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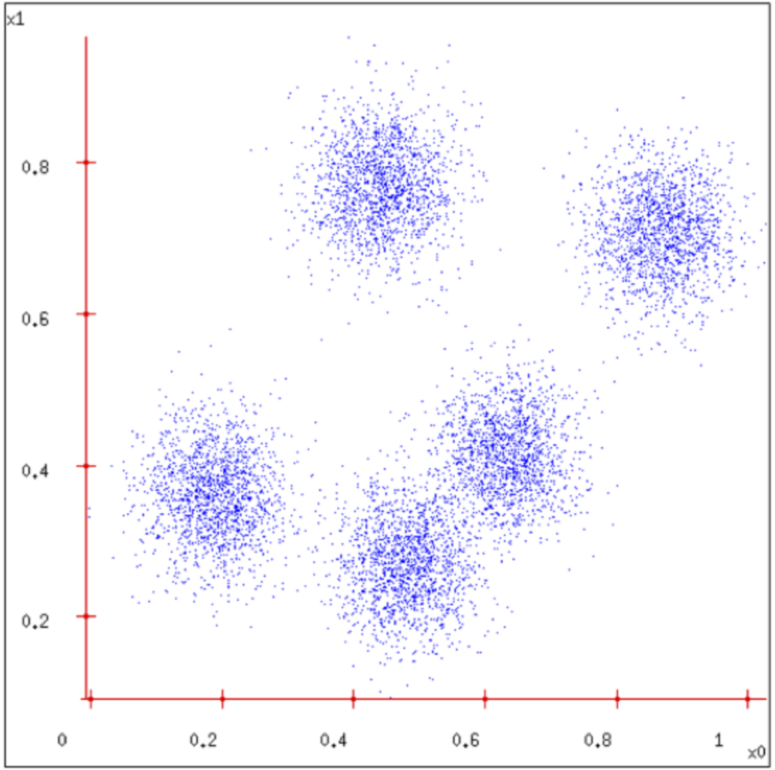
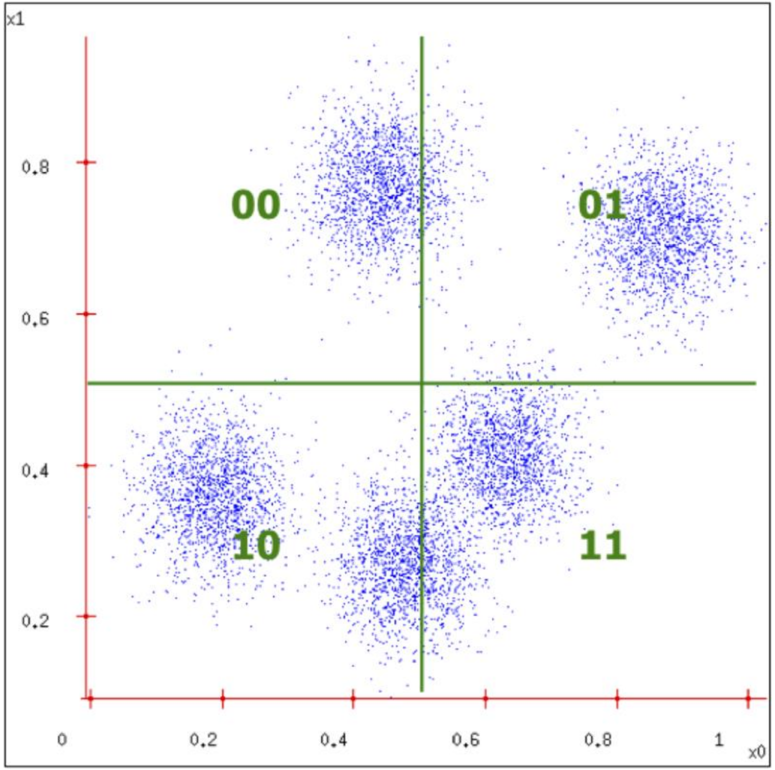
Introduction to Machine Learning

k-Means and k-medoids Clustering

Some Data



Grid Clustering



Expectation Maximization

A local search process where we estimate parameters and then adjust them to increase likelihood of correctness

Example – Find one of the roots of $x^5 - 3x^2 + 2x - 17 = 0$.

- Rewrite as $x = (3x^2 - 2x + 17)^{1/5}$.
- "Guess" that $x = 1$.
- Substitute into right hand side and recalculate, $x = 1.7826$.
- Repeat until convergence

$$1 \to 1.7826 \to 1.8716 \to 1.8845 \to 1.8864 \to 1.8866 \to 1.8867 \to \cdots$$

The proof sets up what we call a "contraction map."

EM for Clustering

- Bivariate Gaussians with equal variance
- *k*-means clustering

- **Assumptions**
  - We have *k* multi-variate Gaussian/spherical clusters.
  - Each cluster has an unknown mean vector: $\langle \boldsymbol{\mu}_1, \ldots \boldsymbol{\mu}_k \rangle$.
  - We do not know which Gaussian generated which data point.
- We can apply EM to find the cluster means.
- We can use the cluster means to assign the points.

k-Means Clustering

Example

- Let $k = 2$.
- Describe a generated instance as $y_i = \langle x_i, z_{i1}, z_{i2} \rangle$, where $z_{ij} = 1$ means x_i was generated by cluster j.
- Begin by guessing values for $h = \langle \mu_1, \mu_2 \rangle$ at random.

