Lattice QCD **sign problem** as an **inverse problem**

Francesco Di Renzo (University of Parma and INFN)

SIGN25

Bern, 20/01/2025

+ SIGN25 +

In collaboration with P. Dimopoulos, M. Aliberti and D. Gavriel (Parma)
Bielefeld Parma Collaboration (… K. Zambello …)

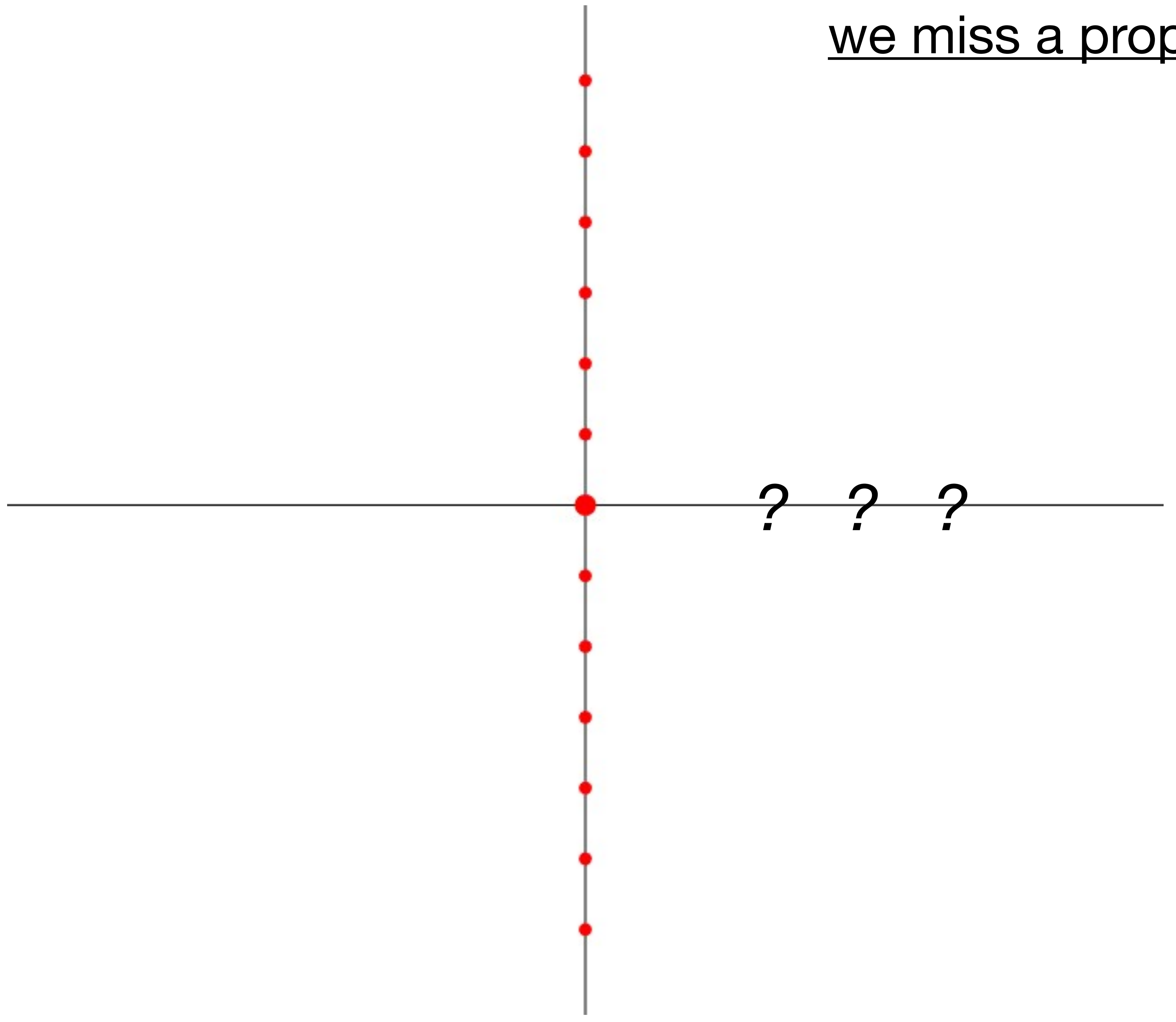
UNIVERSITÀ DI PARMA

INFN Istituto Nazionale di Fisica Nucleare

SIGN PROBLEM for finite density Lattice QCD:

we miss a properly defined (positive) measure in the path integral! … no MC simulation

(… but everything is fine on the imaginary axis)



Complex chemical potential plane

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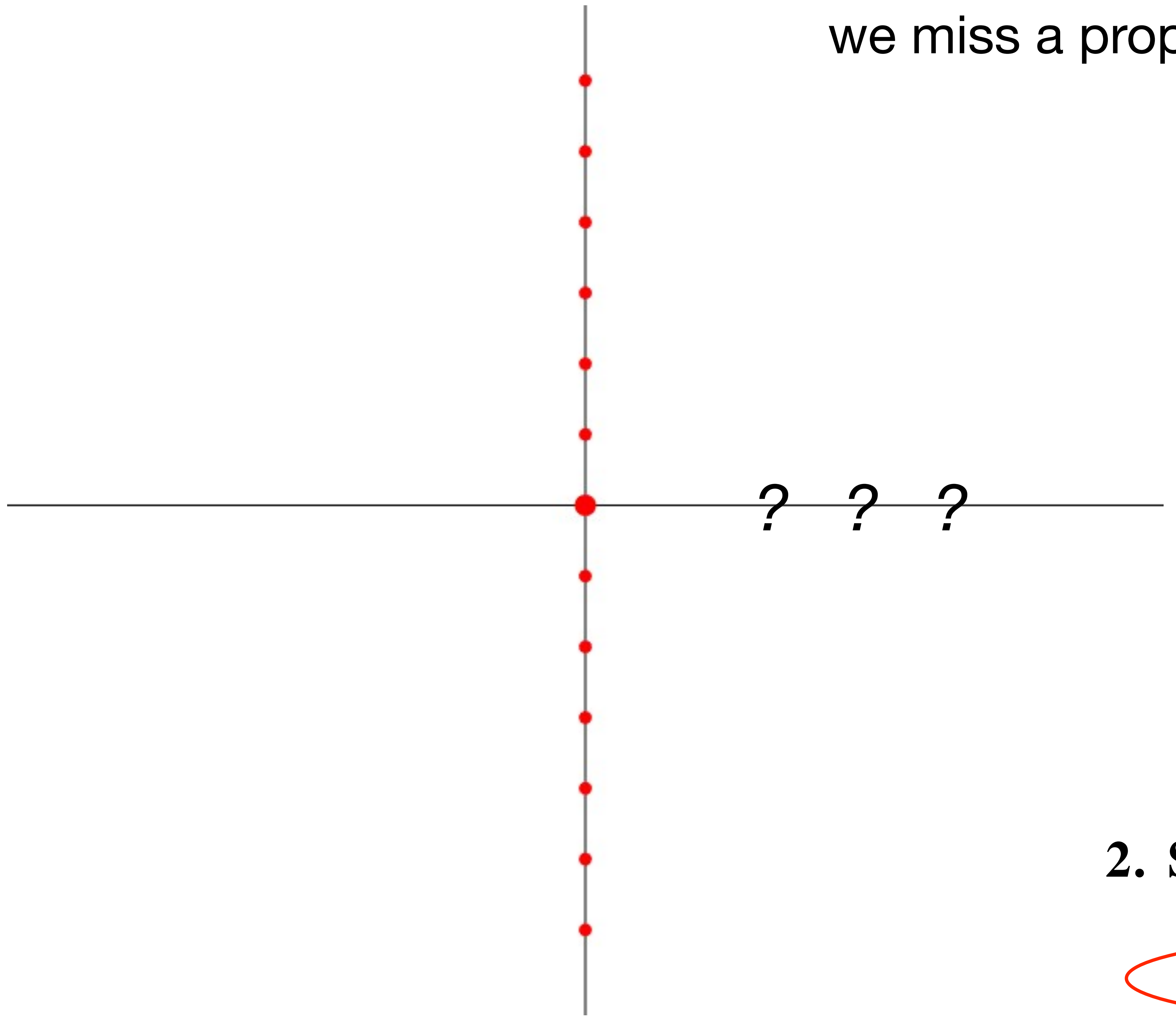

PROCEEDINGS OF SCIENCE

Simulating QCD at finite density

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2. Sign problem

The sign problem is a necessary evil, unavoidable as soon as one integrates out the fermion fields and expresses the partition function in terms of the gauge fields. Analytic integration over each fermion species gives a factor $\det(\not{D}+m+\mu\gamma_0)$, where $\not{D}$ is the massless Dirac operator and the last term appears when the chemical potential μ is non-zero. Now, $\not{D}$ satisfies γ_5-hermiticity: $\gamma_5\not{D}\gamma_5 = \not{D}^\dagger$, so that

$$\gamma_5(\not{D}+m+\mu\gamma_0)\gamma_5 = \not{D}^\dagger + m - \mu\gamma_0 = (\not{D}+m-\mu^*\gamma_0)^\dagger \tag{2.1}$$

Taking the determinant on both sides gives $\det(\not{D}+m+\mu\gamma_0) = \det^*(\not{D}+m-\mu^*\gamma_0)$, which constrains the determinant to be real only if μ is zero or pure imaginary.

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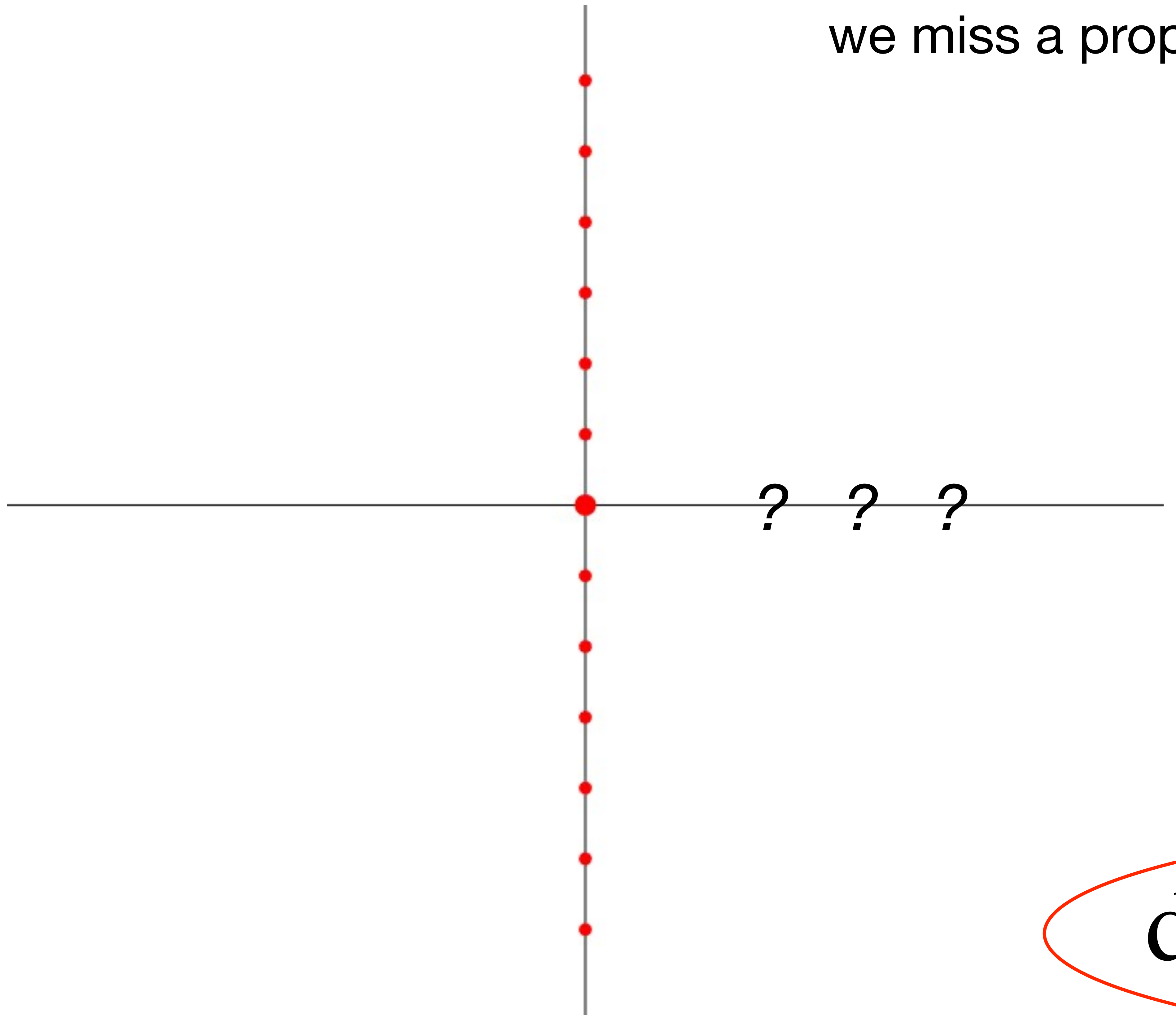

$$\gamma_5(\not{D}+m+\mu\gamma_0)\gamma_5 = \not{D}^\dagger + m - \mu\gamma_0 = (\not{D}+m-\mu^*\gamma_0)^\dagger$$

$$\det(\not{D}+m+\mu\gamma_0) = \det{}^*(\not{D}+m-\mu^*\gamma_0)$$

Fermionic determinant is REAL only for ZERO or IMAGINARY values of the chemical potential!

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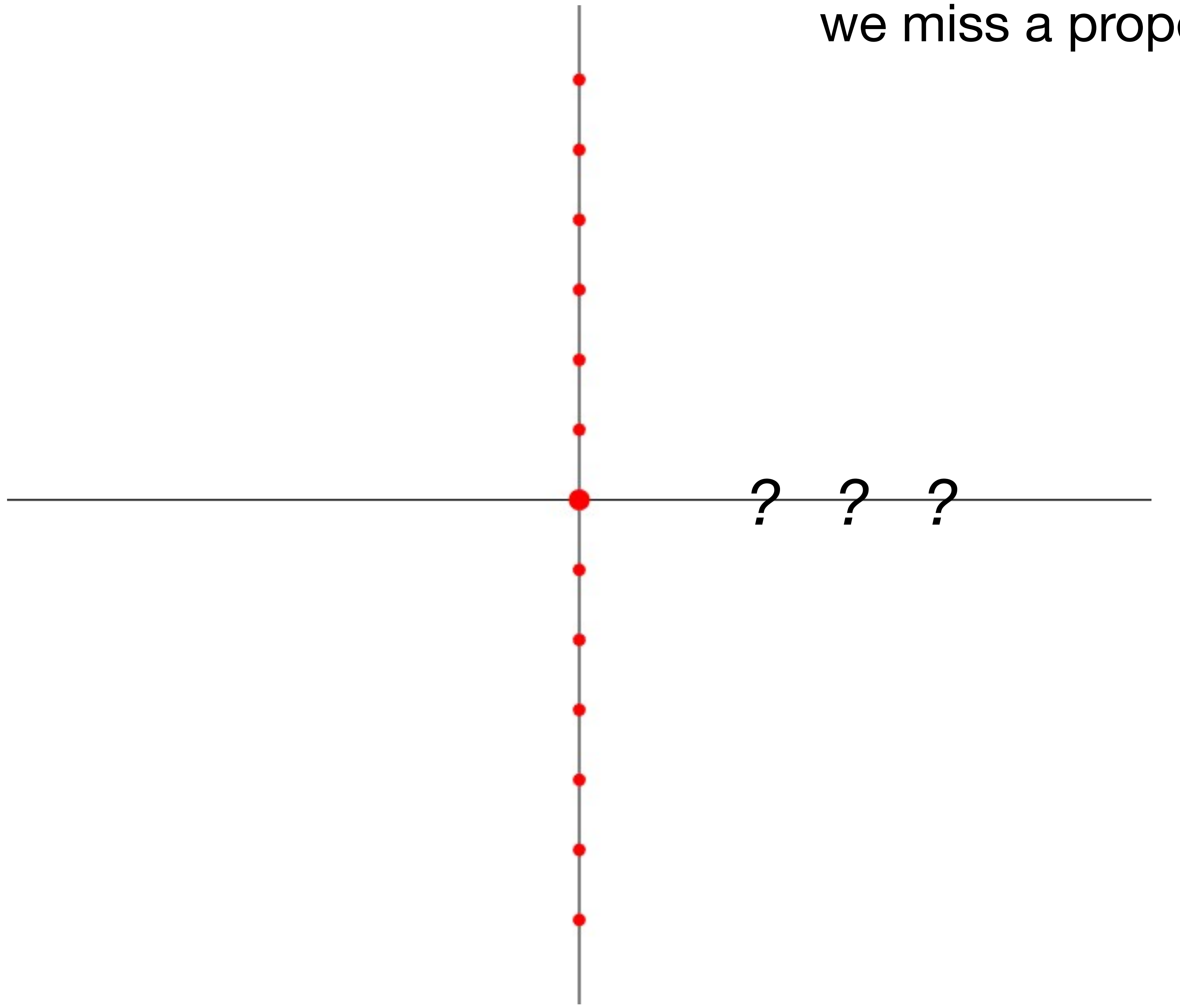

Mainly two working solutions:

- Compute Taylor expansions at $\mu_B = 0$
- Compute on the imaginary axis $\mu_B = i\mu_I$

The two solutions are obviously related … and both imply (strictly speaking) an ANALYTIC CONTINUATION

There are tensions in between differente results for Taylor coefficients in the literature…

Agenda

- An invitation (1. sign problem...)
- An invitation (2. analytic continuation from **multi-point Padé)**
- The sign problem as an **inverse problem** ...
- ... and something more on **other inverse problems** ...
- WORK IN PROGRESS!

