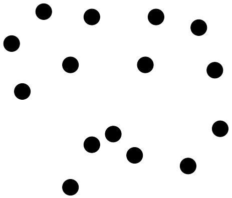
Outline

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**

Data Clustering

Input: point set $X \subseteq \mathbb{R}^d$, $|X| = n$
number of clusters k



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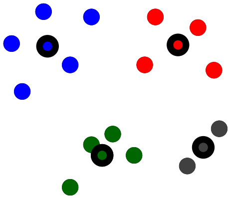

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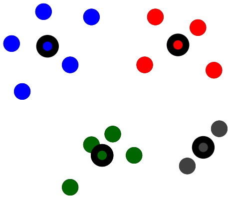

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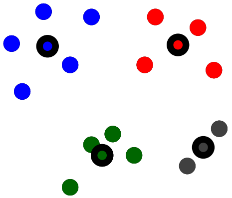


Theory: The problem is NP-hard, but a PTAS exists.
(running time is exponential in k)

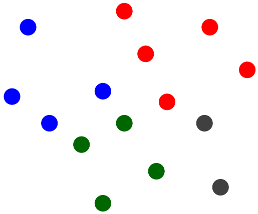
Practice: k-Means Method.

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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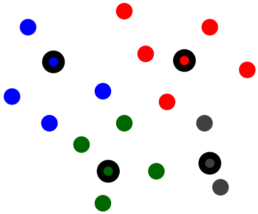

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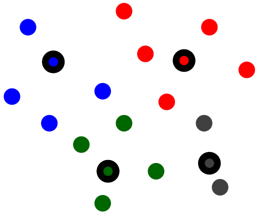

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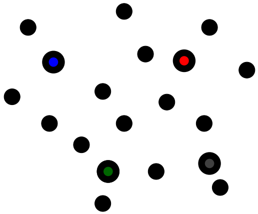

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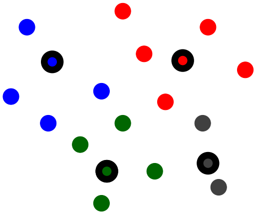

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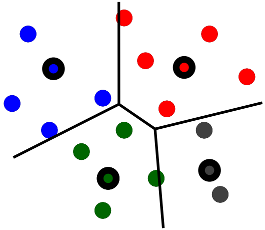

k-Means Method

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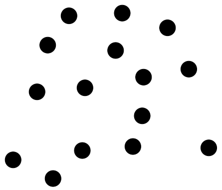

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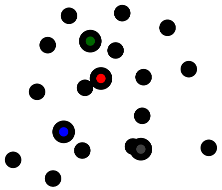

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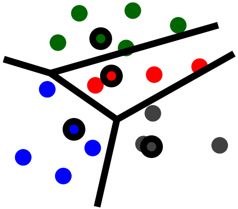

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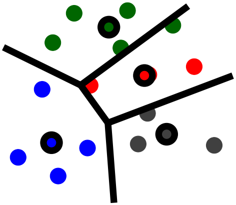

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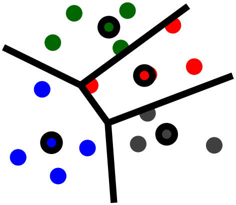

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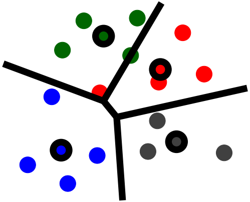

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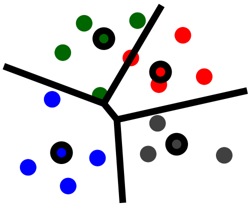

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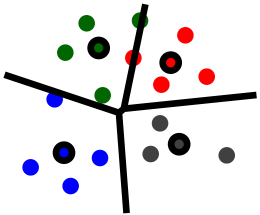

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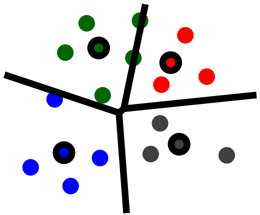

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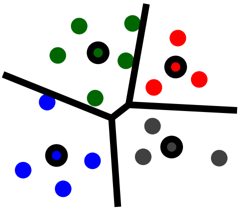

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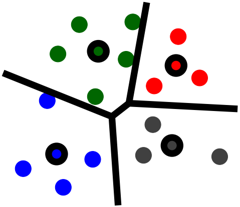

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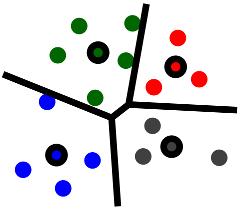

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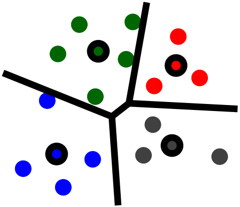

"by far the most popular clustering algorithm used in scientific and industrial applications" (Berkhin 2002)

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

Running Time

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

No clustering can occur twice.

