## Closed Forms for Numerical Loops

## Zachary Kincaid ${ }^{1}$ Jason Breck ${ }^{2}$ John Cyphert ${ }^{2}$ Thomas Reps ${ }^{2,3}$

${ }^{1}$ Princeton University $\quad{ }^{2}$ University of Wisconsin-Madison $\quad{ }^{3}$ GrammaTech, Inc
January 16, 2019

## Loop summarization

The problem: given a loop, compute a formula that represents its behavior.
while (i < n):
i := i + 2
j := j + 1

## Loop summarization

The problem: given a loop, compute a formula that represents its behavior.


## Loop summarization

The problem: given a loop, compute a formula that represents its behavior.

$$
\begin{gathered}
i=j=0 \wedge n>0 \wedge \\
\text { while }(\mathrm{i}<\mathrm{n}): \\
\mathrm{i}:=\mathrm{i}+2 \\
\mathrm{j}:=\mathrm{j}+1
\end{gathered} \quad \exists k \in \mathbb{N} .\left(\begin{array}{l}
i^{\prime}=i+2 k \\
\wedge \\
j^{\prime}=j+k \\
\wedge \\
n^{\prime}=n \\
\wedge \\
i^{\prime} \geq n \wedge\left(k \geq 1 \Rightarrow i^{\prime} \leq n+1\right) \\
\wedge \neg\left(2 j^{\prime}=i^{\prime}\right)
\end{array}\right)
$$

Summary can be used to answer questions about program behavior

- Is $\{i=j=0 \wedge n>0\}$ loop $\{2 j=i\}$ valid?

Today: Linear loops
non-deterministic
while ( *):
$\mathrm{x}:=A \mathrm{x}$

$$
A \in \mathbb{Q}^{n \times n}
$$

Today: Linear loops
while ( $\times$ ):
$\mathrm{x}:=A \mathrm{x}$

```
A\in\mathbb{Q}
```

- In the paper: affine \& solvable polynomial loops [Rodríguez-Carbonell \& Kapur, ISAAC 2004].


## Why linear loops?

- Natural problem


## Why linear loops?

- Natural problem
- Practical applications
- Any loop can be approximated by a linear loop [KBCR POPL'18]
- Summary for the approximation gives invariants for the loop


## Approximating general loops [KBCR POPL'18]

binary-search(A, target):
lo $=1$, hi $=\operatorname{size}(A)$, ticks $=0$
while (lo <= hi):
ticks++;
mid $=10+(h i-l o) / 2$
if $A[m i d]==$ target:
return mid
Not a linear transformation
else if $A[m i d]$ < target: lo = mid+1
else :

$$
\text { hi }=\text { mid-1 }
$$

## Approximating general loops [KBCR POPL'18]

binary-search (A, target):
lo = 1, hi = size(A), ticks = 0
while (lo <= hi):
ticks++;
mid $=10+(h i-l o) / 2$
if $A[m i d]==$ target:
return mid
else if A[mid] < target:
lo = mid+1
else :
hi = mid-1

## Approximating general loops [KBCR POPL'18]


else :
hi = mid-1

## Approximating general loops [KBCR POPL'18]

binary-search (A, target)
lo = 1 , hi = size(A) while (lo <= hi):
ticks++;
mid = lo + (hi-lo)
if $A[m i d]==$ target return mid
else if A[mid] < target:
lo = mid+1
else :
hi = mid-1

## Approximating general loops [KBCR POPL'18]

binary-search (A, target):
lo = 1, hi = size(A), ticks = 0
while (lo <= hi):
ticks++;
mid = lo + (hi-lo)/2
if $A[m i d]==$ target:
return mid
else if A[mid] < target:

$$
\exists k \in \mathbb{N} .\left(\begin{array}{c}
x^{\prime}=x+k z \\
\wedge y^{\prime}=(1 / 2)^{k} y \\
\wedge z^{\prime}=z
\end{array}\right)
$$

lo = mid+1
else :
hi $=$ mid-1

## Approximating general loops [KBCR POPL'18]

binary-search (A, target):
lo $=1$. hi $=\operatorname{size}(\mathrm{A})$. ticks $=0$
$\exists k \in \mathbb{N} .\binom{$ ticks $=$ ticks $+k}{\wedge h i^{\prime}-l o^{\prime} \leq(1 / 2)^{k}(h i-l o)}$
if A [mid] $==$ target return mid

$$
\exists k \in \mathbb{N} .\left(\begin{array}{c}
x^{\prime}=x+k z \\
\wedge y^{\prime}=(1 / 2)^{k} y \\
\wedge z^{\prime}=z
\end{array}\right)
$$

else if A[mid] < target:
lo = mid+1
else :
hi $=$ mid-1

## Hasn't this problem already been solved?

Given a square matrix $A \in \mathbb{Q}^{n \times n}$, can compute $A^{k}$ symbolically

Entries of $A^{k}$ are exponential polynomials:



Camille Jordan

## Hasn't this problem already been solved?

Given a square matrix $A \in \mathbb{Q}^{n \times n}$, can compute $A^{k}$ symbolically

Entries of $A^{k}$ are exponential polynomials:



Camille Jordan
while(*):
$\mathrm{x}:=A \mathbf{x}$


## No.

Skolem's problem (variant):
Given an exponential-polynomial fover the algebraic numbers, does there exists some $n \in \mathbb{N}$ such that $f(k)=0$ ?