E Step: (Expectation)

$$E[z_{ij}] = \frac{P(x_i|\mu_j)}{\sum_{k=1}^{2} P(x_i|\mu_k)} = \frac{\exp\left[-\frac{1}{2\sigma}(x_i - \mu_j)^2\right]}{\sum_{k=1}^{2} \exp\left[-\frac{1}{2\sigma}(x_i - \mu_k)^2\right]}$$

M Step: (Maximization, $h' = \langle \mu_1', \mu_2' \rangle$)

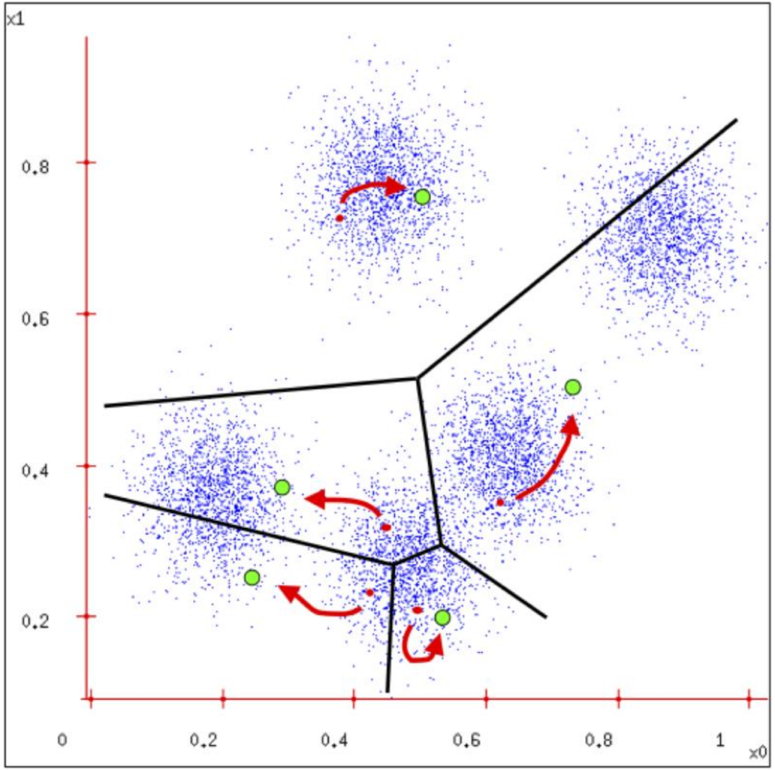
$$\mu_j = \frac{\sum_{i=1}^{m} E[z_{ij}] x_i}{\sum_{i=1}^{m} E[z_{ij}]}$$

k-Means Clustering

Algorithm 10.3 K-Means Clustering

```
function KMeans(𝒟, k)
    initialize μ_1, ..., μ_k randomly
    repeat
        for all x_i ∈ 𝒟 do
            c ← arg min_{μ_j} d(x_i, μ_j)        ▷ d() is the distance between x_i and μ_j.
            assign x_i to the cluster c
        end for
        recalculate all μ_j based on new clusters
    until no change in μ_1, ..., μ_k
    return μ_1, ..., μ_k
end function
```

Illustrating *k*-Means



Another Illustration of *k*-Means

1 2 3 5 6 7 10

$K = 2$

$$\underbrace{1\ 2\ 3\ 5}_{2.5} \qquad \underbrace{6\ 7\ 10}_{7.67}$$

$$\underbrace{1\ 2\ 3}_{2} \qquad \underbrace{3\ 6\ 7\ 10}_{7.5}$$

K-Medoids

- Representative object or member of a data set
- Different objective functions
  - *K*-means

$$J(\mathcal{C}) = \sum_{j=1}^{K} \sum_{x_i \in \mathcal{C}} \left(x_i - c_j\right)^2$$

  - *K*-medoids

$$J(\mathcal{C}) = \sum_{j=1}^{K} \sum_{x_i \in \mathcal{C}} \left(x_i - m_j\right)^2$$

Partitioning Around Medoids (PAM)

Algorithm 10.4 K-Medoids Clustering

function KMEDOIDS-PAM($\mathcal{D}, k$)
    select $\mathbf{m}_1, \ldots, \mathbf{m}_k$ randomly
    repeat
        for all $\mathbf{x}_i \in \mathcal{D}$ **do**
            $c \leftarrow \arg\min_{\mathbf{m}_j} d(\mathbf{x}_i, \mathbf{m}_j)$ $\triangleright$ $d()$ is the distance between $\mathbf{x}_i$ and $\mathbf{m}_j$.
            assign $\mathbf{x}_i$ to the cluster c
        end for
        $distortion_{k\text{-medoids}} = \sum_{j=1}^{k} \sum_{i \in ownedby(\mathbf{c}_j)} (\mathbf{x}_i - \mathbf{m}_j)^2$
        for all $\mathbf{m}_i \in \mathbf{m}$ **do**
            for all $\mathbf{x}_j \in \mathcal{D}$ where $\mathbf{x}_j \notin \mathbf{m}$ **do**
                swap $\mathbf{m}_i$ and $\mathbf{x}_j$
                $distortion'_{k\text{-medoids}} = \sum_{j=1}^{k} \sum_{i \in ownedby(\mathbf{c}_j)} (\mathbf{x}_i - \mathbf{m}_j)^2$
                if $distortion_{k\text{-medoids}} \leq distortion'_{k\text{-medoids}}$ **then**
                    swap back
                end if
            end for
        end for
    until no change in $\mathbf{m}_1, \ldots, \mathbf{m}_k$
    return $\mathbf{m}_1, \ldots, \mathbf{m}_k$
end function

