k-Means has Polynomial Smoothed Complexity

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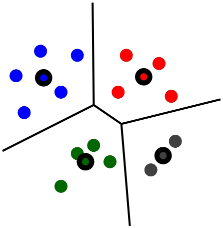

Pearls of Algorithms
Winter 2010/11

Data Clustering

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Input: set of objects X

Ouput: partition of X into k classes $C_1, \ldots, C_k$

Goal: maximize similarity among objects in the same class

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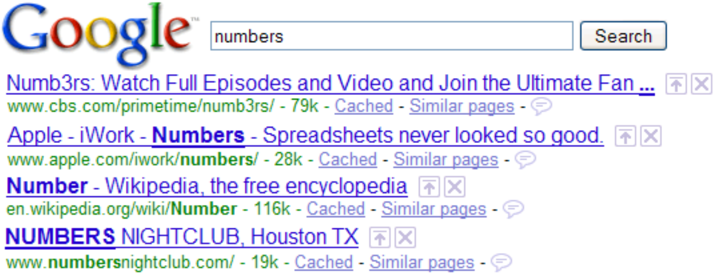
First Example: Clustering of Web Pages



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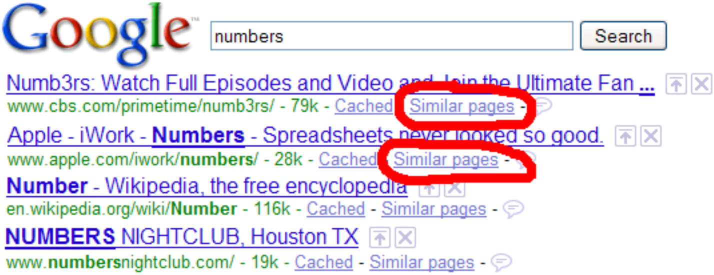

Data Clustering — Further Examples

Second Example: Color Reduction

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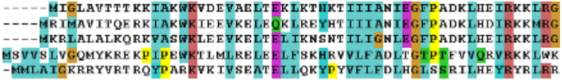
Third Example: Protein Clustering



Outline

Main Questions

1. **Data Clustering**
   What is the *k*-means method?
2. **Smoothed Analysis**
   What can we do when worst case analysis is too pessimistic?
3. **Smoothed Analysis of the *k*-Means Method**
   What is the smoothed complexity of the *k*-means method?
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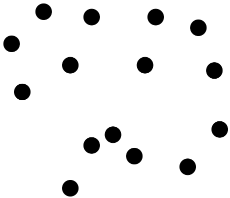
number of clusters k



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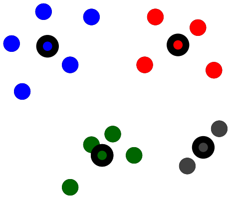

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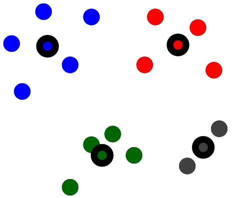

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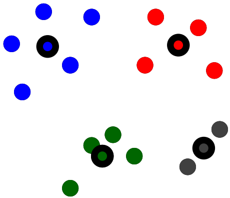


Theory: The problem is NP-hard, but a PTAS exists.
(running time is exponential in k)

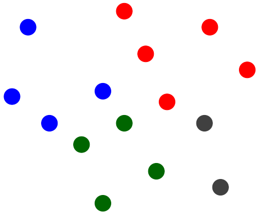
Practice: k-Means Method.

k-Means Method

Local search based on two observations:

1. clusters C_i fixed

$\Rightarrow$ centers $c_i = \frac{1}{|C_i|} \sum_{x \in C_i} x$



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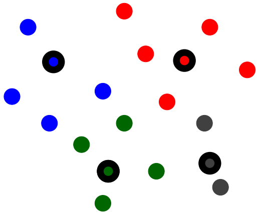

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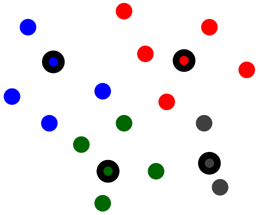

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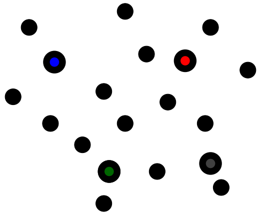

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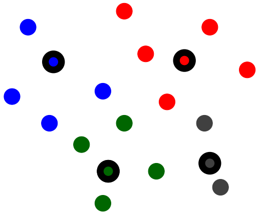

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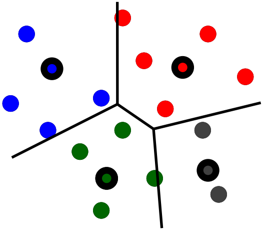

