NumericalCertification
-- certifying roots of polynomial systems on Macaulay2

Author

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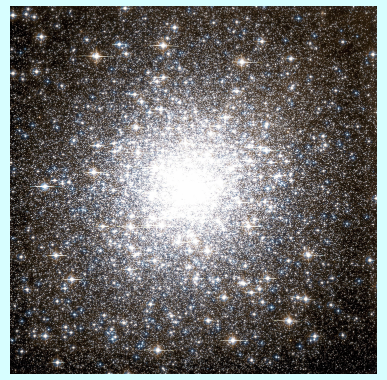
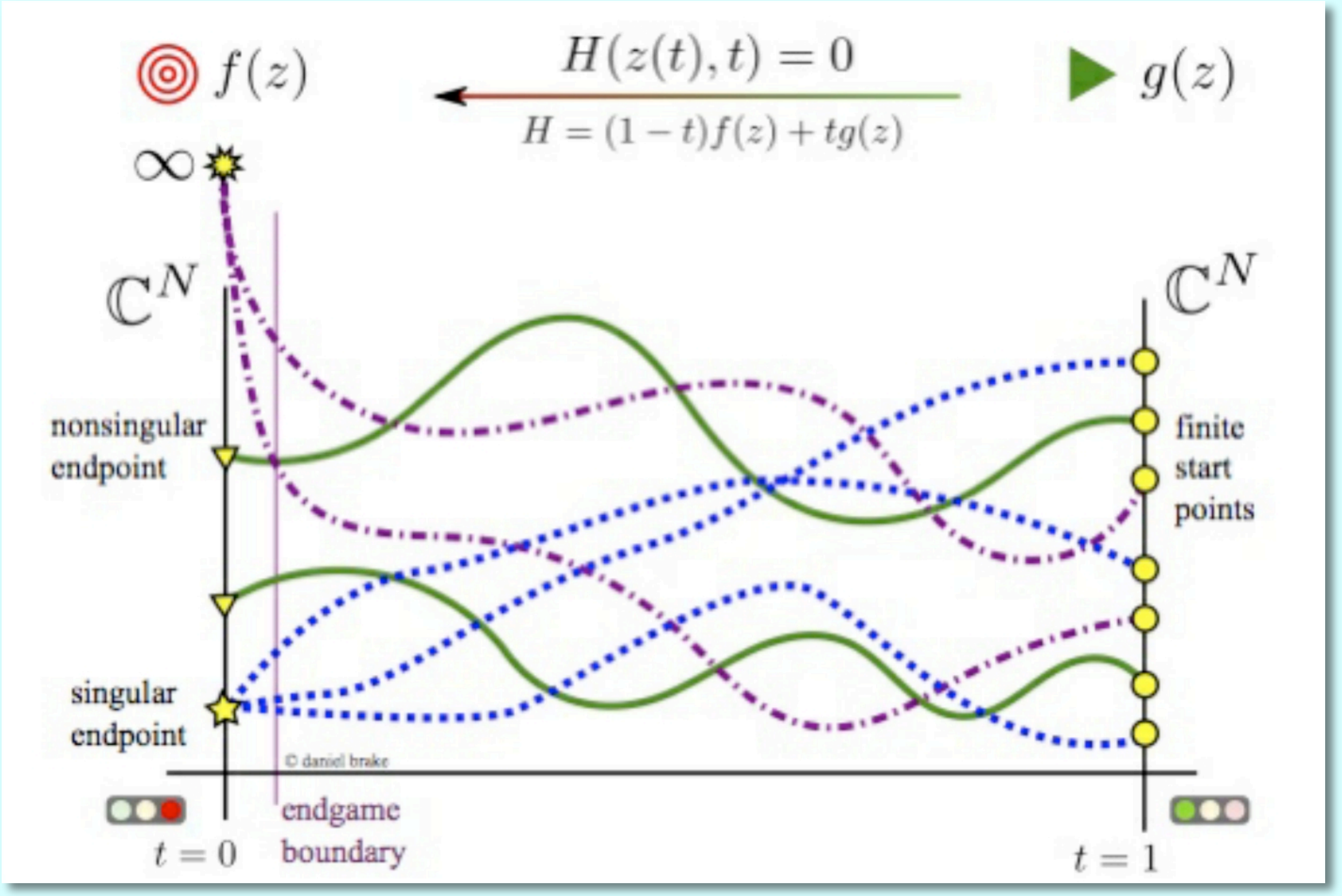
Event

