Linguagem Chapel

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17 de junho de 2015

Timeline

1. **Introdução**
2. **Chapel**
   - Instalação e configuração
   - Tipos de dados
   - Semelhanças com outras linguagens
   - Data Parallelism
   - Task Paralleism
   - Multi-locale Paralleism
   - The Model and the Problem
   - The Integrated Approach
3. **Bad News: Hardness Results**
   - Hardness of PP-Partitioning of Haplotype Matrices
   - Hardness of PP-Partitioning of Genotype Matrices
4. **Good News: Tractability Results**
   - Perfect Path Phylogenies
   - Tractability of PPP-Partitioning of Genotype Matrices

Soma de matrizes

Quantas linhas são necessários para a sua implementação?

Soma de matrizes

OpenMP

```
1 #pragma omp shared( A , B , C , chunk ){
2     #pragma omp for schedule( static , chunk )
3     for( i = 0 ; i < N ; i++)
4         for( j = 0 ; j < N ; j++)
5             C[ i ][ j ] = A[ i ][ j ] + B[ i ][ j ] ;
6 }
```

Soma de matrizes

CUDA

```
1 const int BlockSizeX = 32 ;
2 const int Factor = 4 ;
3 const int BlockSizeY = BlockSizeX / Factor ;
4 __global__ void add( int* C , int* A , int* B , const int N ){
5     int col = blockIdx.x * BlockSizeX + threadIdx.x ;
6     int row = blockIdx.y * BlockSizeX + threadIdx.y * Factor ;
7     for( i = 0 ; i < Factor ; i++)
8         C[ ( row + i ) * N + col ] = A[ ( row + i ) * N + col ] + B[
              ( row + i ) * N + col ] ;
9 }
```

Soma de matrizes

OpenMPI

```
1 MPI_Comm_size( MPI_COMM_WORLD , &npes ) ;
2 MPI_Comm_rank( MPI_COMM_WORLD , &myrank ) ;
3 if( myrank == ROOT )
4     for( target = 0 ; target < npes ; i++){
5         MPI_Send( A+N*target , N , MPI_INT , target , target ,
              MPI_COMM_WORLD ) ;
6         MPI_Send( B+N*target , N , MPI_INT , target , target ,
              MPI_COMM_WORLD ) ;
7     }
8 MPI_Recv( myA , N , MPI_INT , ROOT , myrank , MPI_COMM_WORLD , &
      status ) ;
9 MPI_Recv( myB , N , MPI_INT , ROOT , myrank , MPI_COMM_WORLD , &
      status ) ;
10 for( i = 0 ; i < N ; i++) myC[ i ] = myA[ i ] + myB[ i ] ;
11 MPI_Send( myC , N , MPI_INT , ROOT , 0 , MPI_COMM_WORLD ) ;
12 if( myrank == ROOT )
13     for( sender = 0 ; sender < npes ; sender++)
14         MPI_Recv( C+N*sender , N , MPI_INT , sender , 0 ,
              MPI_COMM_WORLD , &status ) ;
```

Soma de matrizes

Linhas

- OpenMP: 6
- CUDA: 9
- OpenMPI: 14

Então, quantas linhas são necessários com Chapel?

Our formalization of haplotyping.

Inputs

- A genotype matrix G.
- The rows of the matrix are individuals / taxa.
- The columns of the matrix are SNP sites / characters.
- The problem is directed: one haplotype is known.
- The input is biallelic: there are only two homozygous states (0 and 1) and one heterozygous state (2).

Outputs

- A haplotype matrix H.
- Pairs of rows in H explain the rows of G.
- The haplotypes in H form a perfect phylogeny.

We can do perfect phylogeny haplotyping efficiently, but . . .