Decidability of Skolem's problem is unknown!


## No.

Skolem's problem (variant):
Given an exponential-polynomial fover the algebraic numbers, does there exists some $n \in \mathbb{N}$ such that $f(k)=0$ ?

Decidability of Skolem's problem is unknown!


Essential problem: algebraic numbers.

## Outline

Starting point of this work: avoid algebraic numbers
(1) Periodic rational matrices have closed forms over $\mathbb{Q}$.

- Computable in polytime


## Outline

Starting point of this work: avoid algebraic numbers
(1) Periodic rational matrices have closed forms over $\mathbb{Q}$.

- Computable in polytime

2) All matrices have best periodic-rational approximations.

## Outline

Starting point of this work: avoid algebraic numbers
(1) Periodic rational matrices have closed forms over $\mathbb{Q}$.

- Computable in polytime

2) All matrices have best periodic-rational approximations.
(3) Exponential-polynomial arithmetic over $\mathbb{Q}$ is decidable.

## Closed forms for linear loops

## Known:

- Eigenvalues of $A$ are rational $\Rightarrow A^{k}$ can be expressed in exponential-polynomial arithmetic over $\mathbb{Q}$.


## Known:

- Eigenvalues of $A$ are rational $\Rightarrow A^{k}$ can be expressed in exponential-polynomial arithmetic over $\mathbb{Q}$.
- [Boigelot PhD thesis '99]: $A$ generates a finite monoid $\Rightarrow A^{k}$ can be expressed in Presburger arithmetic.

Known:

- Eigenvalues of $A$ are rational $\Rightarrow A^{k}$ can be expressed in exponential-polynomial arithmetic over $\mathbb{Q}$.
- [Boigelot PhD thesis '99]: $A$ generates a finite monoid $\Rightarrow A^{k}$ can be expressed in Presburger arithmetic.
Common generalization: A matrix $A$ is periodic rational if there is some power $p$ such that $A^{p}$ has rational eigenvalues.

Known:

- Eigenvalues of $A$ are rational $\Rightarrow A^{k}$ can be expressed in exponential-polynomial arithmetic over $\mathbb{Q}$.
- [Boigelot PhD thesis '99]: $A$ generates a finite monoid $\Rightarrow A^{k}$ can be expressed in Presburger arithmetic.
Common generalization: A matrix $A$ is periodic rational if there is some power $p$ such that $A^{p}$ has rational eigenvalues.
- A periodic rational $\Rightarrow$ can express closed form as

$$
\left(\exists k \in \mathbb{N} . \mathbf{x}^{\prime}=A^{k} \mathbf{x}\right) \equiv\left(\exists k \in \mathbb{N} . \bigvee_{\text {Rational eigenvalues }}^{\left.\substack{p-1} \equiv i \bmod p \wedge \mathbf{x}^{\prime}=\left(A^{p}\right)^{\lfloor k / p\rfloor} A^{i} \mathbf{x}\right)}\right.
$$

- Problem: Rational period of a matrix might be exponential in its size - Expressing closed form takes exponential space!
- Problem: Rational period of a matrix might be exponential in its size
- Expressing closed form takes exponential space!
- Solution: periodic rational spectral decomposition


## Periodic rational spectral decomposition (PRSD)

Let $A \in \mathbb{Q}^{n \times n}$ be a square rational matrix. A periodic rational spectral decomposition of $A$ is a set of triples

$$
\left\{\left\langle p_{1}, \lambda_{1}, \mathbf{v}_{1}\right\rangle, \ldots,\left\langle p_{m}, \lambda_{m}, \mathbf{v}_{m}\right\rangle\right\} \subset \mathbb{N} \times \mathbb{Q} \times \mathbb{Q}^{n}
$$

such that

- for each $i, \mathbf{v}_{i}$ is a generalized eigenvector of $A^{p_{i}}$, with eigenvalue $\lambda_{i}$.


