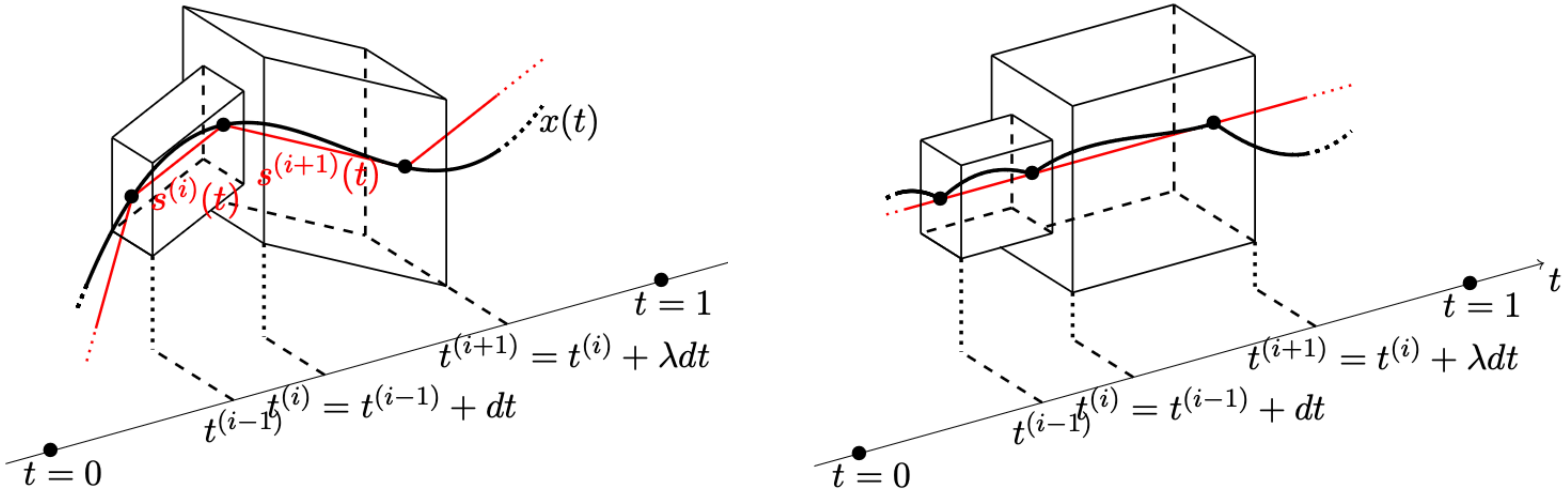
Certified homotopy tracking using the Krawczyk method

Joint work with Tim Duff



Kisun Lee (Clemson University) - kisunl@clemson.edu

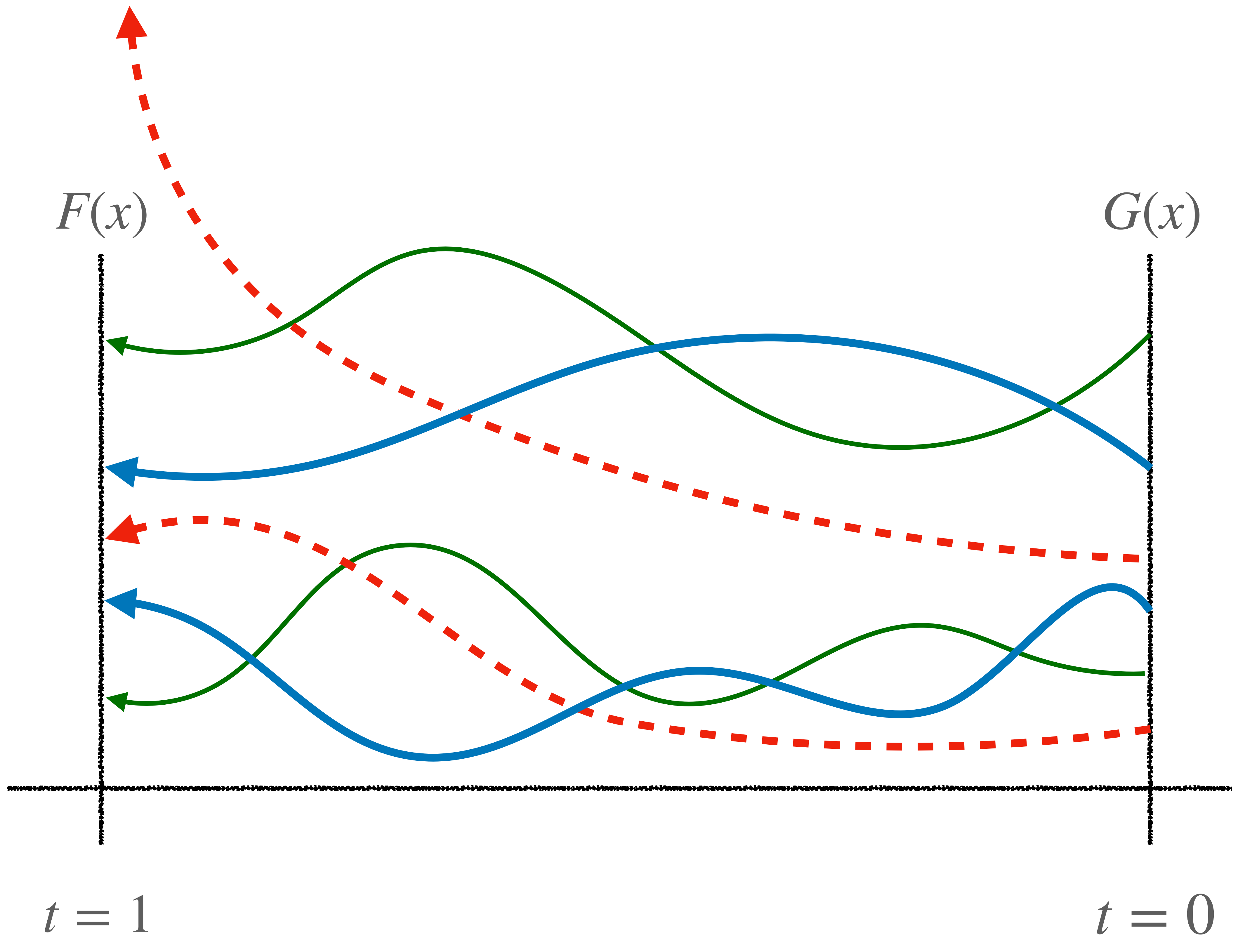
The International Symposium on Symbolic and Algebraic Computation (ISSAC) 2024

Homotopy continuation

Finding solutions by tracking homotopy

$$H(t, x) = (1 - t)\gamma G(x) + tF(x), \quad t \in [0,1]$$

Solve F (target system) by constructing a homotopy with G (start system) whose solutions are known



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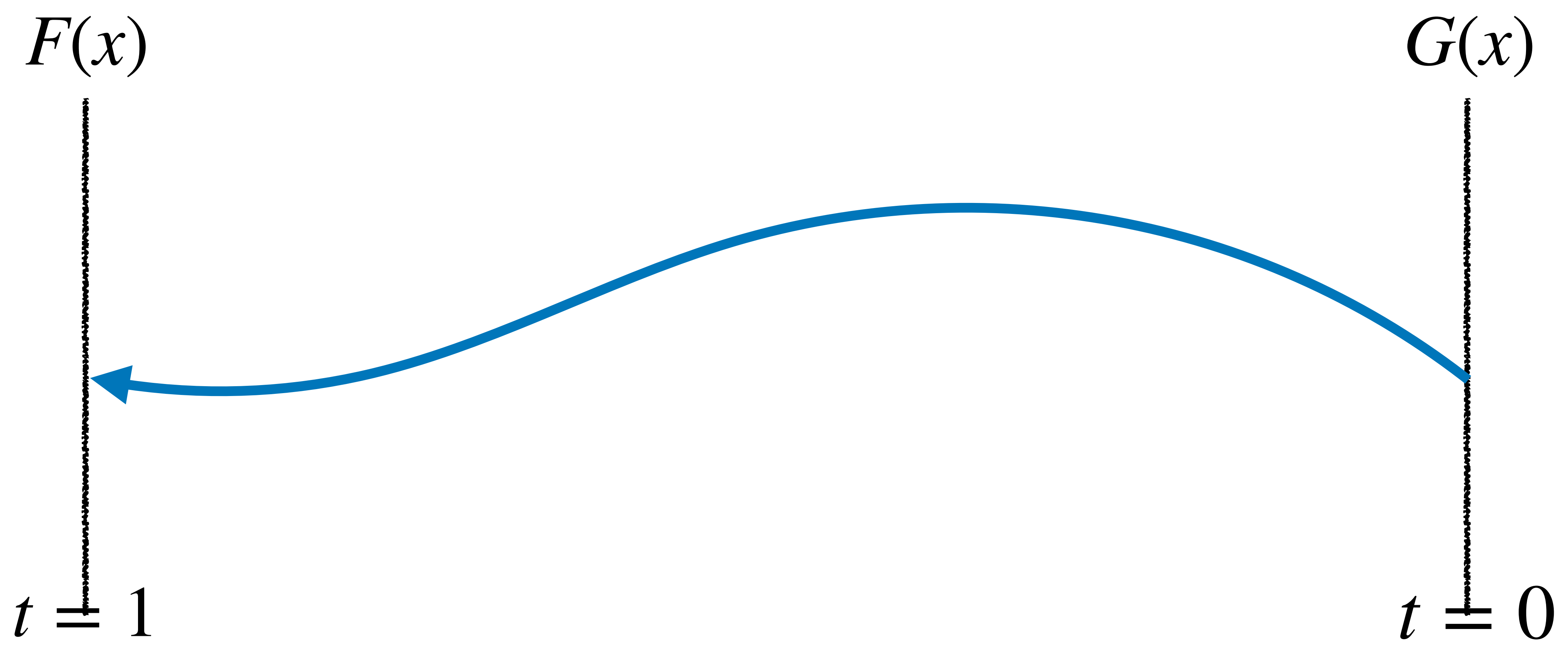


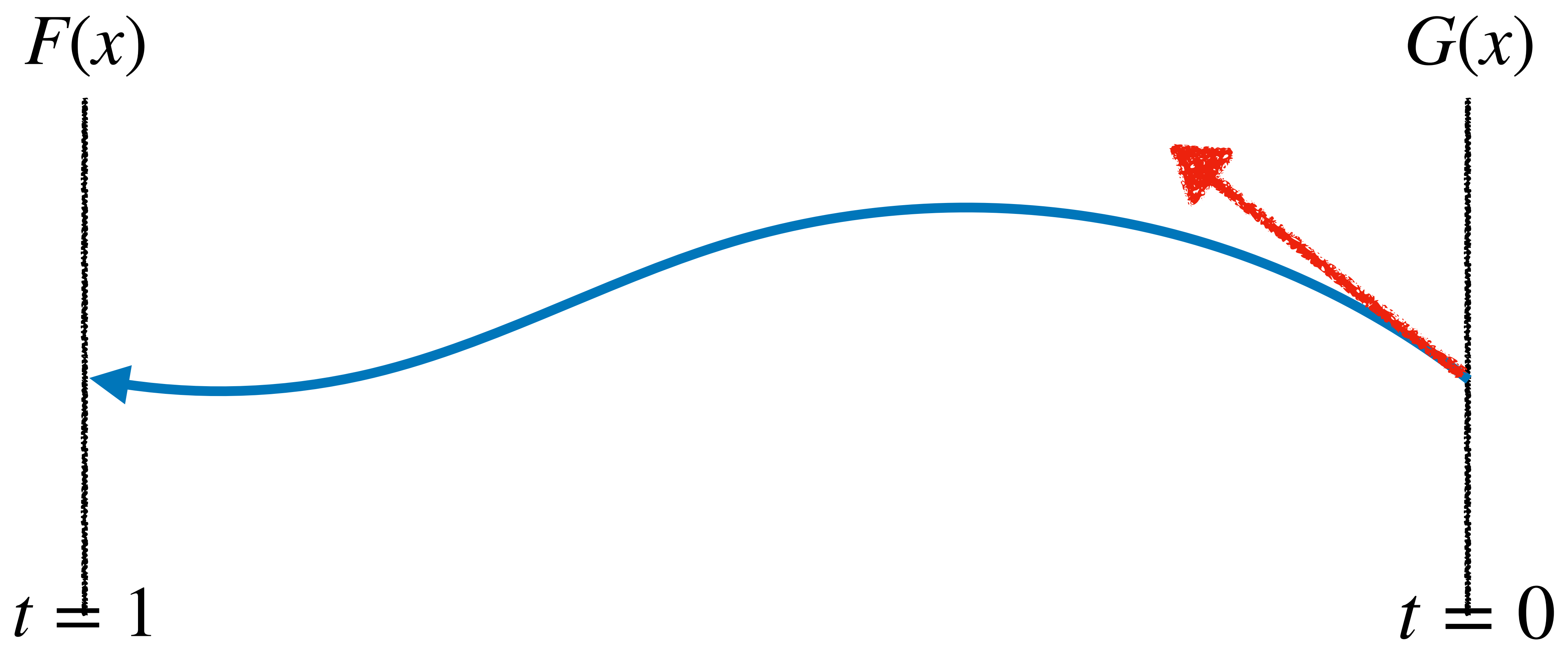
Homotopy continuation

- Predictor step

  Solving ODE

$$x'(t_0) = \left(\partial_x F_t\right)^{-1} \partial_t F_t \Big|_{x=x_0, t=t_0}$$

  to get the prediction.



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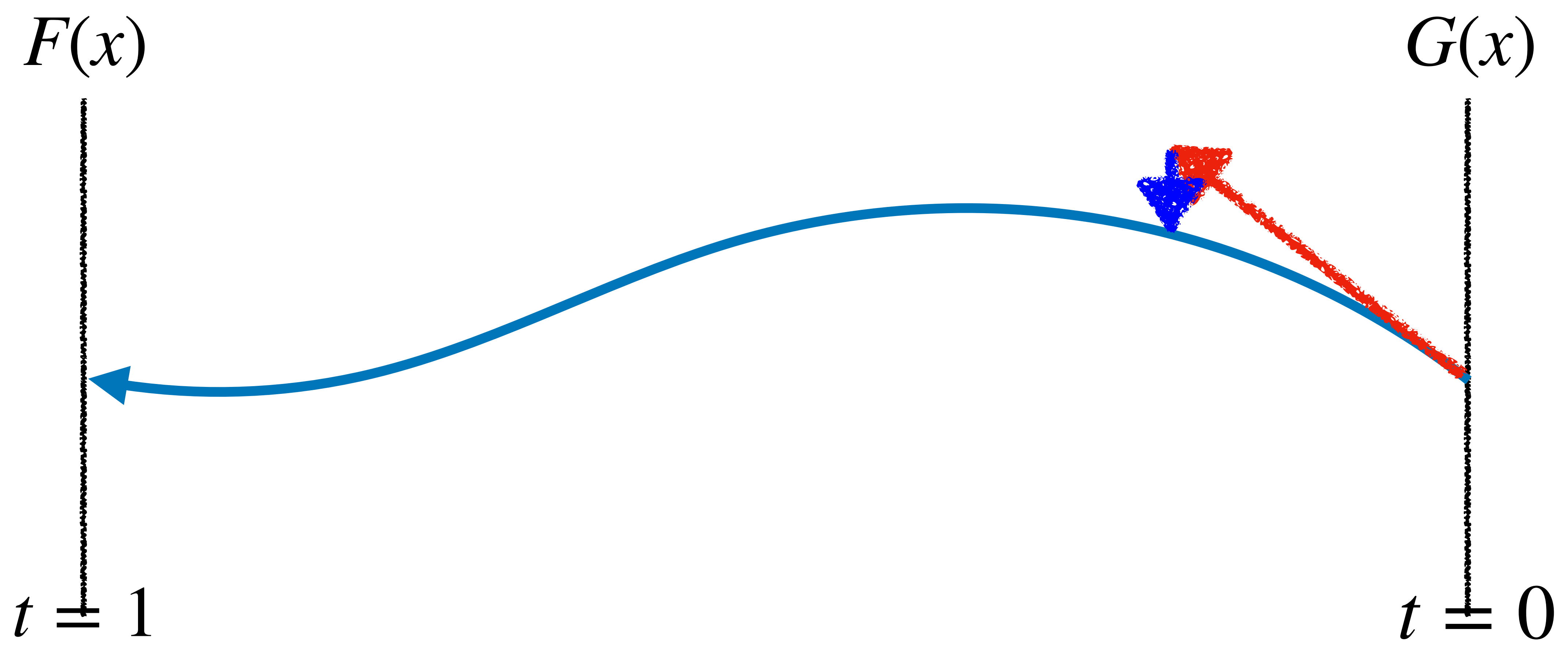

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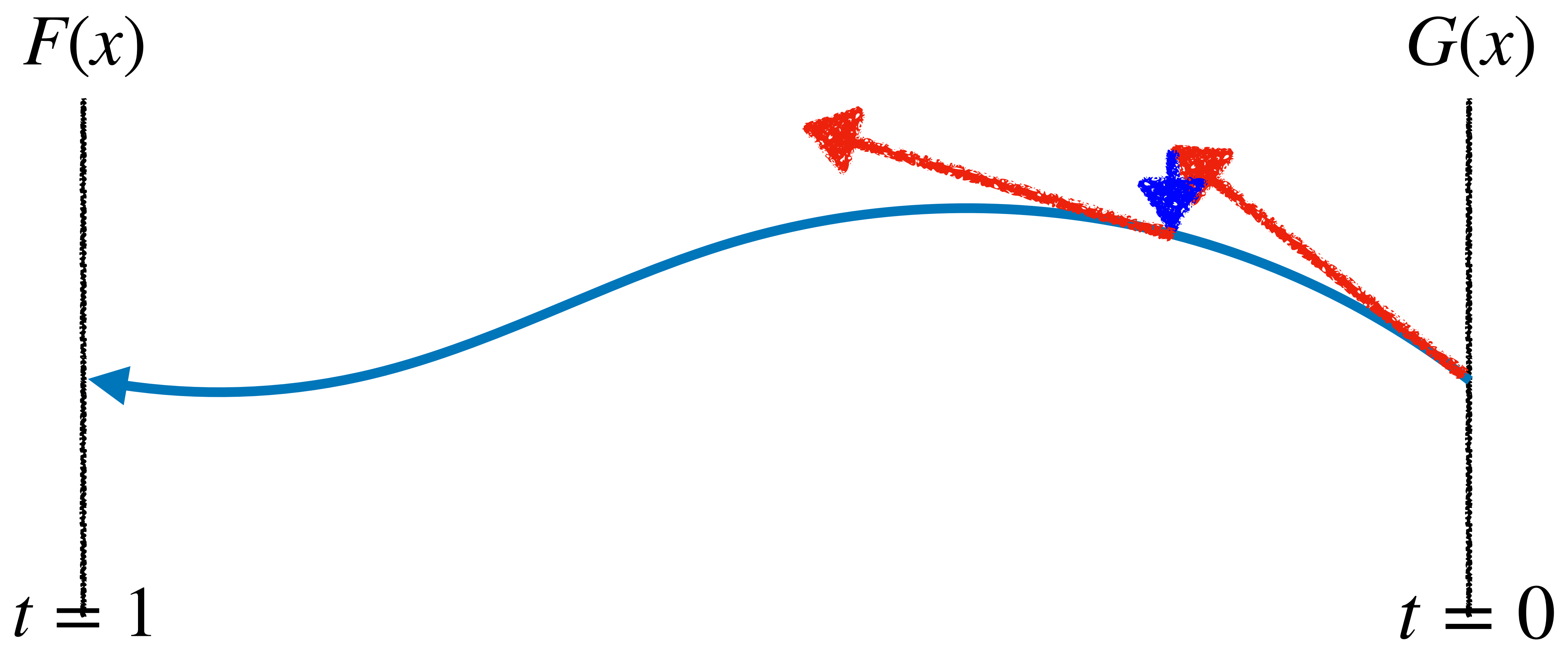

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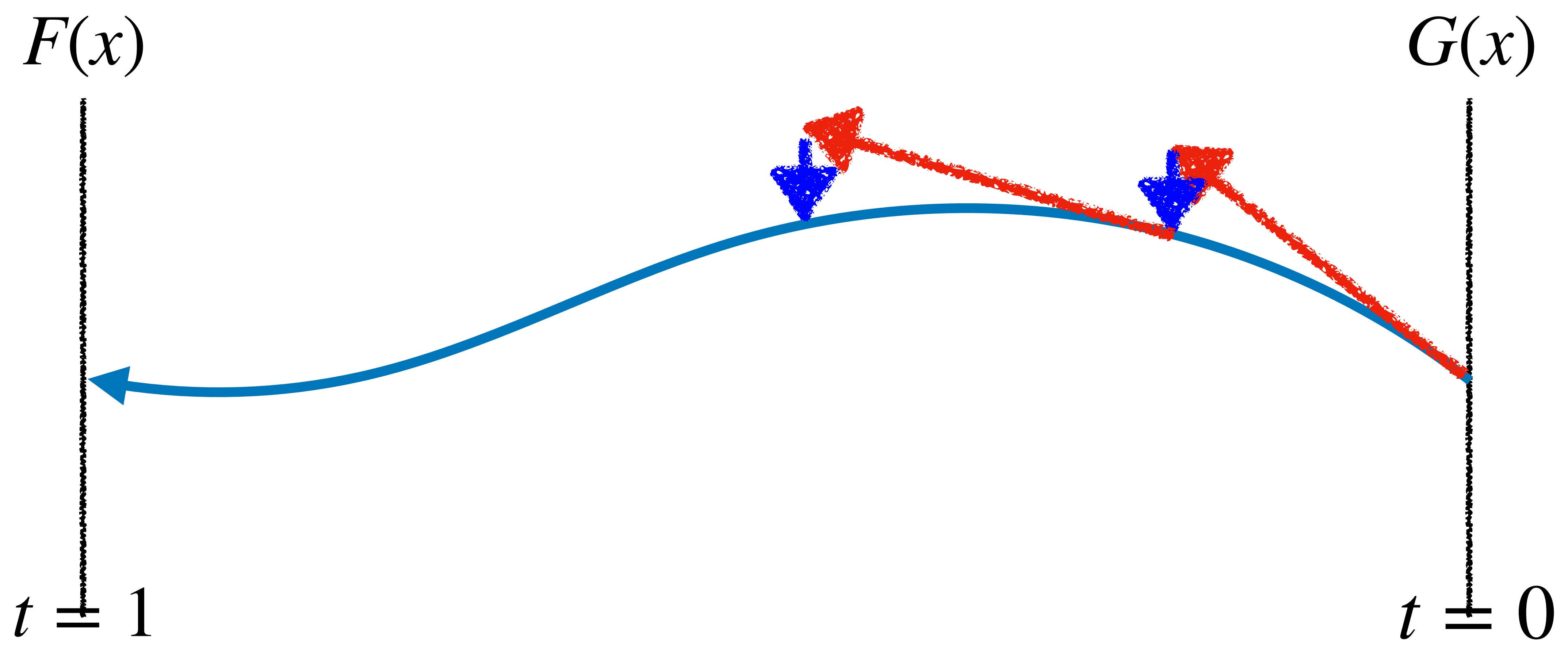

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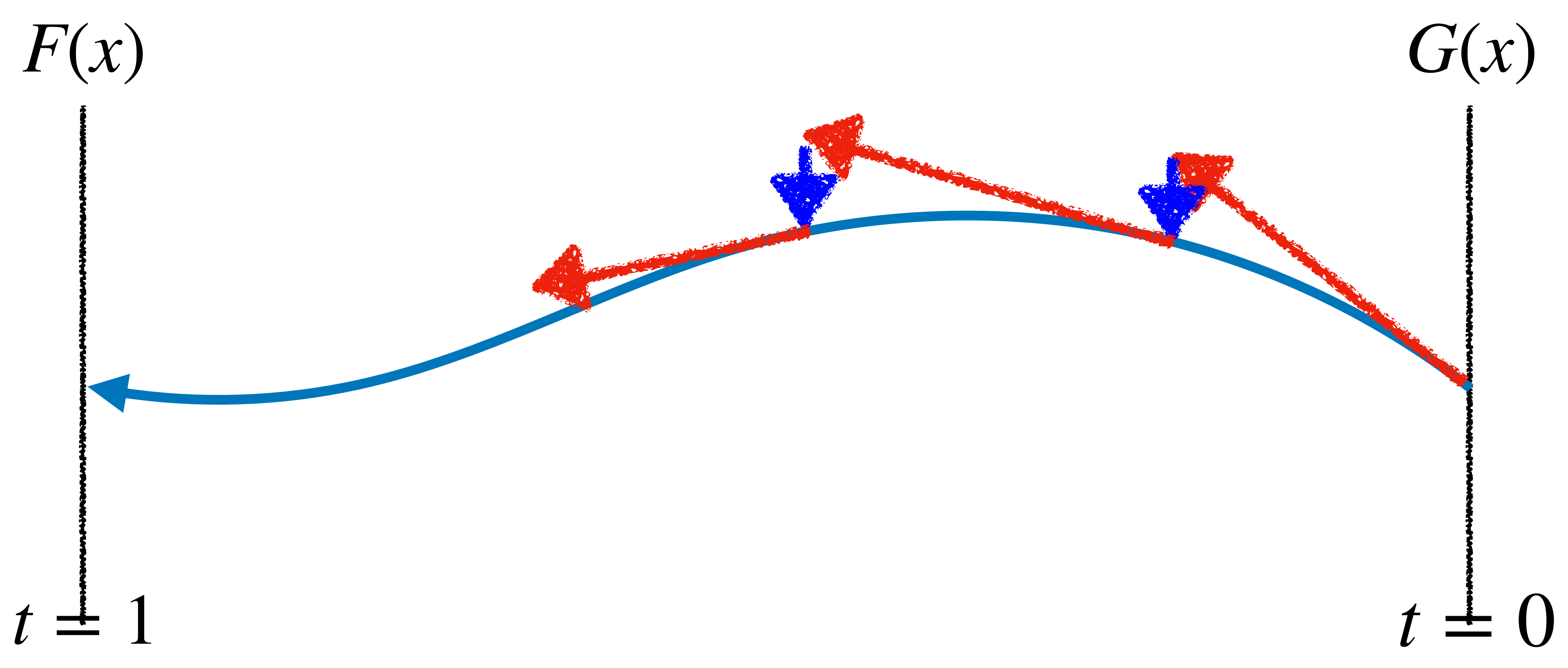

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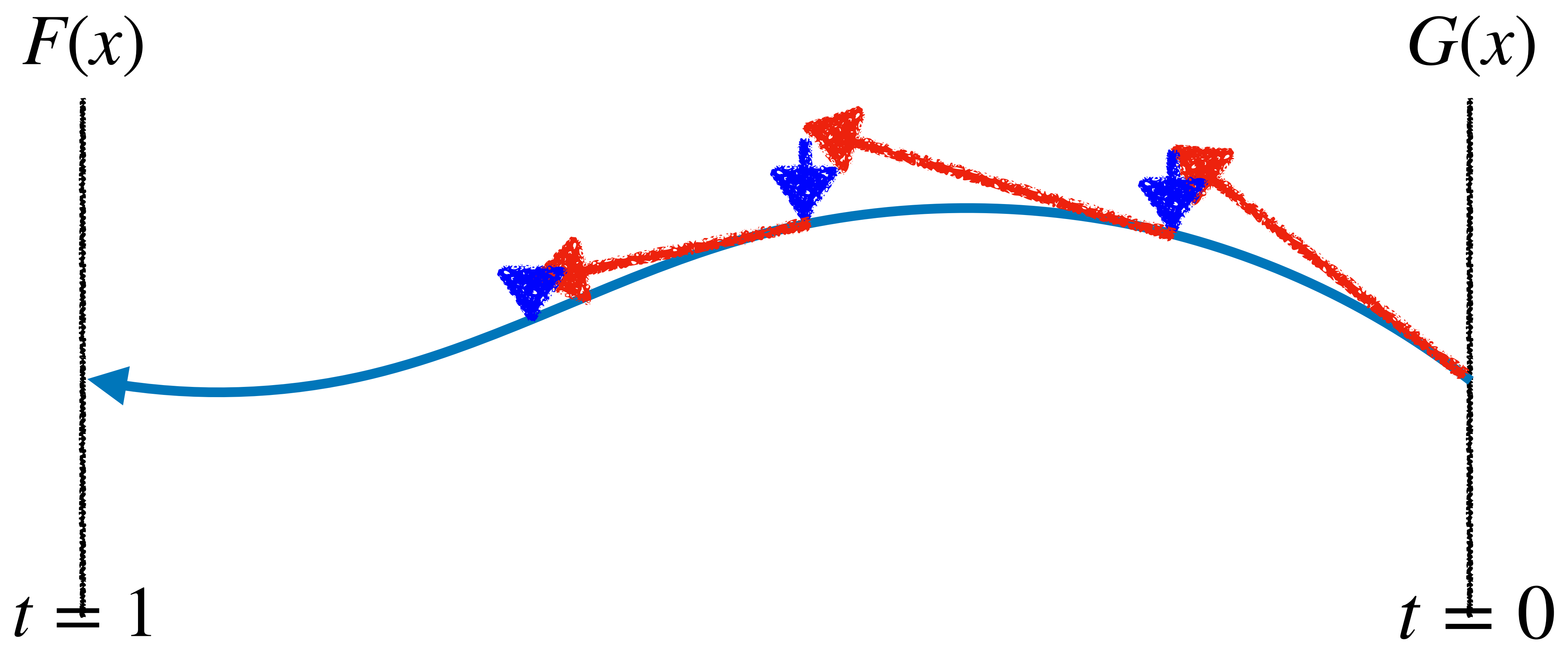