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

[Andrea Vattani (SoCG'09)]

k-Means Method – Theoretical Results

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Local optima can be arbitrarily bad.

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[Andrea Vattani (SoCG'09)]

Quality

Local optima can be arbitrarily bad.

$\Rightarrow$ Huge discrepancy between theory and practice.
(Focus of this talk: running time.)

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   What is the *k*-means method?
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   What can we do when worst case analysis is too pessimistic?
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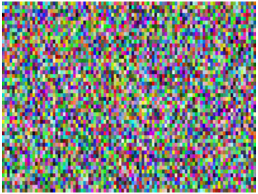

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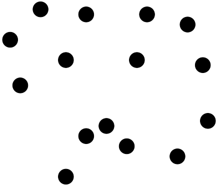

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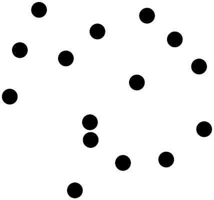

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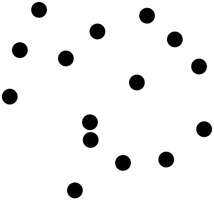

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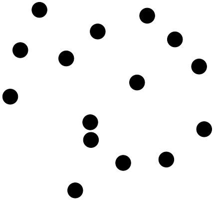

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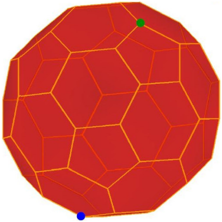
- models, e.g., measurement errors or numerical imprecision
- Smoothed compl. low $\Rightarrow$ bad performance unlikely in practice

Smoothed Analysis introduced for the Simplex Method:

- Linear Programming:
  $\max c \cdot x$ such that $Ax \leq b$



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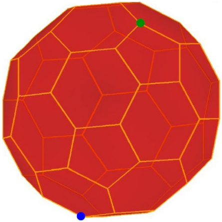

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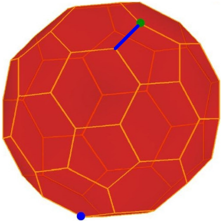

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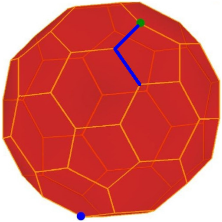

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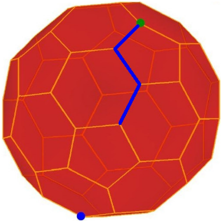

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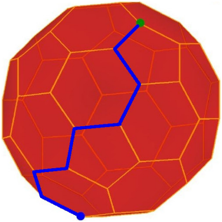

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- Linear Programming:
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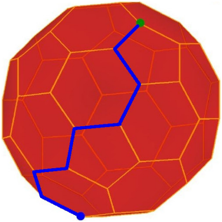

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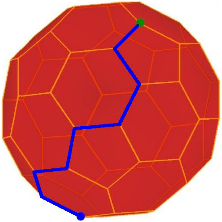

Theorem [Spielman, Teng 2001]

The smoothed running time of the simplex method with shadow vertex pivot rule is polynomial in n, m, and $1/\sigma$.

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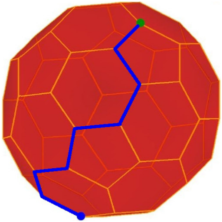

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- In 2006, Roman Vershynin improved bound from $O^*\left(m^{86}n^{55}\sigma^{-30}\right)$ to $O\left(\max\{n^5\log^2 m, n^9\log^4 n, n^3\sigma^{-4}\}\right)$.
- Further results on condition number of matrices, interior-point method, Gaussian elimination, etc.

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Model: Every point is perturbed by independent d-dimensional Gaussian with standard deviation σ.

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Arthur, Vassilvitskii (FOCS 2006)

Smoothed number of iterations is **at most** $\text{poly}(n^k, 1/\sigma)$.

Manthey, Röglin (SODA 2009)

Smoothed number of iterations is **at most**

- $\text{poly}(n^{\sqrt{k}}, 1/\sigma)$
- $k^{kd} \cdot \text{poly}(n, 1/\sigma)$

Smoothed Analysis of k-Means

Model: Every point is perturbed by independent d-dimensional Gaussian with standard deviation σ.

$$T(n, \sigma) = \max_{X, |X|=n} \mathbf{E}(\#\text{Iterations}(\text{per}_\sigma(X)))$$

Arthur, Vassilvitskii (FOCS 2006)

Smoothed number of iterations is **at most** $\text{poly}(n^k, 1/\sigma)$.