1. Data may be missing.
   - This makes the problem NP-complete . . .
   - . . . even for very restricted cases.

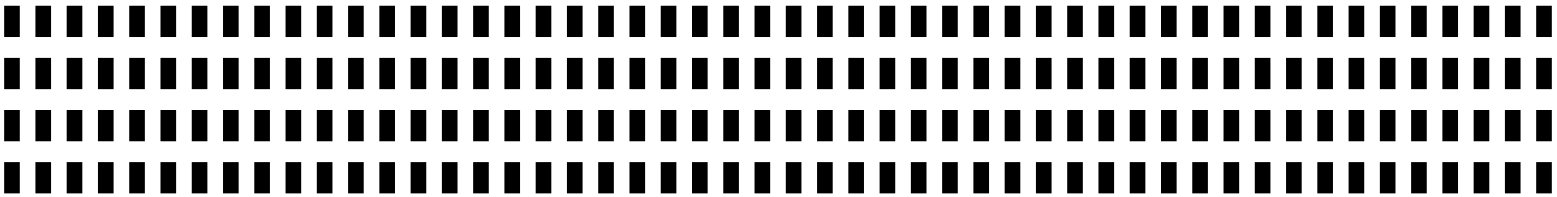
   Solutions:
   - Additional assumption like the rich data hypothesis.
2. No perfect phylogeny is possible.
   - This can be caused by chromosomal crossing-over effects.
   - This can be caused by incorrect data.
   - This can be caused by multiple mutations at the same sites.

   Solutions:
   - Look for phylogenetic networks.
   - Correct data.
   - Find blocks where a perfect phylogeny is possible.

How blocks help in perfect phylogeny haplotyping.

1. Partition the site set into overlapping contiguous blocks.
2. Compute a perfect phylogeny for each block and combine them.
3. Use dynamic programming for finding the partition.

Genotype matrix



no perfect phylogeny

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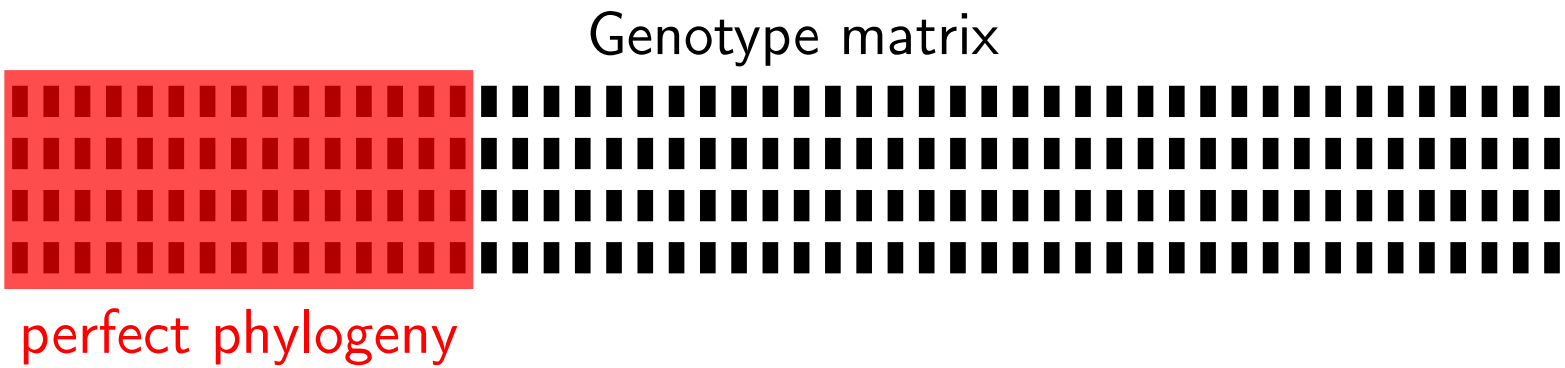

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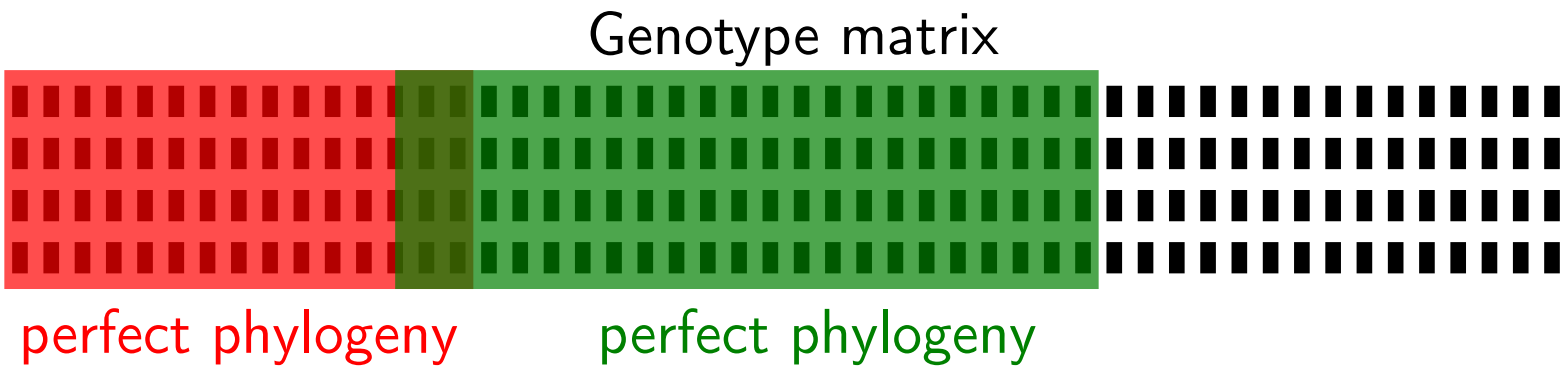