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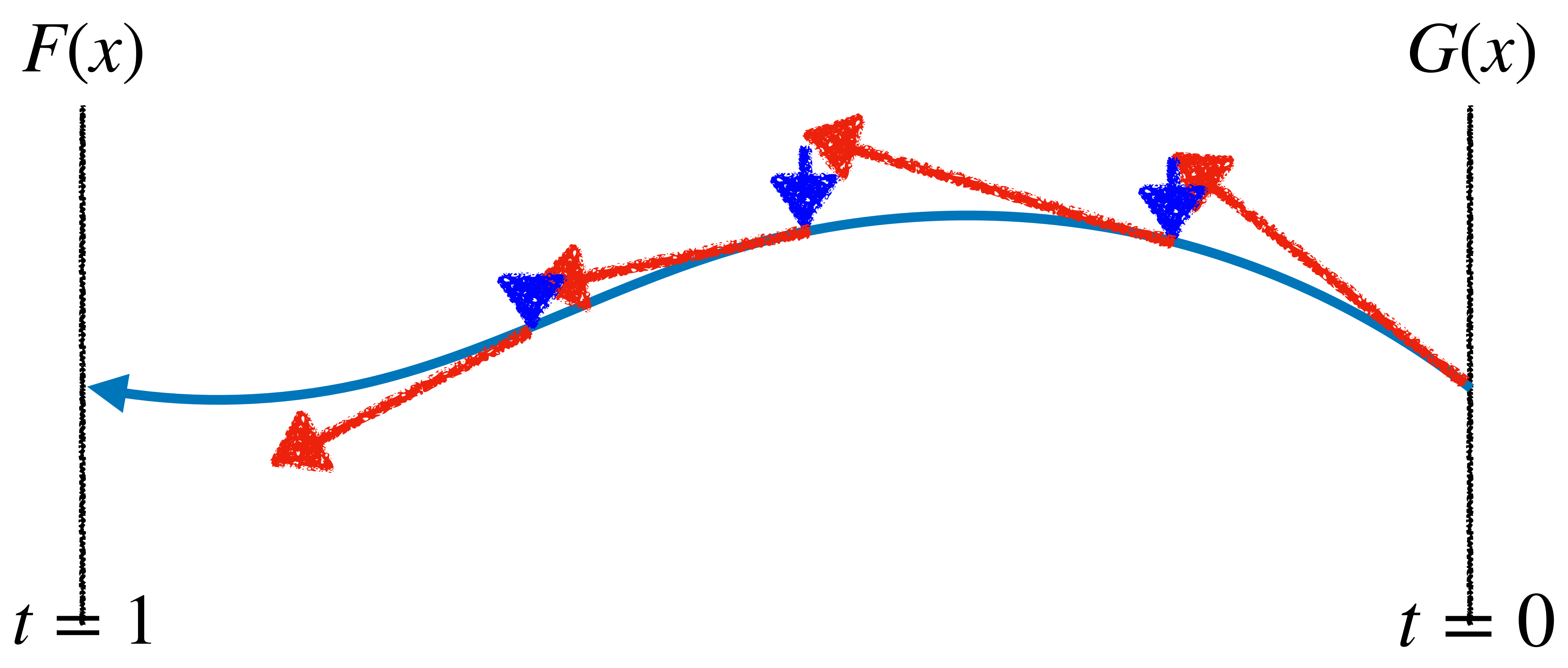

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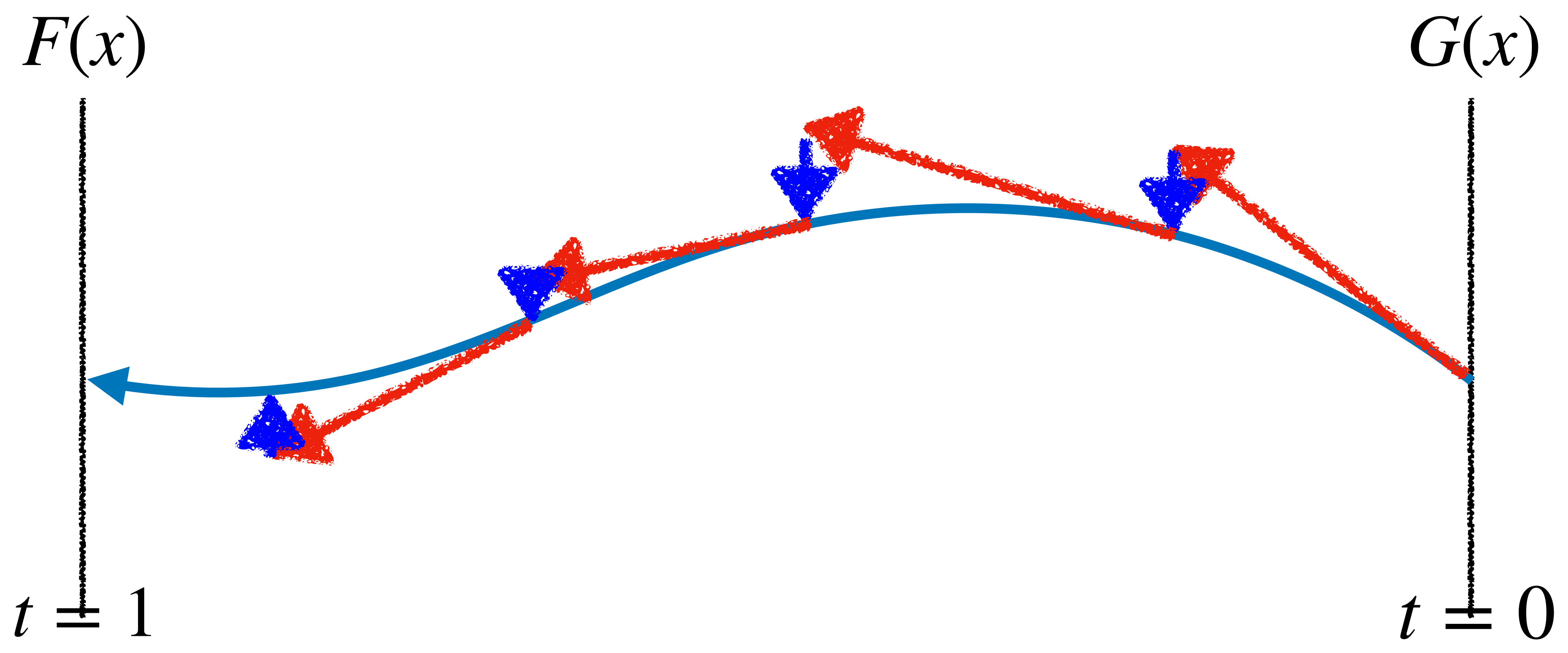

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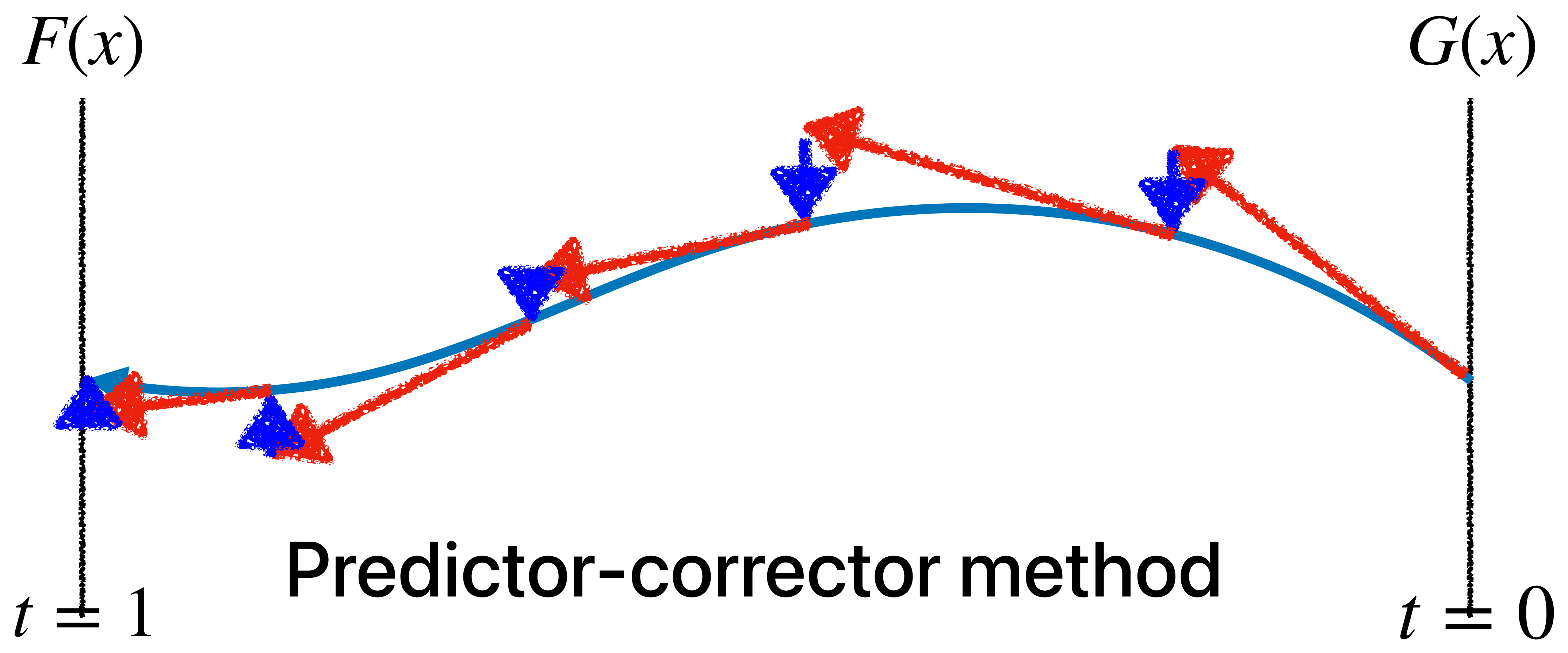

Predictor-corrector method

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(*a posteriori* certification)

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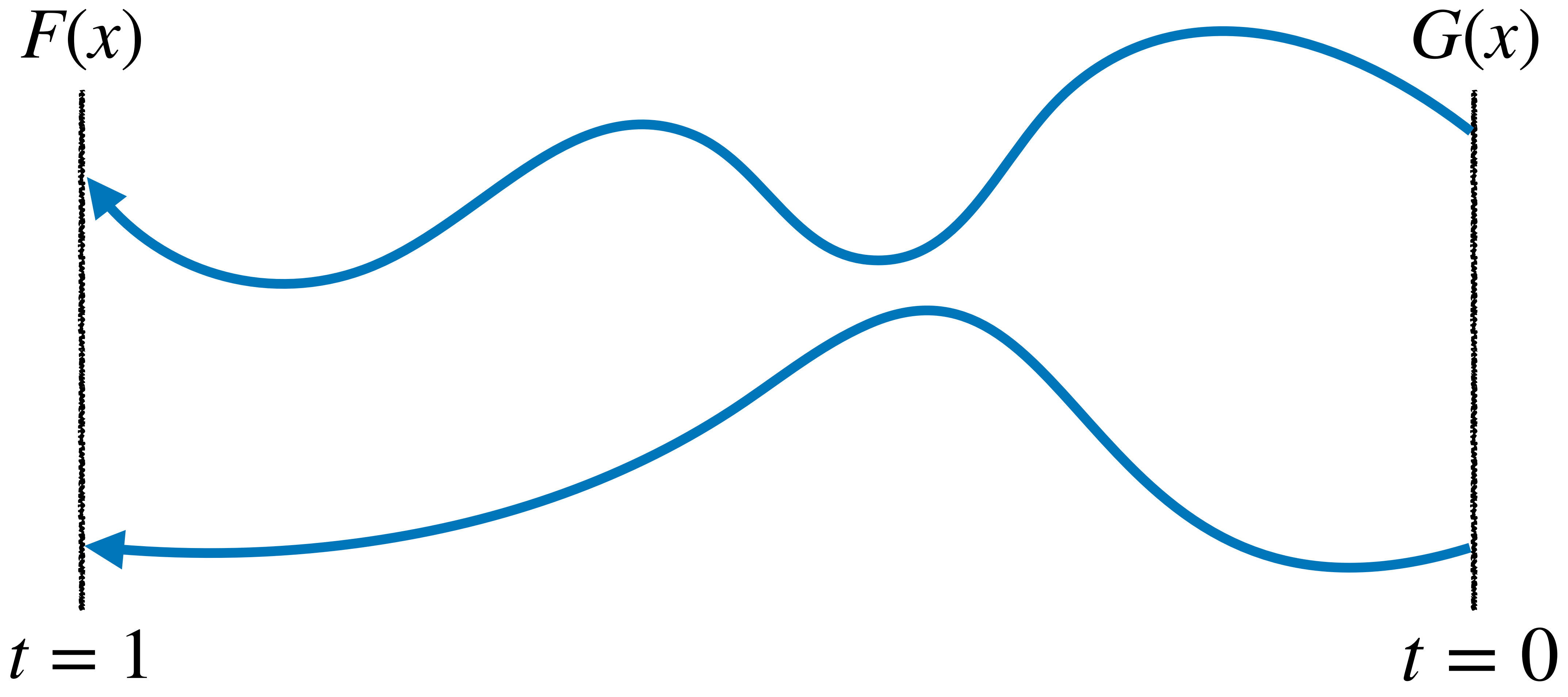
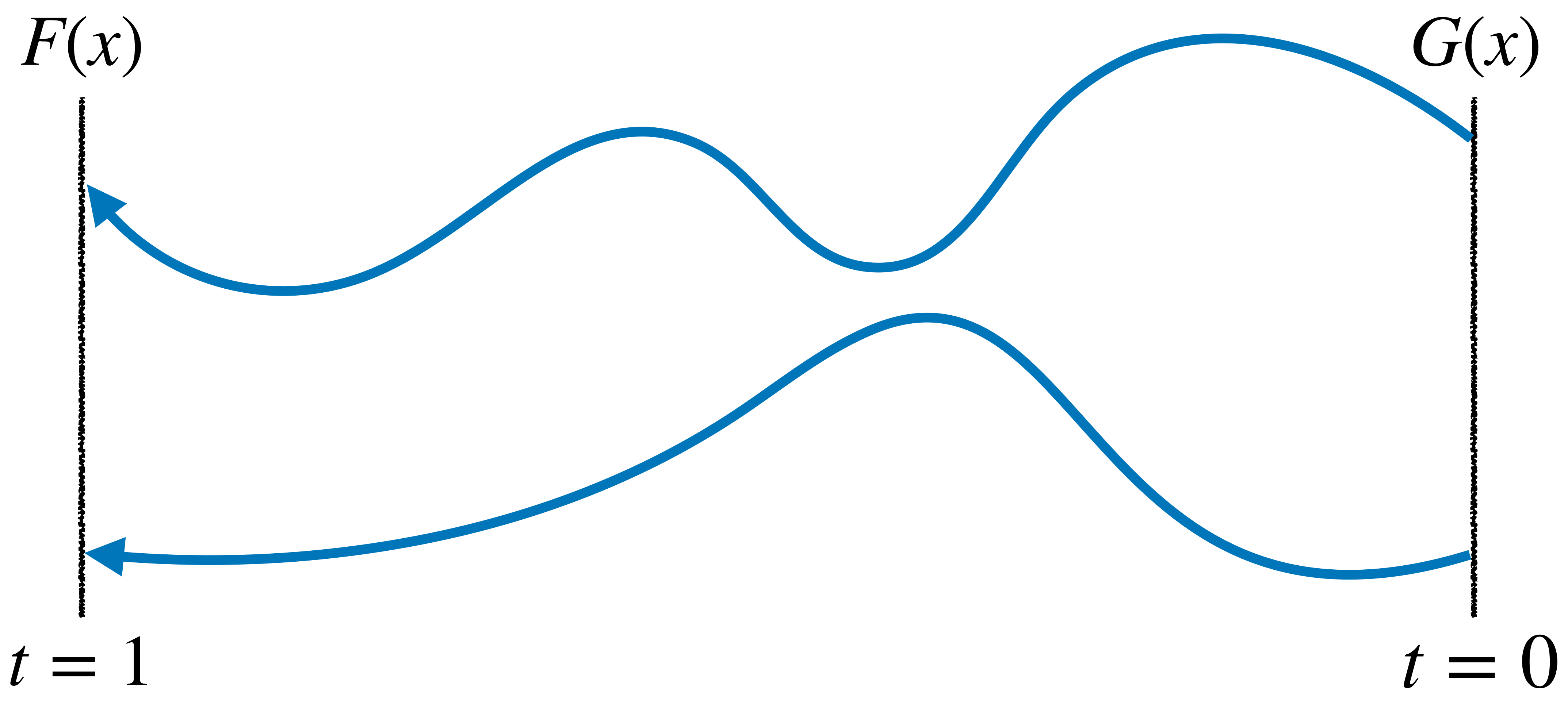
- In some algorithms or computations (e.g. monodromy or Galois group computation), the order and correspondence of solutions are important

Why certified homotopy tracking?



Why certified homotopy tracking?

- Scenario 1) Path jumping



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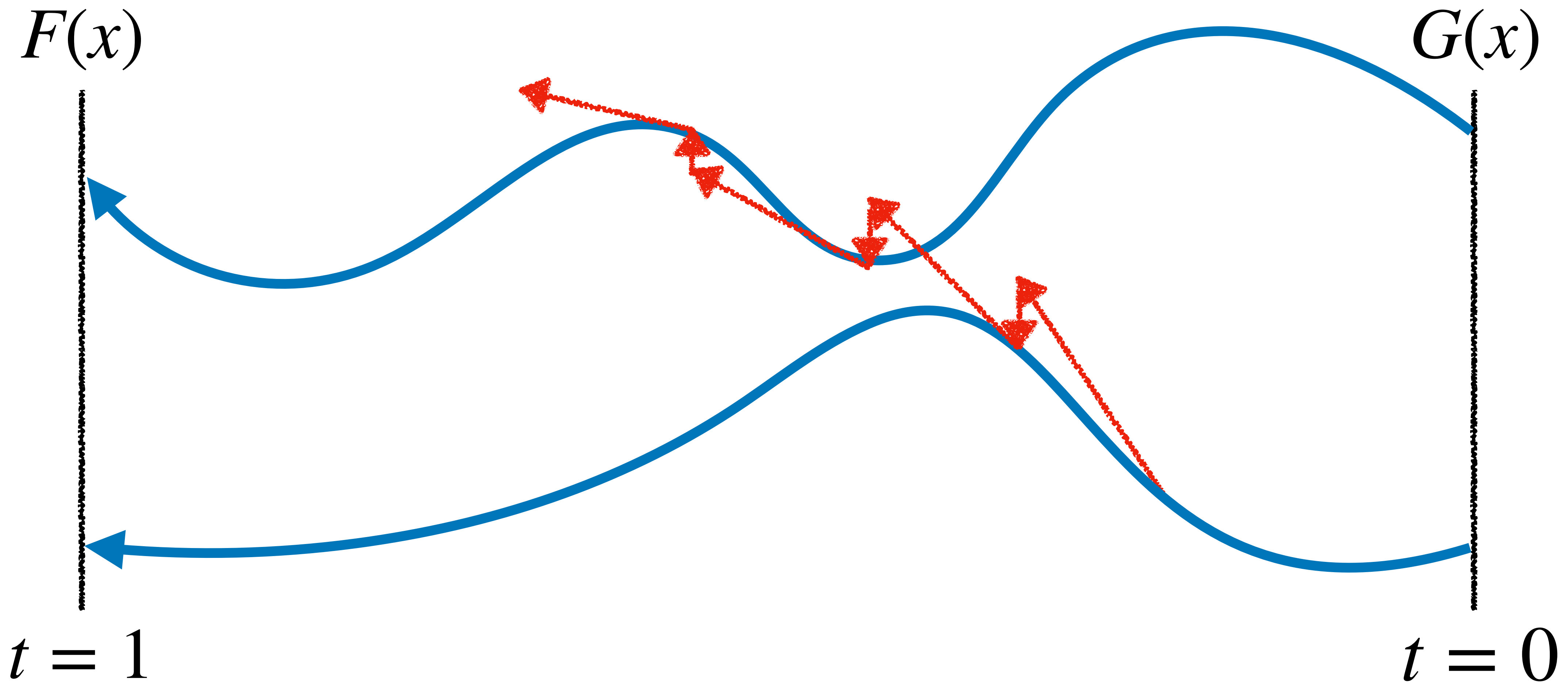

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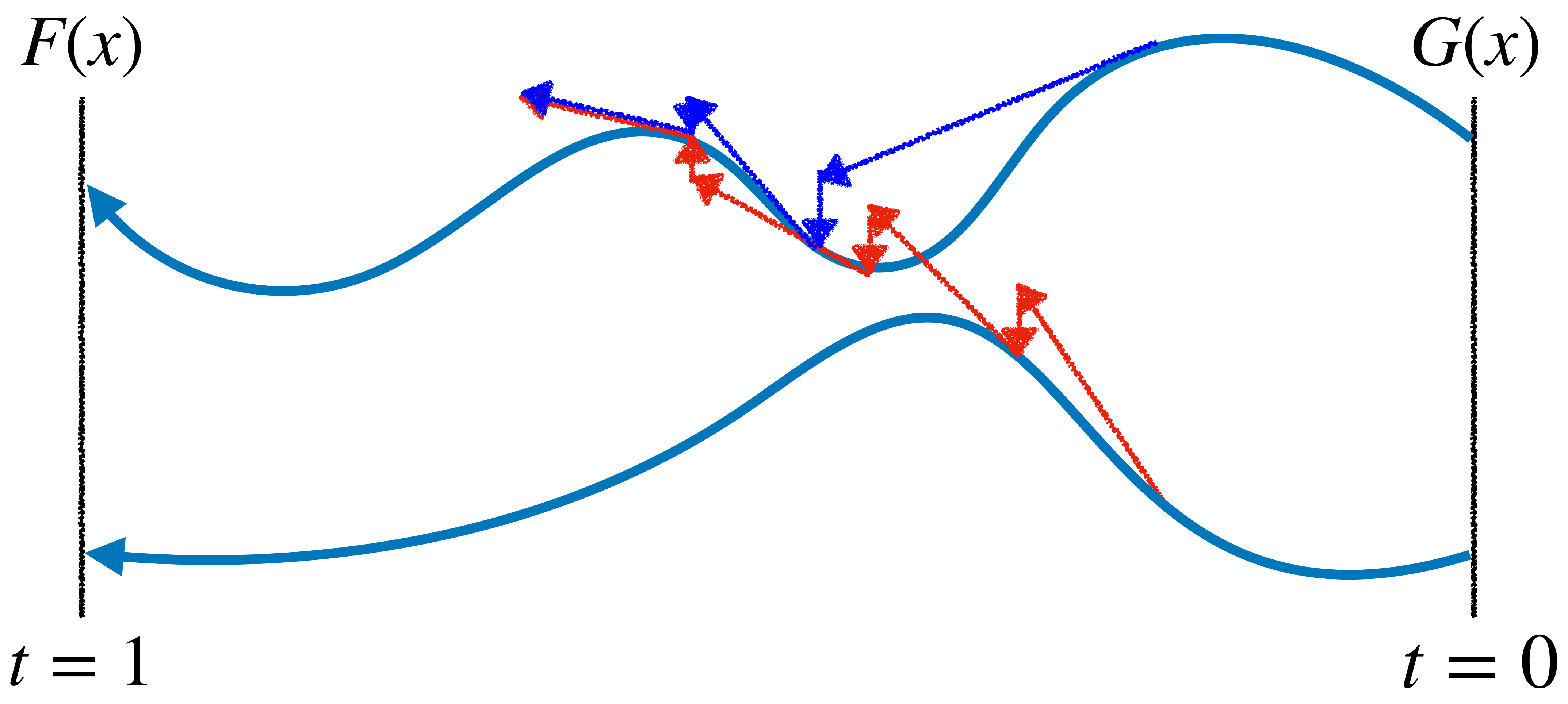
Path jumping may result in false multiple solutions and a lost solution.



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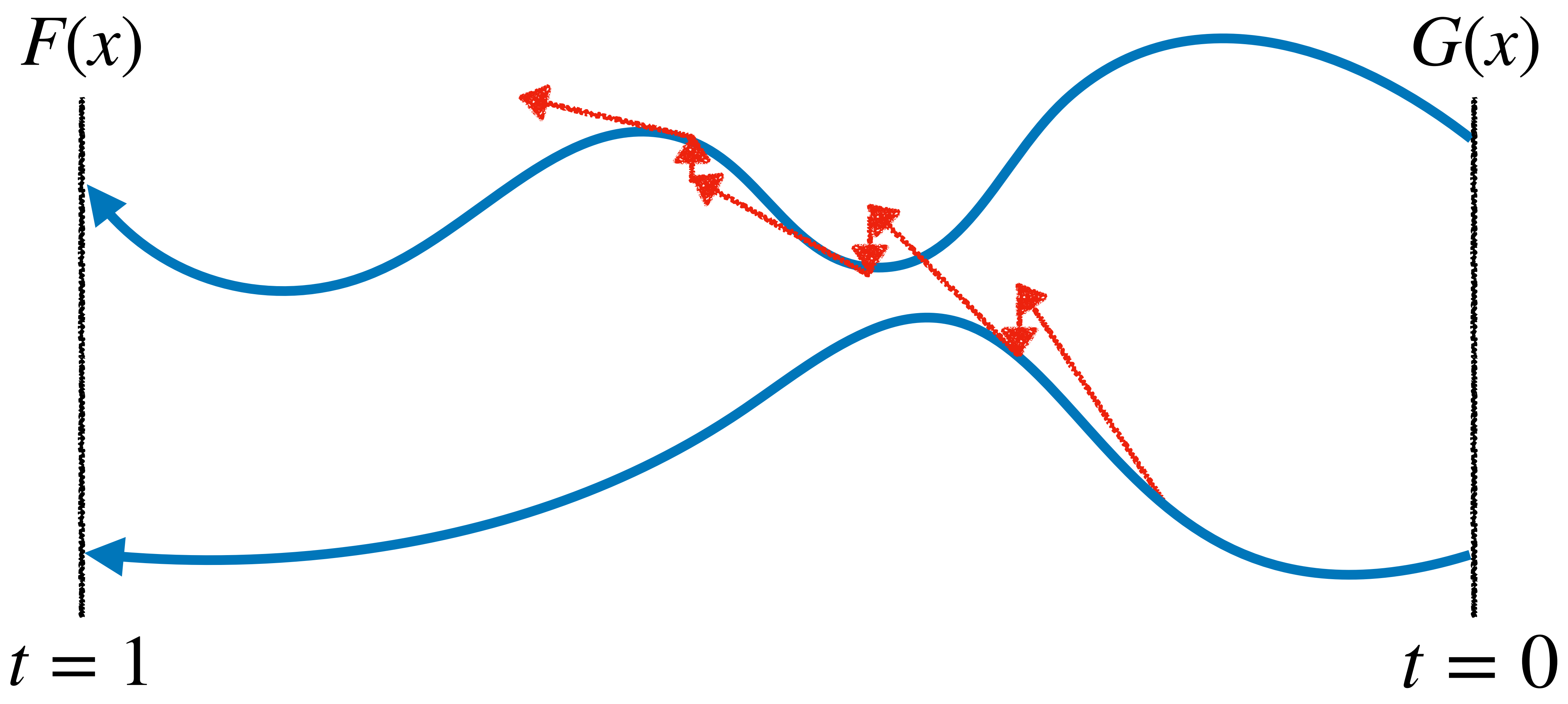