- Macaulay2 conference at CSU
- May 29th 2022



Numerical algebraic geometry

-- Use numerical techniques to approach problems in algebraic geometry

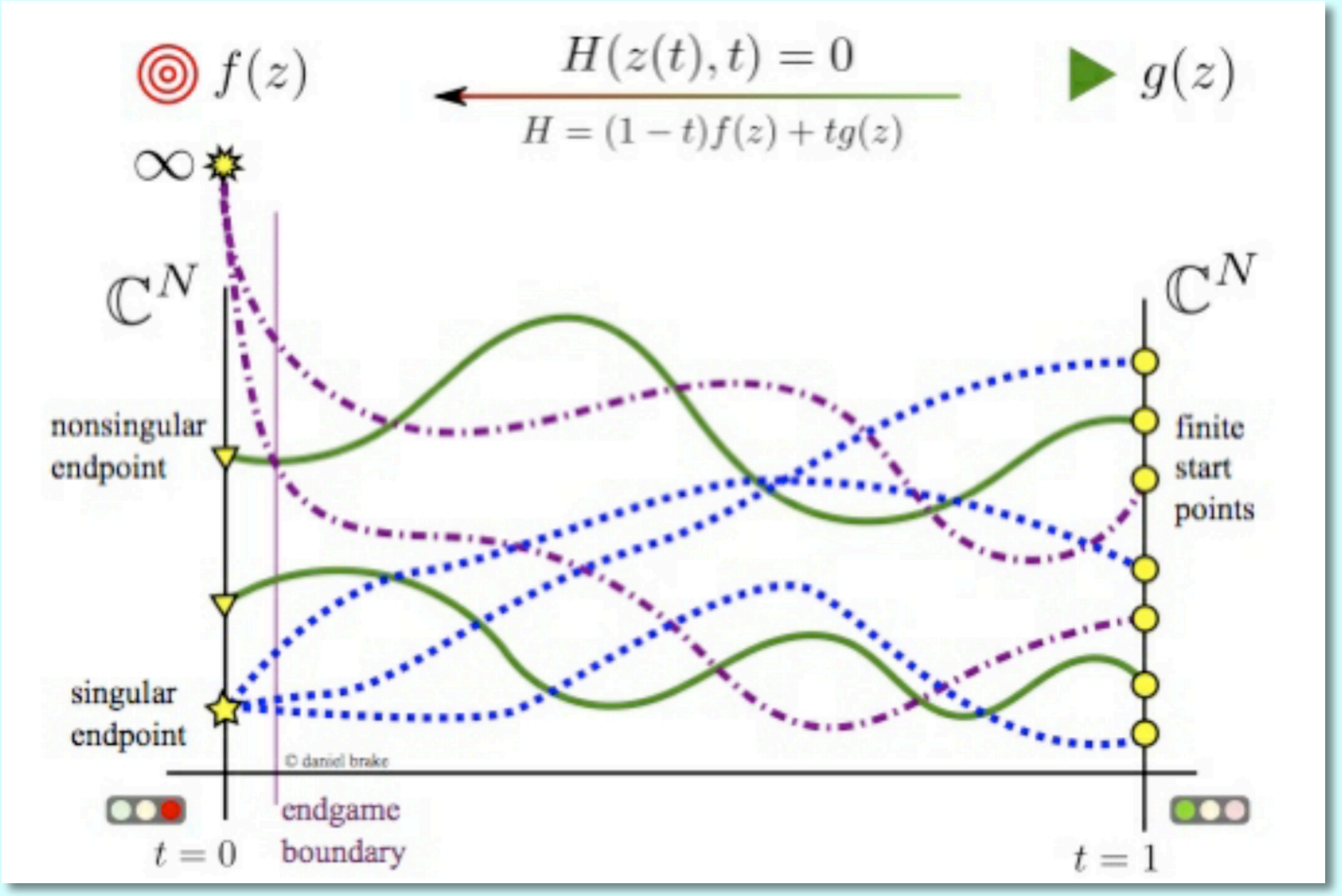


https://ofloveandhate-pybertini.readthedocs.io/en/feature-readthedocs_integration/intro.html#