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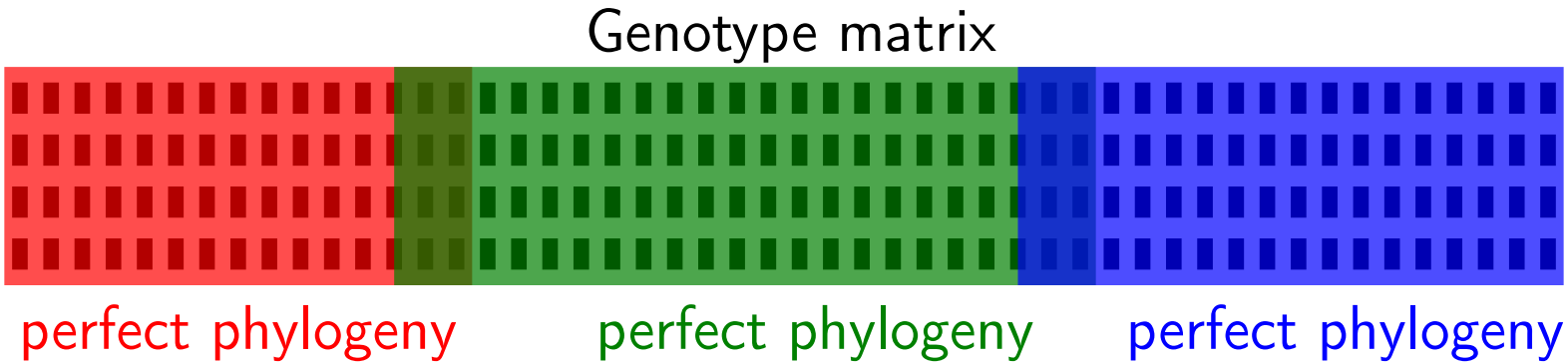
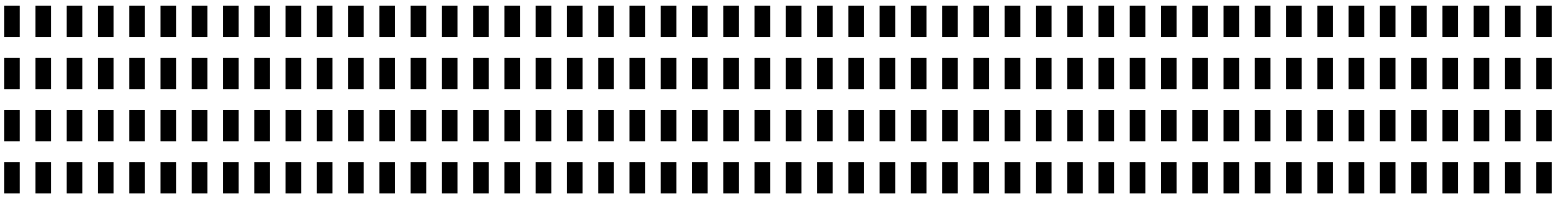


Objective of the integrated approach.

1. Partition the site set into noncontiguous blocks.
2. Compute a perfect phylogeny for each block and combine them.
3. Compute partition while computing perfect phylogenies.