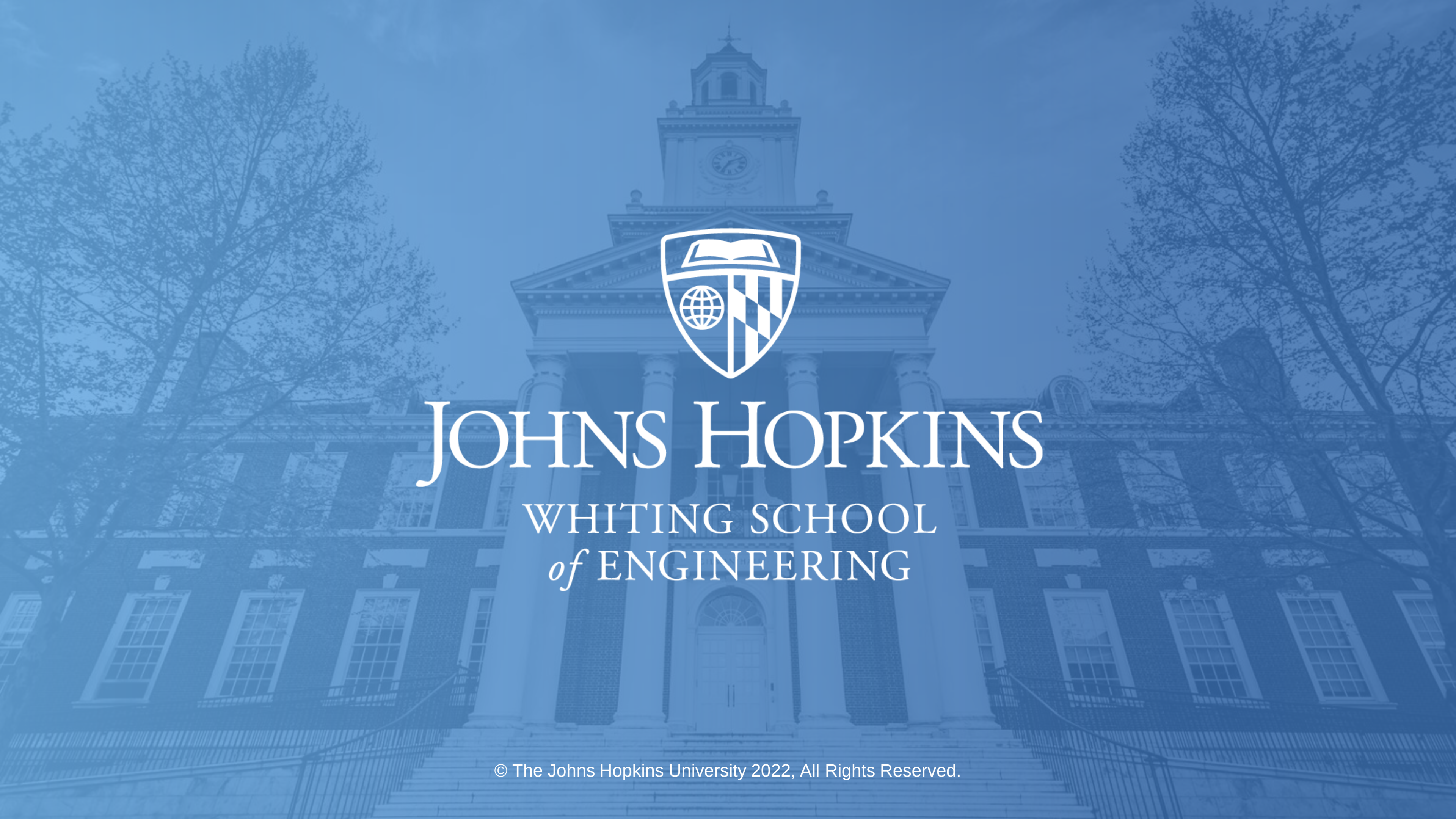
Fuzzy *c*-Means

- A method to create “soft” clusters, where f is a level of ”fuzzification” in the range $1 \ldots n$
  - $f = 1$ indicates “crisp” clusters
  - $f > 1$ indicates ”soft” clusters
- Objective function

$$J(\mathcal{C}) = \sum_{i=1}^{n} \sum_{j-1}^{c} w_j(x_i)^f \left\| c_j - x_i \right\|^2$$

$$w_j(x_i) = \frac{1}{\sum_{k=1}^{c} \left(\frac{\left\| c_j - x_i \right\|}{\left\| c_k - x_i \right\|} \right)^{2/(f-1)}}$$

$$c_j = \frac{\sum_{i=1}^{n} w_j(x_i)^f x_i}{\sum_{i=1}^{n} w_j(x_i)^f}$$



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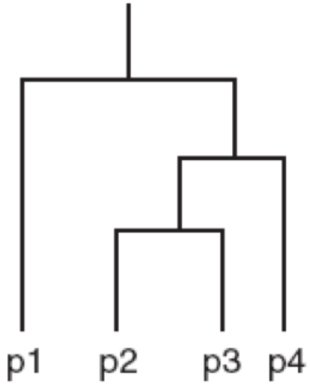
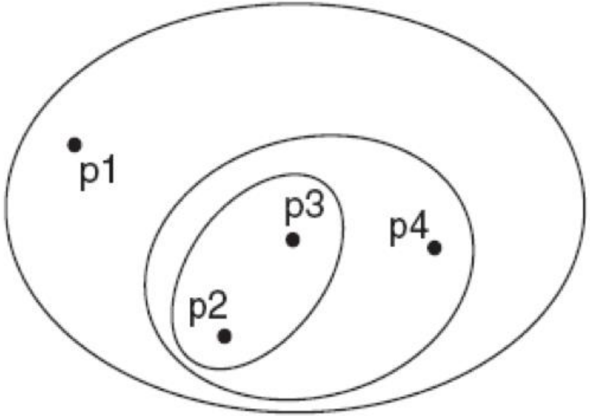
Introduction to Machine Learning

