Smale's Alpha Theory — Verifying Newton's Method

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Newton's Method

Let $f : \mathbb{C} \to \mathbb{C}$ be a polynomial. Define,

$$N(f, x_0) = \begin{cases} x_0 - f(x_0)/f'(x_0) & \text{if } f'(x_0) \neq 0, \\ x_0 & \text{if } f'(x_0) = 0. \end{cases}$$

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Convergence

$$\lim_{k \to \infty} N^k(f, x_0) = \xi \text{ a root of } f$$

Example

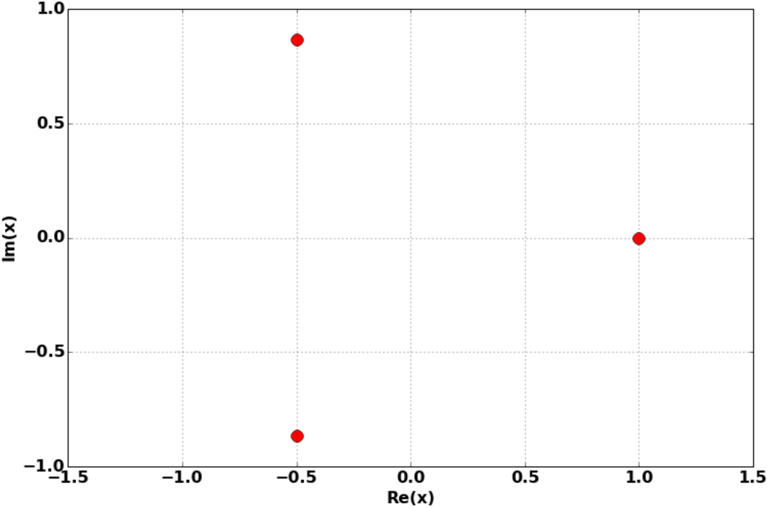
Roots of a Simple Cubic

$$f(x) = x^3 - 1$$

Actual roots:

$$\xi_k = e^{2\pi i k/3}, \text{for } k = 0, 1, 2.$$

Example: Actual Roots



Example: What is a “Good Guess”?

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- white region $\to$ guesses converging to ξ_0,
- grey region $\to$ guesses converging to ξ_1,
- black region $\to$ guesses converging to ξ_2,

(Apply Newton’s Method to each guess until we reach a root.)

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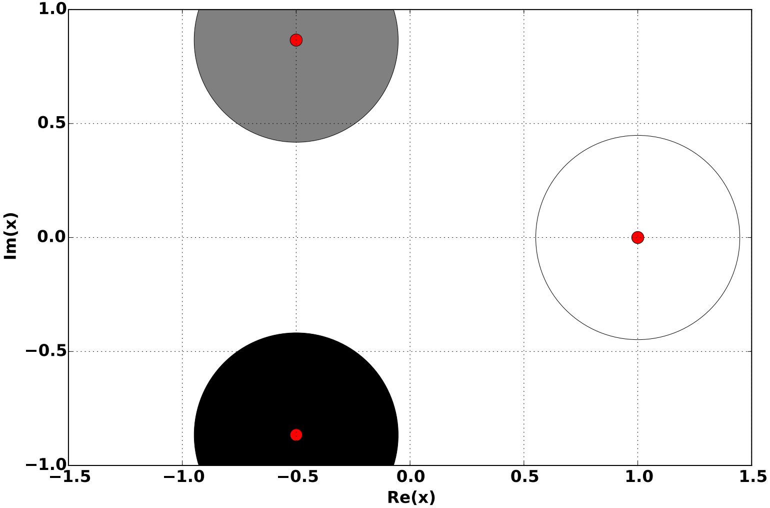

