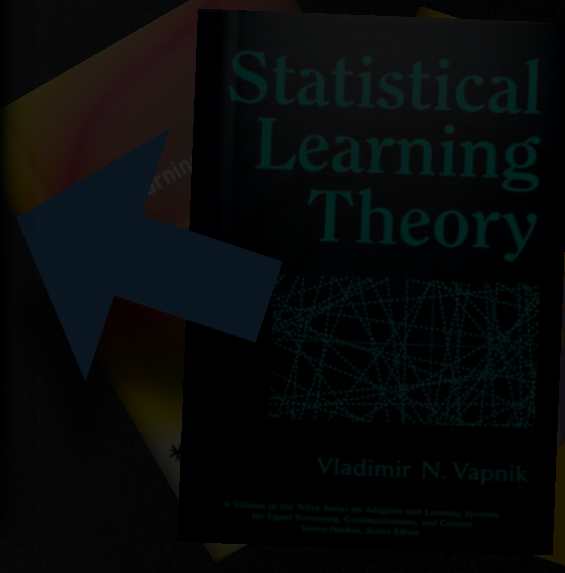

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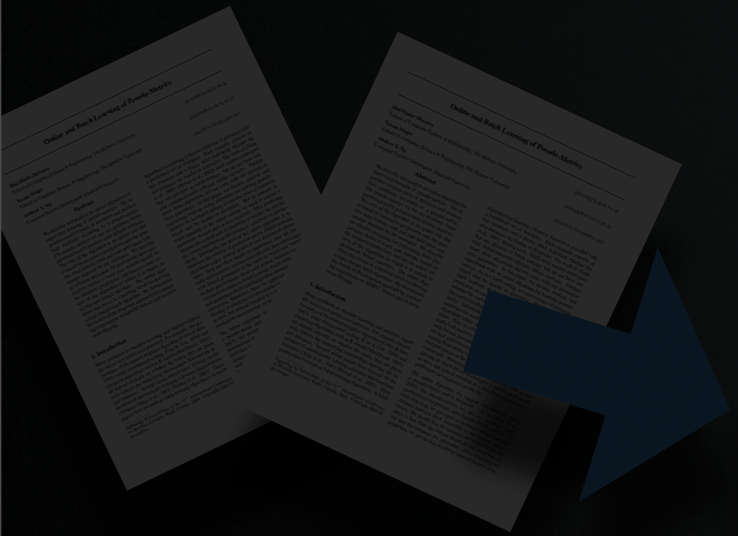

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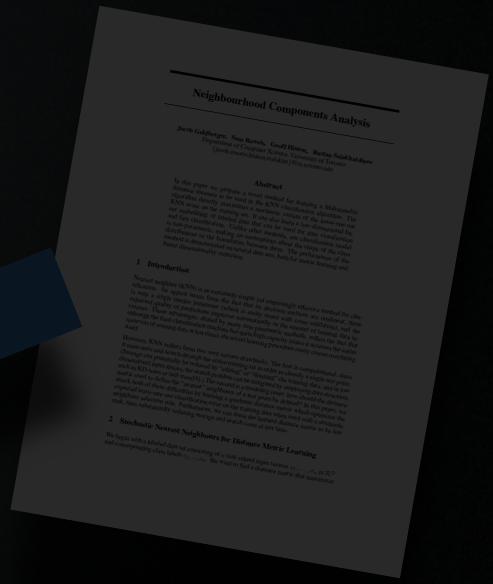

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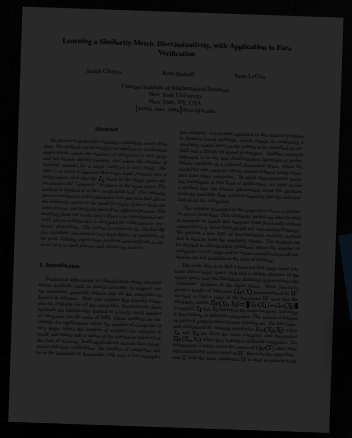

