CUDA and GPU programming: an opportunity for scientists

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May 27, 2009

Why learn GPU programming?

What problems are appropriate for the GPU?

Case study: backtracking

Where to next?

Hardware

- Moore's Law:
  - clock speeds no longer rapidly increasing.
  - massively multicore architectures circumvent this problem.
- Change of paradigm from single threaded applications to parallel and stream processing.
- Double precision on GPUs now supported.
- Major players NVIDIA, AMD, Intel, all serious about GPGPU (general purpose GPU programming).

Software

- CUDA: not a high level language, but an appropriate level for the hardware. Much easier to learn than graphics APIs such as OpenGL.
- For easy problems, CUDA is easy to apply (many problems are easy).
- OpenCL: similar to CUDA, code will run on variety of hardware.
- Details may change, but broad brush-strokes and techniques will remain same. Skills developed now won't go to waste.

- Improving hardware and software make GPU computing very attractive, large benefits for not too large time investment.
- Discontinuity in Moore's Law - one-off opportunity (until quantum computing!).
- Grab low hanging fruit while you can (implement embarrassingly parallel algorithms).
- As time goes by, more applications will be ported to GPU hardware.
- *Desktop supercomputer*: workstation with Tesla GPUs can be as powerful as a CPU cluster.
- Soon, CPU / GPU clusters will be common.
- If current trends continue, will become widespread paradigm in high performance computing.

- Easiest problems: embarrassingly parallel, e.g.
  - Computer graphics.
  - Simulation of large physical systems via molecular dynamics.
  - Large graphs / networks.
  - Numerical integration.
  - Many more.
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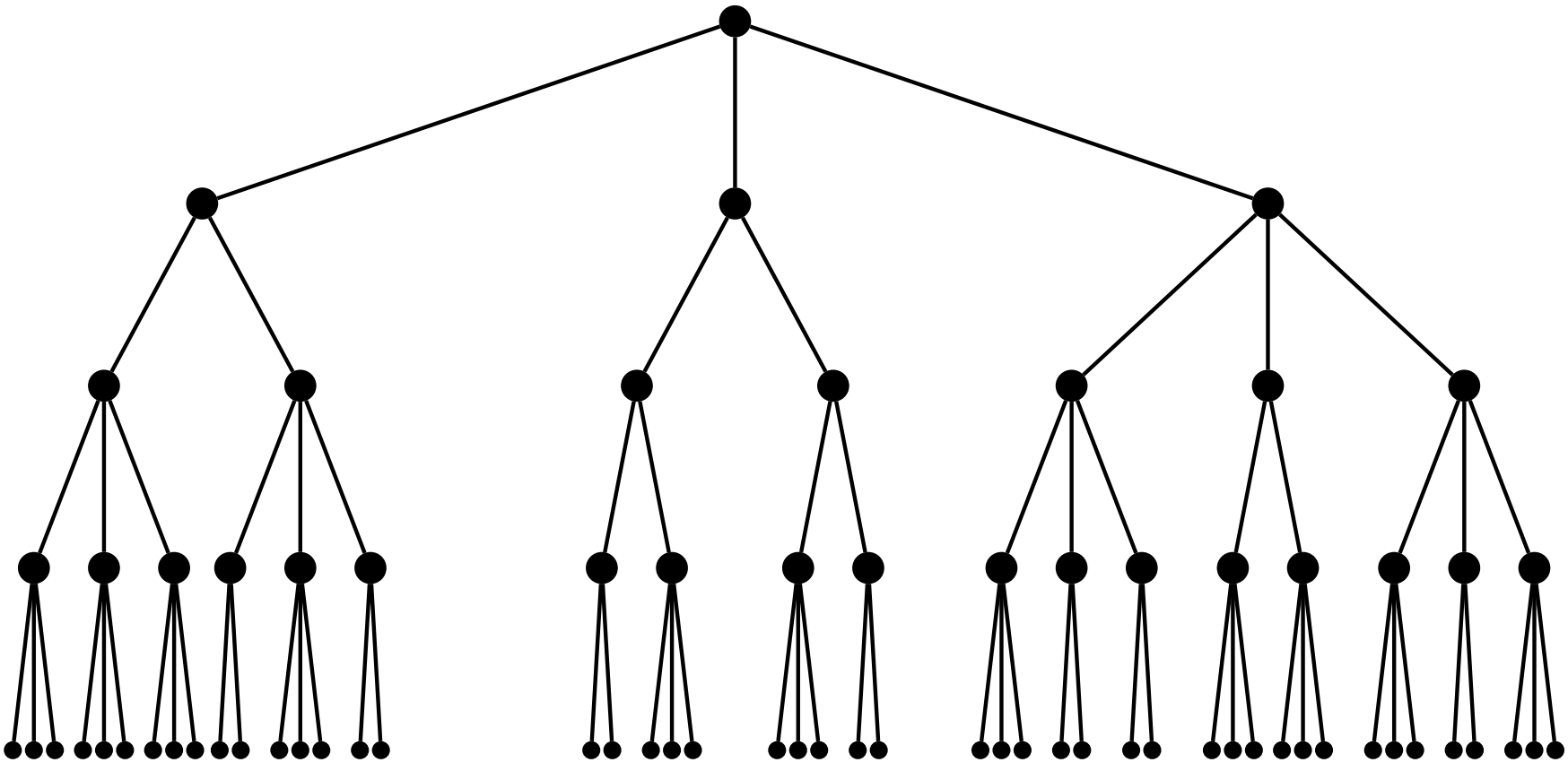
. . . with sufficient ingenuity.

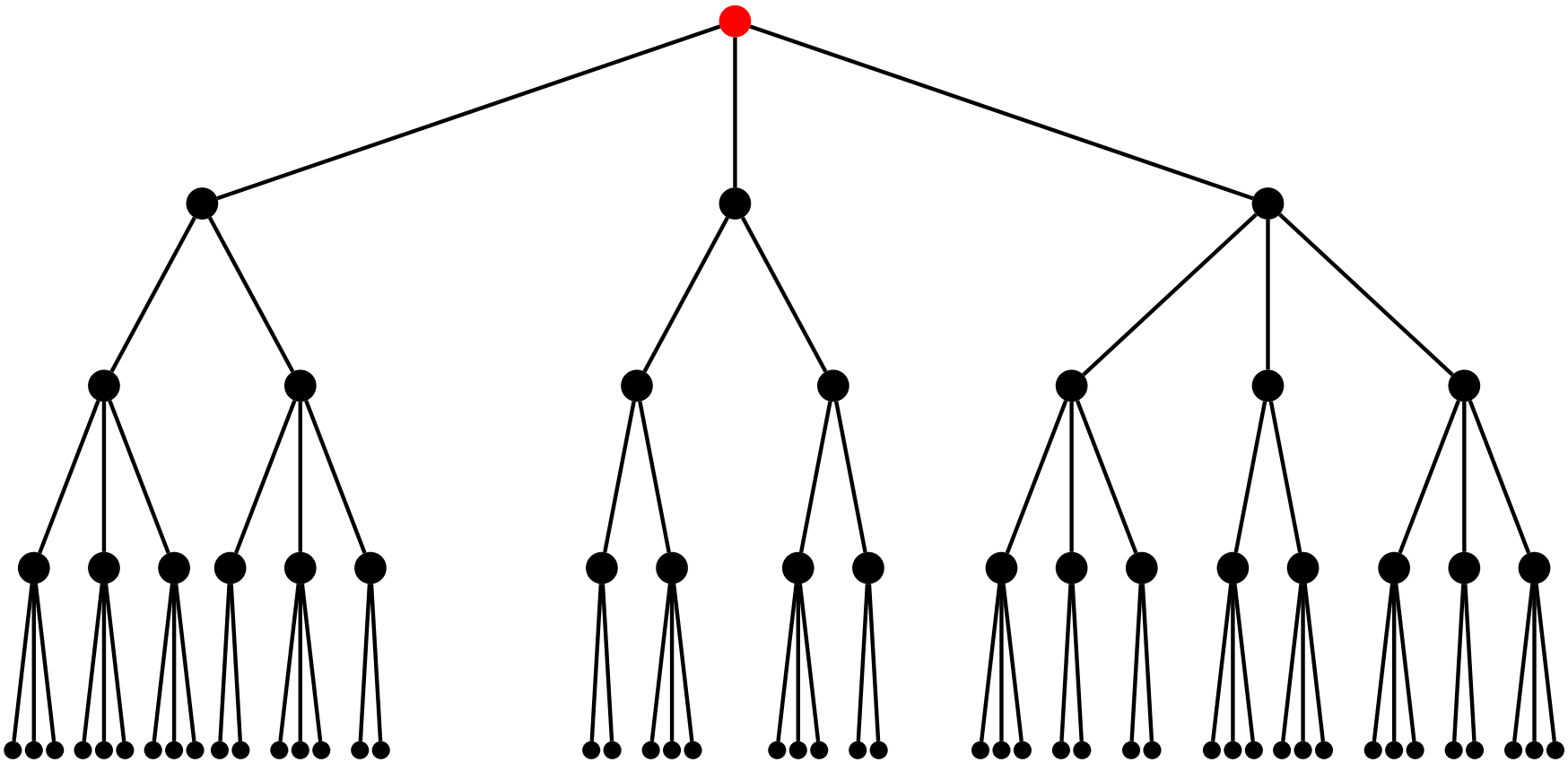
My research

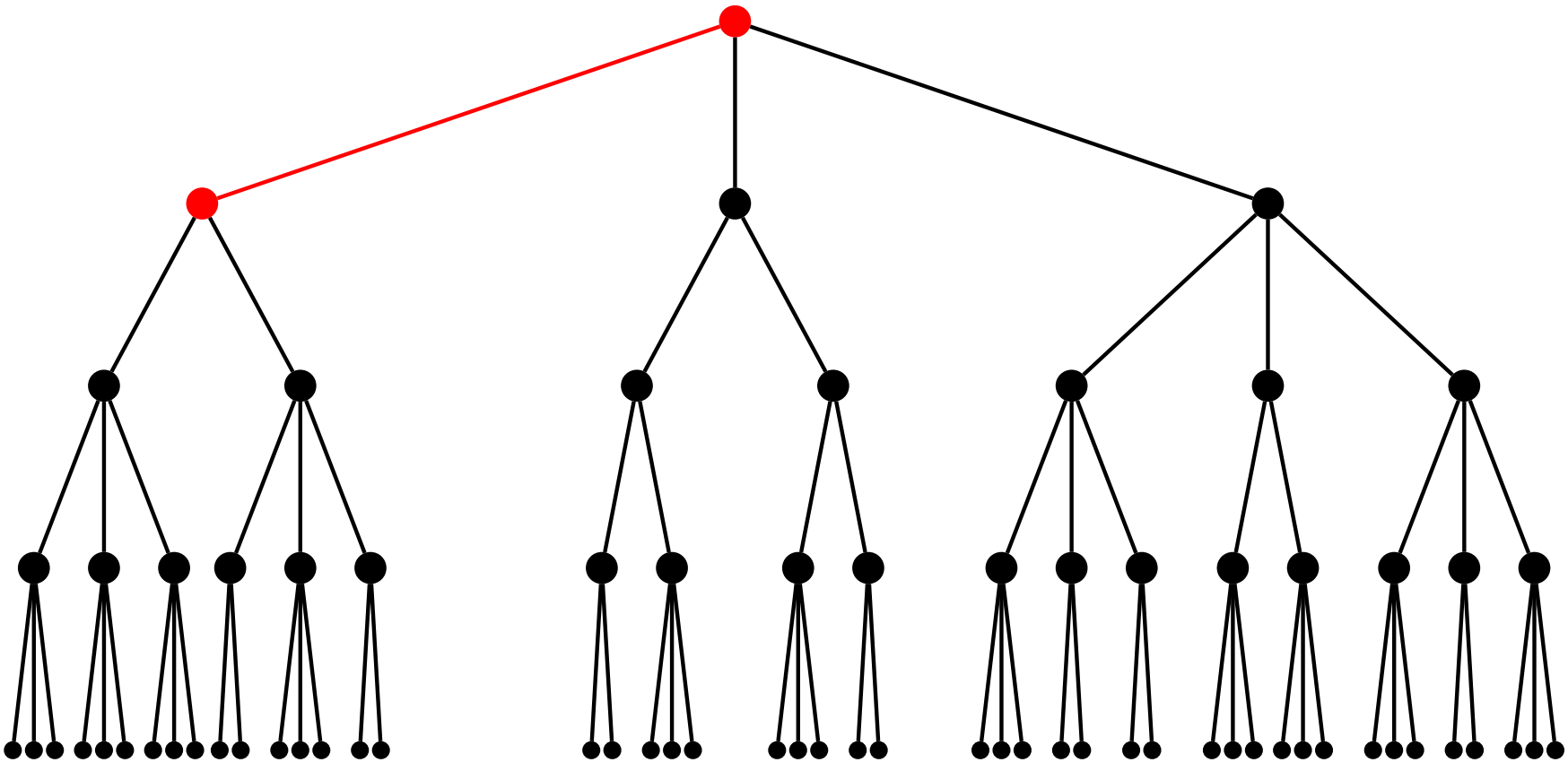
- Monte Carlo integration - embarrassingly parallel, but not what I'm interested at the moment.
- Monte Carlo simulation of self-avoiding walks - complicated algorithm, too hard.
- Self-avoiding walk enumeration via backtracking - ok?

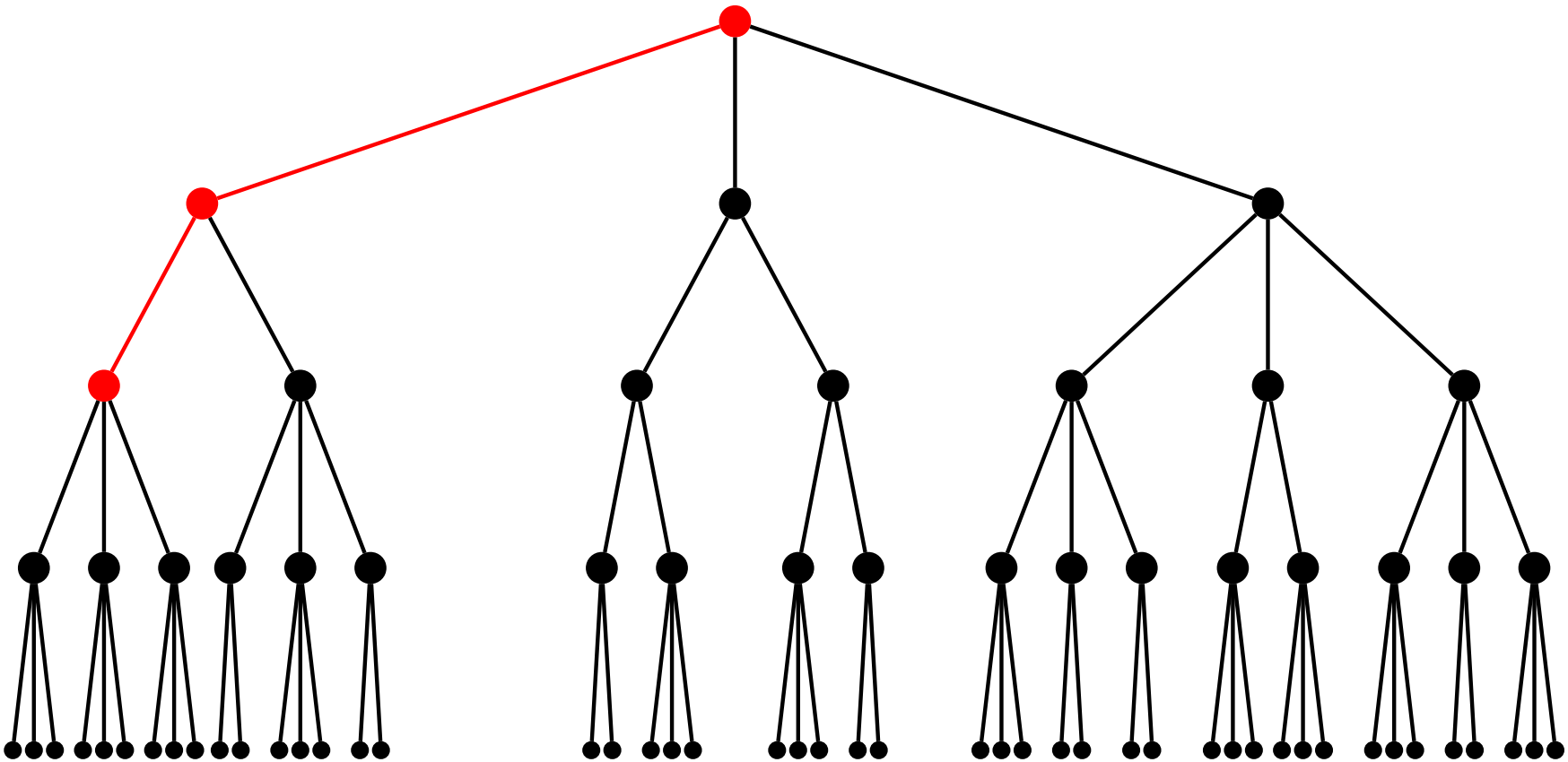
Backtracking

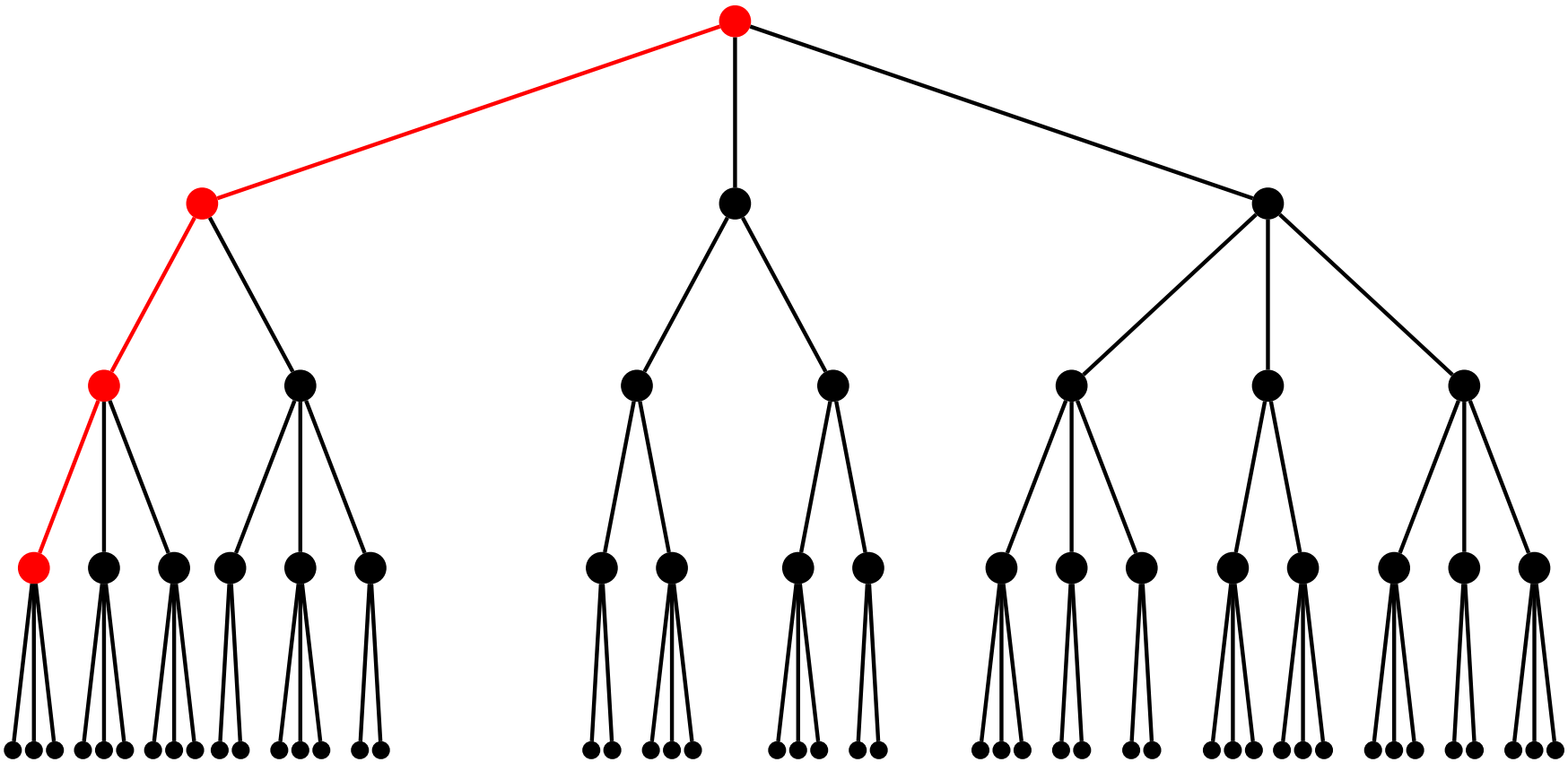
- Exhaustively generate 'objects' by incrementally building up on smaller objects.
- e.g. binary strings of 3 digits:
  $\{empty\} \to 0 \to 00 \to 000 \to 00 \to 001 \to 00 \to 0 \to 01 \to 010 \to 01 \to 011 \to \cdots$
- $\equiv$ depth first search.
- Each object has a unique parent, this defines the *backtracking tree*.

