MDSteer: Steerable and Progressive Multidimensional Scaling

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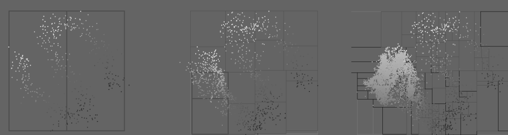

Outline

- Dimensionality Reduction
- Previous Work
- MDSteer Algorithm
- Results and Future Work

Dimensionality Reduction

- mapping multidimensional space into space of fewer dimensions
  – typically 2D for infovis
  – keep/explain as much variance as possible
  – show underlying dataset structure
- multidimensional scaling (MDS)
  – minimize differences between interpoint distances in high and low dimensions

Dimensionality Reduction Example

- Isomap: 4096 D to 2D [Tenenbaum 00]

[A Global Geometric Framework for Nonlinear Dimensionality Reduction. Tenenbaum, de Silva and Langford. *Science* 290 (5500): 2319-2323, 22 December 2000, isomap.stanford.edu]

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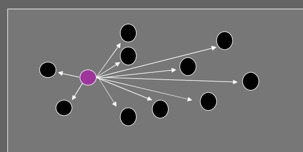
Previous Work

- MDS: iterative spring model (infovis)
  – [Chalmers 96, Morrison 02, Morrison 03]
  – [Amenta 02]
- eigensolving (machine learning)
  – Isomap [Tenenbaum 00], LLE [Roweis 00]
  – charting [Brand 02]
  – Laplacian Eigenmaps [Belkin 03]
- many other approaches
  – self-organizing maps [Kohonen 95]
  – PCA, factor analysis, projection pursuit

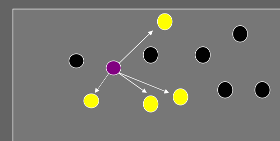
Naive Spring Model

- repeat for all points
  - compute spring force to all other points
    - difference between high dim, low dim distance
  - move to better location using computed forces
- compute distances between all points
  - $O(n^2)$ iteration, $O(n^3)$ algorithm



Faster Spring Model [Chalmers 96]

- compare distances only with a few points
  - maintain small local neighborhood set



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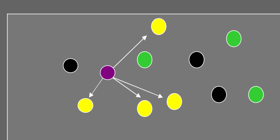
  - each time pick some randoms, swap in if closer



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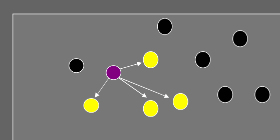
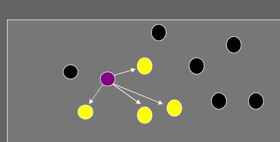


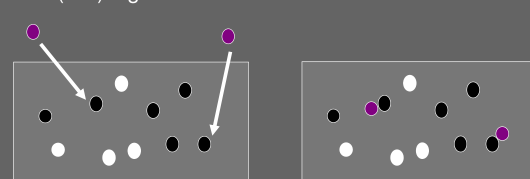
Faster Spring Model [Chalmers 96]

- compare distances only with a few points
  - maintain small local neighborhood set
  - each time pick some randoms, swap in if closer
- small constant: 6 locals, 3 randoms typical
  - $O(n)$ iteration, $O(n^2)$ algorithm



Parent Finding [Morrison 2002, 2003]

- lay out a root(n) subset with [Chalmers 96]
- for all remaining points
  - find “parent”: laid-out point closest in high D
  - place point close to this parent
- $O(n^{5/4})$ algorithm



Scalability Limitations

- high cardinality and high dimensionality: still slow
  - motivating dataset: 120K points, 300 dimensions
  - most existing software could not handle at all
  - 2 hours to compute with $O(n^{5/4})$ HIVE [Ross 03]
- real-world need: exploring huge datasets
  - last year's questioner wanted tools for millions of points
- strategy
  - start interactive exploration immediately
    - progressive layout
  - concentrate computational resources in interesting areas
    - steerability
  - often partial layout is adequate for task