## Periodic rational spectral decomposition (PRSD)

Let $A \in \mathbb{Q}^{n \times n}$ be a square rational matrix. A periodic rational spectral decomposition of $A$ is a set of triples

$$
\left\{\left\langle p_{1}, \lambda_{1}, \mathbf{v}_{1}\right\rangle, \ldots,\left\langle p_{m}, \lambda_{m}, \mathbf{v}_{m}\right\rangle\right\} \subset \mathbb{N} \times \mathbb{Q} \times \mathbb{Q}^{n}
$$

such that

- for each $i, \mathbf{v}_{i}$ is a generalized eigenvector of $A^{p_{i}}$, with eigenvalue $\lambda_{i}$.
- $\left\{\mathbf{v}_{1}, \ldots, \mathbf{v}_{m}\right\}$ is linearly independent


## Periodic rational spectral decomposition (PRSD)

Let $A \in \mathbb{Q}^{n \times n}$ be a square rational matrix. A periodic rational spectral decomposition of $A$ is a set of triples

$$
\left\{\left\langle p_{1}, \lambda_{1}, \mathbf{v}_{1}\right\rangle, \ldots,\left\langle p_{m}, \lambda_{m}, \mathbf{v}_{m}\right\rangle\right\} \subset \mathbb{N} \times \mathbb{Q} \times \mathbb{Q}^{n}
$$

such that

- for each $i, \mathbf{v}_{i}$ is a generalized eigenvector of $A^{p_{i}}$, with eigenvalue $\lambda_{i}$.
- $\left\{\mathbf{v}_{1}, \ldots, \mathbf{v}_{m}\right\}$ is linearly independent
- Informally: $\left\{\mathbf{v}_{1}, \ldots, \mathbf{v}_{m}\right\}$ is maximal

Let $A$ be a matrix with $\operatorname{PRSD}\left\{\left\langle p_{1}, \lambda_{1}, \mathbf{v}_{1}\right\rangle, \ldots,\left\langle p_{m}, \lambda_{m}, \mathbf{v}_{m}\right\rangle\right\}$.

- $\left(\mathbf{x}^{\prime}=A^{k} \mathbf{x}\right)$ takes exponential space, but

Let $A$ be a matrix with $\operatorname{PRSD}\left\{\left\langle p_{1}, \lambda_{1}, \mathbf{v}_{1}\right\rangle, \ldots,\left\langle p_{m}, \lambda_{m}, \mathbf{v}_{m}\right\rangle\right\}$.

- $\left(\mathbf{x}^{\prime}=A^{k} \mathbf{x}\right)$ takes exponential space, but
- for any $i,\left(\mathbf{v}_{i}^{T} \mathbf{x}^{\prime}=\mathbf{v}_{i}^{T} A^{k} \mathbf{x}\right)$ can be computed in polytime
- Intuition: break up period.

Each $\mathbf{v}_{i}$ is an easy-to-compute projection

Let $A$ be a matrix with $\operatorname{PRSD}\left\{\left\langle p_{1}, \lambda_{1}, \mathbf{v}_{1}\right\rangle, \ldots,\left\langle p_{m}, \lambda_{m}, \mathbf{v}_{m}\right\rangle\right\}$.

- $\left(\mathbf{x}^{\prime}=A^{k} \mathbf{x}\right)$ takes exponential space, but
- for any $i,\left(\mathbf{v}_{i}^{T} \mathbf{x}^{\prime}=\mathbf{v}_{i}^{T} A^{k} \mathbf{x}\right)$ can be computed in polytime
- Intuition: break up period.

Each $\mathbf{v}_{i}$ is an easy-to-compute projection

## $A$ is periodic rational

## State-space can be recovered from projections

$$
\left(\mathbf{x}^{\prime}=A^{k} \mathbf{x}\right) \equiv\left(\bigwedge_{i=1}^{m} \mathbf{v}_{i}^{T} \mathbf{x}^{\prime}=\mathbf{v}_{i}^{T} A^{k} \mathbf{x}\right)
$$

## Approximating linear loops

Let $A$ be a matrix with $\operatorname{PRSD}\left\{\left\langle p_{1}, \lambda_{1}, \mathbf{v}_{1}\right\rangle, \ldots,\left\langle p_{m}, \lambda_{m}, \mathbf{v}_{m}\right\rangle\right\}$.

- Set $V=\left[\begin{array}{llll}\mathbf{v}_{1} & \mathbf{v}_{2} & \ldots & \mathbf{v}_{m}\end{array}\right]^{T}$.

Let $A$ be a matrix with $\operatorname{PRSD}\left\{\left\langle p_{1}, \lambda_{1}, \mathbf{v}_{1}\right\rangle, \ldots,\left\langle p_{m}, \lambda_{m}, \mathbf{v}_{m}\right\rangle\right\}$.