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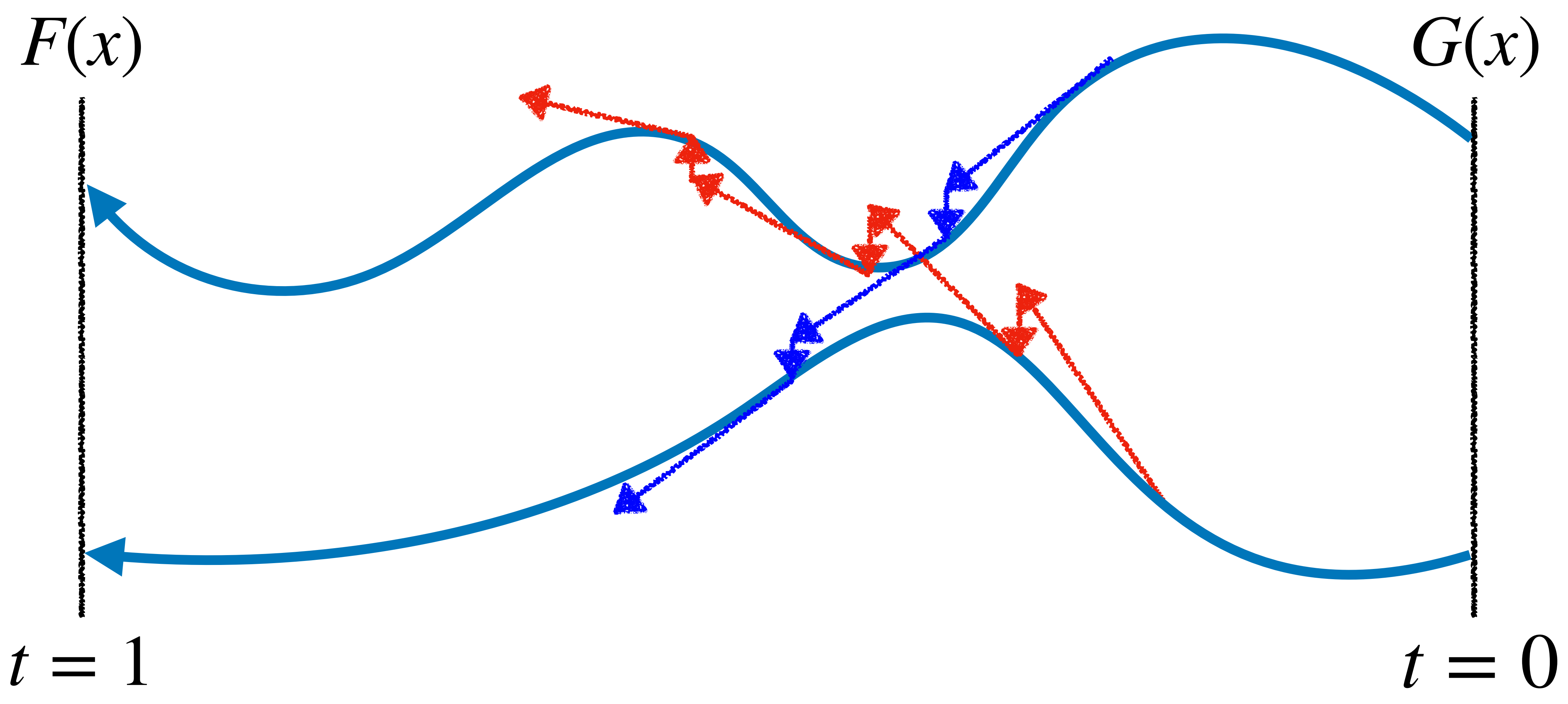

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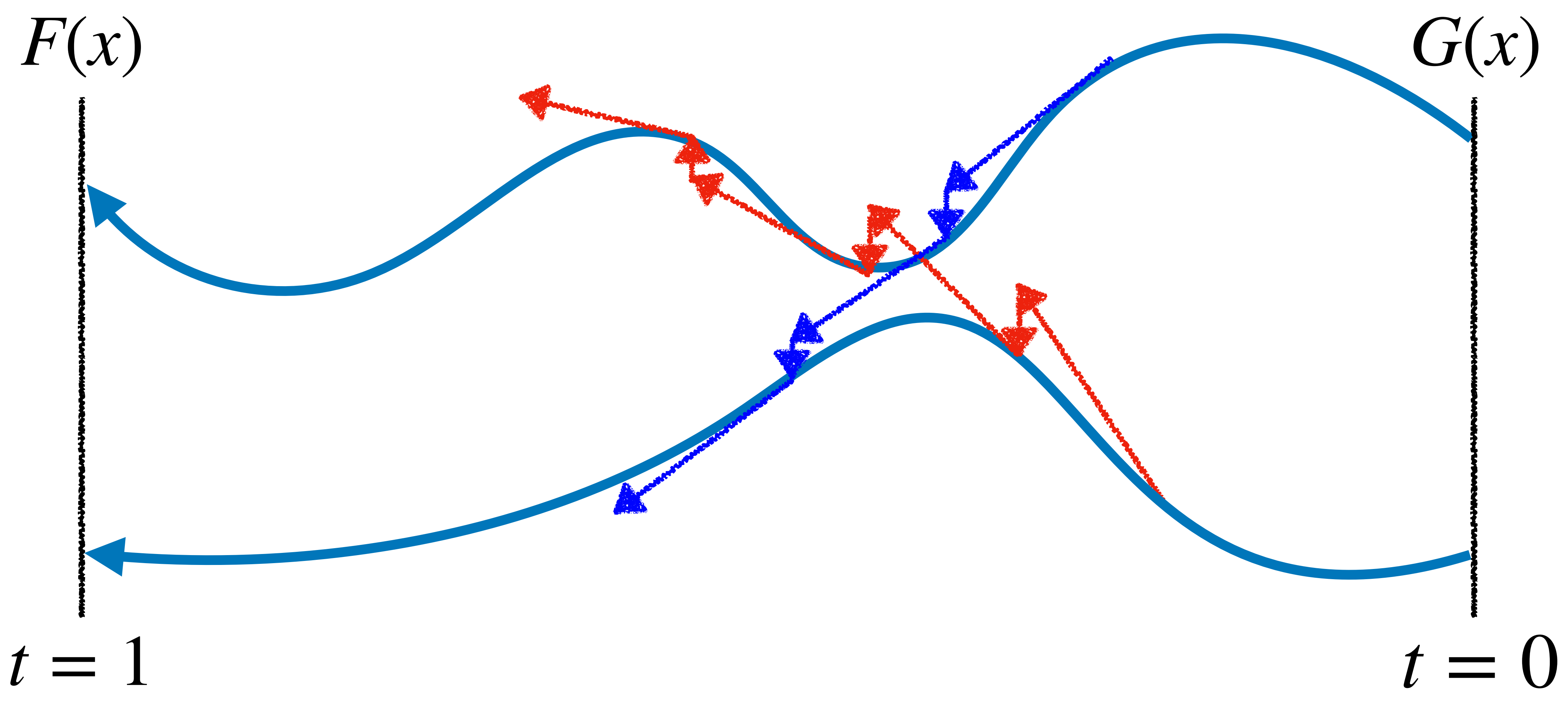

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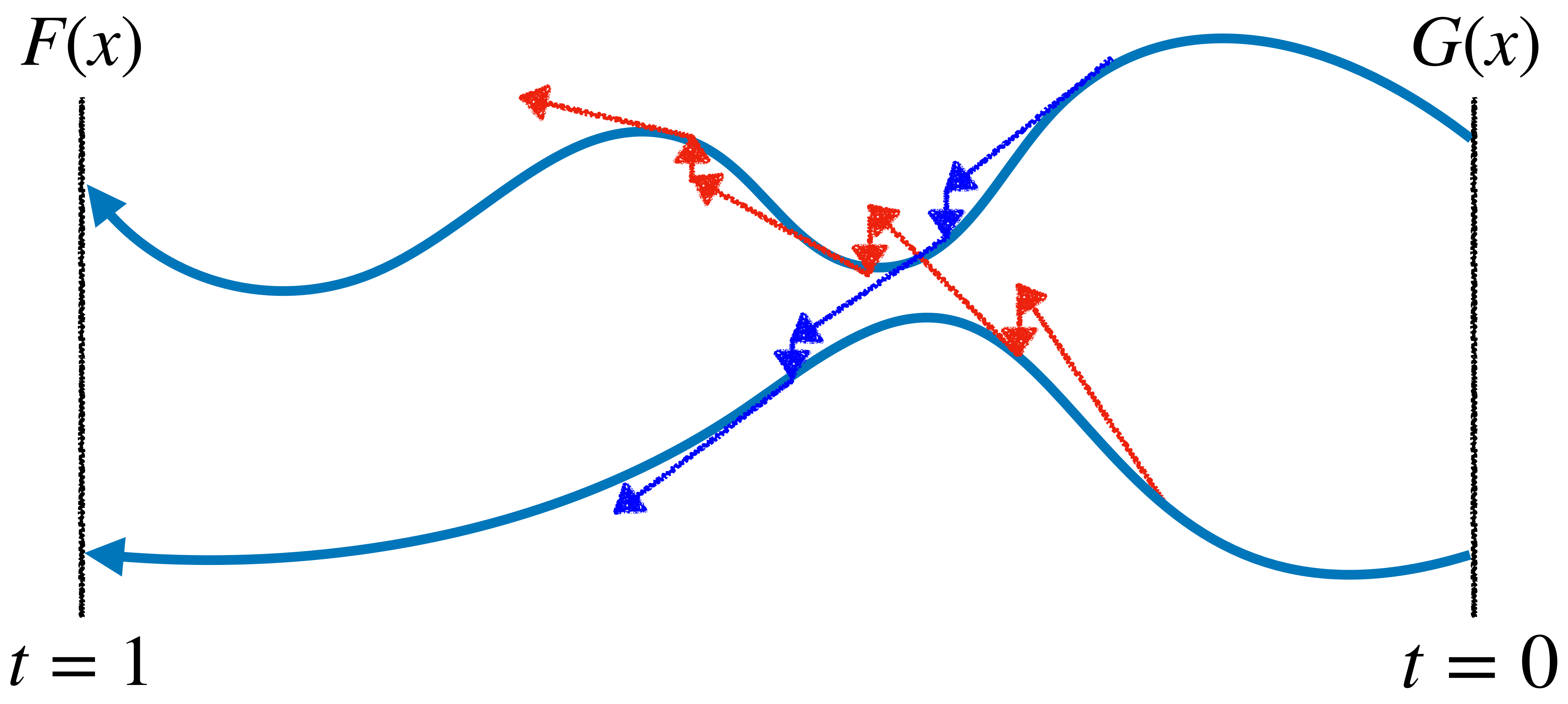
- Scenario 2) Path crossing

  Path crossing loses correspondence between the start solution and the target solution.

  Crucial for some algorithms (e.g. monodromy), and hard to detect.



Why certified homotopy tracking?

- Certified homotopy guarantees tracking the same path from start to finish without jumping or crossing

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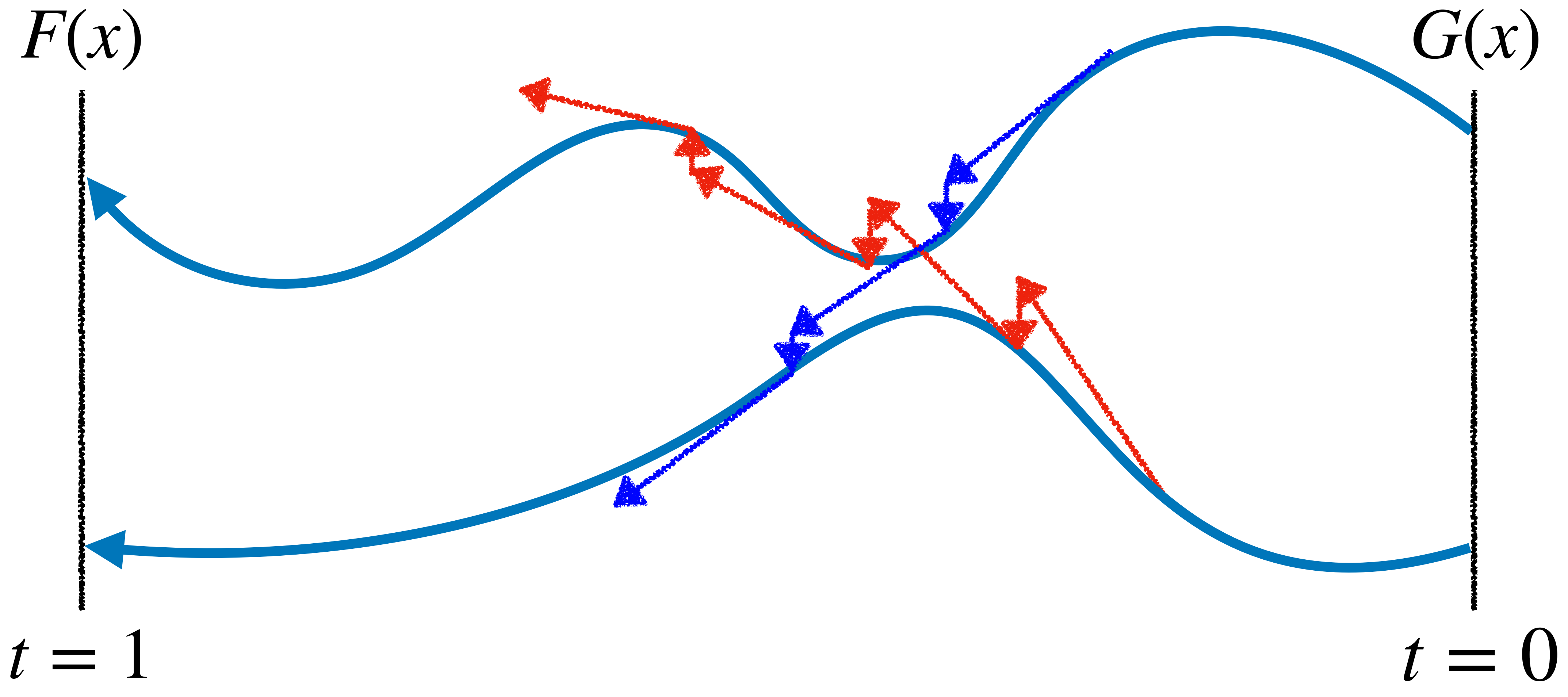

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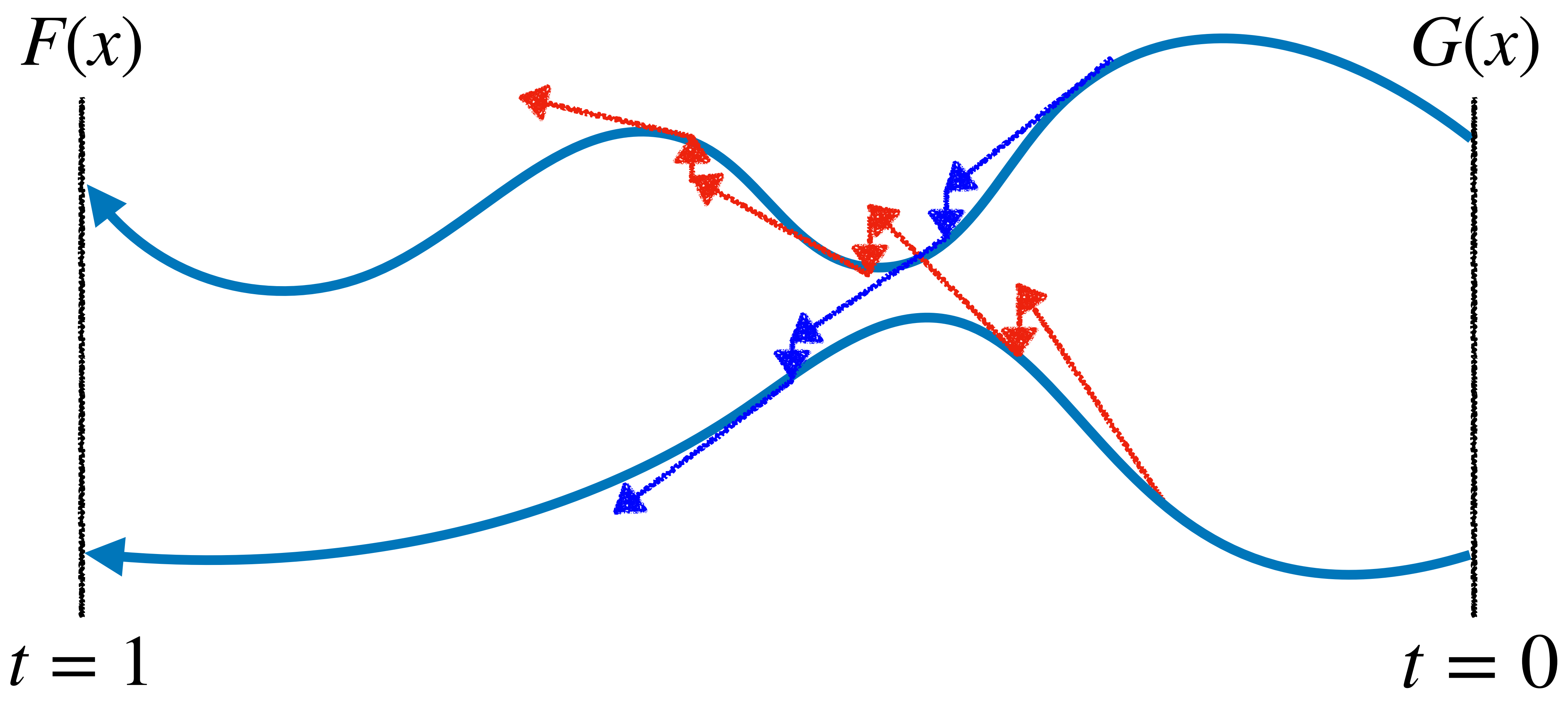

Interval arithmetic

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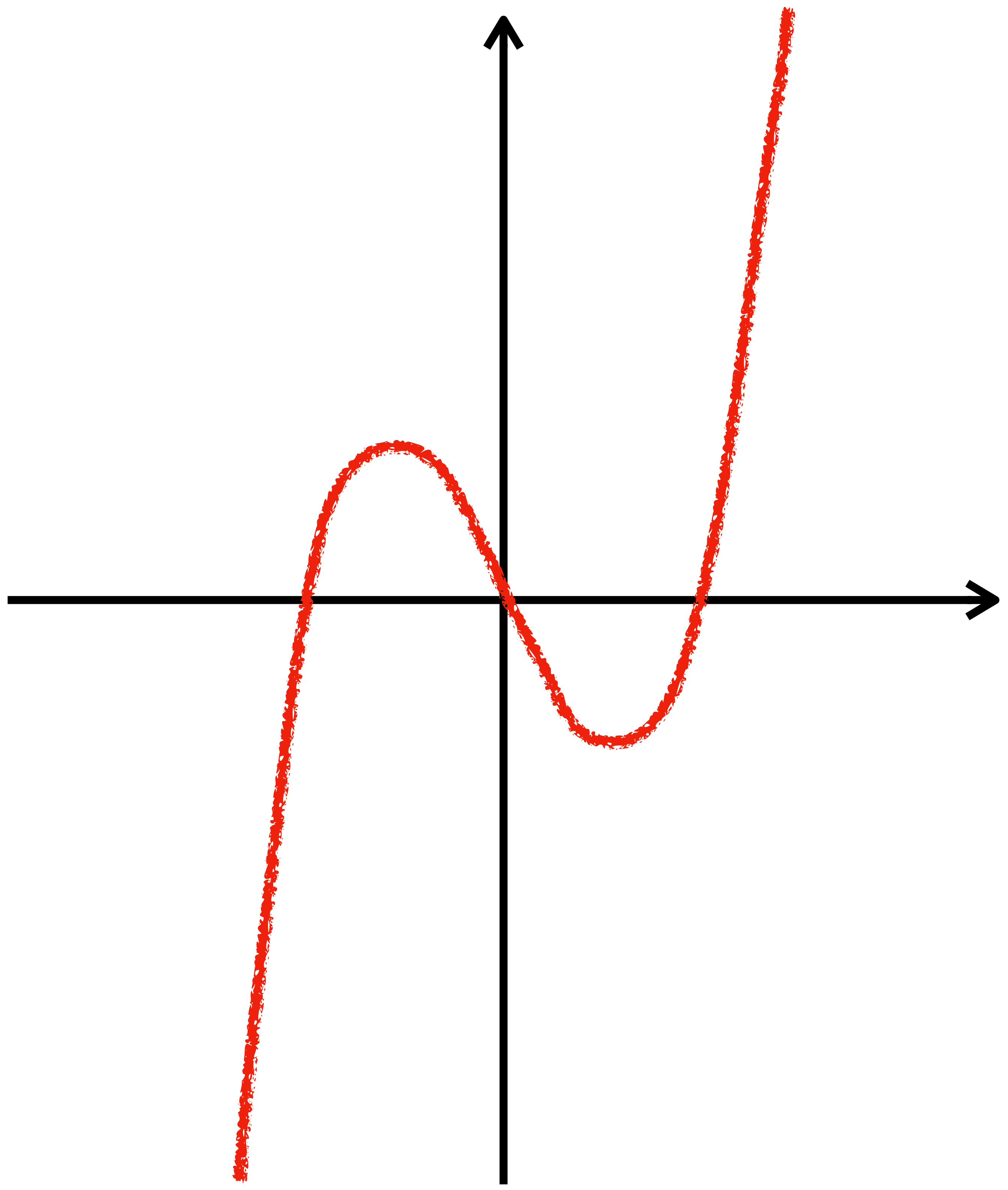

Interval arithmetic

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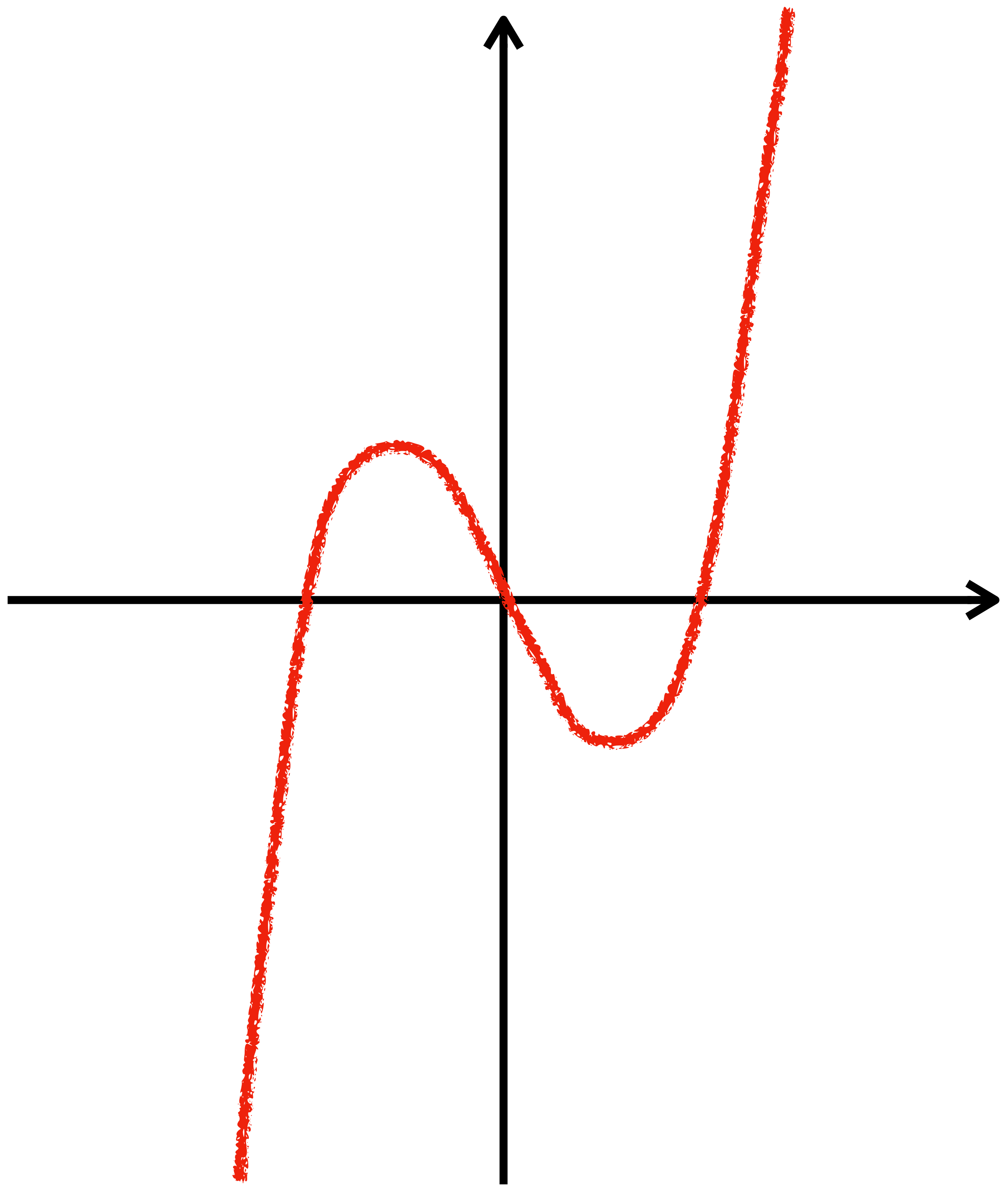
  for an arithmetic operator $\odot$, define

  $$[a, b] \odot [c, d] = \{x \odot y \mid x \in [a, b], y \in [c, d]\}$$

  for conservative and guaranteed computation



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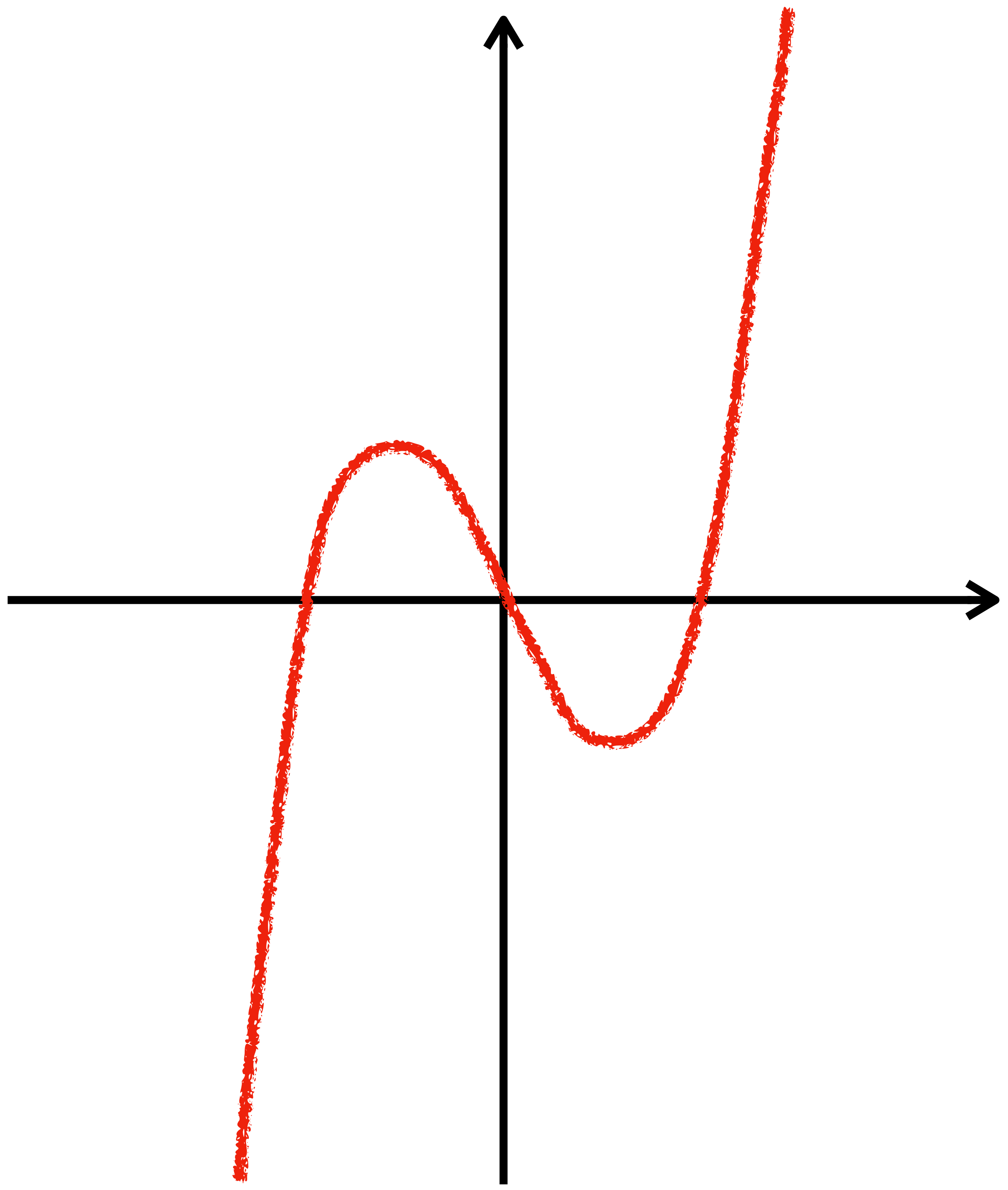
  ex) $f(x) = x^3 - 2x$ on $x \in [-2,2]$.