Genotype matrix



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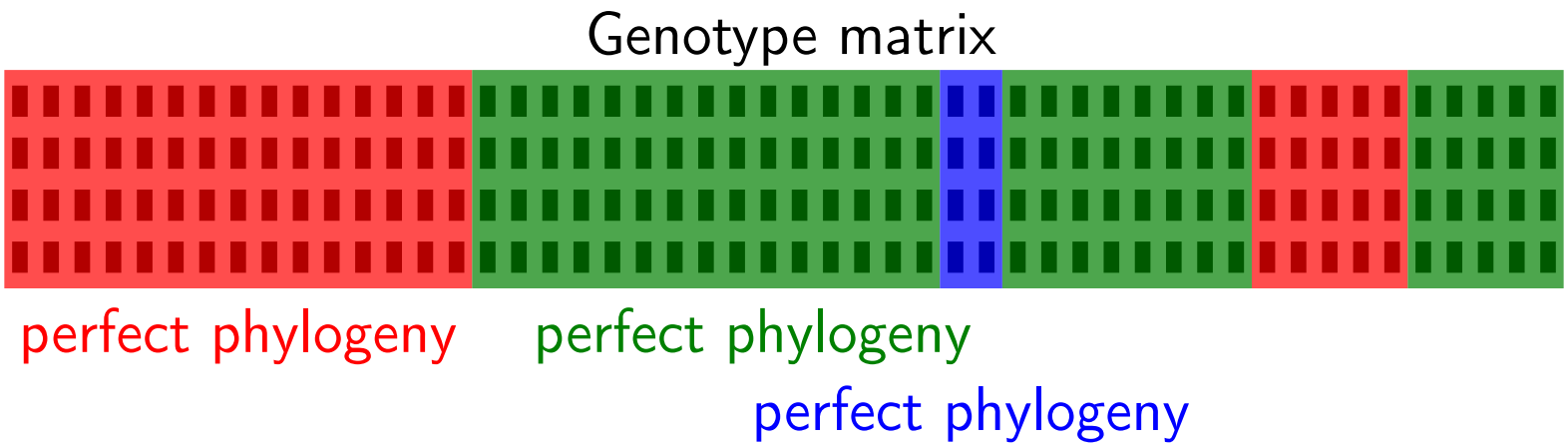


The formal computational problem.

We are interested in the computational complexity of the function χ_{PP}:

- It gets genotype matrices as input.
- It maps them to a number k.
- This number is minimal such that the sites can be covered by k sets, each admitting a perfect phylogeny.
  (We call this a pp-partition.)

Finding pp-partitions of haplotype matrices.

We start with a special case:

- The inputs M are already haplotype matrices.
- The inputs M do not allow a perfect phylogeny.
- What is $\chi_{\mathsf{PP}}(M)$?

Example

$$M: \begin{matrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \end{matrix}$$

No perfect phylogeny is possible.

Finding pp-partitions of haplotype matrices.

We start with a special case:

- The inputs M are already haplotype matrices.
- The inputs M do not allow a perfect phylogeny.
- What is $\chi_{\text{PP}}(M)$?

Example

M:

0	0	0	1
0	1	0	0
1	0	0	0
0	1	0	0
1	0	0	0
0	1	0	1
1	1	0	0
0	0	1	0
1	0	1	0

Perfect phylogeny
Perfect phylogeny
$\chi_{\text{PP}}(M) = 2$.

Bad news about pp-partitions of haplotype matrices.

Theorem

Finding optimal pp-partition of haplotype matrices is equivalent to finding optimal graph colorings.

Proof sketch for first direction.

1. Let G be a graph.
2. Build a matrix with a column for each vertex of G.
3. For each edge of G add four rows inducing the submatrix $\begin{pmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix}$.
4. The submatrix enforces that the columns lie in different perfect phylogenies. □

Implications for pp-partitions of haplotype matrices.

Corollary

If $\chi_{\mathrm{PP}}(M) = 2$ for a haplotype matrix M, we can find an optimal pp-partition in polynomial time.

Corollary

Computing χ_{PP} for haplotype matrices is

- NP-*hard*,
- *not fixed-parameter tractable, unless* P = NP,
- *very hard to approximate.*

Finding pp-partitions of genotype matrices.

Now comes the general case:

- The inputs M are genotype matrices.
- The inputs M do not allow a perfect phylogeny.
- What is $\chi_{\mathrm{PP}}(M)$?

Example

$$M: \begin{matrix} 2 & 2 & 2 & 2 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 2 & 2 & 0 \\ 1 & 1 & 0 & 0 \end{matrix}$$

No perfect phylogeny is possible.

Finding pp-partitions of genotype matrices.

Now comes the general case:

- The inputs M are genotype matrices.
- The inputs M do not allow a perfect phylogeny.
- What is $\chi_{\text{PP}}(M)$?