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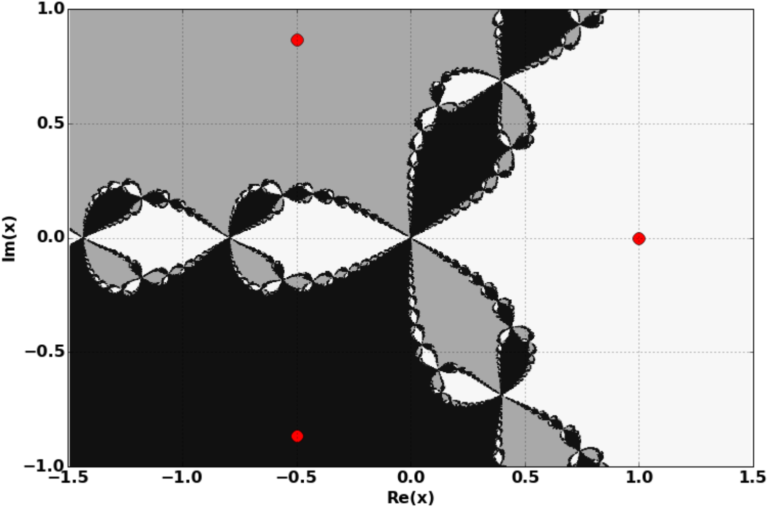

There are many terrible guesses.

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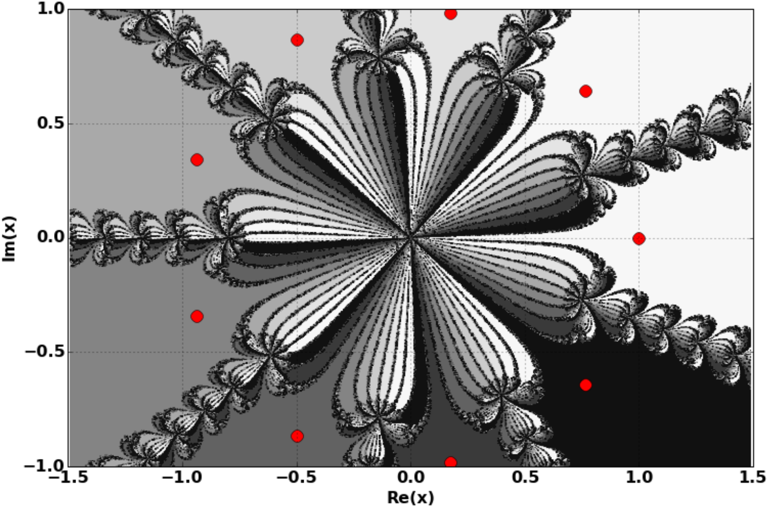
(Even guesses closer to some roots converge to other roots.)

Example: Roots of $f(x) = x^9 - 1$



Two Questions

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But...

...can we do these a priori? *(w/o knowing location of roots)*

Terminology

Let $f : \mathbb{C} \to \mathbb{C}$ be a polynomial.

- Define: $x \in \mathbb{C}$ is an **approximate solution** to f with **associated solution** $\xi \in \mathbb{C}$ if

$$\left| N^{(k)}(f, x) - \xi \right| \leq \left(\tfrac{1}{2}\right)^{2^k - 1} |x - \xi|$$

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- approximate solutions converge quadratically to their associated soltuions
- *"x lies inside the quadratic convergence region of ξ"*

Quadratic Convergence Region

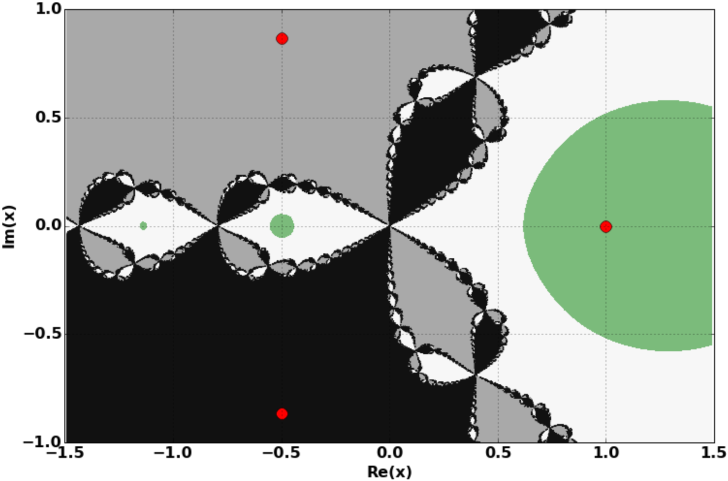

Figure: Quadratic convergence region of $\xi = 1$ for $f(x) = x^3 - 1$.

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Determine if x is an **approximate solution**.