  Then, $f(x) \in [-2,2]^3 - 2 \cdot [-2,2] = [-12,12]$

  (much larger than the actual image $[-4,4]$)



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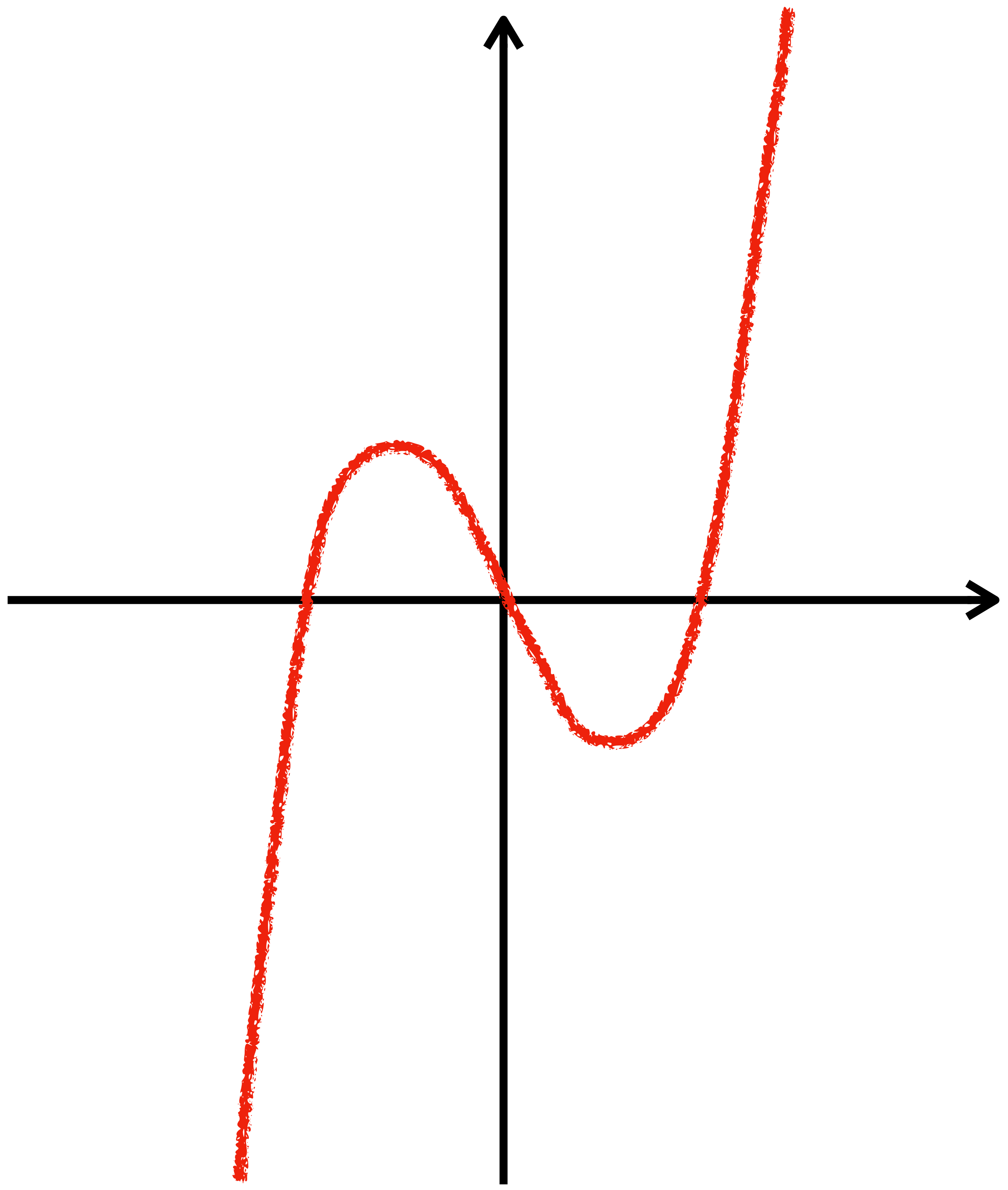
  If a certain property is true for $[-12,12]$,

  then it is true for any point in the actual image of $f(x)$ over $[-2,2]$



Krawczyk method

Combine interval arithmetic and Newton's method. Define the **Krawczyk operator**

$$K_{x,Y}(I) = x - YF(x) + \left(Id - Y \square \frac{dF}{dx}(I) \right)(I - x)$$

F : a square differentiable system of polynomial equations

I : an interval

$\square F(I) \supset \{F(x) \mid x \in I\}$: an interval extension of F over I

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2. If I has a solution and $\sqrt{2}\|Id - Y\Box\frac{dF}{dx}(I)\| < 1$, then there is a solution of F in I, and it is unique (**uniqueness** of a solution)

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Therefore, I contains a root of F (which is $(\sqrt{2}, 1)$), uniquely.

Q. Can we use the Krawczyk method for certified homotopy tracking?

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A. Consider the Krawczyk method **“for a system with parameters”**

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Combine interval arithmetic and Newton's method.
Define the **Krawczyk operator**

$$K_{x,Y}(I,T) = x - Y \square H(x,T) + \left(Id - Y \square \frac{\partial H(I,T)}{\partial x} \right)(I - x)\,.$$

$H(x,t)$: a homotopy with a parameter t from $\mathbb{C}^n \times [0,1]$ to $\mathbb{C}^n$

(e.g. $H(x,t) = t\gamma G(x) + (1-t)F(x)$)

I : an interval

T : an interval contained in $[0,1]$

Krawczyk method

Combine interval arithmetic and Newton's method. Define the **Krawczyk operator**

$$K_{x,Y}(I,T) = x - Y \,\square\, H(x,T) + \left(Id - Y \,\square\, \frac{\partial H(I,T)}{\partial x}\right)(I - x)\,.$$

$H(x,t)$: a homotopy with a parameter t from $\mathbb{C}^n \times [0,1]$ to $\mathbb{C}^n$

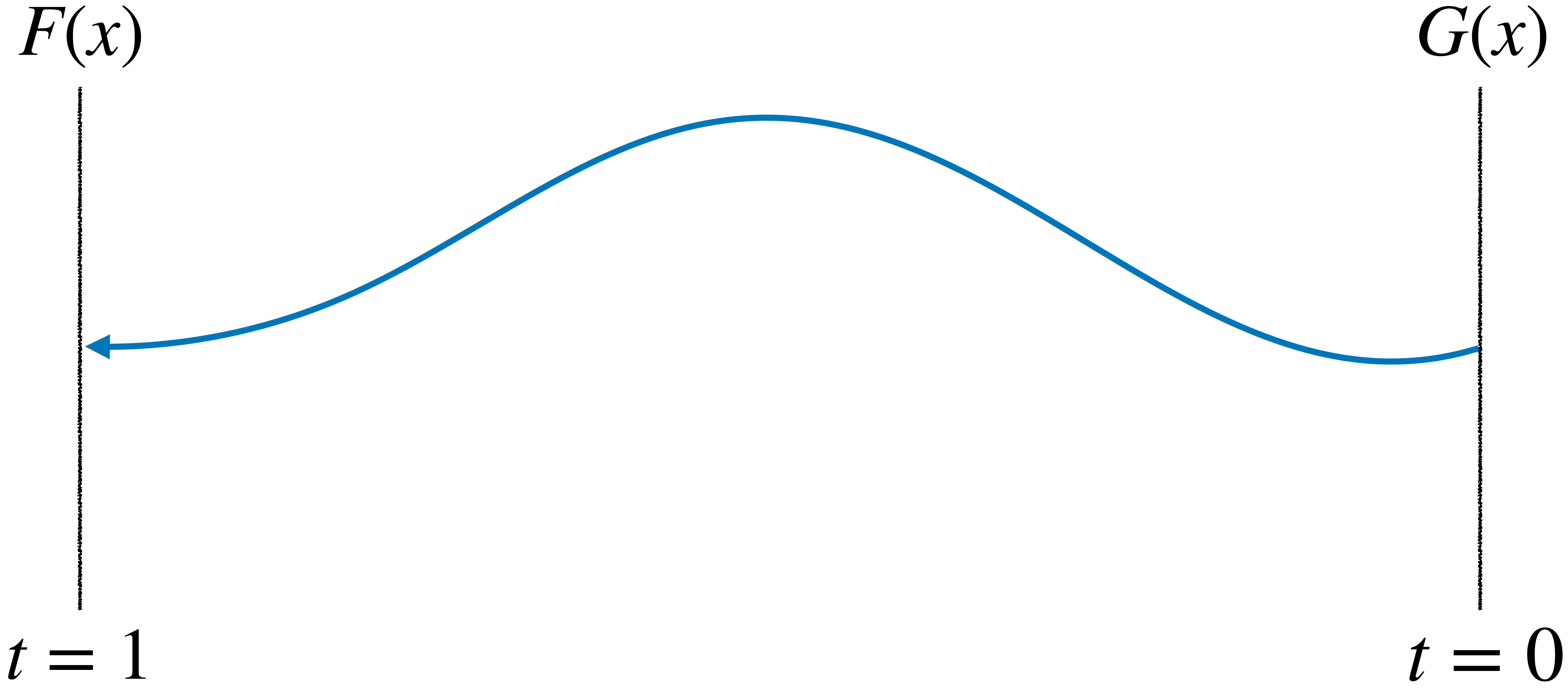
(e.g. $H(x,t) = t\gamma G(x) + (1-t)F(x)$)

I : an interval

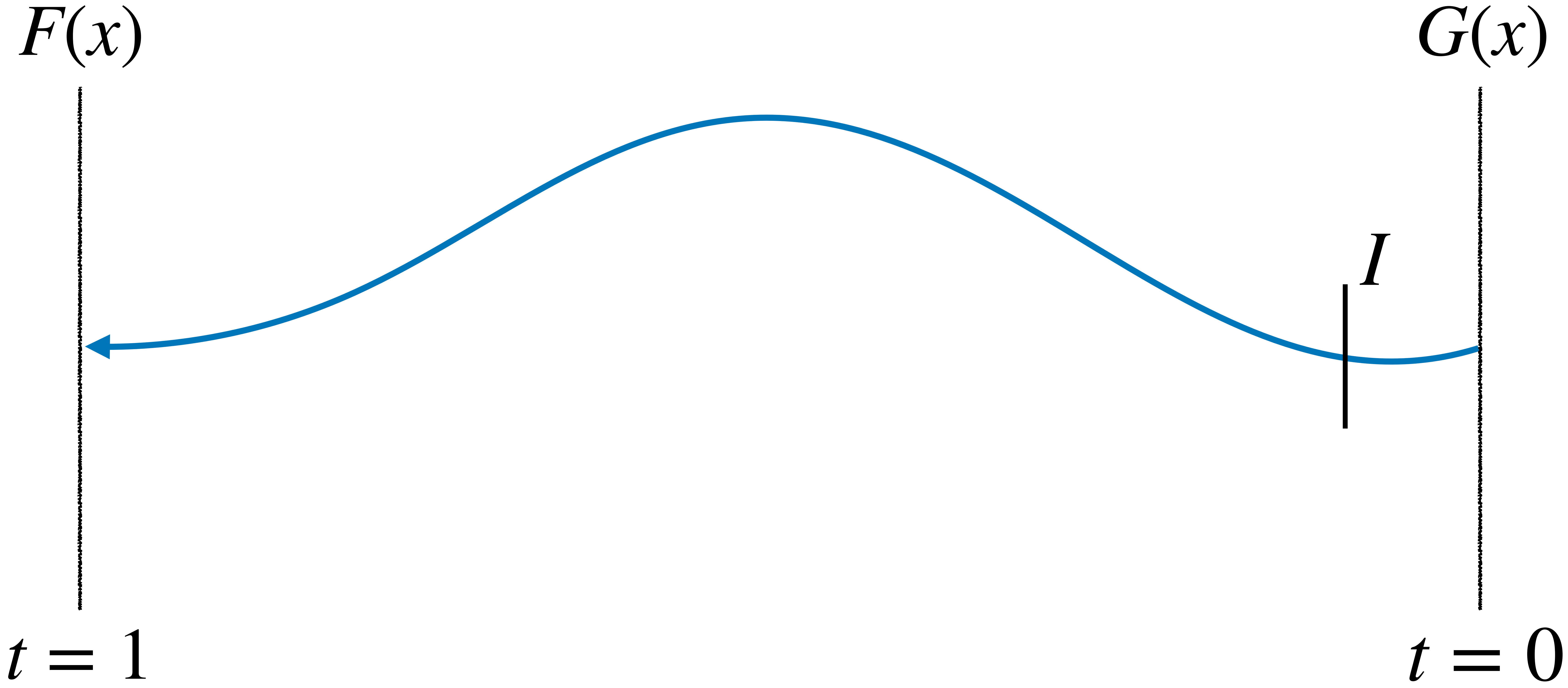
T : an interval contained in $[0,1]$

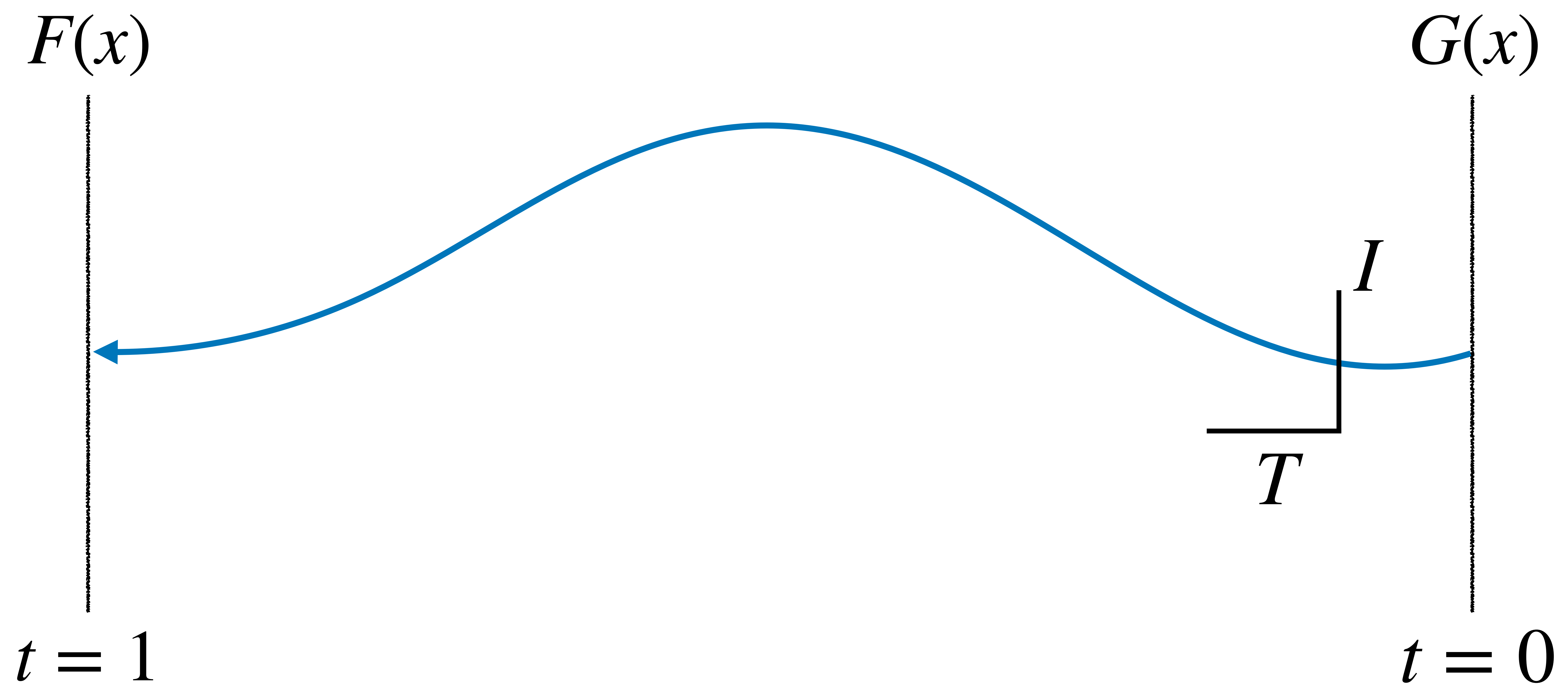
Theorem (Duff-L.) For the Krawczyk operator, the following hold :

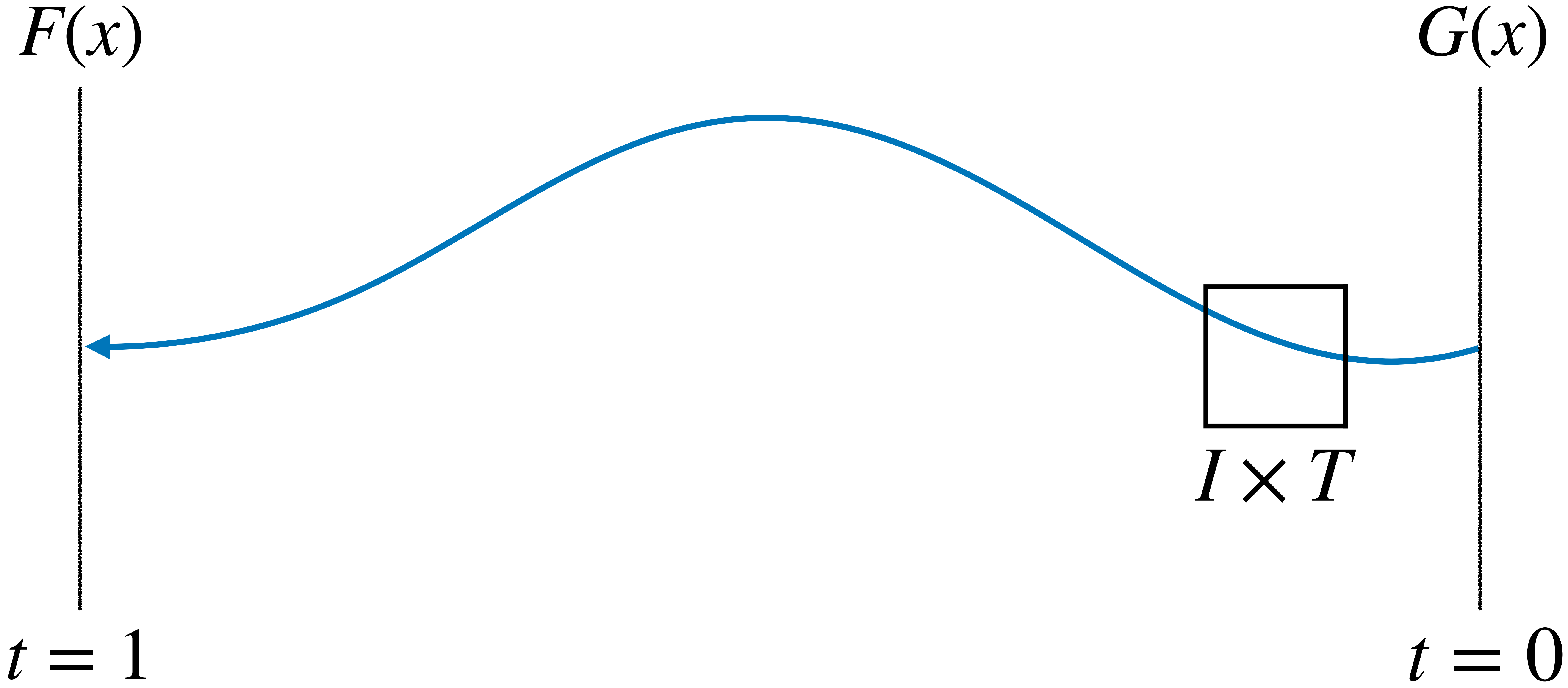
1. If $K_{x,Y}(I,T) \subset I$, then there is a solution of $H(x,t)$ in I for all $t \in T$ (**existence** of a solution path)
2. If I has a solution and $$\sqrt{2}\left\| Id - Y \,\square\, \frac{\partial H(I,T)}{\partial x} \right\| < 1,$$ then for all $t \in T$, there is a solution of F in I, and it is unique (**uniqueness** of a solution path)