Example

M:

2	2	2	2
1	0	0	0
0	0	0	1
0	0	1	0
0	2	2	0
1	1	0	0

Perfect phylogeny

Perfect phylogeny

$\chi_{\text{PP}}(M) = 2$.

Bad news about pp-partitions of haplotype matrices.

Theorem

Finding optimal pp-partition of genotype matrices is at least as hard as finding optimal colorings of 3-uniform hypergraphs.

Proof sketch.

1. Let G be a 3-uniform hypergraph.
2. Build a matrix with a column for each vertex of G.
3. For each hyperedge of G add four rows inducing the submatrix $\begin{pmatrix} 2 & 2 & 2 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$.
4. The submatrix enforces that the three columns do not all lie in the same perfect phylogeny. □

Implications for pp-partitions of genotype matrices.

Corollary

Even if we know $\chi_{\mathsf{PP}}(M) = 2$ *for a genotype matrix* M*, finding a pp-partition of any fixed size is still*

- NP-*hard*,
- *not fixed-parameter tractable, unless* P = NP,
- *very hard to approximate.*

Automatic optimal pp-partitioning is hopeless, but...

- The hardness results are worst-case results for highly artificial inputs.
- Real biological data might have special properties that make the problem tractable.
- One such property is that perfect phylogenies are often perfect path phylogenies:
  In HapMap data, in 70% of the blocks where a perfect phylogeny is possible a perfect path phylogeny is also possible.

Example of a perfect path phylogeny.

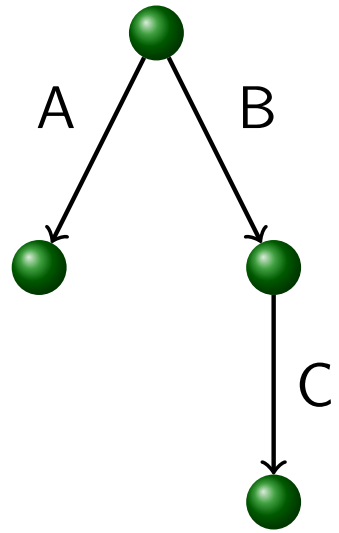
Genotype matrix

	A	B	C
	2	2	2
G:	0	2	0
	2	0	0
	0	2	2

Haplotype matrix

	A	B	C
	1	0	0
	0	1	1
	0	0	0
H:	0	1	0
	0	0	0
	1	0	0
	0	0	0
	0	1	1

Perfect path phylogeny



The modified formal computational problem.

We are interested in the computational complexity of the function χ_{PPP}:

- It gets genotype matrices as input.
- It maps them to a number k.
- This number is minimal such that the sites can be covered by k sets, each admitting a perfect path phylogeny.
  (We call this a ppp-partition.)

Good news about ppp-partitions of genotype matrices.

Theorem

Optimal ppp-partitions of genotype matrices can be computed in polynomial time.

Algorithm

1. Build the following partial order:
   - Can one column be above the other in a phylogeny?
   - Can the columns be the two children of the root of a perfect path phylogeny?
2. Cover the partial order with as few compatible chain pairs as possible. For this, a maximal matching in a special graph needs to be computed.

▸ The algorithm in action

Summary

- Finding optimal pp-partitions is intractable.
- It is even intractable to find a pp-partition when just two noncontiguous blocks are known to suffice.
- For perfect path phylogenies, optimal partitions can be computed in polynomial time.

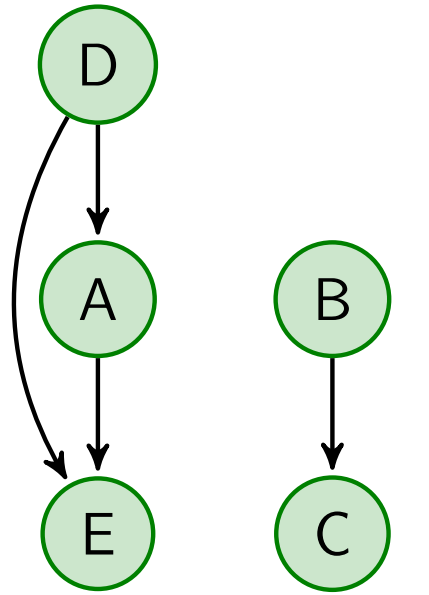
The algorithm in action.

Computation of the partial order.