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- **Smale's Alpha Theory**: sufficient conditions for x to be in *some* quadratic convergence region

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$$\beta(f,x) := |x - N(f,x)| = \left|f(x)/f'(x)\right|$$
$$\gamma(f,x) := \max_{k\geq 2}\left|\frac{f^{(k)}(x)/f'(x)}{k!}\right|^{\frac{1}{k-1}}$$

Question #1: Converging to a Given Root

Smale Theorem #1

If $f : \mathbb{C} \to \mathbb{C}$ is a polynomial and $x \in \mathbb{C}$ such that

$$\alpha(f, x) \leq \frac{13 - 3\sqrt{17}}{4} \approx 0.157671$$

then x is an **approximate solution** to f.

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Additionally,

$$|x - \xi| \leq 2\beta(f, x)$$

where ξ is the **associated solution** to x.

Alpha Region

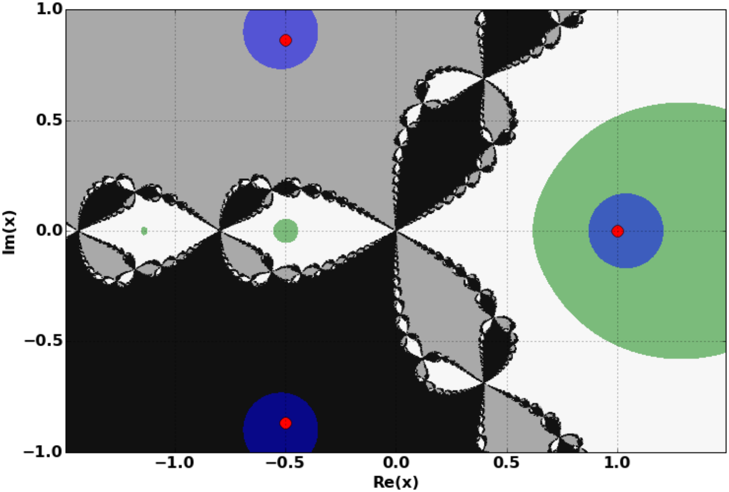

Figure: Region where $\alpha(f, x) < 0.157\ldots$ for $f(x) = x^3 - 1$.

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  - doesn't say which root (but β gives us an idea)
  - alpha region much smaller than quad. conv. region

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then

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- **Homework:** prove this

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- **fact:** polynomial roots vary continuously as function of coefficients

$$\text{roots “above” } x : \qquad y_1(x),\ y_2(x),\ y_3(x)$$

Example: $f(x, y) = y^3 - x$

Let x_i range from $x_0 = 1$ to $x_N = 8$:

$$y_1(1) = 1$$
$$y_2(1) = e^{2\pi i/3}$$
$$y_3(1) = e^{4\pi i/3}$$
$$\vdots$$
$$y_1(8) = 2$$
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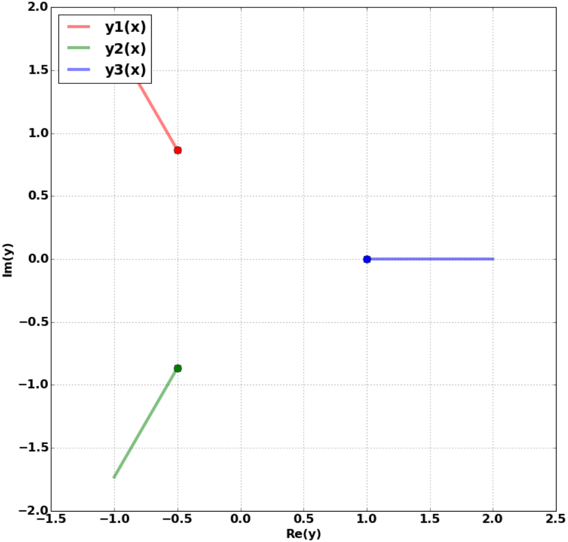

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Let x_i range along the complex circle

$$x(t) = e^{2\pi i t} - 2$$
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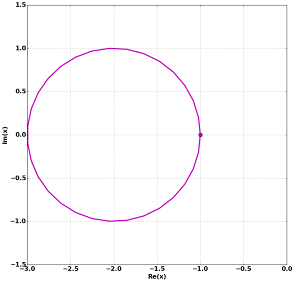