- Homotopy continuation

Numerical algebraic geometry

-- Use numerical techniques to approach problems in algebraic geometry



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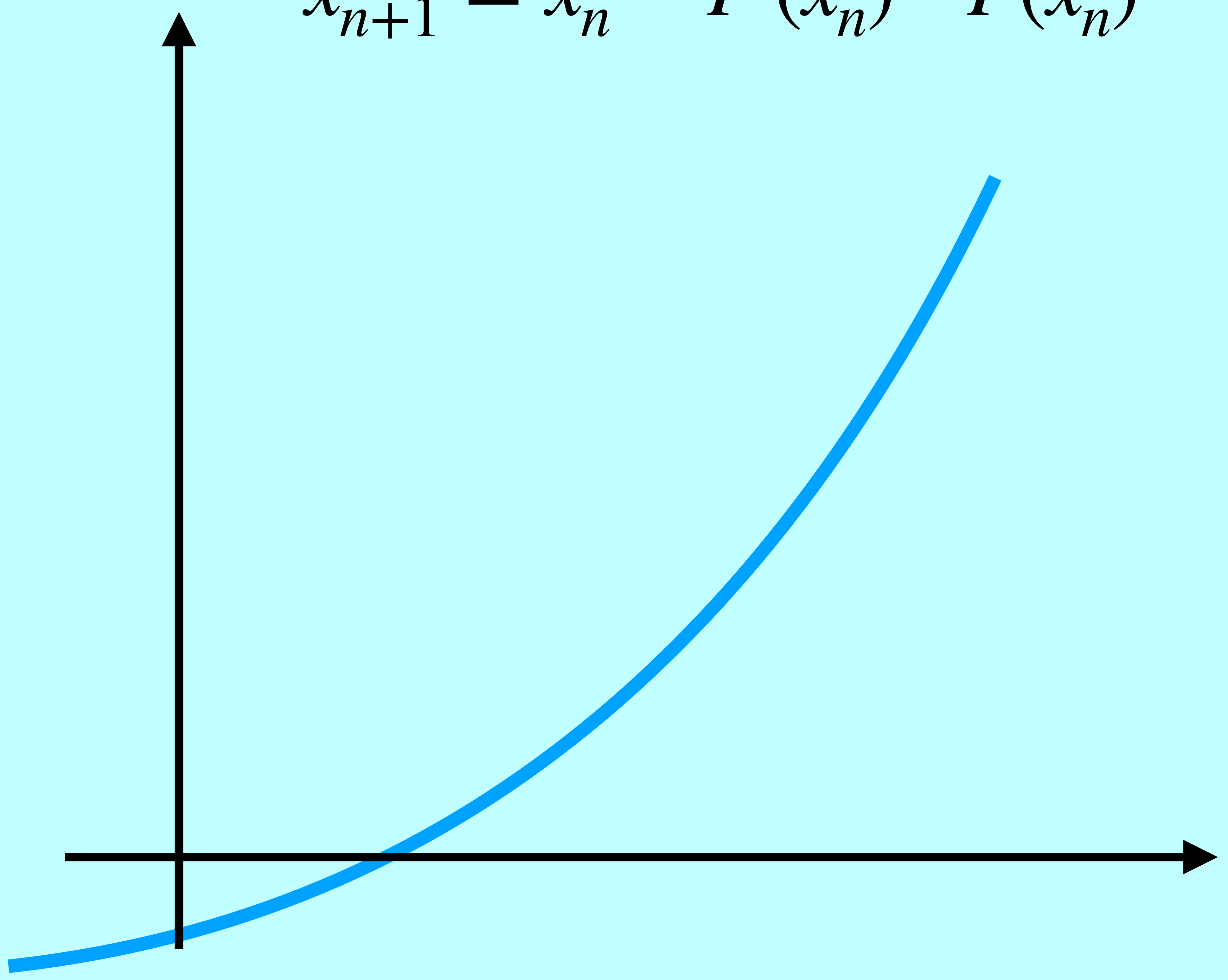
- Homotopy continuation
- Mostly rely on heuristic : Certification is needed

Newton's method -- Use tangent lines to approximate a root

$$x_{n+1} = x_n - F'(x_n)^{-1}F(x_n)$$



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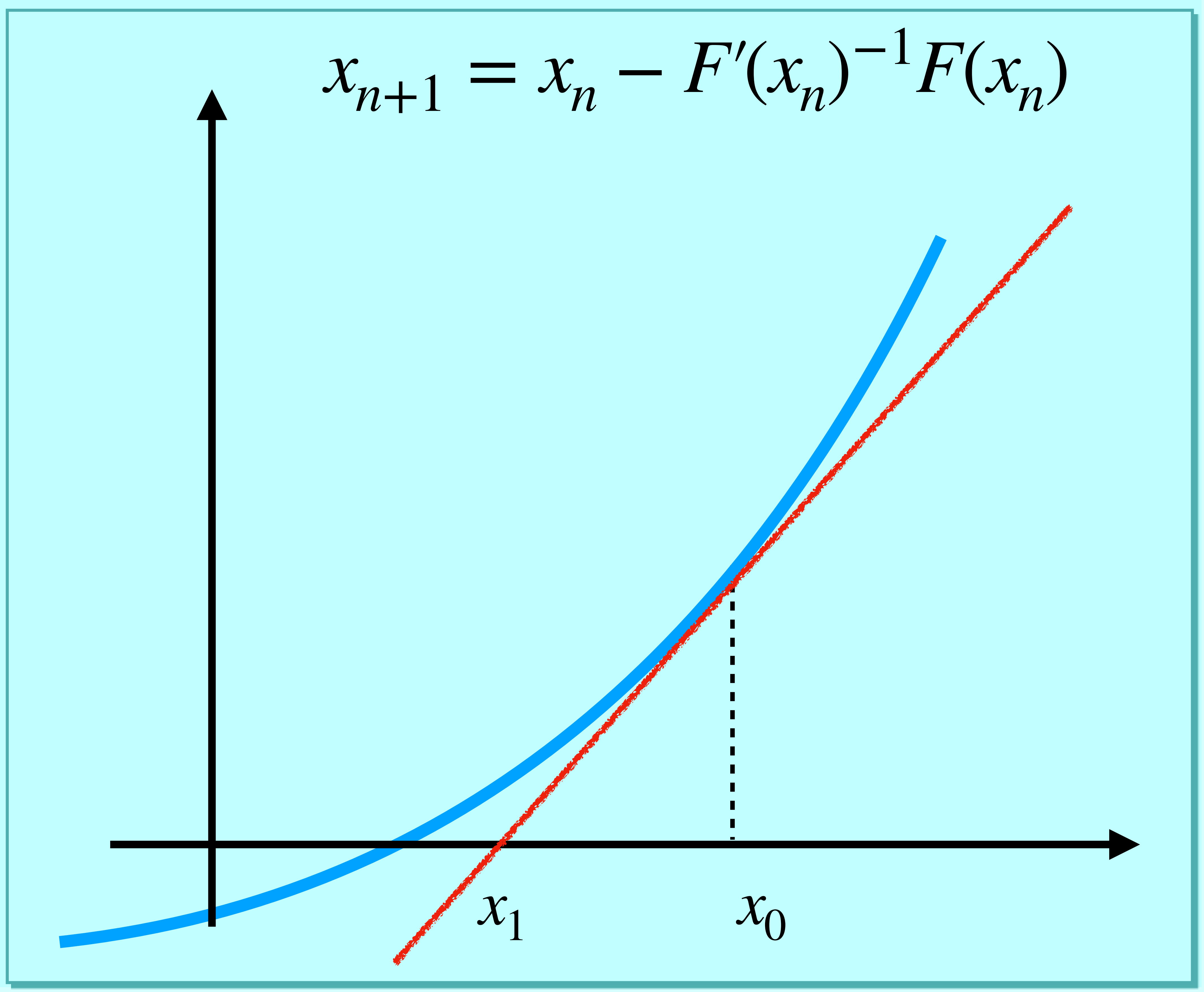