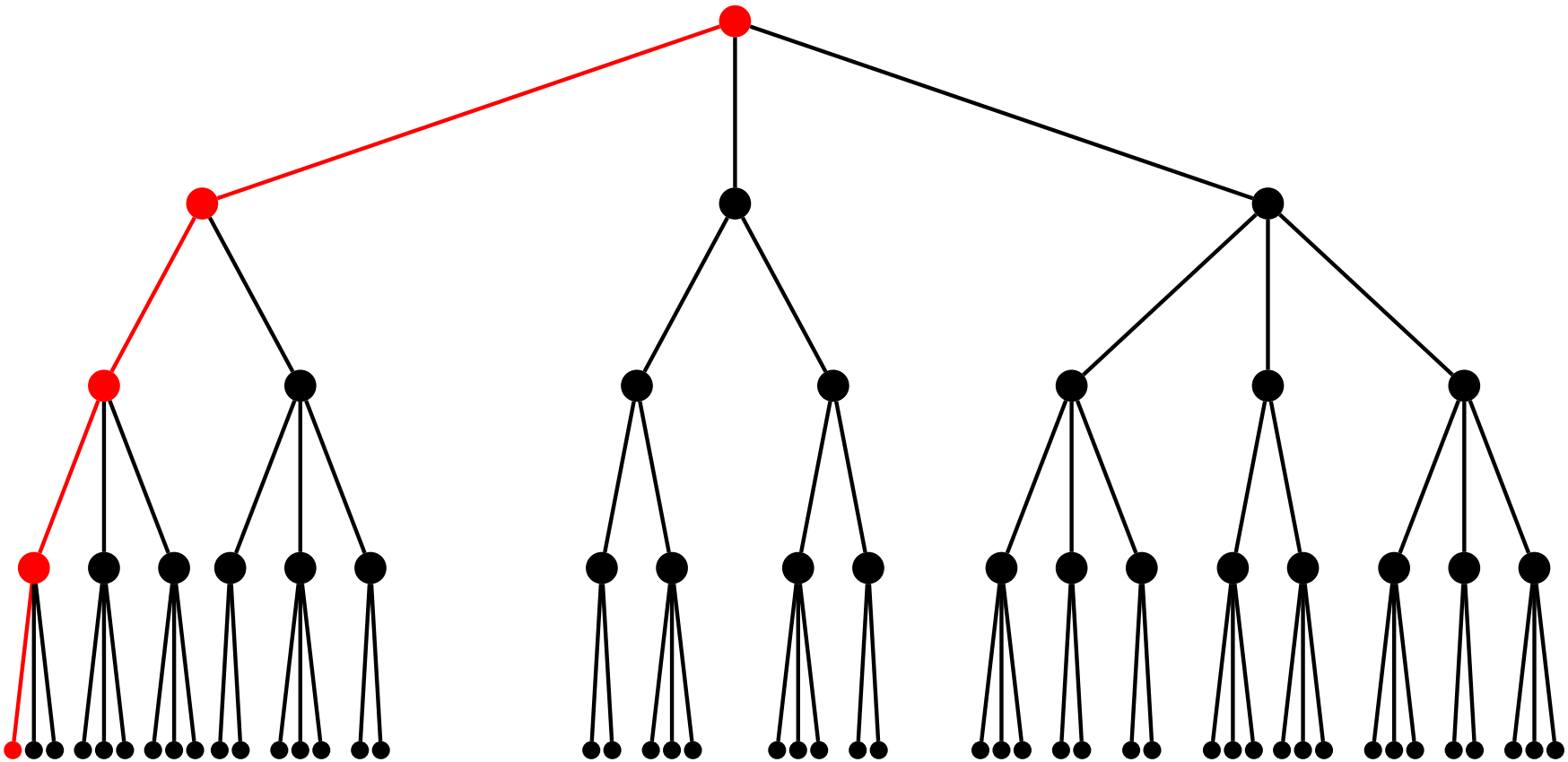


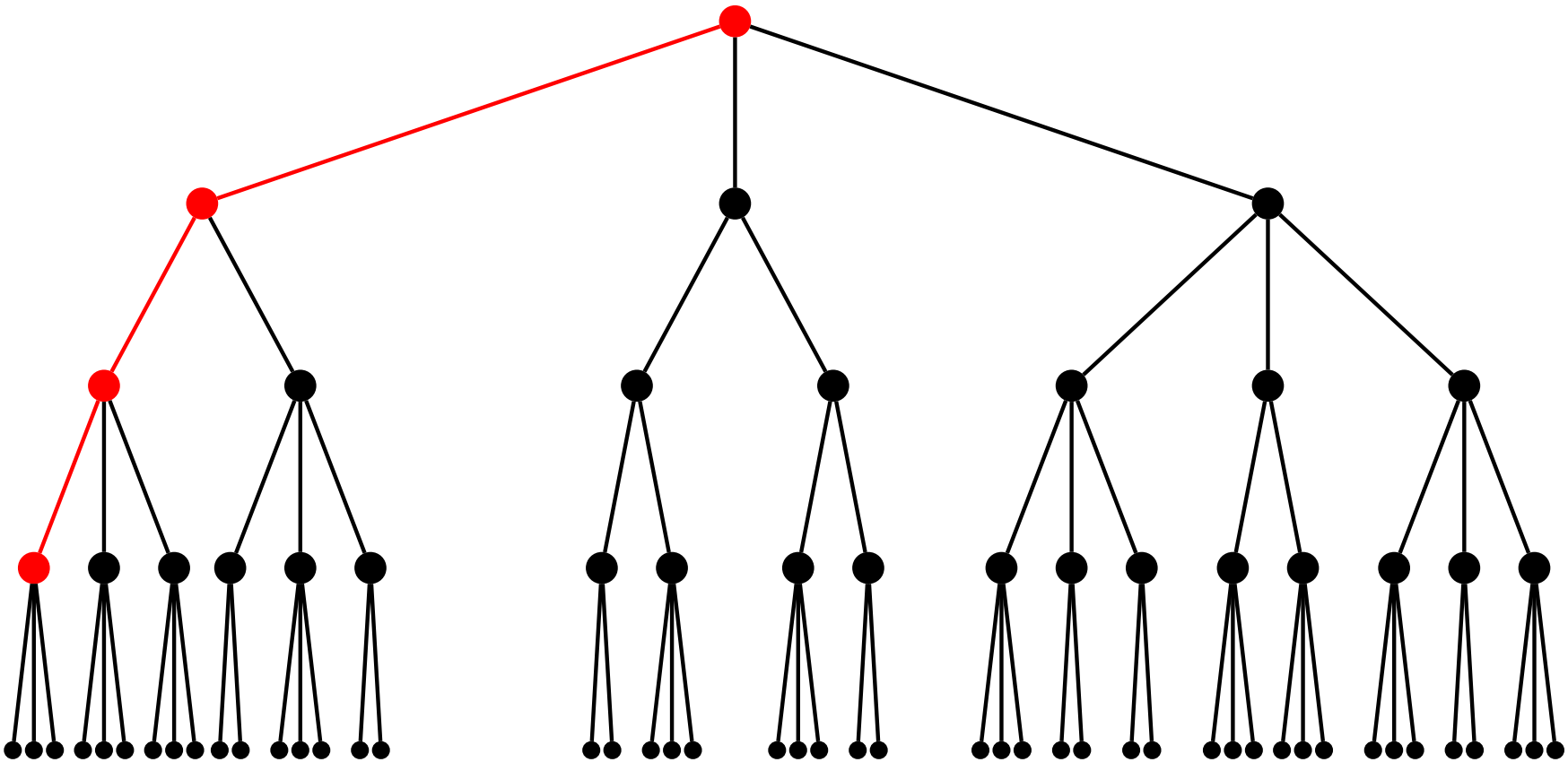


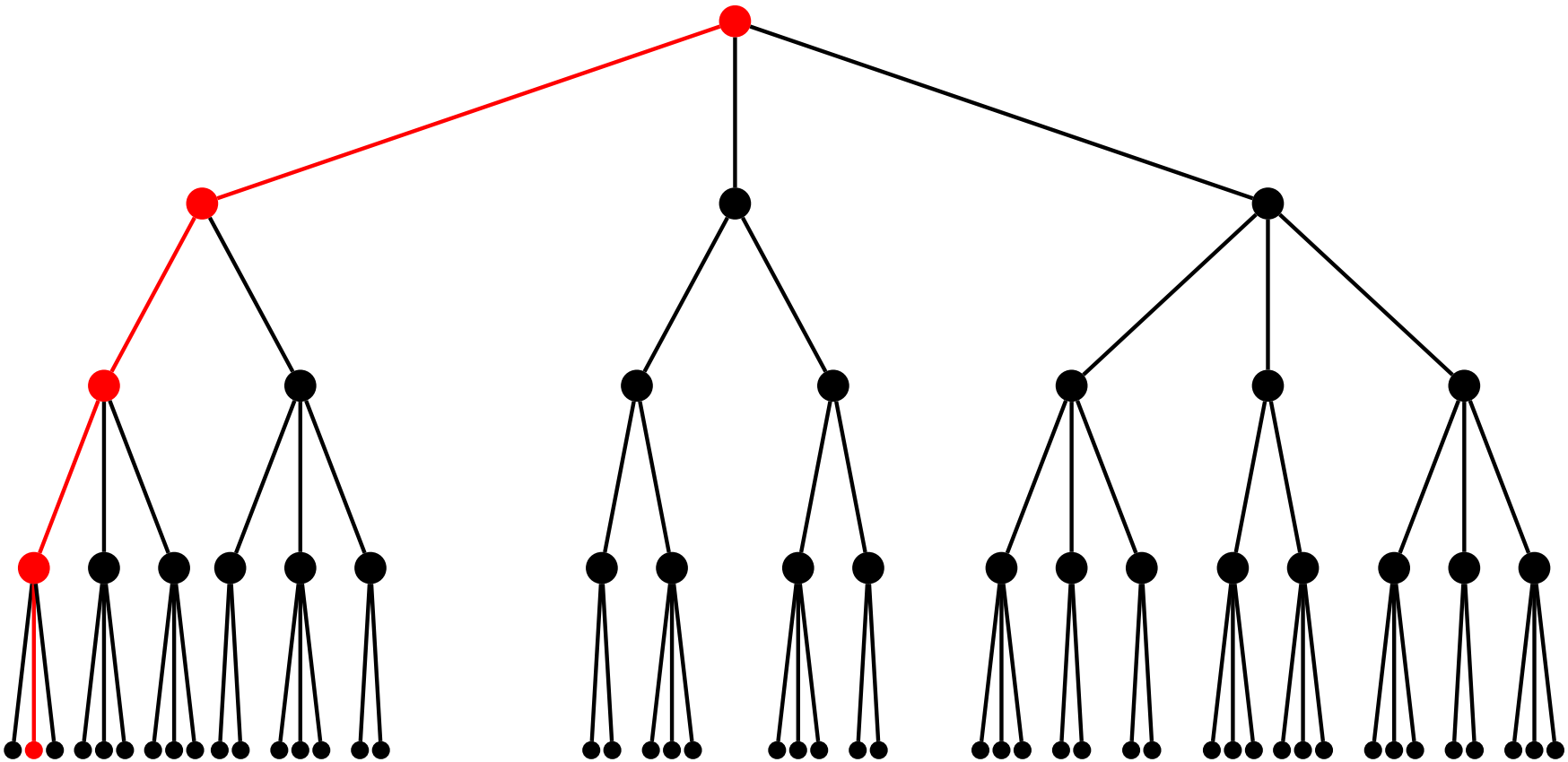


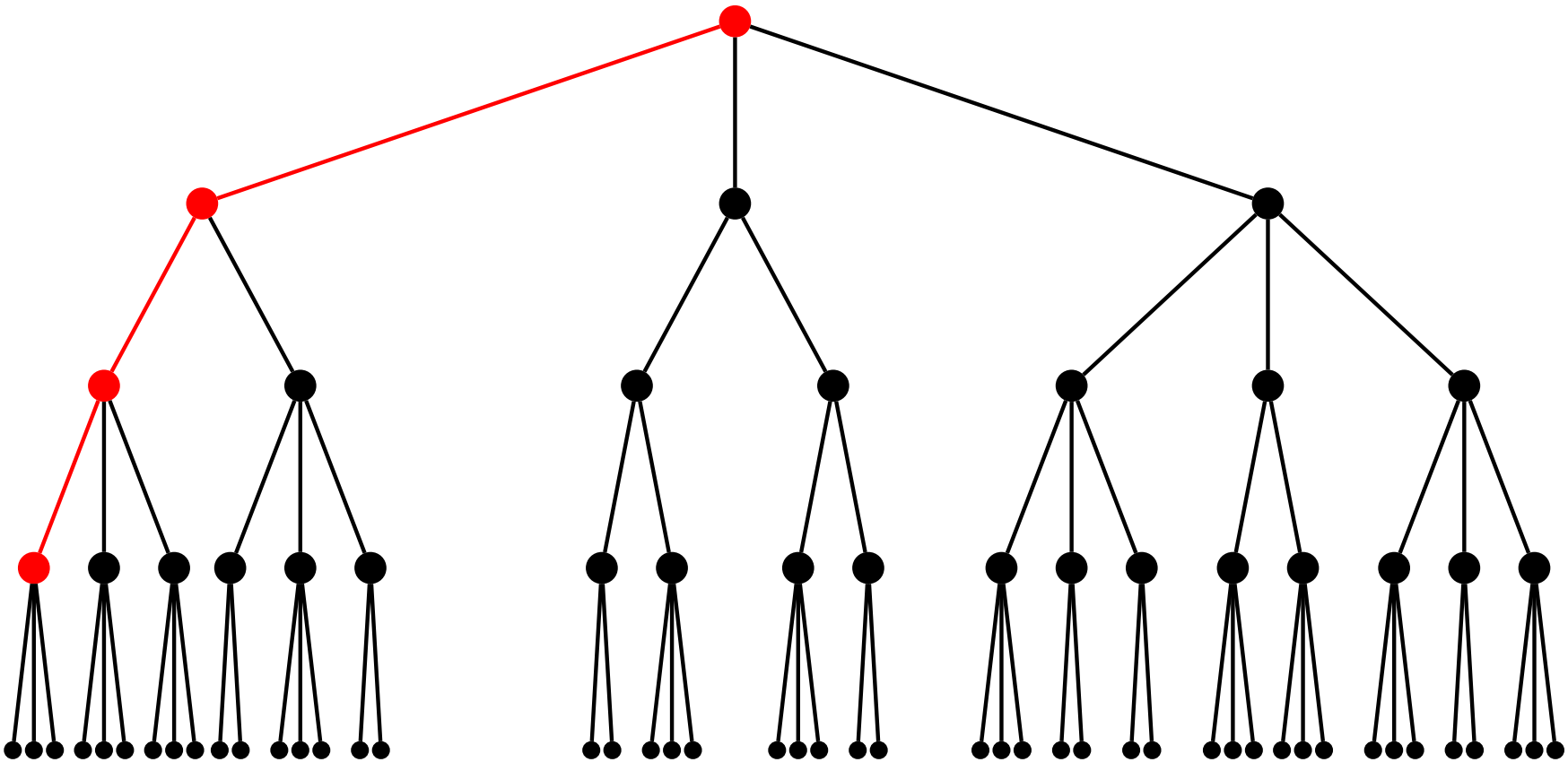


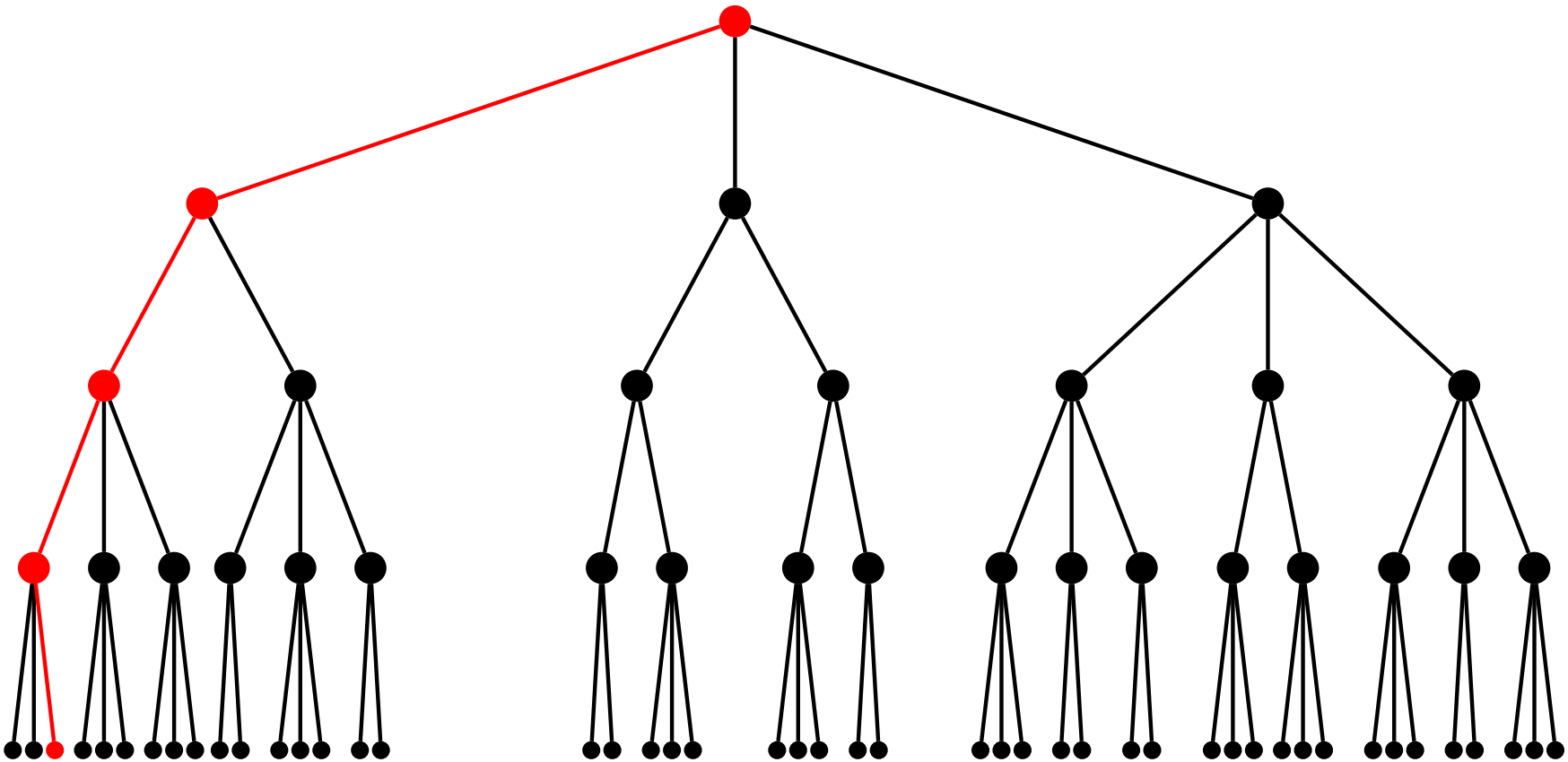


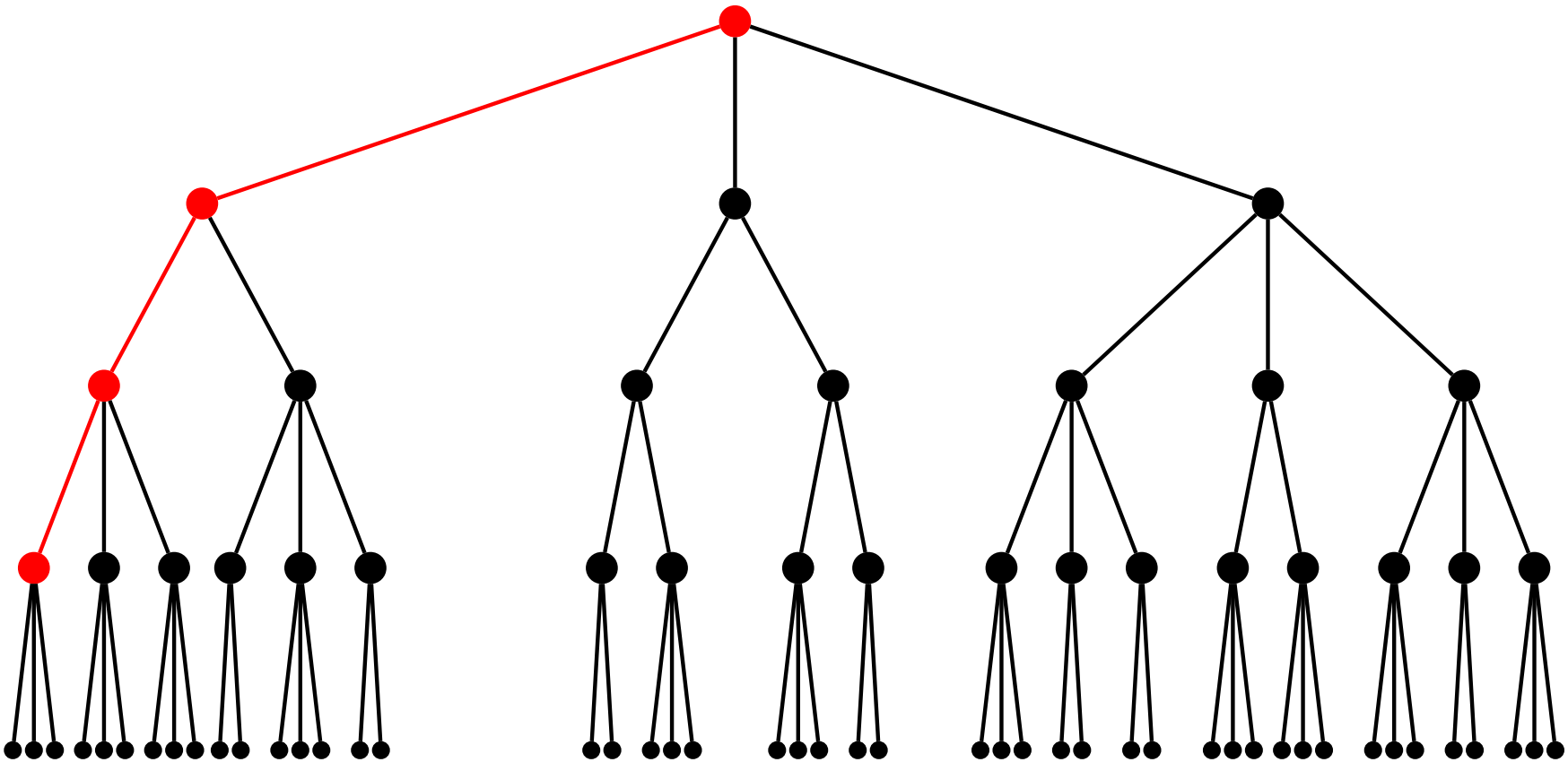


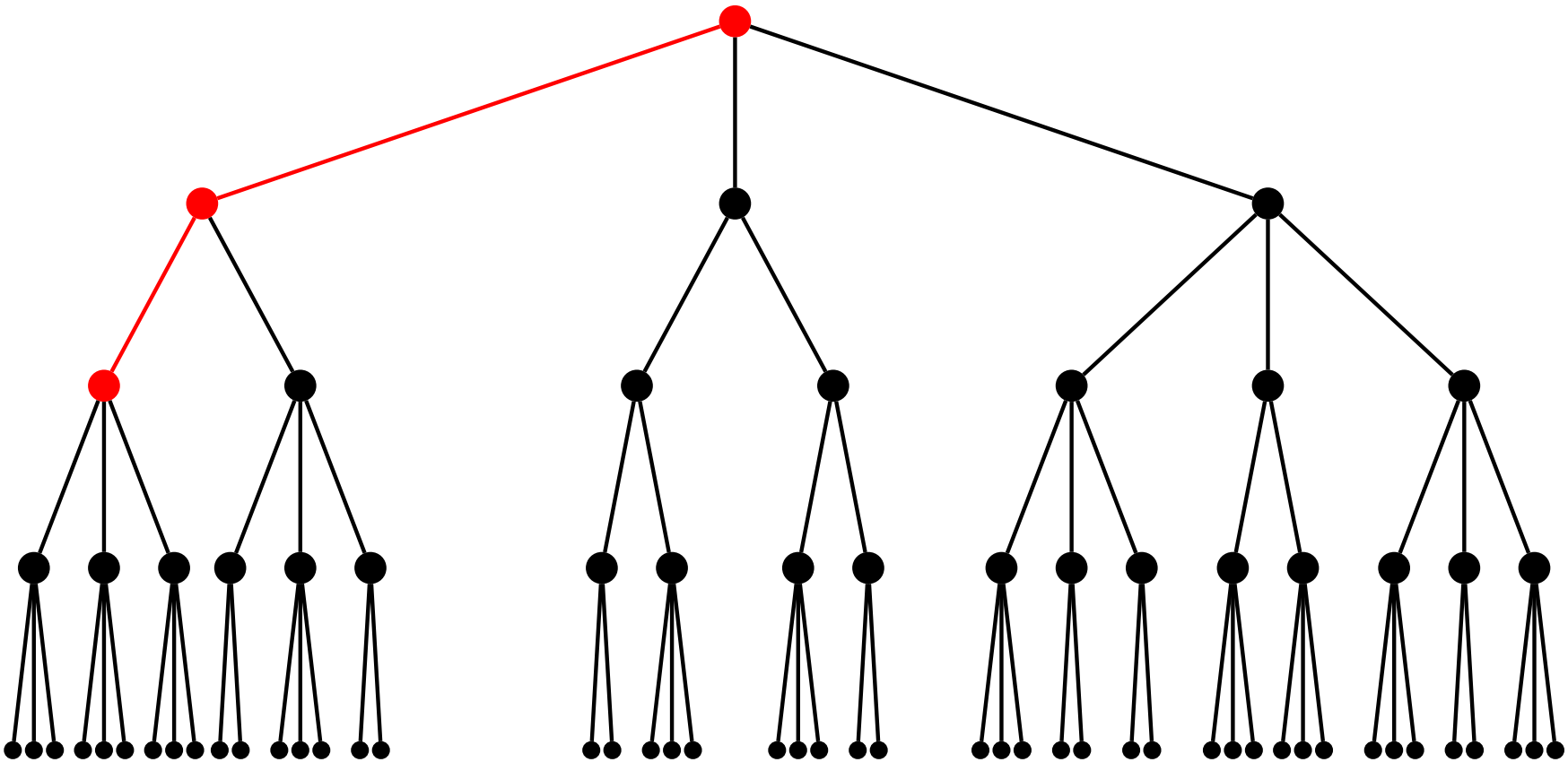


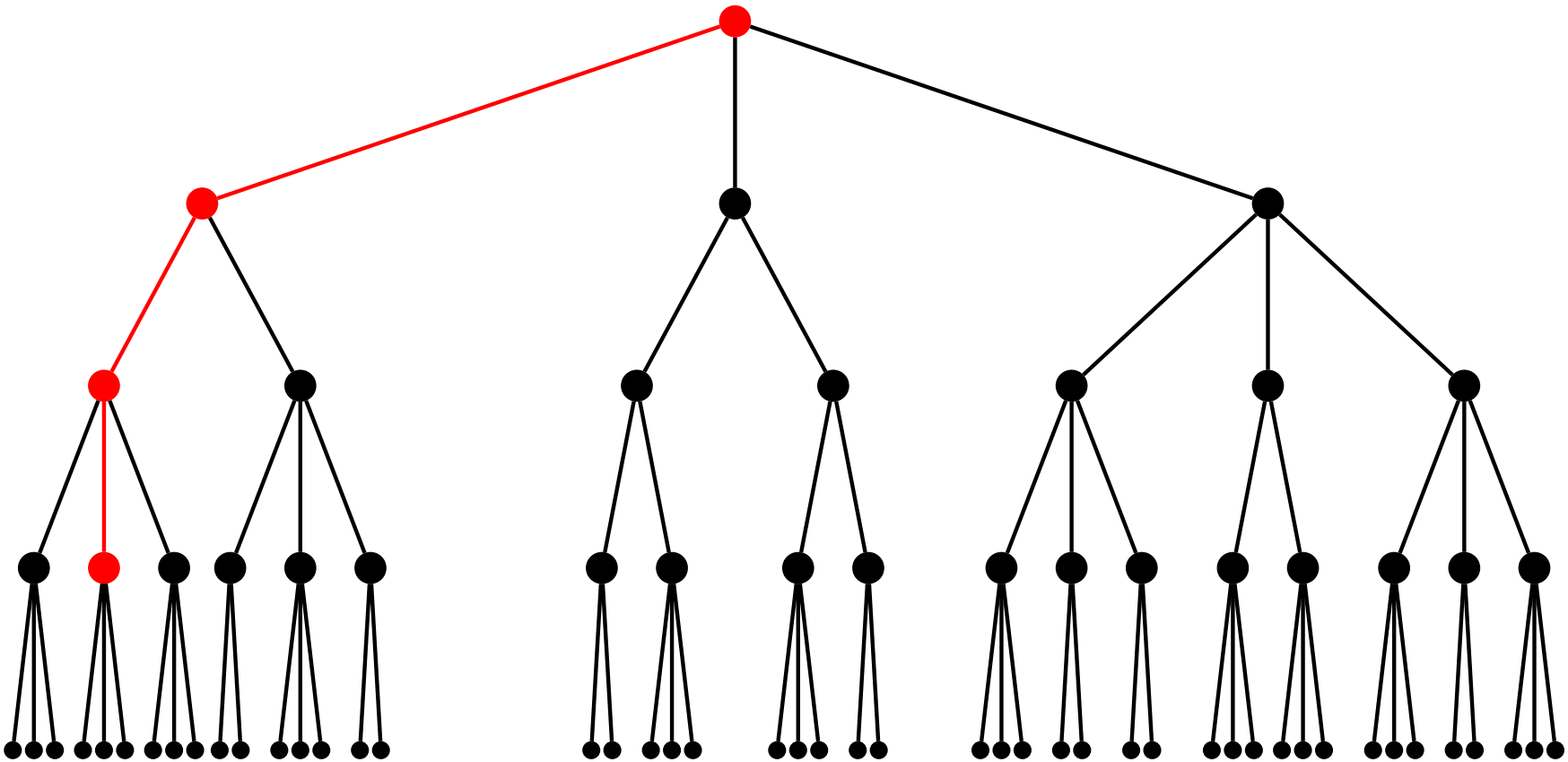


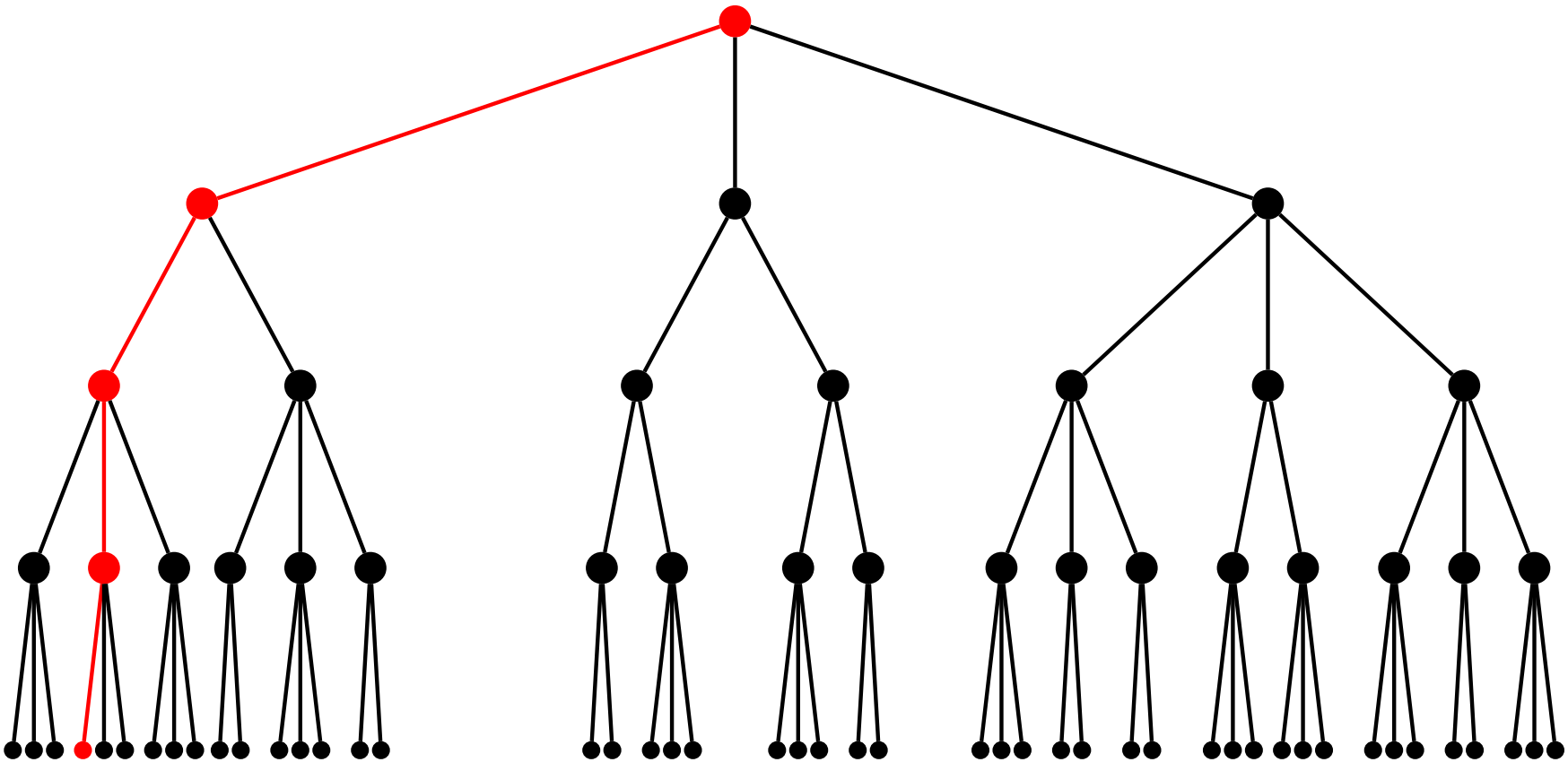


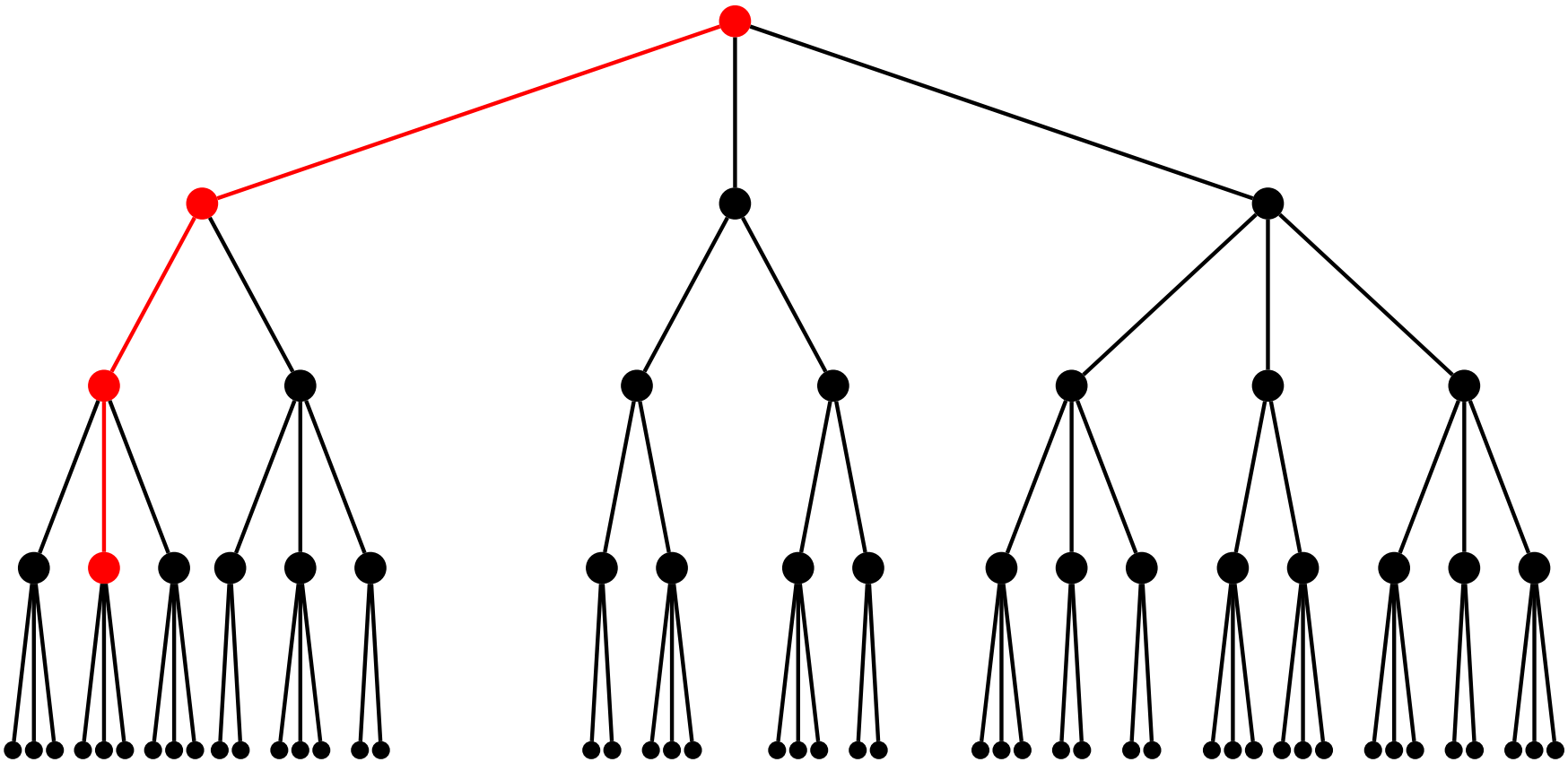


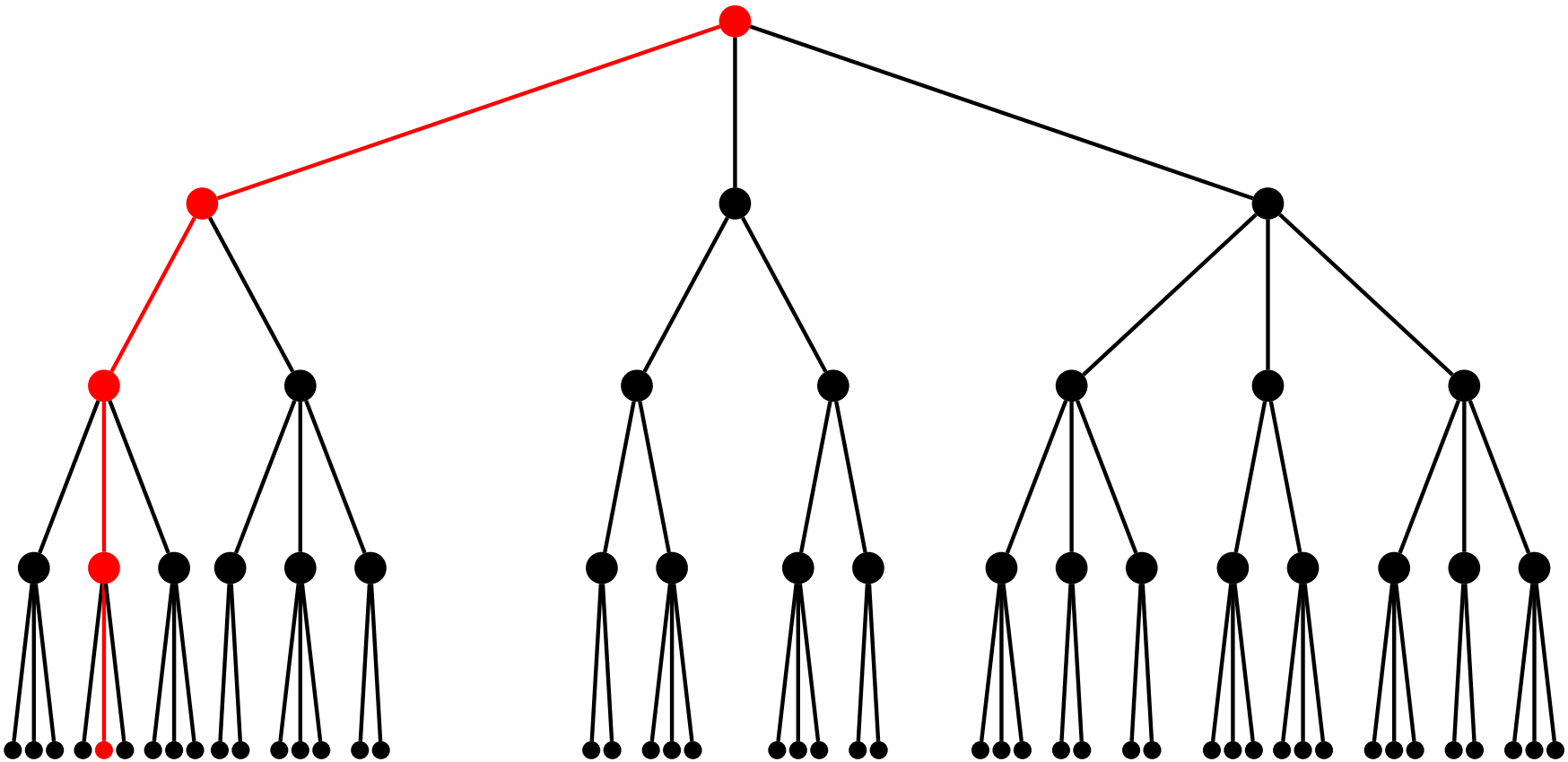


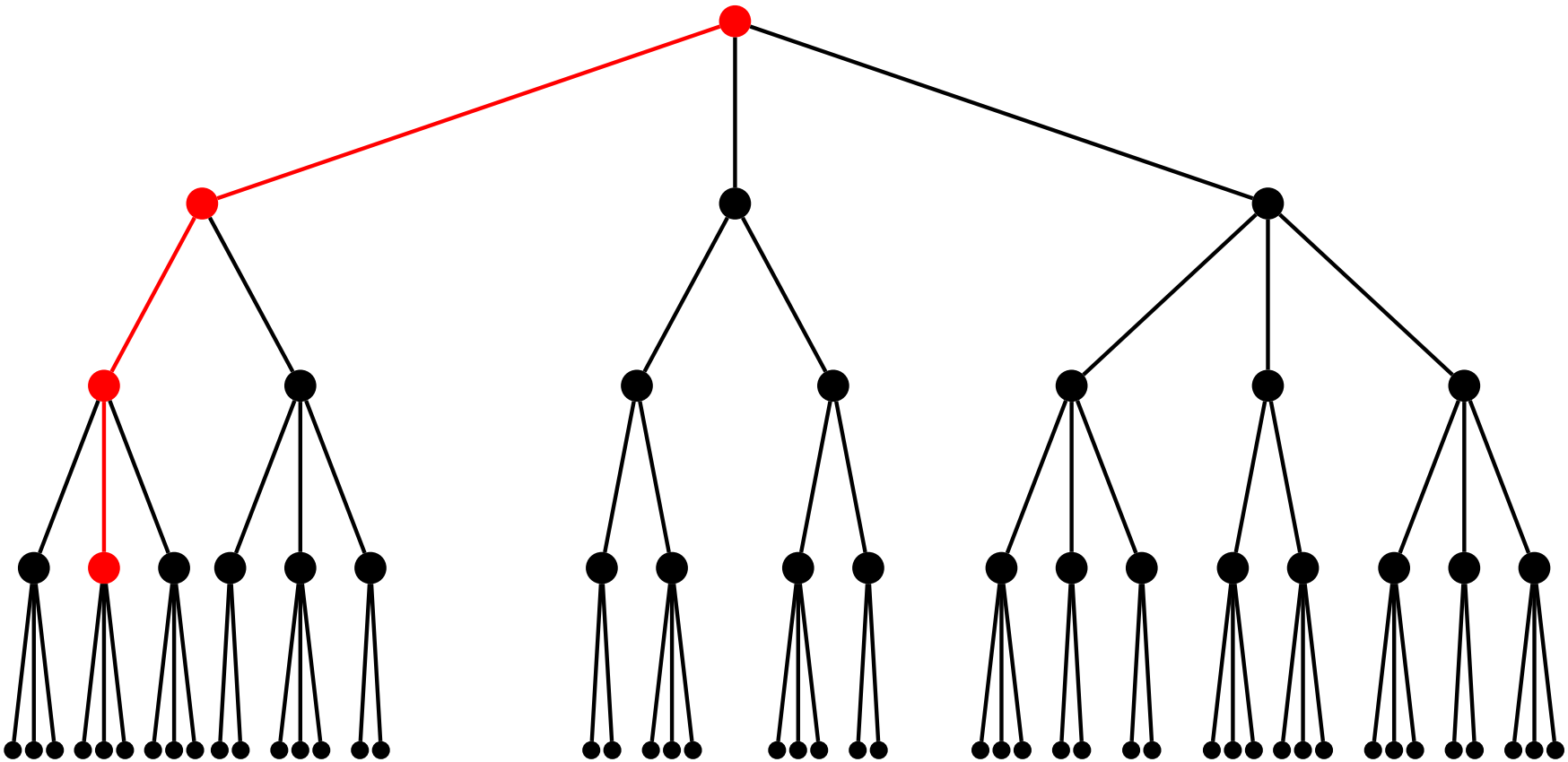