Until a few moths ago, if you had asked me about analytic continuation, I would have told you a few words on multi-point PADÈ

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Suppose you know the values of a function (and of its derivatives) at a number of points

$$\ldots\ ,\ f(z_k)\,,\ f'(z_k)\,,\ \ldots,\ f^{(s-1)}(z_k)\,,\ \ldots \qquad k = 1 \ldots N$$

If you want to approximate the function with a rational function

$$R^m_n(z) = \frac{P_m(z)}{\tilde{Q}_n(z)} = \frac{P_m(z)}{1 + Q_n(z)} = \frac{\sum_{i=0}^{m} a_i\, z^i}{1 + \sum_{j=1}^{n} b_j\, z^j}$$

the obvious requirement is that

$$R^{m\,(j)}_n(z_k) = f^{(j)}(z_k) \qquad k = 1 \ldots N, \quad j = 0 \ldots s-1$$

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$$R_n^{m\,(j)}(z_k) = f^{(j)}(z_k) \qquad k = 1\ldots N, \quad j = 0\ldots s-1$$

This is the starting point for a ***multi-point Padè approximation***: solve the linear system

$$\ldots$$

$$P_m(z_k) - f(z_k)Q_n(z_k) = f(z_k)$$

$$P'_m(z_k) - f'(z_k)Q_n(z_k) - f(z_k)Q'_n(z_k) = f'(z_k)$$

$$\ldots$$

from which we want to get the unknown

$$\{a_i \,|\, i = 0\ldots m\} \quad \{b_j \,|\, j = 1\ldots n\} \qquad n+m+1 = N\,s$$

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Any useful …?

Yes! LATTICE QCD at IMAGINARY values of the baryonic chemical potential

PHYSICAL REVIEW D **105,** 034513 (2022)

Contribution to understanding the phase structure of strong interaction matter: Lee-Yang edge singularities from lattice QCD

P. Dimopoulos,[1] L. Dini,[2] F. Di Renzo,[1] J. Goswami,[2] G. Nicotra,[2] C. Schmidt,[2] S. Singh,[1,*] K. Zambello,[1] and F. Ziesché[2]

… where we computed and “multi-point Padè approximated”

$$\chi^B_n(T,V,\mu_B) = \left(\frac{\partial}{\partial\hat{\mu}_B}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$
$$= \left(\frac{1}{3}\frac{\partial}{\partial\hat{\mu}_l} + \frac{1}{3}\frac{\partial}{\partial\hat{\mu}_s}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$

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Any useful ...?

Yes! LATTICE QCD at IMAGINARY values of the baryonic chemical potential

... a natural analytic continuation to real chemical potential!

... and not only that: singularities!

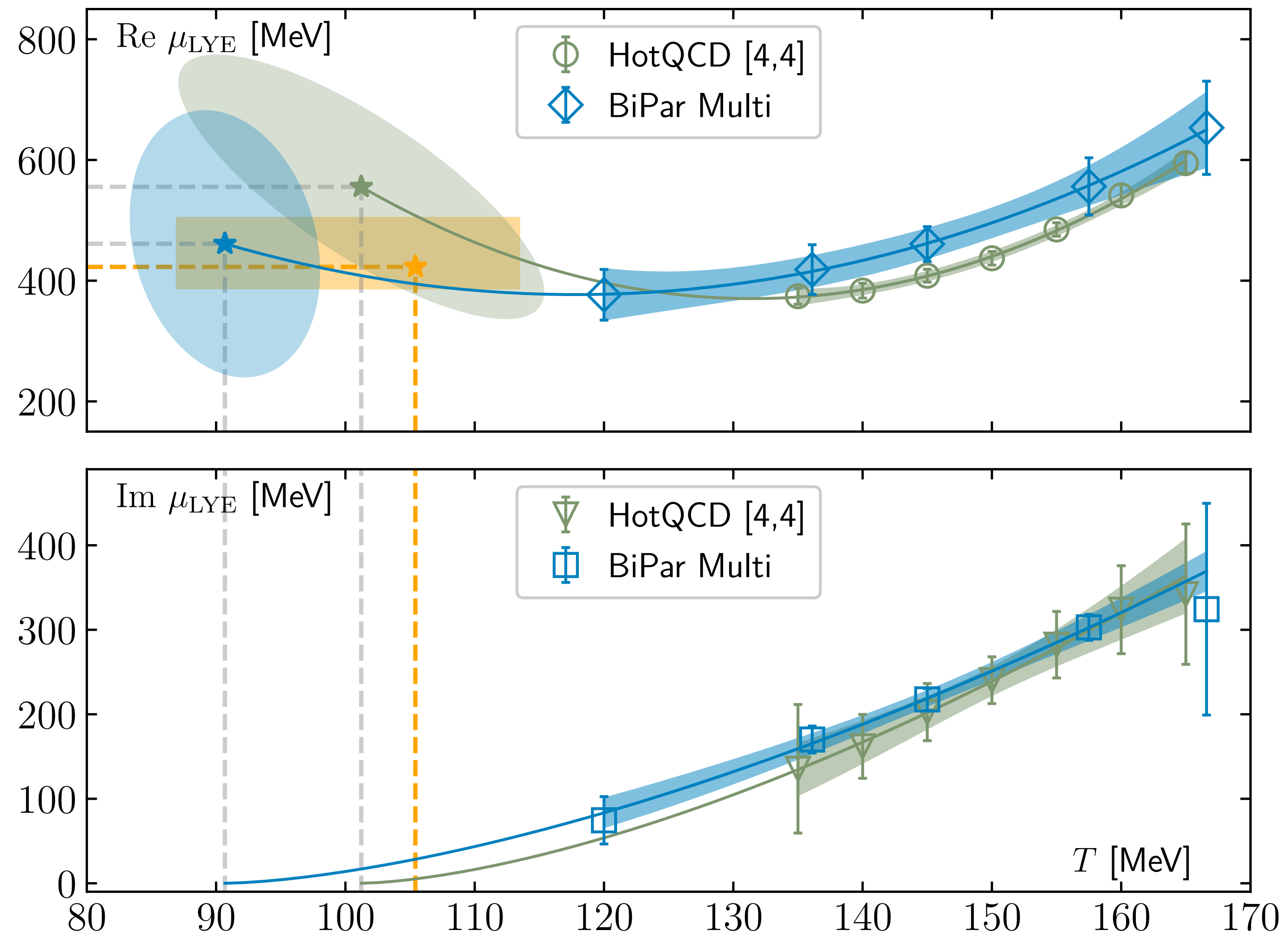
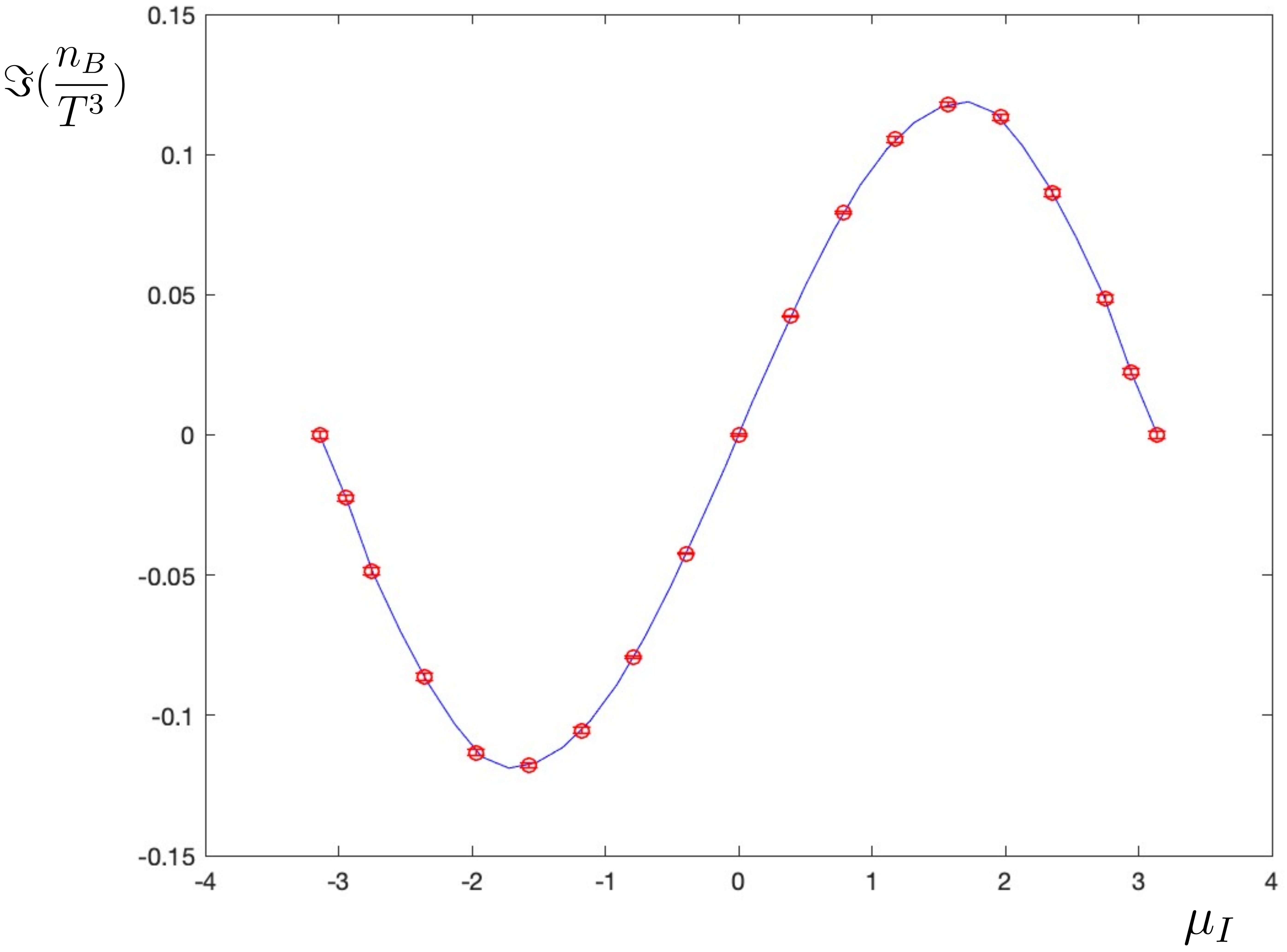


FIG. 4. Scaling fits for the LYE singularities related to the CEP. Green data come from a [4,4] Padé from Ref. [7]. Blue data come from the multi-point Padé. *Top*: Scaling of the real part. *Bottom*: Scaling of the imaginary part. The ellipses shown in the top panel represent the 68% confidence region deduced from the covariance matrix of the fit. The orange box indicates the AIC weighted estimate (6).

In the following we will play with a few Bielefeld Parma Collaboration data
2+1 HISQ at physical quarks mass, at fixed cutoff ($N_\tau = 6$)

...so, let's look at analytic continuation of our PADÈ approximant

$T = 157.5\ (\sim 155)$ MeV



... which is pretty simple (we will be concerned with the number density):

you take your rational function, which describes very well data at IMAGINARY VALUES of μ_B

CAVEAT: errors on data points are there ... no error shown on the interpolating function (*as for now* ...)

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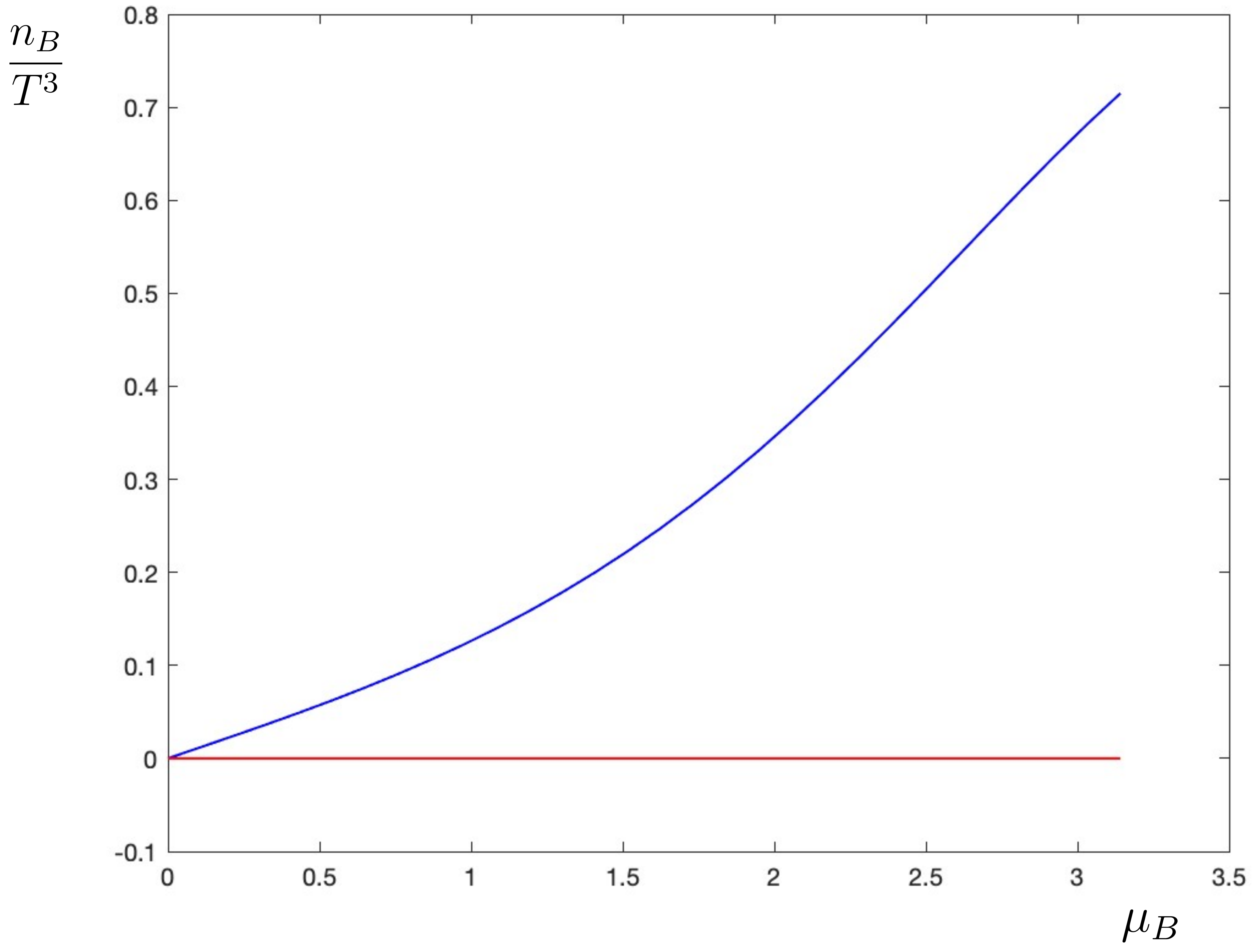

... which is pretty simple (we will be concerned with the number density):

you take your rational function, which describes very well data at IMAGINARY VALUES of μ_B

... and you simply compute it for REAL VALUES of μ_B

CAVEAT: no error shown as for now ... here we are concerned with *trends*... FIXED CUTOFF!

