Solving fixed-point equations by derivation tree analysis

### Javier Esparza

### Technische Universität München

# Joint work with Stefan Kiefer and Michael Luttenberger

#### We study systems of equations of the form

$$X_1 = f_1(X_1, \dots, X_n)$$
  

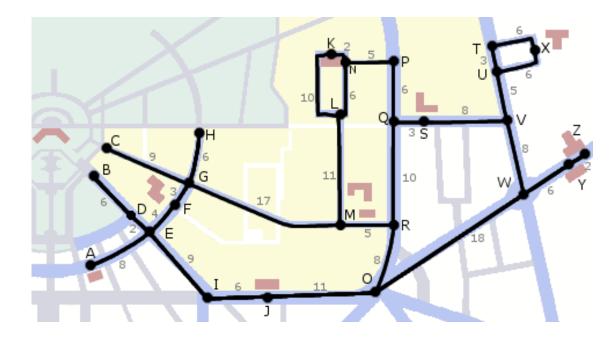
$$X_2 = f_2(X_1, \dots, X_n)$$
  

$$\dots$$
  

$$X_n = f_n(X_1, \dots, X_n)$$

where the  $f_i$ 's are "polynomial expressions".

# Shortest paths



Lengths  $d_i$  of shortest paths from vertex 0 to vertex *i* in graph G = (V, E) are the largest solution of

$$d_i = \min_{(i,j)\in E} (d_i, d_j + w_{ji})$$

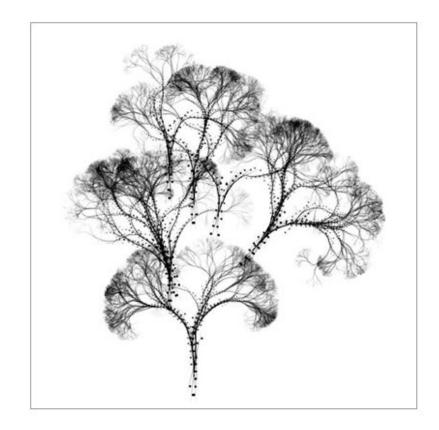
where  $w_{ij}$  is the distance from *i* to *j*.

#### Context-free grammar

 $egin{array}{rcl} X & 
ightarrow & ZX \mid Z \ Y & 
ightarrow & aYa \mid ZX \ Z & 
ightarrow & b \mid aYa \end{array}$ 

Languages generated from X, Y, Z are the least solution of

 $L_X = (L_Z \cdot L_X) \cup L_Z$   $L_Y = (\{a\} \cdot L_Y \cdot \{a\}) \cup (L_Z \cdot L_X)$  $L_Z = \{b\} \cup (\{a\} \cdot L_Y \cdot \{a\})$ 



<sup>235</sup>U ball of radius *D*, spontaneous fission. Probability of a chain reaction is  $(1 - p_0)$ , where  $p_{\alpha}$  for  $0 \le \alpha \le D$  is least solution of

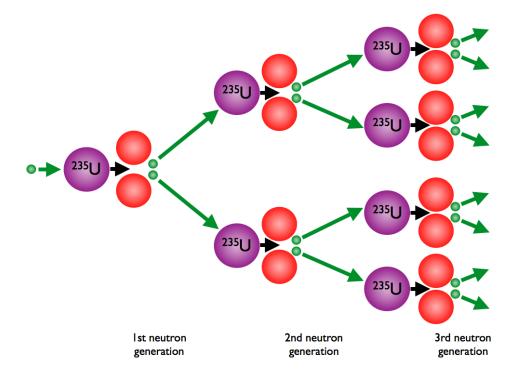
$$p_{\alpha} = k_{\alpha} + \int_{0}^{D} R_{\alpha,\beta} f(p_{\beta}) d\beta$$

for constants  $k_{\alpha}$ ,  $R_{\alpha,\beta}$  and polynomial f(x).

Discretizing the interval [0, D] we get

$$p_i = k_i + \sum_{j=1}^n r_{i,j} f(p_j)$$

for constants  $k_i$ ,  $r_{i,j}$ .



- Stochastic theory:Stationary distribution of Markov chainsExtinction probability of branching processes
- Physics: Heat equation Electrostatic equilibrium
- Biology: RNA structure prediction Population dynamics
- Computer science: Dataflow equations (abstract interpretation) Reputation systems Provenance in databases

### Semiring $(C, +, \times, 0, 1)$ :

(C, +, 0) is a commutative monoid $\times$  distributes over + $(C, \times, 1)$  is a monoid $0 \times a = a \times 0 = 0$ 

#### $\omega$ -continuity:

the relation  $a \sqsubseteq b \Leftrightarrow \exists c : a + c = b$  is a partial order  $\sqsubseteq$ -chains have limits

Examples: nonnegative integers and reals plus  $\infty$ , min-plus (tropical), languages, complete lattices, multisets, Viterbi ...