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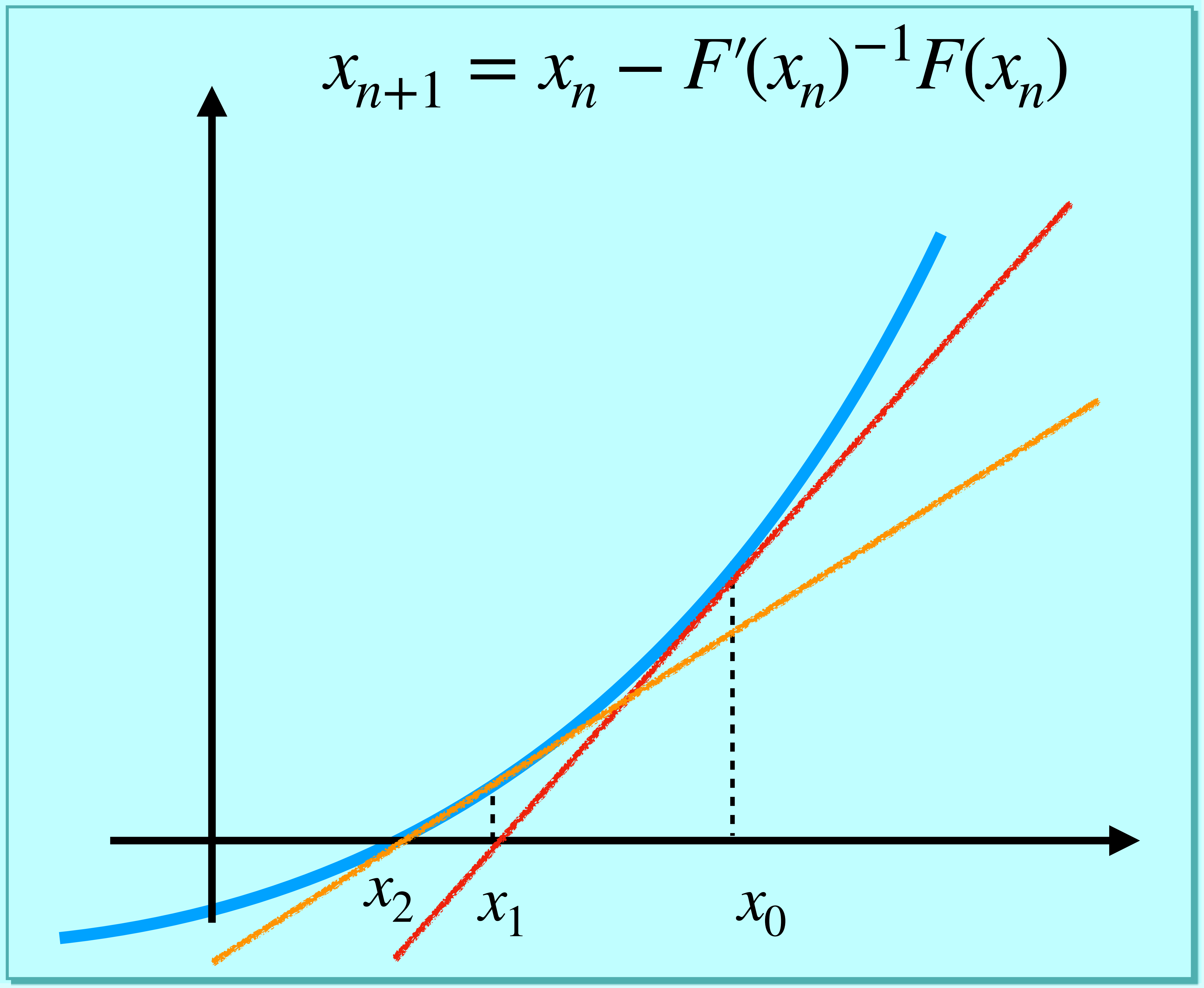