Genotype matrix

	A	B	C	D	E
	2	2	2	2	2
G:	0	1	2	1	0
	1	0	0	1	2
	0	2	2	0	0

Partial order



Partial order: $\longrightarrow$

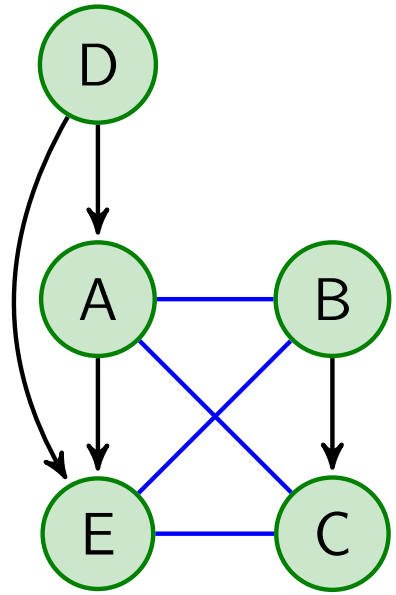
The algorithm in action.

Computation of the partial order.

Genotype matrix

	A	B	C	D	E
	2	2	2	2	2
G:	0	1	2	1	0
	1	0	0	1	2
	0	2	2	0	0

Partial order



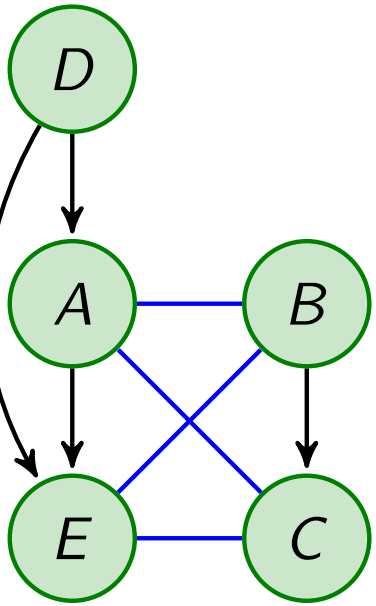
Partial order: $\longrightarrow$

Compatible as children of root: ——

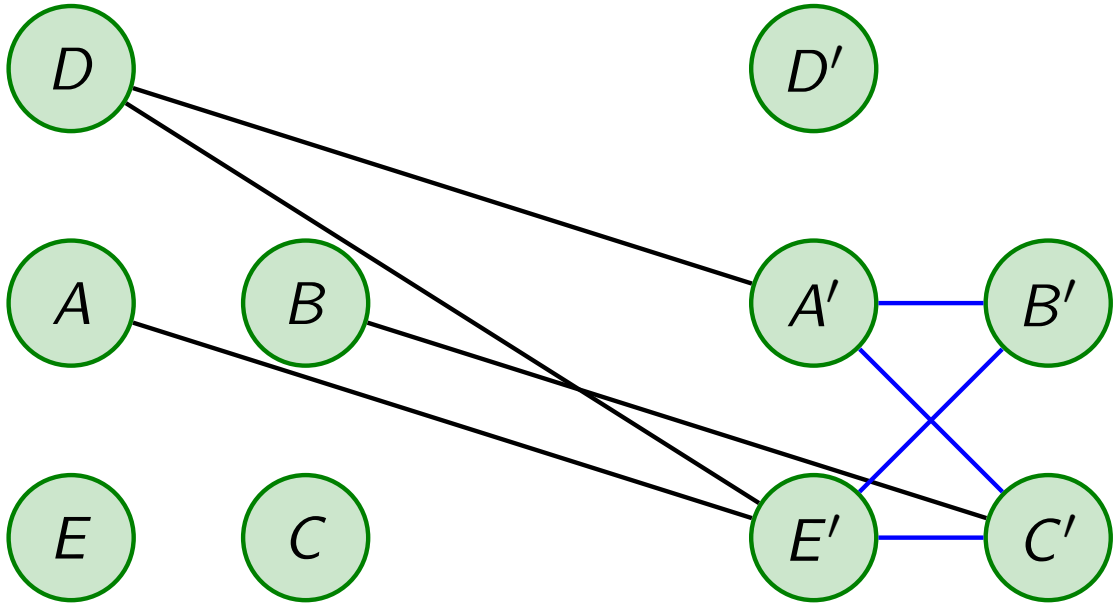
The algorithm in action.

The matching in the special graph.