In the rest of the talk: semiring  $\equiv \omega$ -continuous semiring.

Develop generic solution methods valid for all semirings, or at least for large classes.

- Generic implementations.
- Exchange of algorithms and proof techniques between numerical mathematics, algebraic computation and language theory.

Develop generic solution methods valid for all semirings, or at least for large classes.

- Generic implementations.
- Exchange of algorithms and proof techniques between numerical mathematics, algebraic computation and language theory.

In this talk: brief survey of our work on derivation tree analysis.

Theorem [Klee 38, Tars 55, Kui 97]: A system f of fixed-point equations over a semiring has a least solution  $\mu f$  w.r.t. the natural order  $\sqsubseteq$ . This least solution is the supremum of the Kleene approximants, denoted by  $\{k_i\}_{i>0}$ , and given by

> $k_0 = f(0)$  $k_{i+1} = f(k_i)$ .

Basic algorithm for calculation of  $\mu f$ : compute  $k_0, k_1, k_2, \ldots$  until either  $k_i = k_{i+1}$  or the approximation is considered adequate.

Set interpretations: Kleene iteration never terminates if  $\mu f$  is an infinite set.

•  $X = \{a\} \cdot X \cup \{b\}$   $\mu f = a^*b$ 

Kleene approximants are finite sets:  $k_i = (\epsilon + a + ... + a^i)b$ 

Real semiring: convergence can be very slow.

•  $X = 0.5 X^2 + 0.5$   $\mu f = 1 = 0.99999...$ 

"Logarithmic convergence": k iterations give  $O(\log k)$  correct digits.

$$k_n \le 1 - \frac{1}{n+1}$$
  $k_{2000} = 0.9990$ 

An equation X = f(X) over a semiring induces a context-free grammar Gand a valuation V An equation X = f(X) over a semiring induces a context-free grammar Gand a valuation V

Example:  $X = 0.25X^2 + 0.25X + 0.5$ 

Grammar:  $X \rightarrow aXX \mid bX \mid c$ 

Valuation: V(a) = 0.25, V(b) = 0.25, V(c) = 0.5

An equation X = f(X) over a semiring induces a context-free grammar Gand a valuation V

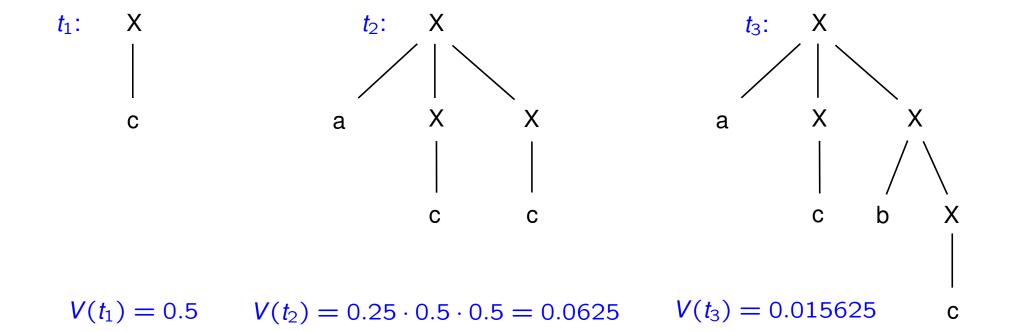
Example:  $X = 0.25X^2 + 0.25X + 0.5$ 

Grammar:  $X \rightarrow aXX \mid bX \mid c$ Valuation: V(a) = 0.25, V(b) = 0.25, V(c) = 0.5

*V* extends to derivation trees and sets of derivation trees:

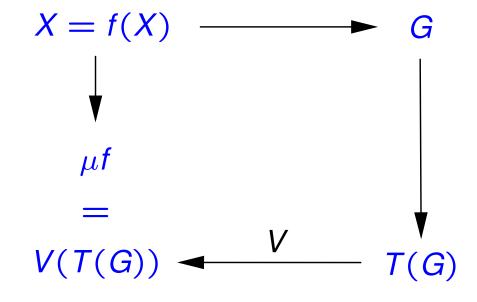
V(t) := ordered product of the leaves of t V(T) :=  $\sum_{t \in T} V(t)$ 

#### $X \rightarrow aXX \mid bX \mid c$ V(a) = V(b) = 0.25, V(c) = 0.5



 $V({t_1, t_2, t_3}) = 0.5 + 0.0625 + 0.015625 = 0.578125$ 

Fundamental Theorem [Boz99,EKL10]: Let *G* be the grammar for X = f(X), and let T(G) be the set of derivation trees of *G*. Then  $\mu f = V(T(G)) \stackrel{def}{=} V(G)$ 



Use language-theoretic results about the

set of derivation trees of the associated context-free grammar

to derive approximation or solution algorithms for the

system of equations.