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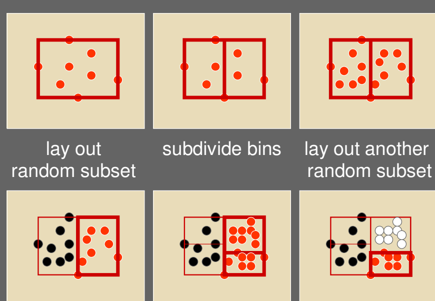
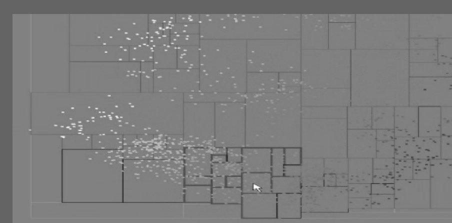
MDSteer Overview



lay out random subset | subdivide bins | lay out another random subset

user selects active region of interest | more subdivisions and layouts | user refines active region

Video 1



Algorithm Outline

lay out initial subset of points

loop {

    lay out some points in active bins

        - precise placement of some

    subdivide bins, rebin all points

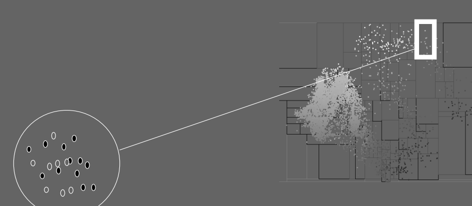
        - coarse placement of all

        - gradually refined to smaller regions

}

Bins

- screen-space regions
  - placed points: precise lowD placement with MDS
  - unplaced points: rough partition using highD distances

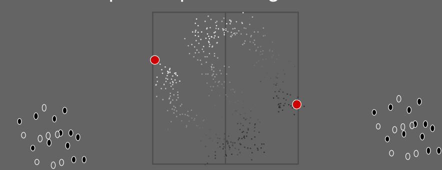


Bins

- incremental computation
  - unplaced points partitioned
  - cheap estimate of final position, refine over time
- interaction
  - user activates screen-space regions of interest
- steerability
  - only run MDS on placed points in active bins
  - only seed new points from active bins
- partition work into equal units
  - roughly constant number of points per bin
  - as more points added, bins subdivided

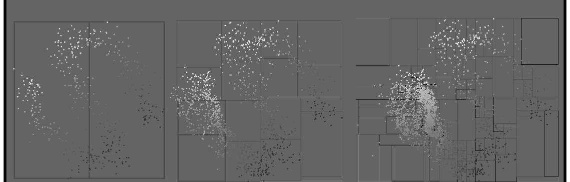
Rebinning

- find min and max representative points
  - alternate between horizontal and vertical
- split bin halfway between them
- rebin placed points: lowD distance from reps
- rebin unplaced points: highD distance from reps



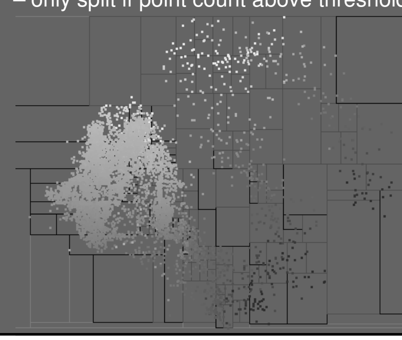
Recursive Subdivision

- start with single top bin
  - contains initial root(n) set of placed points
- subdivide when each new subset placed



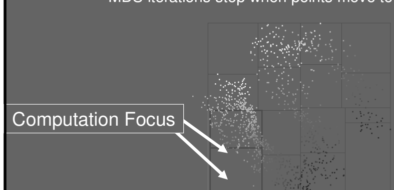
Irregular Structure

- split based on screen-space point locations
- only split if point count above threshold



Steerability

- user selects screen-space bins of interest
- screen space defines "interesting"
  - explore patterns as they form in lowD space
  - points can move between bins in MDS placement
    - MDS iterations stop when points move to inactive bins