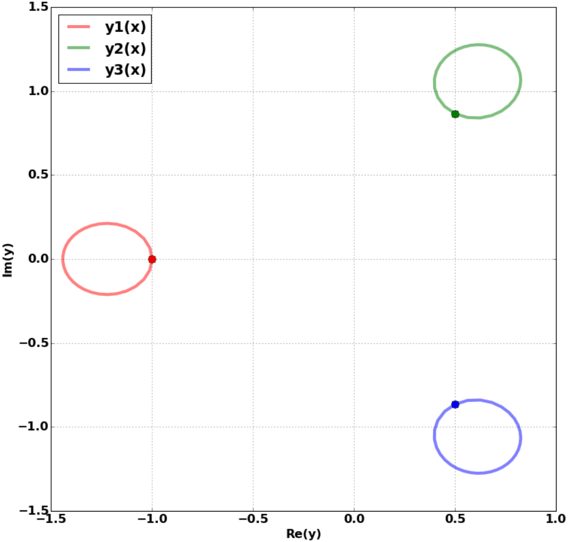

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- **Important:** must satisfy

  $$y_1(x_i) = y_1^{(i)} \quad \text{and} \quad y_1(x_{i+1}) = y_1^{(i+1)}$$

Example: $f(x, y) = y^3 - 2x^3y + x^7$

Let x_i range along the complex circle

$$x(t) = e^{2\pi it} - 2$$
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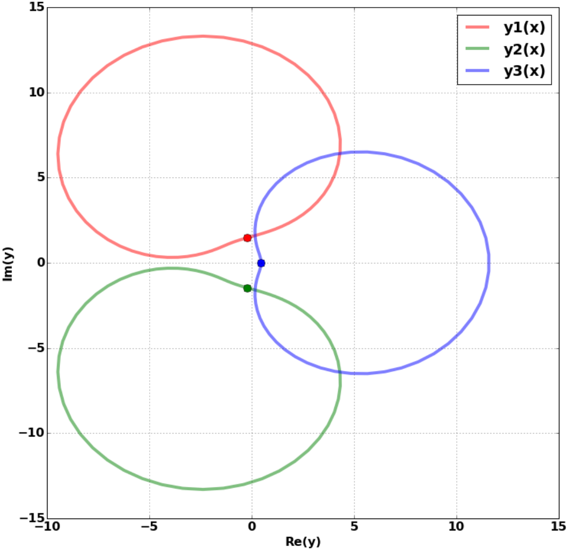
64 different x-values

small Δx means $y^{(i)}$ are good guesses for $y^{(i+1)}$



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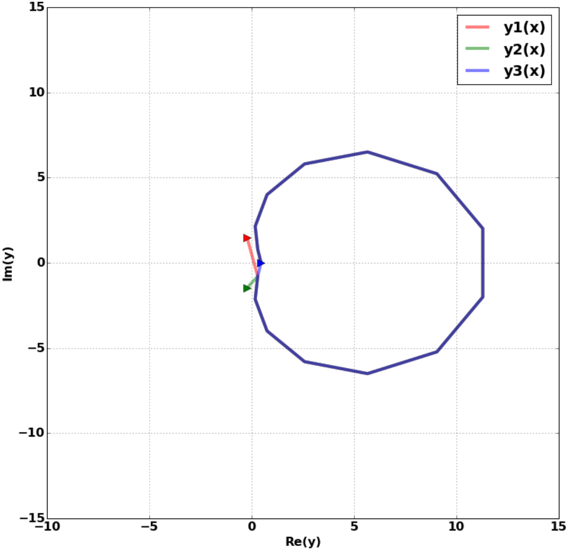
16 different x-values

Something wrong happened. (Too large Δx.)



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  - each $y_j^{(i)}$ will converge to *distinct* $y_j^{(i+1)}$ **(Use Smale Theorem #2)**

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Output: ordered y-roots $y^{i+1} = \left(y_1^{(i+1)}, \ldots, y_d^{(i+1)}\right)$ above x_{i+1}.