Let G be the grammar for X = f(X).

An unfolding of G is a sequence  $U^1, U^2, U^3, \ldots$  of grammars such that

- $T(U^i) \cap T(U^j)$  for every  $i \neq j$ , and
- there is a bijection between  $\bigcup_{i=1}^{\infty} T(U^i)$  and T(G) that preserves the yield.

From  $U^1, U^2, U^3, \ldots$  we get another sequence  $G^1, G^2, G^3, \ldots$  such that  $T(G^j) = \bigcup_{i=1}^j T(U^i)$ 

Let Op be the operator on the semiring such that

- $V(G^1) = Op(0)$  and
- $V(G^{i+1}) = Op(V(G^i))$  for every  $i \ge 1$

By the fundamental theorem we get  $\mu f = \sup_{i=1}^{\infty} Op^{i}(0)$ 

Op yields a procedure to approximate  $\mu f$ .

.

 $G: X \rightarrow aXX \mid bX \mid c$ .

.

 $G: X \rightarrow aXX \mid bX \mid c$  .

 $X^{\langle 1 
angle} o c$ 

 $G: X \rightarrow aXX \mid bX \mid c$  .

 $X^{\langle 1 
angle} 
ightarrow c$ 

 $X^{[1]} \rightarrow X^{\langle 1 \rangle}$ 

$$G: X \rightarrow aXX \mid bX \mid c$$
 .

$$X^{\langle 1 
angle} o c$$

$$X^{[1]} \rightarrow X^{\langle 1 \rangle}$$

 $X^{\langle k \rangle} \rightarrow aX^{\langle k-1 \rangle}X^{\langle k-1 \rangle} \mid aX^{[k-2]}X^{\langle k-1 \rangle} \mid aX^{\langle k-1 \rangle}X^{[k-2]} \mid bX^{\langle k-1 \rangle}$ 

.

$$G: X \rightarrow aXX \mid bX \mid c$$
 .

$$X^{\langle 1 
angle} 
ightarrow c$$

$$X^{[1]} \rightarrow X^{\langle 1 \rangle}$$

 $\begin{array}{lll} X^{\langle k \rangle} & \to & a X^{\langle k-1 \rangle} X^{\langle k-1 \rangle} \mid a X^{[k-2]} X^{\langle k-1 \rangle} \mid a X^{\langle k-1 \rangle} X^{[k-2]} \mid b X^{\langle k-1 \rangle} \\ \\ X^{[k]} & \to & X^{\langle k \rangle} \mid X^{[k-1]} \end{array}$ 

$$G: X \rightarrow aXX \mid bX \mid c$$
 .

$$X^{\langle 1 
angle} 
ightarrow c$$

$$X^{[1]} \rightarrow X^{\langle 1 \rangle}$$

 $U^{i}$  ( $G^{i}$ ) is the grammar with  $X^{\langle i \rangle}$  ( $X^{[i]}$ ) as axiom.

"Taking values" we get:

$$V(U^{k}) = V(a) \cdot V(U^{k-1})^{2} + V(a) \cdot V(G^{k-2}) \cdot V(U^{k-1})$$
  
+  $V(a) \cdot V(U^{k-1}) \cdot V(G^{k-2}) + V(b) \cdot V(U^{k-1})$   
 $V(G^{k}) = V(G^{k-1}) + V(U^{k})$ 

and since  $f(X) = V(a) \cdot X^2 + V(b) \cdot X + V(c)$ 

$$V(G^{1}) = f(0)$$
  
$$V(G^{i+1}) = f(V(G^{i})) \text{ for every } i \ge 1$$

Kleene approximation corresponds to evaluating the derivation trees of *G* by increasing height.

$$G: X \rightarrow aXX \mid bX \mid c$$
 .

Recall the approximation by height

 $X^{\langle k \rangle} \rightarrow aX^{\langle k-1 \rangle} X^{\langle k-1 \rangle} | aX^{[k-2]} X^{\langle k-1 \rangle} | aX^{\langle k-1 \rangle} X^{[k-2]} | bX^{\langle k-1 \rangle}$ 

To capture more trees we allow linear recursion.