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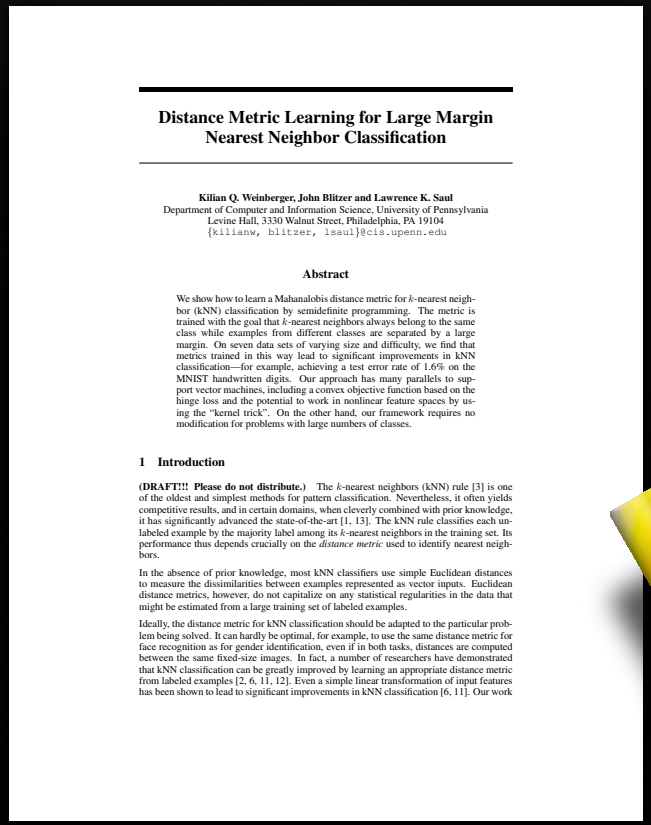

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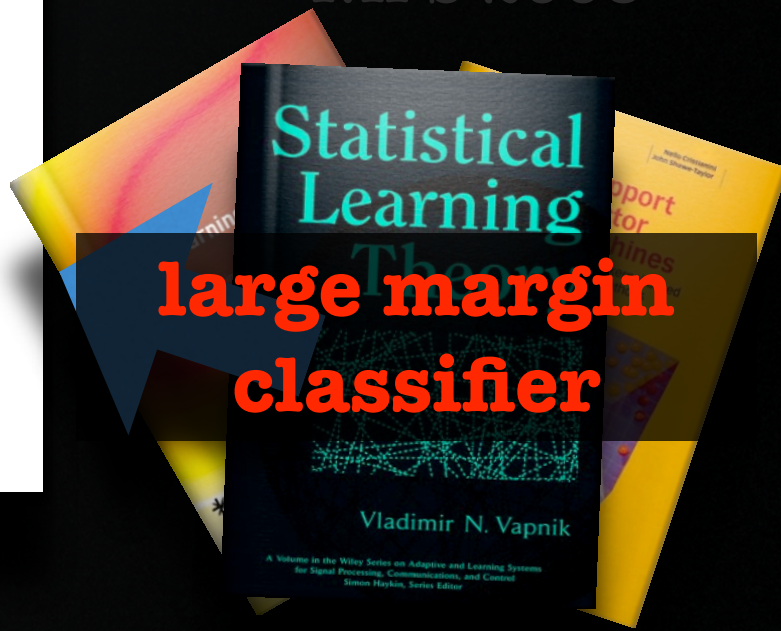
(DRAFT!!! Please do not distribute.) The k-nearest neighbors (kNN) rule [3] is one of the oldest and simplest methods for pattern classification. Nevertheless, it often yields competitive results, and in certain domains, when cleverly combined with prior knowledge, it has significantly advanced the state-of-the-art [1, 13]. The kNN rule classifies each unlabeled example by the majority label among its k-nearest neighbors in the training set. Its performance thus depends crucially on the *distance metric* used to identify nearest neighbors.