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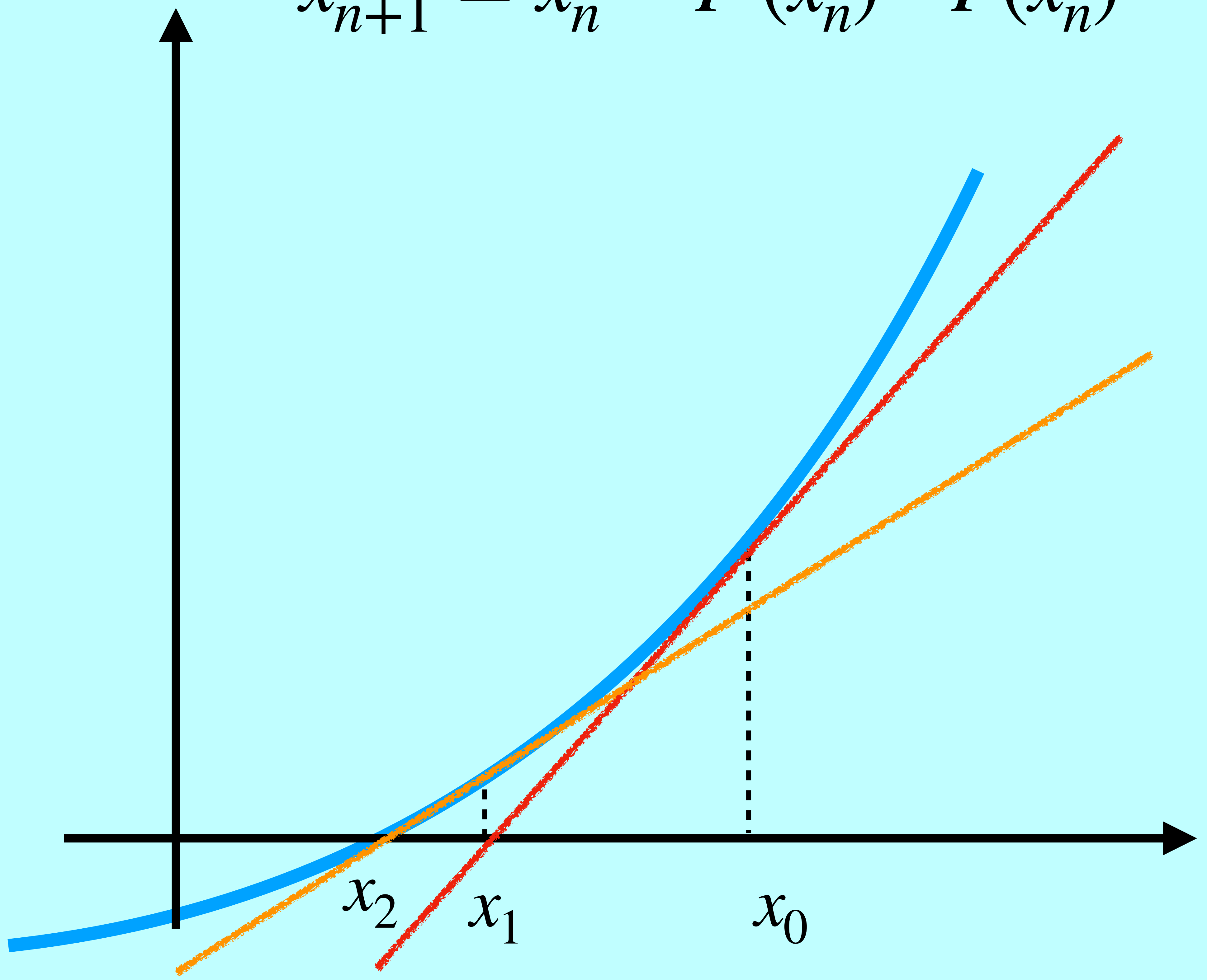