 $X^{\langle k \rangle} \rightarrow aX^{\langle k-1 \rangle}X^{\langle k-1 \rangle} \mid aX^{[k-1]}X^{\langle k \rangle} \mid aX^{\langle k \rangle}X^{[k-1]} \mid bX^{\langle k-1 \rangle}$ 

 $U^i$  ( $G^i$ ) defined as before.

$$X^{\langle k \rangle} \rightarrow aX^{\langle k-1 \rangle} X^{\langle k-1 \rangle} \mid aX^{[k-1]} X^{\langle k \rangle} \mid aX^{\langle k \rangle} X^{[k-1]} \mid bX^{\langle k-1 \rangle}$$

 $V(U^{i})$  is the least solution of the linear equation

$$X = V(a) \cdot V(U^{i-1})^2 + V(a) \cdot V(G^{i-1}) \cdot X$$
  
+  $V(a) \cdot X \cdot V(G^{i-1}) + V(b) \cdot X$ 

Iterative approximation of V(G):

- $V(G^1)$  = least solution of  $X = V(b) \cdot X + V(c)$
- $V(G^{i+1}) = V(G^{i}) + V(U^{i+1})$  for every  $i \ge 1$

Recipe to approximate  $\mu f$  by solving linear equations.

Consider equations X = f(X) on the real semiring

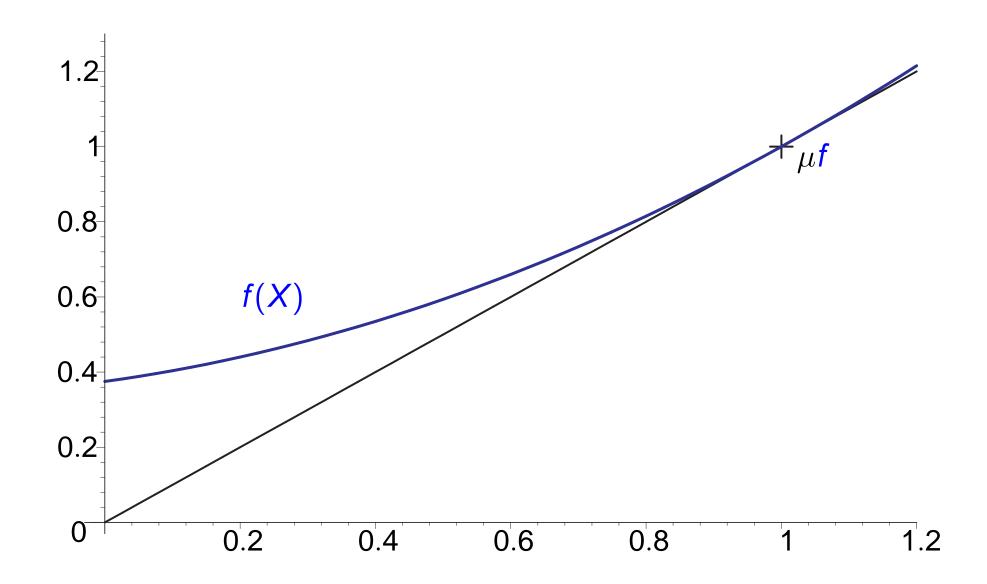
Let g(X) = f(X) - X. Then  $\mu f$  is a zero of g(X).