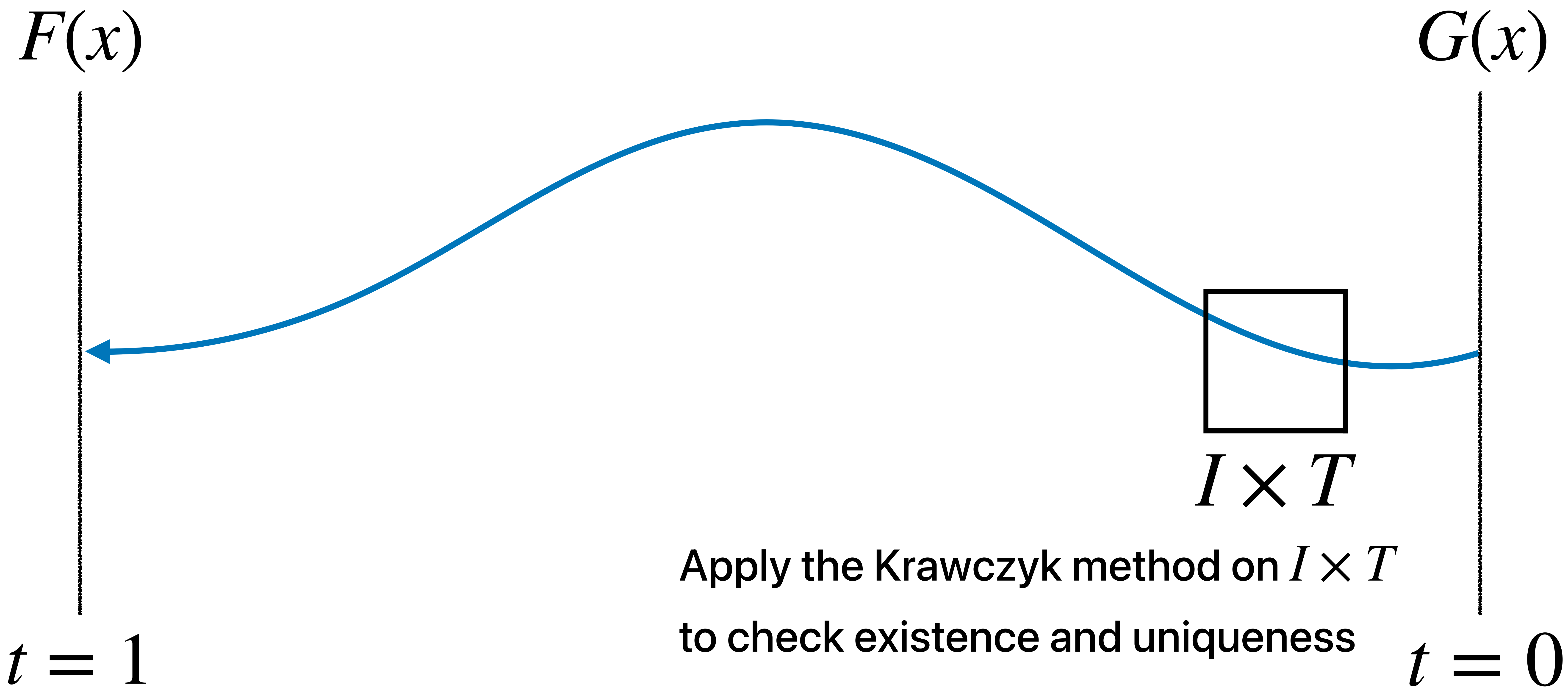


$F(x)$
$G(x)$
$t = 1$
$t = 0$

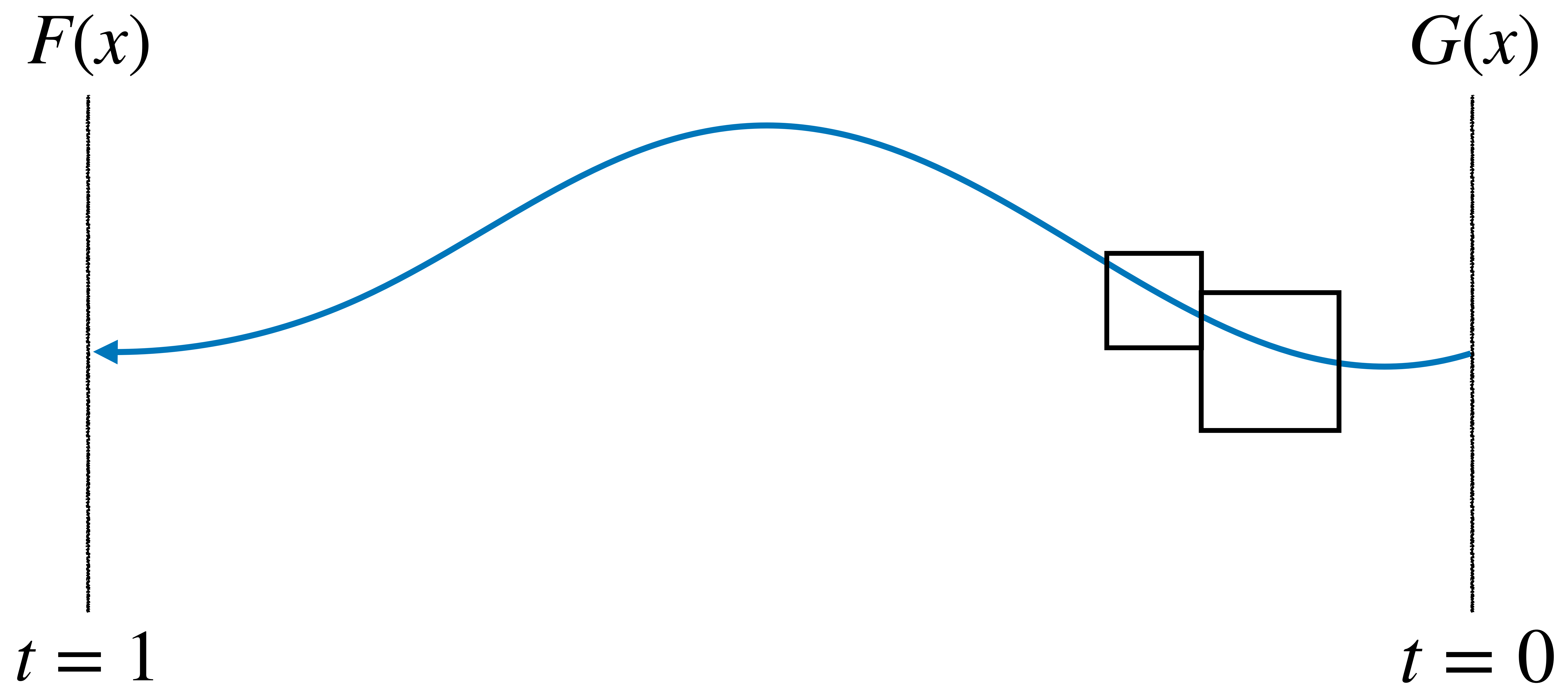

$F(x)$
$G(x)$
I
$t = 1$
$t = 0$


$F(x)$
$G(x)$
I
T
$t = 1$
$t = 0$

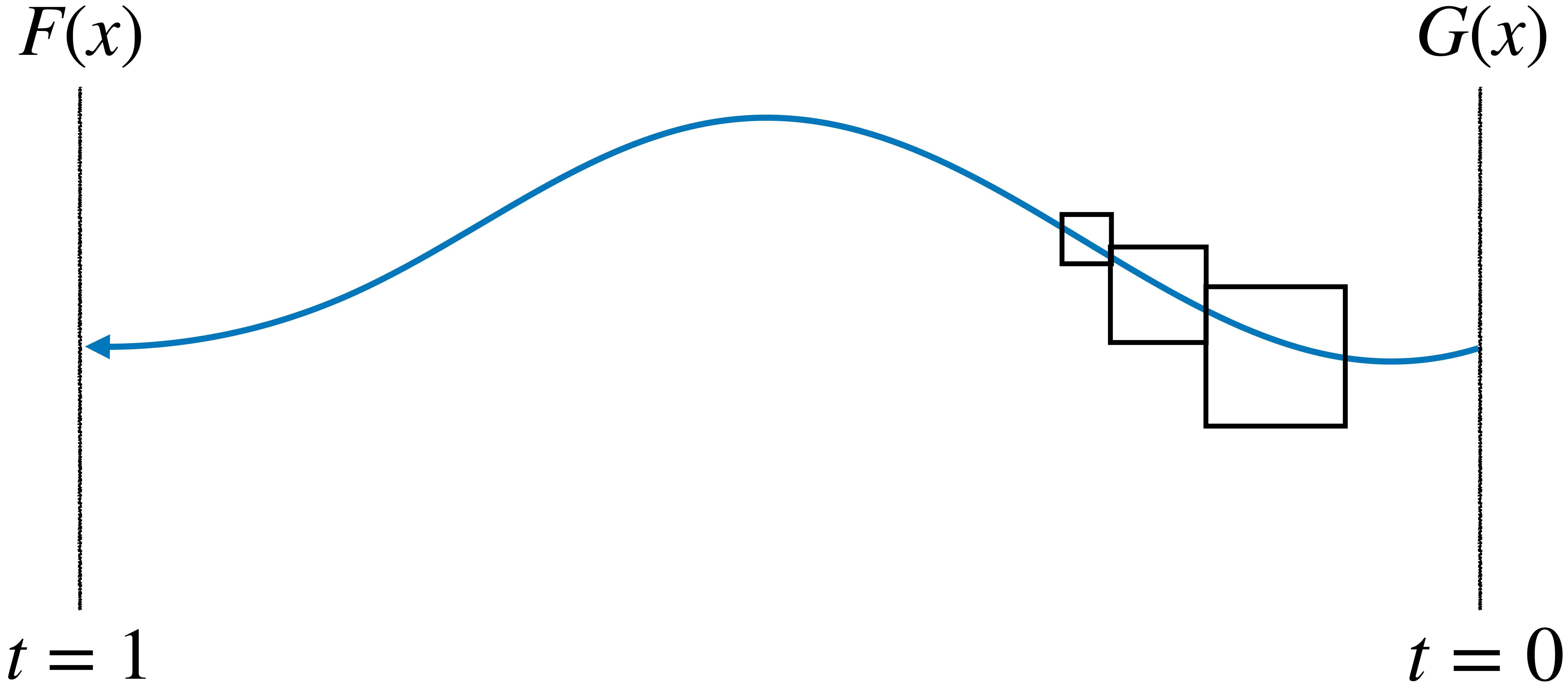

$F(x)$
$G(x)$
$I \times T$
$t = 1$
$t = 0$

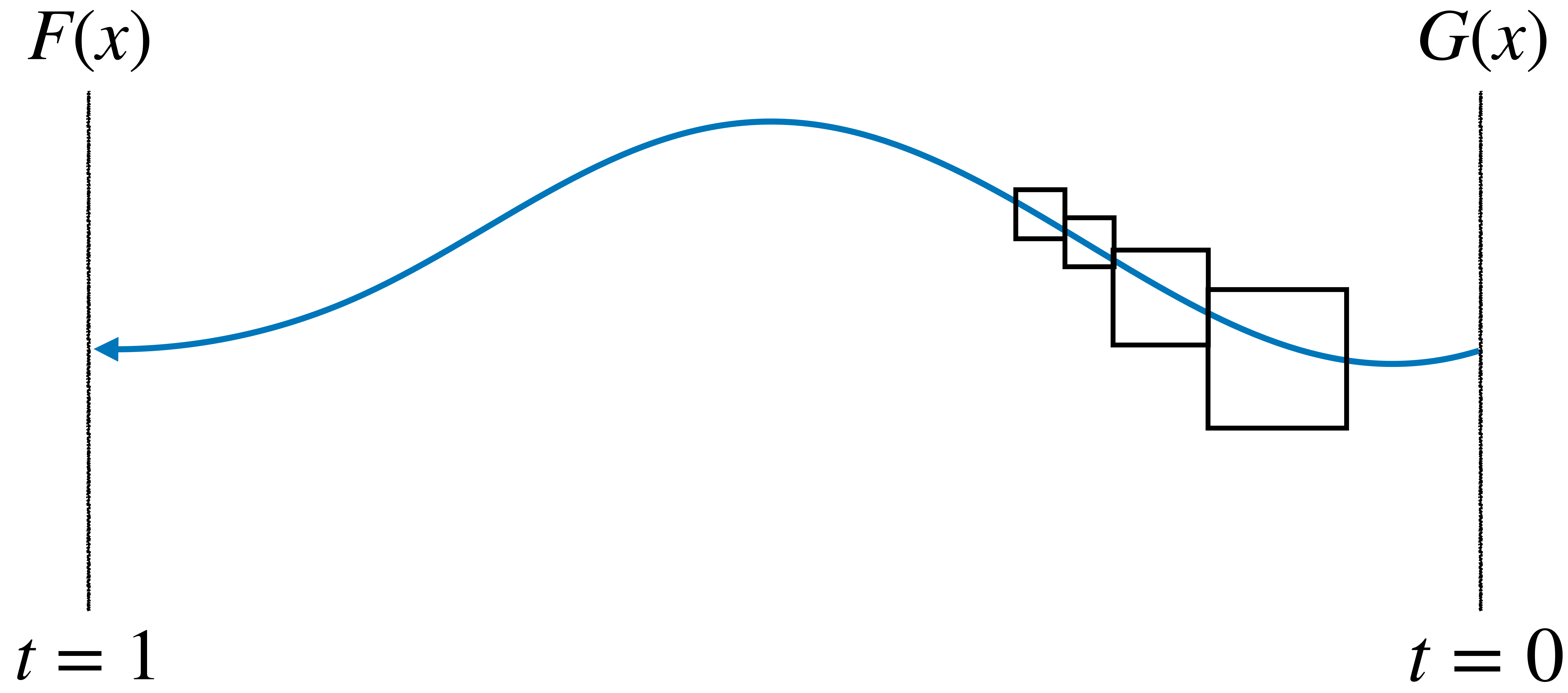


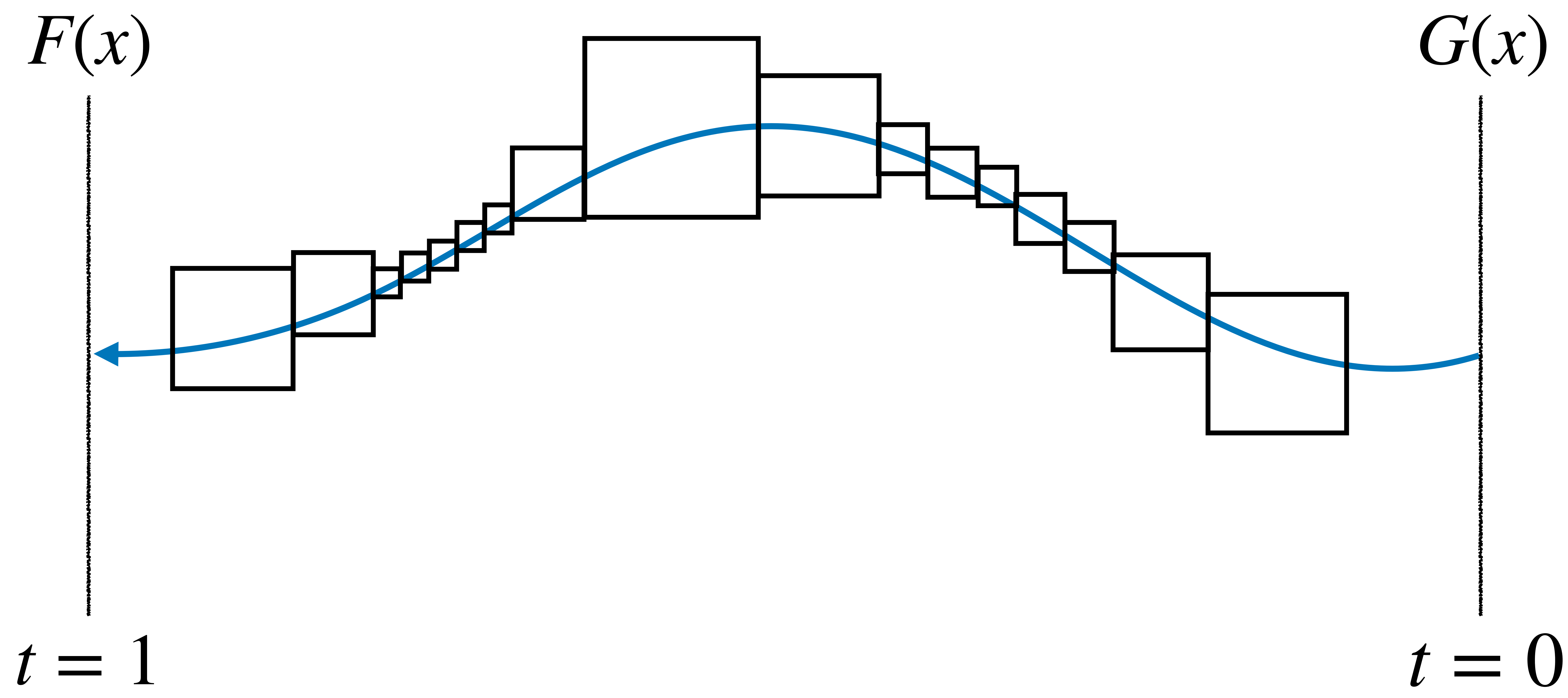
$F(x)$
$G(x)$
$I \times T$
Apply the Krawczyk method on $I \times T$
to check existence and uniqueness
$t = 1$
$t = 0$

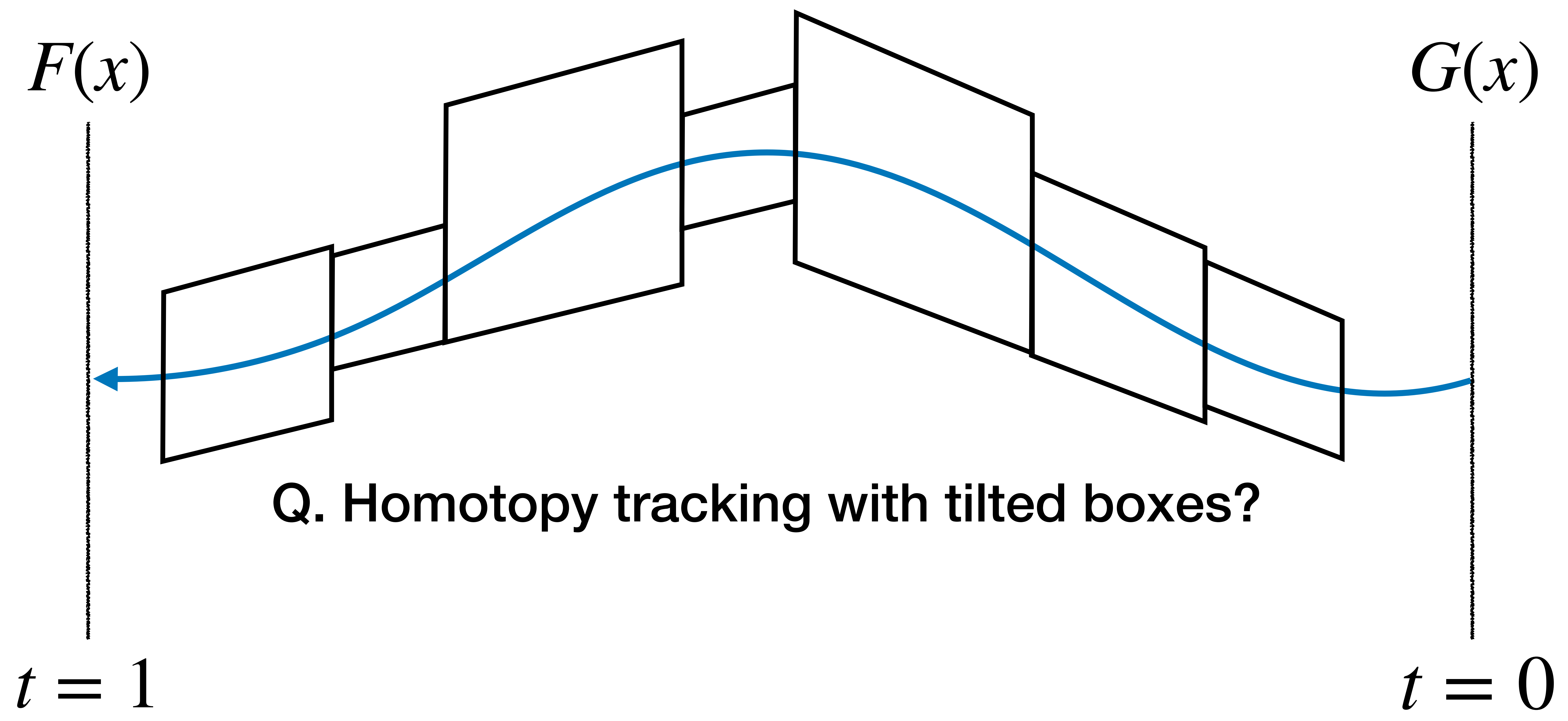


$F(x)$
$G(x)$
$t = 1$
$t = 0$


$F(x)$
$G(x)$
$t = 1$
$t = 0$


$F(x)$
$G(x)$
$t = 1$
$t = 0$

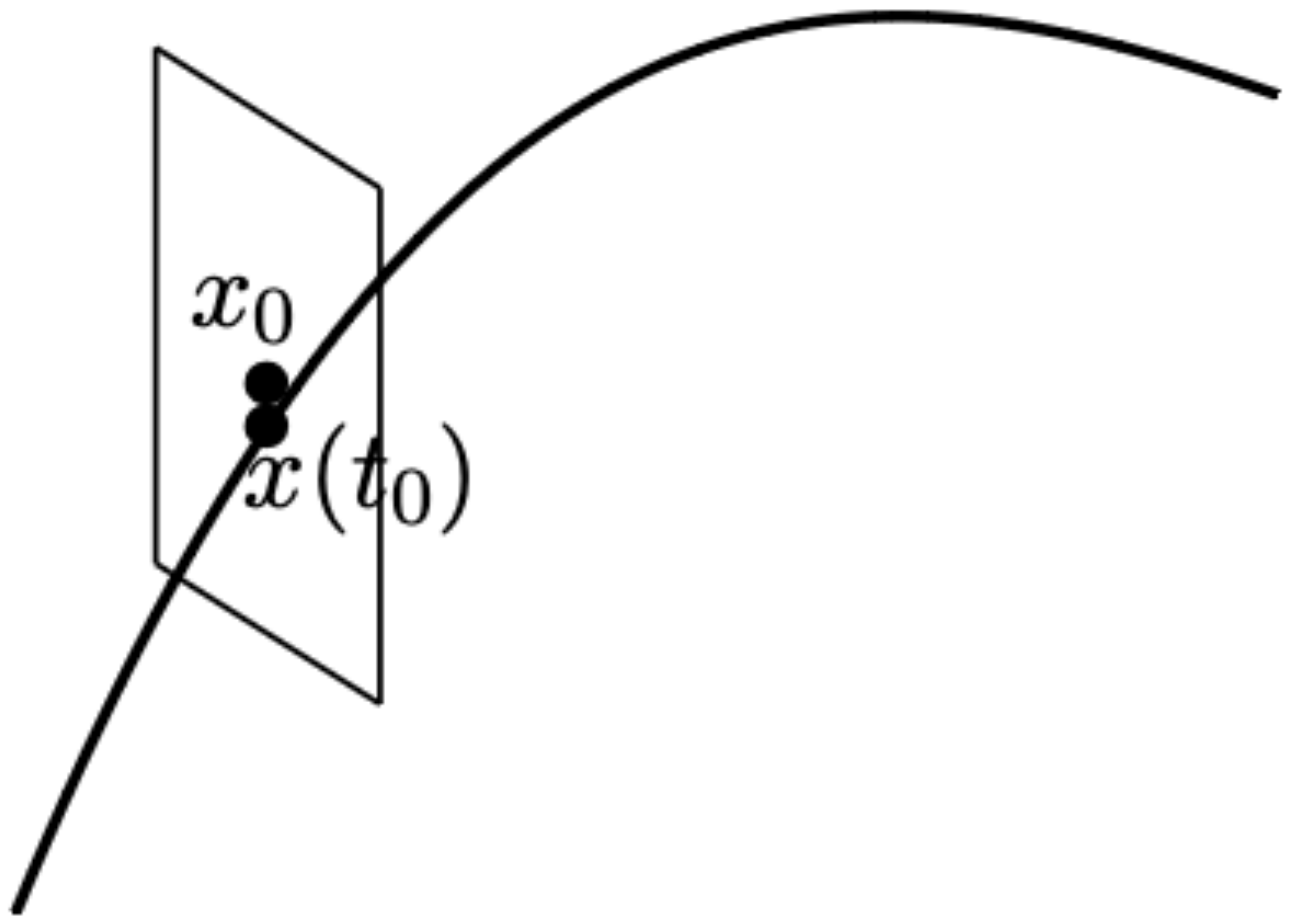

$F(x)$
$G(x)$
$t = 1$
$t = 0$



$F(x)$
$G(x)$
Q. Homotopy tracking with tilted boxes?
$t = 1$
$t = 0$

Preconditioning

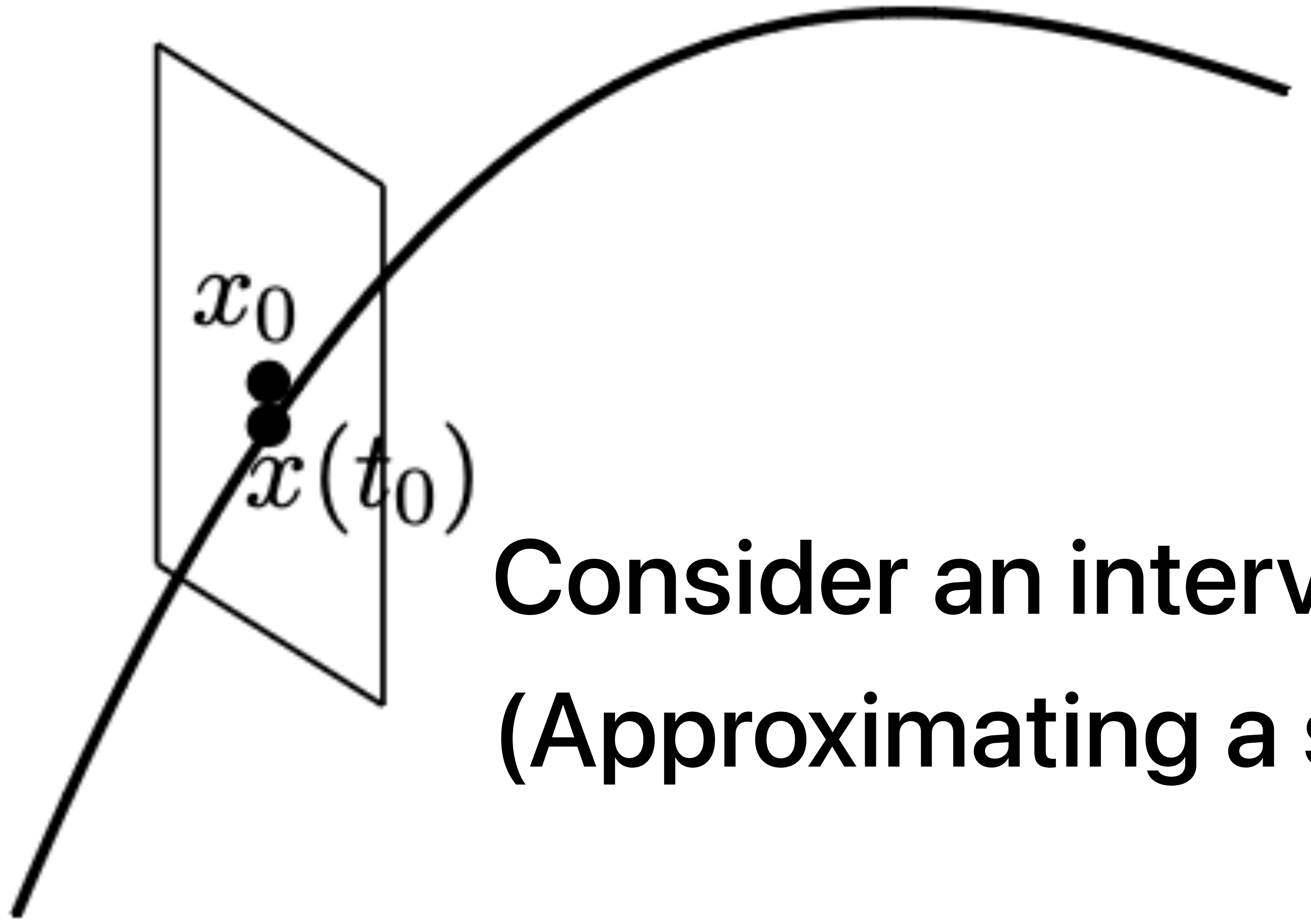
Constructing a tilted interval box



Solution path $x(t)$
from $t = 0$ to $t = 1$

Preconditioning

Constructing a tilted interval box



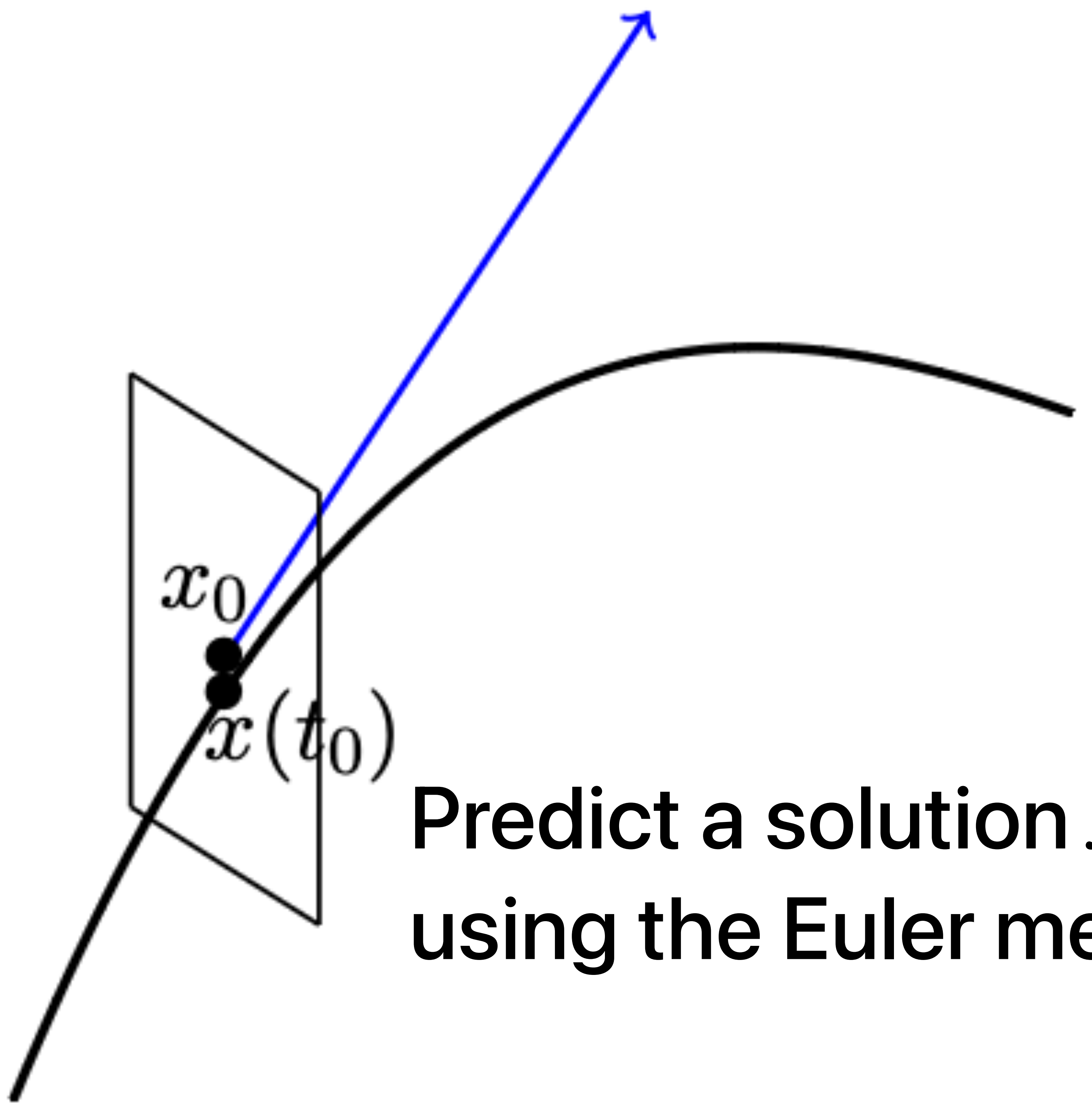
Solution path $x(t)$
from $t = 0$ to $t = 1$

Consider an interval box I centered at x_0

(Approximating a solution at $t = t_0$)