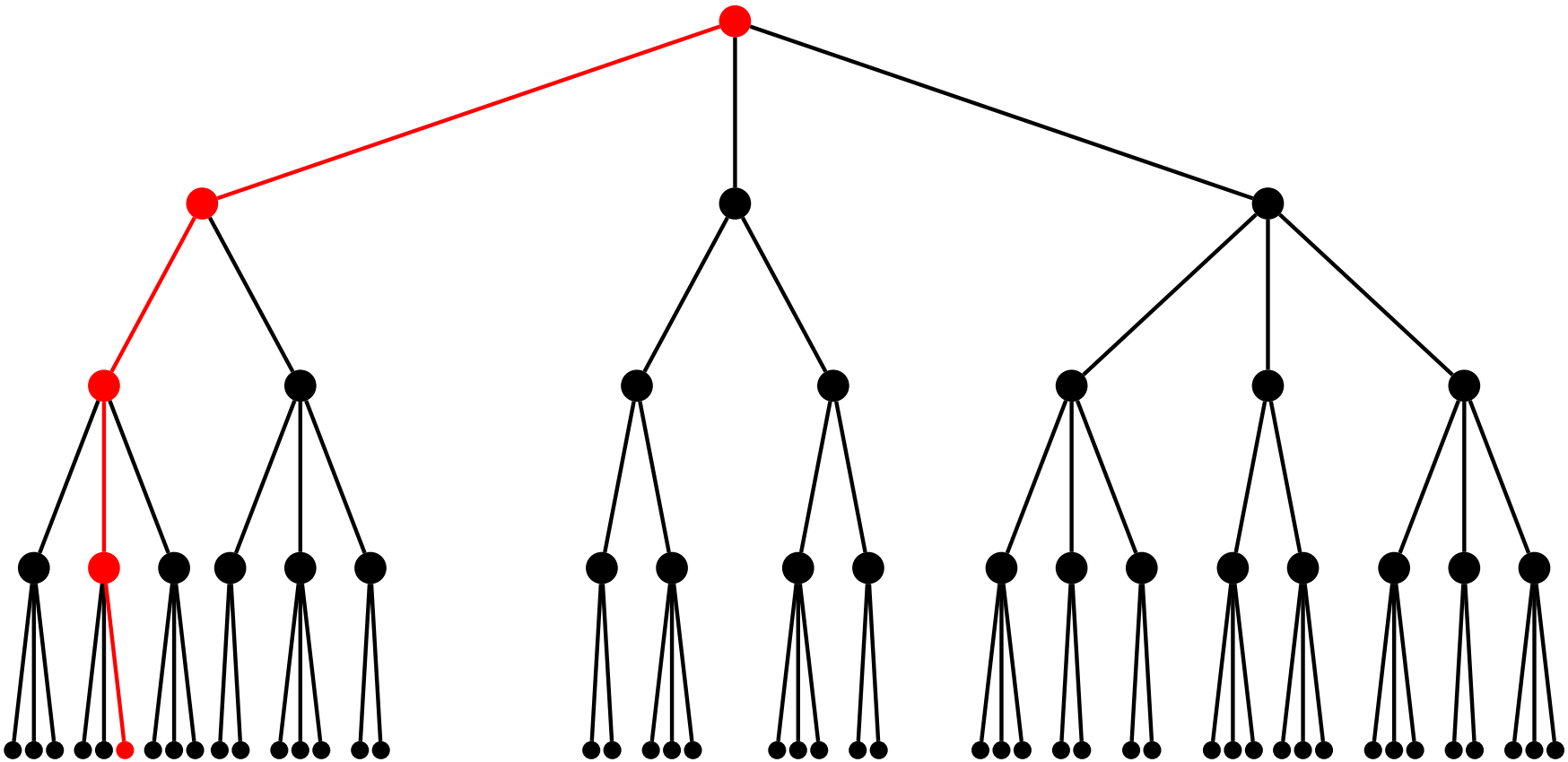


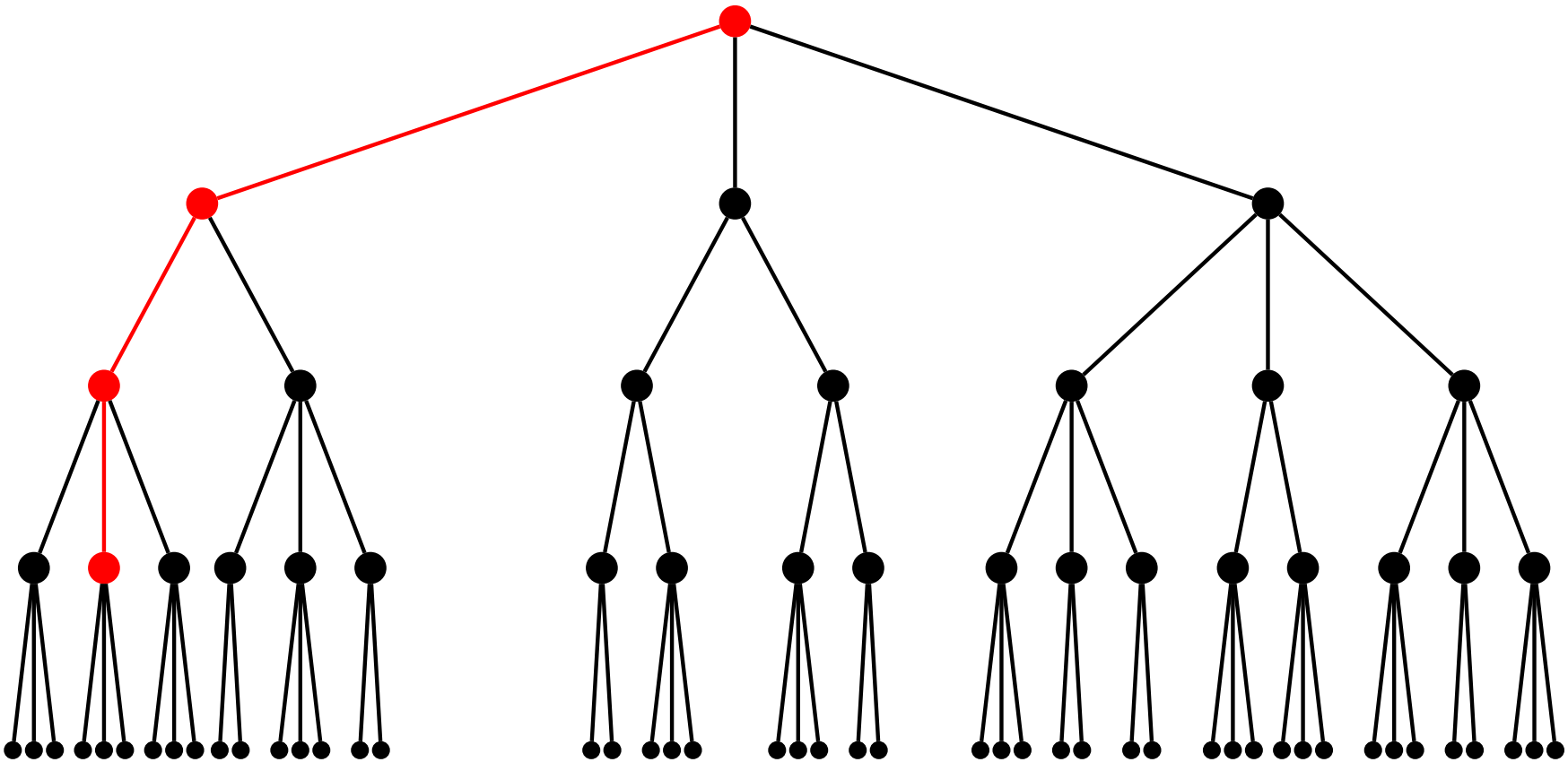


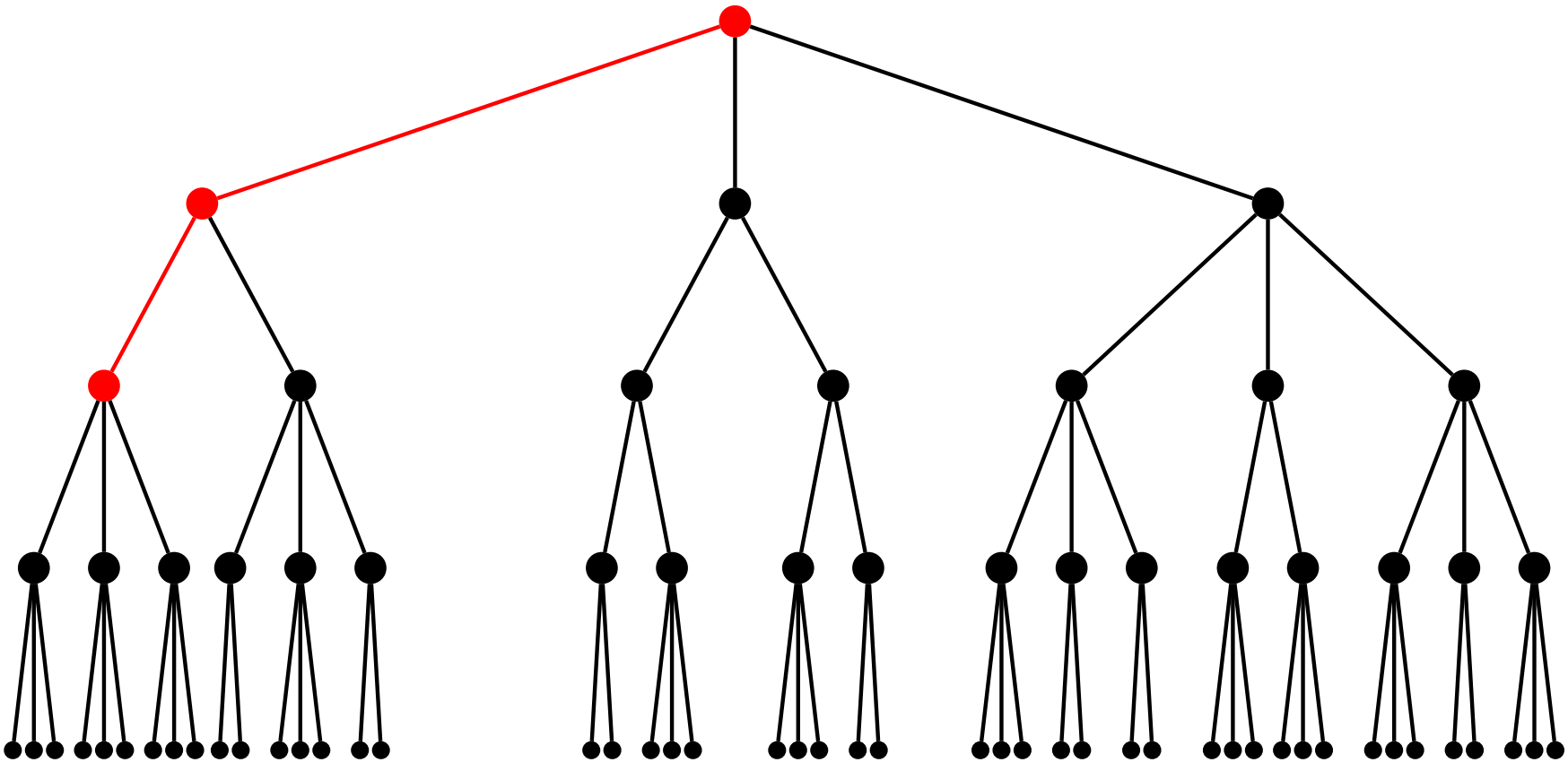


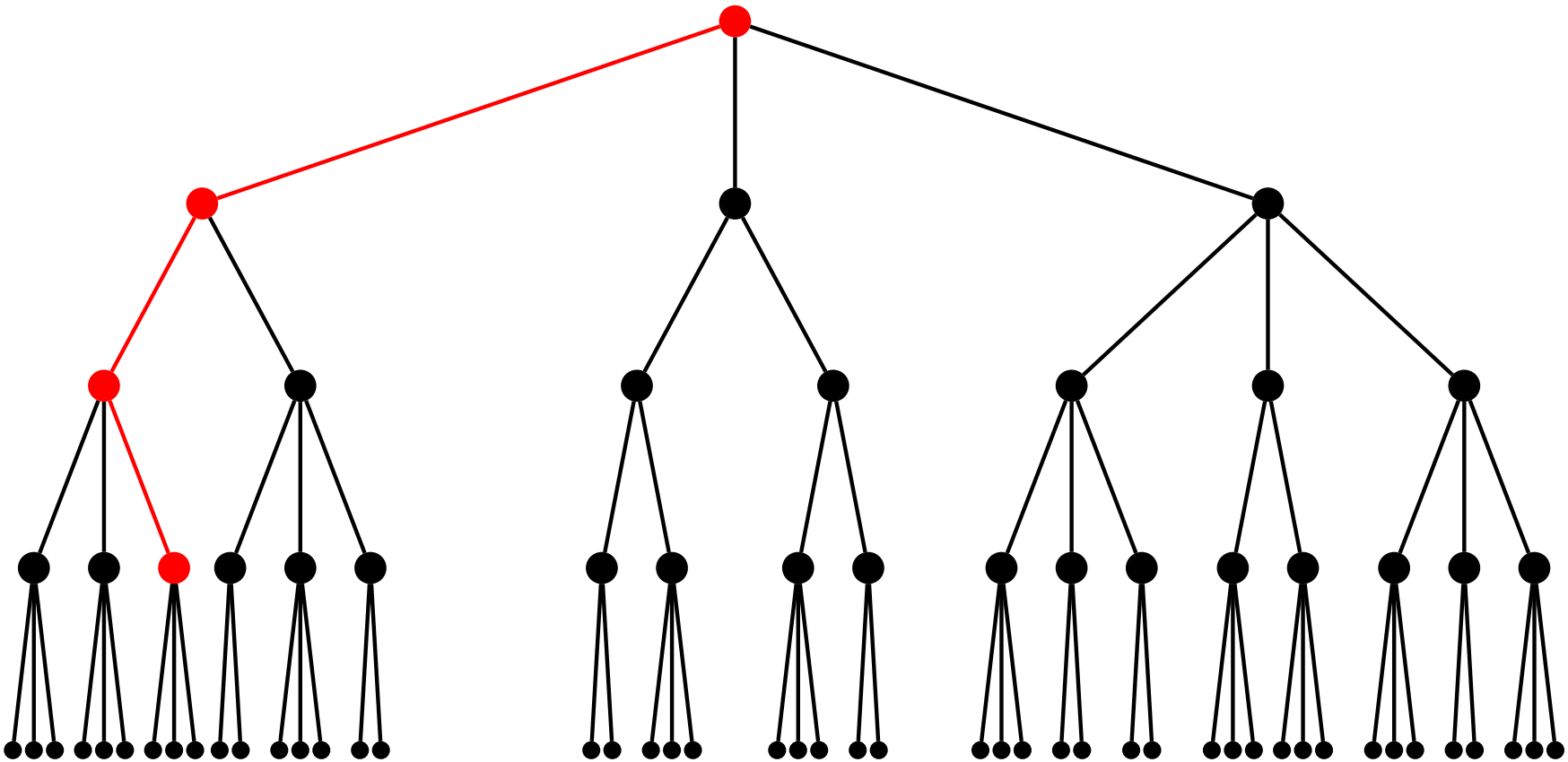


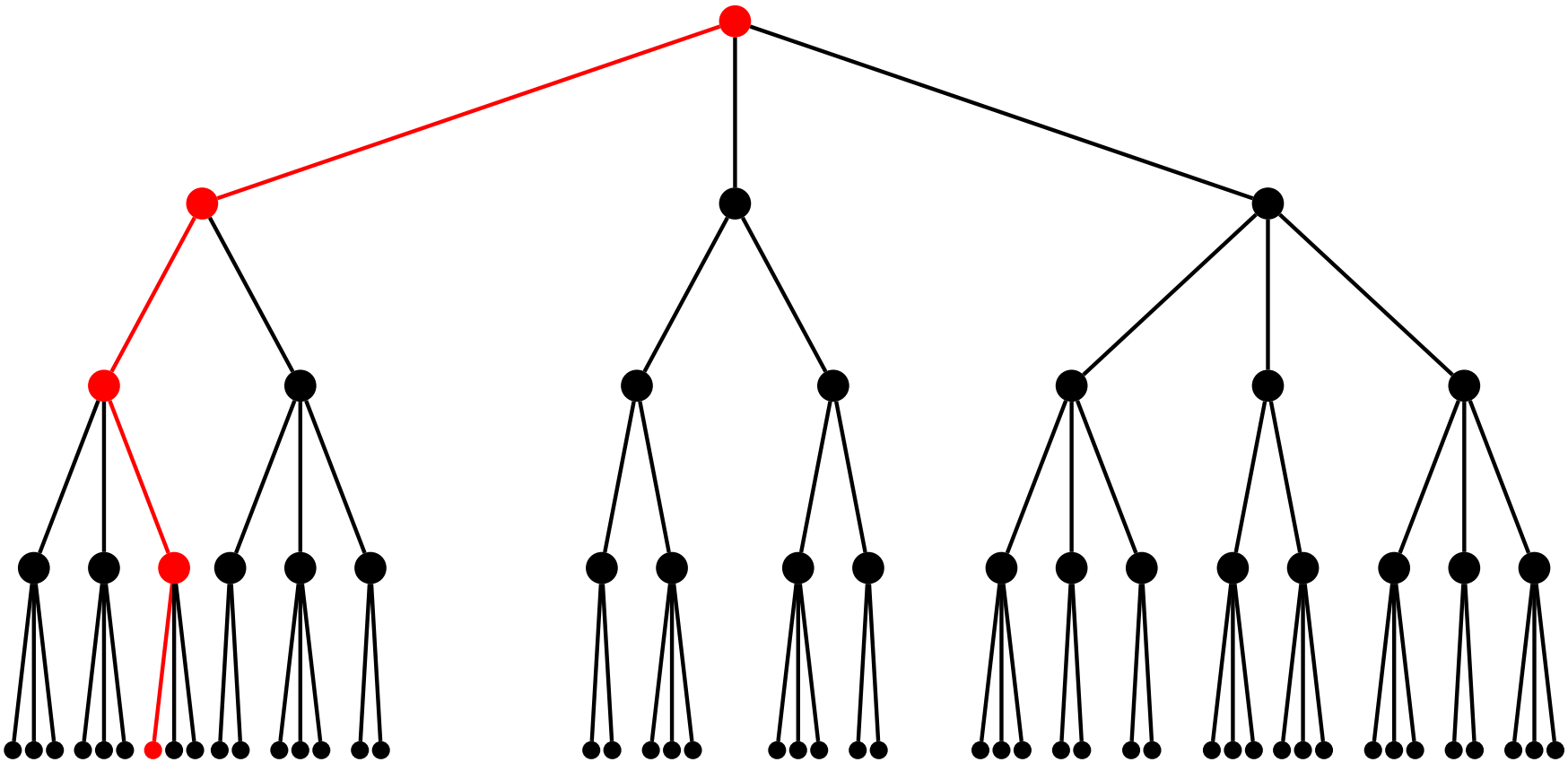


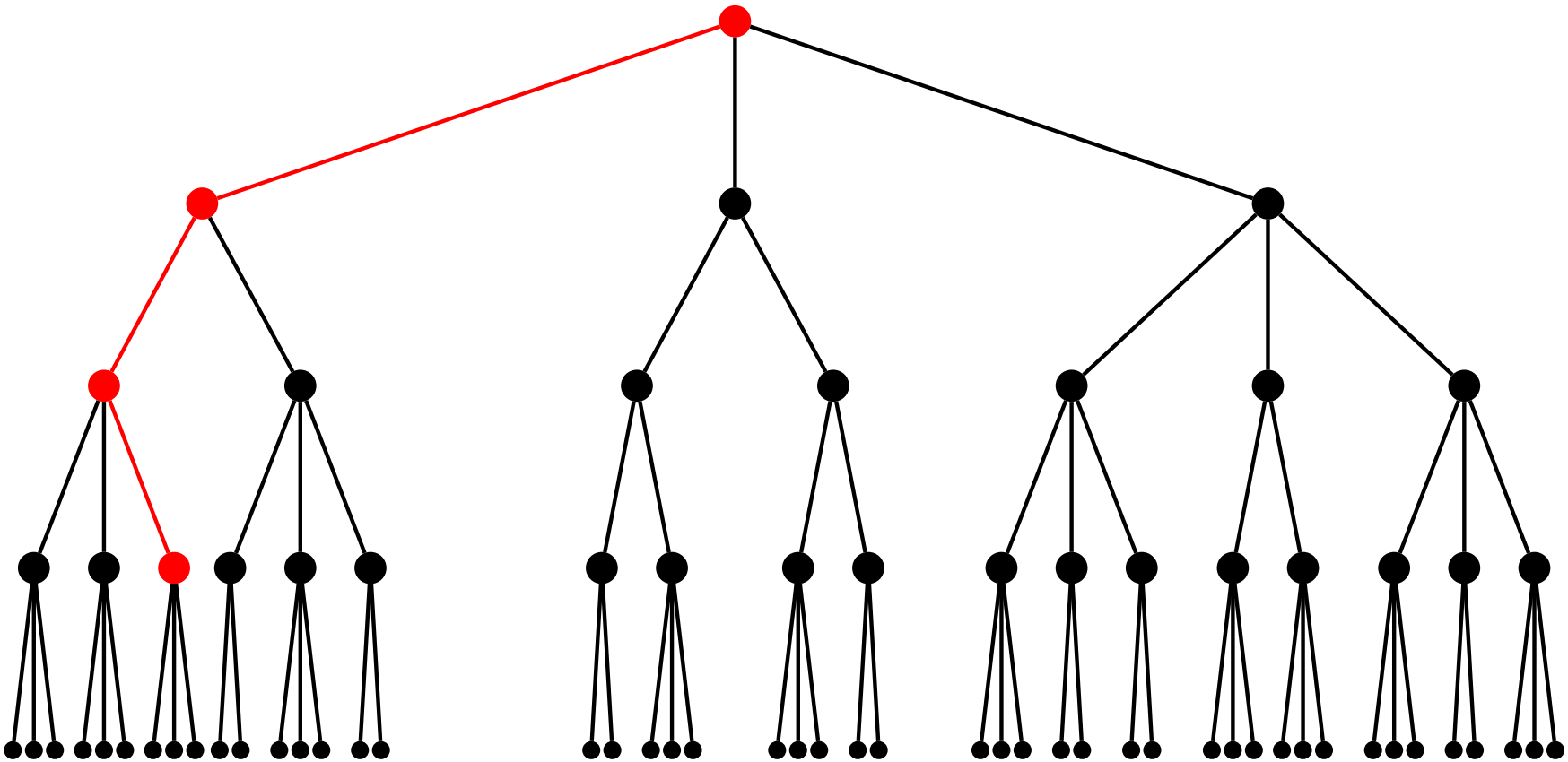


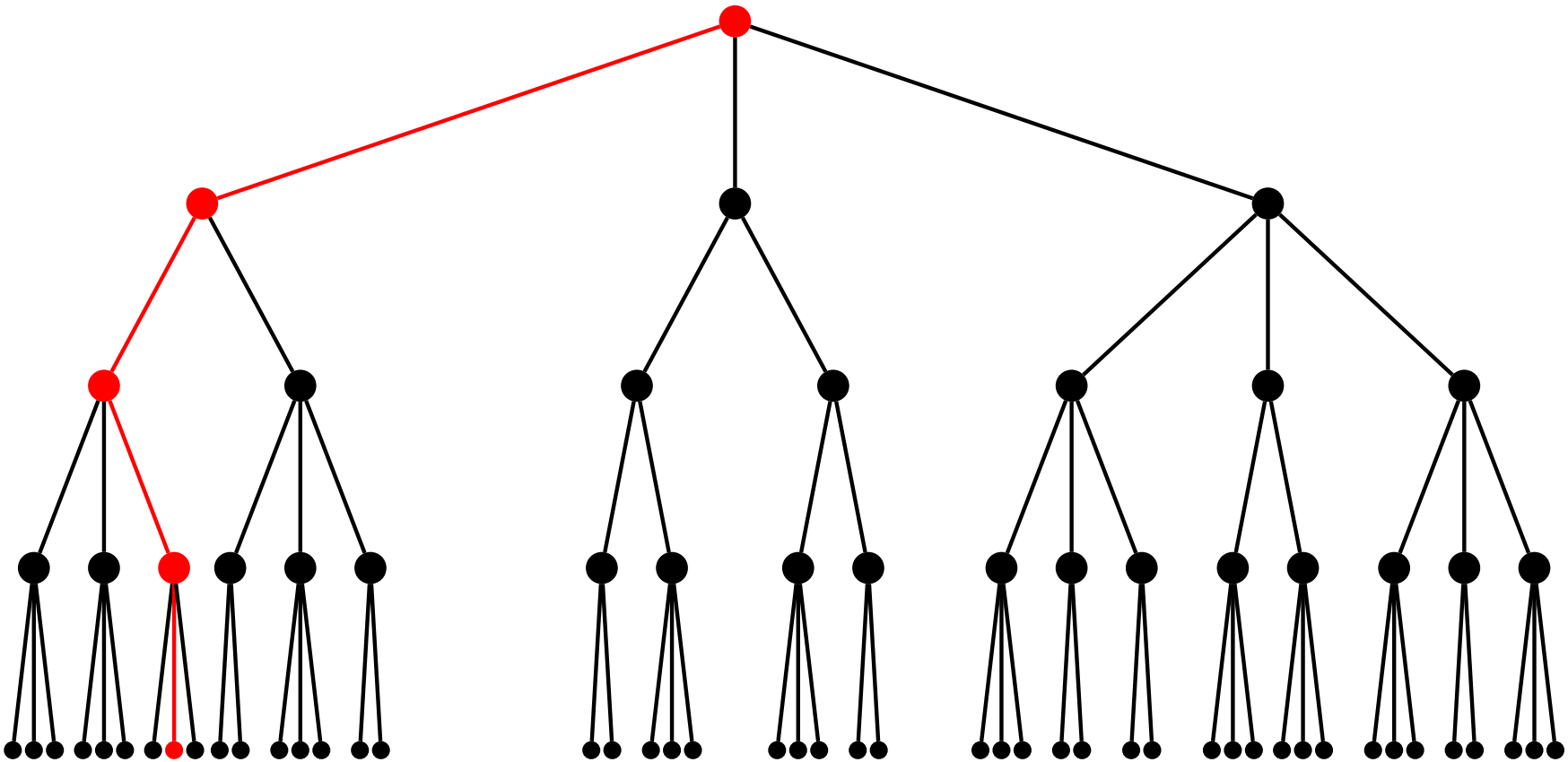


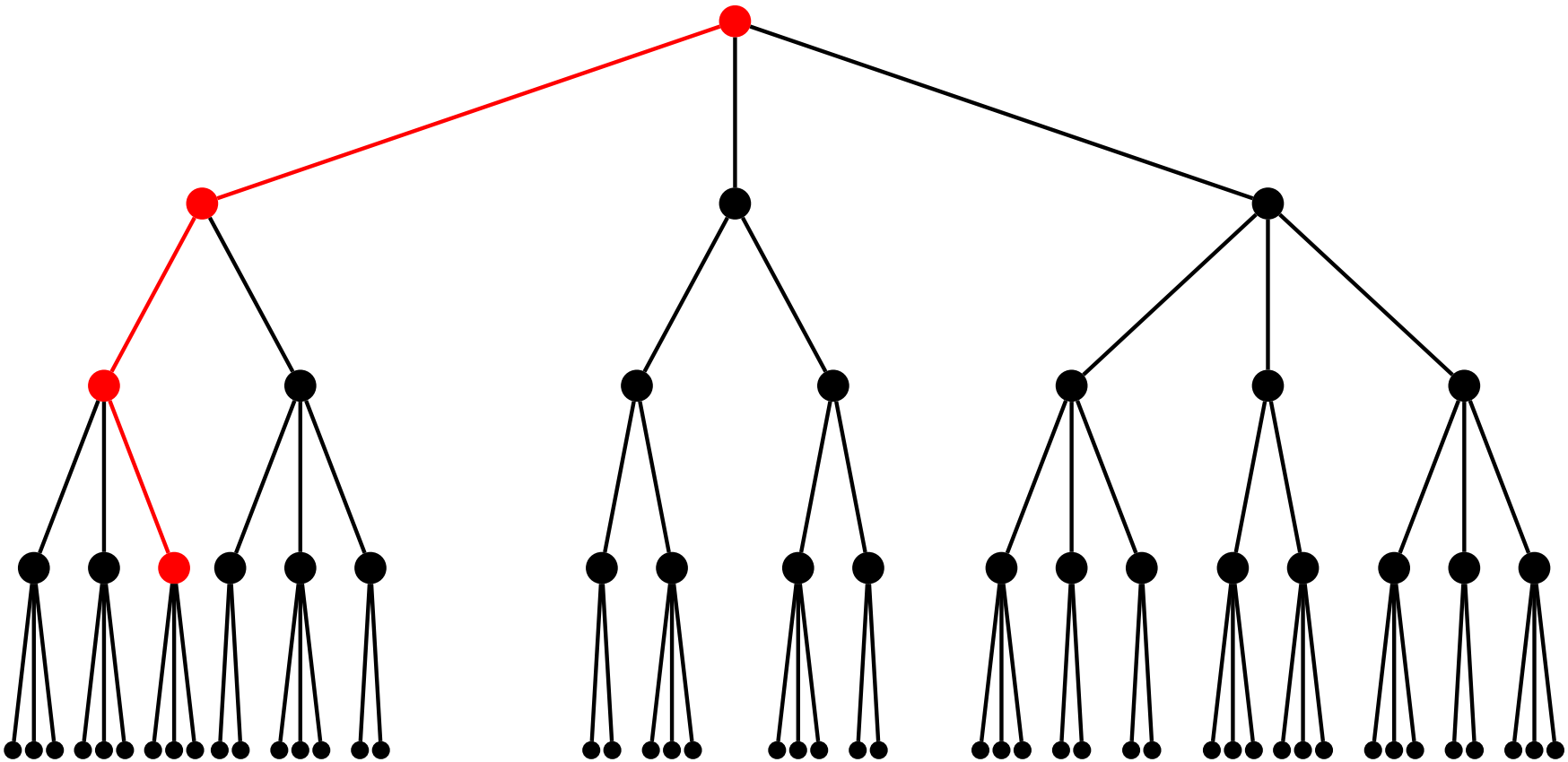


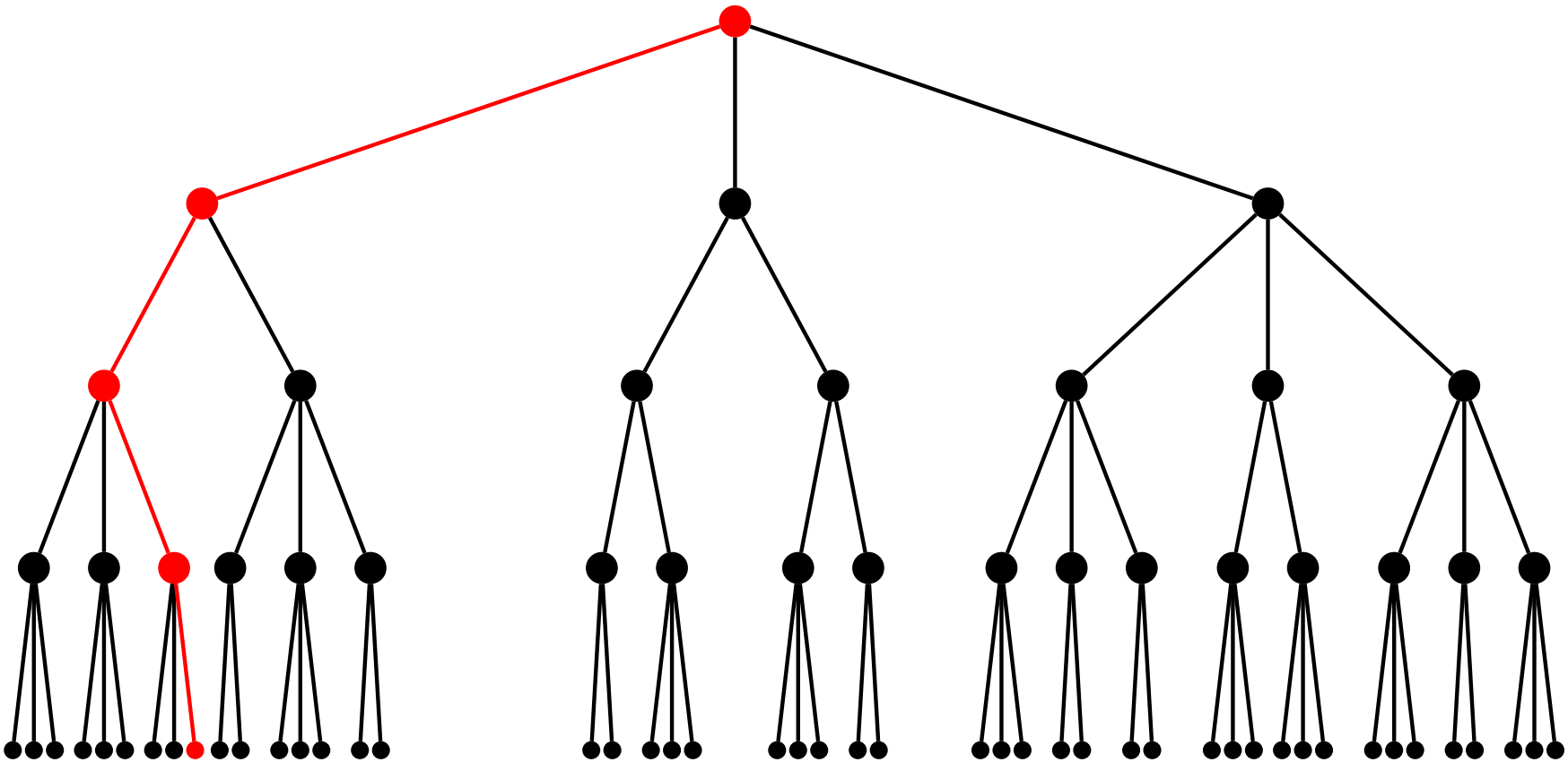


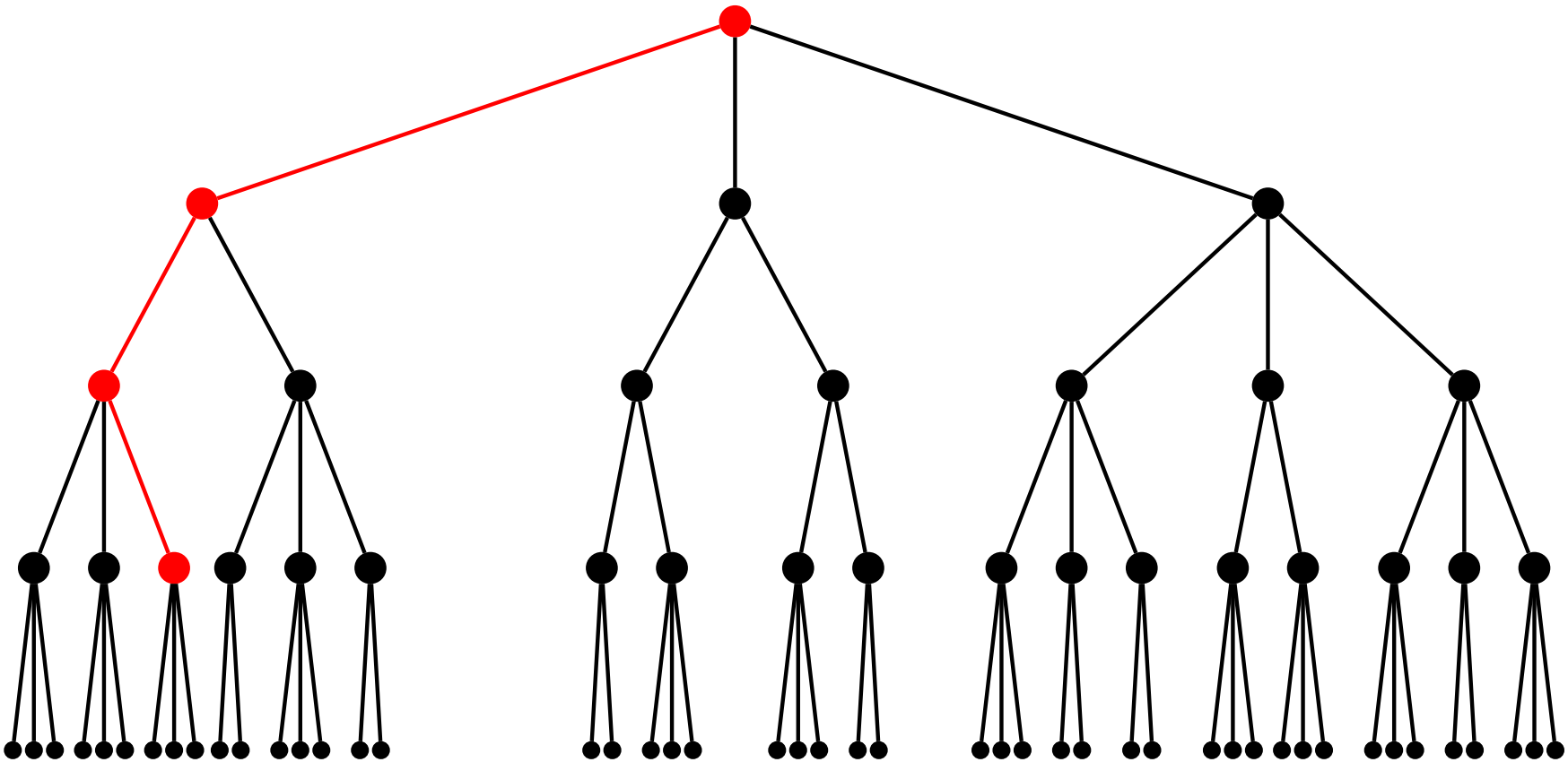


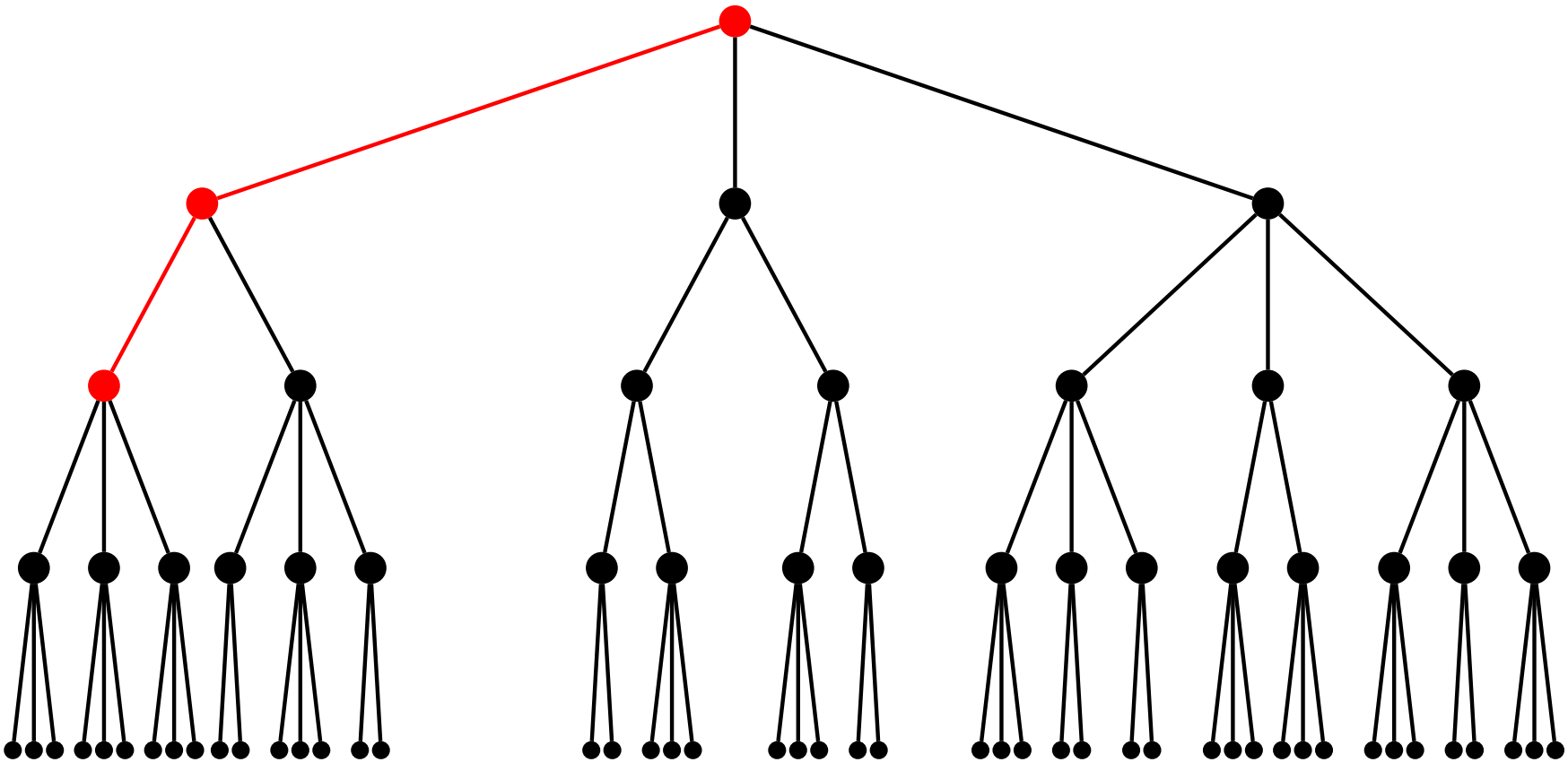


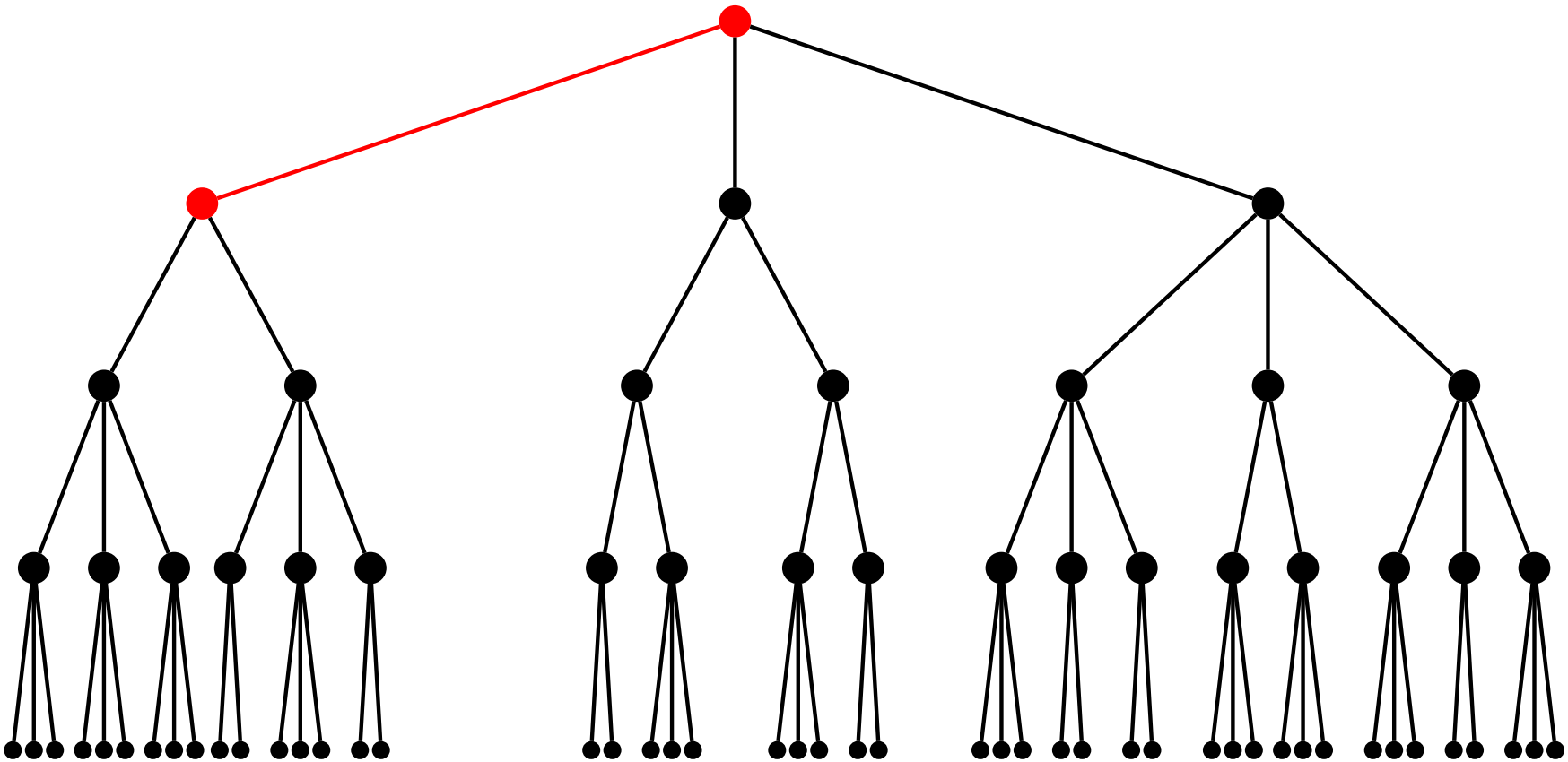