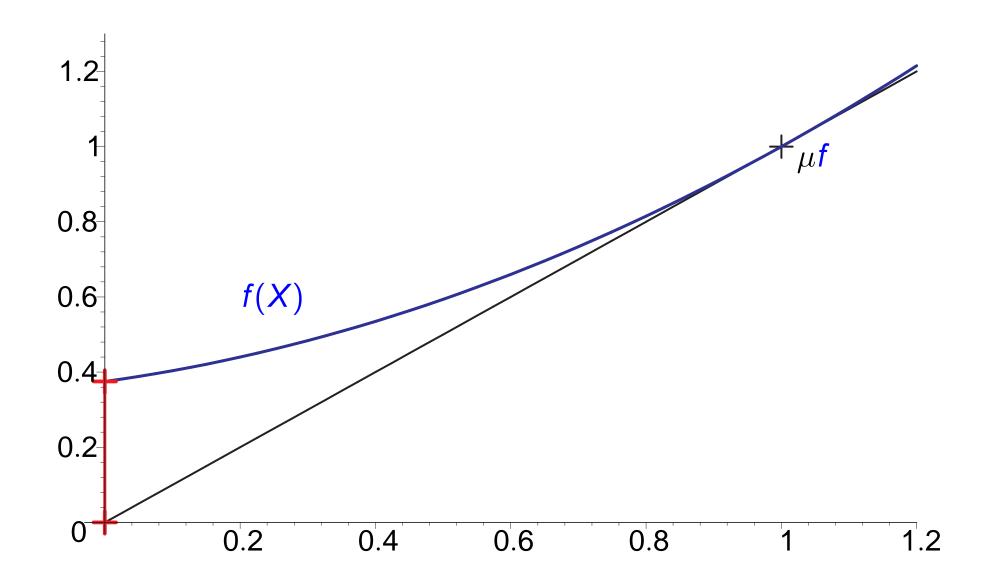
Simple arithmetic yields

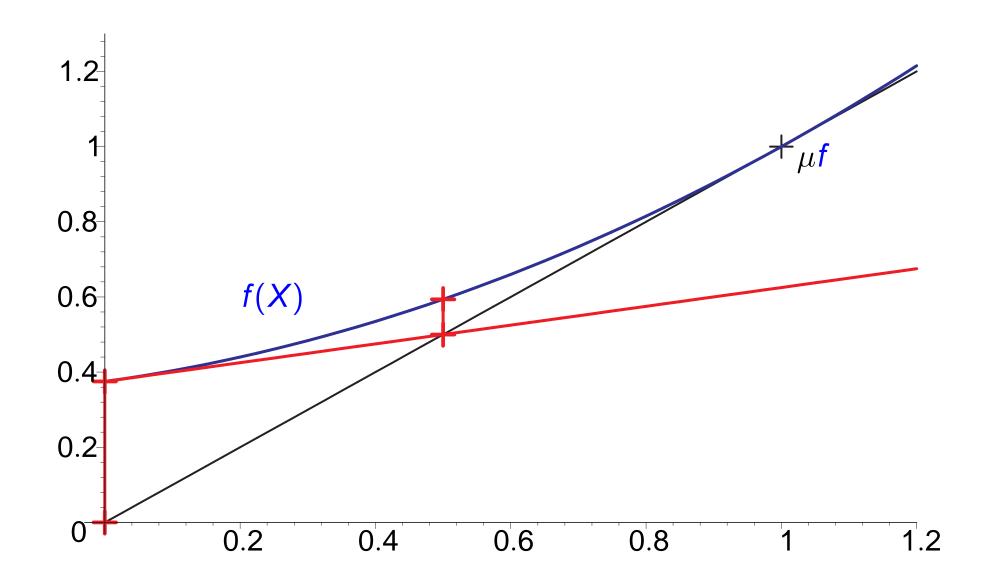
$$V(G^{i+1}) = V(G^{i}) - \frac{g(V(G^{i}))}{g'(V(G^{i}))}$$

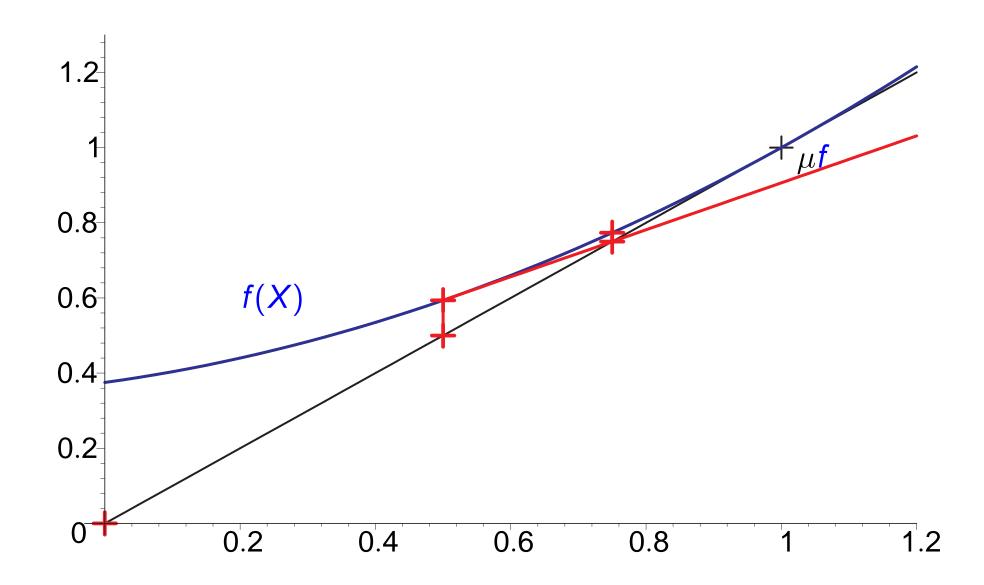
where g'(X) is the derivative of g.