Partial order



Matching graph

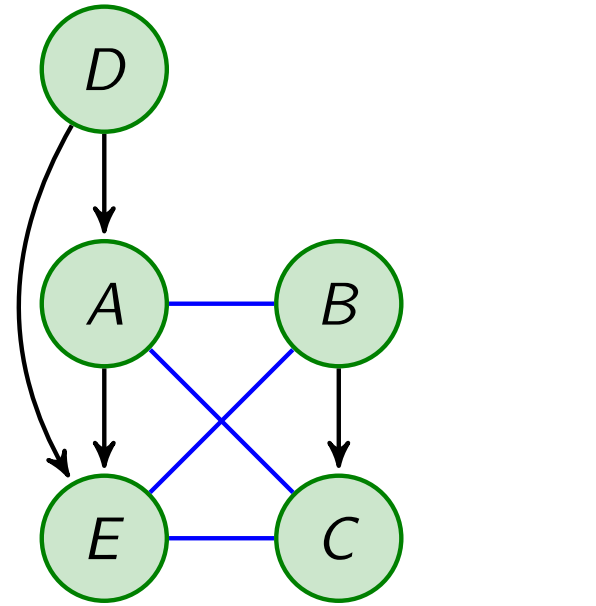


◂ Return

The algorithm in action.

The matching in the special graph.

Partial order



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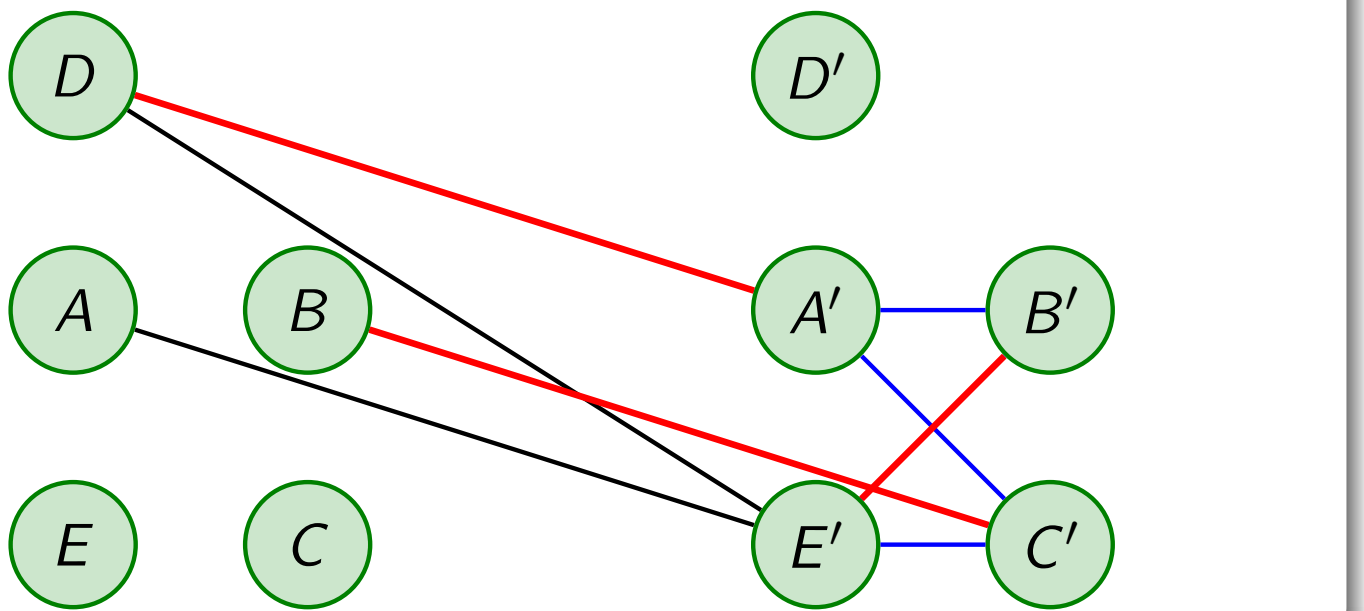


