Minimizing Potential Energy in Constrained Physical Systems and Applications to Graph Drawing

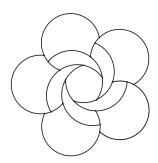
Agenda

- Introduction
 - Problem Statement
 - Motivation
 - Related Work
- Minimizing Potential Energy
- Drawing Graphs with Circular Arcs

Christian Schnorr

Problem Statement

- Create drawings of arbitrary input graphs
 - Drawn edges as circular arcs
 - Use few geometric entities by drawing entire paths as a single circular arc
 - Visually appealing drawings

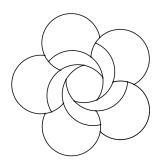


Motivation

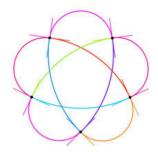
- Drawings with few geometric entities are
 - easier to parse
 - easier to remember
- Drawings can be subject to any form of constraint
 - Soft constraints: violation decreases drawing's quality
 - Hard constraints: violation renders drawing invalid
 - Traditional force-directed algorithms may violate constraints

Christian Schnorr

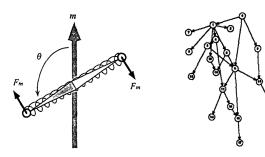
- "Drawing Graphs with Few Arcs" (2015)
 - Lower and upper bounds of required entities
 - Only very specific classes of graphs



- "Force-directed Lombardi-style Graph Drawing" (2011)
 - Attempt to improve angular resolution
 - Soft constraint

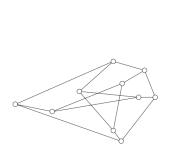


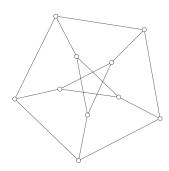
- Magnetic-spring algorithm (1994)
 - Attempt to align edges with a magnetic field
 - Soft constraint



Christian Schnorr

- PrEd (1999)
 - Preserves edge crossing properties
 - Hard constraint
 - Does not reduce the number of degrees of freedom





Agenda

- Introduction
- Minimizing Potential Energy
 - Generalized Coordinates
 - Forces and Potential Energy
 - Force-Directed Algorithms
 - Explicit Energy Function
- Drawing Graphs with Circular Arcs

Christian Schnorr

Generalized Coordinates

- System of *n* particles with position vectors $\vec{r_i} \in \mathbb{R}^2$
 - Unconstrained systems: 2*n* degrees of freedom
 - Constrained systems: $\leq 2n$ degrees of freedom
- **Constraints** introduce dependencies between $\vec{r_i}$
 - Holonomic constraints $f_k(\vec{r_1}, ..., \vec{r_n}) \equiv 0$
 - Holonomic constraints reduce number of degrees of freedom
- Generalized coordinates q_j
 - Determine position vectors $\vec{r_i} = \vec{r_i}(q_1, \dots, q_m)$
 - Independent variables
 - Implicitly satisfy holonomic constraints
 - $\mathbf{m} = \mathbf{m}$ number of degrees of freedom

Christian Schnorr

Forces and Potential Energy

$$W := \int -\vec{F}_{res}(\vec{r}) \, d\vec{r} \tag{2.1}$$

- Restoring force \vec{F}_{res} points towards equilibrium
- One must do work against \vec{F}_{res} to displace system from equilibrium
- Potential energy $U = U_0 + W$

Forces and Potential Energy

$$\vec{F}_i := -\frac{\partial U}{\partial \vec{r}_i} \tag{2.2}$$

- Potential energy U is a function of position vectors $\vec{r_i}$
- \vec{F}_i are directed towards lower energy levels
- Duality of potential energy and restoring forces

 Christian Schnorr
 April 25th, 2017
 12 / 30

Force-Directed Algorithms

- **Explicit** restoring forces $\vec{F_i}$
- Potential energy *U* implicitly defined
- (Infinitesimal) displacements in direction of restoring forces reduce potential energy

Force-Directed Algorithms

- Restoring forces $\vec{F_i}$ act on particles
- \blacksquare Generalized forces Q_i
 - Translate restoring forces to generalized coordinates q_i

$$Q_j := \sum_{i=1}^n \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j}, \qquad j = 1, \dots, m$$
 (2.3)

$$\stackrel{(2.2)}{=} -\frac{\partial U}{\partial q_j} \tag{2.4}$$

 (Infinitesimal) displacements in the direction of generalized forces reduce potential energy

(ロ) (個) (注) (注) (注) つくぐ

Christian Schnorr April 25th, 2017

Explicit Energy Function

- Hard to find restoring forces that yield desired features in equilibrium
- Explicit potential energy $U \colon \mathbb{R}^m \to \mathbb{R} \cup \{\infty\}$
 - Easy to specify which features are desirable in equilibrium
 - Should be continuous and locally differentiable
- Generic optimization of U
 - Derivative-based optimization: e.g. Newton's method
 - Derivative-free optimization: e.g. Hill climbing