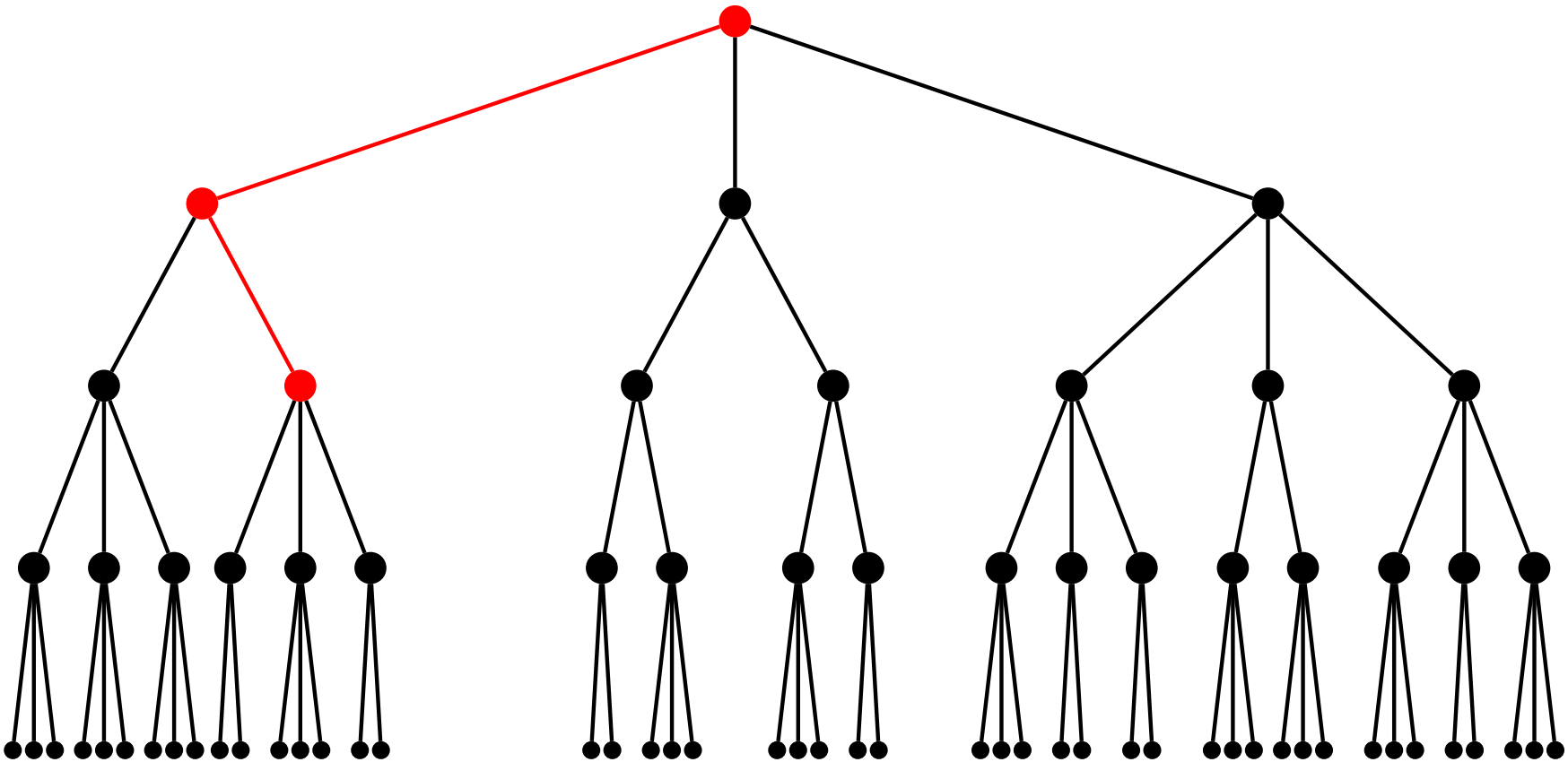


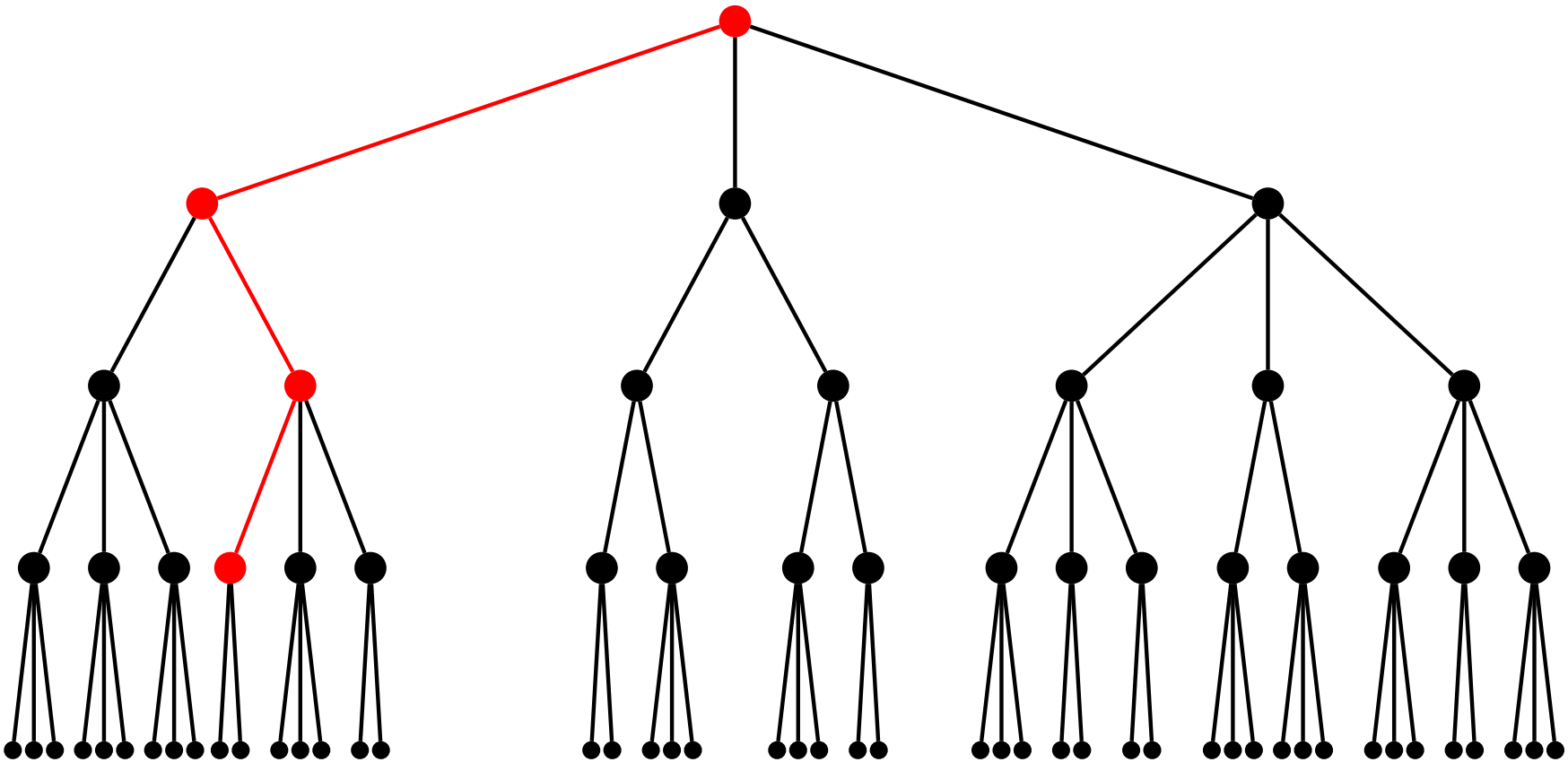


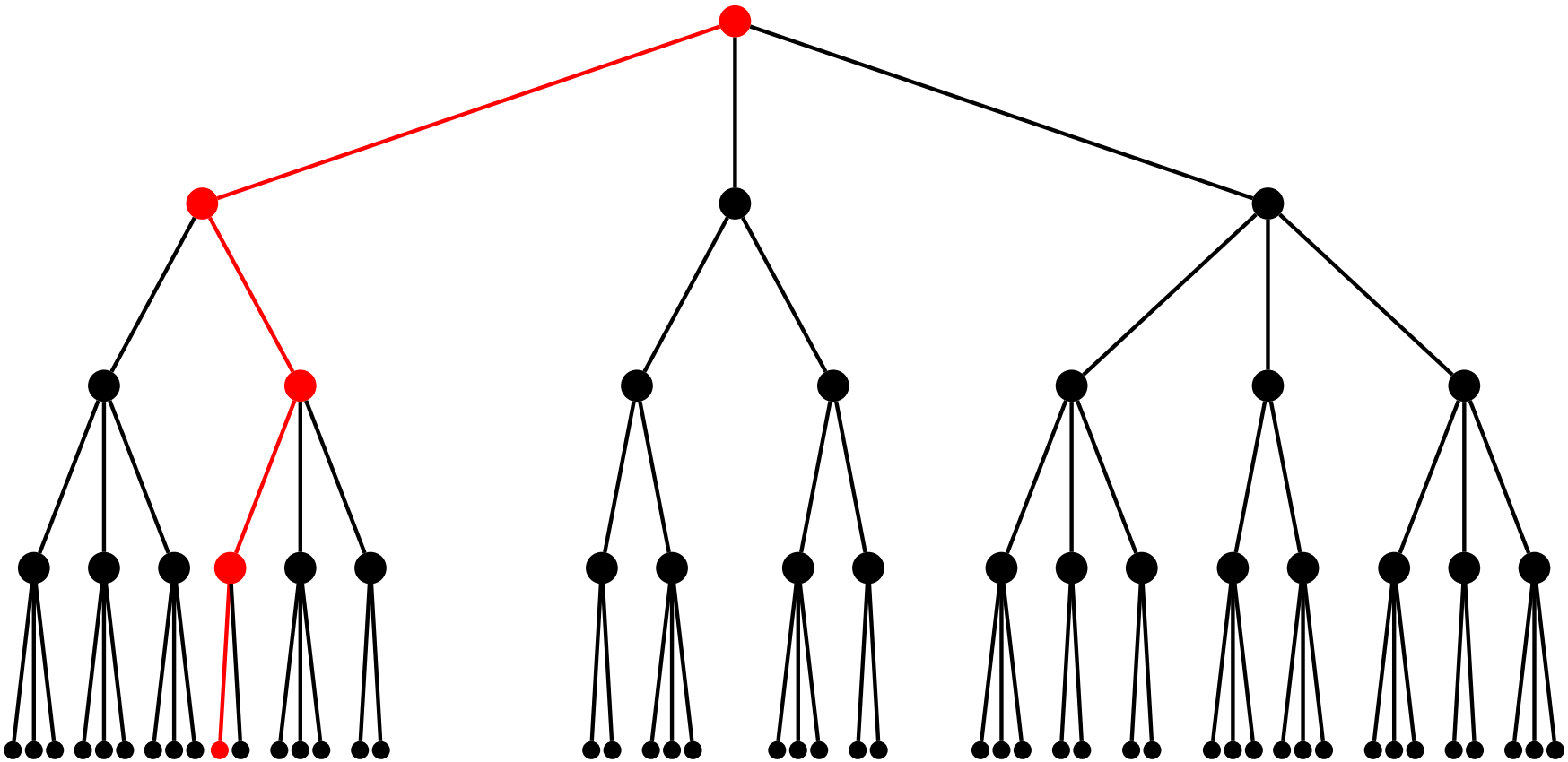


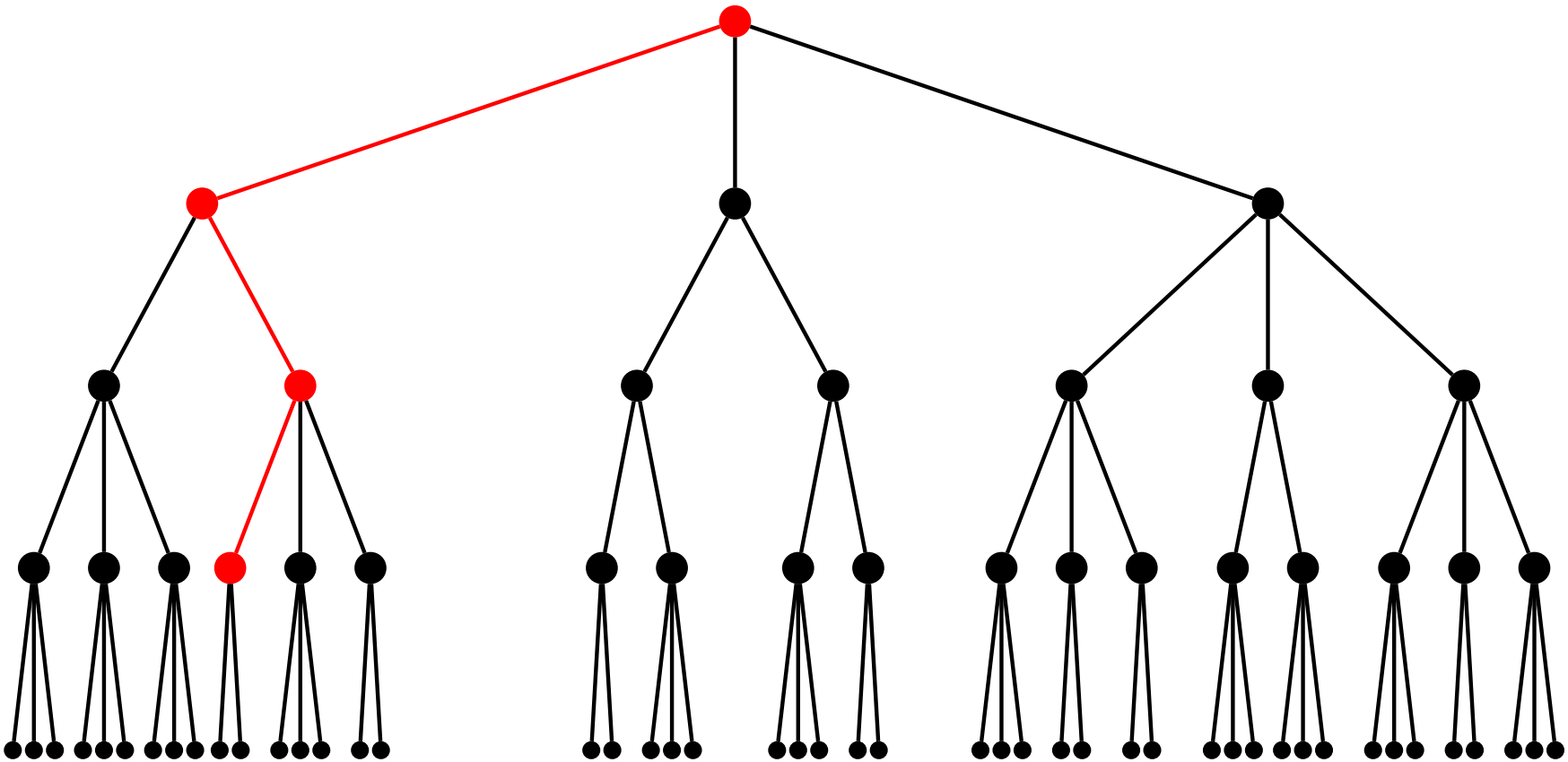


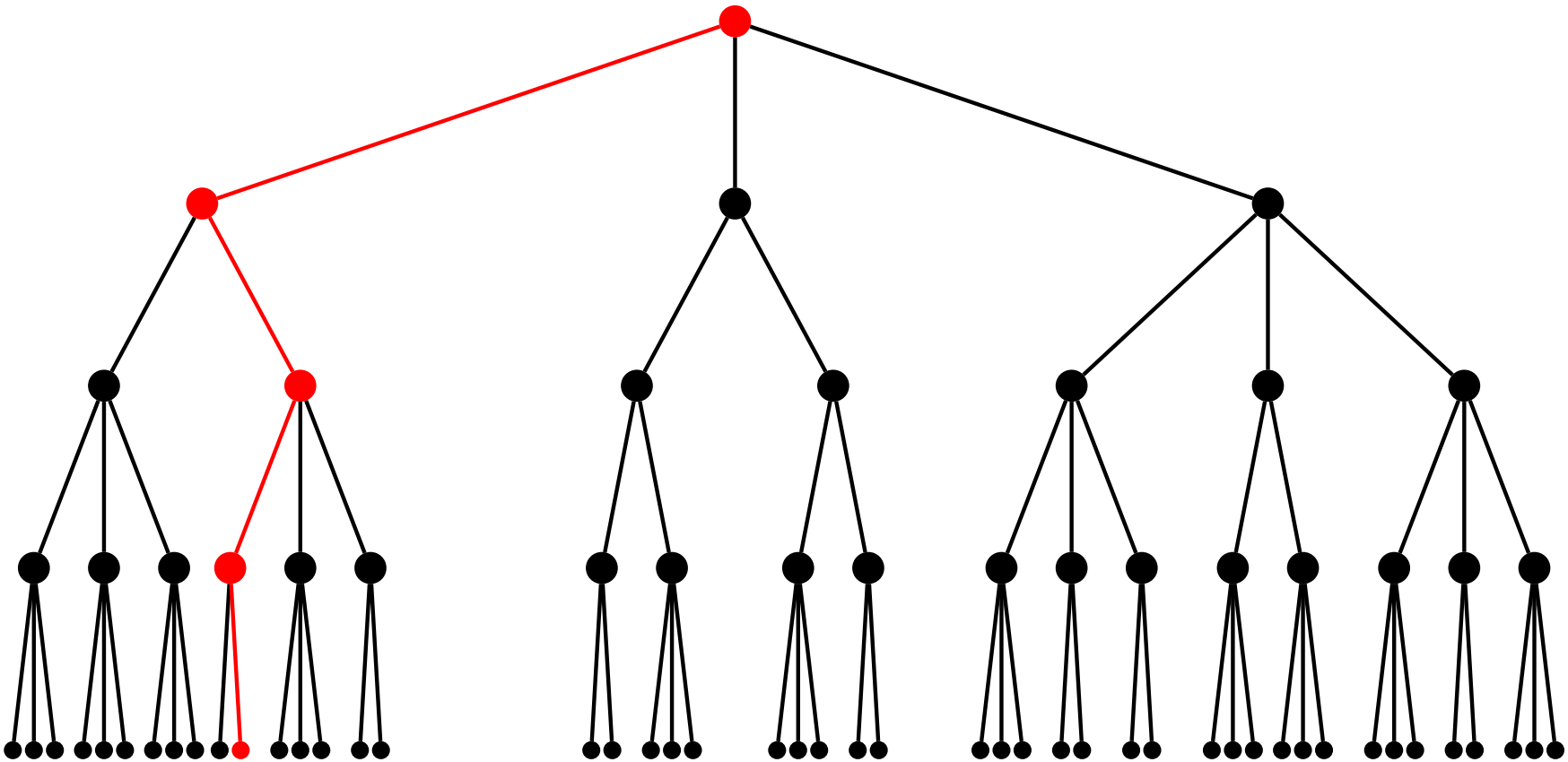


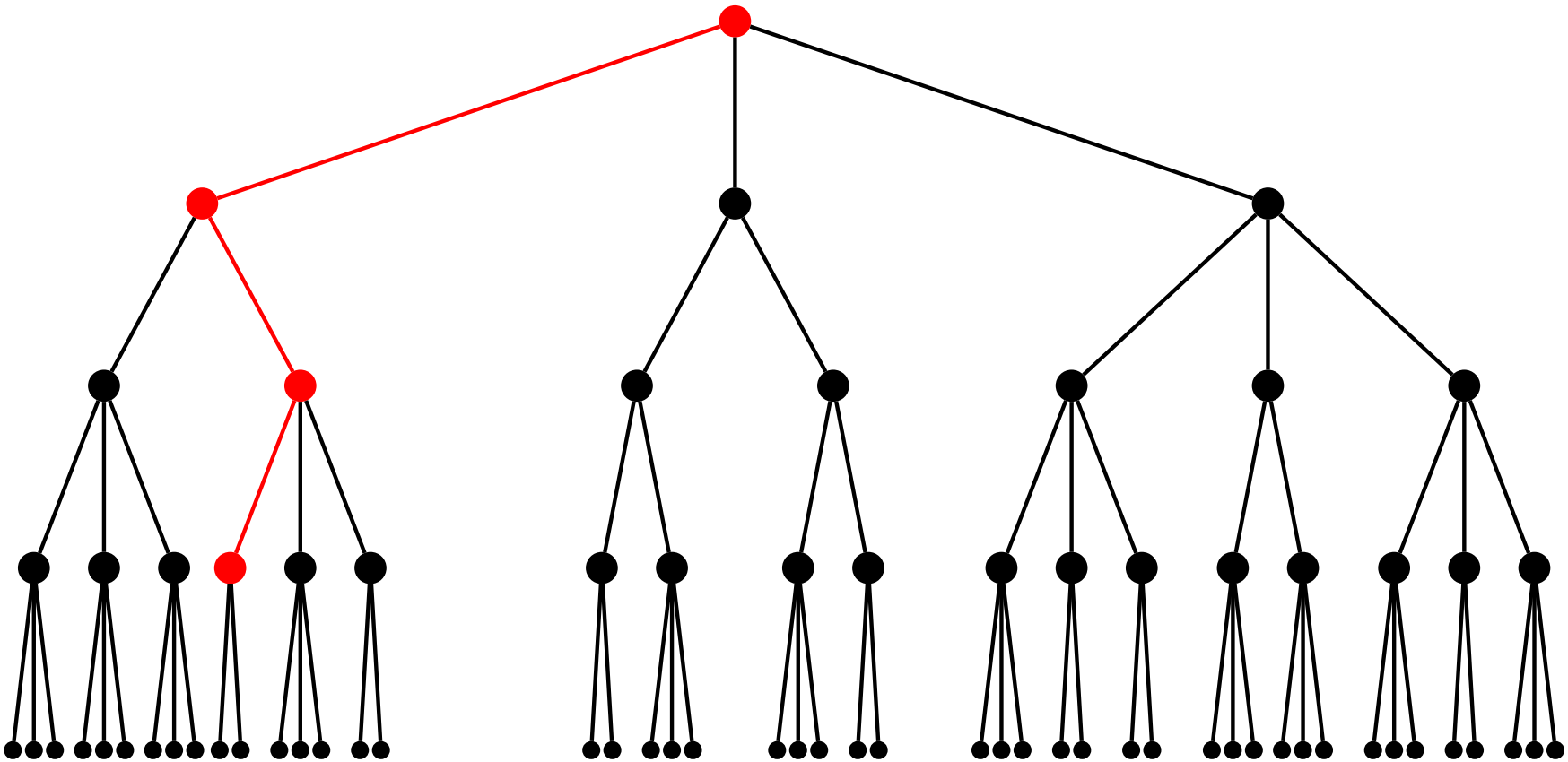


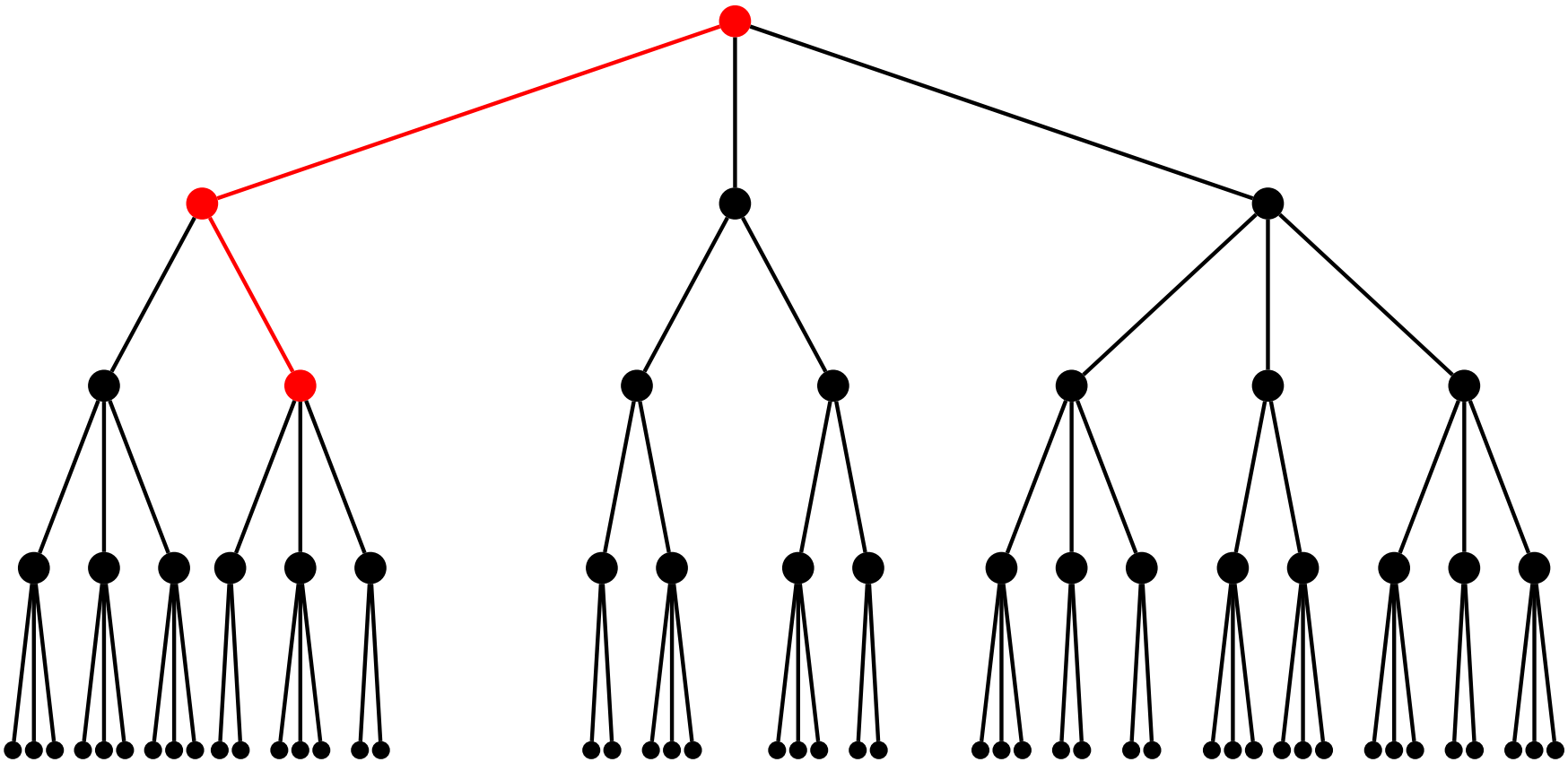


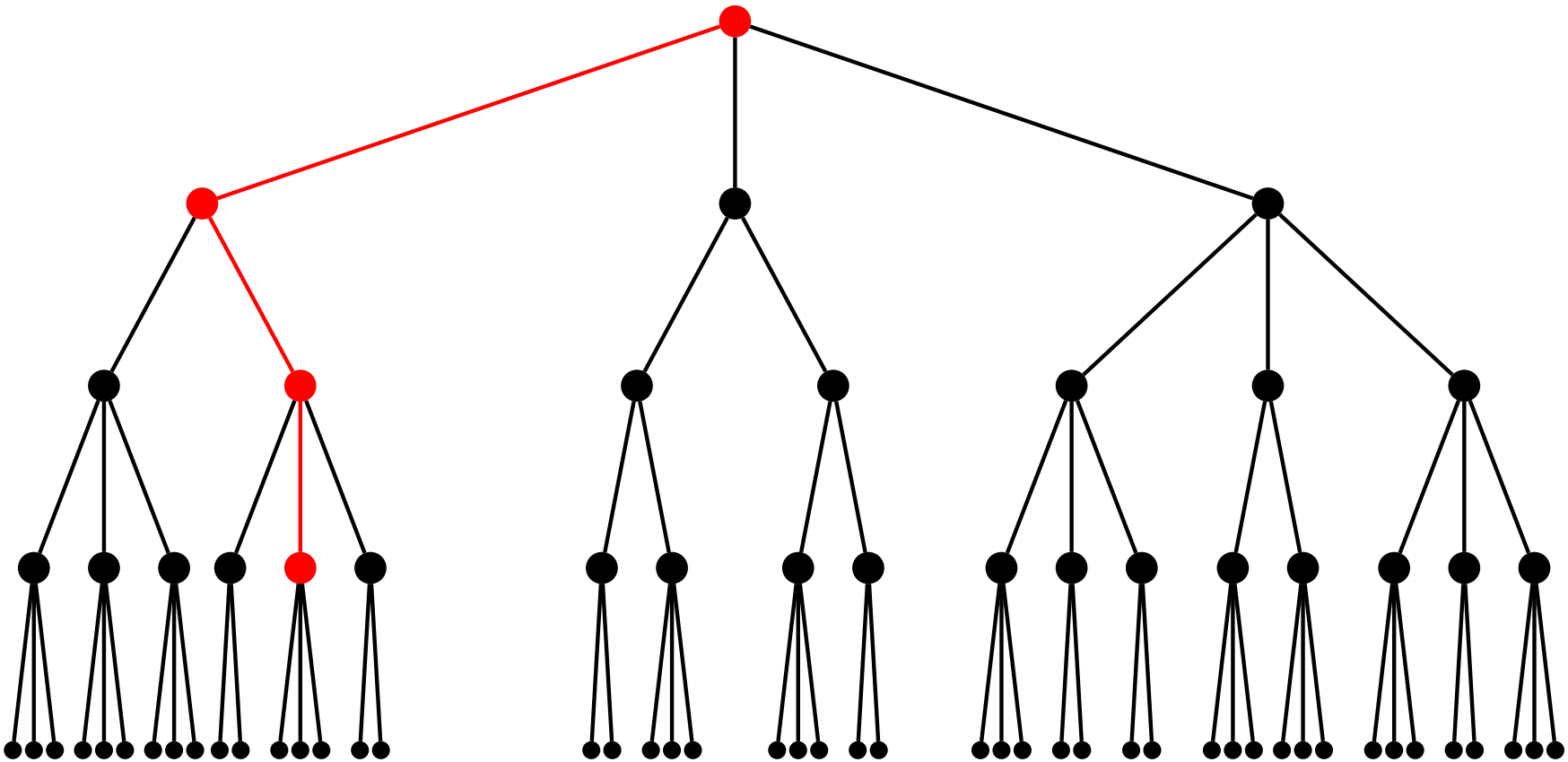






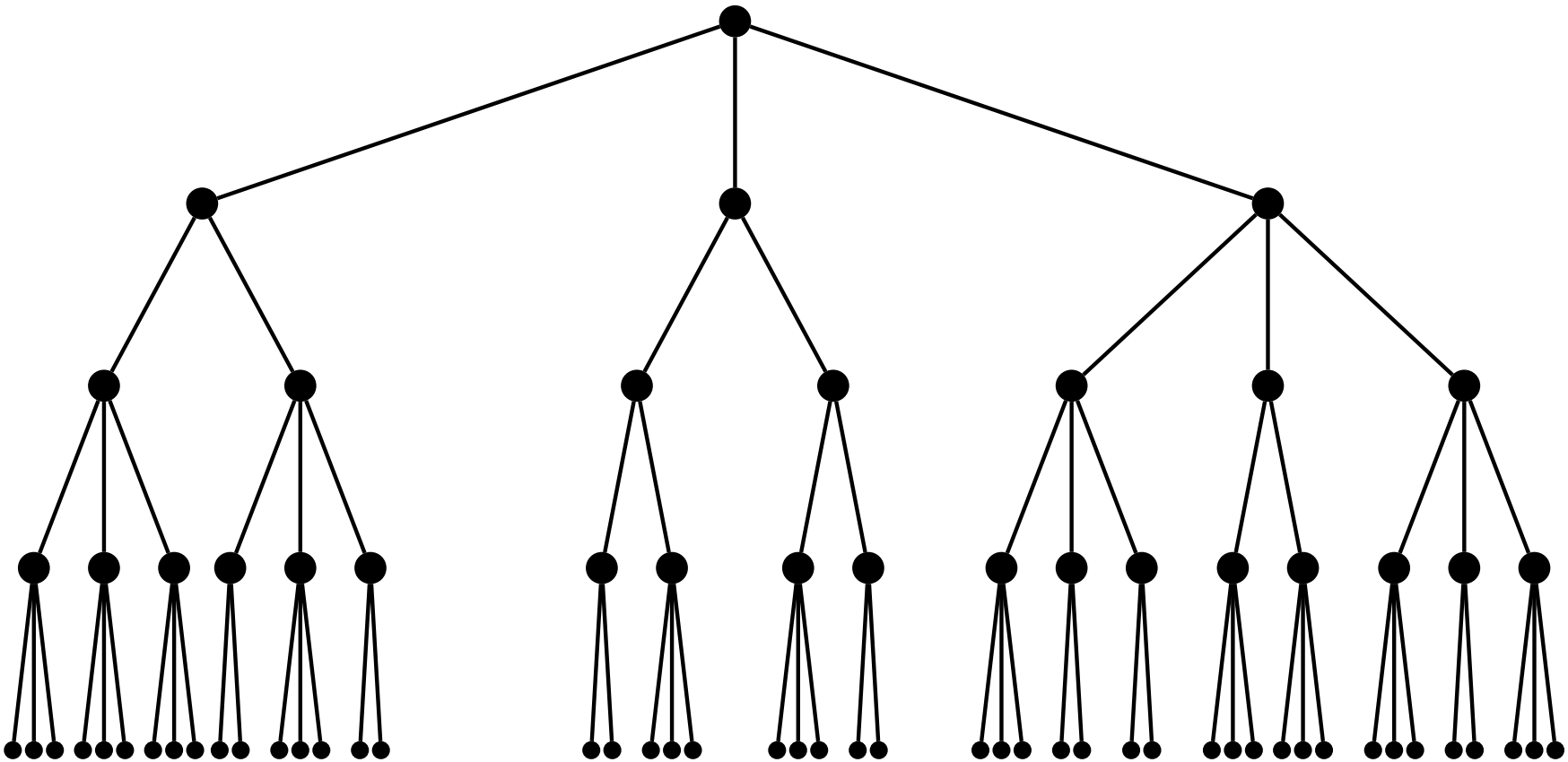


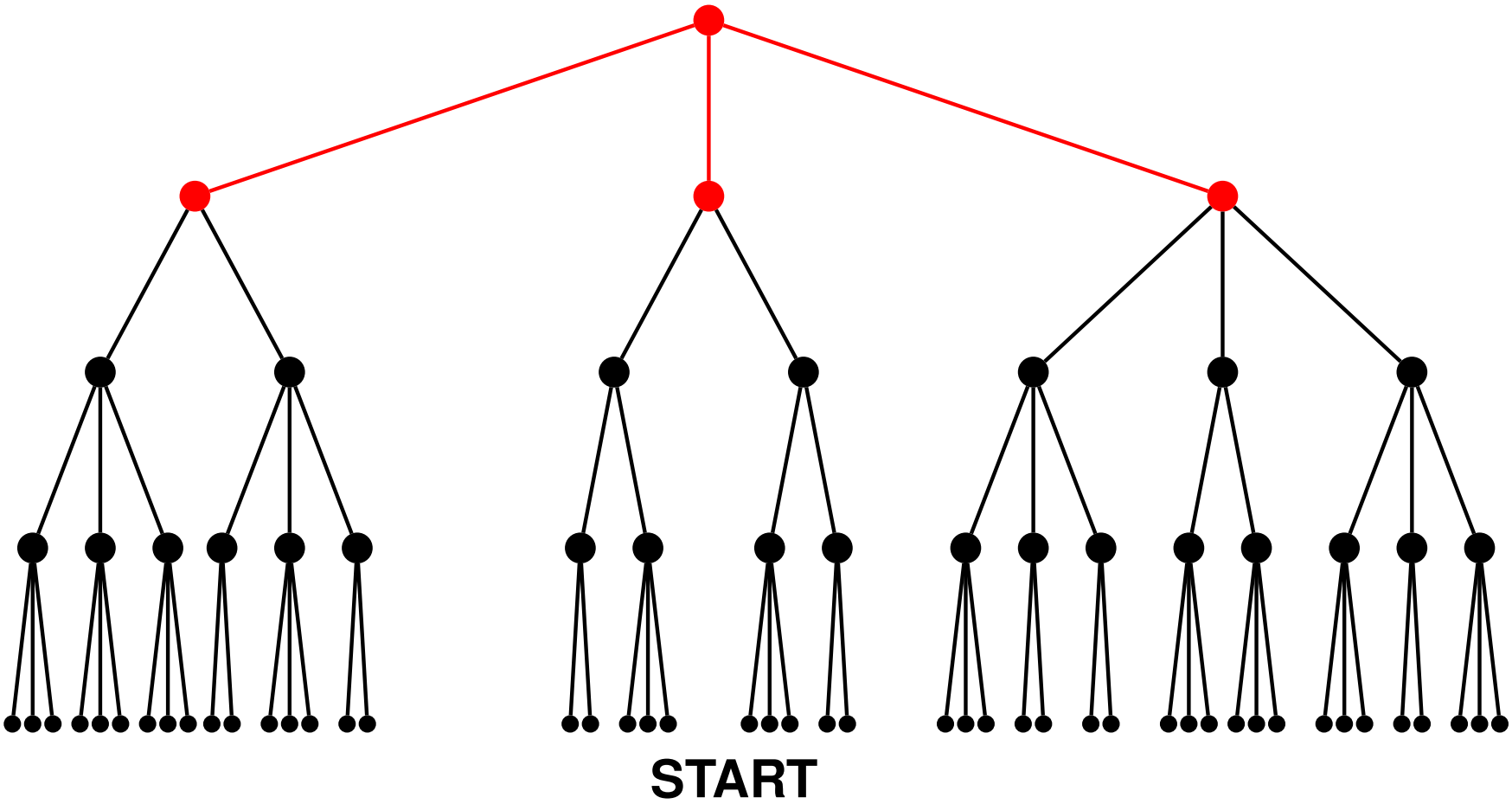




To adapt this problem to GPU some issues need to be resolved:

- Parallelize $\Rightarrow$ split backtracking tree at a fixed depth (easy).
- No recursion $\Rightarrow$ stack implementation.
- SIMT architecture (Single Instruction Multiple Thread) $\Rightarrow$ need to eliminate branching, as much as possible.
- SIMT $\Rightarrow$ ensure most threads doing useful work most of the time.
- Memory model $\Rightarrow$ for this application need to fit all variables in shared memory (effectively 512B) and registers.

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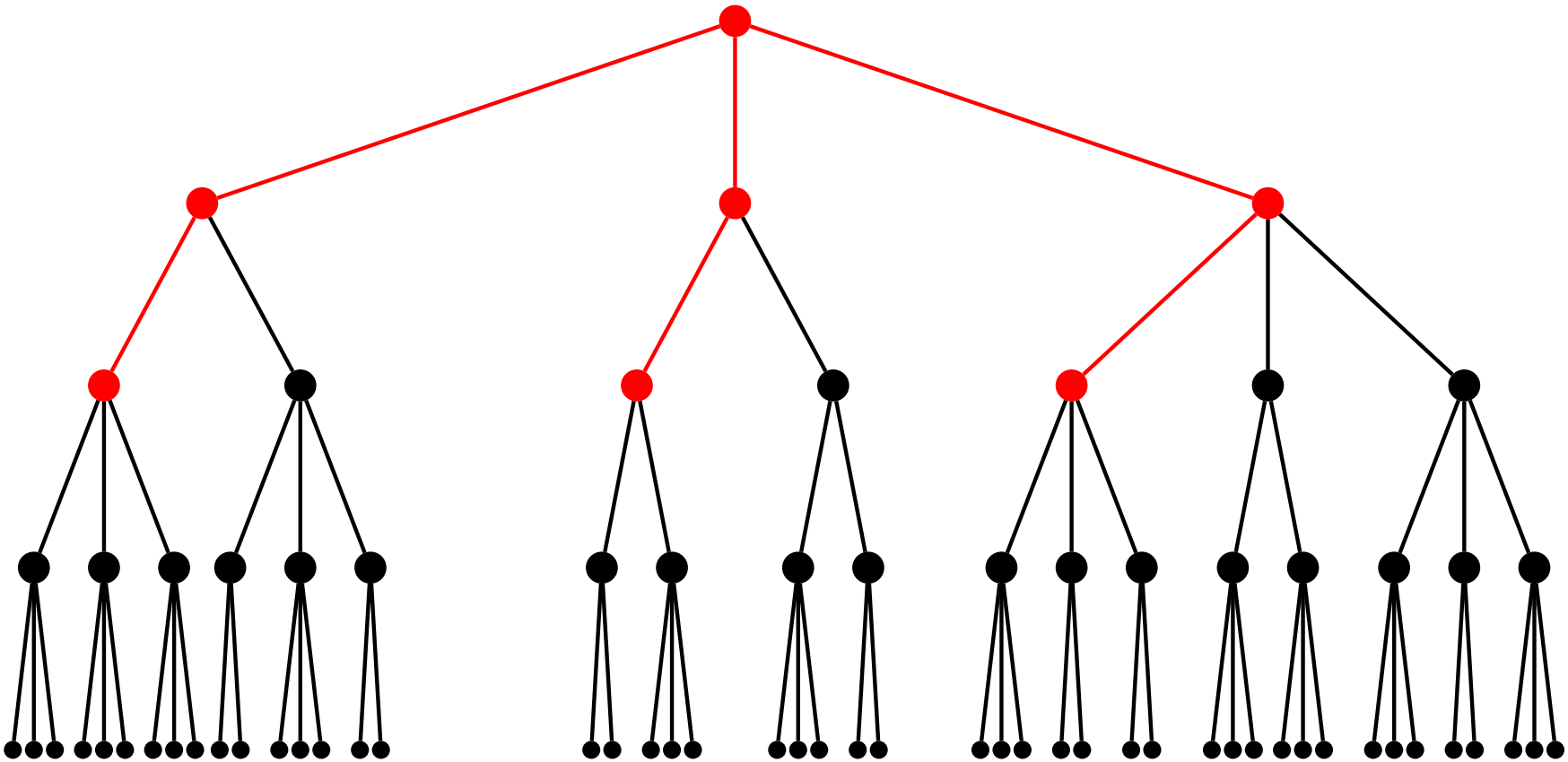