Steerability

- approximate partitioning
  - point destined for bin A may be in bin B's unplaced set
  - will not be placed unless B is activated
- allocation of computation time
  - user-directed: MDS placement in activated areas
  - general: rebinning of all points to refine partitions
  - rebinning cost grows with
    - dimensionality
    - cardinality
- traditional behavior possible, just select all bins

Algorithm Loop Details

```
until all points in selected bins are placed {
    add sampleSize points from selected bins
    until stress stops shrinking {
        for all points in selected bins {
            run [Chalmers96] iteration
            calculate stress } }
    divide all bins in half
    rebin all points }
```

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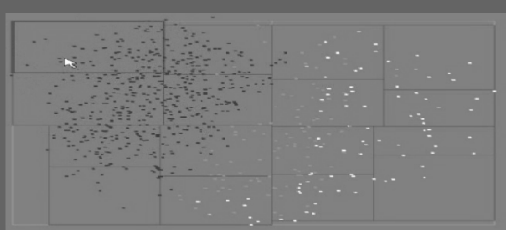
Video 2



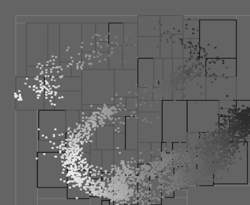
Comparison

Standard MDS

- all points placed
- hours to compute for big data (100K points, 300 dim)

MDSteer

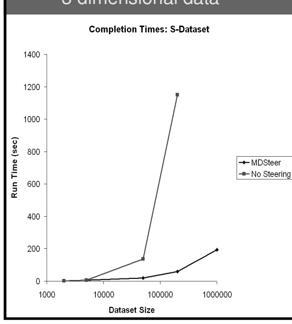
- user-chosen subset of points placed
- progressive, steerable
- immediate visual feedback



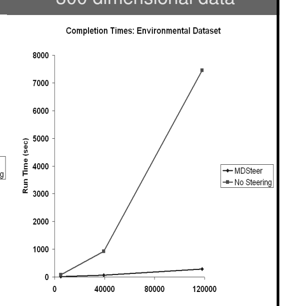
Results: Speed

- unsurprisingly, faster since fewer points placed

3 dimensional data



300 dimensional data

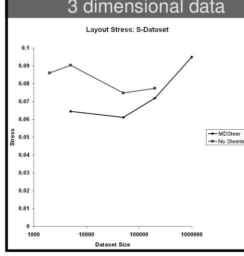


Results: Stress

$$Stress = \frac{\sum_{i<j}(d_{ij} - p_{ij})^2}{\sum_{i<j} p_{ij}^2}$$

- difference between high dimensional distance and layout distances
  - one measure of layout quality
- d_{ij} – high dim distance between i and j
- p_{ij} – layout distance between i and j

3 dimensional data



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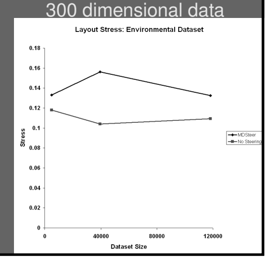
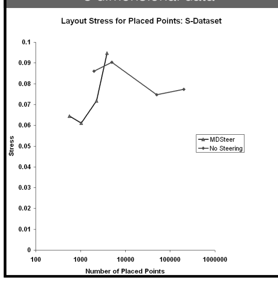


Results: Stress For Placed Points

- placed << total during interactive session
- passes sanity check: acceptable quality

3 dimensional data



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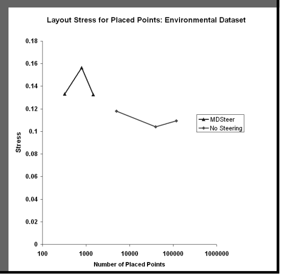
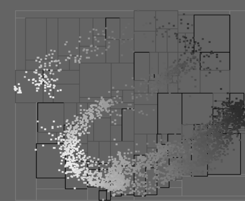


Contributions

- first steerable MDS algorithm
  - progressive layout allows immediate exploration
  - allocate computational resources in lowD space



Future Work

- fully progressive
  - gradual binning
  - automatic expansion of active area
- dynamic/streaming data
- steerability
  - find best way to steer
  - steerable eigensolvers?
- manifold finding

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