Preconditioning

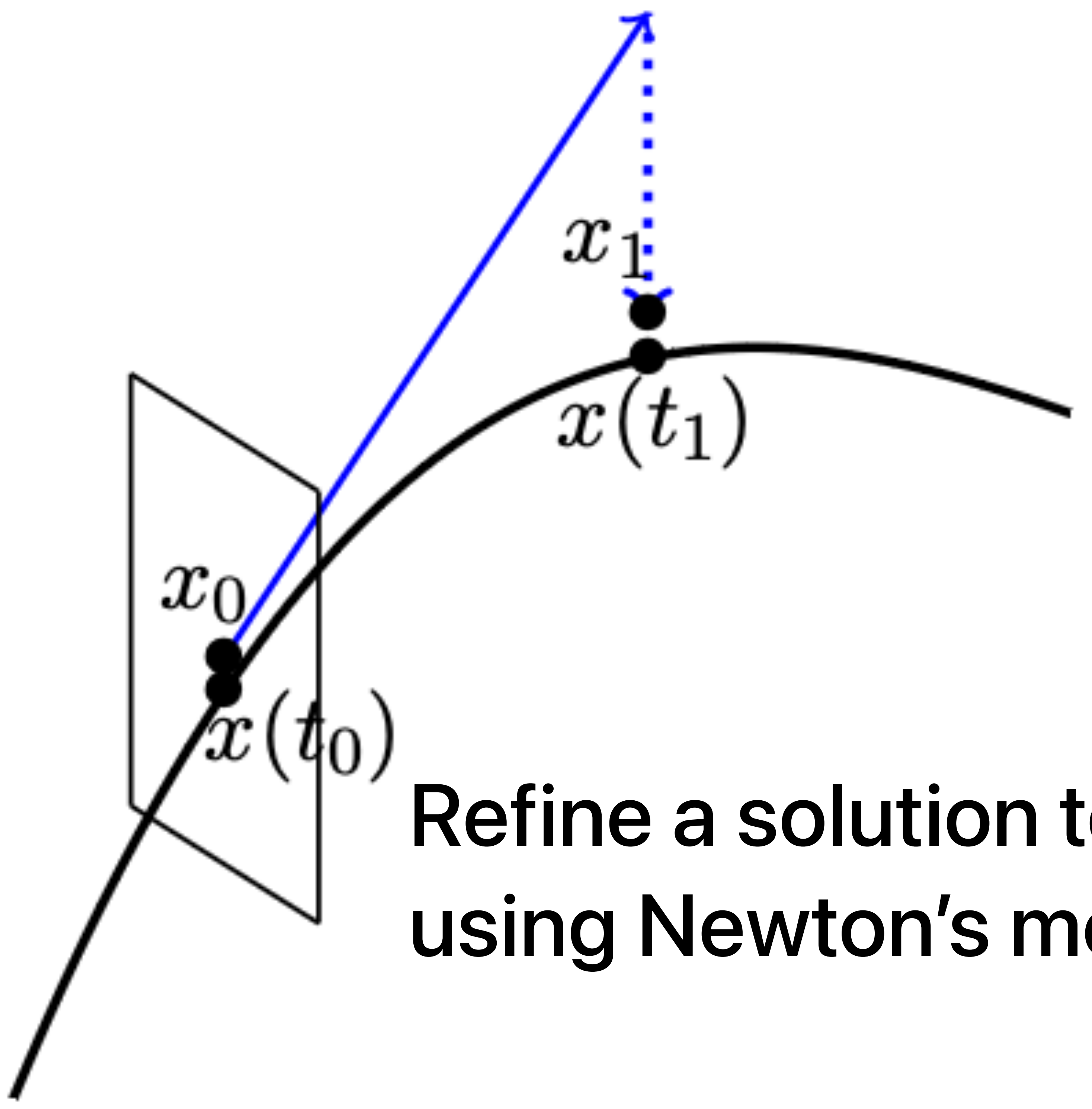
Constructing a tilted interval box



Predict a solution $x(t_1)$
using the Euler method for example

Preconditioning

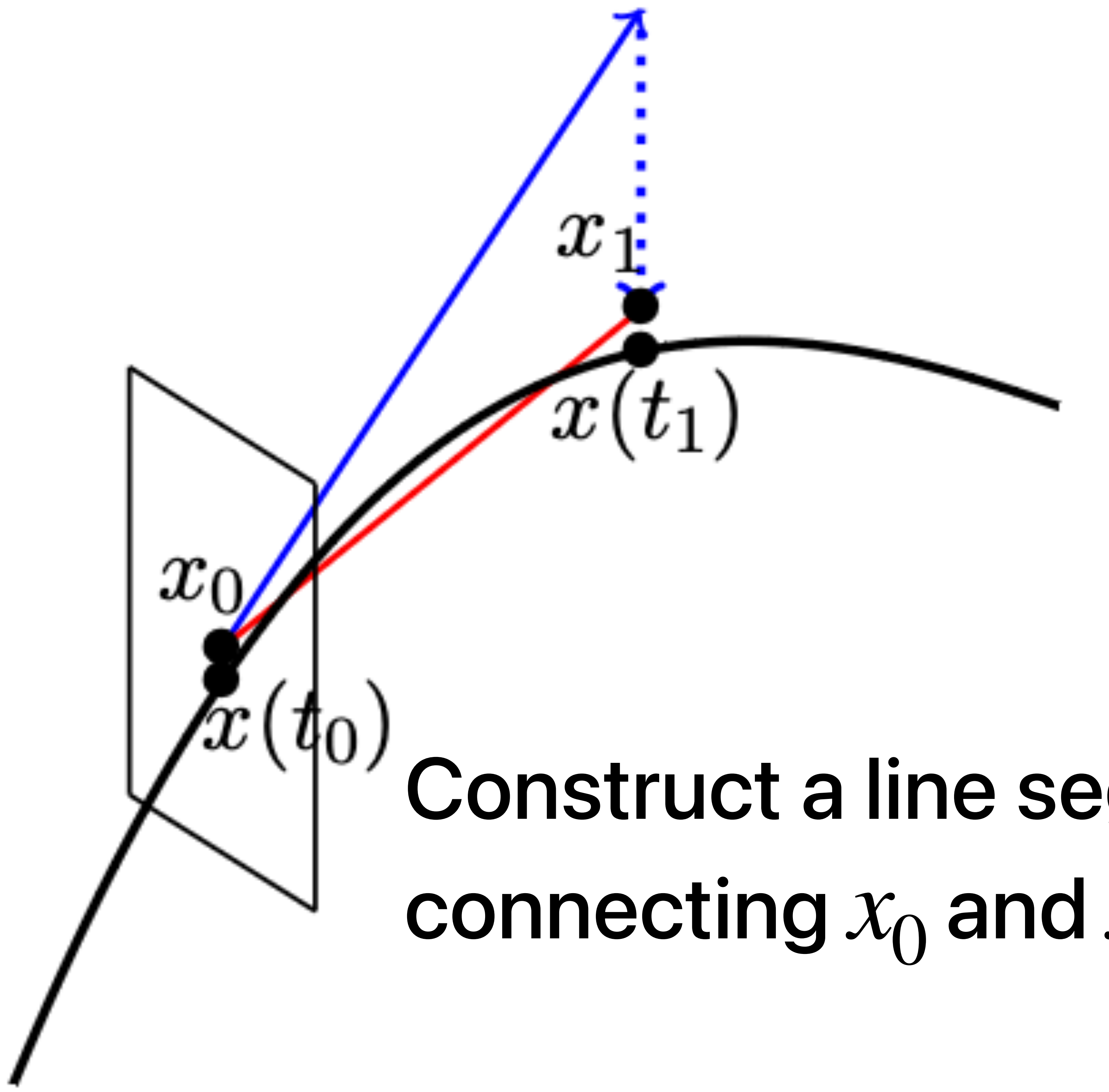
Constructing a tilted interval box



Refine a solution to get x_1
using Newton's method

Preconditioning

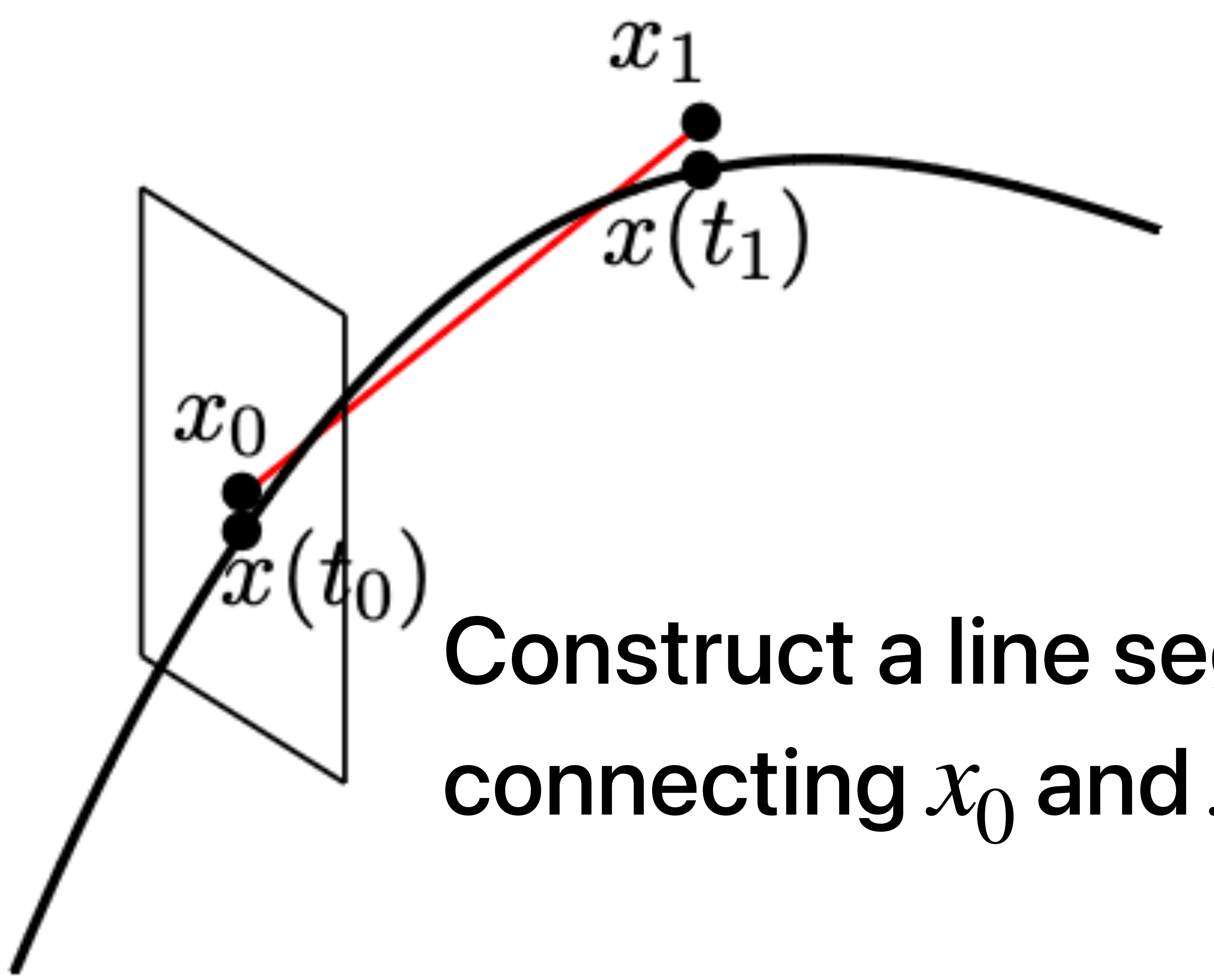
Constructing a tilted interval box



Construct a line segment connecting x_0 and x_1

Preconditioning

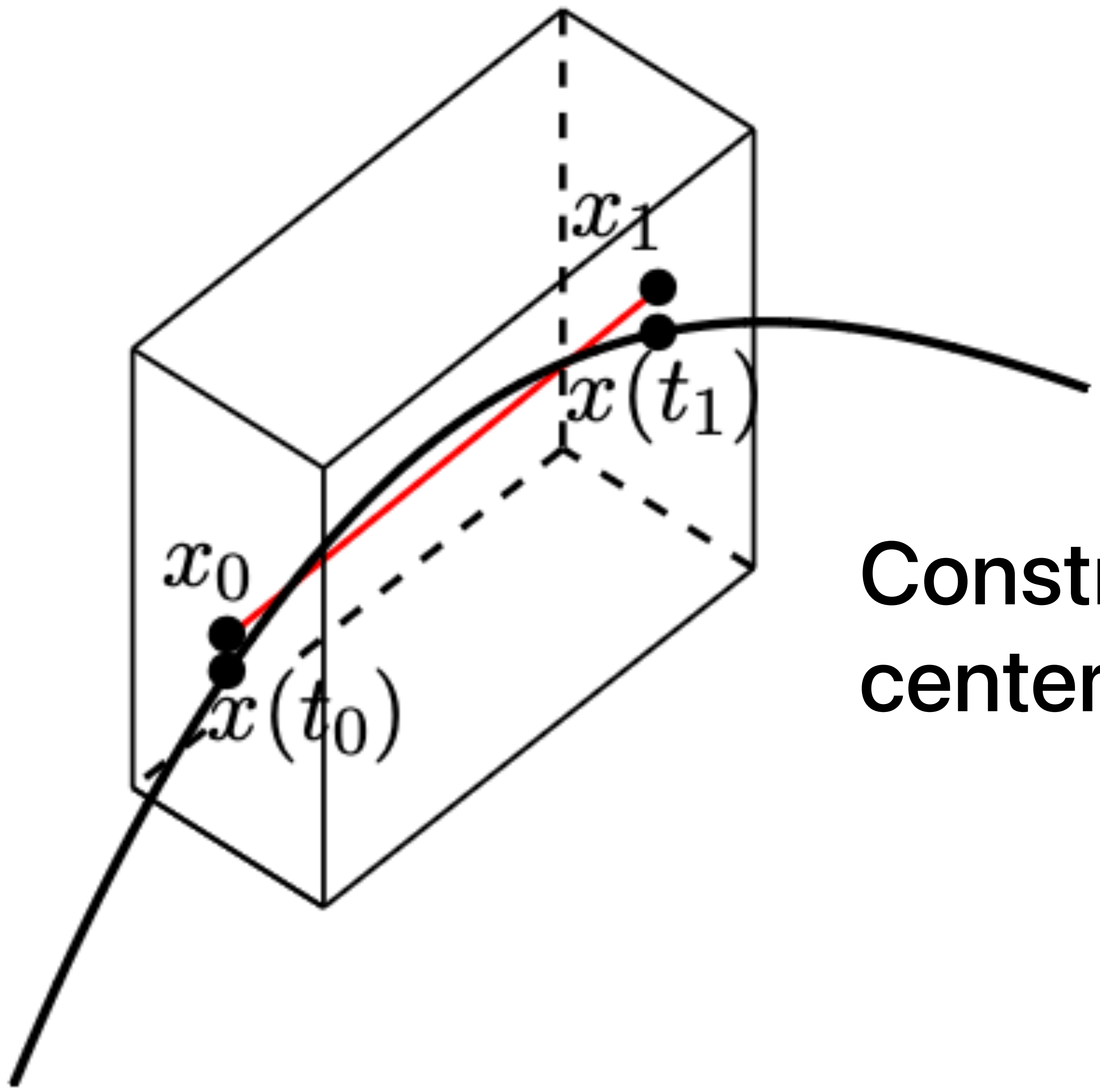
Constructing a tilted interval box



Construct a line segment connecting x_0 and x_1

Preconditioning

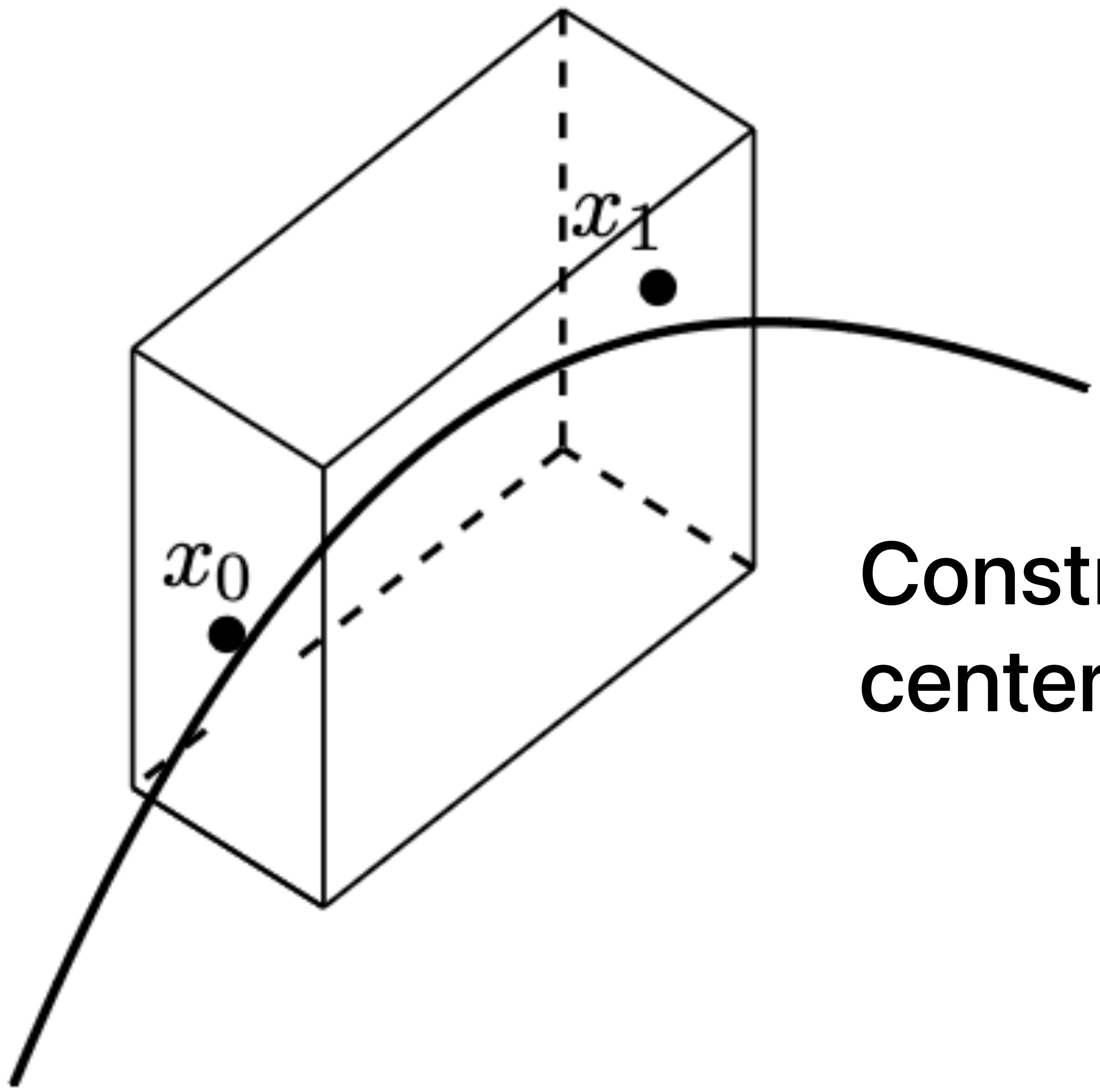
Constructing a tilted interval box



Construct a tilted interval box
centered at the line segment

Preconditioning

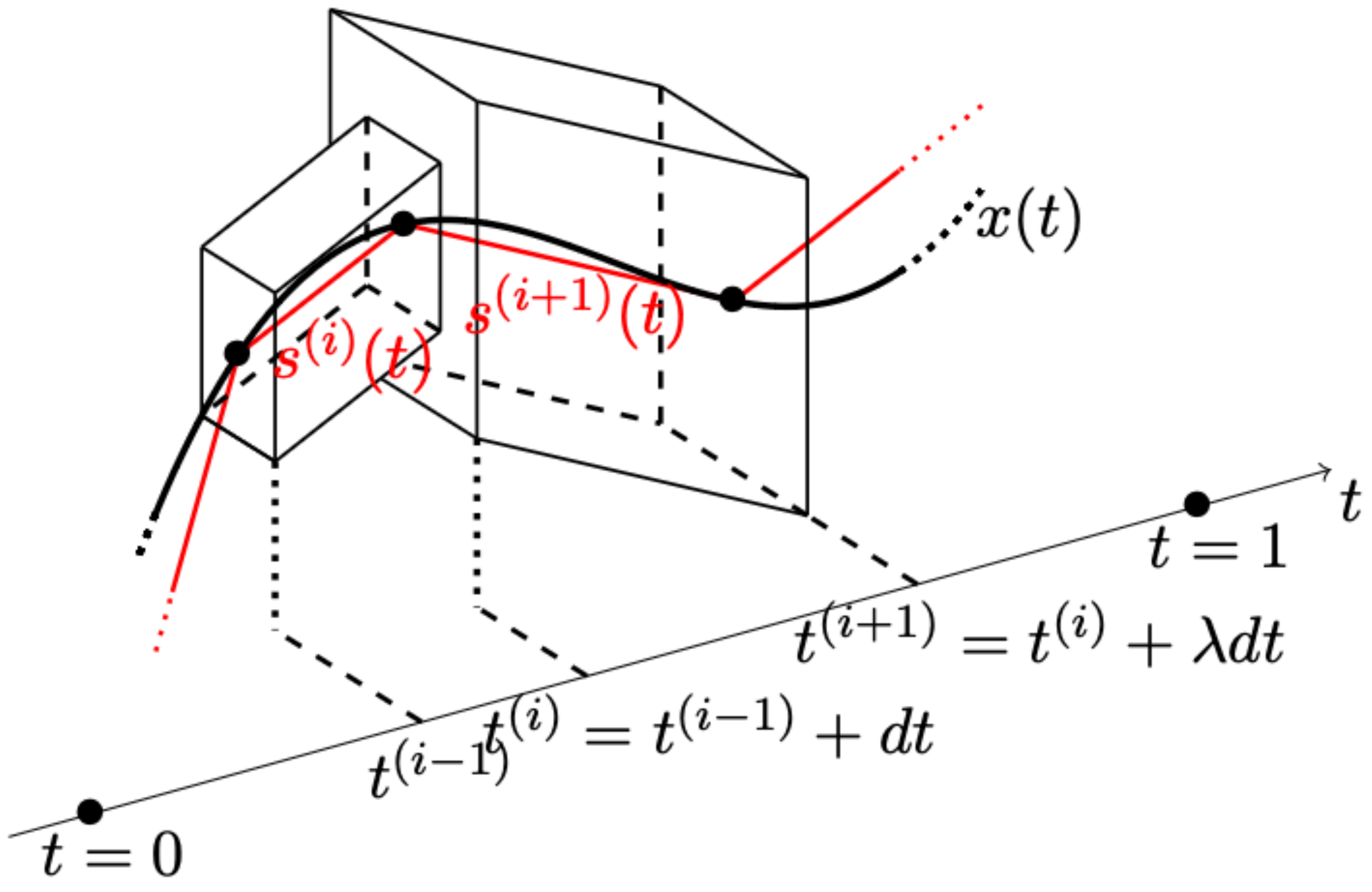
Constructing a tilted interval box



Construct a tilted interval box centered at the line segment

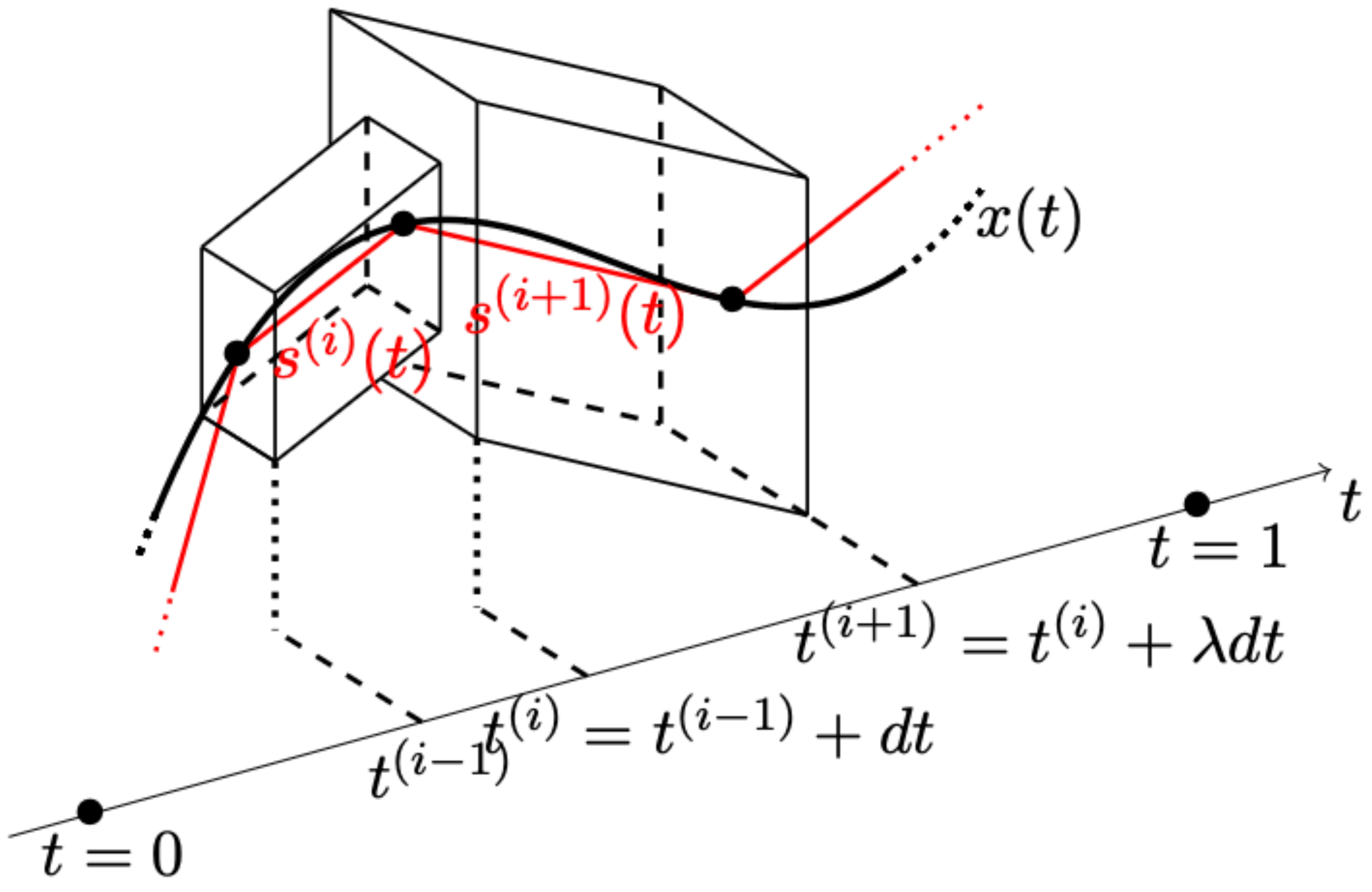
Preconditioning

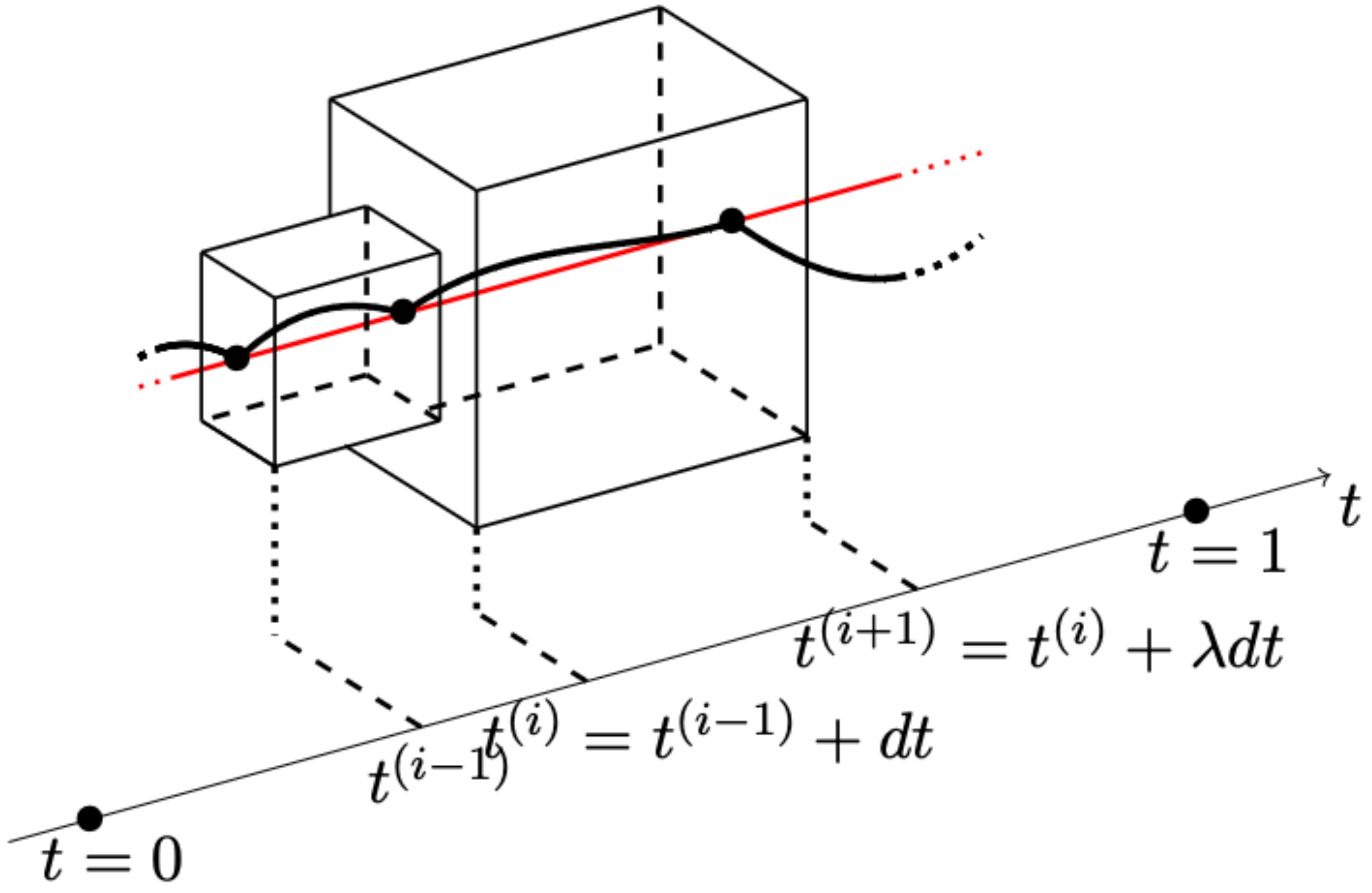
Constructing a tilted interval box



Preconditioning

Constructing a tilted interval box





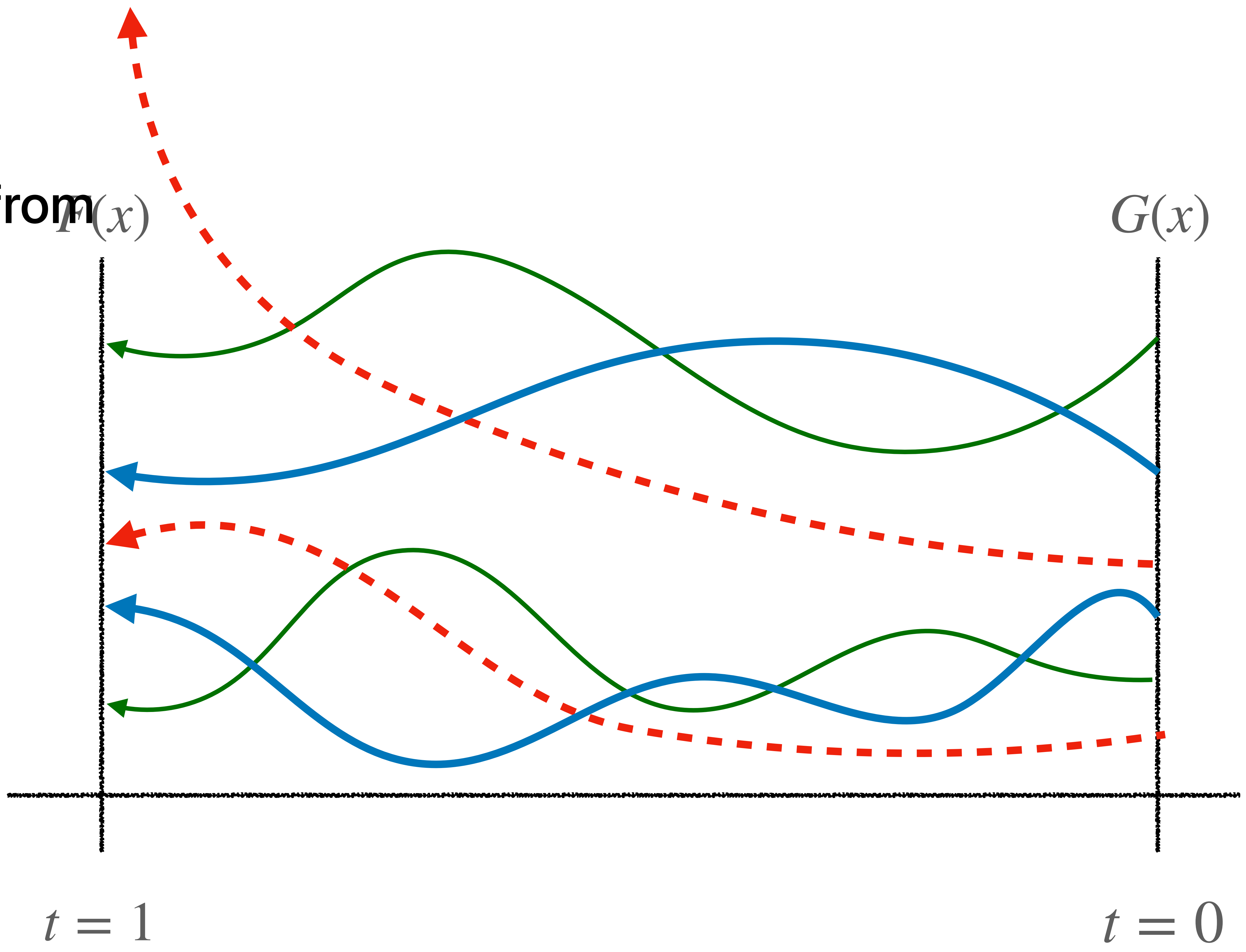
After the construction, apply the shearing map to make the rectangular interval box to avoid overestimation from interval arithmetic

Algorithm

Algorithm

Input :