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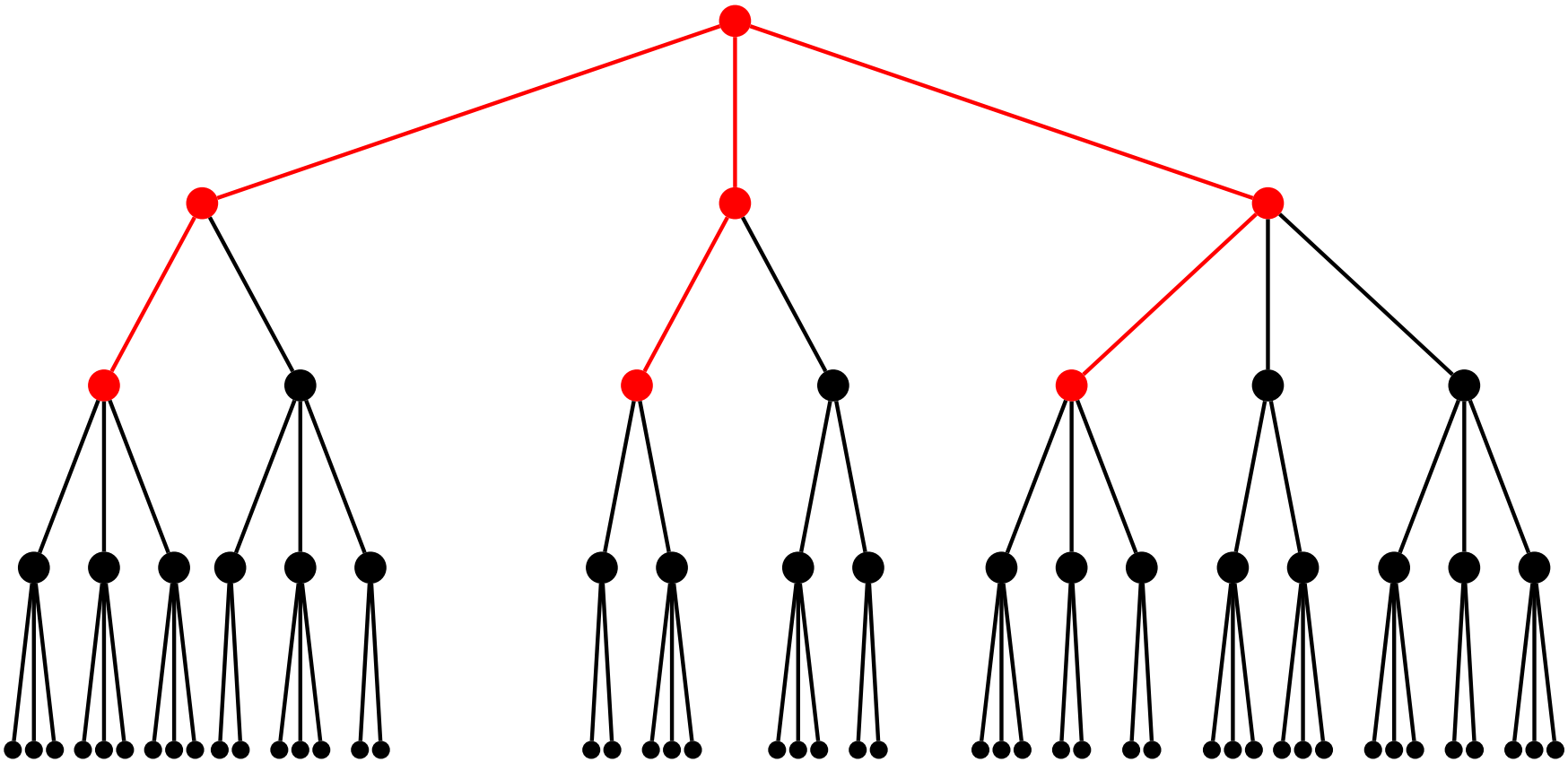
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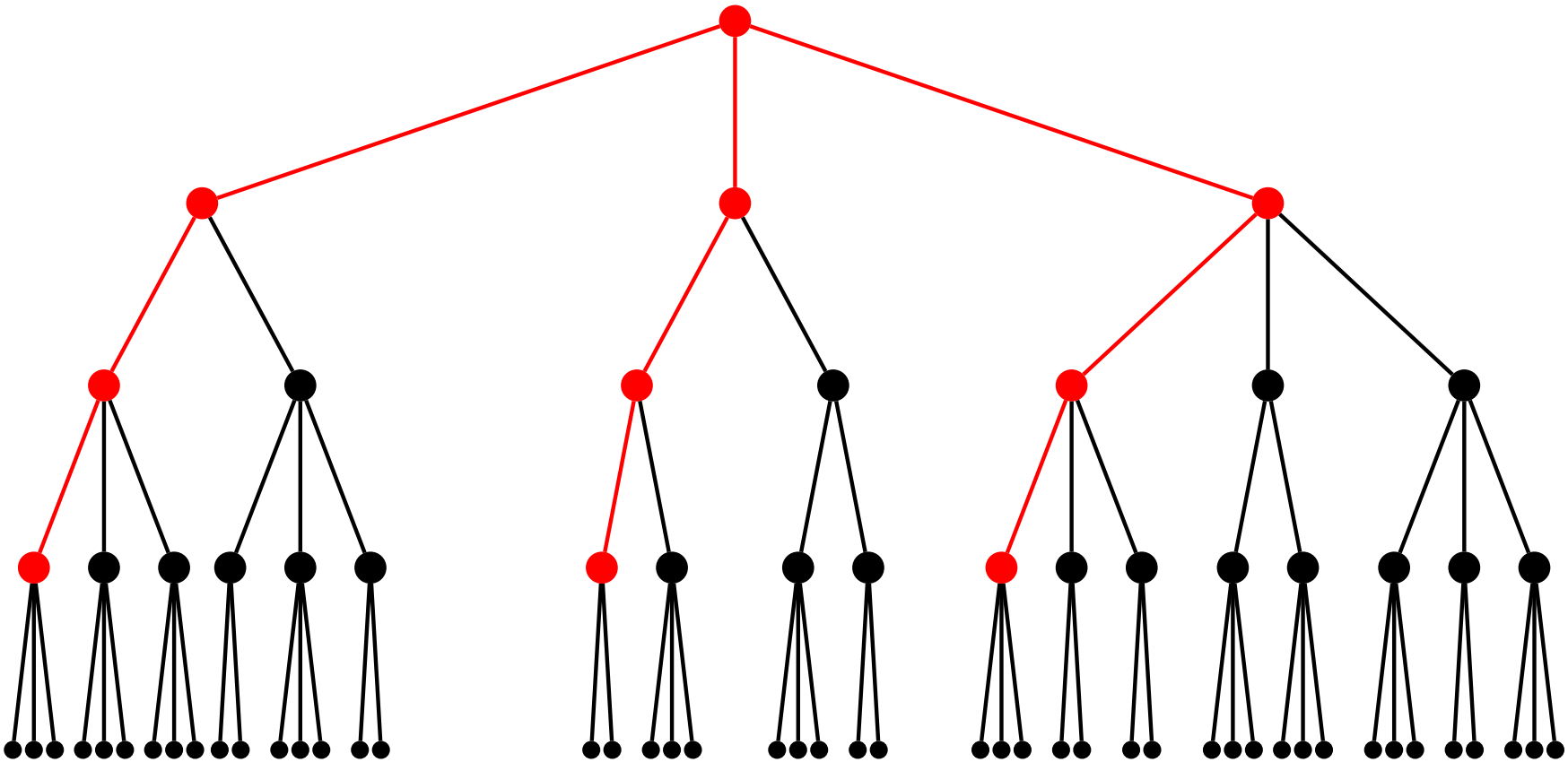

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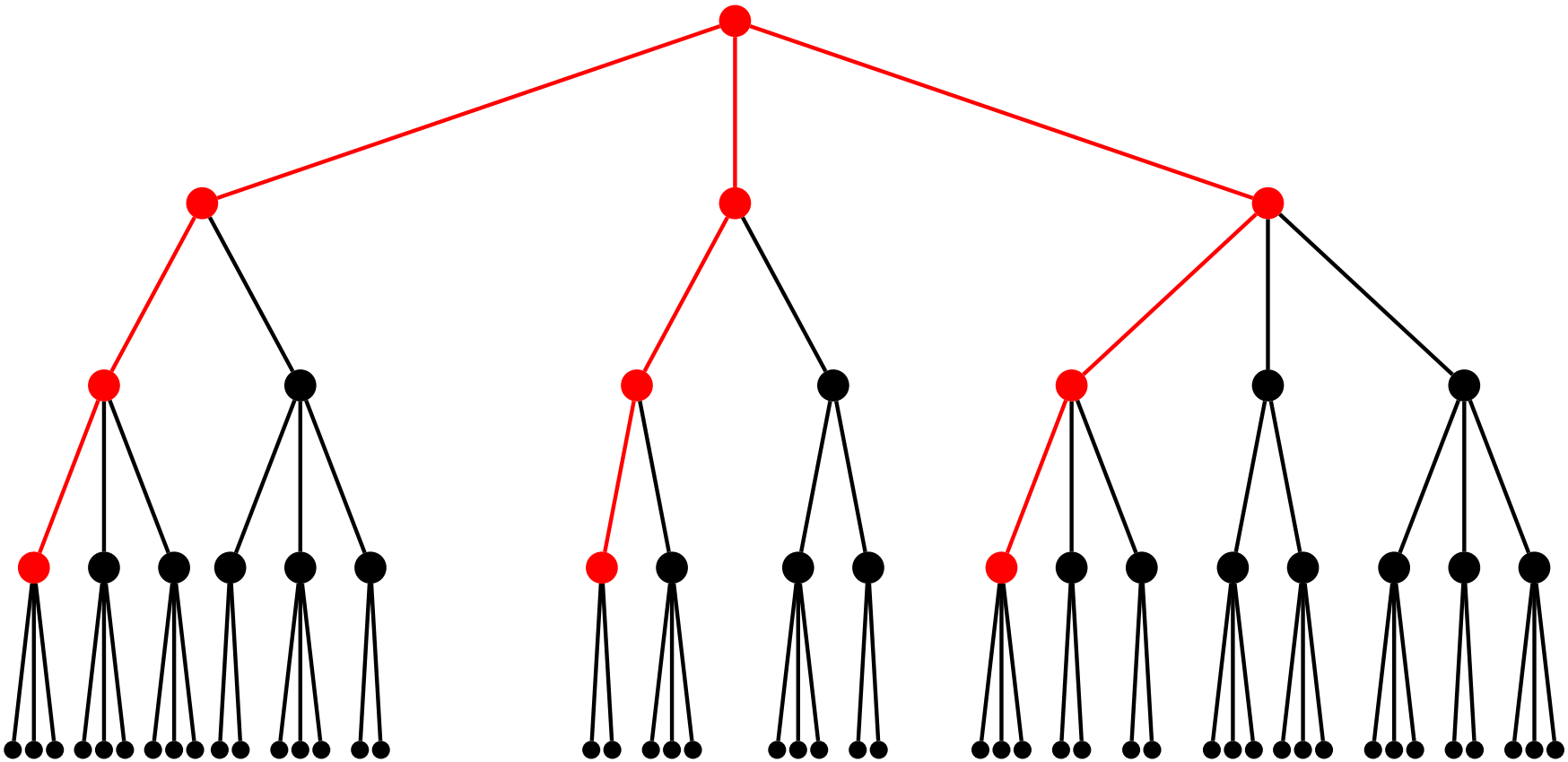
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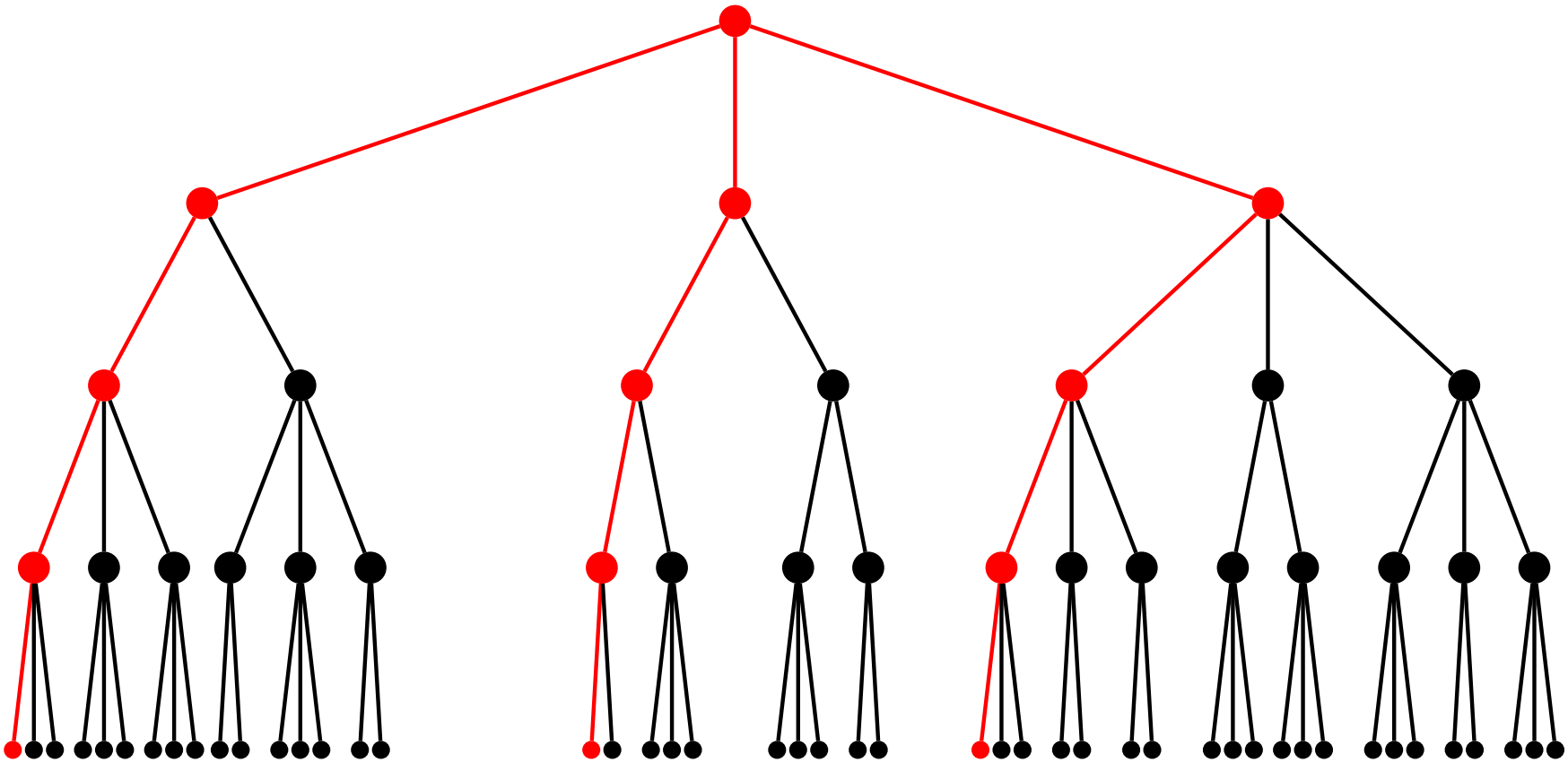

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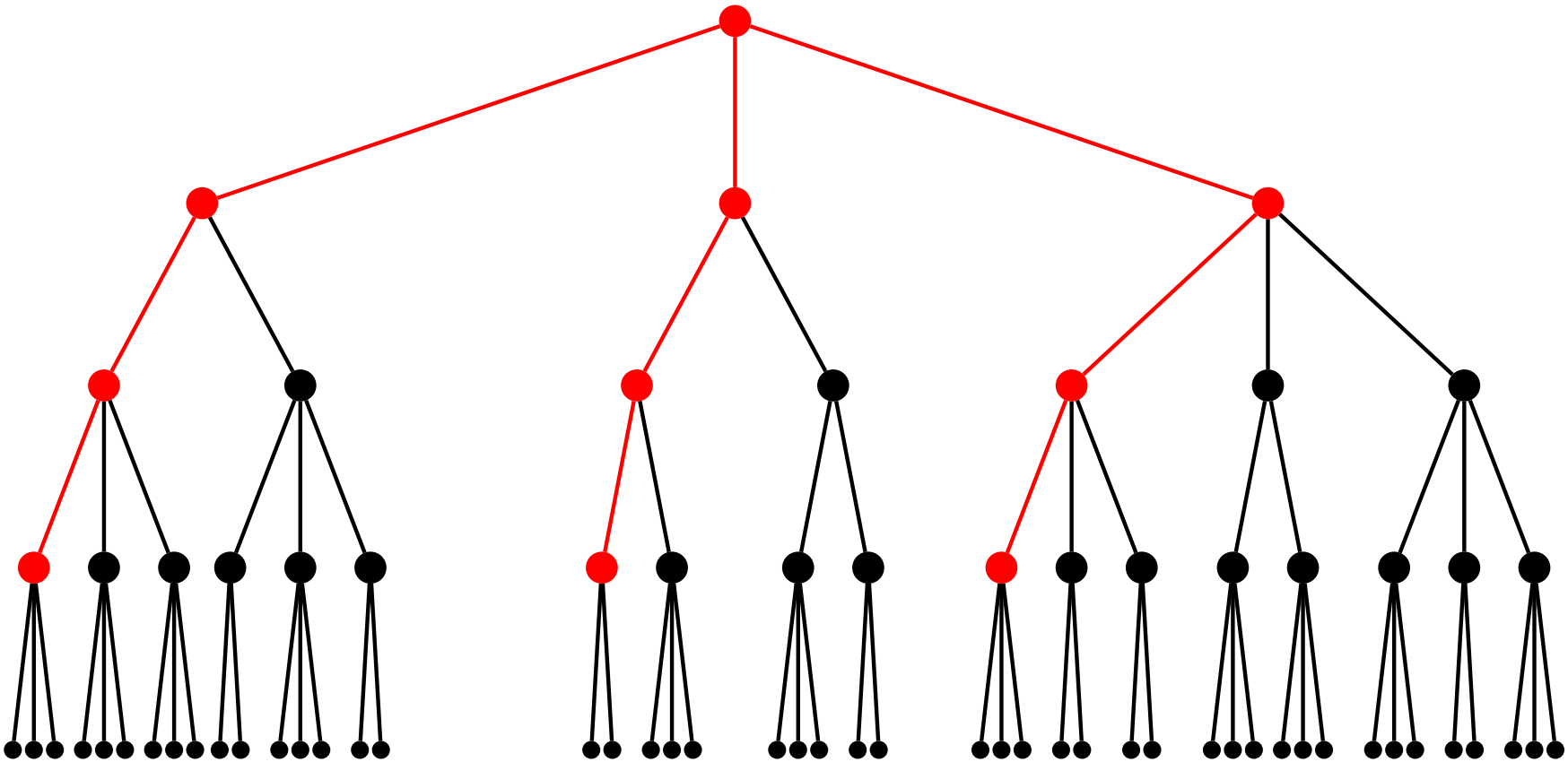
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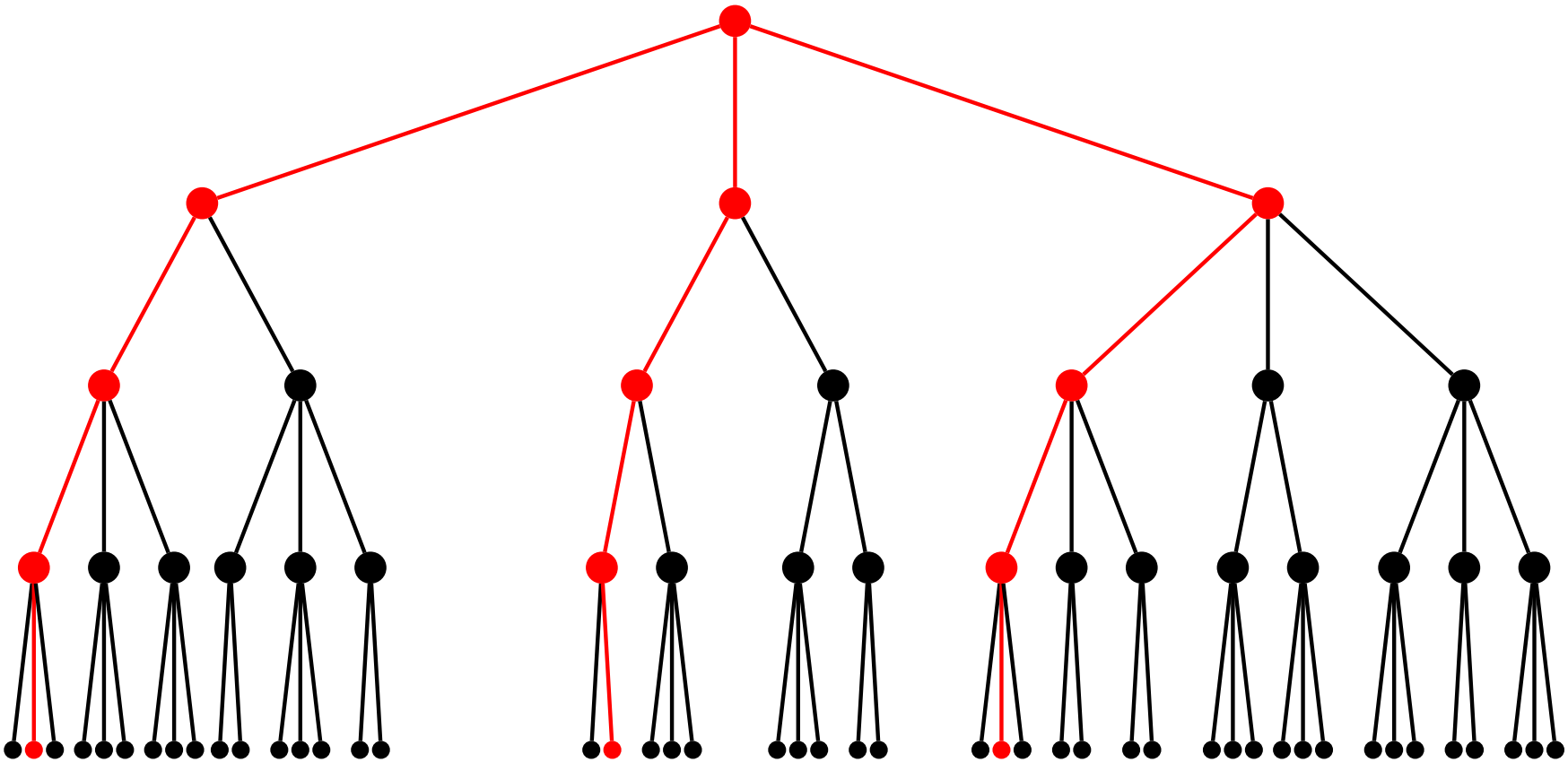

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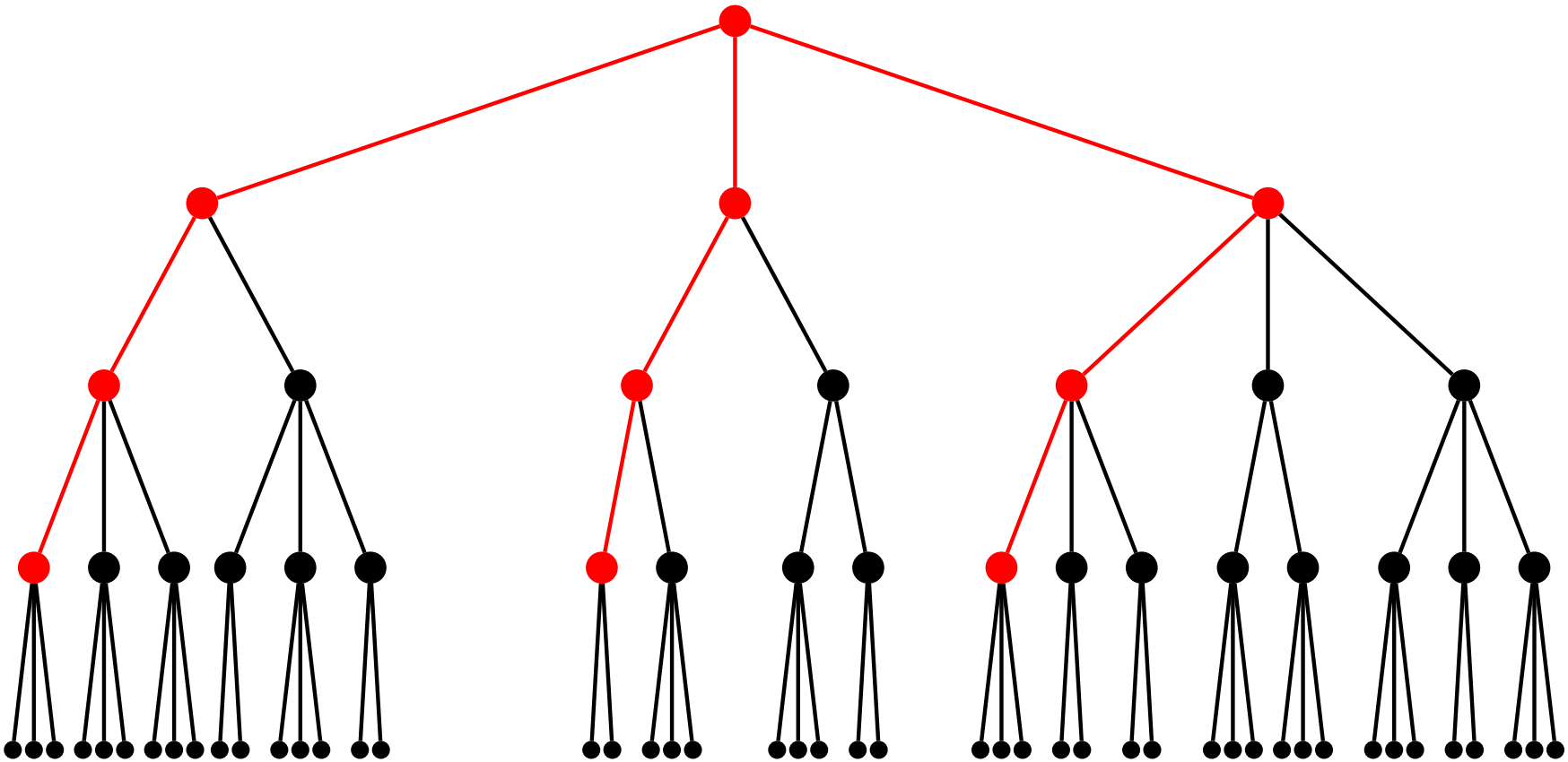
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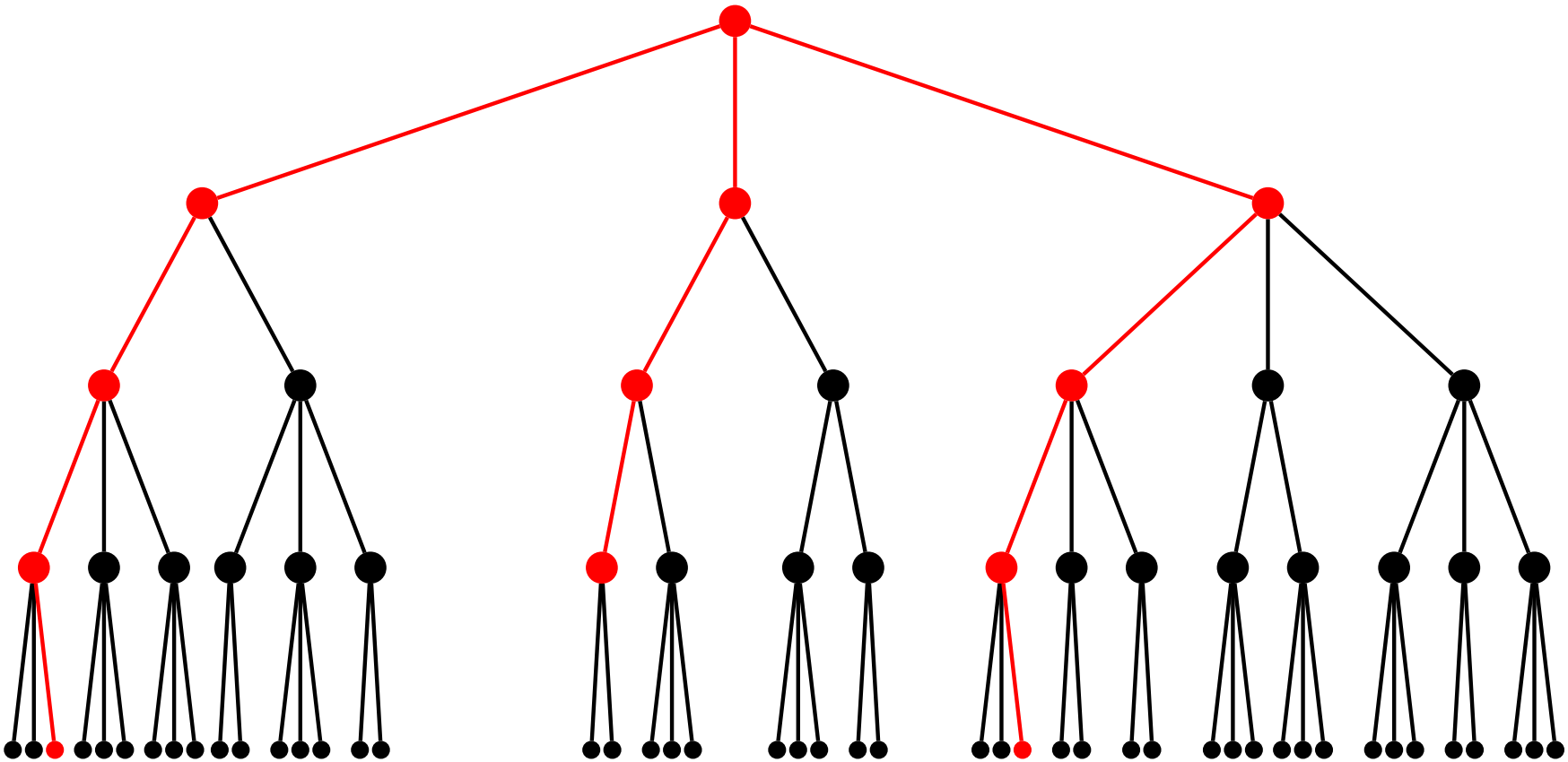