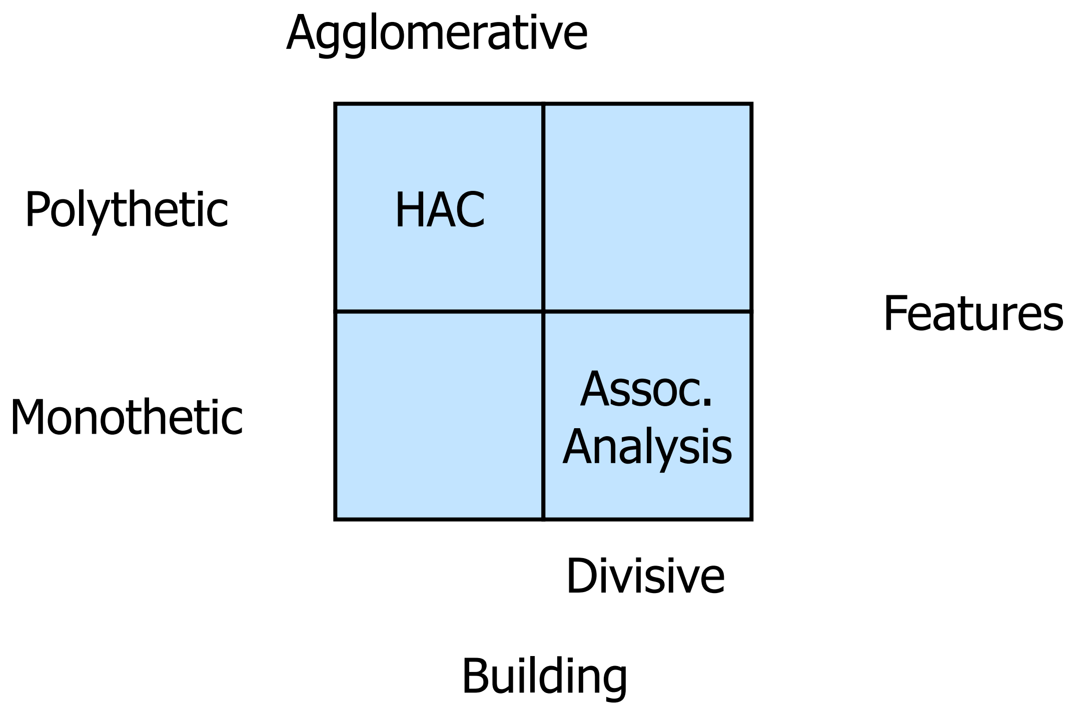
Hierarchical Agglomerative Clustering

Dendrogram

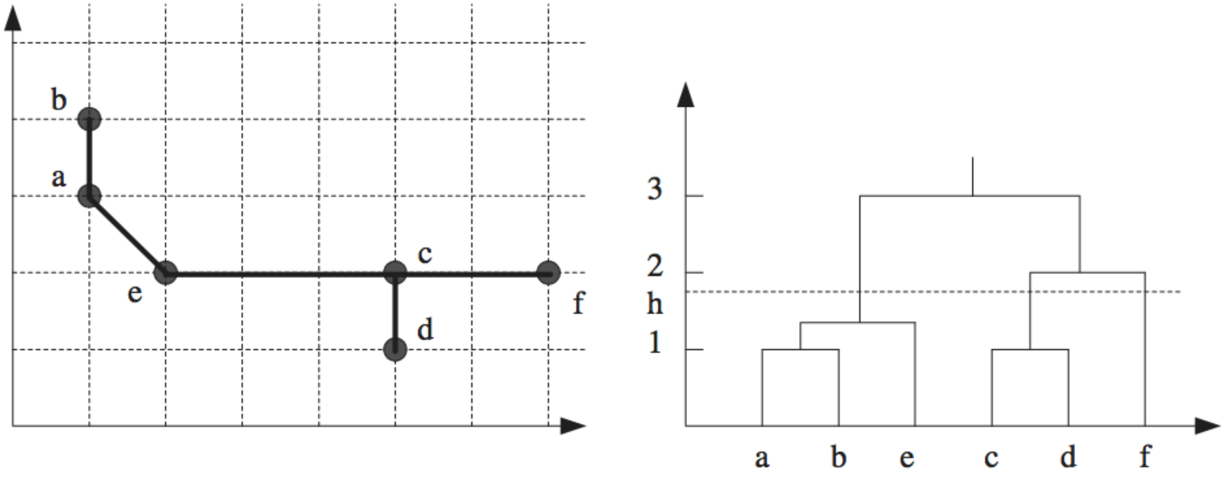




Agglomerative vs Divisive



Hierarchical Agglomerative Clustering



Association Analysis

- Recall

$$\chi^2 = \sum_{i=1}^{n} \frac{(O_i - E_i)^2}{E_i}$$

- Binary → Normalized
- F_{ij} is the j^{th} attribute of the i^{th} data point
- F_{ik} is the k^{th} attribute of the i^{th} data point

$$a_{jk} = \sum\nolimits_{x_i} F_{ij} \times F_{ik}$$

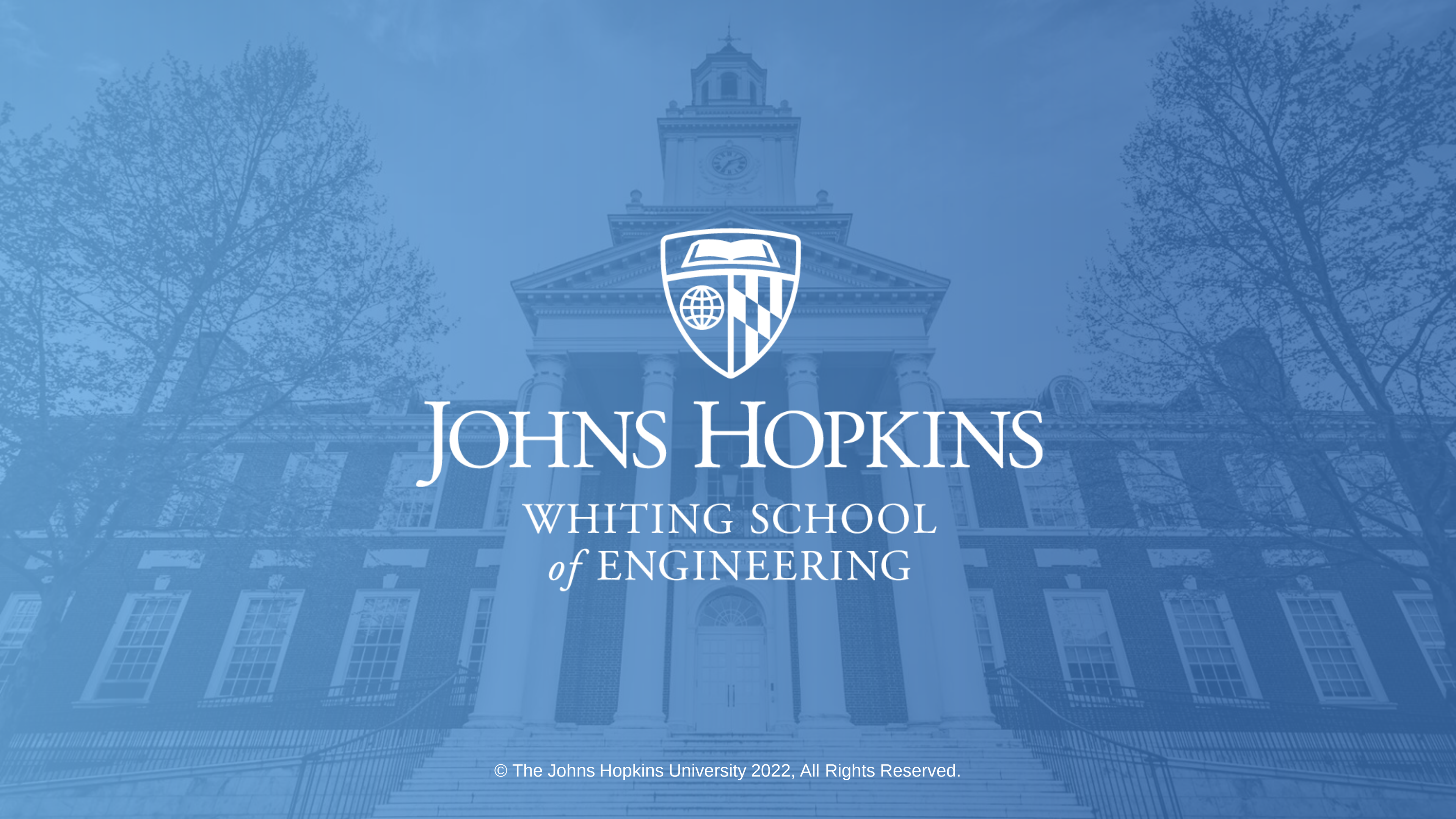
$$b_{jk} = \sum\nolimits_{x_i} (1 - F_{ij}) \times F_{ik}$$