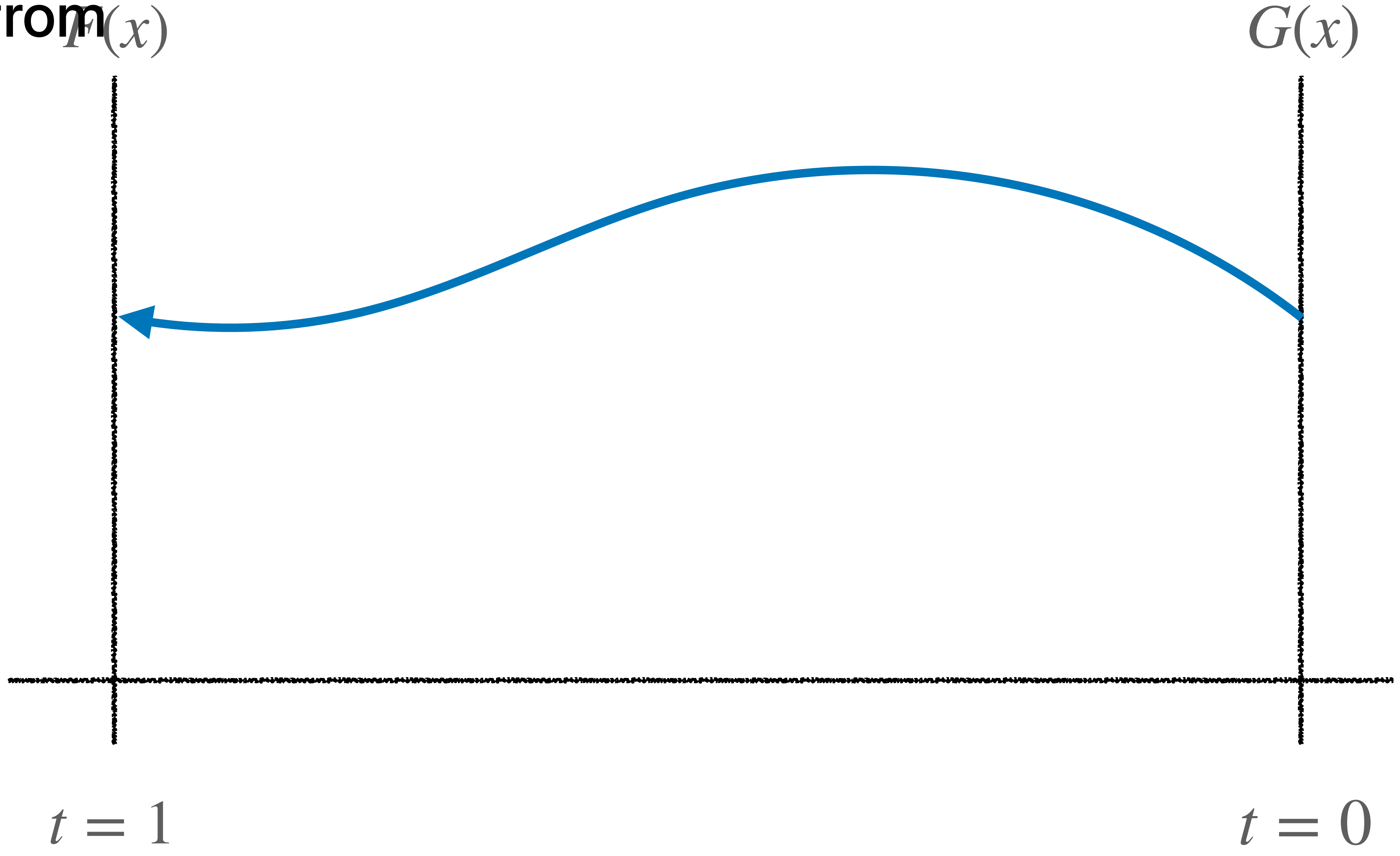
- $H(x,t) = F(x;p(t))$ a parameter homotopy from $t=0$ to $t=1$



Algorithm

Input :

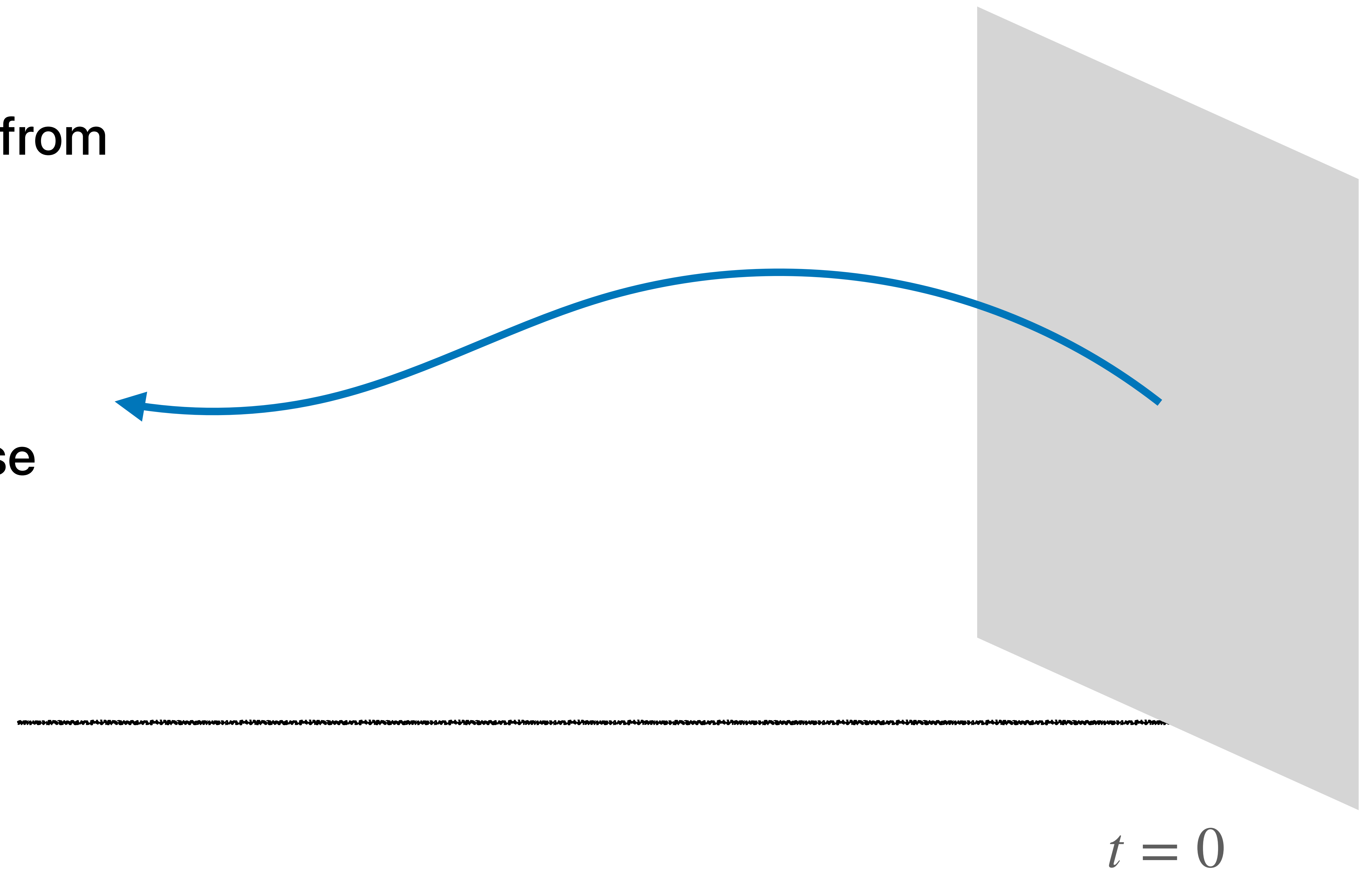
- $H(x,t) = F(x;p(t))$ a parameter homotopy from $t=0$ to $t=1$
- $x(t)$: a nonsingular solution path in $\mathbb{C}^n$



Algorithm

Input :

- $H(x,t) = F(x; p(t))$ a parameter homotopy from $t=0$ to $t=1$
- $x(t)$: a nonsingular solution path in $\mathbb{C}^n$
- I_r : a square interval box with a radius r whose midpoint $x_0 = m(I_r)$ approximates $x(0)$



Algorithm

Input :

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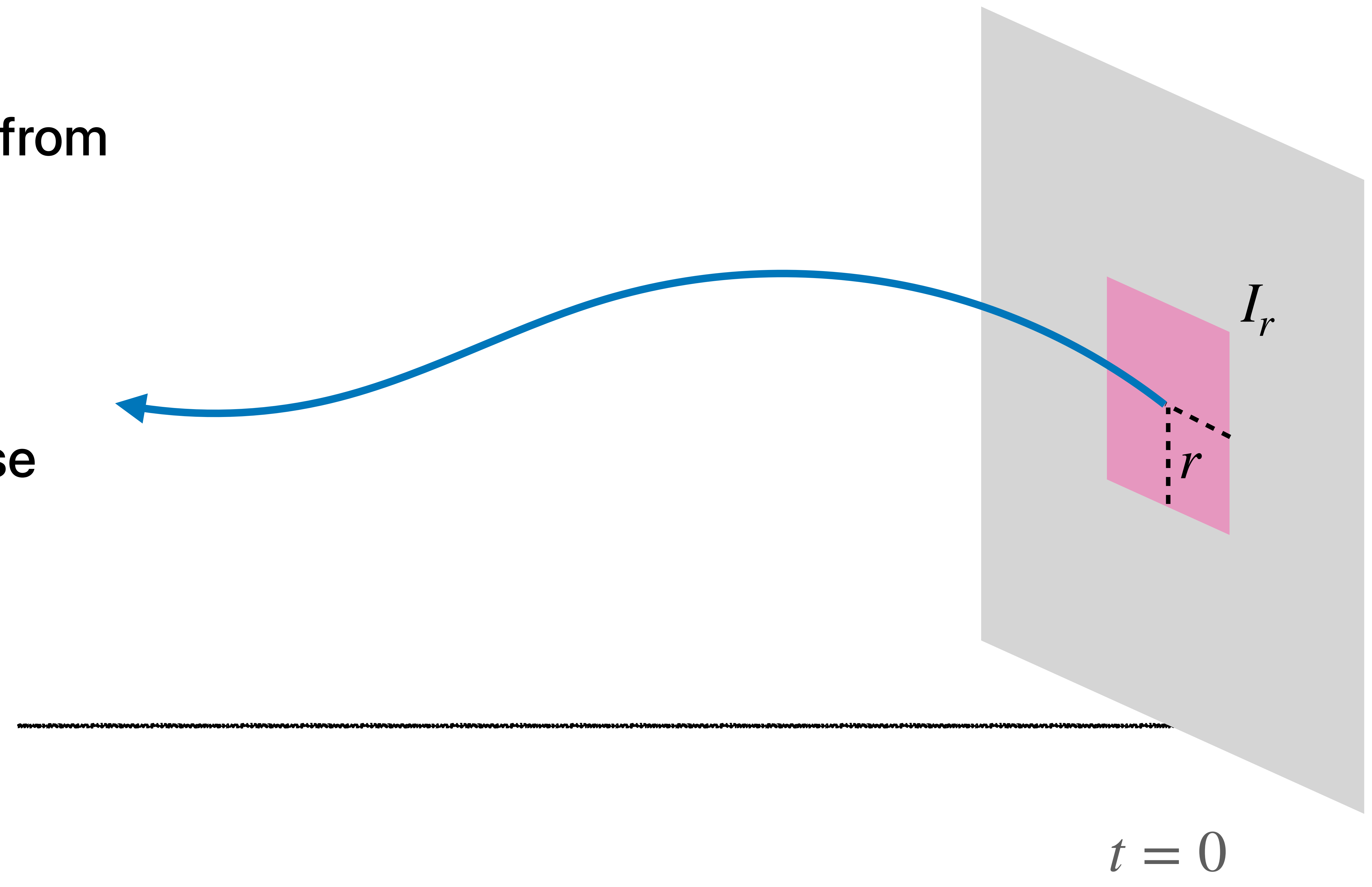

Algorithm

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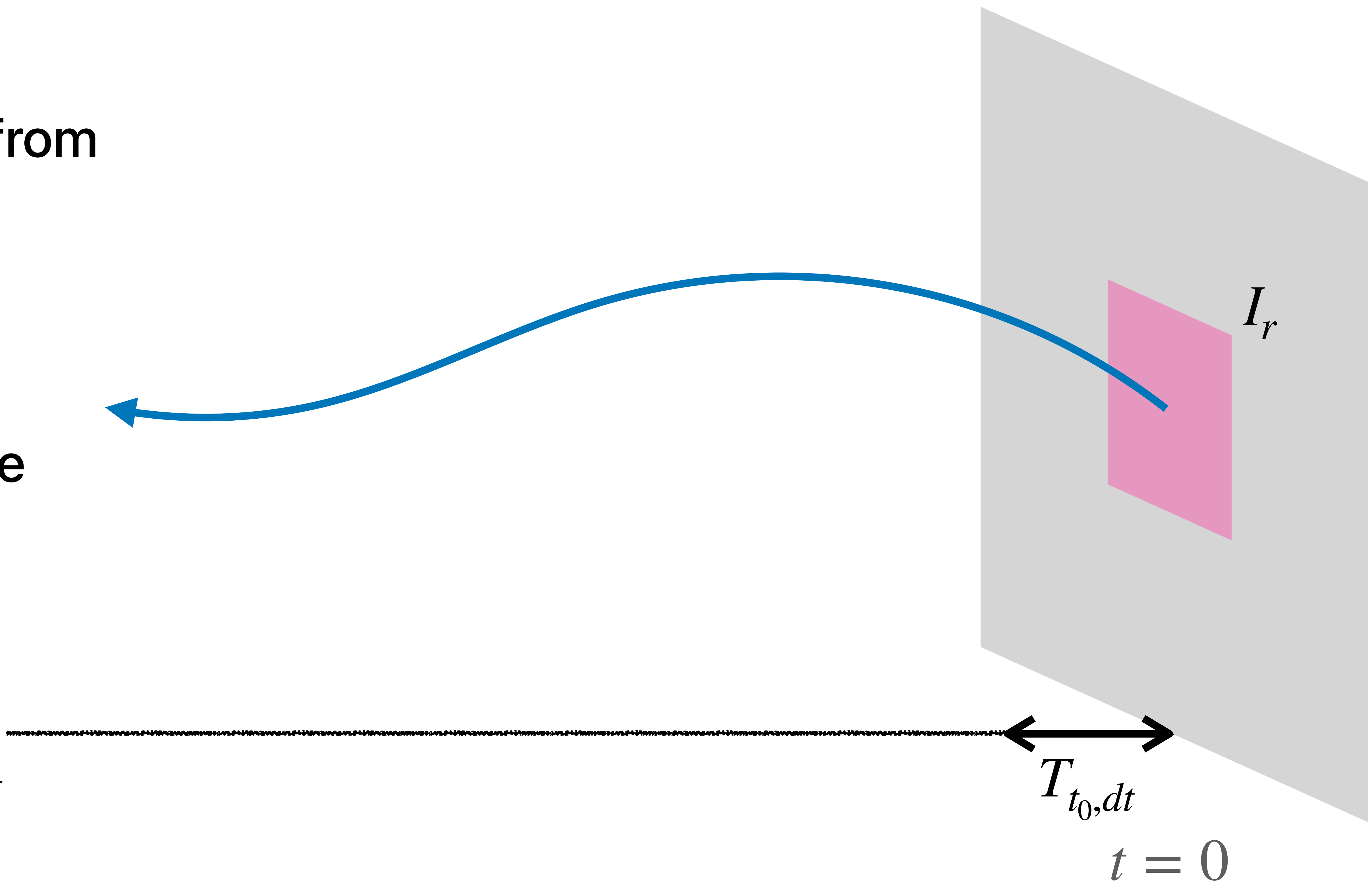
- $x(t)$: a nonsingular solution path in $\mathbb{C}^n$
- I_r : a square interval box with a radius r whose midpoint $x_0 = m(I_r)$ approximates $x(0)$
- $dt \in (0,1)$: the initial step size
- $T_{t_0,dt} = [t_0, t_1]$ where $t_0 = 0$ and $t_1 = t_0 + dt$



Algorithm

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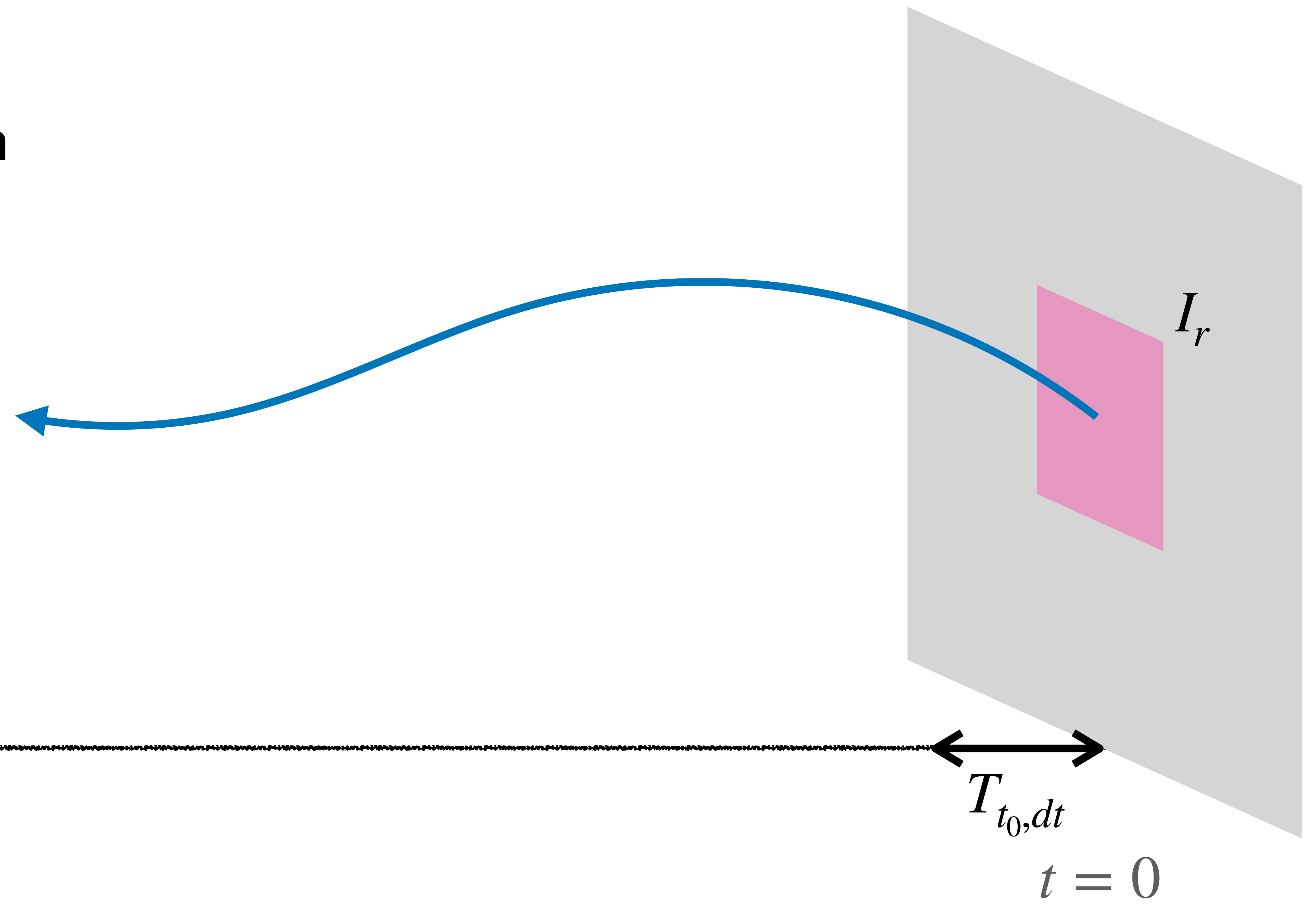
- $T_{t_0,dt} = [t_0, t_1]$ where $t_0 = 0$ and $t_1 = t_0 + dt$
- $\lambda > 1$: a scaling constant



Algorithm

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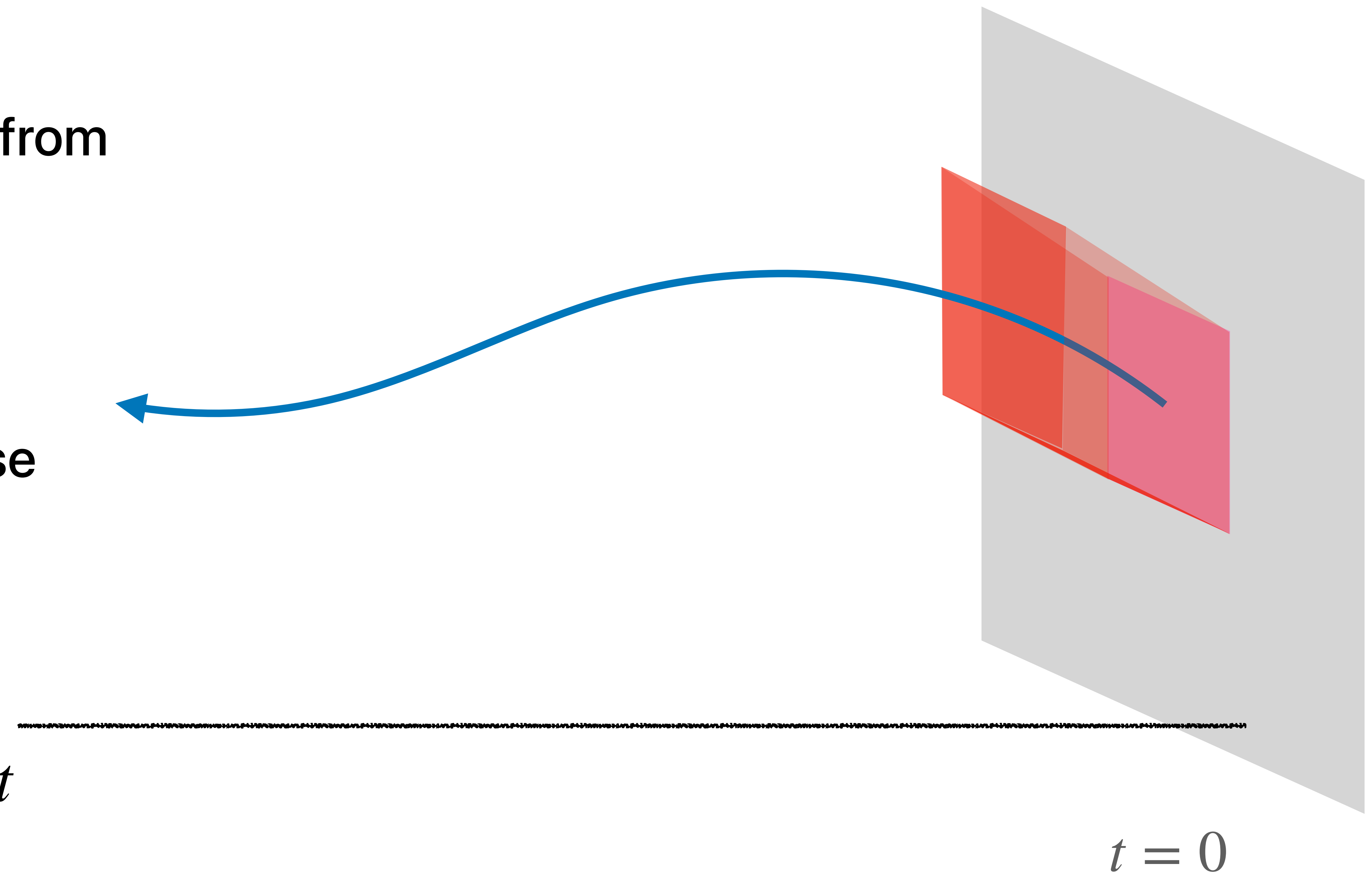

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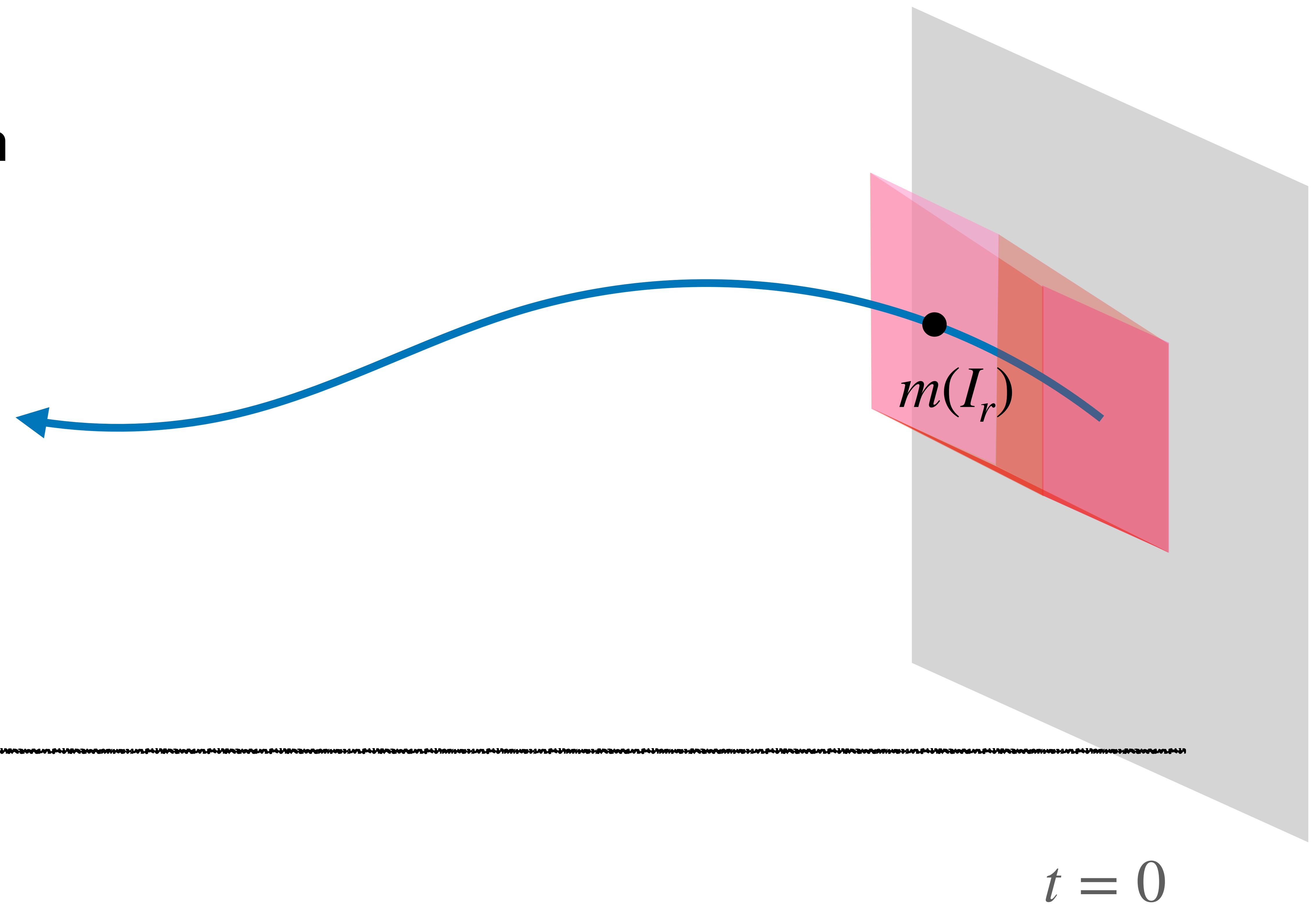

Algorithm

Input :

- $H(x,t) = F(x;p(t))$ a parameter homotopy from $t = 0$ to $t = 1$
- $x(t)$: a nonsingular solution path in $\mathbb{C}^n$
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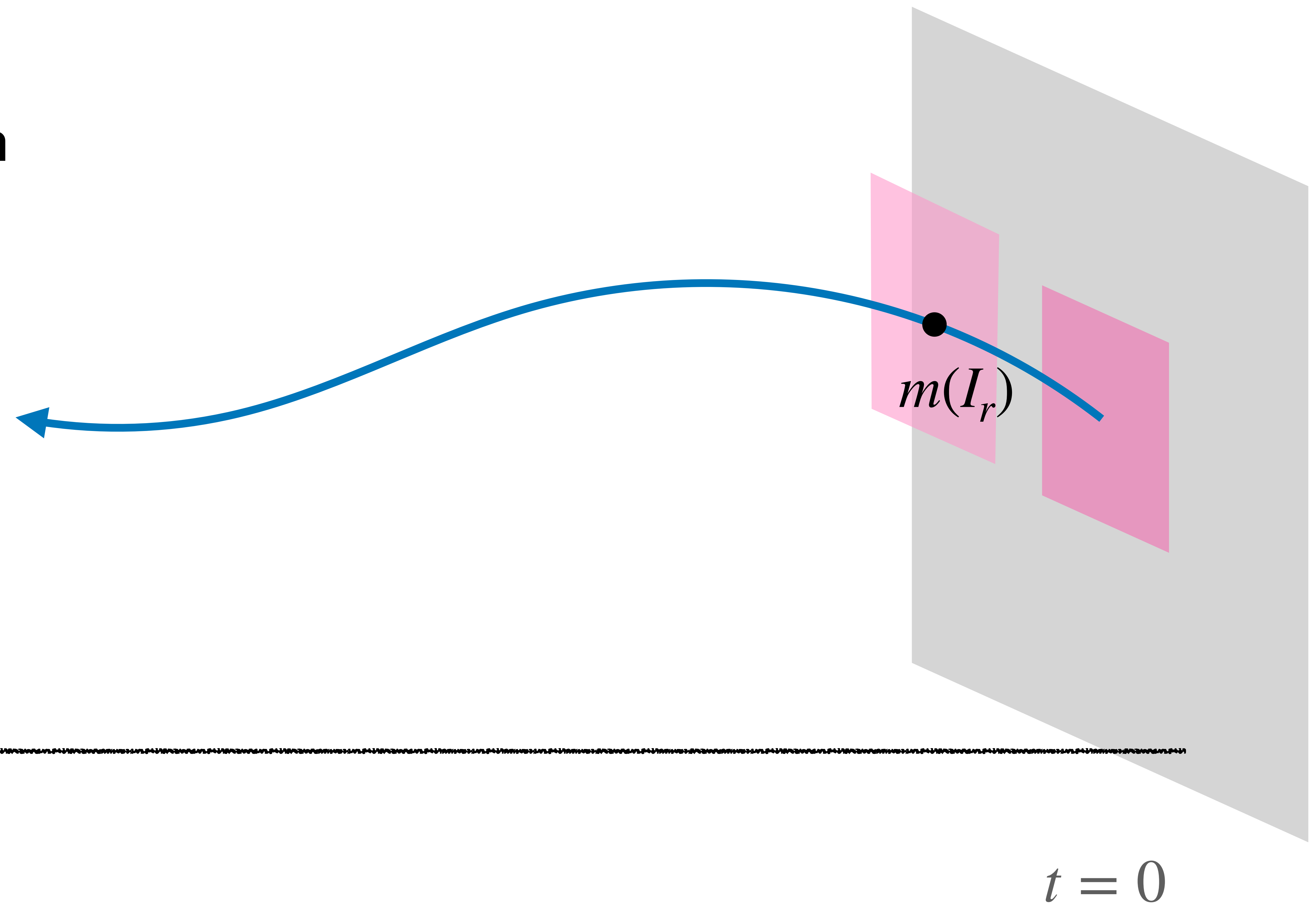