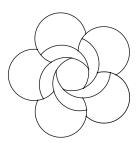
Christian Schnorr

Agenda

- Introduction
- Minimizing Potential Energy
- Drawing Graphs with Circular Arcs
 - Definitions
 - Existence of Drawings
 - Graph Decomposition
 - Generalized Coordinates
 - Potential Energy
 - Results
 - Demo

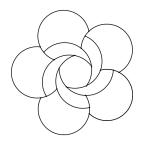
Definitions

- Drawing of *G* with circular arcs
 - Every edge $e \in E$ drawn as a circular arc Γ_e
 - No vertices coincide
 - No edges overlap
 - No edge intersects any vertices other than its endpoints



Definitions

- Given a set $\Pi = \{P_1, \dots, P_k\}$ of edge-disjoint paths
 - $V(\Pi) := V(P_1) \cup \ldots \cup V(P_k)$
 - $E(\Pi) := E(P_1) \uplus \ldots \uplus E(P_k)$
- Drawing of Π with circular arcs
 - Drawing of $G := (V(\Pi), E(\Pi))$ with circular arcs
 - Each path $P \in \Pi$ is drawn as a circular arc Γ_P



- Circles are determined by three distinct points
- Necessary condition: $|V(P_i) \cap V(P_i)| \le 2 \quad \forall i \ne j$
 - Condition is not sufficient!

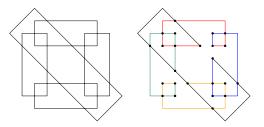


Figure: An arrangement of pseudocircles that is not circleable (left) and a derived arrangement of pseudo circular arcs (right).

4 D > 4 B > 4 E > 4 E > 9 Q (>

19 / 30

Christian Schnorr April 25th, 2017

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{int}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \emptyset, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm

a

Figure: Greedy drawing of $\Pi = (abcde, bfghd, gijkl, jmc)$

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{int}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \emptyset, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm

a

Figure: Greedy drawing of $\Pi = (abcde, bfghd, gijkl, jmc)$

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{int}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \emptyset, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm

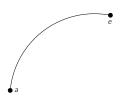


Figure: Greedy drawing of $\Pi = (abcde, bfghd, gijkl, jmc)$

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{int}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \emptyset, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm

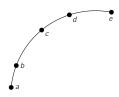


Figure: Greedy drawing of $\Pi = (abcde, bfghd, gijkl, jmc)$

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{int}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \emptyset, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm

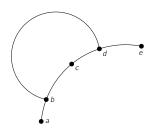


Figure: Greedy drawing of $\Pi = (abcde, bfghd, gijkl, jmc)$

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{int}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \emptyset, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm

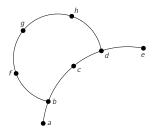


Figure: Greedy drawing of $\Pi = (abcde, bfghd, gijkl, jmc)$

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{int}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \emptyset, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm

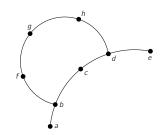


Figure: Greedy drawing of $\Pi = (abcde, bfghd, gijkl, jmc)$

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{int}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \emptyset, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm

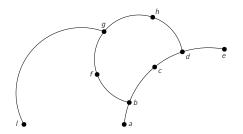


Figure: Greedy drawing of $\Pi = (abcde, bfghd, gijkl, jmc)$

 Christian Schnorr
 April 25th, 2017
 20 / 30

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{\text{int}}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \varnothing, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm

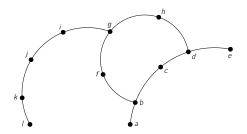


Figure: Greedy drawing of $\Pi = (abcde, bfghd, gijkl, jmc)$

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{int}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \emptyset, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm

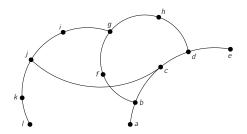


Figure: Greedy drawing of $\Pi = (abcde, bfghd, gijkl, jmc)$

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{int}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \emptyset, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm

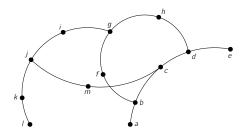


Figure: Greedy drawing of $\Pi = (abcde, bfghd, gijkl, jmc)$

- Greedily realizable sequence of paths Π
 - Ordered sequence of edge-disjoint paths $\Pi = (P_1, \dots, P_k)$
 - $V_{int}(P_i) \cap V(P_1 \cup \ldots \cup P_{i-1}) = \emptyset, \quad i = 2 \ldots k$
 - Permits drawing with circular arcs using greedy algorithm
- Characterization of vertices with respect to Π
 - Constrained vertices $V_c(\Pi)$: first appear as a path's endpoint
 - Unconstrained vertices $V_{\rm u}(\Pi)$: first appear as a path's internal vertex

21 / 30

Christian Schnorr April 25th, 2017

Graph Decomposition

- Trivial decomposition $\Pi = E$ valid
- Non-trivial (greedy) graph decomposition
 - Idea: append edges to working path until current head has been used before
 - Runtime: $\Theta(|V| + |E|)$

22 / 30

Christian Schnorr April 25th, 2017

Generalized Coordinates

- Generalized coordinates
 - $x: V_{\mu}(\Pi) \to \mathbb{R}$
 - $y: V_{\mu}(\Pi) \to \mathbb{R}$
 - φ : $\Pi \rightarrow (-180^\circ, 180^\circ)$
 - $p: V_c(\Pi) \to (0,1)$

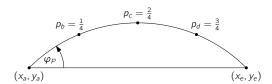


Figure: Generalized coordinates for a single path P = abcde with equi-length edges.