$$c_{jk} = \sum\nolimits_{x_i} F_{ij} \times (1 - F_{ik})$$

$$d_{jk} = \sum\nolimits_{x_i} (1 - F_{ij}) \times (1 - F_{ik})$$

$$\chi^2_{jk} = \frac{(ad - bc)^2}{(a-b)(a-c)(b-d)(c-d)}$$

$$F_{split} = \operatorname{argmax} \sum\nolimits_{k=1}^{d} \chi^2_{jk}$$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Introduction to Machine Learning

Density-based Clustering

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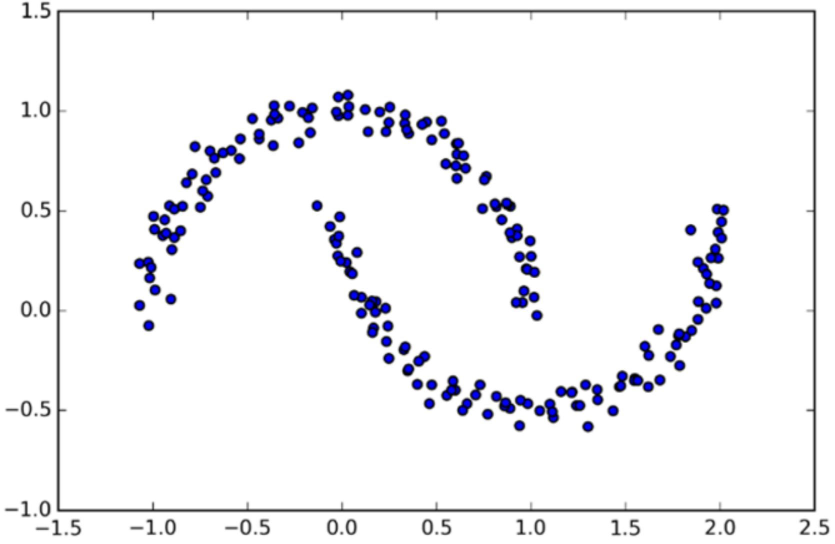
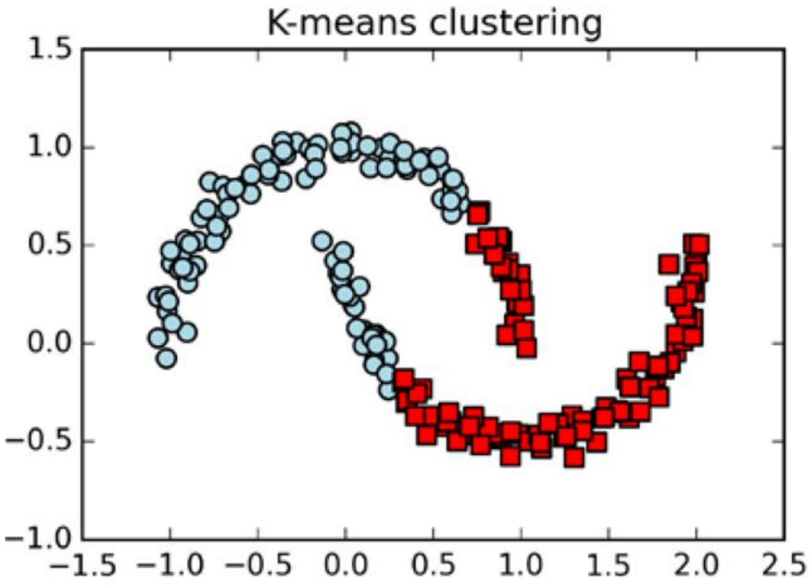
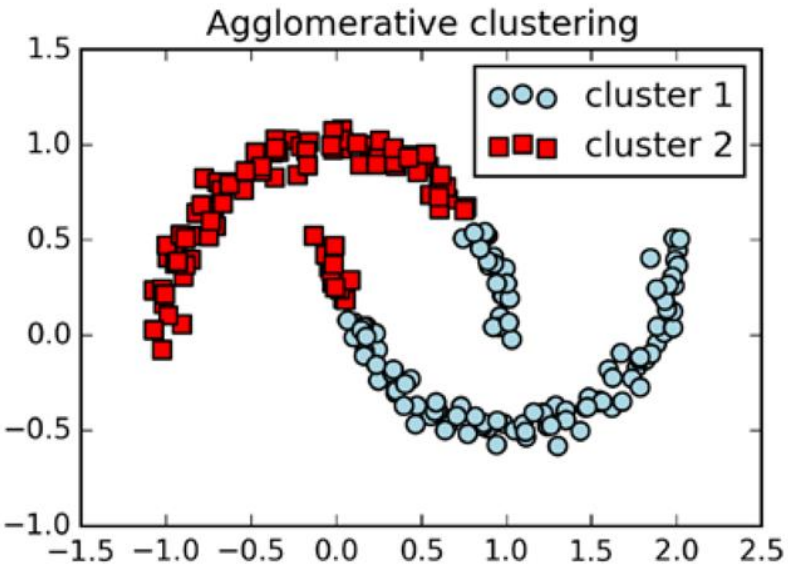
A Motivating Example