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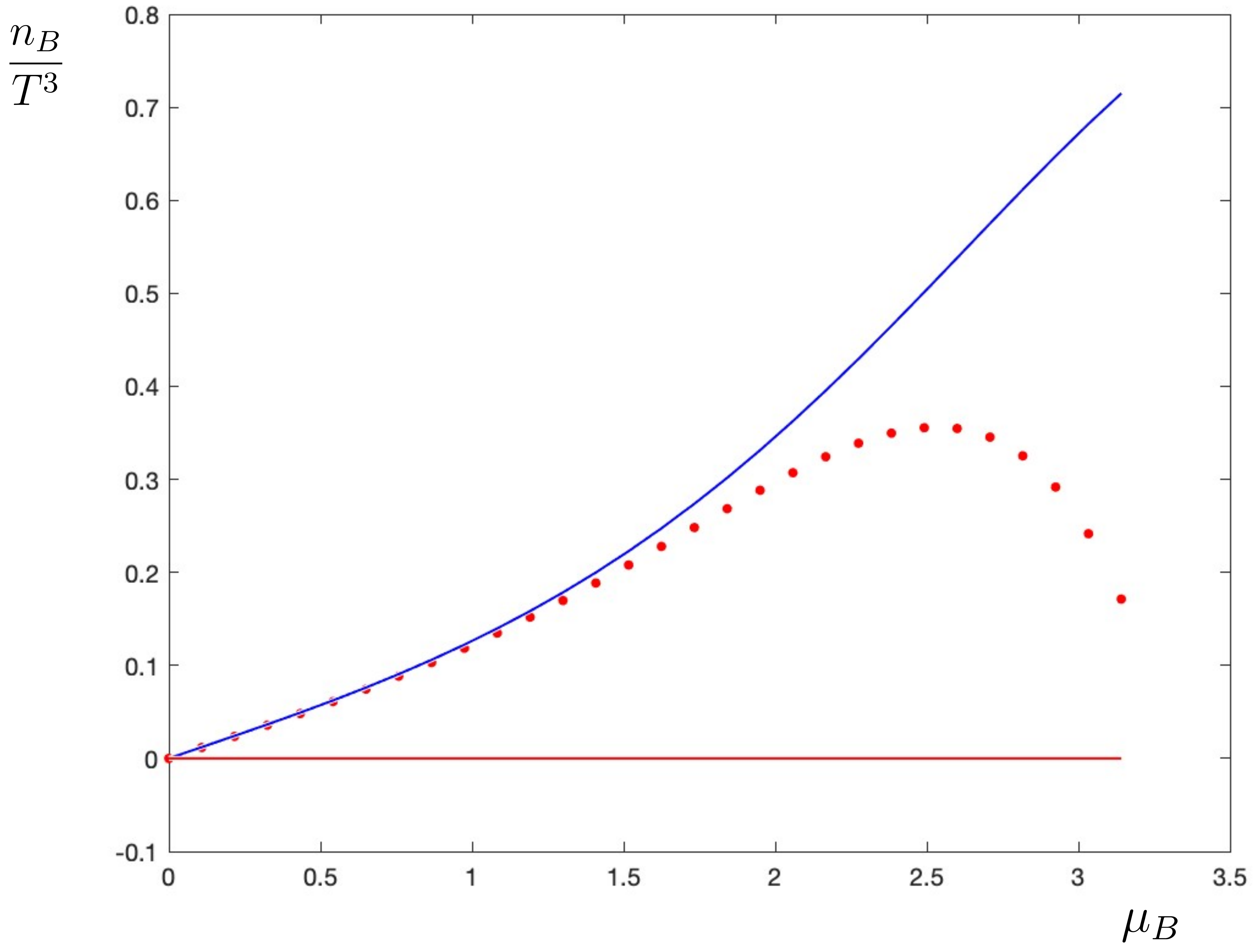

... which is pretty simple (we will be concerned with the number density):

you take your rational function, which describes very well data at IMAGINARY VALUES of μ_B

... and you simply compute it for REAL VALUES of μ_B

You can compare the result with HotQCD results

PHYSICAL REVIEW D **105,** 074511 (2022)

Taylor expansions and Padé approximants for cumulants of conserved charge fluctuations at nonvanishing chemical potentials

D. Bollweg,[1] J. Goswami,[2] O. Kaczmarek,[2] F. Karsch,[2] Swagato Mukherjee,[3] P. Petreczky,[3] C. Schmidt,[2] and P. Scior[3]

(HotQCD Collaboration)

CAVEAT: no error shown as for now ... here we are concerned with *trends*... FIXED CUTOFF!

Finite density QCD as an inverse problem

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… *aka* How to trade a difficult problem for another (even more?) difficult one …

What does ANALYTICITY mean? … (analytic functions aka olomorphic…)

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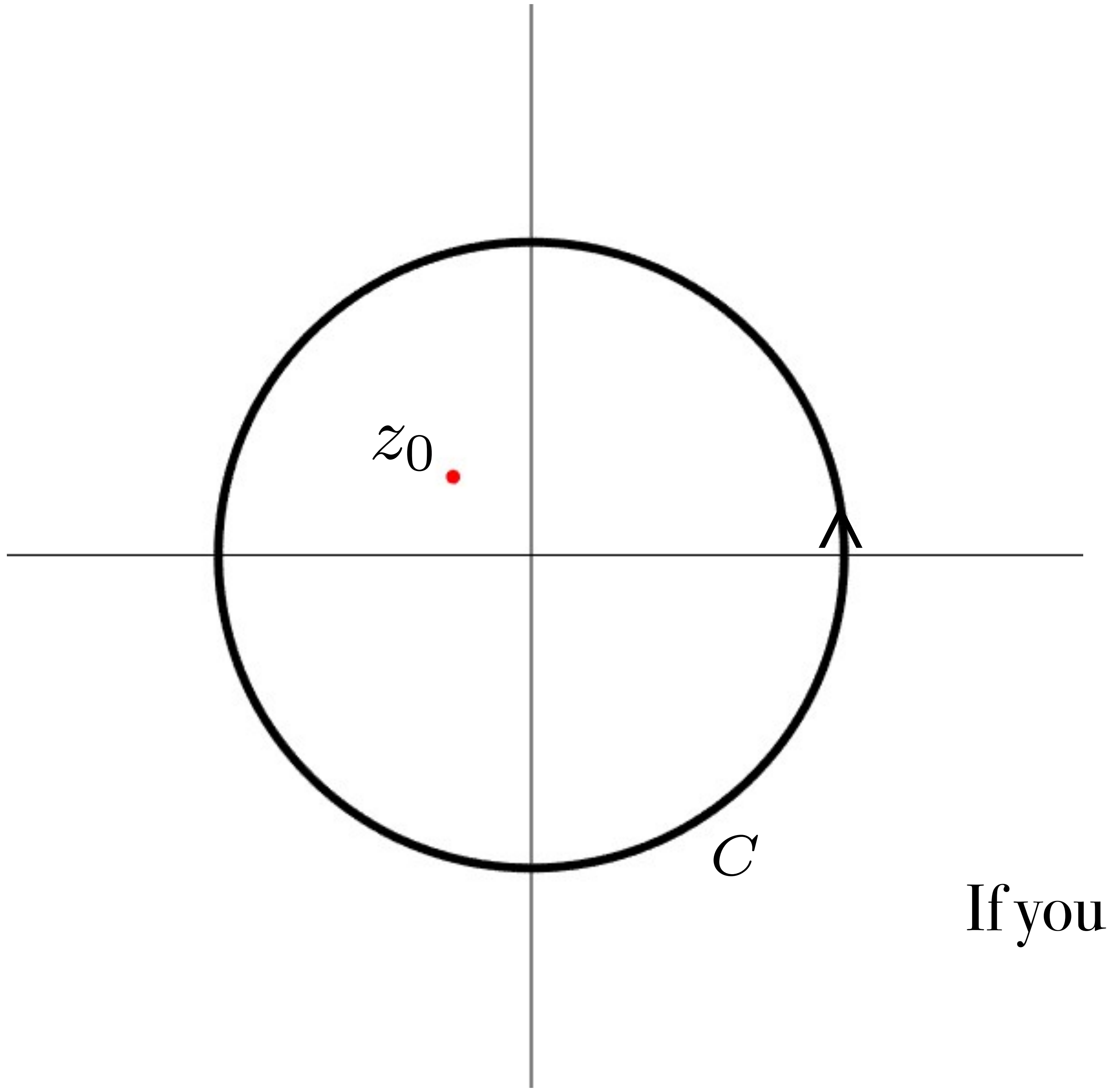
One simple way of thinking of it is that *you can perfectly know such functions from an apparently limited amount of information.*

What does ANALYTICITY mean? … (analytic functions aka olomorphic…)



CAUCHY FORMULA

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0}\, dz$$

If you know the function on the contour, you can compute it at any point inside… sounds good!

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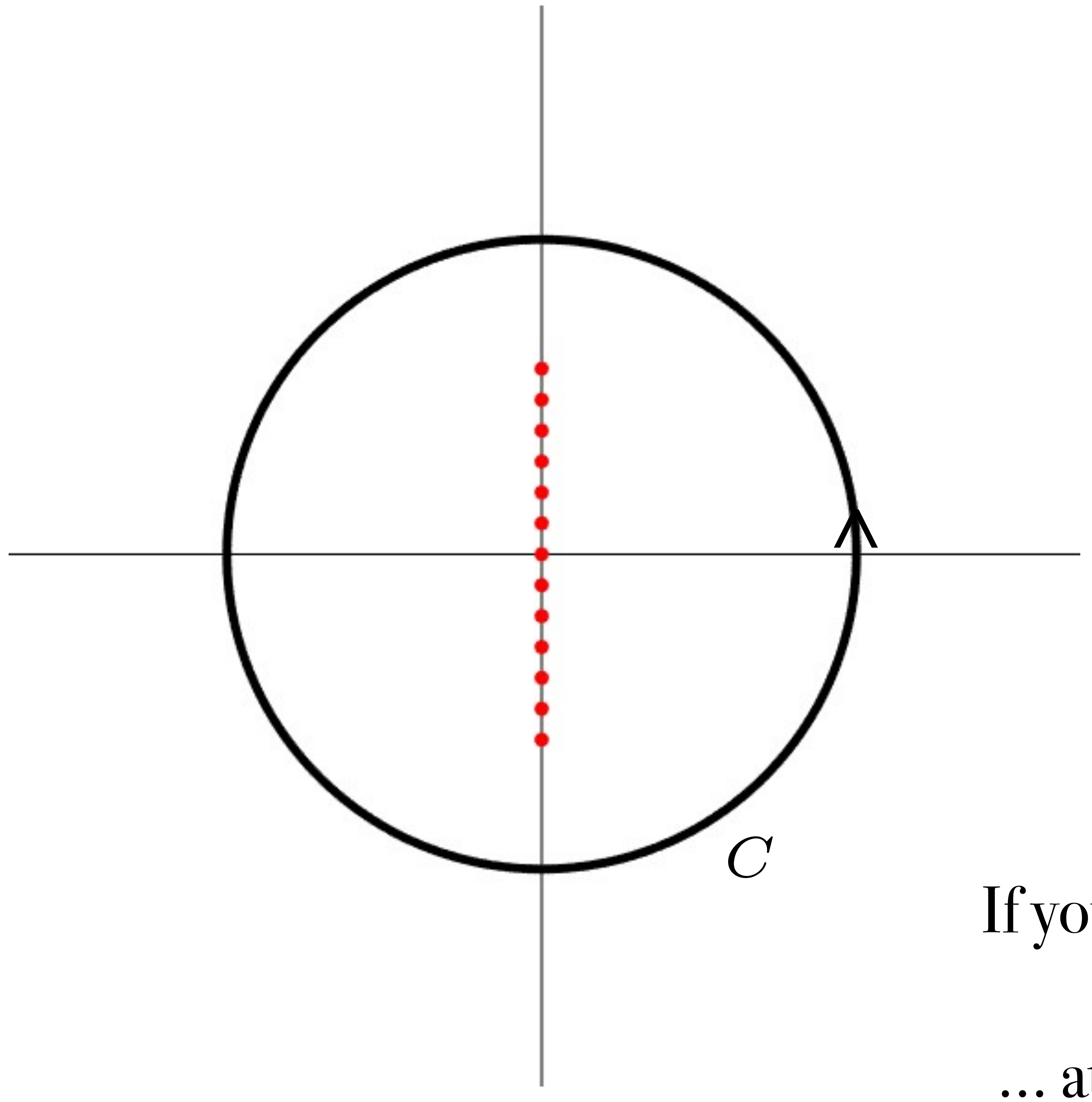

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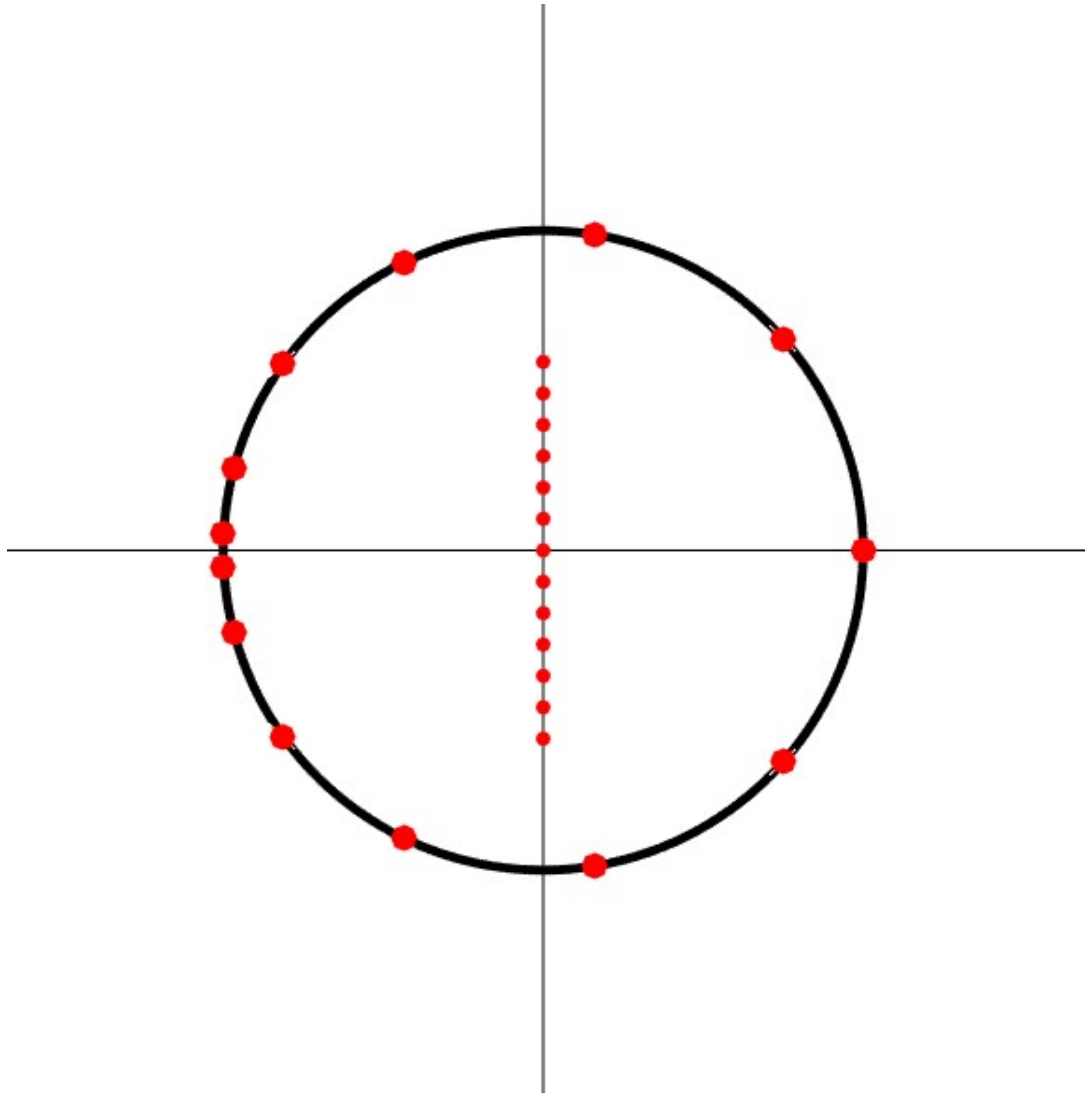
... at any point, including the (only) ones we can compute (on the imaginary axis) in our case...

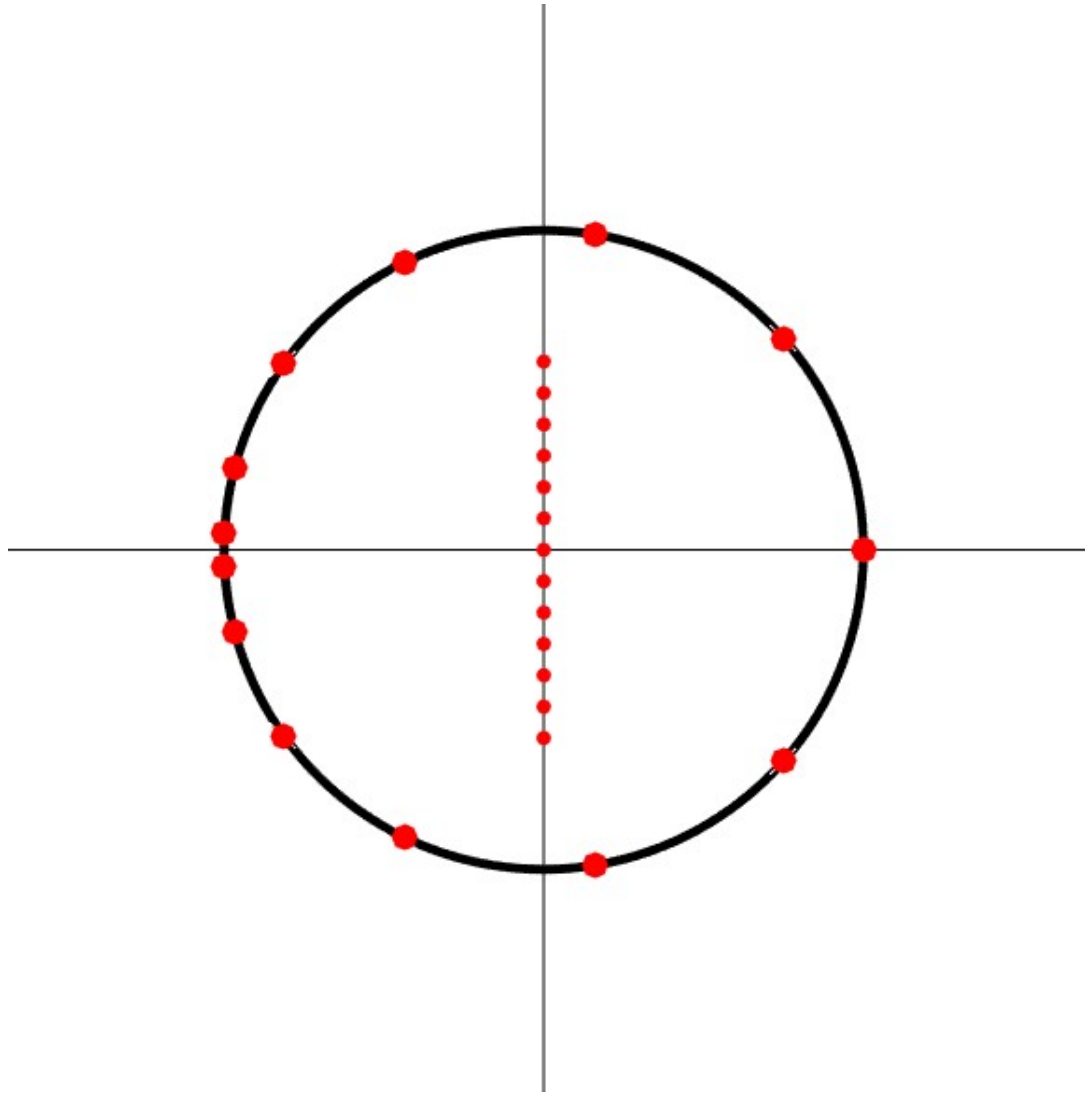


With your favourite QUADRATURE method ... you can go numeric!