(ロ) (部) (注) (注) 注 のQの

Generalized Coordinates

$$\label{eq:continuous_problem} \begin{split} & \text{foreach } v \in V_u(\Pi) \text{ do } \\ & \mid \vec{r}(v) \leftarrow (x(v), y(v)) \\ & \text{end} \\ & \\ & \text{foreach } P = (v_1, \dots, v_n) \in \Pi \text{ do } \\ & \mid \Gamma(P) \leftarrow \mathsf{CircularArc}(\vec{r}(v_1), \vec{r}(v_n), \varphi(P)) \\ & \quad \text{foreach } v \in (v_2, \dots, v_{n-1}) \text{ do } \\ & \mid \vec{r}(v) \leftarrow \Gamma(P).\mathsf{pointForProgress}(p(v)) \\ & \quad \text{end} \\ & \text{end} \end{split}$$

Algorithm 1: Transformation to Cartesian coordinates $\vec{r}(v)$

Potential Energy

- Vertex-Vertex repulsion
 - Repulsive force based on Coulomb's law
 - $F_{\text{rep}}(d) := c_1 \cdot \frac{1}{d^2}$

$$U_{\mathsf{rep}}(u,v) \coloneqq \int\limits_{-\infty}^{d(u,v)} -F_{\mathsf{rep}}(s) \, ds$$

- Vertex-Vertex attraction
 - Attractive force based on logarithmic spring
 - $F_{\rm att}(I) := -c_2 \cdot k \cdot \ln\left(\frac{I}{k}\right)$

$$U_{\mathsf{att}}(e) \coloneqq \int\limits_{k}^{I(\Gamma_e)} -F_{\mathsf{att}}(s) \, ds$$

Potential Energy

- Order of vertices on a path
 - Prevents intra-path overlapping edges

$$U_{\mathrm{ord}}(P) \coloneqq egin{cases} 0 & ext{if edges } e \in E(P) ext{ do not overlap} \\ \infty & ext{otherwise} \end{cases}$$

- Vertex-Path repulsion
 - Prevents unwanted vertex-edge intersections
 - Prevents inter-path overlapping edges

$$U_{\mathrm{int}}(v,P) \coloneqq egin{cases} c_3 \cdot rac{1}{d(v,\Gamma_P)} & \mathrm{if} \ d(v,\Gamma_P)
eq 0 \\ \infty & \mathrm{otherwise} \end{cases}$$

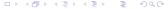
26 / 30

Christian Schnorr April 25th, 2017

Potential Energy

$$U := \sum_{\{u,v\} \in V^2} U_{\mathsf{rep}}(u,v) + \sum_{e \in E} U_{\mathsf{att}}(e) + \sum_{P \in \Pi} U_{\mathsf{ord}}(P) + \sum_{\substack{v \in V, P \in \Pi \\ v \notin V(P)}} U_{\mathsf{int}}(v,P)$$

- Can be evaluated in $\mathcal{O}(|V|^2 + |E| + |V| \cdot |\Pi|)$
- Optimization using hill climbing



27 / 30

Christian Schnorr April 25th, 2017

Results

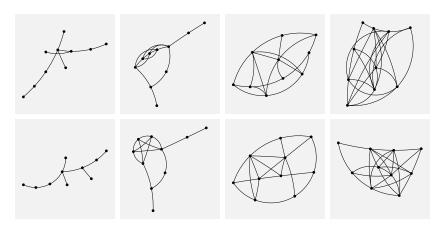


Figure: Drawings of graphs with 10 vertices and 9/15/20/25 edges; each with (bottom) and without (top) user adjustments.

Results

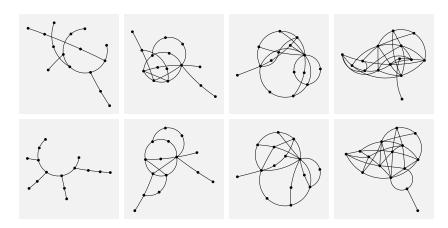


Figure: Drawings of graphs with 15 vertices and 14/20/25/35 edges; each with (bottom) and without (top) user adjustments.

 Christian Schnorr
 April 25th, 2017
 29 / 30

Demo

■ This slide is boring.



Christian Schnorr April 25th, 2017