K-Means

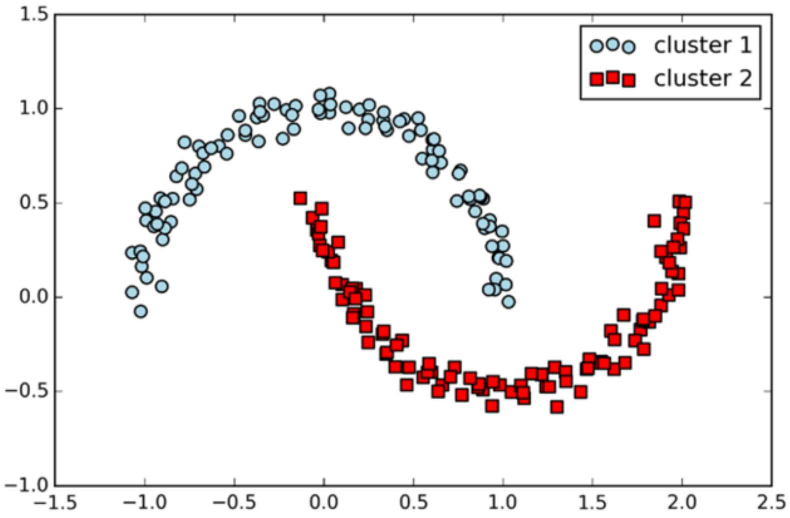


HAC

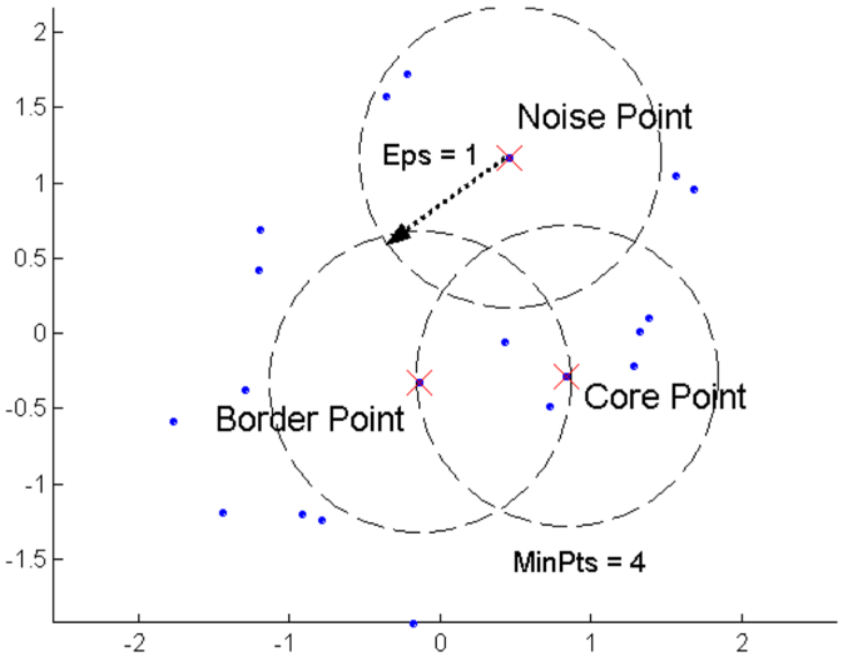


Agglomerative clustering
cluster 1
cluster 2
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5

Density-based Clustering



Point Categorization



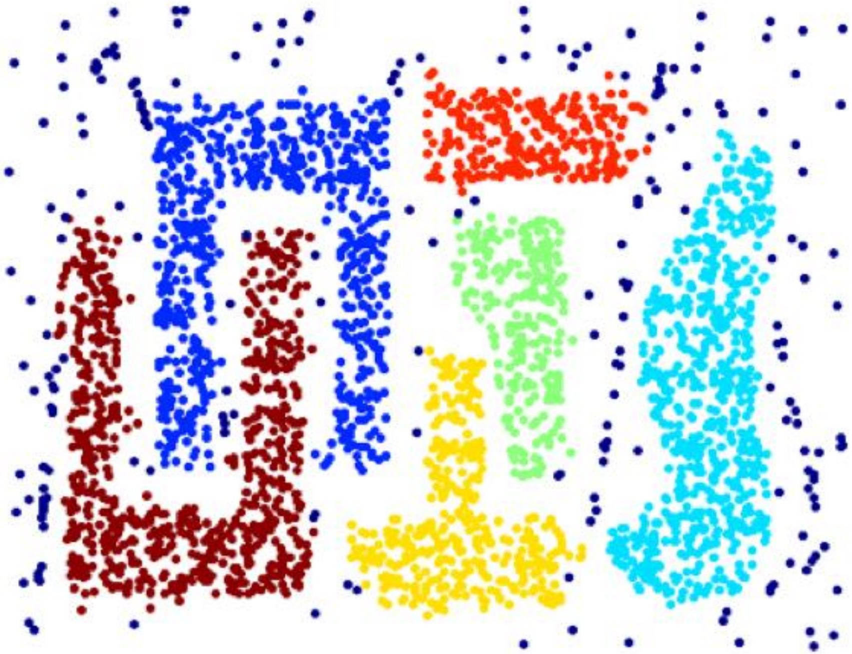
DBSCAN

Algorithm 2 DB-Scan

```
function DB-SCAN(𝒟)
    currClustLbl ← 1
    for all p ∈ Core do do
        if clustLbl[p] = "Unknown" then
            currClustLbl ← currClustLbl + 1
            clustLbl[p] ← currClustLbl
        end if
        for all p′ ∈ θ-neighborhood do
            if clustLbl[p′] = "Unknown" then
                clustLbl[p′] ← currClustLbl
            end if
        end for
    end for
    return clustLbl
end function
```