De facto, you would like to think of Legendre quadrature

$$f(z_0) = \frac{1}{2\pi} \int_0^{2\pi} \frac{f(R\,e^{i\theta})\,R\,e^{i\theta}}{R\,e^{i\theta} - z_0}\, d\theta \simeq \frac{1}{2\pi} \sum_{k=1}^{n} w_k \frac{f(R\,e^{i\theta_k})\,R\,e^{i\theta_k}}{R\,e^{i\theta_k} - z_0}$$

$$y_i = \frac{1}{2\pi} \sum_{k=1}^{n} w_k \frac{R\,e^{i\theta_k}}{R\,e^{i\theta_k} - z_i}\, \hat{f}_k\,, \quad i = 1, 2, \ldots, n$$



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... and then you are ready for your (BRAVE) INVERSE PROBLEM!

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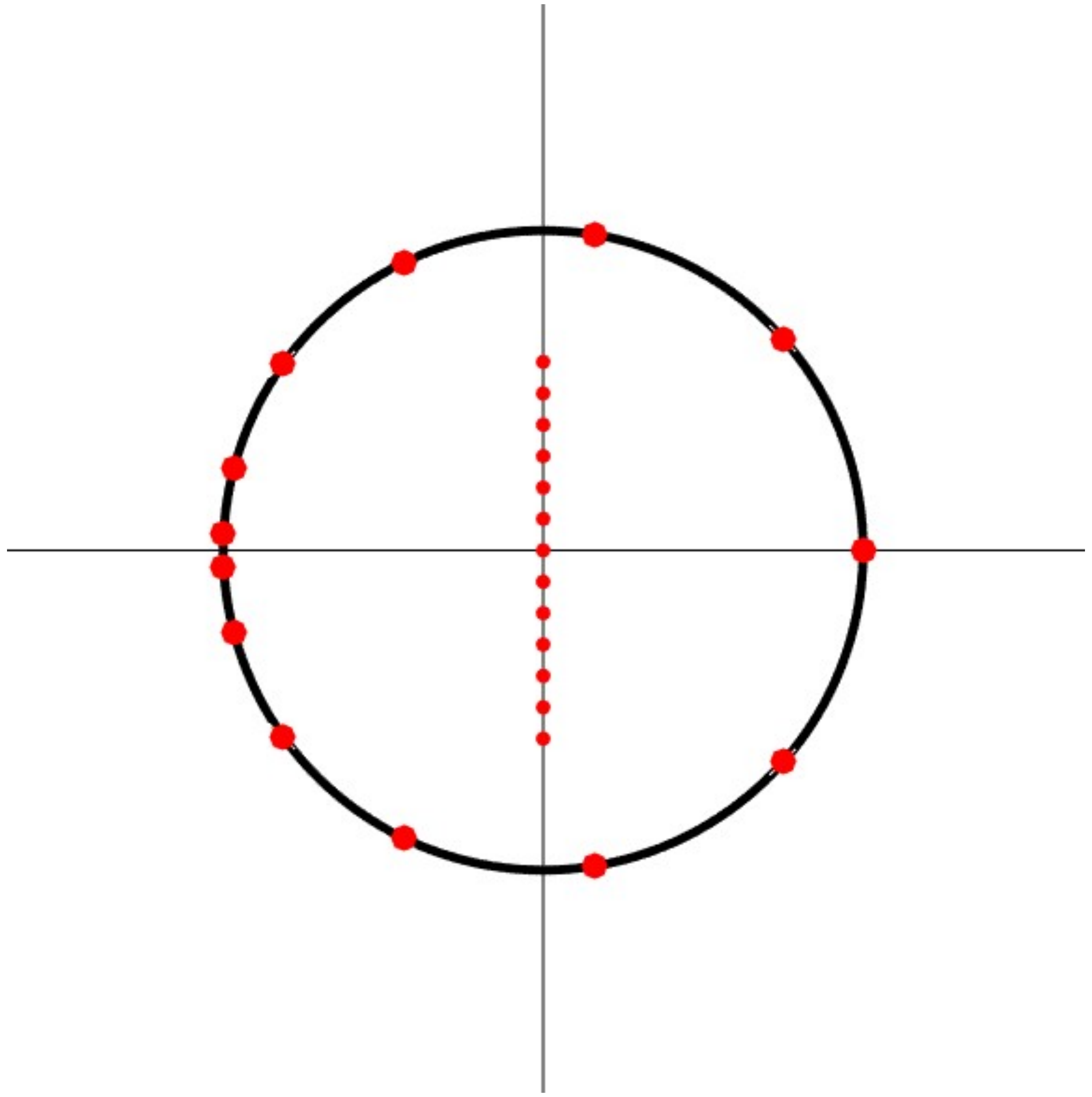

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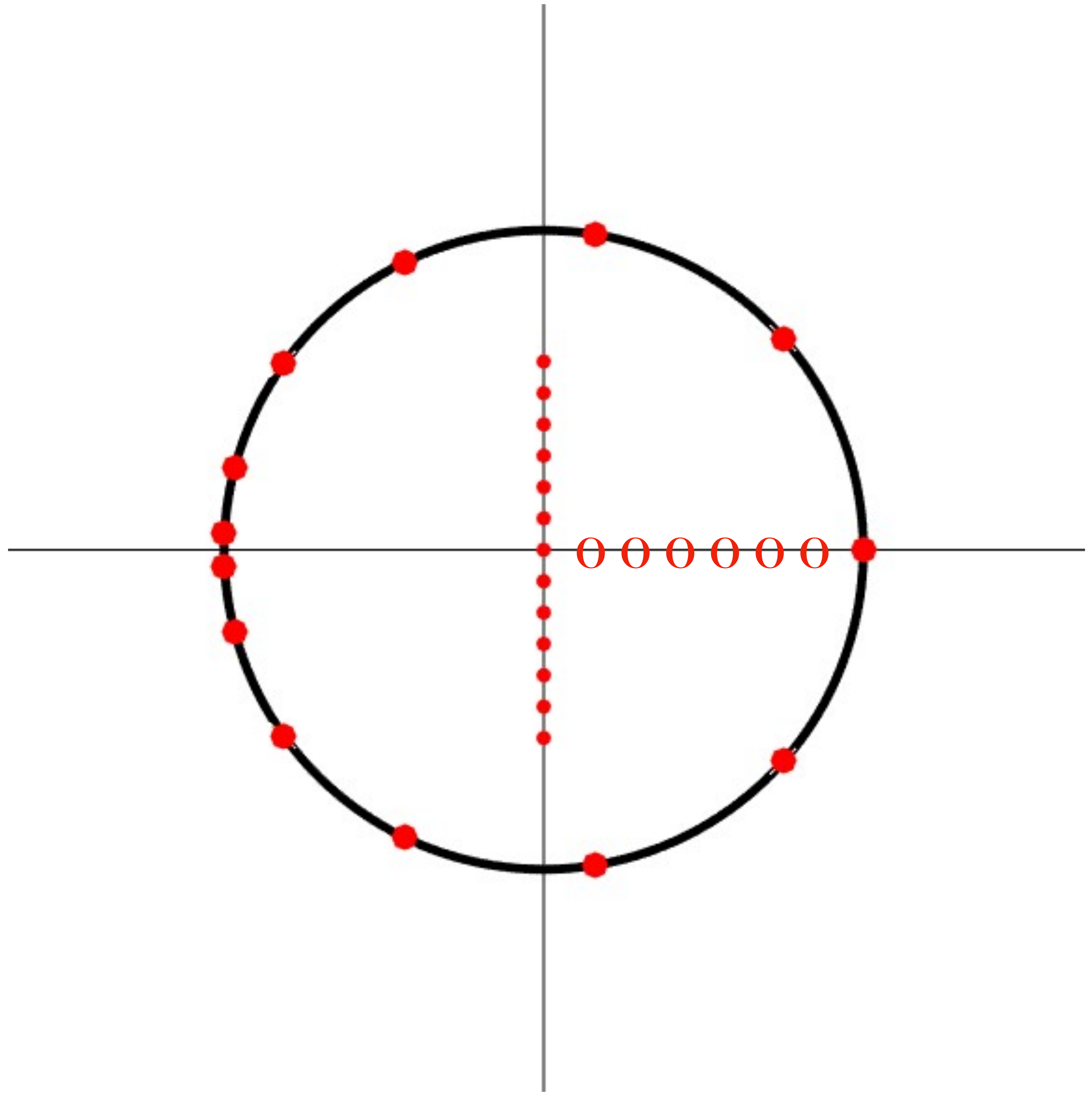
$$A_{ik} = \frac{1}{2\pi} w_k \frac{R\,e^{i\theta_k}}{R\,e^{i\theta_k} - z_i}$$

$$A\,\mathbf{x} = \mathbf{b}$$

SOLVE for the $\hat{f}_k$!



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... and when you have solved your (BRAVE) INVERSE PROBLEM(!) ...

$$A_{ik} = \frac{1}{2\pi}\,w_k\,\frac{R\,e^{i\theta_k}}{R\,e^{i\theta_k} - z_i}$$

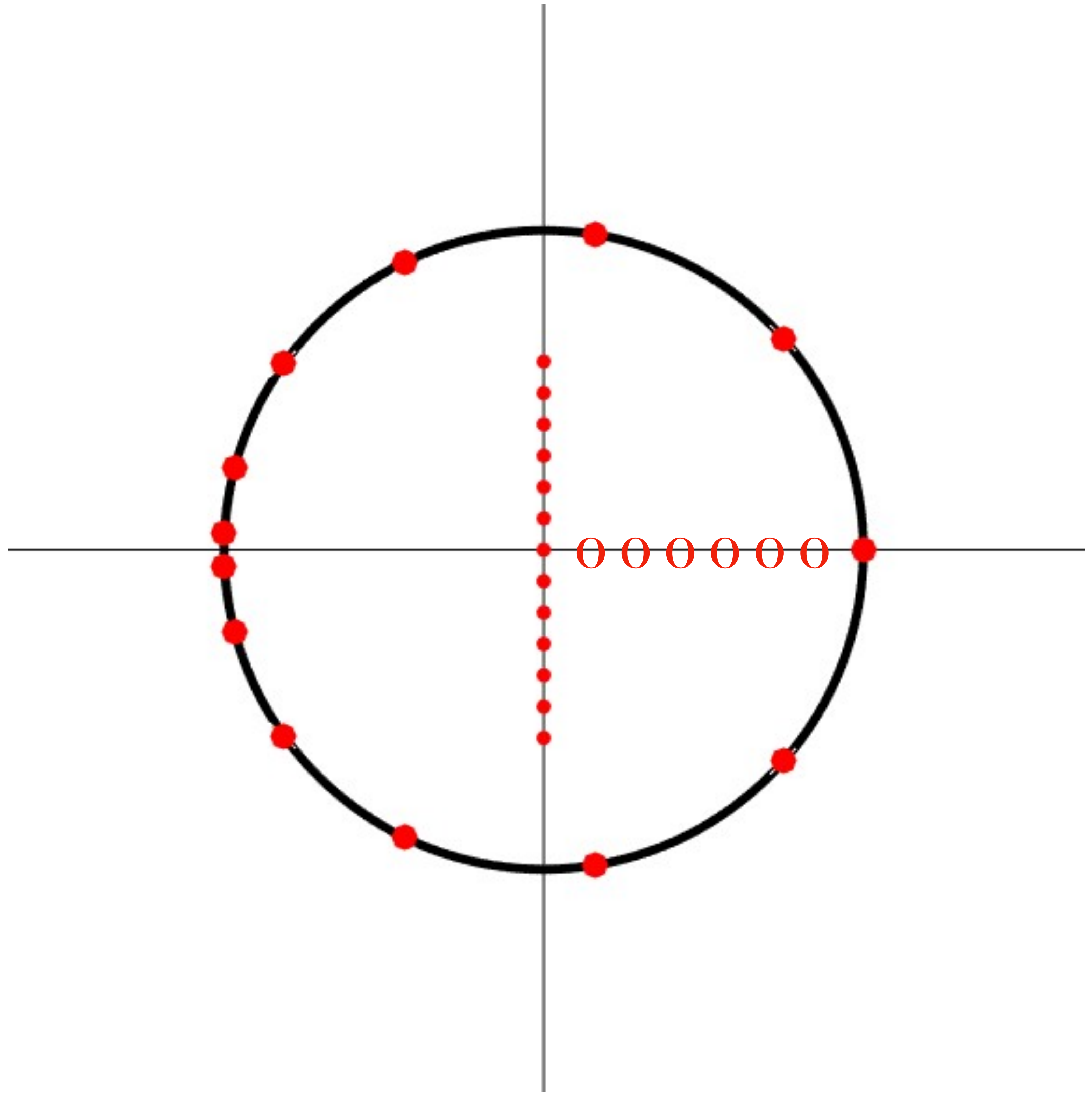
$$A\,\mathbf{x} = \mathbf{b}$$

SOLVE for the $\hat{f}_k$!

Once you have the values on the contour, you can compute on the REAL AXIS! (o o o o o o)

With your favourite QUADRATURE method ... you can go numeric!

De facto, you would like to think of Legendre quadrature



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... a BRAVE INVERSE PROBLEM!...

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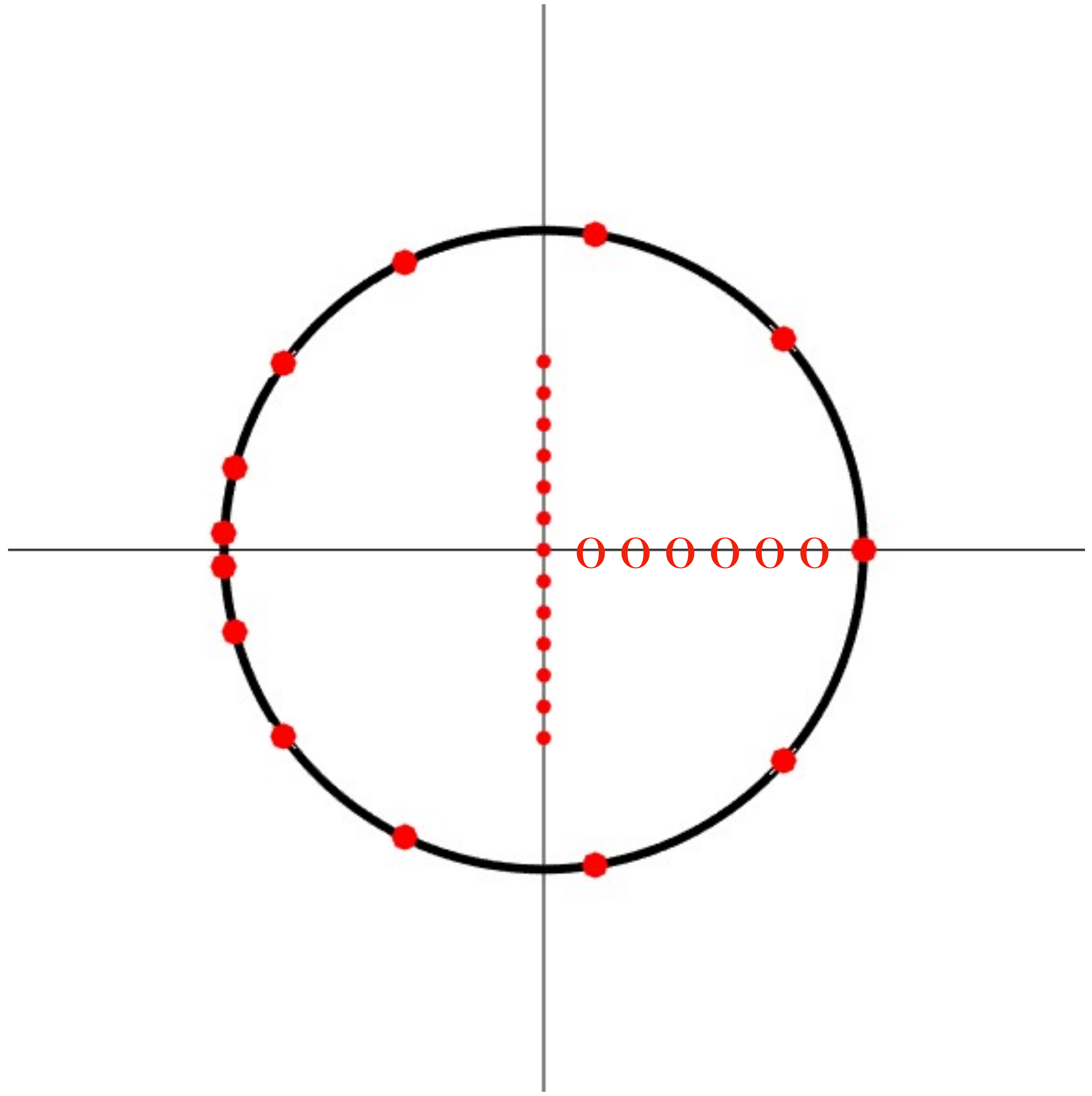
$$A\,\mathbf{x} = \mathbf{b}$$

SOLVE for the $\hat{f}_k$!