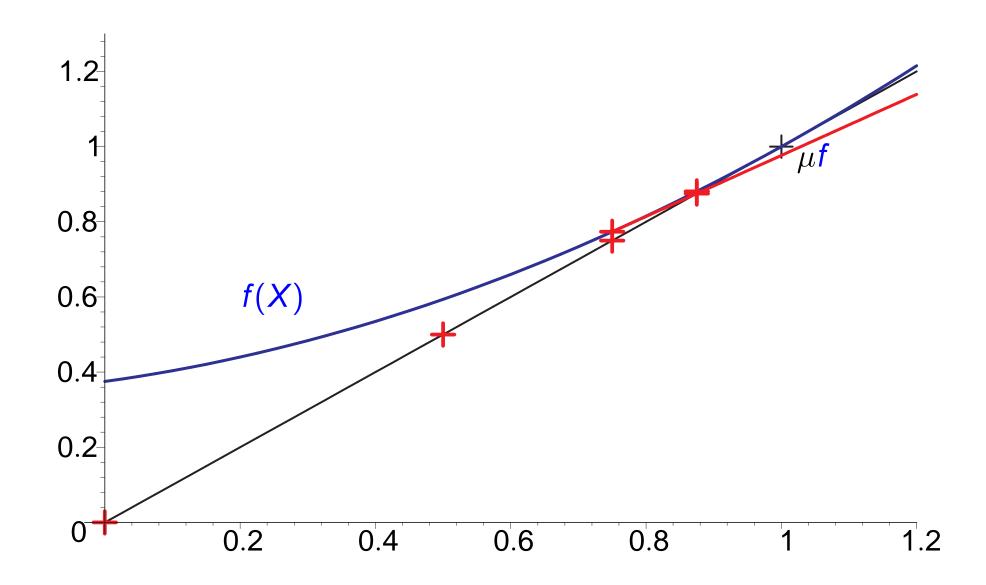
This is Newton's method for approximating a zero of a differentiable function.

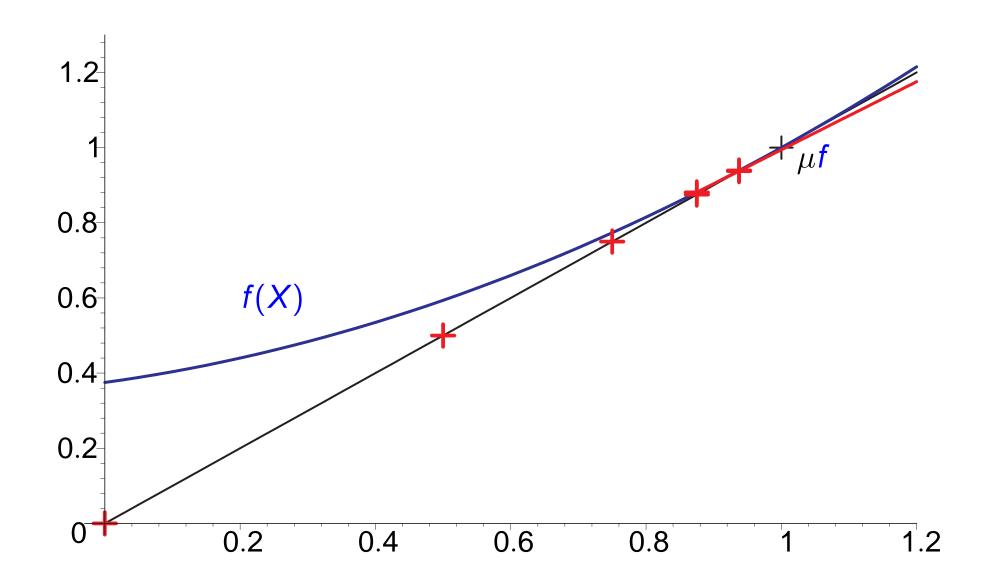










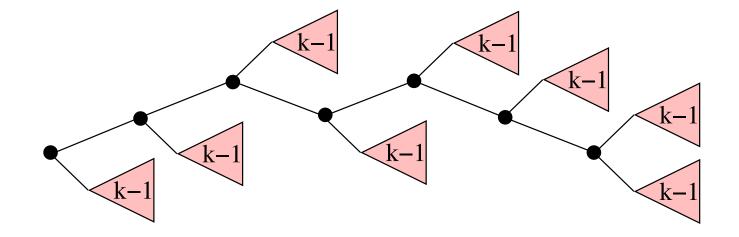


 $X^{\langle k \rangle} \rightarrow aX^{\langle k-1 \rangle} X^{\langle k-1 \rangle} \mid aX^{[k-1]} X^{\langle k \rangle} \mid aX^{\langle k \rangle} X^{[k-1]} \mid bX^{\langle k-1 \rangle}$ 

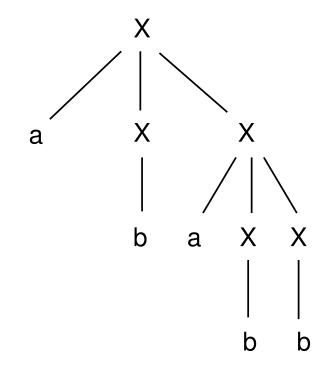
Say a tree of G has dimension k if it is derived from  $U^k$ 

A derivation tree has dimension 0 if it has one node.