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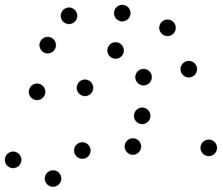

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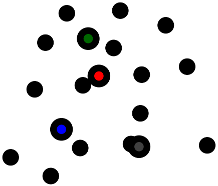

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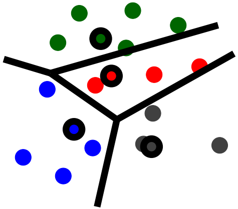

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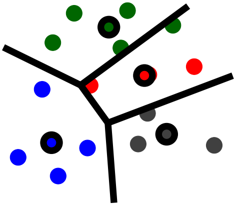

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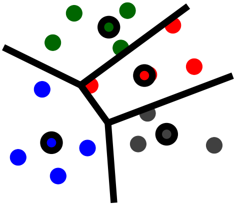

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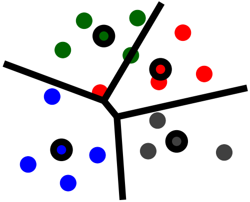

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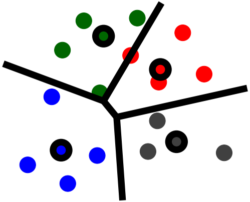

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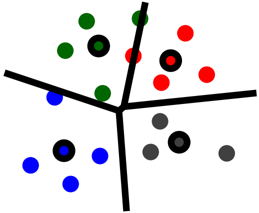

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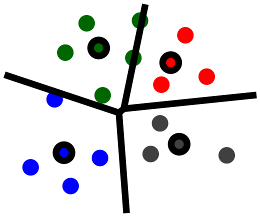

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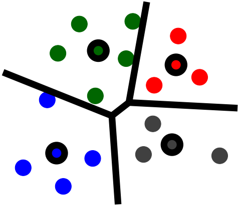

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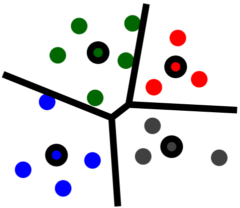

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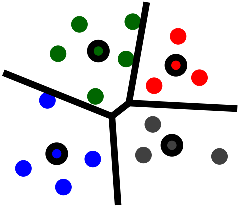

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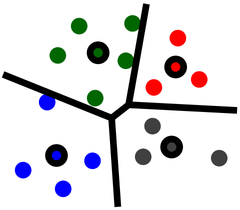

"by far the most popular clustering algorithm used in scientific and industrial applications" (Berkhin 2002)

"in practice the number of iterations is generally much less than the number of points" (Duda et al. 2001)

k-Means Method – Theoretical Results

Running Time

Upper Bound: **At most $(k^2 n)^{kd}$ iterations.**

No clustering can occur twice.

Lower Bound: **At least $2^{\Omega(k)}$ iterations** for $d \geq 2$.

[Andrea Vattani (SoCG'09)]

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Local optima can be arbitrarily bad.

$\Rightarrow$ Huge discrepancy between theory and practice.

(Focus of this talk: running time.)

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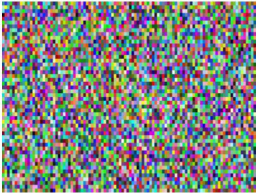

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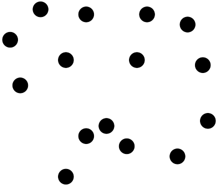

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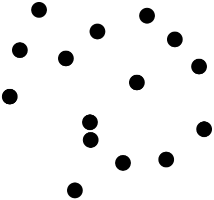

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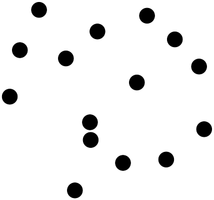

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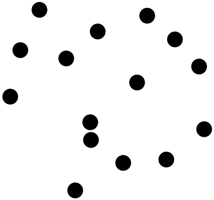

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- models, e.g., measurement errors or numerical imprecision
- Smoothed compl. low $\Rightarrow$ bad performance unlikely in practice

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Arthur, Vassilvitskii (FOCS 2006)

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Manthey, Röglin (SODA 2009)

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Our Result (FOCS 2009)

Smoothed number of iterations is $\mathrm{poly}(n, 1/\sigma)$.

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Lemma

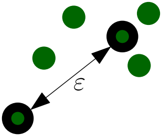
For $d \geq 2$, for every $X \subseteq [0, 1]^d$, in the model of smoothed analysis:

$$\mathbf{E}\left[\frac{1}{\Delta}\right] = \mathrm{poly}(n, 1/\sigma) \ .$$

$$\Rightarrow \max_{X, |X|=n} \mathbf{E}(\#\mathrm{Iterations}(\mathrm{per}_\sigma(X))) = \mathrm{poly}(n, 1/\sigma) \ .$$

When does the potential drop?