A very SIMPLE idea! ... a NAIVE one ... INVERSE PROBLEM!!!



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$$A\,\mathbf{x} = \mathbf{b}$$

SOLVE for the $\hat{f}_k$!

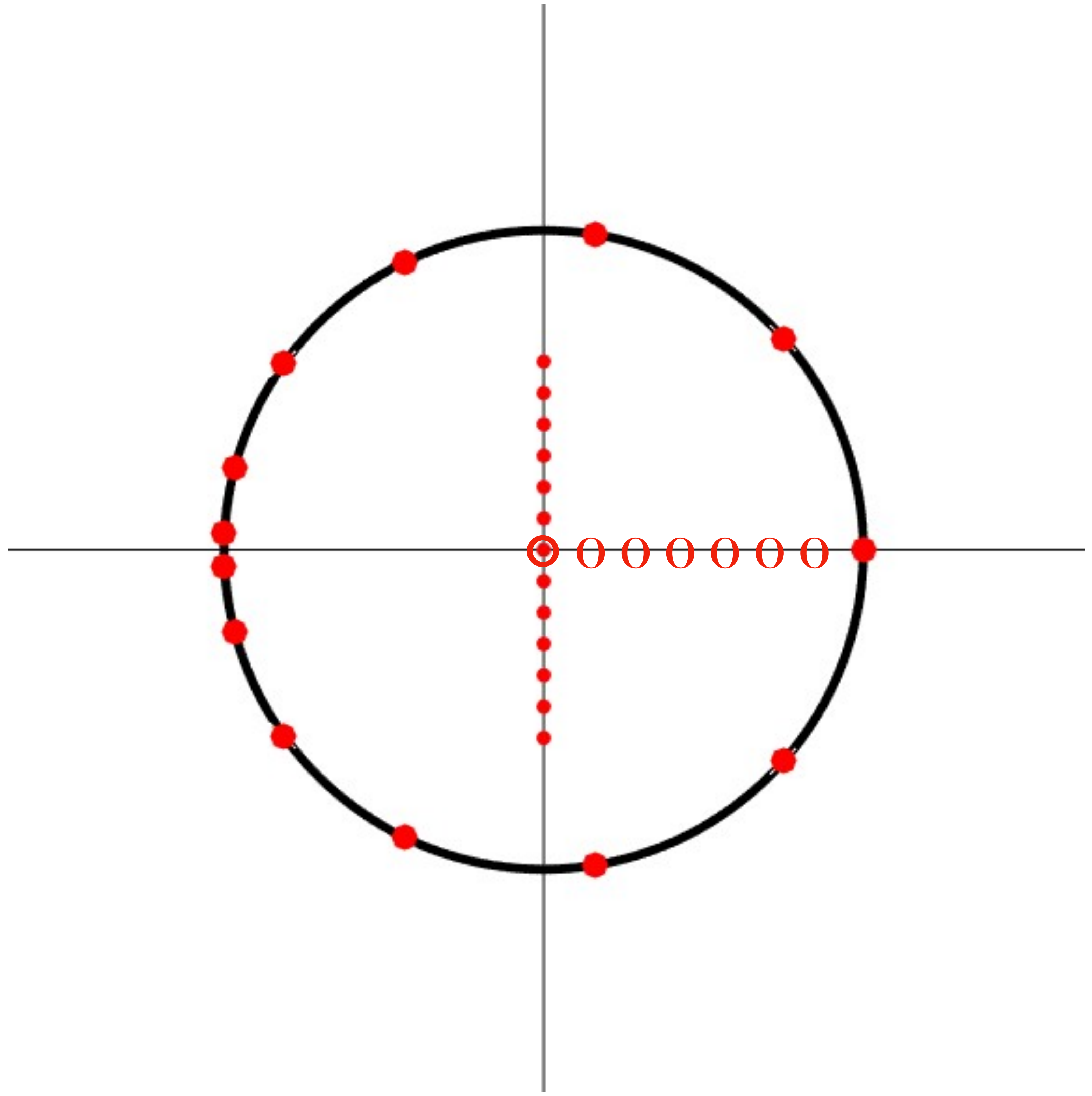
Can we hope it could work? ... are we afraid it should not?

... and it could(?)/should(?) not for a combination of

(a) bad condition number of the linear system

(b) the quadrature formula being NOT exact

Much care is needed ... and so we will perform some tests...



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$$A\,\mathbf{x} = \mathbf{b}$$

SOLVE for the $\hat{f}_k$!

Not the end of the story … Obviously, it is a good (CHEAP) idea to also remember Cauchy formula for derivatives

$$f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{n+1}}\, dz = \frac{n!}{2\pi i} \int_0^{2\pi} \frac{f(R\, \exp(i\theta))\, R\, \exp(i\theta)}{(R\, \exp i\theta - z_0)^{n+1}}\, d\theta$$

LOOK! … we tackled a funny inverse problem, a non-standard one … other are very much investigated!

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SOMETHING ELSE you can do with the inverse problem machinery:
we can play the same game for inverse Laplace transform ...

You know this ...

$$f(s) = \int_0^\infty e^{-ts}\, F(t)\, dt$$

You want this ...

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You want this ...

We slightly rephrase the problem ...

$$f(s) = \int_0^\infty e^{-t}\, e^{-t(s-1)}\, F(t)\, dt$$

... and we can play the same game ...

$$f(s) = \int_0^\infty e^{-t}\, e^{-t(s-1)}\, F(t)\, dt \;\sim\; \sum_j w_j\, e^{-t_j(s-1)}\, F(t_j)$$

This time, Laguerre quadratures ...

... A brave attempt, but with a rational ...

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HARD ... from a limited amount of information you want to get an infinite one...

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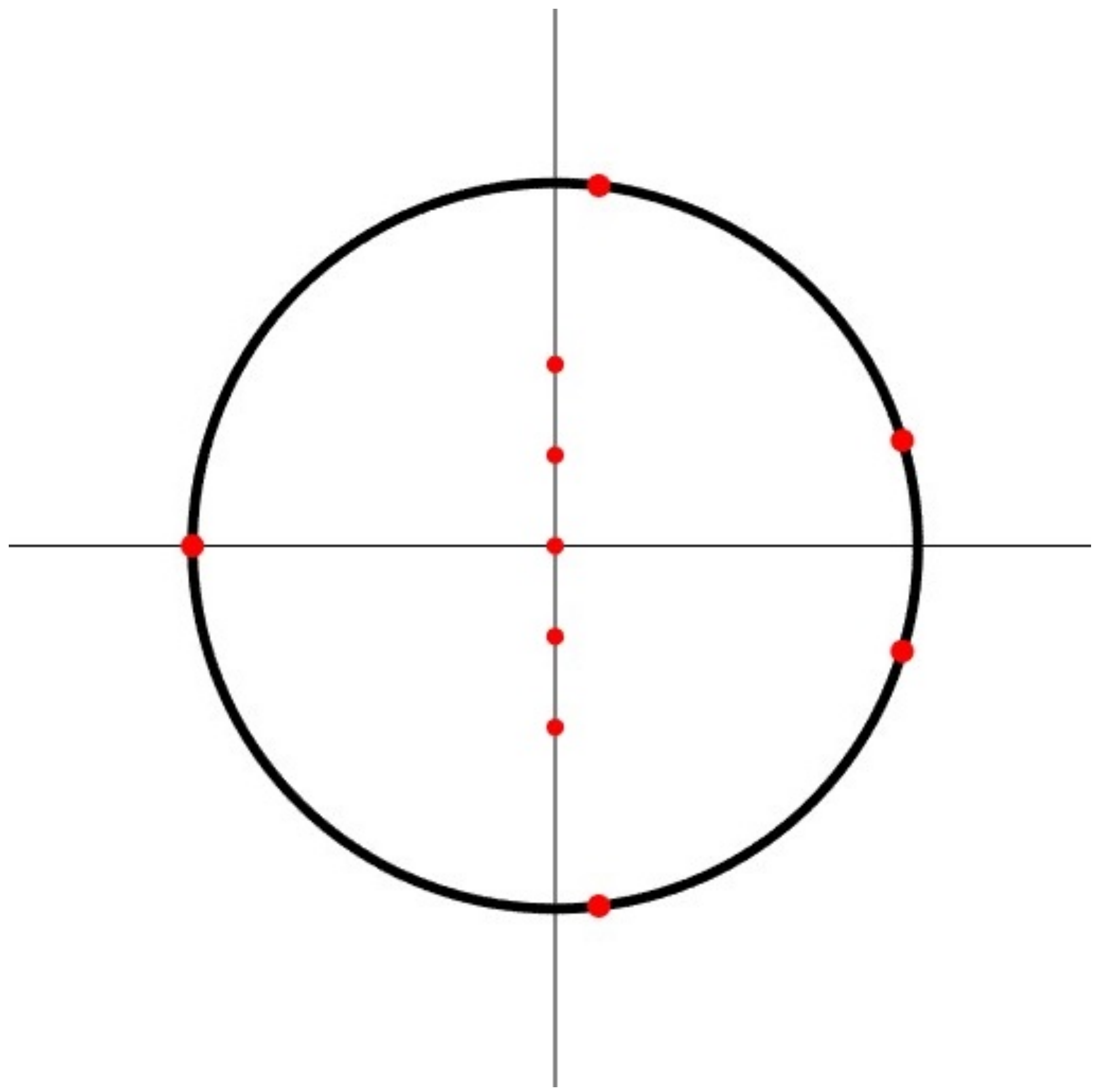
Actually, both for (anti)Laplace and for the Cauchy formula, we provide n values and try to get n as well ... e.g.



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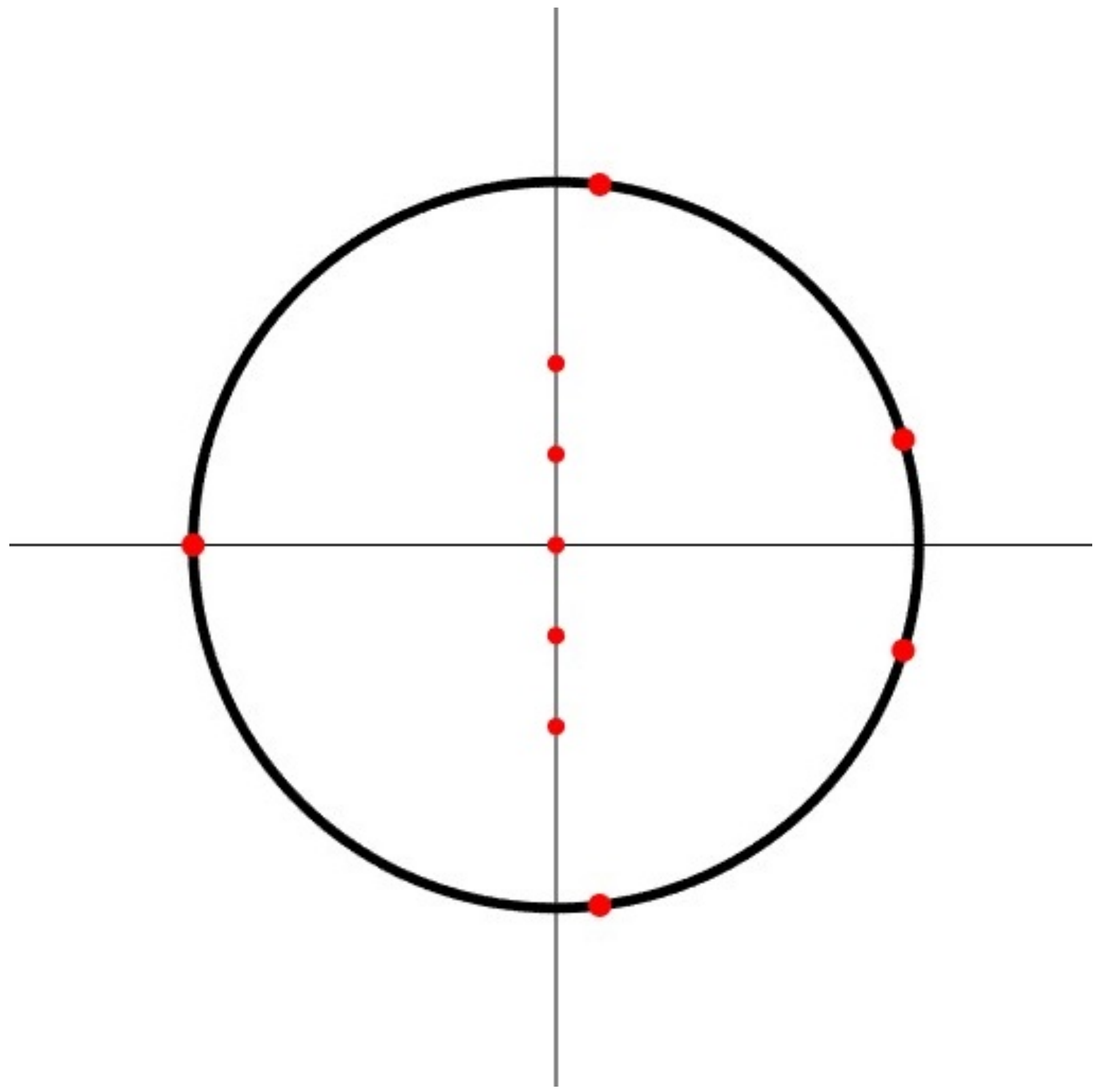