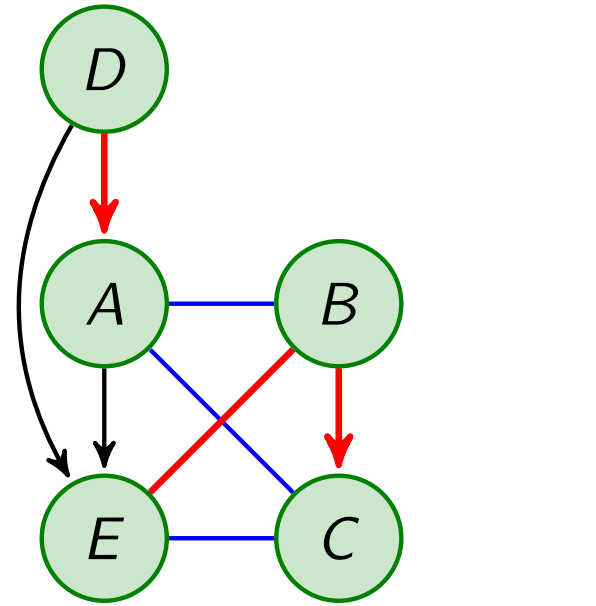
A maximal matching in the matching graph

◂ Return

The algorithm in action.

The matching in the special graph.

Partial order



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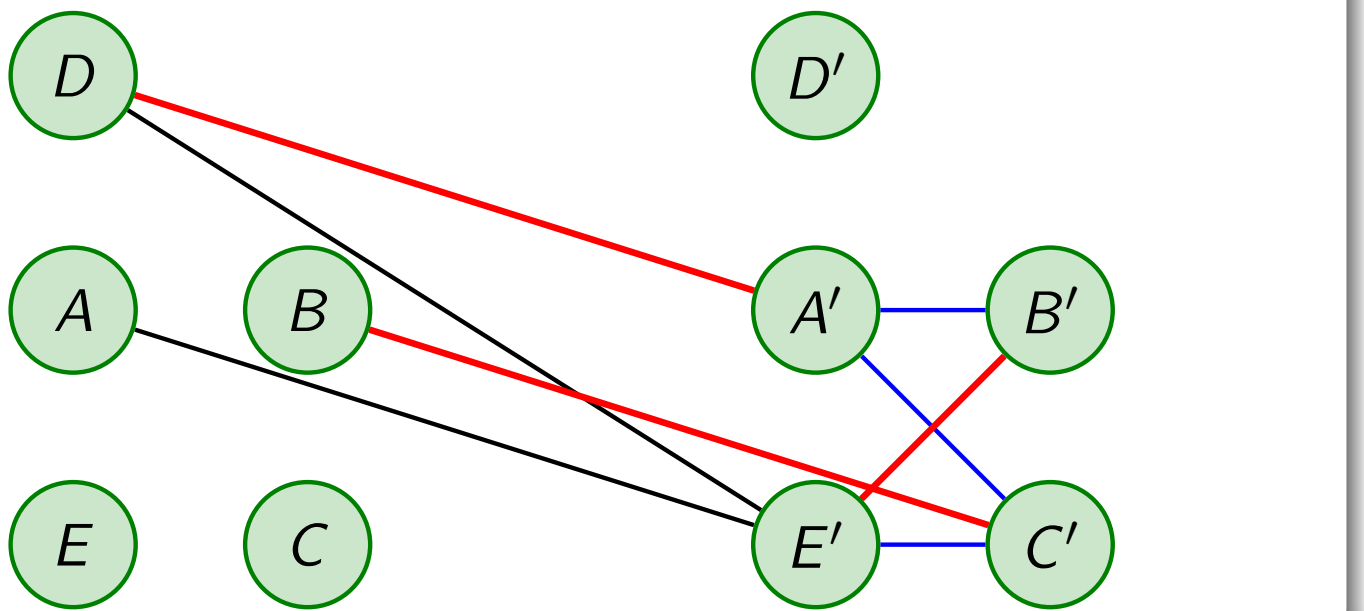

A maximal matching in the matching graph induces perfect path phylogenies.

◂ Return

Simple slide with three points shown all at once

- Point 1
- Point 2
- Point 3

Simple slide with three points shown in succession

- Point 1 (Click “Next Page” to see Point 2)

Simple slide with three points shown in succession

- Point 1 (Click “Next Page” to see Point 2)
- Point 2

Simple slide with three points shown in succession

- Point 1 (Click “Next Page” to see Point 2)
- Point 2
- Point 3

Slide with two columns: items and a graphic

- First item

Slide with two columns: items and a graphic

- First item
- Second item

Slide with two columns: items and a graphic

- First item
- Second item
- ...