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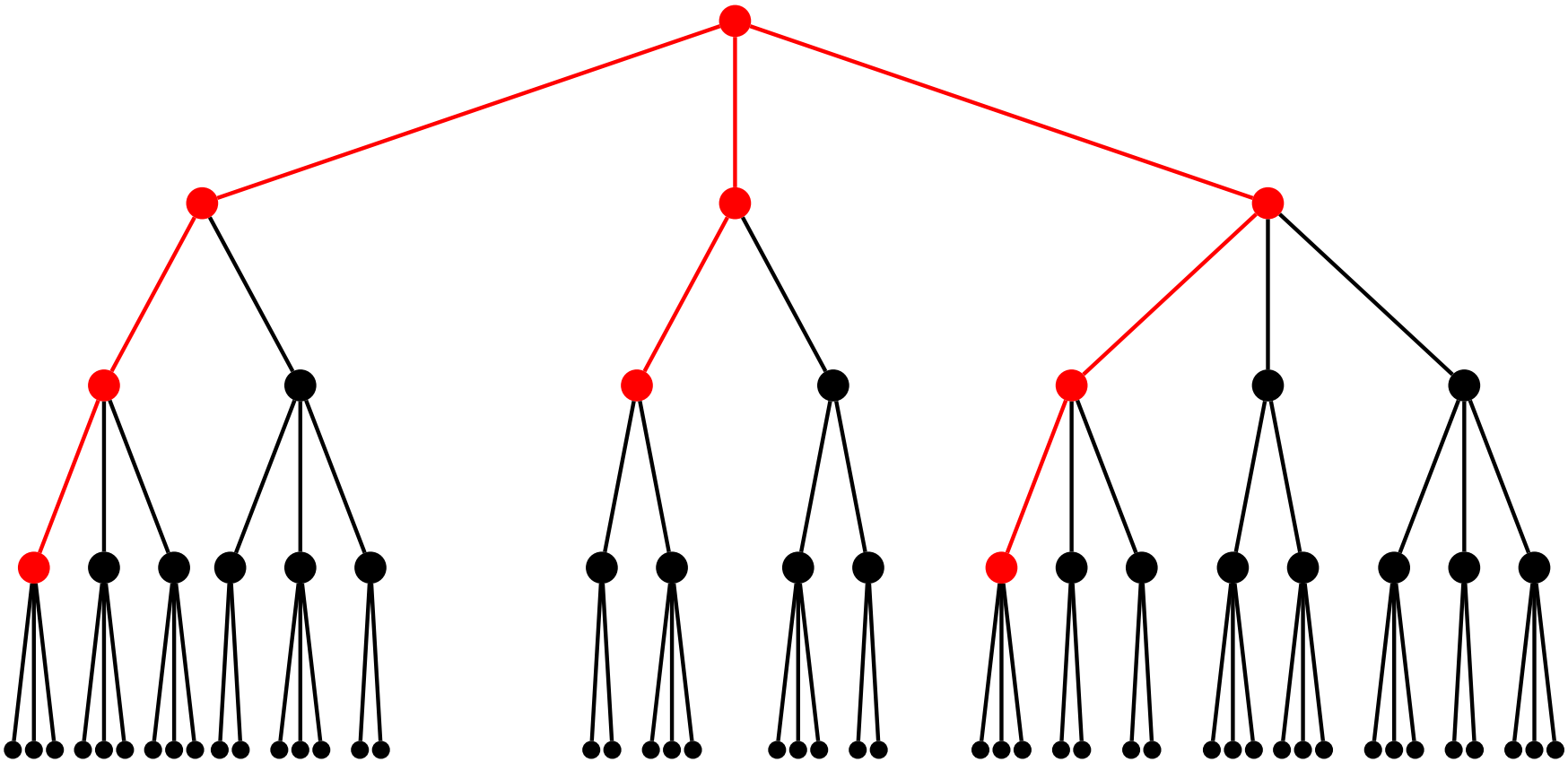
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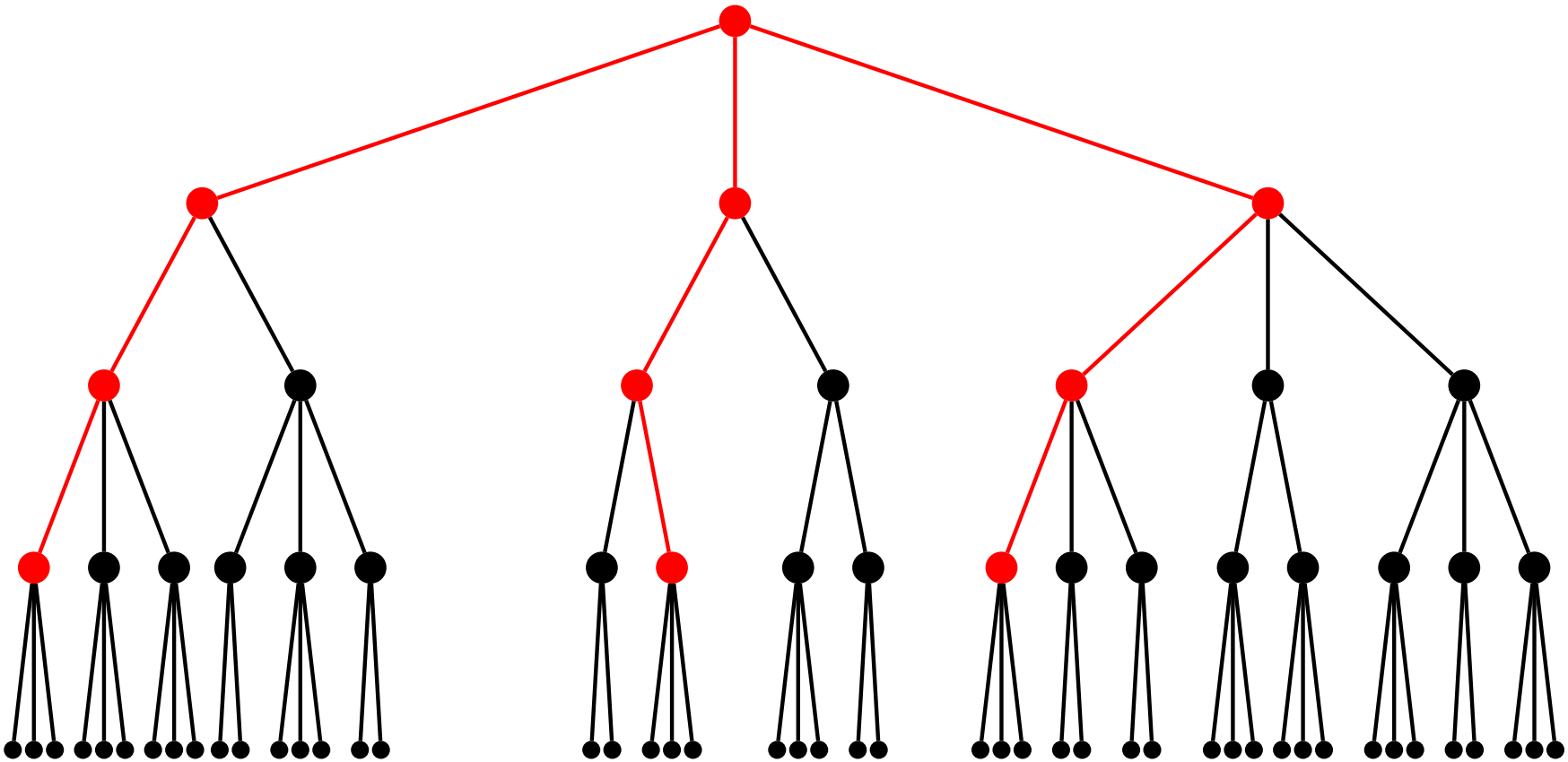

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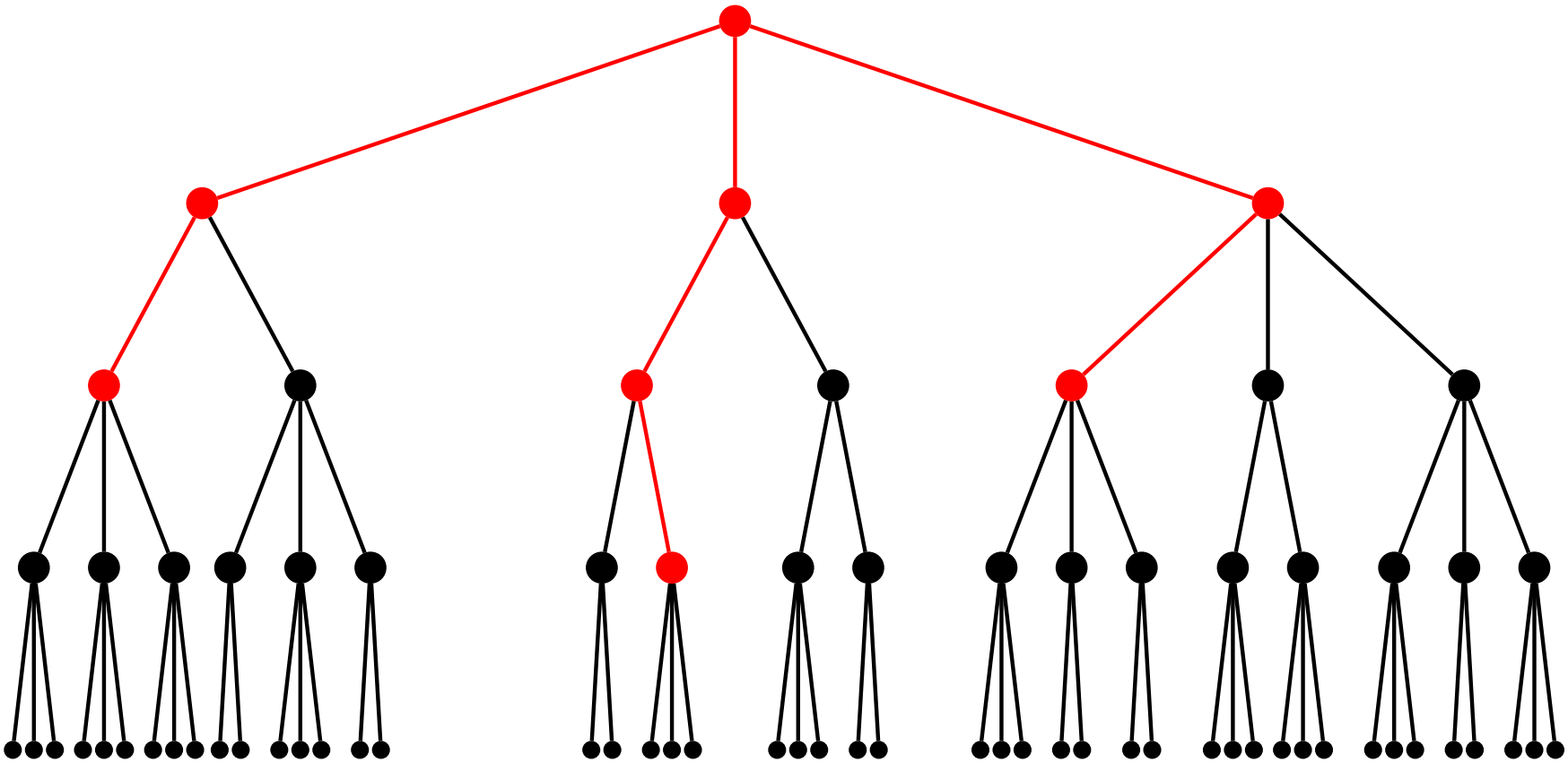
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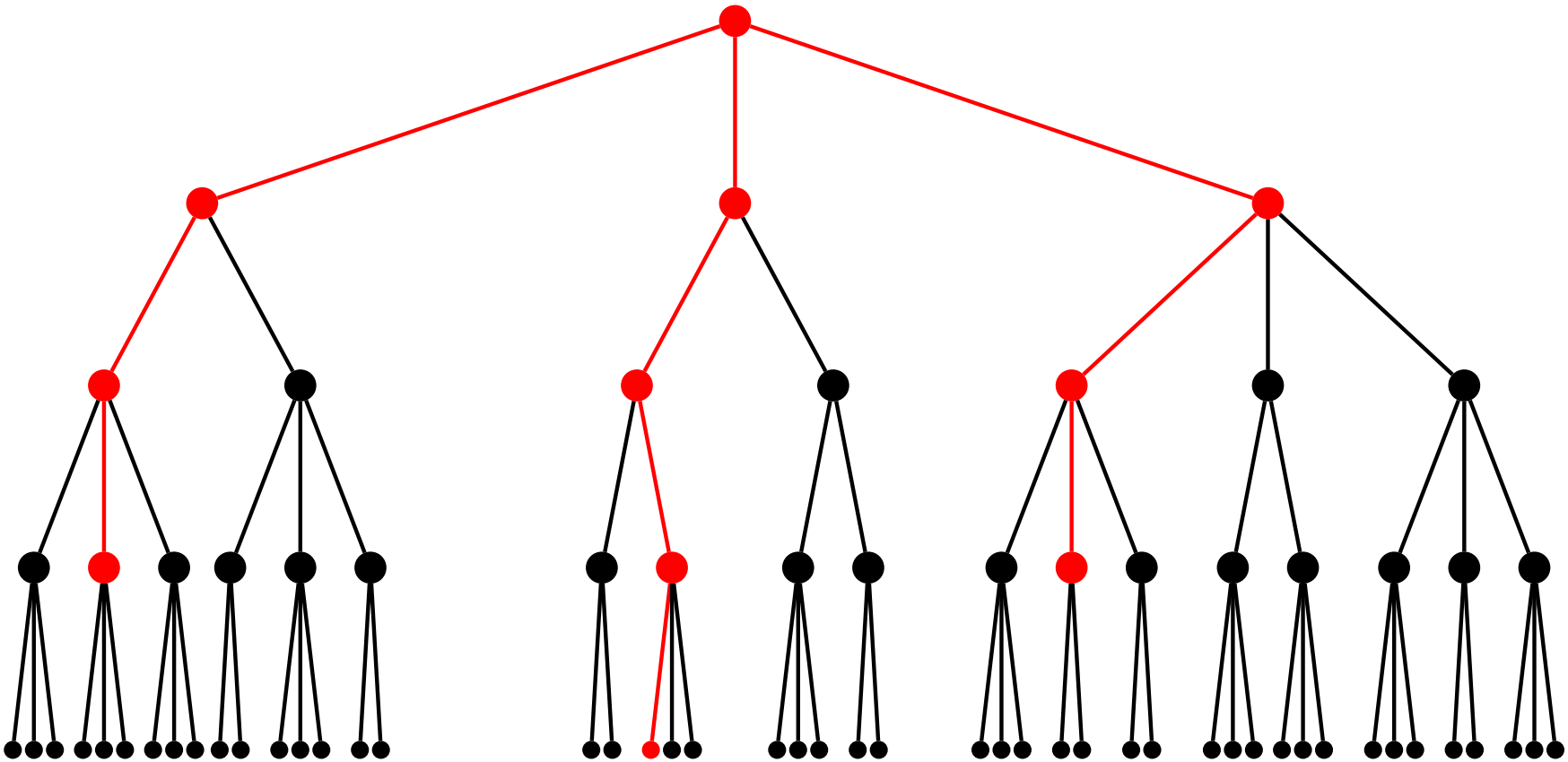

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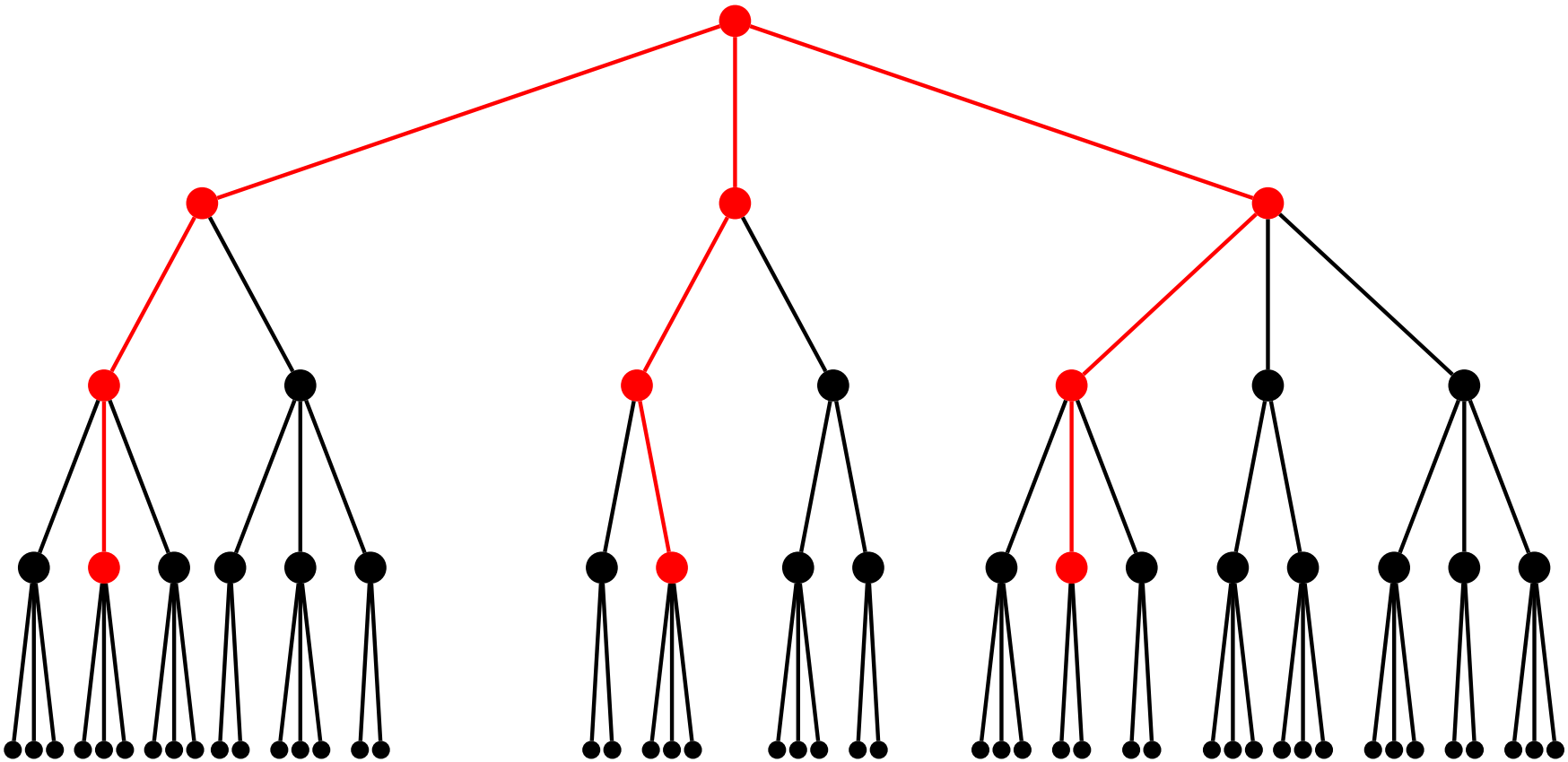
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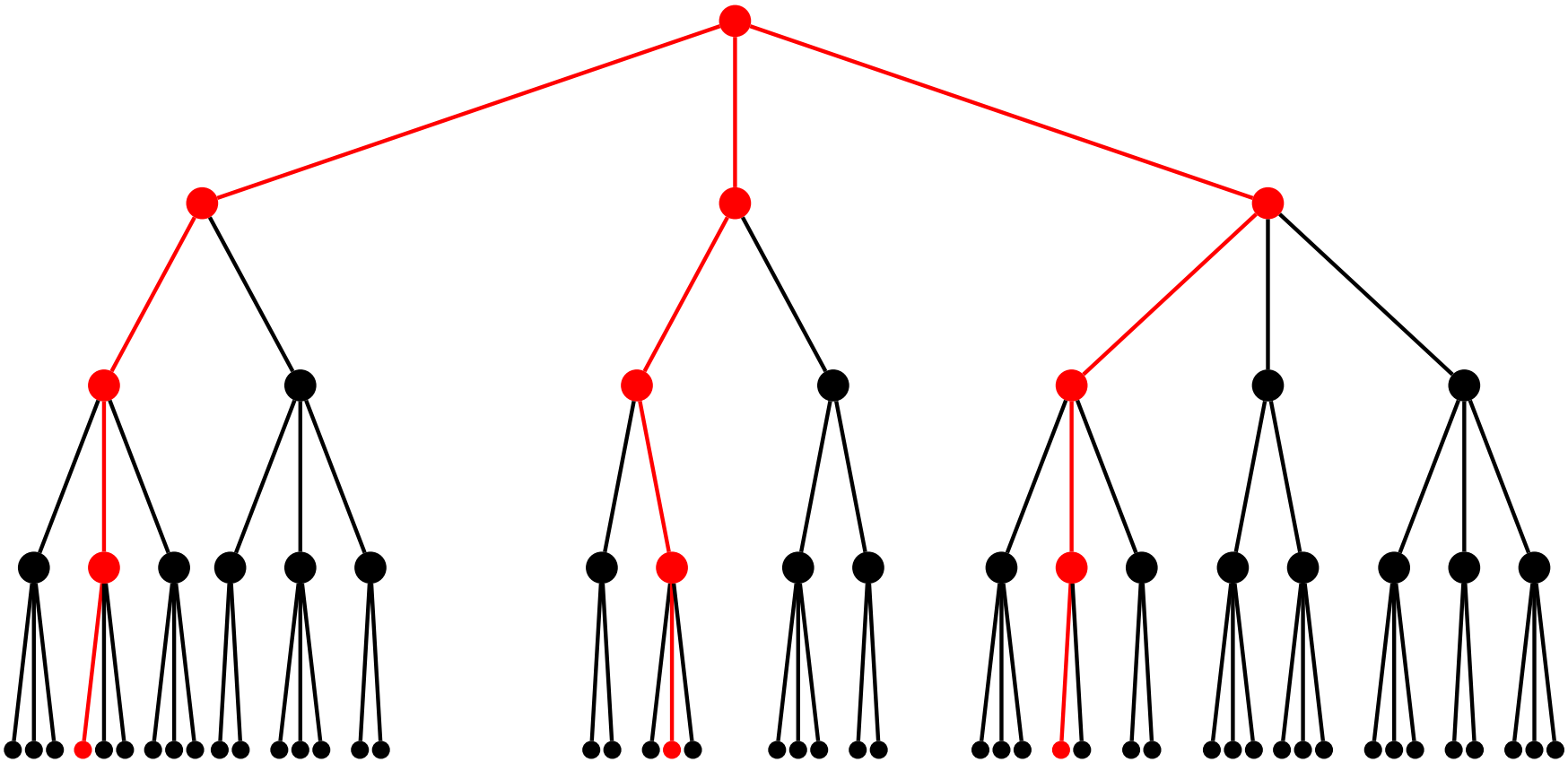

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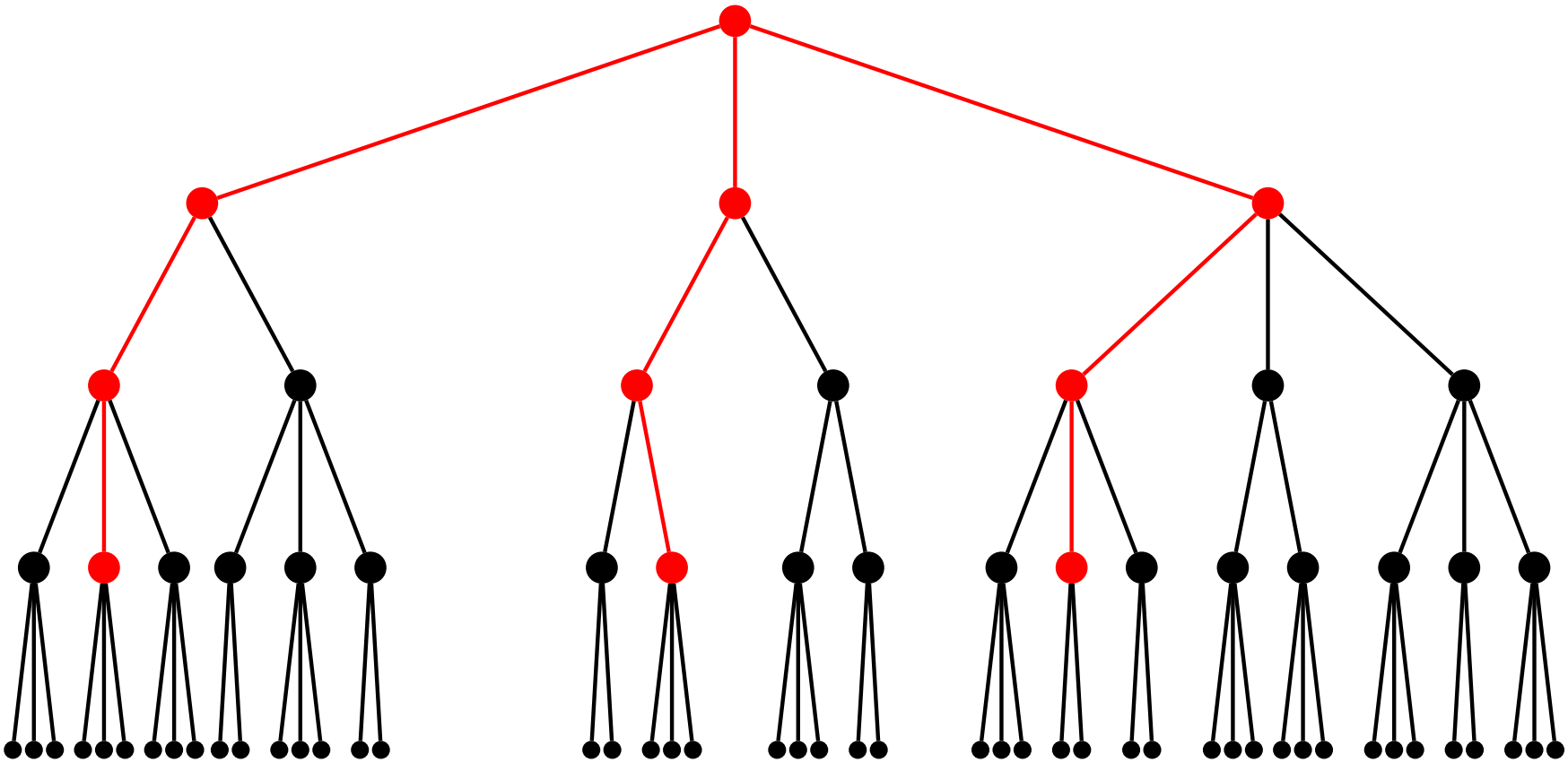
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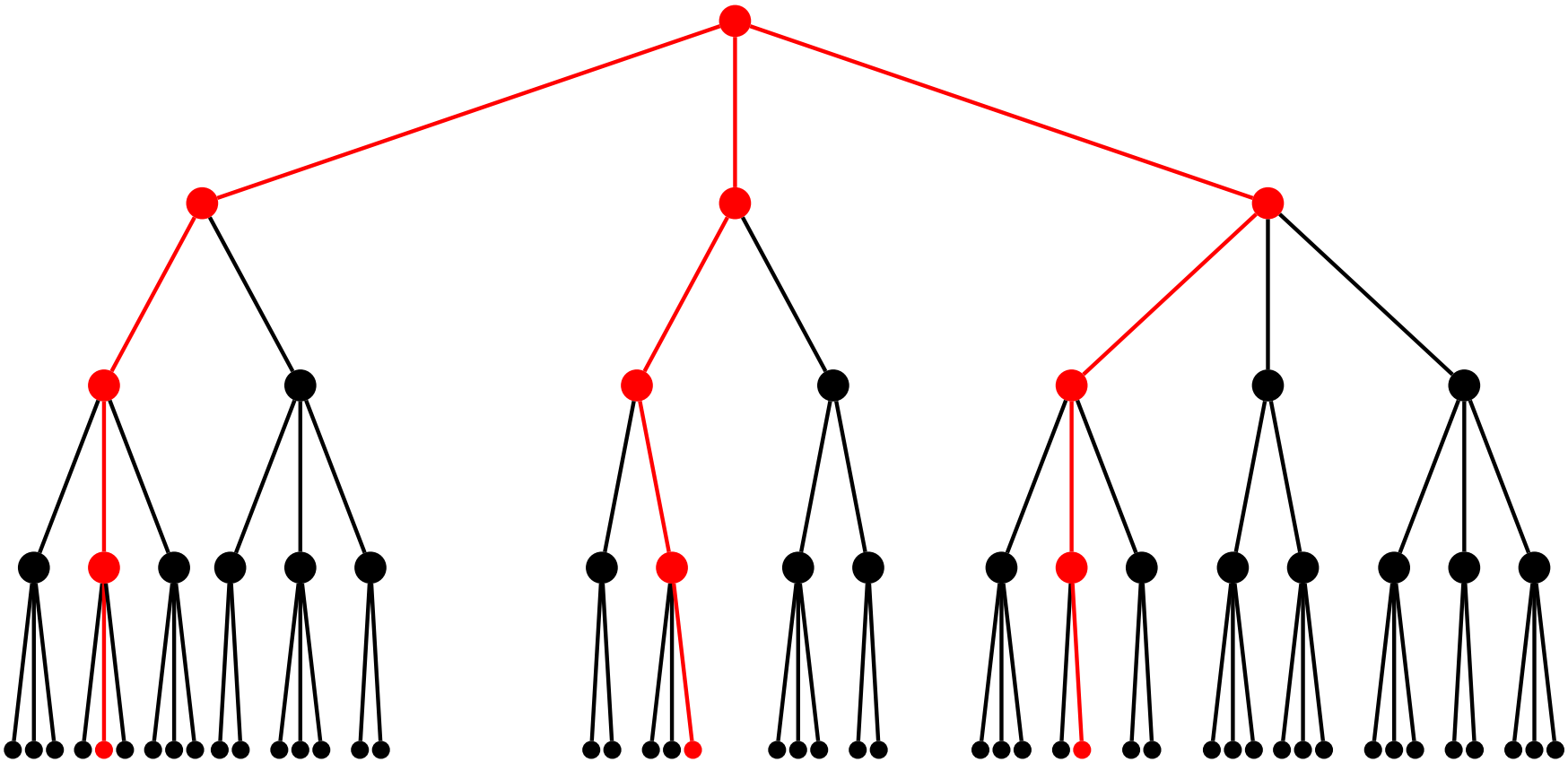

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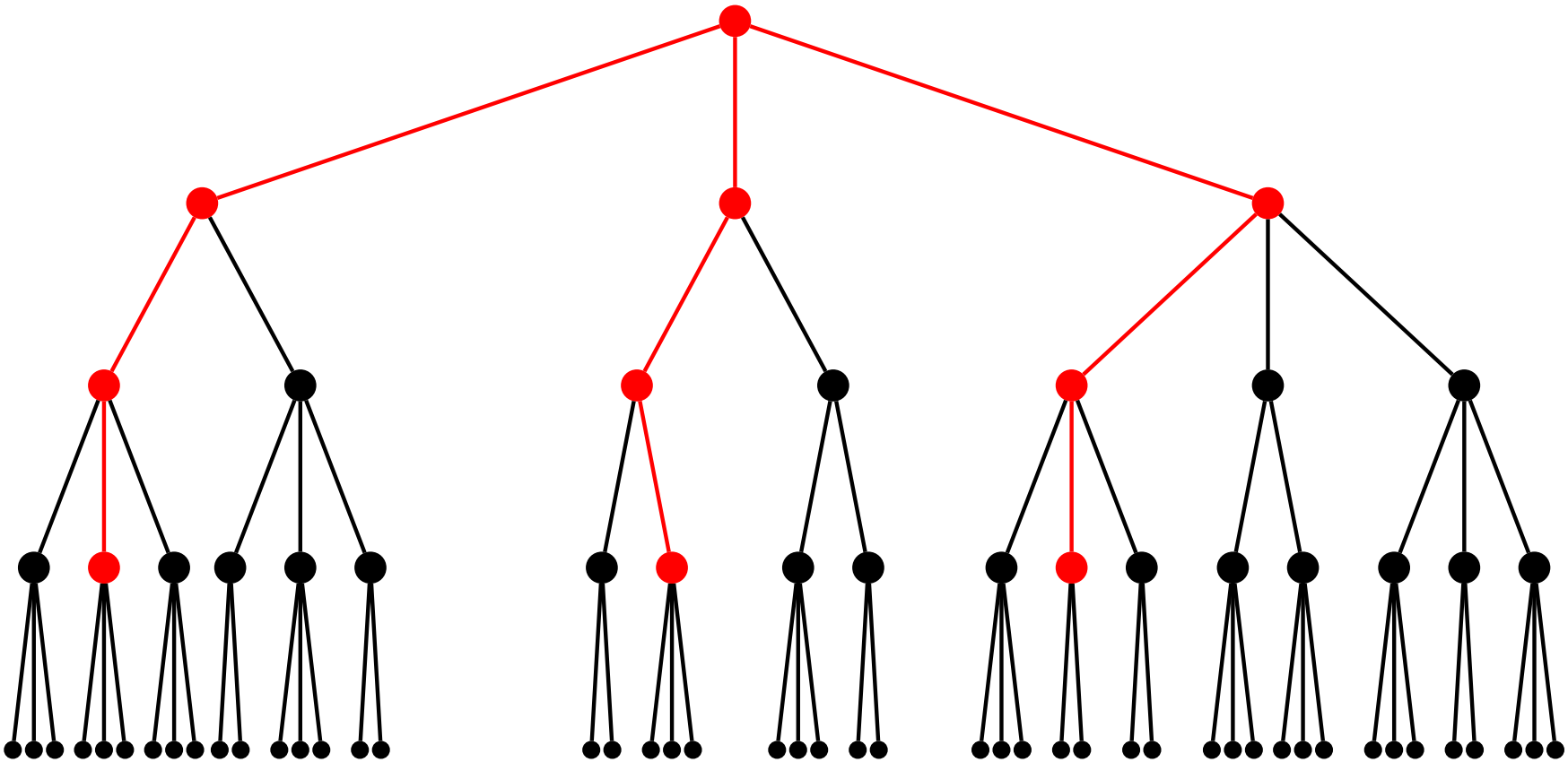
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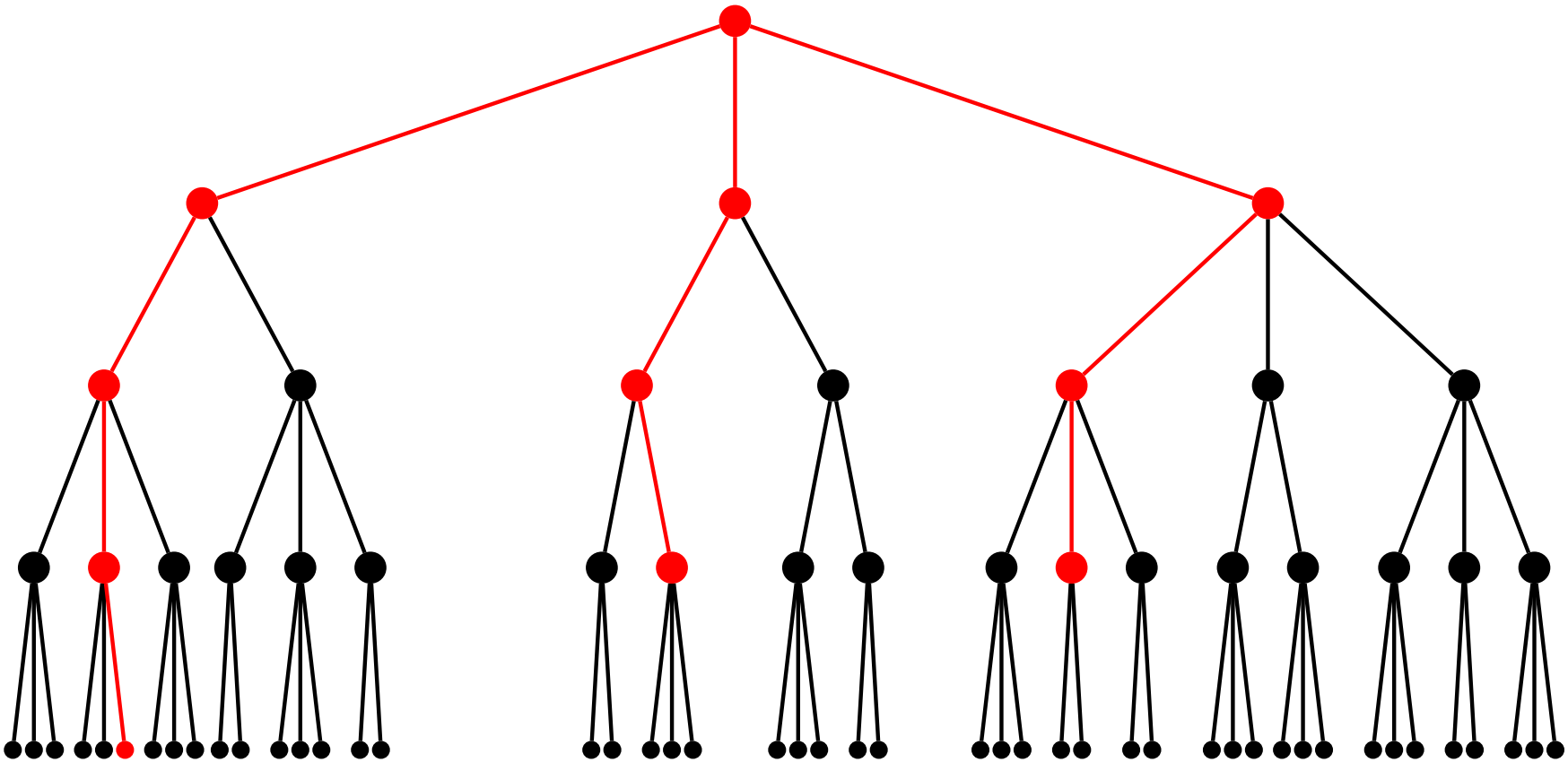