Manthey, Röglin (SODA 2009)

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Our Result (FOCS 2009)

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General Approach

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Lemma

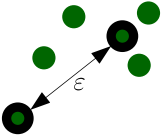
For $d \geq 2$, for every $X \subseteq [0, 1]^d$, in the model of smoothed analysis:

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

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

When does the potential drop?

1) center moves by ε



$\Rightarrow$ improvement by ε^2

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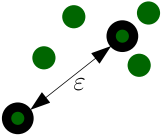

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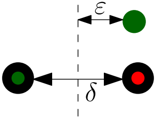

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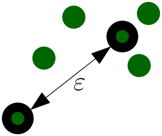

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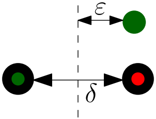

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How large is Δ?

Configuration $\mathcal{C}$ is **ε-bad** if $\Phi(\mathcal{C}) - \Phi(\text{succ}(\mathcal{C})) \leq \varepsilon$.
Naive approach: Union Bound over all configurations.

$$\mathbf{Pr}\left[\exists \text{Configuration } \mathcal{C} : \mathcal{C} \text{ is } \varepsilon\text{-bad}\right] \leq \sum_{\text{Configuration } \mathcal{C}} \mathbf{Pr}\left[\mathcal{C} \text{ is } \varepsilon\text{-bad}\right]$$

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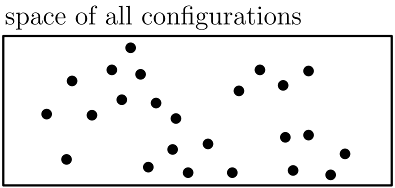

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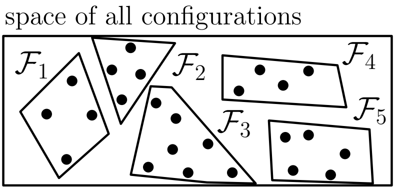

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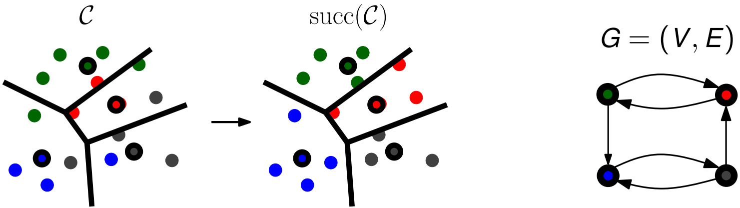
Transition Graph $G = (V, E)$:

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



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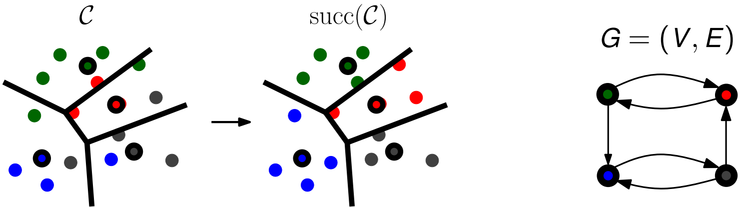

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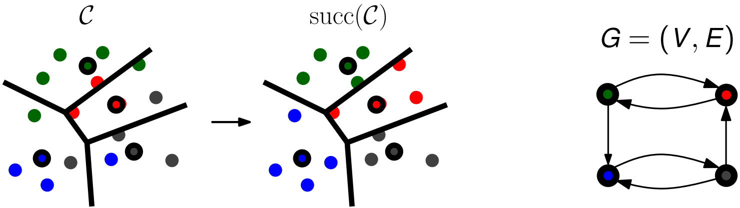

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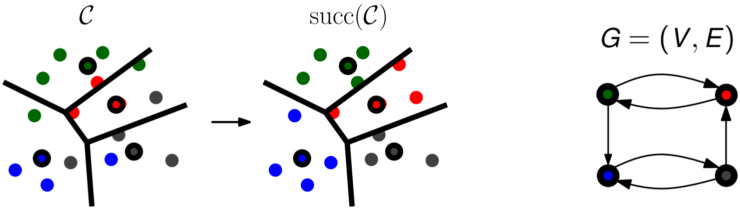

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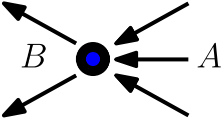

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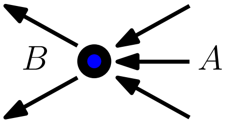

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small potential drop $\Rightarrow$ $\mathrm{cm}(C)$ must be close to $\mathrm{approx}(A, B)$

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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**

Text Classification and Bag-of-Words Model:

- S set of all words
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Kullback-Leibler divergence (relative entropy):

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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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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?