- such that $y_j^{(i)} \to y_j^{(i+1)}$ (same position j)

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Algorithm: `analytic`$\big(f,\, x_i,\, x_{i+1},\, y^{(i)}\big)$

1. Check that each $y_j^{(i)}$ is an **approximate solution** to

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using $\alpha(g, y_j^{(i)}) < 0.157\ldots$ If any are not, **refine step**:

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2. Determine if all **approximate solutions** $y_j^{(i)}$ will converge to distinct **associated solutions** $y_j^{(i+1)}$:

$$|y_j^{(i)} - y_k^{(i)}| > 2\left(\beta(f, y_j^{(i)}) + \beta(f, y_k^{(i)})\right), \quad \forall j, k = 1, \ldots, d.$$

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   If any are not, **refine step**.

3. Finally, Newton iterate each $y_j^{(i)}$ to $y_j^{(i+1)}$ and return.

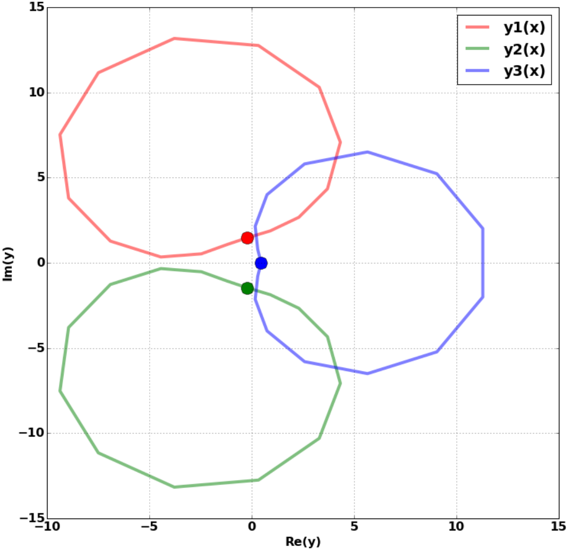
Example: $f(x, y) = y^3 - 2x^3y + x^7$

Let x_i range along the complex circle

$$x(t) = e^{2\pi it} - 2$$
$$t \in [0, 1]$$

16 different x-values

Smale guarantees we converge to the correct roots.



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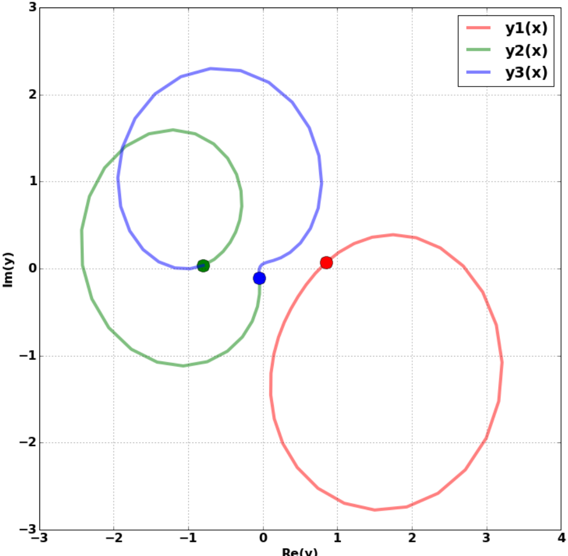
$$x(t) = \frac{1}{2}e^{2\pi it} + \beta$$
$$t \in [0, 1]$$

where

$$\beta \approx -0.8369 - 0.6081j.$$

(Branch point of curve.)



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  - Derivative $f' \to$ Jacobian Df.
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  - Definition of $\gamma(f, x)$: "max $\to$ sup".

Final Remarks

- Works for square systems of polynomials $f : \mathbb{C}^n \to \mathbb{C}^n$.
  - Derivative $f' \to$ Jacobian Df.
- Even works for smooth functions $f : \mathbb{C}^n \to \mathbb{C}^n$.
  - Definition of $\gamma(f, x)$: "max $\to$ sup".
  - Some simpler bounds on γ: results in much smaller α-region.

Thank you

Talk and code available at `www.cswiercz.info`. GitHub repo at `github.com/cswiercz/smale`.

References

- S. Smale, "Newton's method estimates from data at one point", Springer New York, 1986.
- J. D. Hauenstein, F. Sottile, "AlphaCertified: certifying solutions to polynomial systems", ACM Trans. Math. Softw., vol. 38, no. 4, pp. 1-20, 2012.