- Set $V=\left[\begin{array}{llll}\mathbf{v}_{1} & \mathbf{v}_{2} & \ldots & \mathbf{v}_{m}\end{array}\right]^{T}$.
- There exists a unique $B \in \mathbb{Q}^{m \times m}$ with $V A=B V$.
- $B$ is periodic rational

Let $A$ be a matrix with $\operatorname{PRSD}\left\{\left\langle p_{1}, \lambda_{1}, \mathbf{v}_{1}\right\rangle, \ldots,\left\langle p_{m}, \lambda_{m}, \mathbf{v}_{m}\right\rangle\right\}$.

- Set $V=\left[\begin{array}{llll}\mathbf{v}_{1} & \mathbf{v}_{2} & \ldots & \mathbf{v}_{m}\end{array}\right]^{T}$.
- There exists a unique $B \in \mathbb{Q}^{m \times m}$ with $V A=B V$.
- $B$ is periodic rational
- B simulates $A$, and $V$ is a simulation:


Let $A$ be a matrix with $\operatorname{PRSD}\left\{\left\langle p_{1}, \lambda_{1}, \mathbf{v}_{1}\right\rangle, \ldots,\left\langle p_{m}, \lambda_{m}, \mathbf{v}_{m}\right\rangle\right\}$.

- Set $V=\left[\begin{array}{llll}\mathbf{v}_{1} & \mathbf{v}_{2} & \ldots & \mathbf{v}_{m}\end{array}\right]^{T}$.
- There exists a unique $B \in \mathbb{Q}^{m \times m}$ with $V A=B V$.
- $B$ is periodic rational
- B simulates $A$, and $V$ is a simulation:

$B$ is the best periodic-rational approximation of $A$


## Invariant generation pipeline

General loop $\xrightarrow{[\mathrm{KBCR} \text { POPL'18] }}$ Linear loop

## Invariant generation pipeline

## General loop $\xrightarrow{[K B C R \text { POPL'18] }}$ Linear loop $\xrightarrow{\text { This work }}$ Periodic rational linear loop

## Invariant generation pipeline



## Invariant generation pipeline



Reasoning about non-linear arithmetic

## Exponential-polynomial arithmetic is decidable

## Two steps:

(1) Eliminate all symbols except the loop counter (i.e., program variables)

- Key idea: terms are linear over the ring of exponential-polynomials.

$$
\text { - }\left(2^{k} k^{3}-3^{k} k^{2}+140 \cdot 3^{k}\right) x+\left(4^{k} k\right) y+\left(2^{k}\right) z
$$

- Eliminate symbols using linear q.e. [Loos \& Weispfennning '93]


## Exponential-polynomial arithmetic is decidable

## Two steps:

(1) Eliminate all symbols except the loop counter (i.e., program variables)

- Key idea: terms are linear over the ring of exponential-polynomials.

$$
\text { - }\left(2^{k} k^{3}-3^{k} k^{2}+140 \cdot 3^{k}\right) x+\left(4^{k} k\right) y+\left(2^{k}\right) z
$$

- Eliminate symbols using linear q.e. [Loos \& Weispfennning '93]
(2) Find a bound for the loop counter
- Key idea: exponential-polynomials are eventually dominated by the term with largest base (and largest degree)
- E.g., $2^{k} k^{3}-3^{k} k^{2}+140 \cdot 3^{k}$ is eventully negative


## Consequences

Suppose $A$ is periodic rational. The following problems are decidable:

- Is $\{P\}\{$ while $(*): \mathbf{x}:=A \mathbf{x}\}\{Q\}$ valid?

Linear rational arithmetic

## Consequences

Suppose $A$ is periodic rational. The following problems are decidable:

- Is $\{P\}\{\mathbf{w h i l e}(*): \mathbf{x}:=A \mathbf{x}\}\{Q\}$ valid?

Linear rational arithmetic

- Does $(\mathrm{x}:=\underset{\uparrow}{\mathrm{v}} ; \mathbf{w h i l e}(\mathrm{C})$ do $\mathrm{x}:=A \mathrm{x})$ terminate?


## Constant vector

## Experiments

Suite of 101 microbenchmarks from C4B, HOLA, and literature:


Contributions:
(1) Periodic rational linear loops have closed forms over $\mathbb{Q}$.

- Polytime computation of the summary

Contributions:
(1) Periodic rational linear loops have closed forms over $\mathbb{Q}$.

- Polytime computation of the summary

2 Every matrix has a best periodic-rational approximation.

Contributions:
(1) Periodic rational linear loops have closed forms over $\mathbb{Q}$.

- Polytime computation of the summary

2 Every matrix has a best periodic-rational approximation.
(3) Exponential-polynomial arithmetic over $\mathbb{Q}$ is decidable.