A derivation tree has dimension k > 0 if it consists of a spine with subtrees of dimension at most k - 1 (and at least one subtree of dimension k - 1).



The dimension of a derivation tree is the height of the largest full binary tree embeddable in it (ignoring terminals).



Newton approximation corresponds to evaluating the derivation trees of *G* by increasing dimension.

At least as good as Kleene's approximation

For every value v let  $\alpha^{i}(v)$  be the number of trees of  $G^{i}$  with that value, if the number is finite, and  $\alpha^{i}(v) = \infty$  otherwise.

$$V(G^{i}) = \sum_{v} \sum_{i=1}^{\alpha^{i}(v)} v \qquad V(G) = \sum_{v} \sum_{i=1}^{\alpha(v)} v$$

Intuitively:  $\sum_{i=1}^{\alpha(v)} v$  is the "contribution" of v to V(G).  $\sum_{i=1}^{\alpha^{i}(v)} v$  is the "contribution" of v to  $V(G^{i})$ .

We analyze how fast  $\alpha^{i}(v)$  converges to  $\alpha(v)$ .

Theorem (Luttenberger, unpublished): Given a system of *n* equations over a commutative semiring,

 $\alpha^{k \cdot n+1}(\mathbf{v}) \geq \min\{\alpha(\mathbf{v}), \mathbf{k}\}\$ 

for every semiring value v and every  $k \ge 1$ .

In words:  $k \cdot n + 1$  Newton steps "capture" at least k trees of each value v (if there are that many).

Convergence speed for commutative and idempotent semirings

In idempotent semirings v + v = v holds, and so

capturing one single tree of value v amounts to capturing the whole contribution of v to V(G).

Theorem [EKL 10]: Let X = f(X) be a system with *n* equations over an idempotent and commutative semiring. Then  $\mu f = V(G^{n+1})$ .

Stronger version of a theorem by Hopkins and Kozen in LICS'99.

Recall:  $V(U^i)$  is the least solution of

$$X = V(a) \cdot V(U^{i-1})^2 + V(a) \cdot V(G^{i-1}) \cdot X$$
  
+  $V(a) \cdot X \cdot V(G^{i-1}) + V(b) \cdot X$ 

Neither left- nor right linear!

In a commutative and idempotent semiring the equation is equivalent to

$$X = V(a) \cdot V(U^{i-1})^2 + (V(a) \cdot V(G^{i-1}) + V(b)) \cdot X$$

which gives

$$V(U^{i}) = (V(a) \cdot V(G^{i-1}) + V(b))^{*} \cdot V(a) \cdot V(U^{i-1})^{2}$$

A semiring  $S, +, \cdot, 0, 1$  1-bounded if it is idempotent and  $a \sqsubseteq 1$  for every semiring element a.

(Note: commutativity not required)

Example: Viterbi's semiring for computing maximal probabilities.

We use derivation tree analysis to show that for a system on *n* equations (and so *n* variables)

 $\mu f = V(G^n) = f^n(0)$ 

Every tree *t* of height greater than *n* is pumpable: if *t* has yield *w* then there is uvxyz = w and trees  $t^i$  with yield  $uv^ixy^iz = w$  for every  $i \ge 0$ .

$$V(t) + V(t^{0}) = V(uvxyz) + V(uxz)$$

$$\sqsubseteq V(u) \cdot 1 \cdot V(x) \cdot 1 \cdot V(z)$$

$$+ V(u) \cdot V(x) \cdot V(z) \quad (1-\text{boundedness})$$

$$= V(uxz) \quad (\text{idempotence})$$

$$= V(t^{0})$$

So  $t^0$  captures the total contribution of value v.

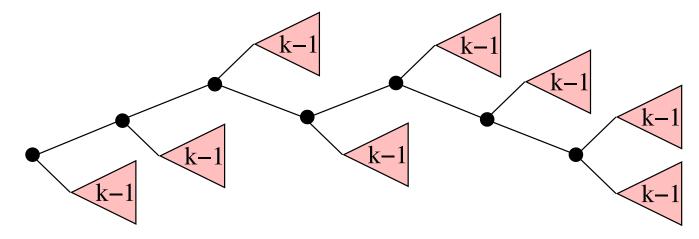
Use now that  $t^0$  has height at most *n*.

A semiring is star-distributive if it is idempotent, commutative, and  $(a + b)^* = a^* + b^*$  for any semiring elements a, b.

Example: tropical semiring.

We use derivation tree analysis to show that for a system on *n* equations  $\mu f$  can be computed by *n* Kleene steps followed by one Newton step.

A derivation tree is a bamboo if it has a path, the stem, such that the height of every subtree not containing a node of the stem is at most *n*.