Another Example

Another Example



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Spectral Clustering

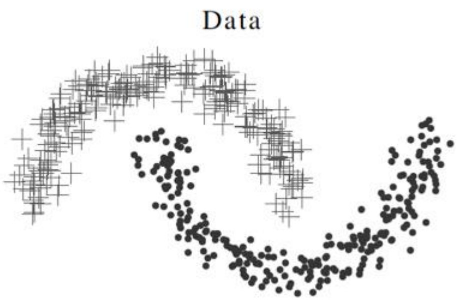
Laplacian Matrix

- **Begin with a similarity matrix,** $\mathbf{M} = \begin{bmatrix} \delta(x_1, x_1) & \cdots & \delta(x_1, x_n) \\ \vdots & \ddots & \vdots \\ \delta(x_n . x_1) & \cdots & \delta(x_n . x_n) \end{bmatrix}$
- The ϵ-neighborhood graph limits points for which $\delta(x_i, x_j)$ is calculated to require that $\delta(x_i, x_j) \leq \epsilon$.
- The k-nearest neighbor graph limits points corresponding to, as the name suggests, the k nearest neighbors of each point.
- These approaches lead to "reduced" similarity matrices, $\mathbf{M}_{\text{reduced}}$.
- The graph Laplacian begins with a diagonal "degree" matrix, $\boldsymbol{\Delta} = \begin{bmatrix} \deg(x_1) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \deg(x_n) \end{bmatrix}$, where $\deg(x_i) = \sum_j \delta(x_i, x_j)$.
- Then the graph Laplacian is $\mathbf{L} = \boldsymbol{\Delta} - \mathbf{M}_{\text{reduced}}$.

Un-normalized Spectral Clustering

1. Construct $\mathbf{M}_{\text{reduced}}$.
2. Construct $\mathbf{L} = \mathbf{\Delta} - \mathbf{M}_{\text{reduced}}$.
3. Find the first k non-zero eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_k$ of $\mathbf{L}$.
4. Construct matrix $\mathbf{U}$ from $\mathbf{u}_1, \ldots, \mathbf{u}_k$.
5. Cluster the *rows* of $\mathbf{U}$ with k-means.
6. Return the row indices grouped by the clusters.

Example Clusters



Normalized (Sym) Spectral Clustering

Two normalized graph Laplacians

$$\mathbf{L}_{\text{sym}} = \mathbf{\Delta}^{-1/2}\mathbf{L}\mathbf{\Delta}^{-1/2} = \mathbf{I} - \mathbf{\Delta}^{-1/2}\mathbf{U}\mathbf{\Delta}^{-1/2}$$

$$\mathbf{L}_{\text{rw}} = \mathbf{\Delta}^{-1/2}\mathbf{L} = \mathbf{I} - \mathbf{\Delta}^{-1/2}\mathbf{U}$$

1. Construct $\mathbf{M}_{\text{reduced}}$.
2. Construct $\mathbf{L} = \mathbf{\Delta} - \mathbf{M}_{\text{reduced}}$.
3. Construct $\mathbf{L}_{\text{sym}} = \mathbf{\Delta}^{-1/2}\mathbf{L}\mathbf{\Delta}^{-1/2}$.
4. Find the first k non-zero eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_k$ of $\mathbf{L}_{\text{sym}}$.
5. Construct matrix $\mathbf{U}$ from $\mathbf{u}_1, \dots, \mathbf{u}_k$.
6. Normalize the rows of $\mathbf{U}$, $\forall i \leq n, \sum_j u_{ij}^2 = 1$.
7. Cluster the *rows* of $\mathbf{U}$ with k-means.
8. Return the row indices grouped by the clusters.

Normalized (RW) Spectral Clustering

Two normalized graph Laplacians

$$\mathbf{L}_{\mathrm{sym}} = \boldsymbol{\Delta}^{-1/2}\mathbf{L}\boldsymbol{\Delta}^{-1/2} = \mathbf{I} - \boldsymbol{\Delta}^{-1/2}\mathbf{U}\boldsymbol{\Delta}^{-1/2}$$
$$\mathbf{L}_{\mathrm{rw}} = \boldsymbol{\Delta}^{-1/2}\mathbf{L} = \mathbf{I} - \boldsymbol{\Delta}^{-1/2}\mathbf{U}$$