1) center moves by ε



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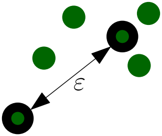

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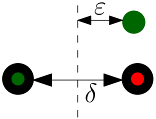

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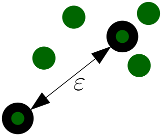

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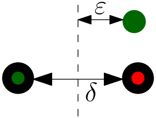

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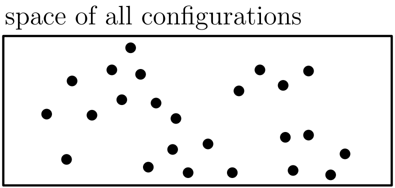

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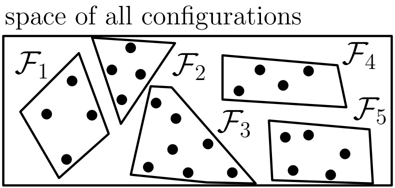

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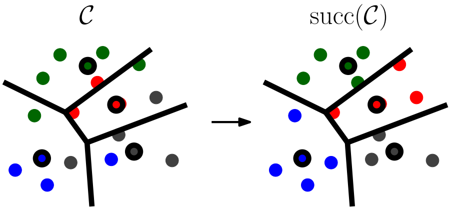
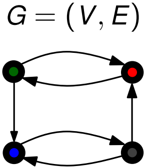
Transition Graph $G = (V, E)$:

V: clusters E: labeled directed edge for each reassigned point





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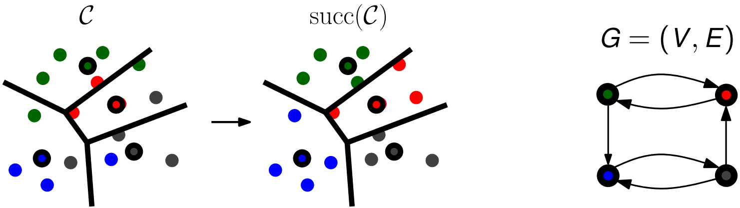

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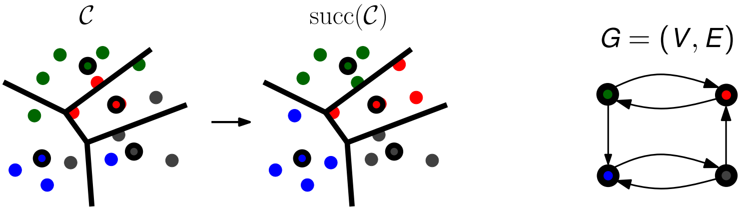

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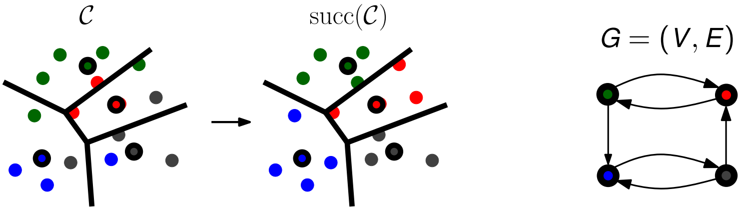

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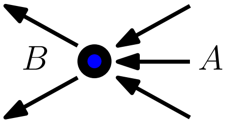

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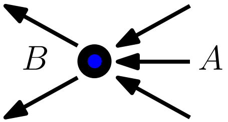

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small potential drop $\Rightarrow$ $\text{cm}(C)$ must be close to $\mathrm{approx}(A, B)$

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Technical Difficulties: Data points are not independent from approx. bisectors, approximate centers not defined for balanced clusters, blueprints must have enough edges, . . .

Outline

Main Questions

1. **Data Clustering**
   What is the *k*-means method?
2. **Smoothed Analysis**
   What can we do when worst case analysis is too pessimistic?
3. **Smoothed Analysis of *k*-Means Method**
   What is the smoothed complexity of the *k*-means method?
4. **Extensions and Conclusions**

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Kullback-Leibler divergence (relative entropy):

$$\mathrm{KLD}(p,q) = \sum_{i=1}^{d} p_i \log\left(\frac{p_i}{q_i}\right)$$

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Bregman divergences are distance measures that generalize squared Euclidean distances and the Kullback-Leibler divergence.

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Polynomial bound does not extend as it uses special properties of Gaussian perturbations.

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Summary:

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Future Research:

- improve exponents for k-means (currently $\approx n^{30}$)
  better understanding of dynamics seems necessary for this
- explanation for good approximation ratio
- better analysis of Bregman divergences
- more systematic theory of smoothed local search
- Are all local search problems in PLS easy in smoothed analysis?

Thank you for your attention!

Questions?