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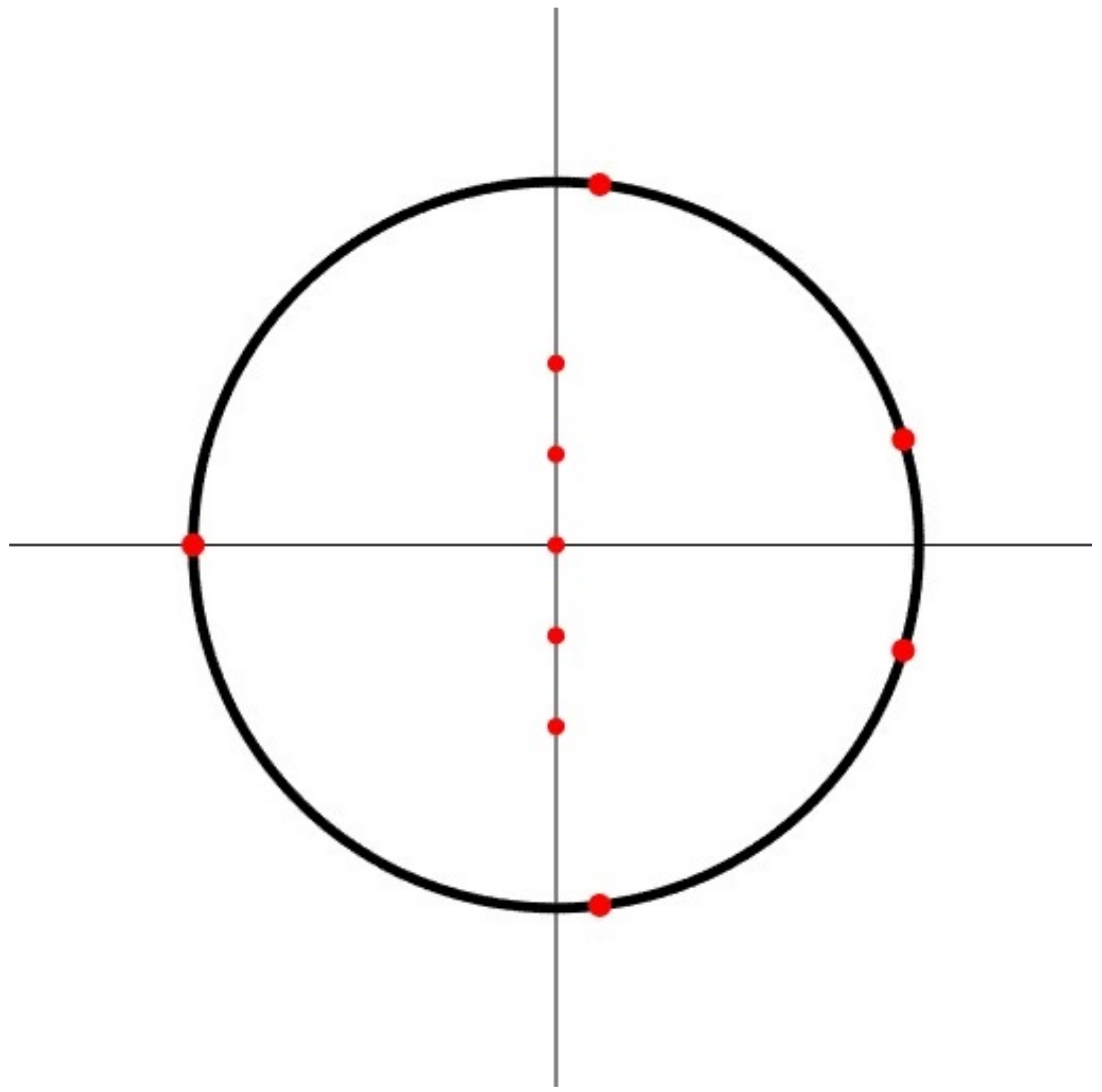
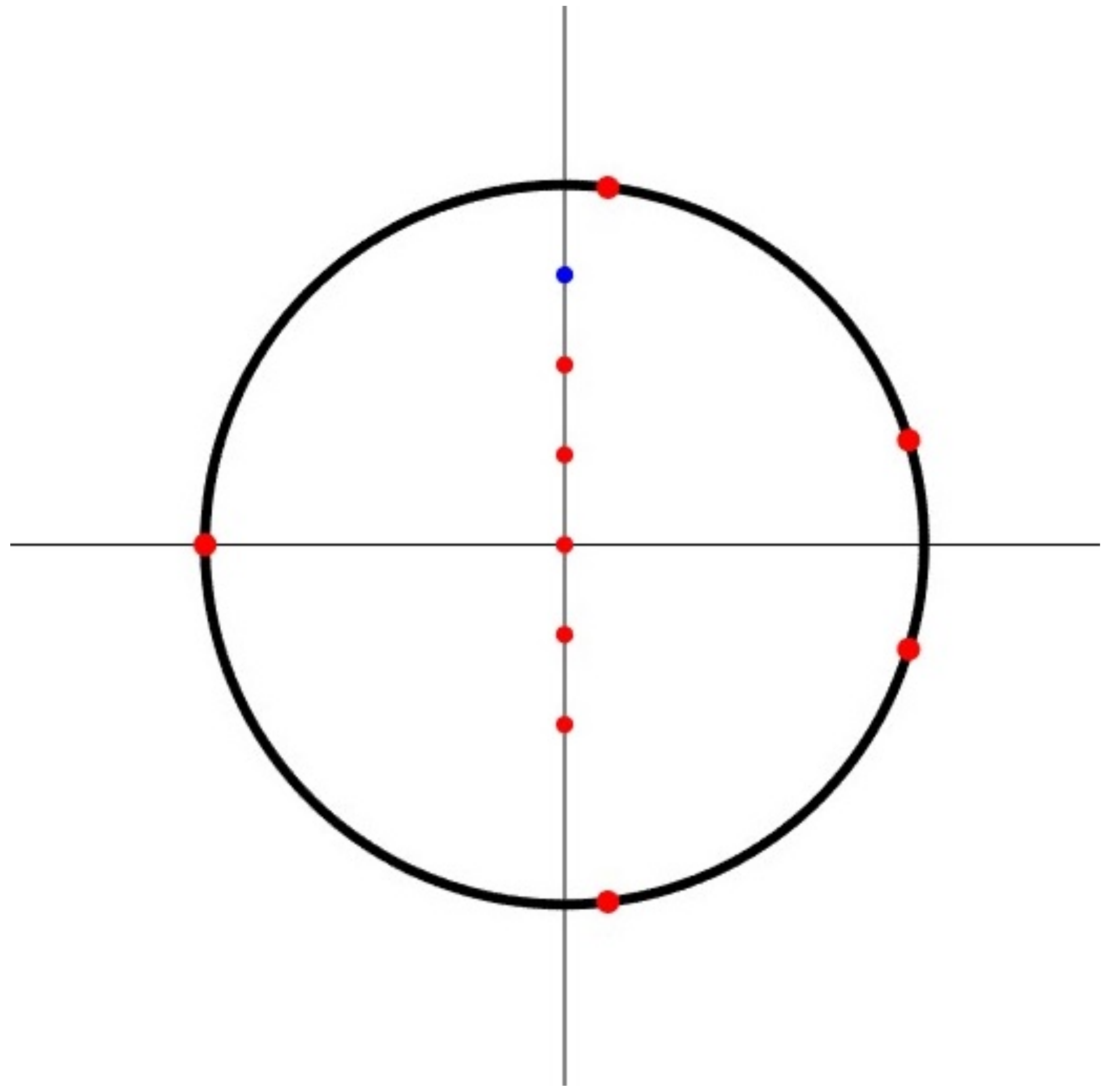


Actually, both for (anti)Laplace and for the Cauchy formula, we provide n values and try to get n as well ... e.g.

... but then ... simply add one (single) point ...



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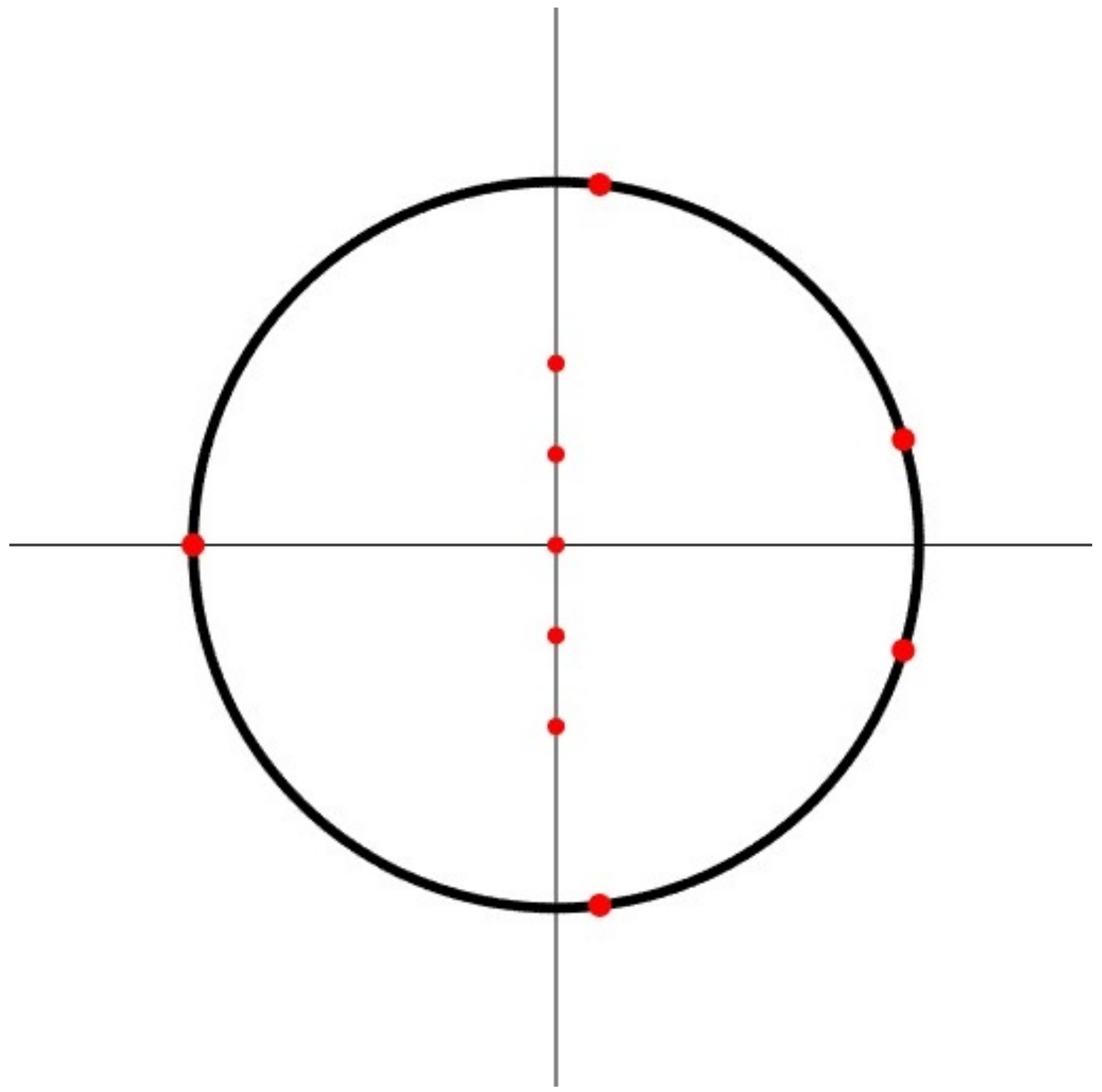

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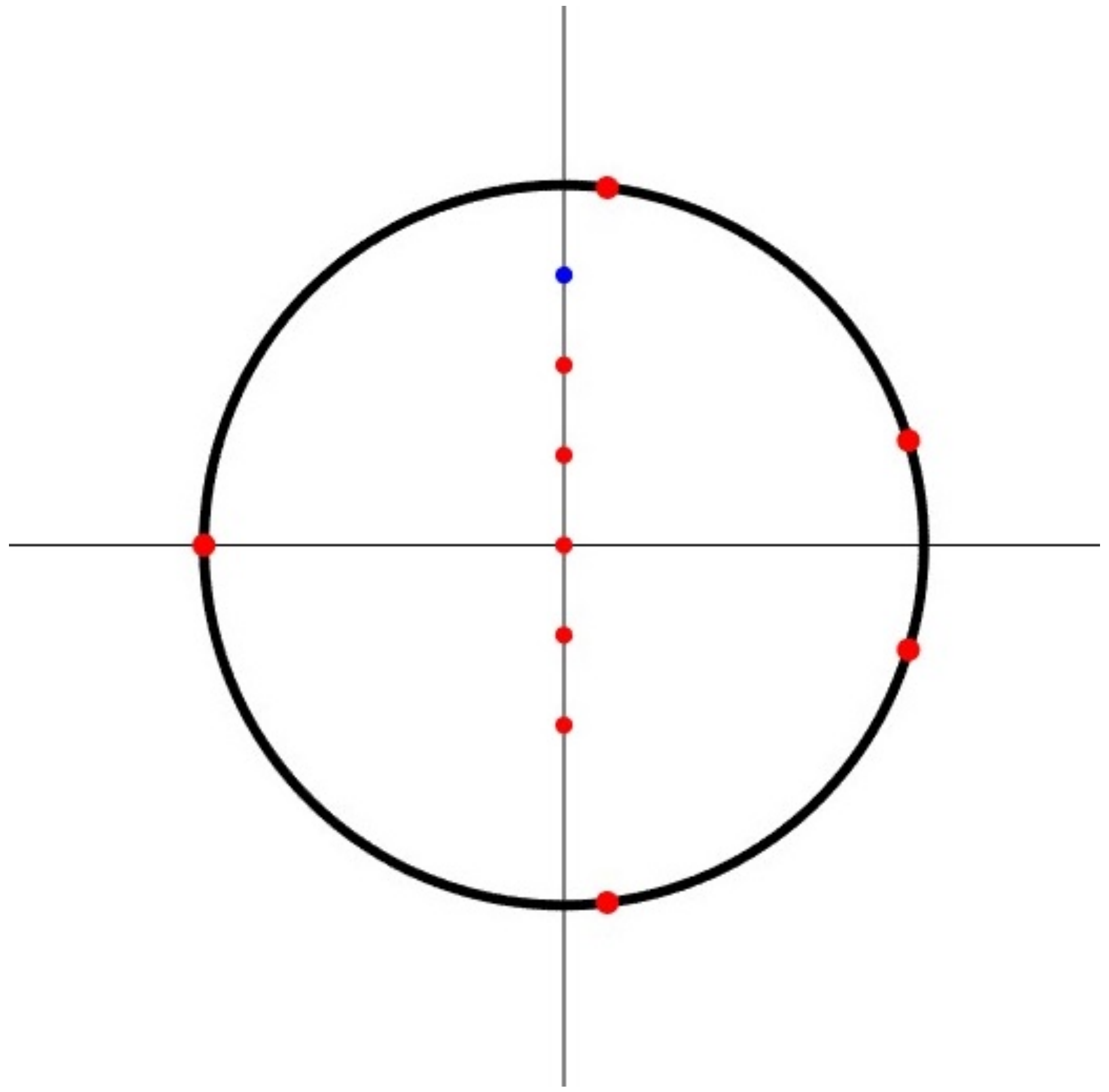

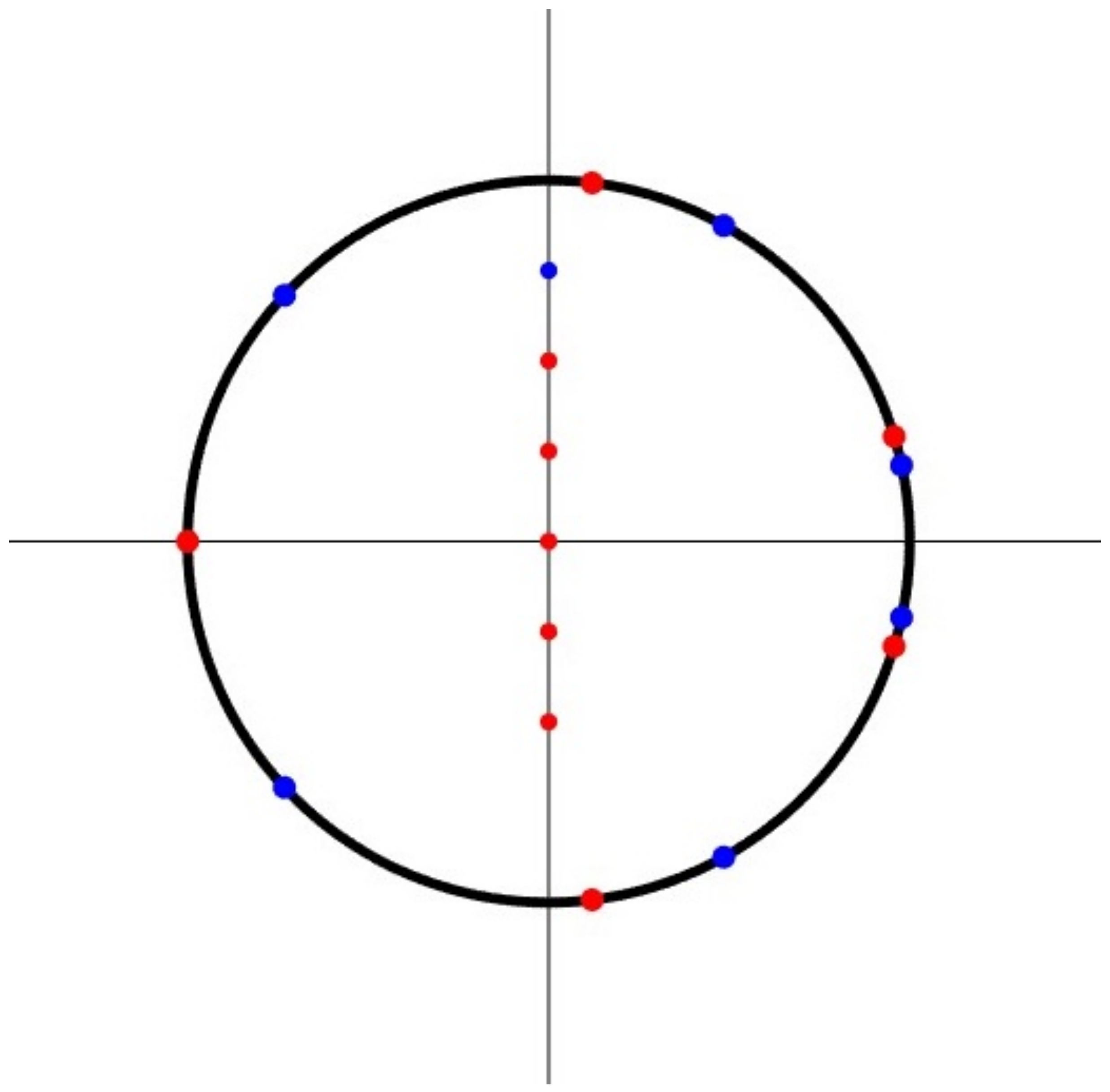

... and you get n+1 new ones!