1. Construct $\mathbf{M}_{\mathrm{reduced}}$.
2. Construct $\mathbf{L} = \boldsymbol{\Delta} - \mathbf{M}_{\mathrm{reduced}}$.
3. Construct $\mathbf{L}_{\mathrm{rw}} = \boldsymbol{\Delta}^{-1/2}\mathbf{L}$.
4. Find the first k non-zero eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_k$ of $\mathbf{L}_{\mathrm{sym}}$.
5. Construct matrix $\mathbf{U}$ from $\mathbf{u}_1, \dots, \mathbf{u}_k$.
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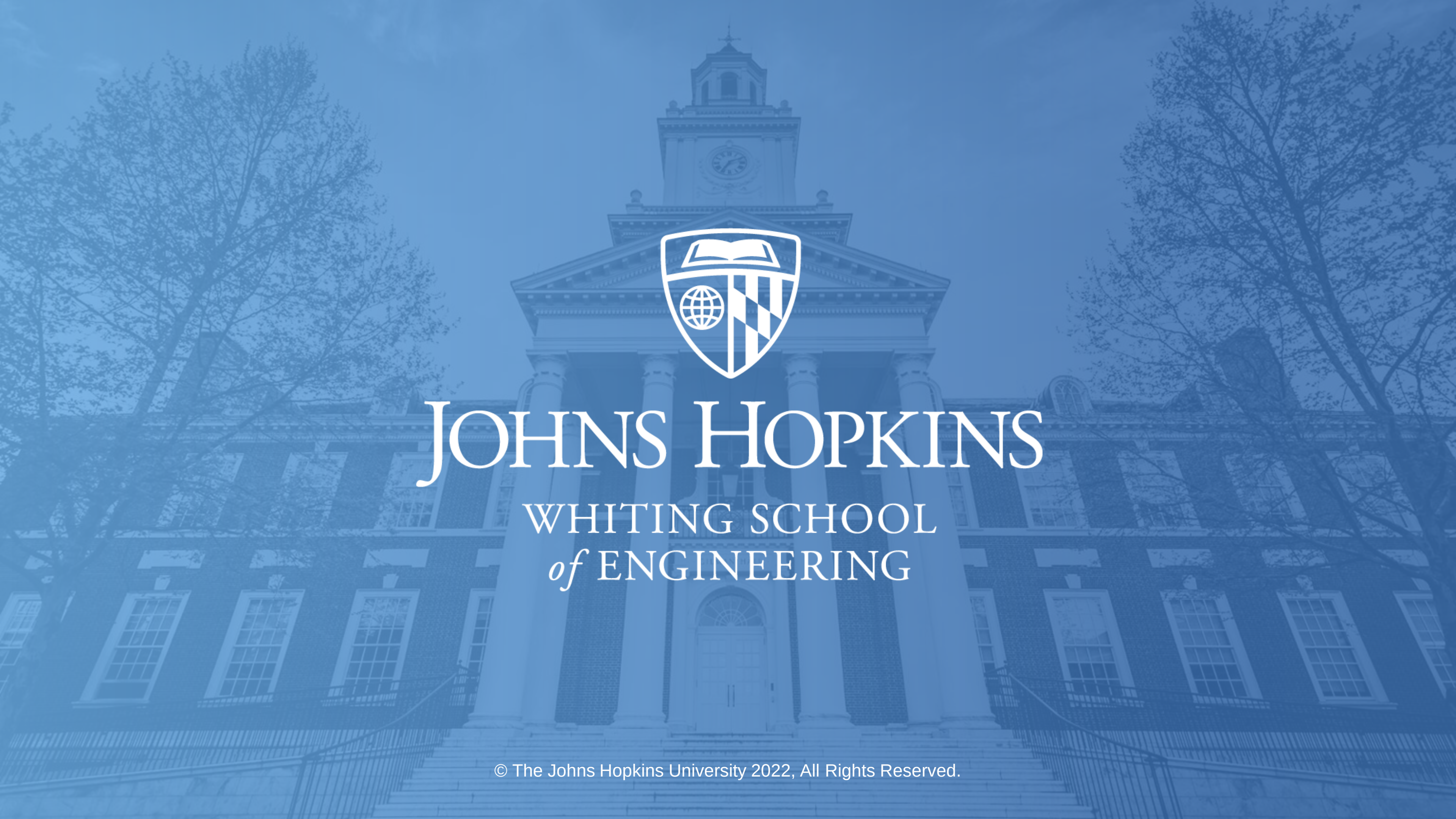

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PAC Learning

Sample Complexity

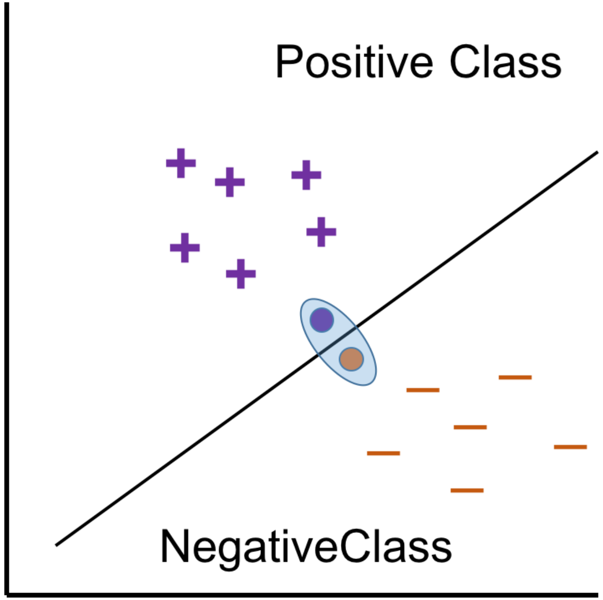
Computational Learning Theory (COLT)

1. What general laws constrain learning?
2. What types of learning problems can be solved in reasonable time/space?
3. When can we trust the output of a learned hypothesis, and by how much can be trust it?

Types of Supervised Learning

- Teacher-annotated learning
    - Probability distribution
    - Inductive learning principle/hypothesis
- Active learning
    - Examples → oracle
    - Oracle provides the label
- Helpful teacher
    - Teacher picks the examples
    - Principle to determine minimum number of examples needed

Learning with a Helpful Teacher



Back to Sample Complexity

- The sample complexity of a learning problem seeks to determine, for a concept,
  - The number of training examples needed to learn the concept
  - Ideally minimize the amount of training required under the associated learning model
- The notion of sample complexity was first posed by Leslie Valiant.

  L. G. Valiant, “A Theory of the Learnable,” *Communications of the ACM*, Volume 27, Issue 11, November 1984, pp. 1134–1142.

- **Def:** A concept *C* is said to be *PAC-Learnable* by learner *L* using hypothesis space *H* if, for all $c \in C$, distributions *D* over *X* of length *n*, ε such that $0 < \varepsilon < 0.5$, and δ such that $0 < \delta < 0.5$, learner *L* will output hypothesis $h \in H$ with probability at least $(1 - \delta)$ such that the true error $error(h) \leq \varepsilon$ in time polynomial in $\frac{1}{\varepsilon}, \frac{1}{\delta}, n$ and $size(c)$.

PAC Learning

- Term first coined by Dana Angluin.
- Many key theorems proven by David Haussler.

$$m \geq \frac{1}{\epsilon}\left(\ln|H| + \ln\frac{1}{\delta}\right)$$

- Example

$$y = f(x_1, \ldots, x_n) = x'_1 \wedge \cdots \wedge x'_k,$$

  - Active learner: n examples
  - Helpful teacher: k examples
  - Teacher annotated: $\frac{1}{\epsilon}\left(\ln n + \ln\frac{1}{\delta}\right)$ examples

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