Newton’s method shows fast convergence

- Quadratic convergence
- Approximates root precisely within few iterations

Newton’s method -- Use tangent lines to approximate a root

Newton’s method shows fast convergence

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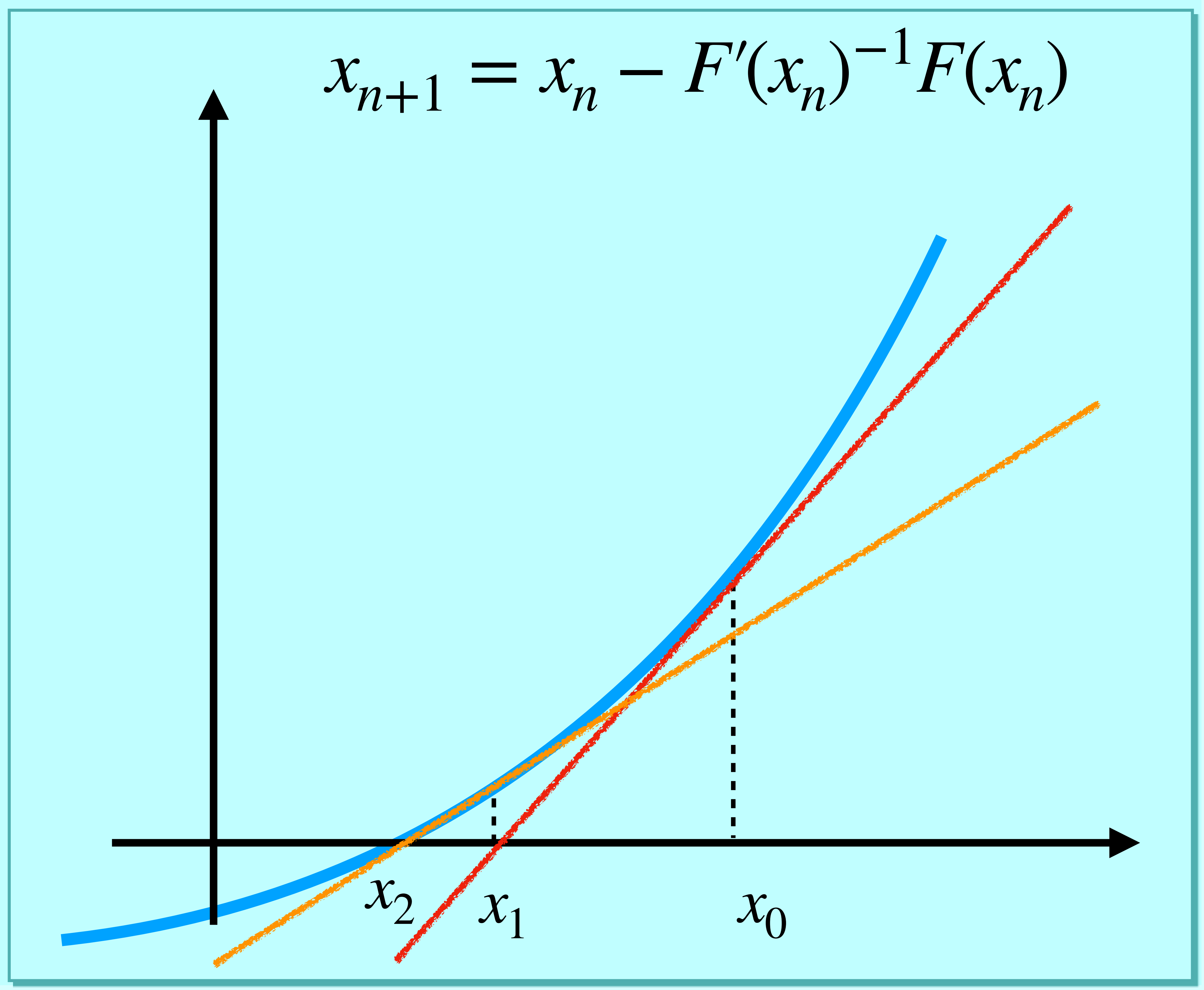
ex) $f(x) = x^2 - 2, \quad x_0 = 1$