Algorithm

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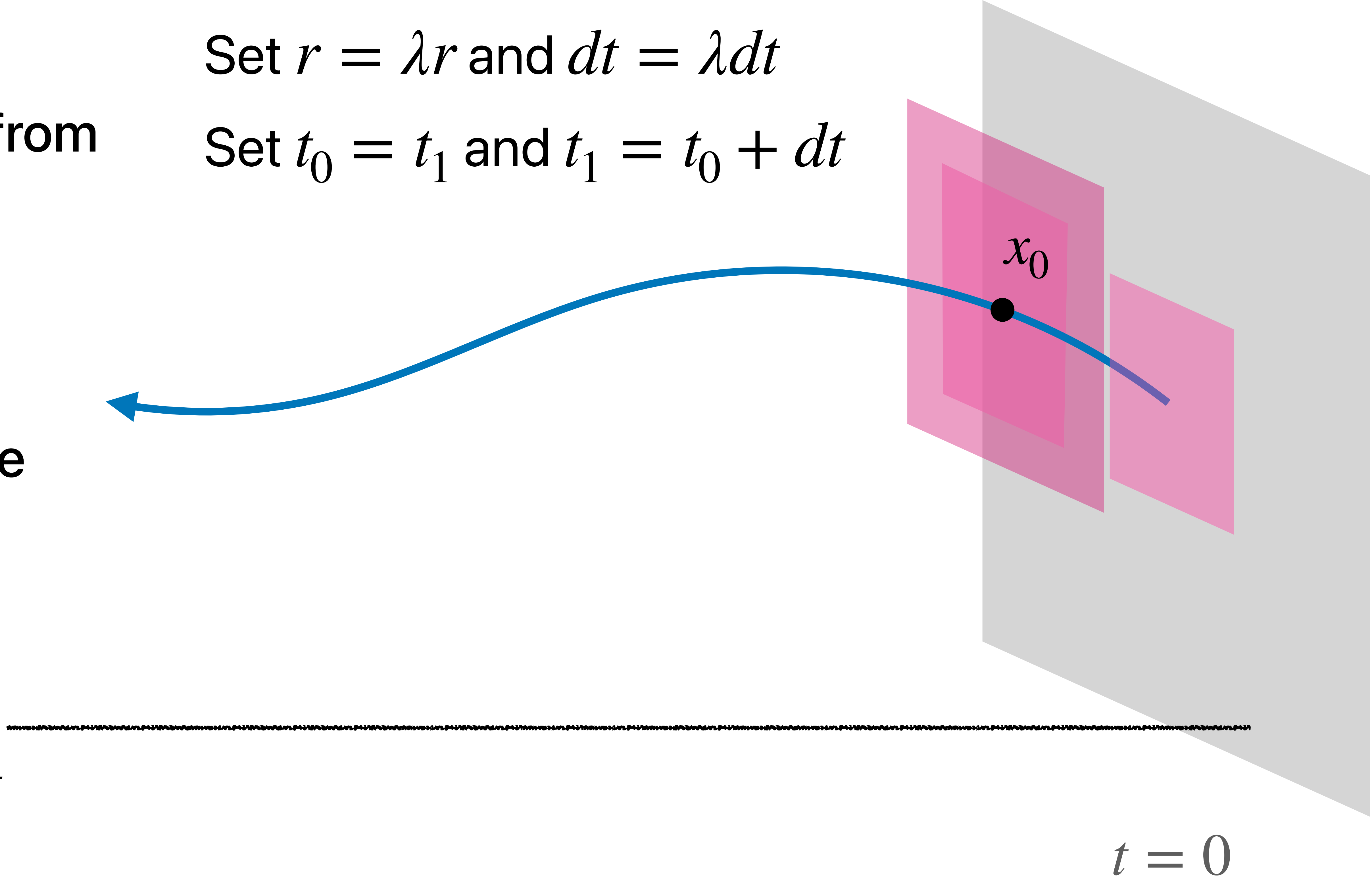
- $dt \in (0,1)$: the initial step size
- $T_{t_0,dt} = [t_0, t_1]$ where $t_0 = 0$ and $t_1 = t_0 + dt$
- $\lambda > 1$: a scaling constant

While $t_0 < 1$ **do**

If Krawczyk test passed **then**

Set $r = \lambda r$ and $dt = \lambda dt$

Set $t_0 = t_1$ and $t_1 = t_0 + dt$



Algorithm

Input :

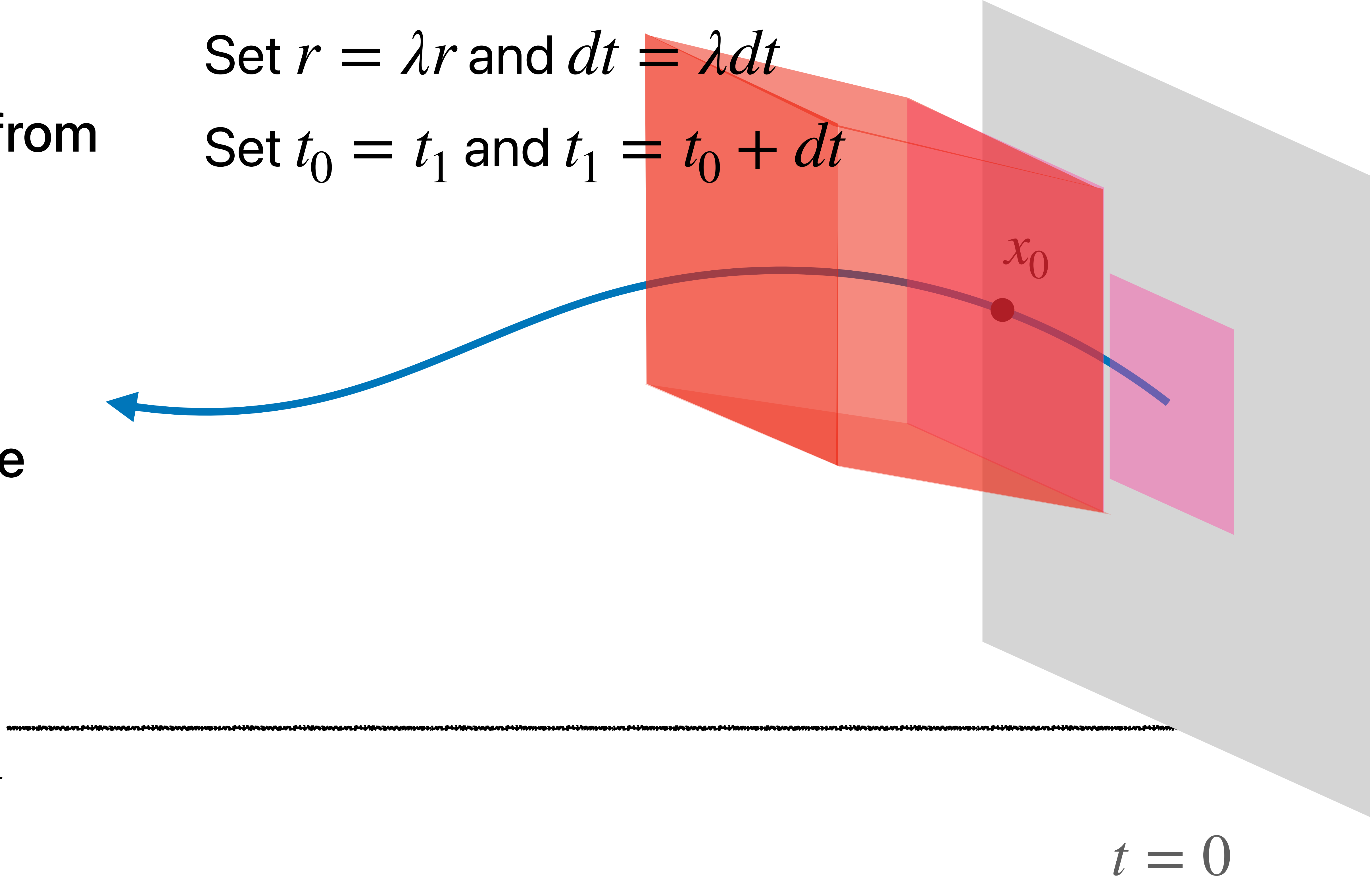
- $H(x,t) = F(x; p(t))$ a parameter homotopy from $t = 0$ to $t = 1$
- $x(t)$: a nonsingular solution path in $\mathbb{C}^n$
- I_r : a square interval box with a radius r whose midpoint $x_0 = m(I_r)$ approximates $x(0)$
- $dt \in (0,1)$: the initial step size
- $T_{t_0,dt} = [t_0, t_1]$ where $t_0 = 0$ and $t_1 = t_0 + dt$
- $\lambda > 1$: a scaling constant

While $t_0 < 1$ **do**

If Krawczyk test passed **then**

Set $r = \lambda r$ and $dt = \lambda dt$

Set $t_0 = t_1$ and $t_1 = t_0 + dt$



Algorithm

Input :

- $H(x, t) = F(x; p(t))$ a parameter homotopy from $t = 0$ to $t = 1$
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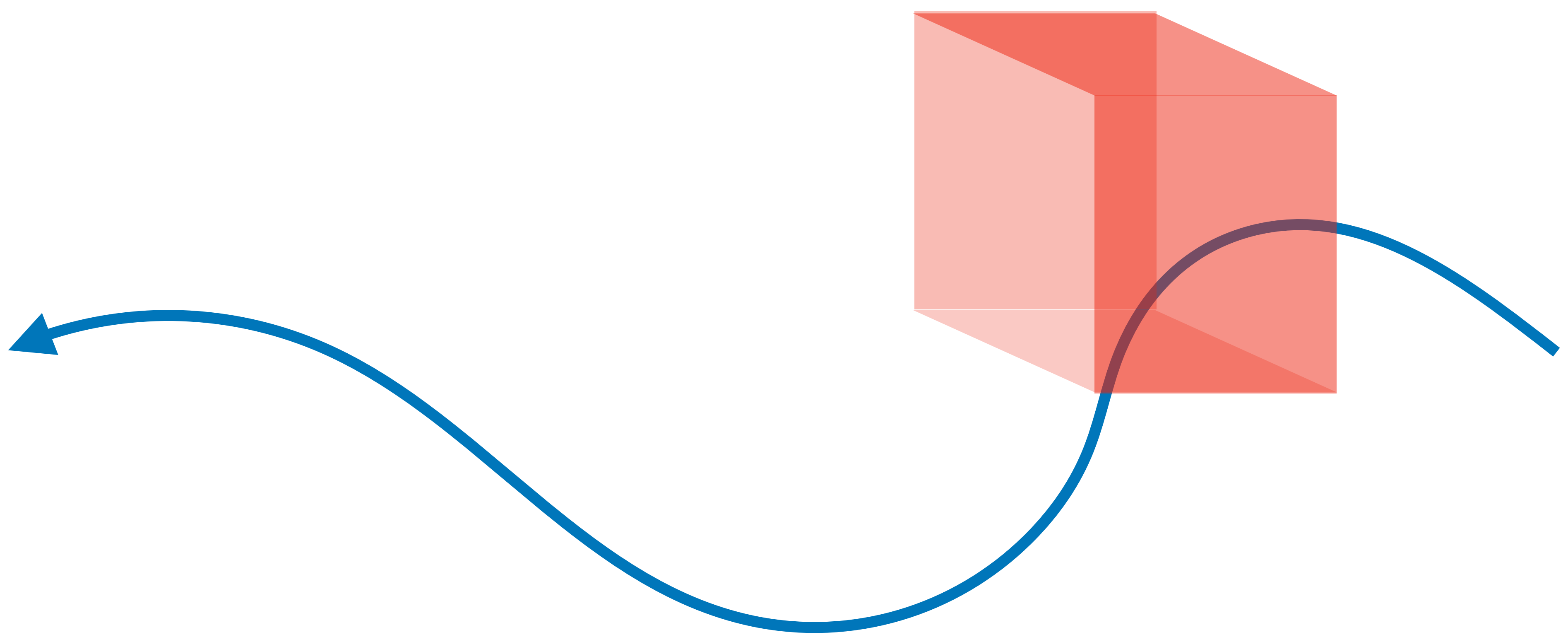
- I_r : a square interval box with a radius r whose midpoint $x_0 = m(I_r)$ approximates $x(0)$
- $dt \in (0,1)$: the initial step size
- $T_{t_0,dt} = [t_0, t_1]$ where $t_0 = 0$ and $t_1 = t_0 + dt$
- $\lambda > 1$: a scaling constant

While $t_0 < 1$ **do**

If Krawczyk test failed **then**



Algorithm

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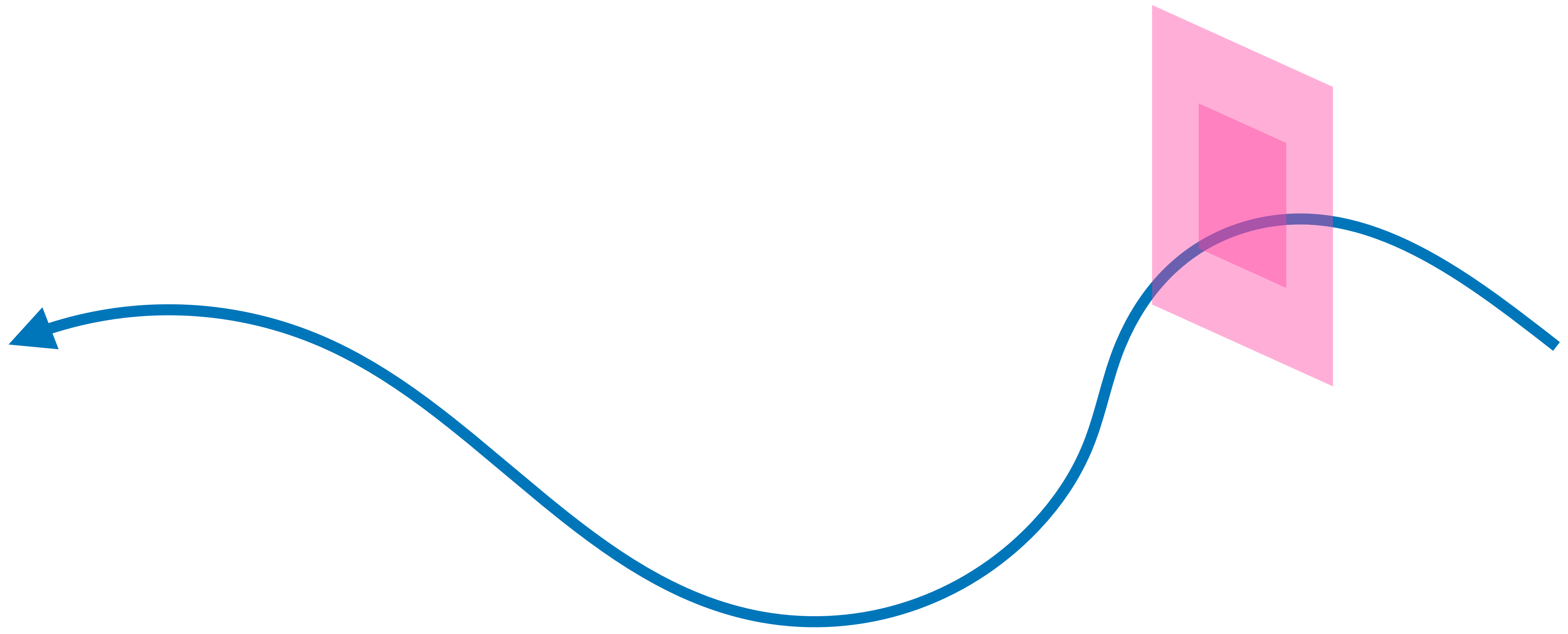
- $H(x, t) = F(x; p(t))$ a parameter homotopy from $t = 0$ to $t = 1$
- $x(t)$: a nonsingular solution path in $\mathbb{C}^n$
- I_r : a square interval box with a radius r whose midpoint $x_0 = m(I_r)$ approximates $x(0)$
- $dt \in (0,1)$: the initial step size
- $T_{t_0,dt} = [t_0, t_1]$ where $t_0 = 0$ and $t_1 = t_0 + dt$
- $\lambda > 1$: a scaling constant

While $t_0 < 1$ **do**

If Krawczyk test failed **then**

Set $r = \dfrac{1}{\lambda} r$ and $dt = \dfrac{1}{\lambda} dt$



Algorithm

Input :

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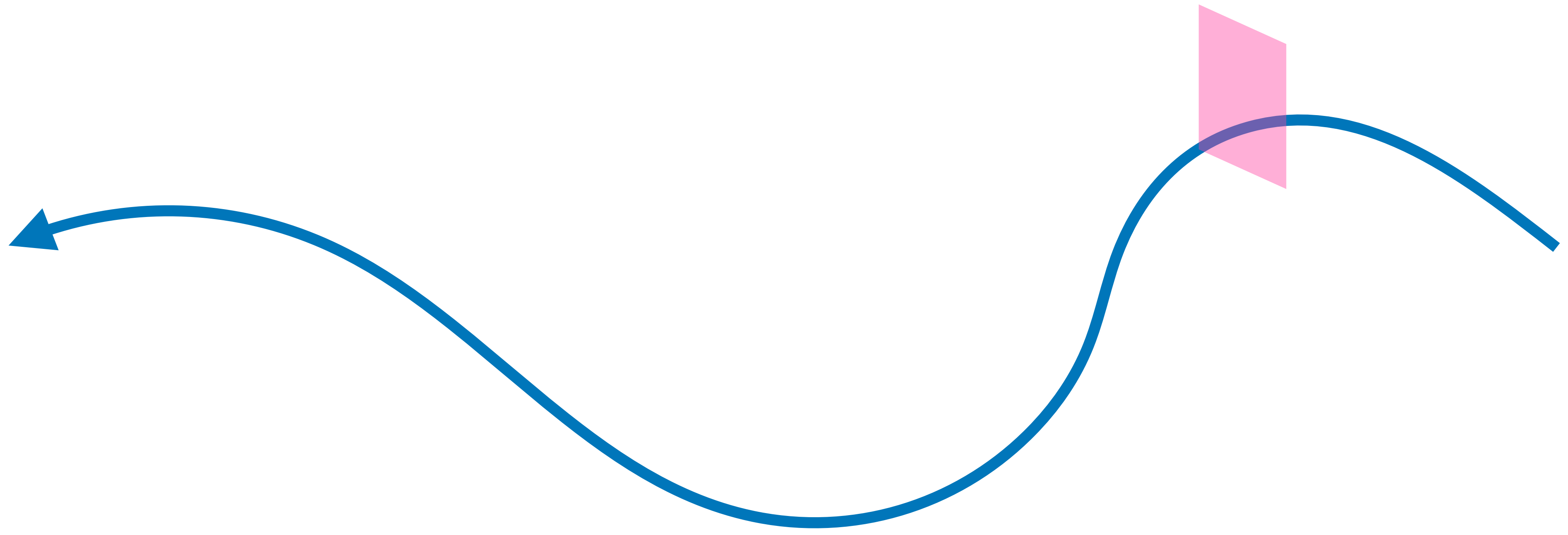
- $x(t)$: a nonsingular solution path in $\mathbb{C}^n$
- I_r : a square interval box with a radius r whose midpoint $x_0 = m(I_r)$ approximates $x(0)$
- $dt \in (0,1)$: the initial step size
- $T_{t_0,dt} = [t_0, t_1]$ where $t_0 = 0$ and $t_1 = t_0 + dt$
- $\lambda > 1$: a scaling constant

While $t_0 < 1$ **do**

If Krawczyk test failed **then**

Set $r = \dfrac{1}{\lambda} r$ and $dt = \dfrac{1}{\lambda} dt$



Algorithm

Input :

- $H(x, t) = F(x; p(t))$ a parameter homotopy from $t = 0$ to $t = 1$
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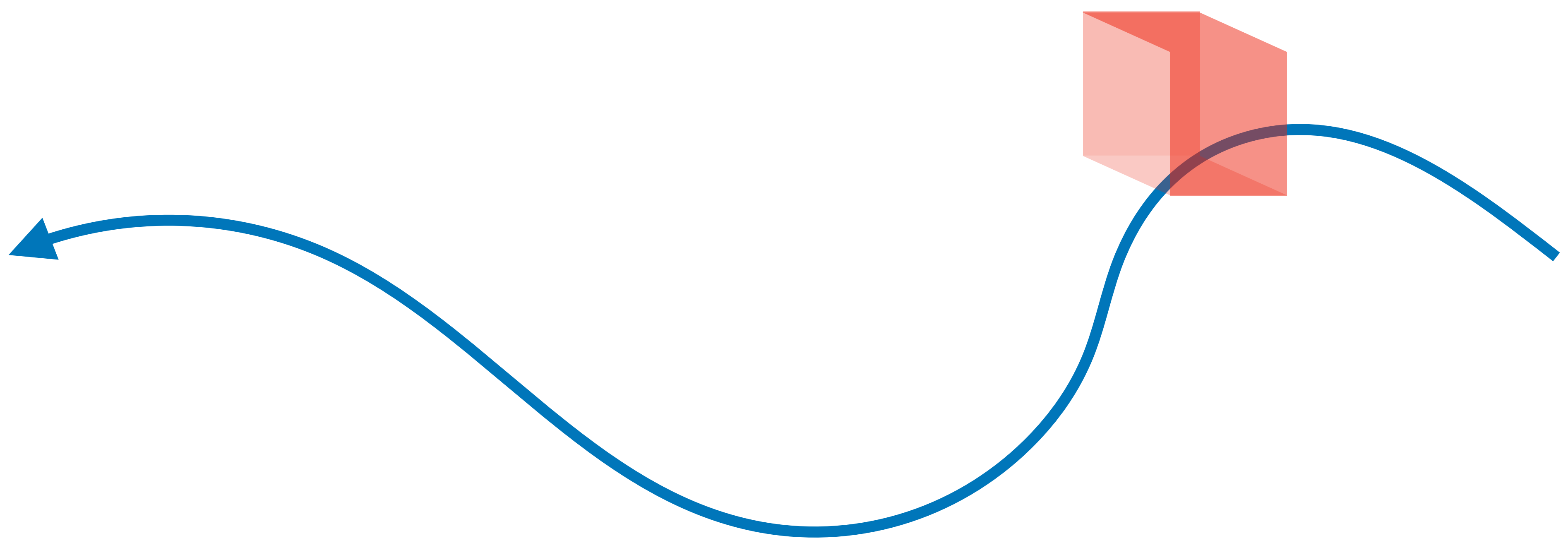
- I_r : a square interval box with a radius r whose midpoint $x_0 = m(I_r)$ approximates $x(0)$
- $dt \in (0,1)$: the initial step size
- $T_{t_0,dt} = [t_0, t_1]$ where $t_0 = 0$ and $t_1 = t_0 + dt$
- $\lambda > 1$: a scaling constant

While $t_0 < 1$ **do**

If Krawczyk test failed **then**

Set $r = \dfrac{1}{\lambda} r$ and $dt = \dfrac{1}{\lambda} dt$



Algorithm

Algorithm 3 Krawczyk homotopy (tilted)

Input:
- A parameter homotopy $H(x,t) = F(x; p(t)) : \mathbb{C}^n \times [0,1] \to \mathbb{C}^n$ analytic in x and linear in p,
- a point x_0 approximating $x(0)$, for some nonsingular solution path $x(t) : [0,1] \to \mathbb{C}^n$ such that $H(x(t), t) = 0$,
- a positive number $r > 0$ for the initial radius,
- a time-step size $dt \in (0,1)$, and
- a scaling constant $\lambda > 1$.

Output: A certified approximation of $x(1)$.

Set $t_0 = 0$ and $t_1 = dt$.
Run **Preconditioning**$(H(x,t), r, t_0, t_1, x_0)$ to compute $x_1, \hat{H}(x,t), I_r$ and $T_{t_0,dt}$.
Compute $Y := \partial_x \hat{H}(0, t_0)^{-1}$.
while $t_0 < 1$ **do**
 Run Krawczyk test with $K_{0,Y}(I_r, T_{t_0,dt})$.
 if Krawczyk test passed **then**
  Set $r = \lambda r$ and $dt = \lambda dt$.
  Refine x_1
  Set $x_0 = x_1, t_0 = t_1$, and $t_1 = t_0 + dt$.
  Run **Preconditioning**$(H(x,t), r, t_0, t_1, x_0)$ to compute $x_1, \hat{H}(x,t), I_r$ and $T_{t_0,dt}$.
  Compute $Y := \partial_x \hat{H}(0, t_0)^{-1}$.
 else
  Set $r = \frac{1}{\lambda} r$ and $dt = \frac{1}{\lambda} dt$.
  Run **Preconditioning**$(H(x,t), r, t_0, t_1, x_0)$ to compute $x_1, \hat{H}(x,t), I_r$ and $T_{t_0,dt}$.
 end if
end while
Find a point x_1 by refining $s(1)$ with the system $H(x,1)$.
Return x_1.

Termination

Theorem (Duff-L.). Let $H(x,t) = t\gamma G(x) + (1-t)F(x)$ be twice differentiable with an exact solution $x^\star$ to $H(x,t_0)$.

Termination

Theorem (Duff-L.). Let $H(x,t) = t\gamma G(x) + (1-t)F(x)$ be twice differentiable with an exact solution $x^\star$ to $H(x,t_0)$. Consider a fixed constant $L \geq \left\| \square\, \partial_x^2 H(I_1, [0,1]) \right\|$.

Termination

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Corollary (Duff-L.). Assuming that $x(t)$ is nonsingular at any $t \in [0,1]$, the tracking terminates in finitely many steps for the homotopy $H(x,t)$.

Implementation detail

Implementation in Macaulay2

Not the optimal version yet due to incomplete implementation of interval arithmetic in M2 (a proof-of-concept implementation)

A scaling constant $\lambda = 3$ is used

Experiments

- Comparison with the known method

  The certified homotopy **(Beltran-Leykin 2012 2013)** is based on alpha theory. Compare the number of steps for each solution path for benchmark problems. The initial radius and step-size, $r = 0.4$ and $dt = 0.1$ were used

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System	# roots	Average	Max	Min	Average(BL 2012)
Random (2,2,2)	8	317.75	509	203	198.5
Random (2,2,2,2)	16	563.25	1257	211	813.812
Random (2,2,2,2,2)	32	675.3125	5119	209	1542.5
Random (2,2,2,2,2,2)	64	1166.421875	5415	267	2211.58

- In many examples, Krawczyk homotopy requires less number of steps in average than **BL 2012**

Experiments

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$(dt, r) = (.2, .4)$	134.75	181	83
$(.4, .4)$	96.5	170	44
$(.6, .4)$	98.625	166	32
$(.8, .4)$	96.75	194	24
$(.9, .4)$	100.5	216	23

	Average	Max	Min
$(.02, .04)$	135.625	189	85
$(.04, .04)$	99.5	175	48
$(.06, .04)$	98.875	171	34
$(.08, .04)$	99.5	195	28
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- The performance of the algorithm depends on the ratio between dt and r (rather than their specific values)

Summary

- Certified homotopy tracking guarantees the correctness of homotopy tracking without path jumping or crossing
- Certified tracking assisted by interval arithmetic may be more competitive to alpha theory-based known methods
- Robust implementation to deal with larger size examples is expected

Thanks For Your Attention!

(https://arxiv.org/abs/2402.07053)