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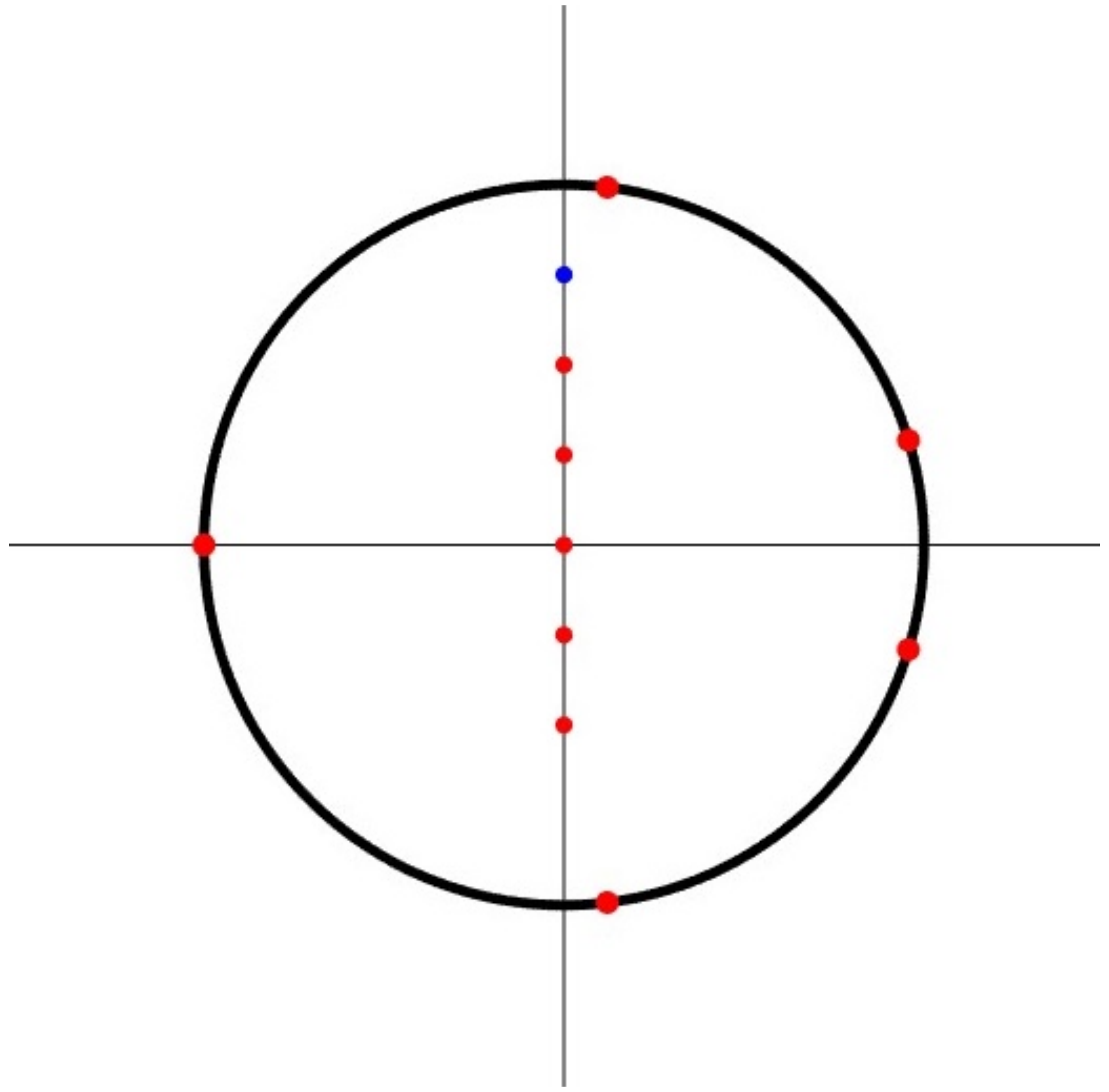

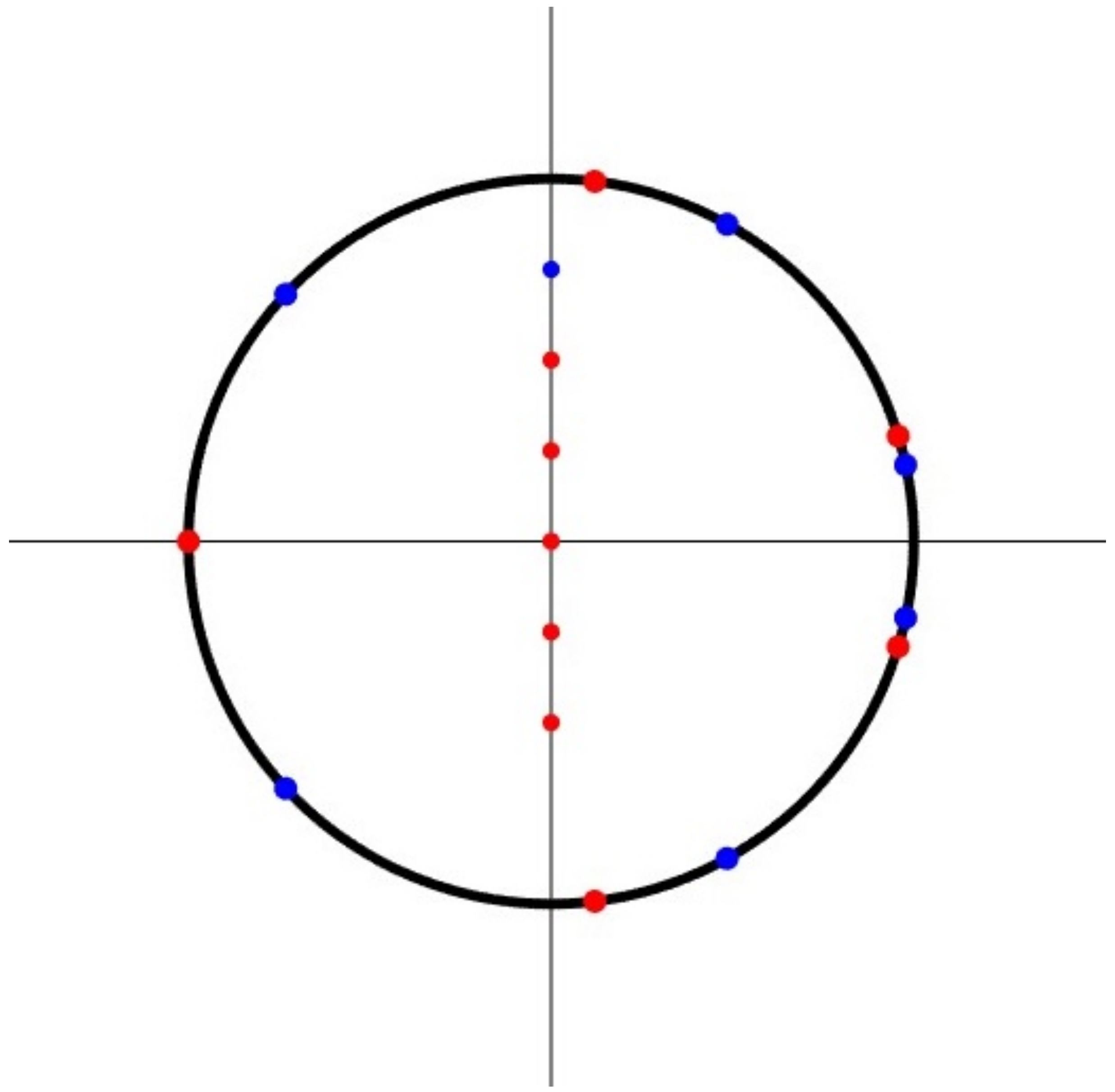

... and you get
n+1 new ones!

... extra tricks we can play ... (Laplace) reparametrization!

$$f(s_j) = \int_0^\infty e^{-ts} F(t)\, dt = t_0 \int_0^\infty e^{-tt_0 s} F(tt_0)\, dt = t_0 \int_0^\infty e^{-t} e^{-t(t_0 s - 1)} F(tt_0)\, dt$$

... we can get quite a number of values! ... actually all those for which the machinery works ...

… (Laplace) reparametrization!

… In the end … DOES IT WORK?!

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Not only we can possibly get quite a number of values … we get a CONSISTENCY ARGUMENT!

$$f(s_j) \sim \sum_k e^{-t_k (t_0\, s - 1)}\, F(t_k\, t_0)\, dt$$

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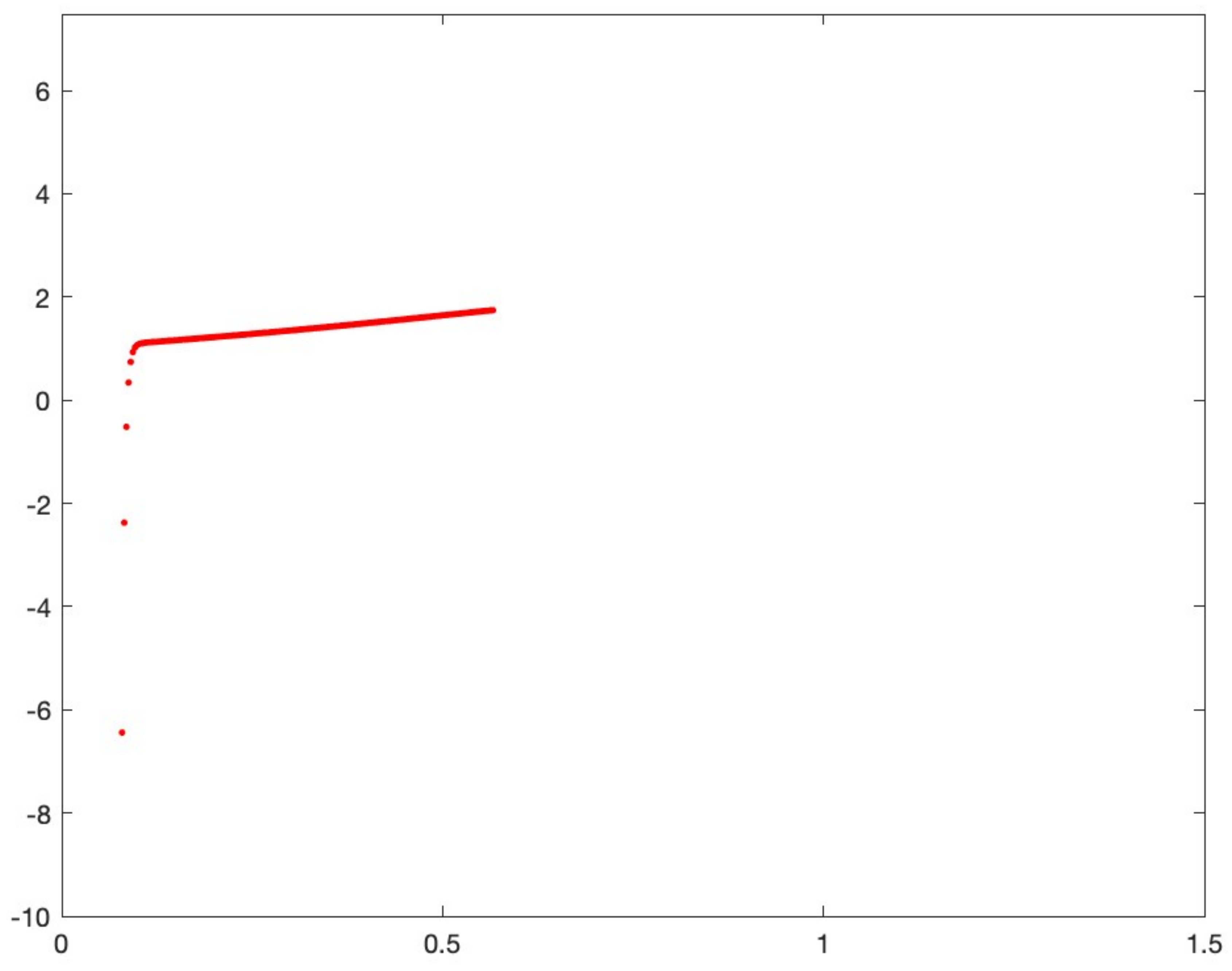
$$k = 2$$



Some CRAZY points

... and ...

a number falling on a SMOOTH line

We said we get a CONSISTENCY ARGUMENT …

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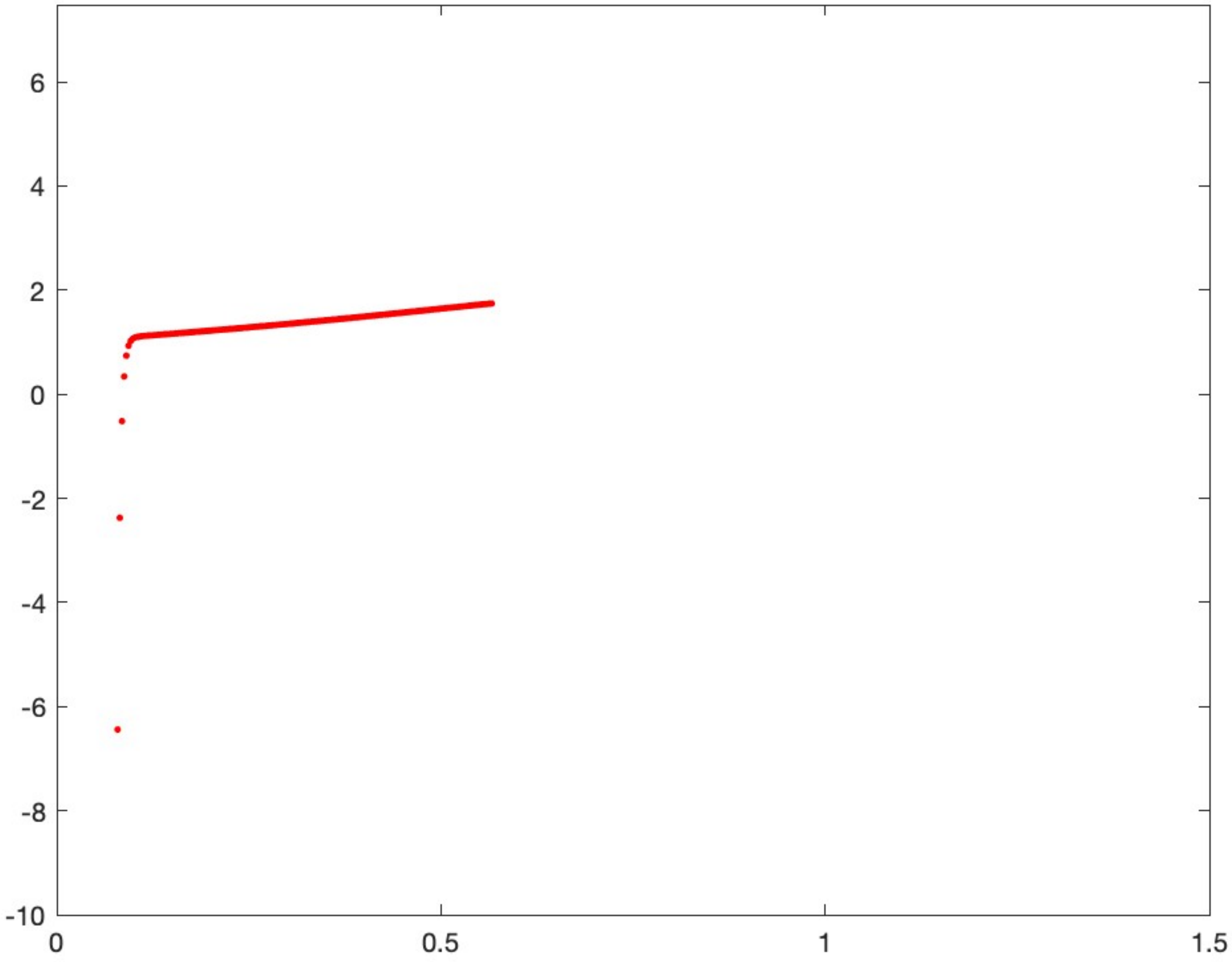

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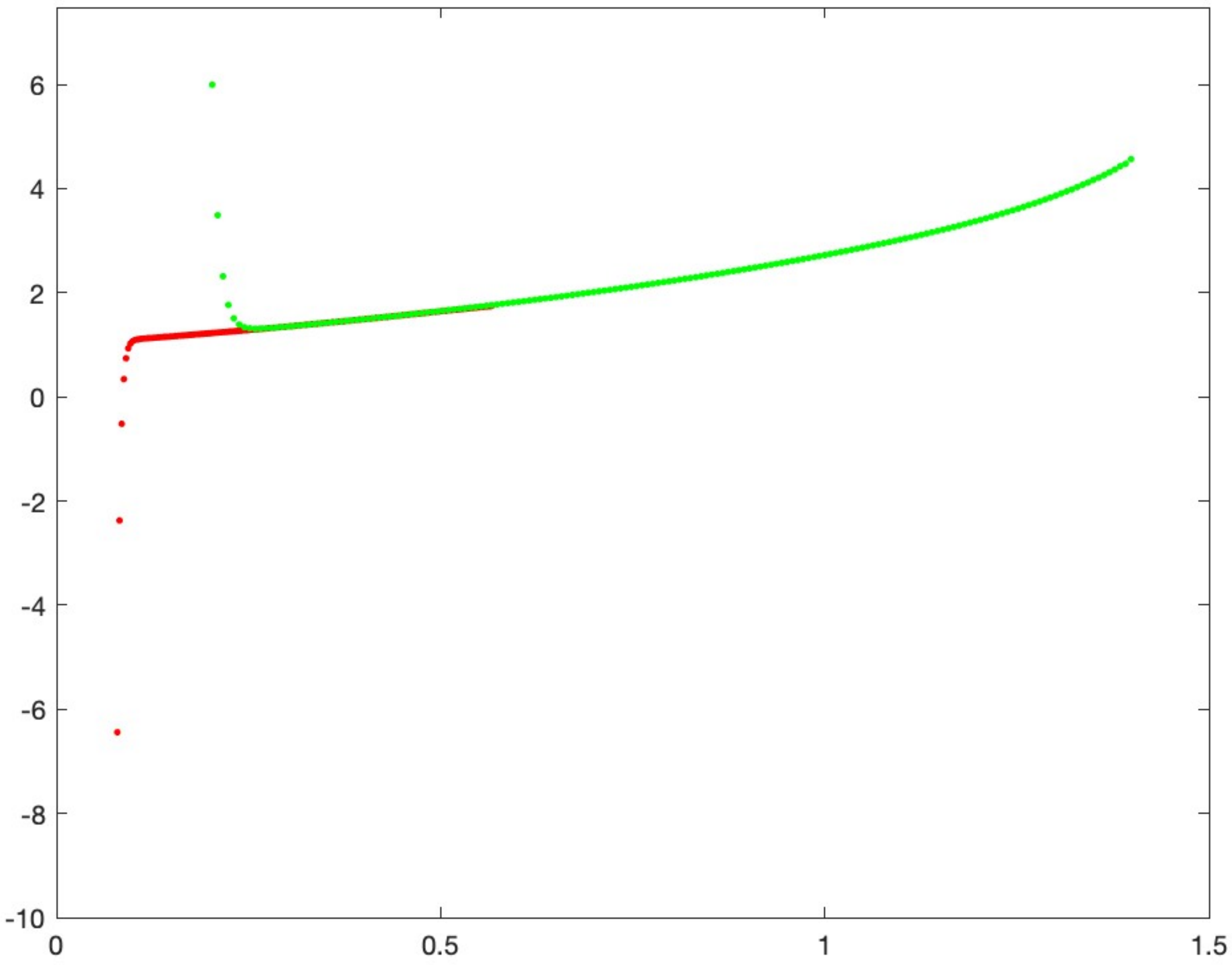
$$k = 2, 3$$