$x_1 = 1.5 \;\; x_2 = 1.4167 \;\; x_3 = 1.414213562$

$$x_4 = 1.4142135623731$$

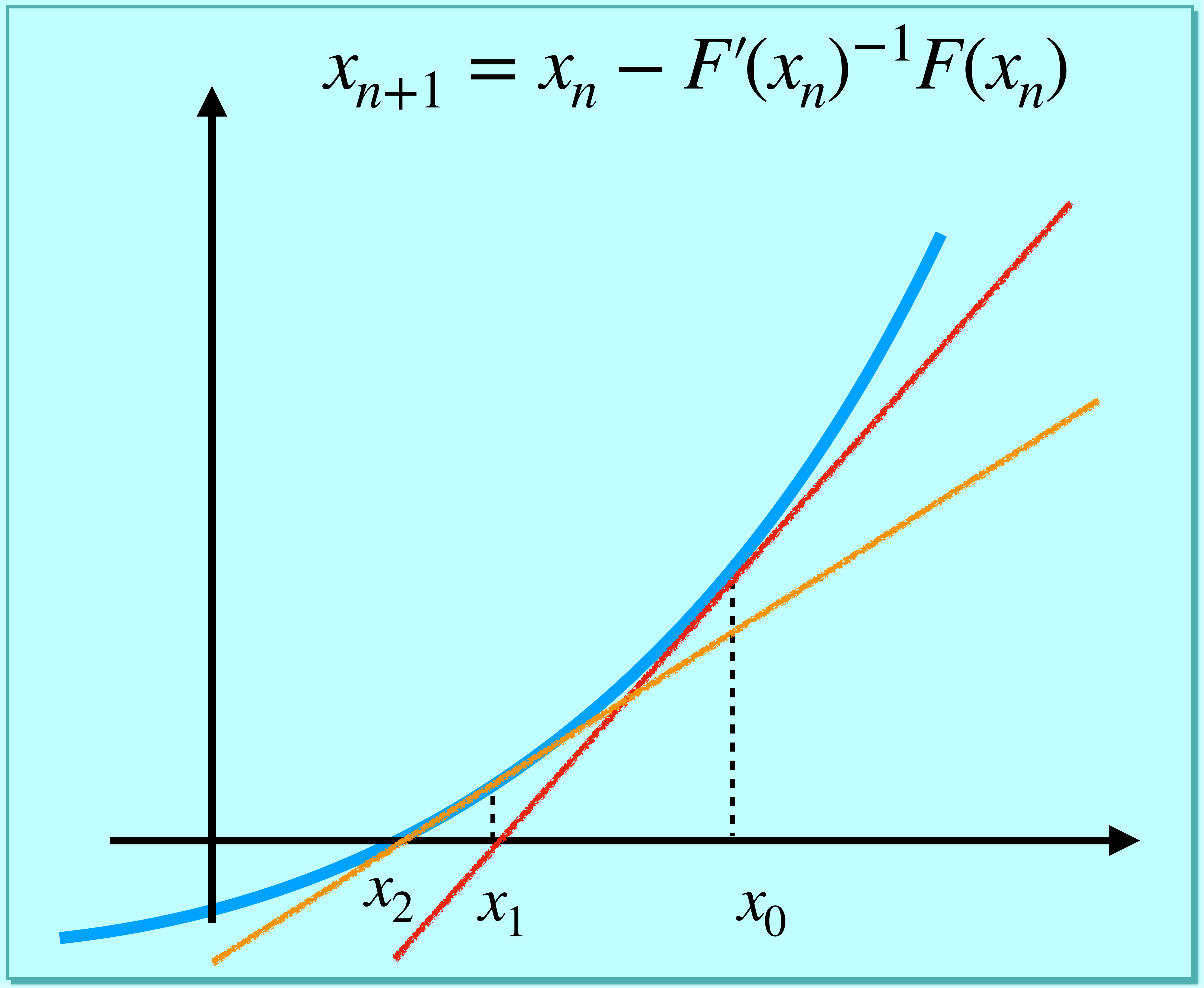
$$\sqrt{2} = 1.4142135623731\cdots$$



Newton's method -- Use tangent lines to approximate a root

Newton's method may fail

- Depends on where to start from.
- Works only for regular roots.

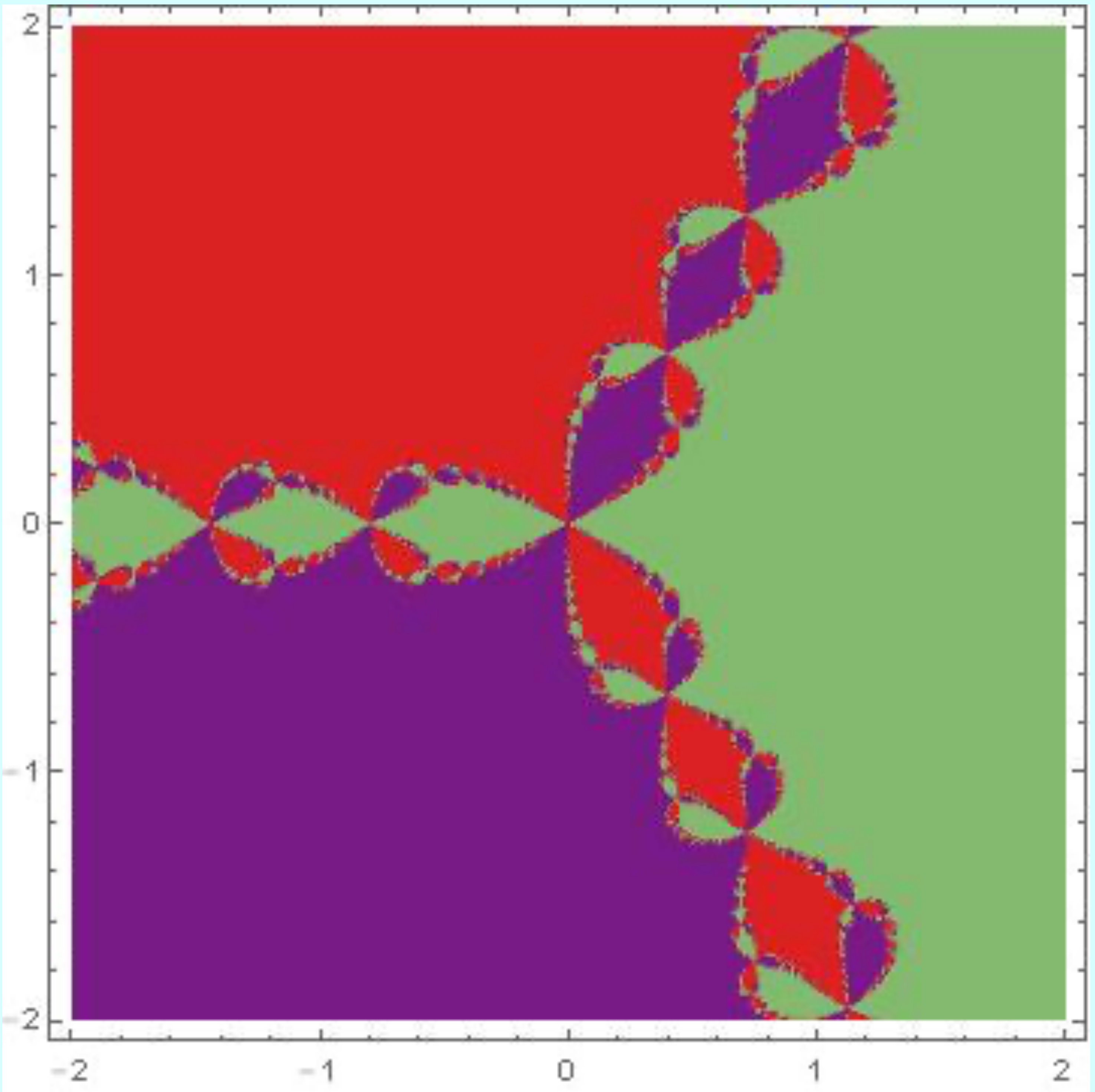


Certifying solutions

Given a point in $\mathbb{C}^n$ (or $\mathbb{R}^n$), apply an algorithm to construct a compact region I to ensure