Proposition: For every tree t there is a bamboo t' such that V(t) = V(t').

Corollary: Bamboos already capture the contribution of all trees.

To compute: *n* Kleene steps for the trees of height at most *n* followed by one Newton step for the bamboos.

## Some applications

 $O(n^3)$  algorithm for computing the throughput of context-free grammars (improving  $O(n^4)$  algorithm by Caucal et al.) [EKL TCS '11].

New algorithm for pattern-based verification of multithreaded procedural programs with fixed number of threads [GMM CAV '10, EG POPL '11].

Very simple algorithm for transforming a context-free grammar into a Parikh-equivalent NFA [EGKL IPL '11].

Threads can spawn new threads with known probabilities.

Execution by one processor. We assume termination with probability 1.

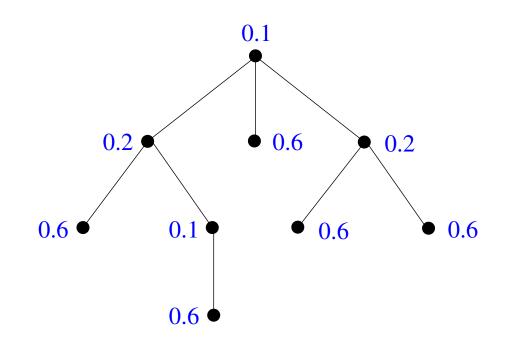
Example (only one type of thread):

$$X \xrightarrow{0.1} \langle X, X, X \rangle \quad X \xrightarrow{0.2} \langle X, X \rangle \quad X \xrightarrow{0.1} X \quad X \xrightarrow{0.6} \epsilon$$

Probability generating function

$$f(X) = 0.1X^3 + 0.2X^2 + 0.1X + 0.6$$

## Describing executions: family trees



Probability of a family tree: product of the probabilities of its nodes.

Execution order depends on a scheduler that chooses a thread from the pool of inactive threads and executes it for one time unit.

Completion space  $S^{\sigma}$  for a scheduler  $\sigma$ : maximal size reached by the pool during execution.

Lemma: The family trees with completion space  $S^{op} = k$  "are" the derivation trees of dimension k.

Theorem [BEKL I&C '11]: The probability  $\Pr[S^{op} \le k]$  of completing execution within space at most *k* is equal to the *k*-th Newton approximant of X = f(X).

In our example:	$\Pr[S^{op} = 1]$	= 2	= 3	= 4	= 5
	0.667	0.237	0.081	0.014	0.001

New connections between analysis and numerical mathematics and TCS, leading to several new algorithms.

Open questions:

- Use language theory to derive convergence bounds of Newton's method over the reals
- Algebraic proof of the convergence speed theorem
- Applications to linear programming ?

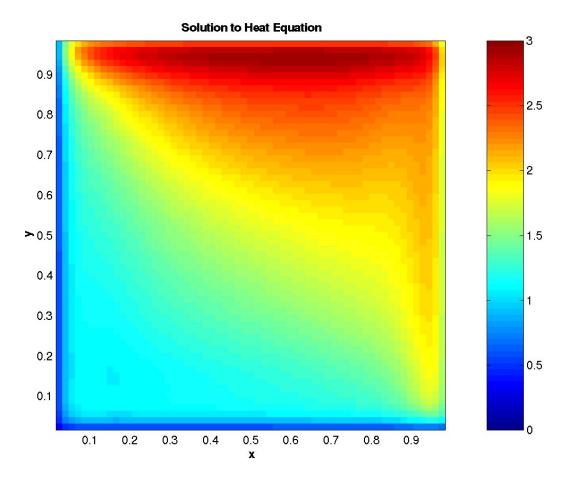
## Heat equation in 2d

$$\frac{\partial u}{\partial t} = h^2 \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

After discretization, temperature at thermal equilibrium is a solution of

$$u_{i,j} = k_{i,j}(u_{i-1,j} + u_{i+1,j} + u_{i,j+1} + u_{i,j-1})$$

for constants  $k_{i,j}$  plus boundary conditions.



Collecting semantics of a program: assigns to each program point *p* the possible values of the memory when the program reaches *p*.

Solution of the equations

$$p_i Store = \bigsqcup_{p_j \in pred(p_i)} f_{ij}(p_j Store)$$

Basis of abstract interpretation

Idempotent semiring: a + a = a

Technique for computing  $\mu f$  algebraically:

- (1) Identify a set  $T \subseteq D$  of trees such that Y(T) can be computed algebraically.
- (2) Show that for every  $t \in D$  there is  $t' \in T$  such that  $Y(t) \sqsubseteq Y(t')$ .

Then by idempotence we have  $\mu f = Y(D) = Y(T)$