In the absence of prior knowledge, most kNN classifiers use simple Euclidean distances to measure the dissimilarities between examples represented as vector inputs. Euclidean distance metrics, however, do not capitalize on any statistical regularities in the data that might be estimated from a large training set of labeled examples.

Ideally, the distance metric for kNN classification should be adapted to the particular problem being solved. It can hardly be optimal, for example, to use the same distance metric for face recognition as for gender identification, even if in both tasks, distances are computed between the same fixed-size images. In fact, a number of researchers have demonstrated that kNN classification can be greatly improved by learning an appropriate distance metric from labeled examples [2, 6, 11, 12]. Even a simple linear transformation of input features has been shown to lead to significant improvements in kNN classification [6, 11]. Our work



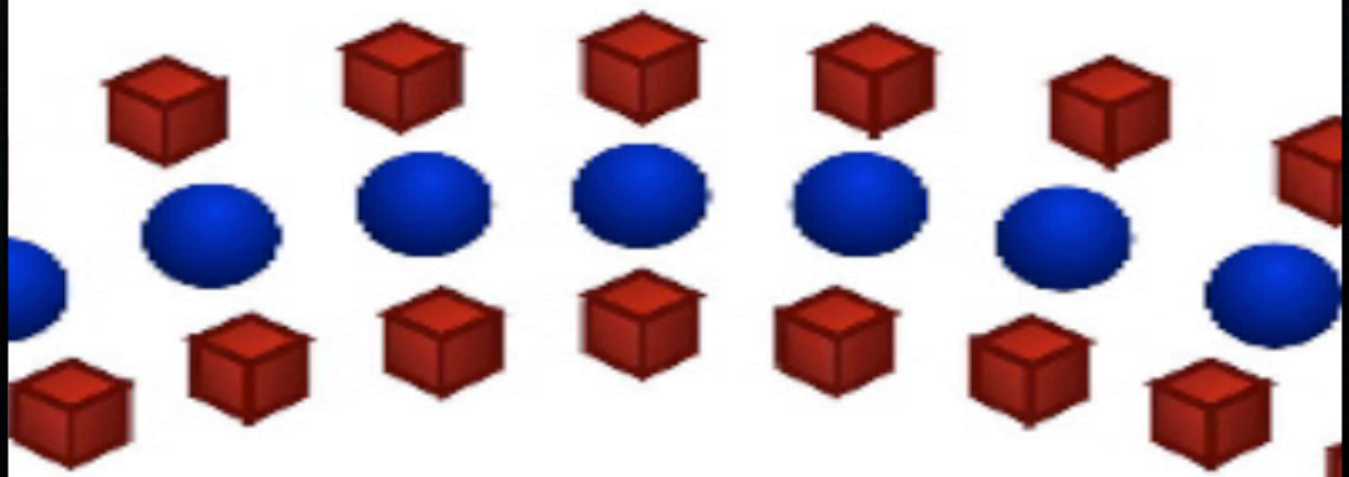
large margin classifier

Vapnik 1998

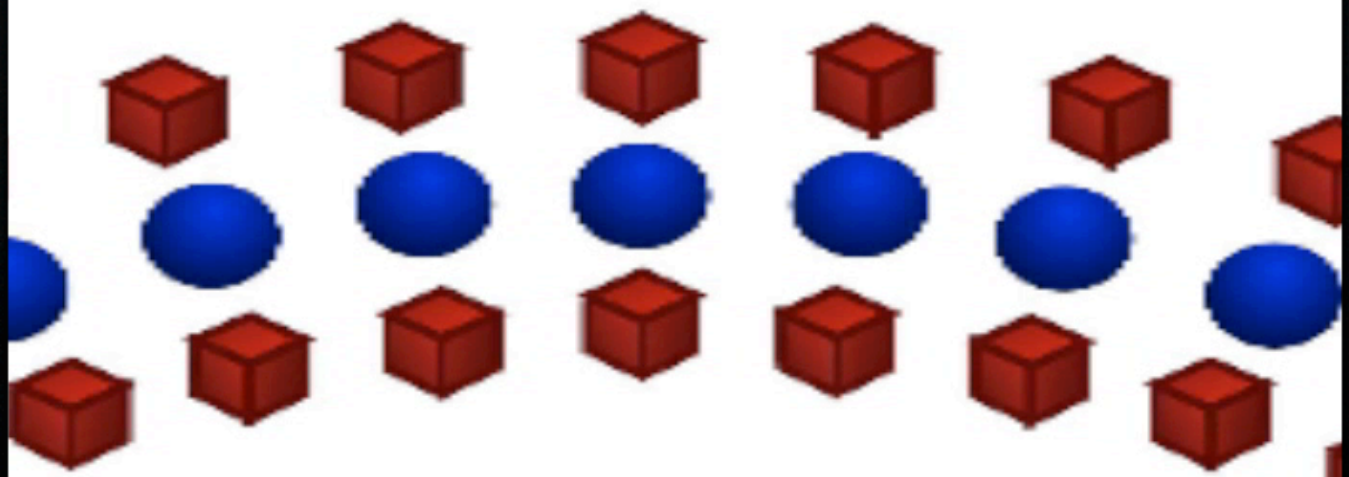
Conclusion

- Novel algorithm for metric learning
- Replaces linear decision boundary in SVM by kNN decision boundary
- Training complexity independent of number of classes (unlike multiclass SVM)
- Optimization is a semidefinite program
- (Can be kernelized)

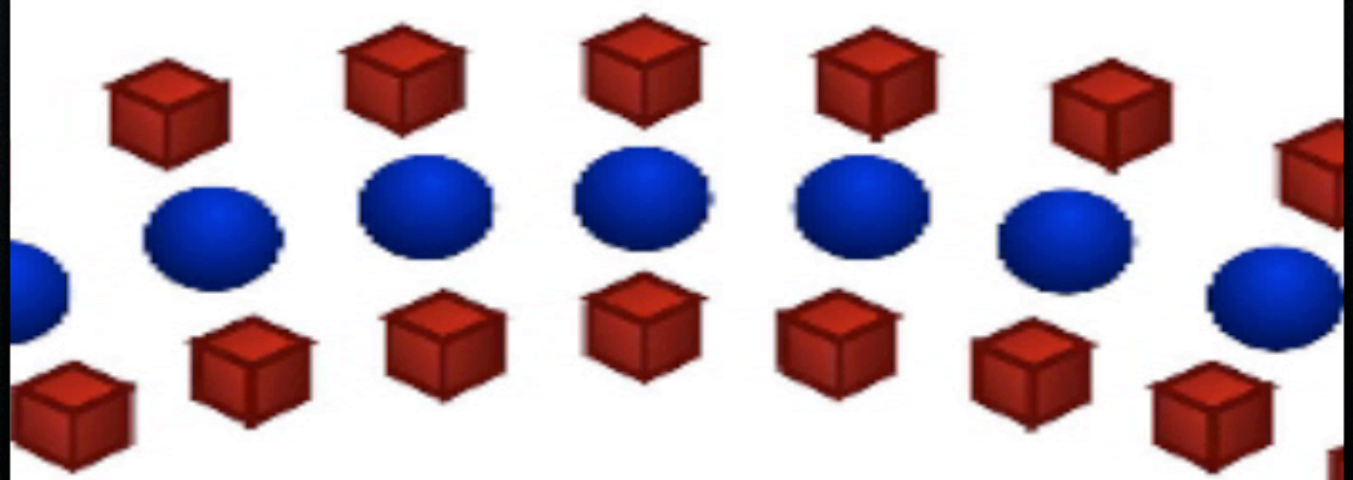
Future work



Future work



Future work



Locally adaptive k-NN that exploits manifold structure

Thank you!!!