1. the existence
2. the uniqueness

of a root of a system in I.



https://mathematica.stackexchange.com/questions/101255/basins-of-attraction-using-newtons-method

Basin of attraction for $z^3 - 1$

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Implementations

- alphaCertified (Hauenstein-Sottile 2012)
- certify in HomotopyContinuation.jl (Breiding-Rose-Timme 2020)

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- NumericalCertification.m2 (Lee 2019)

Two paradigms -- Smale's α-theory

Certify quadratic convergence of a numerical root

Let $x = (x_1, \ldots, x_n) \in \mathbb{C}^n$ a point and $N_F(x) = x - F'(x)^{-1}F(x)$. Define

$$\alpha(F, x) := \beta(F, x)\gamma(F, x)$$

$$\beta(F, x) := \|x - N_F(x)\| = \|F'(x)^{-1}F(x)\|$$

$$\gamma(F, x) := \sup_{k \geq 2} \left\| \frac{F'(x)^{-1}F^{(k)}(x)}{k!} \right\|^{\frac{1}{k-1}}$$

If $\alpha(F, x) < \dfrac{13 - 3\sqrt{17}}{4}$, then x converges quadratically to a root $x^\star$ and $\|x - x^\star\| \leq 2\beta(F, x)$.

Two paradigms -- Smale's α-theory

Proposition (Shub-Smale 1993).

F be a square polynomial system with nonsingular $F'(x)$ at $x \in \mathbb{C}^n$. Define

$$\mu(F,x) := \max\{1, \|F\| \, \|F'(x)^{-1}\Delta_F(x)\|\}$$

with the operator norm. Then,

$$\gamma(F,x) \leq \frac{\mu(F,x)d^{\frac{3}{2}}}{2\|(1,x)\|}$$

where d is the maximum degree of the polynomials.

Two paradigms -- Krawczyk method

Combine interval arithmetic and Newton's method

- Interval arithmetic : For an arithmetic operator $\odot$, define $[a,b] \odot [c,d] = \{x \odot y \mid x \in [a,b], y \in [c,d]\}$

Define the Krawczyk operator

$$K_{x,Y}(I) = x - YF(x) + (Id - Y \square F'(I))(I - x)$$

- I : an interval to certify
- $\square F(I) := \{F(x) \mid x \in I\}$: an interval extension of F over I
- x : a point in I
- Y : an invertible matrix

Two paradigms -- Krawczyk method

Theorem (Krawczyk 1969).

The following holds:

1. If $x^\star \in I$ is a root of F, then $x^\star \in K_{x,Y}(I)$
2. If $K_{x,Y}(I) \subset I$, then there is a root of F in I (existence)
3. If I has a root and $\sqrt{2}||Id - Y \square F'(I)|| < 1$, then there is a root of F in I and it is unique where $|| \cdot ||$ is the maximum operator norm (uniqueness)

Demo 1 -- Regular solution certification

Certifying singular solutions

$$F(x, y, z) = \left[x^3 - y\,z, y^3 - x\,z, z^3 - x\,y\right]$$

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o1 = has 16 regular roots and 1 multiple root at the origin with multiplicity 11.
     Solving F using numerical solver gives a cluster of 11 numerical roots at
     the origin.

o2 = How to certify the cluster of roots?
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Deflation -- Recovering quadratic convergence for singular solutions

Introduce more variables and equations and generate an augmented system with reduced multiplicity.

Deflation -- Recovering quadratic convergence for singular solutions

Deflation (Leykin-Verschelde-Zhao 2006)

- F : a $n \times n$-square polynomial system with an isolated multiple root $x^\star$ such that $\dim \ker F'(x^\star) = \kappa$
- B : a generic $n \times (n - \kappa + 1)$ matrix
- b : a generic vector in $\mathbb{C}^{n-\kappa+1}$.

There is a unique vector $\lambda \in \mathbb{C}^{n-\kappa+1}$ such that $(x^\star, \lambda) \in \mathbb{C}^{2n-\kappa+1}$ is a root with reduced multiplicity of $H = \begin{bmatrix} F \\ F' \cdot B \cdot \lambda \\ b^\top \cdot \lambda - 1 \end{bmatrix}$.

If $(x^\star, \lambda)$ remains singular, iterate the process.
(The algorithm terminates within finitely many iterations.)

Deflation -- Recovering quadratic convergence for singular solutions

Construct a system $F(x) + F'(x) \cdot \lambda$ with a randomly chosen kernel vector λ.

Apply regular solution certification.

Demo 2 -- Singular solution certification

certifySolutions -- certify a given list of solutions

Thank you for your attention!