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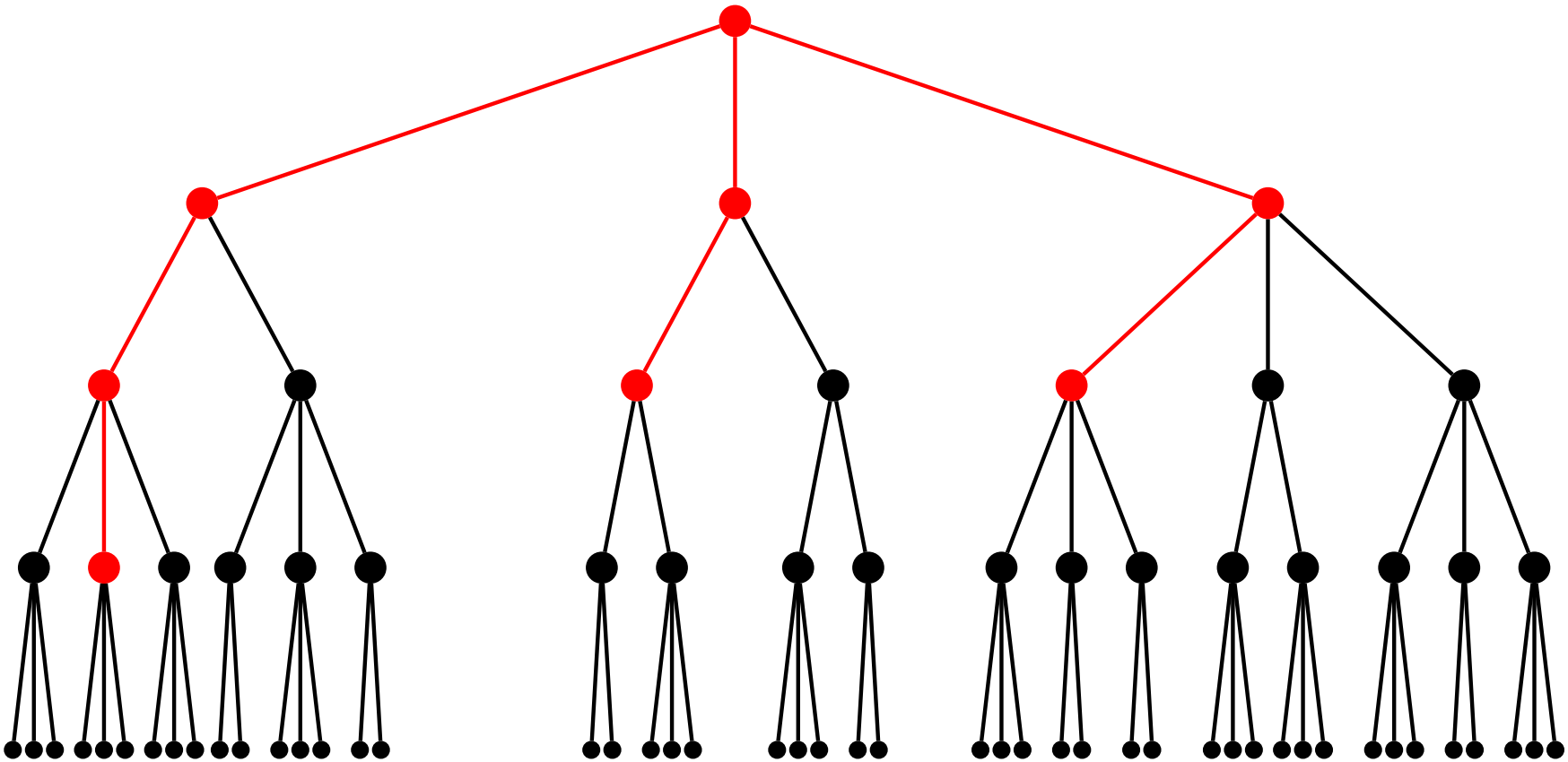
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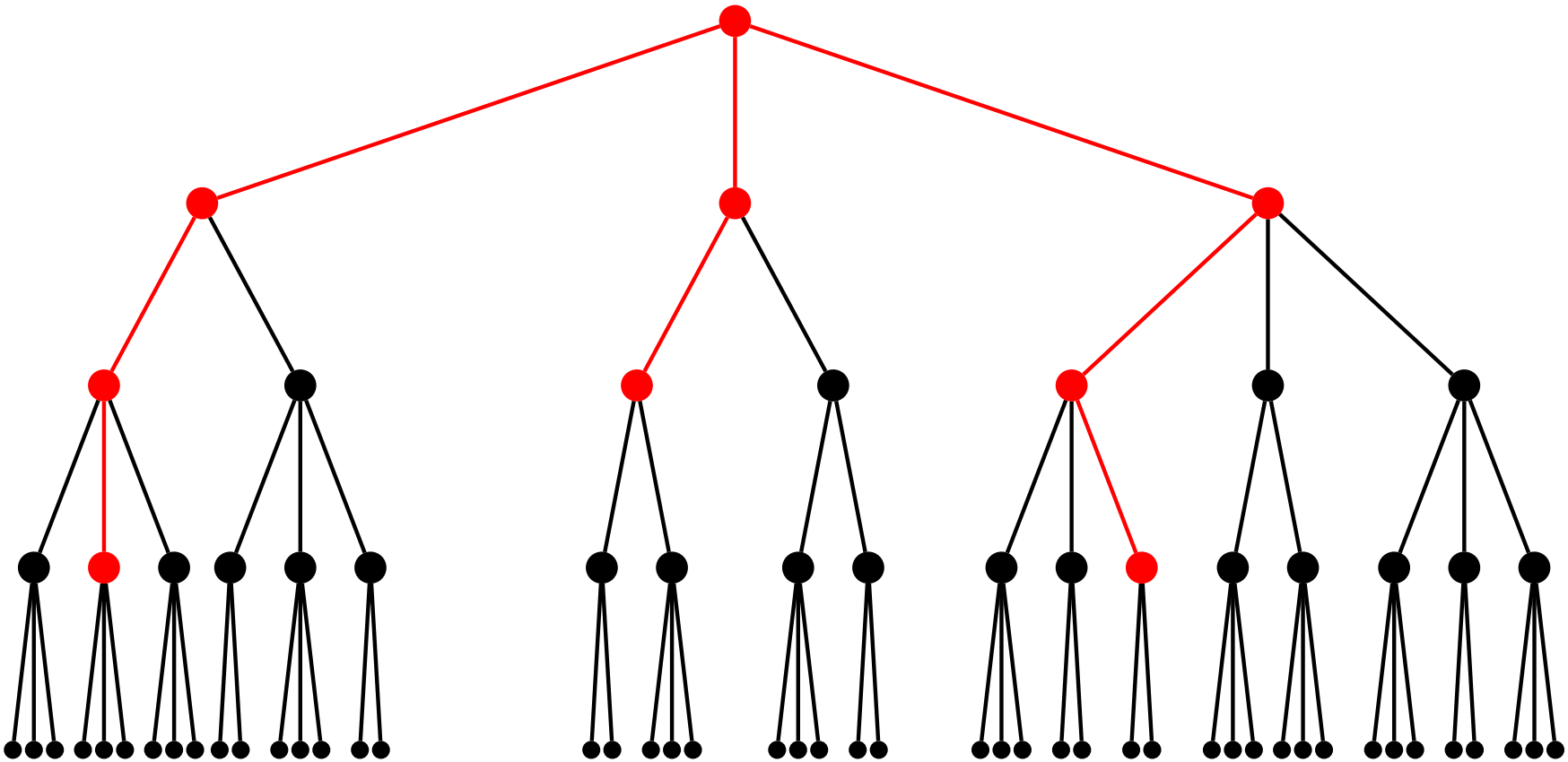
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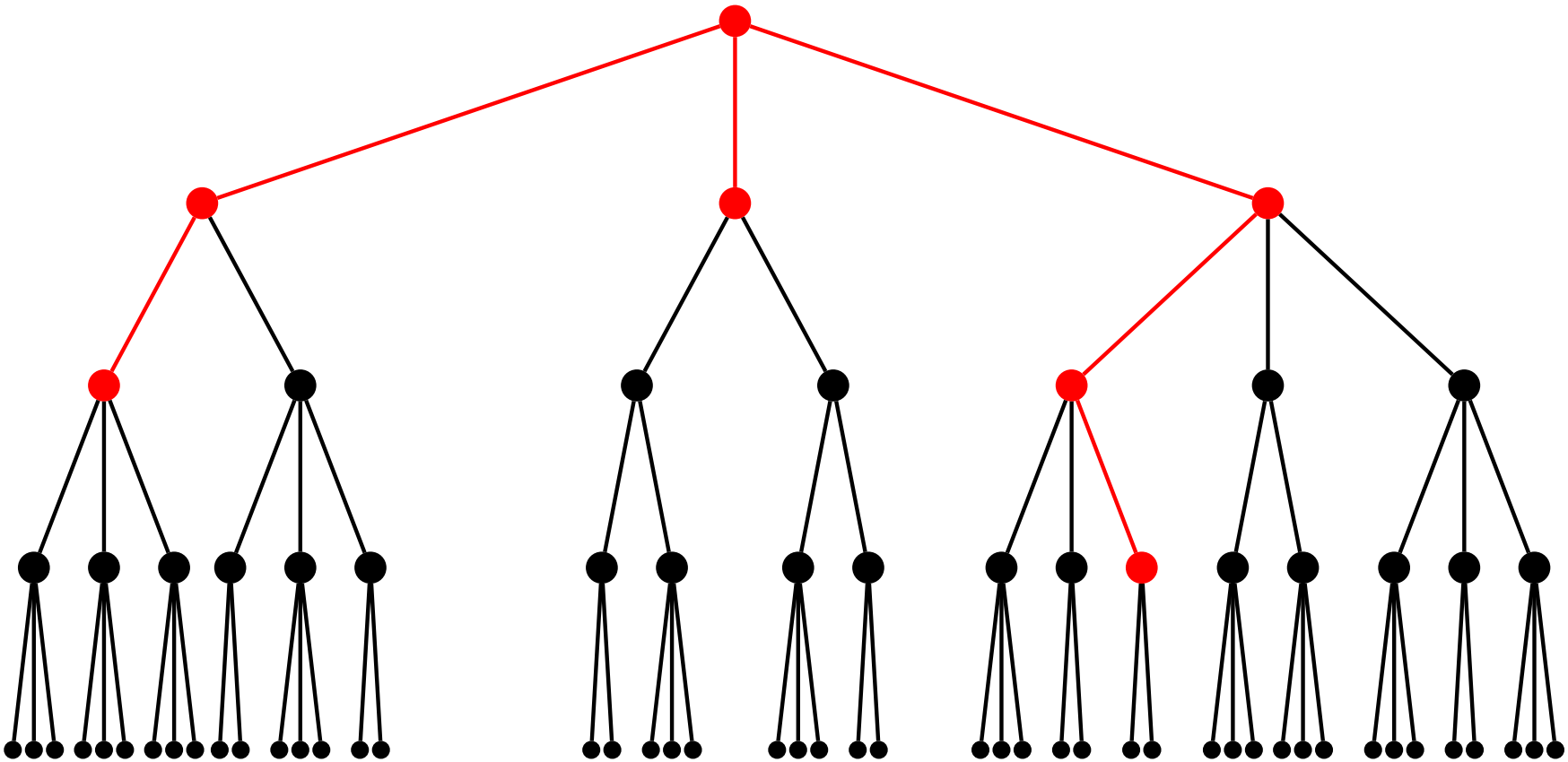
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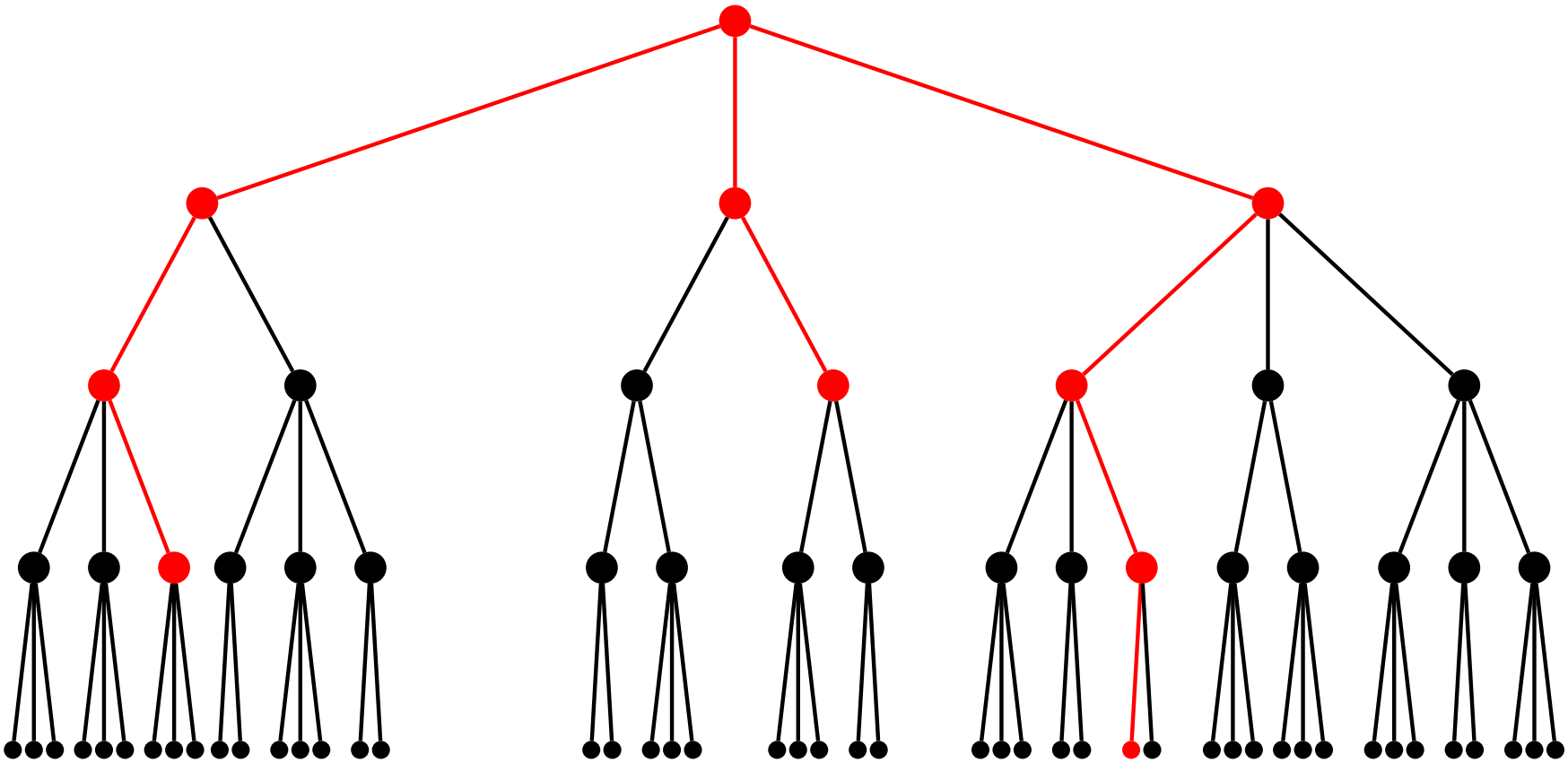

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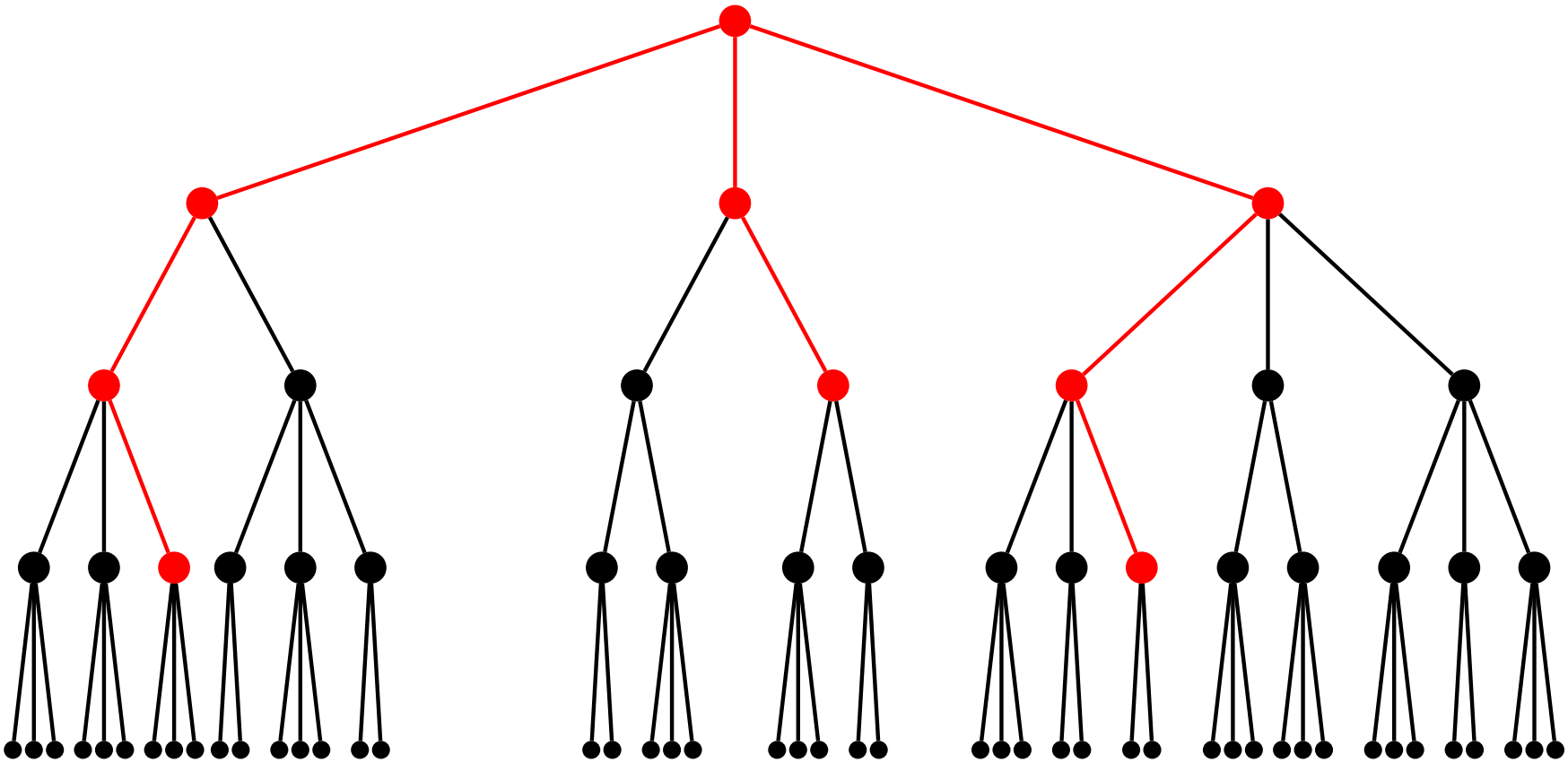
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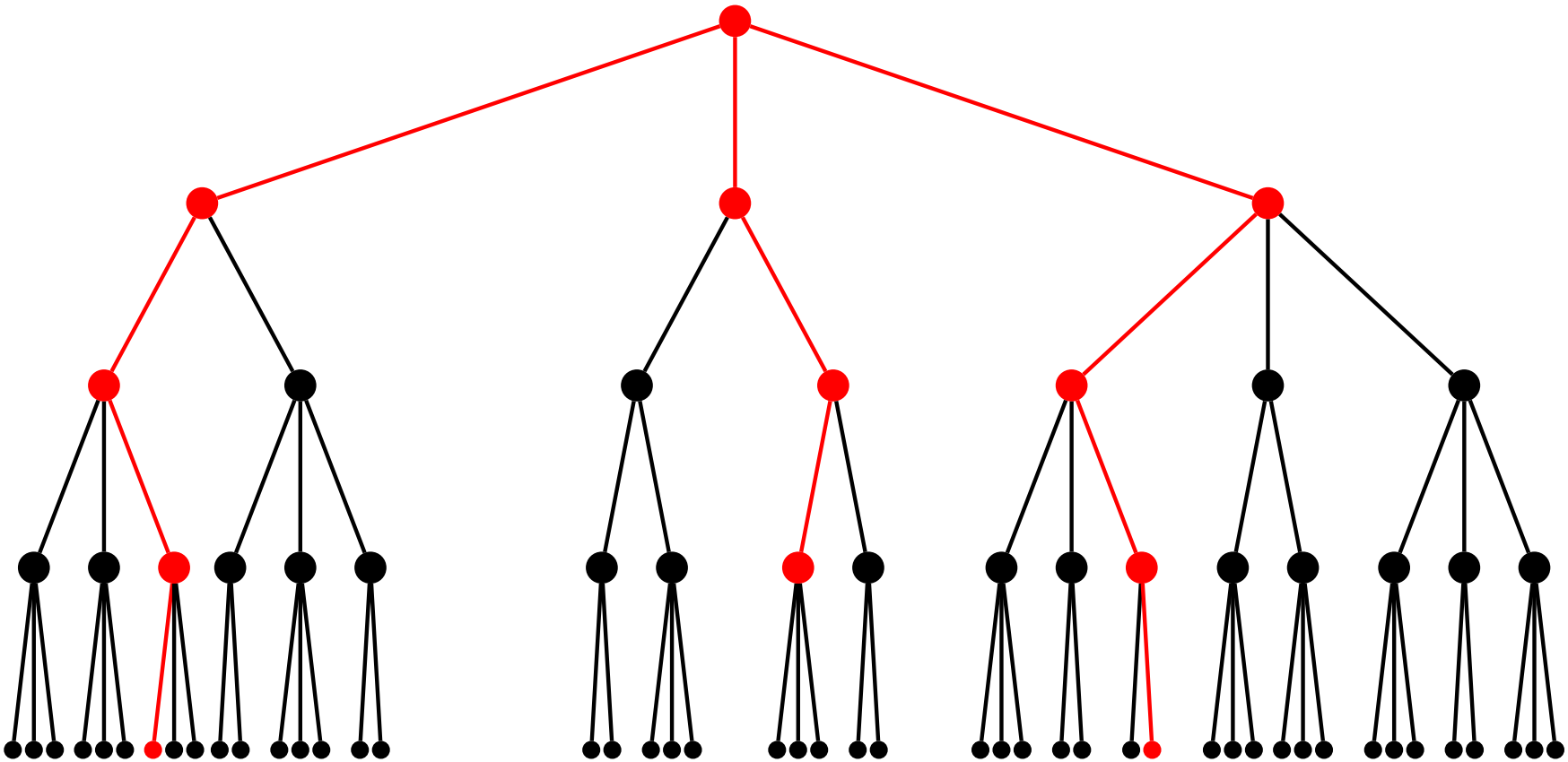

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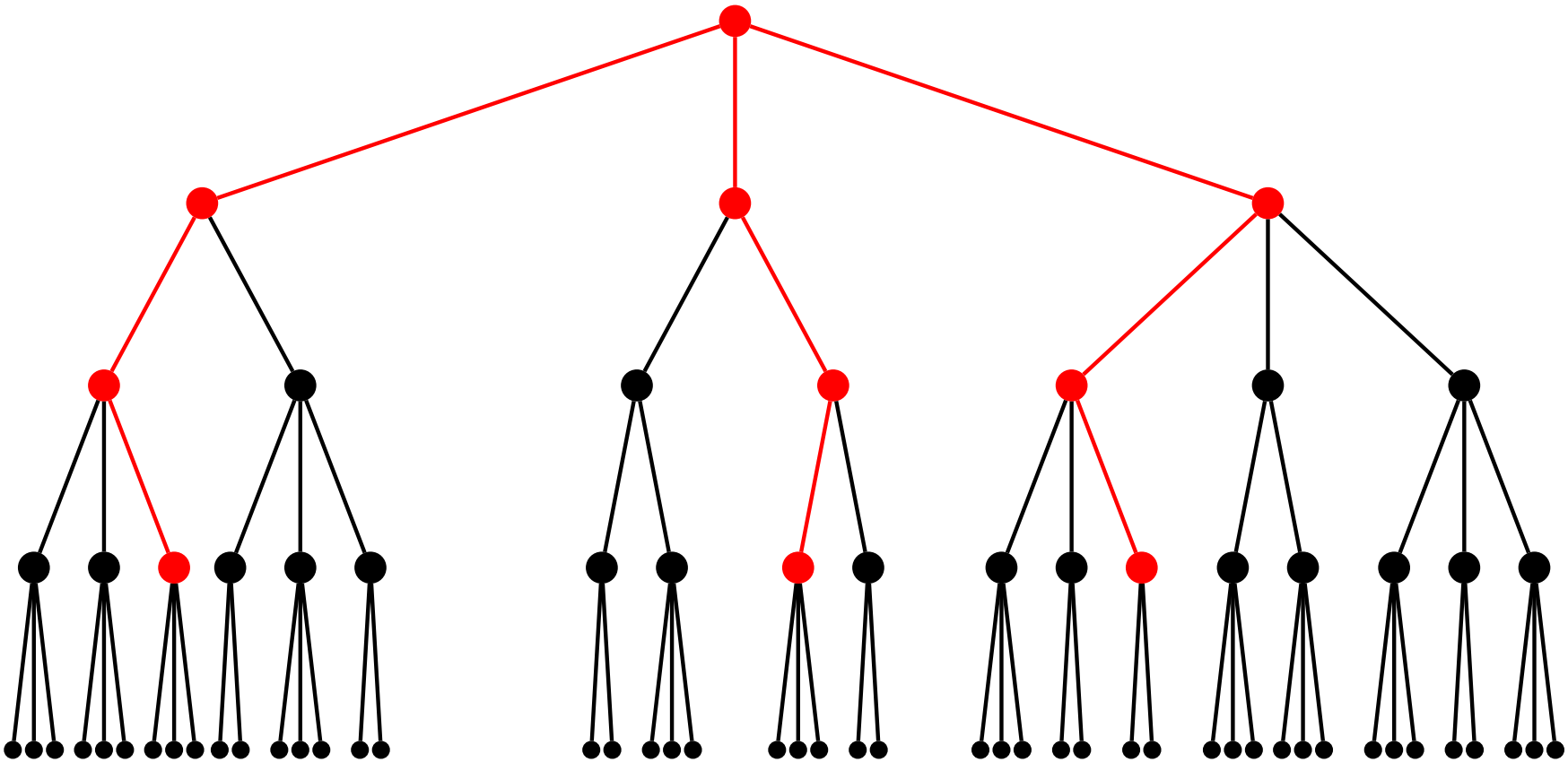
REMOVE

Backtracking - conclusion

- Thinking this way helped me develop a 25% faster C implementation.
- 8 GPU cores = 1 CPU core
- $\Rightarrow$ 240 GPU cores = 30 CPU cores (worth doing).

Backtracking - conclusion

- Thinking this way helped me develop a 25% faster C implementation.
- 8 GPU cores = 1 CPU core
- $\Rightarrow$ 240 GPU cores = 30 CPU cores (worth doing).
- Not the end of the story: additional algorithmic improvements over brute force backtracking possible.
- GPU can't compete without these improvements (better algorithms trump hardware).
- More work, and ingenuity, needed.

Where to next?

- Start programming, even if you can't think of a problem (yet).
- Different from CPU (parallelism, SIMT), will take time to become expert in thinking this way (I'm not).
- Will also give you a different way to consider problems.
- Help form a GPU community? Largest barrier to taking advantage of hardware and software improvements is lack of technical skill.
- See Melbourne University GPU Group http://groups.google.com.au/group/mugpug
- Dave Rawlinson speaking on June 19.