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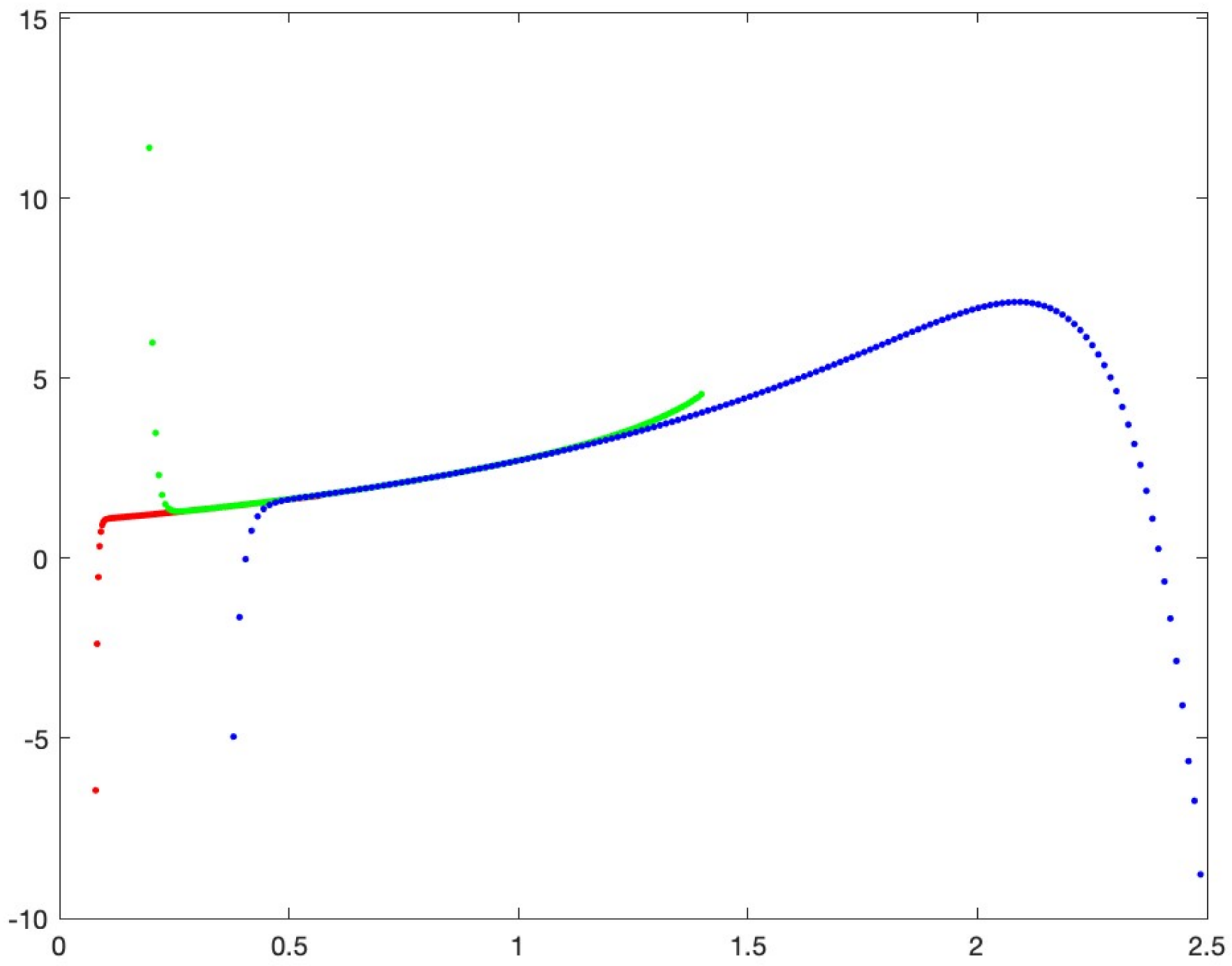

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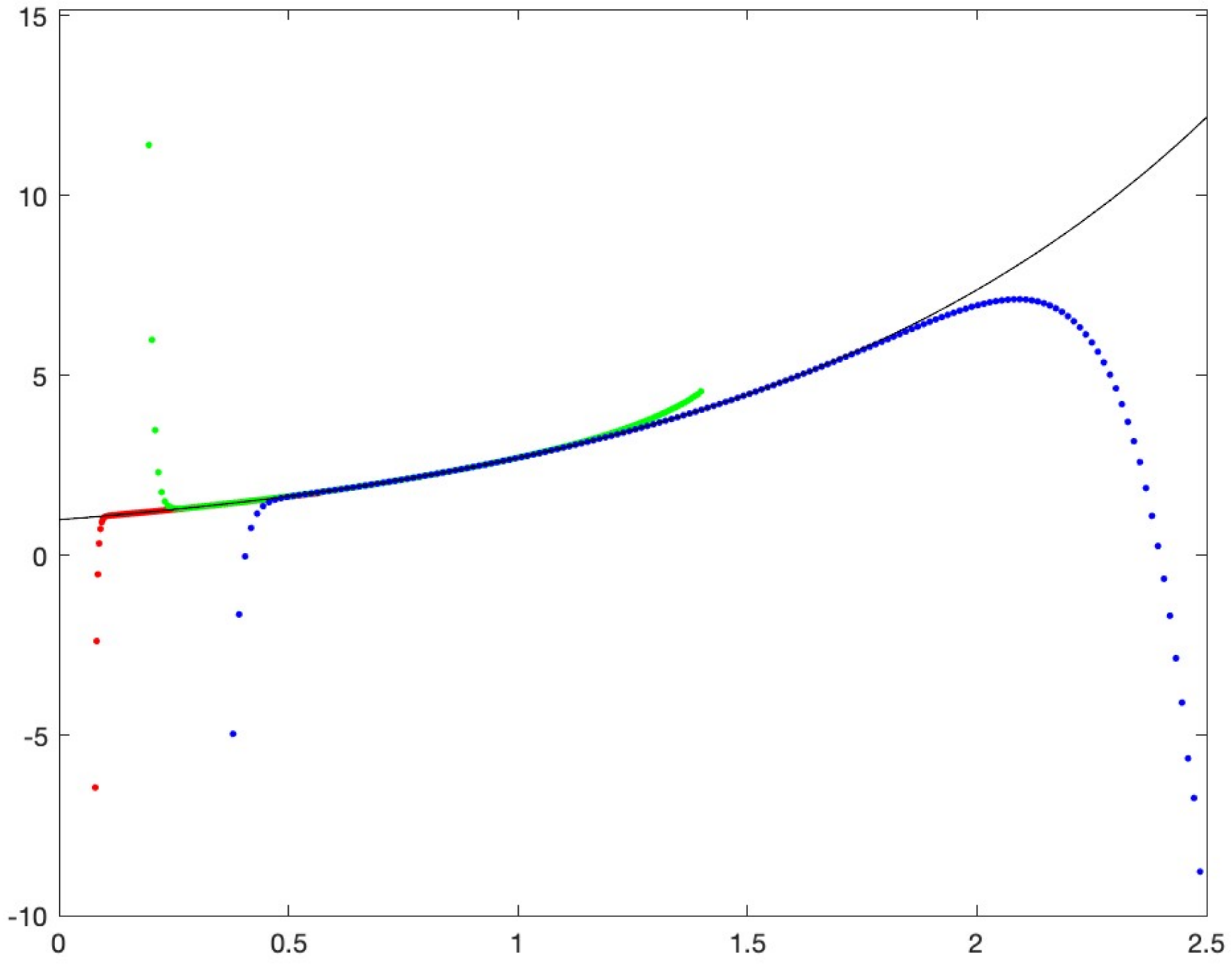
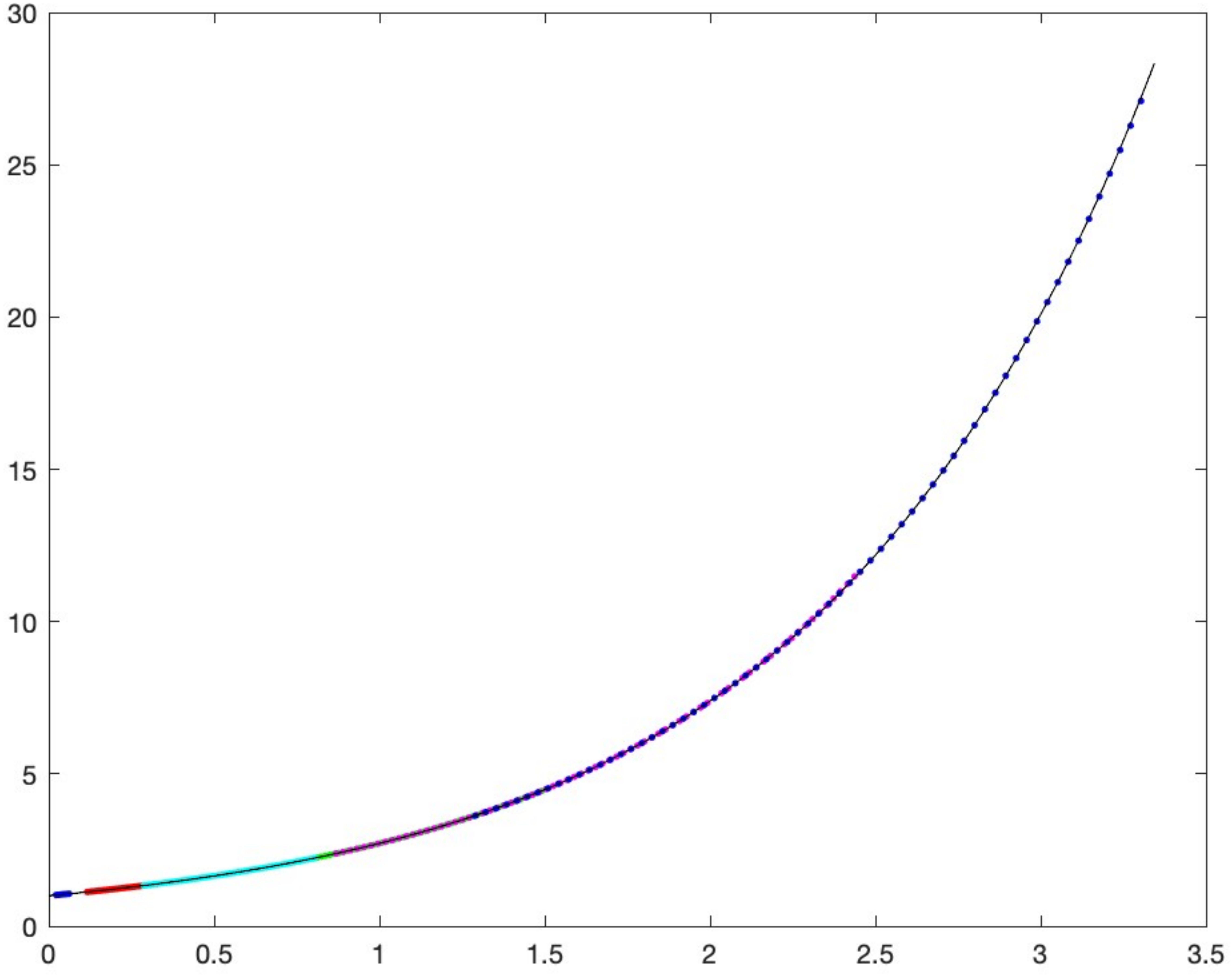
The black line is the EXPONENTIAL ...!



... In the end ... DOES IT WORK?!

... It is fair to say... IT WORKS!

... provided we look for smooth overlaps ...!
(... of course, provided they show up ...)



… but what about the CAUCHY FORMULA?!

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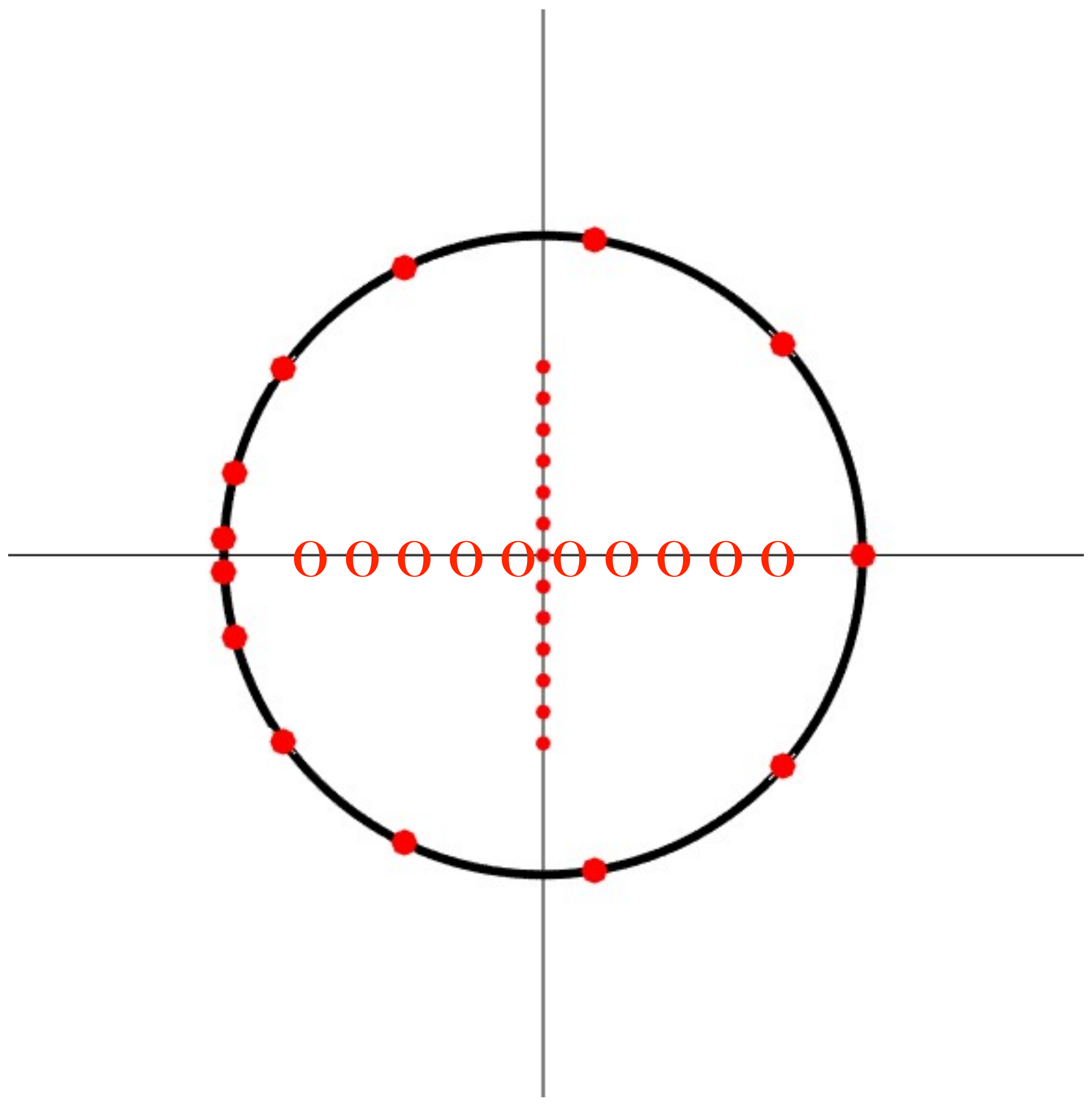
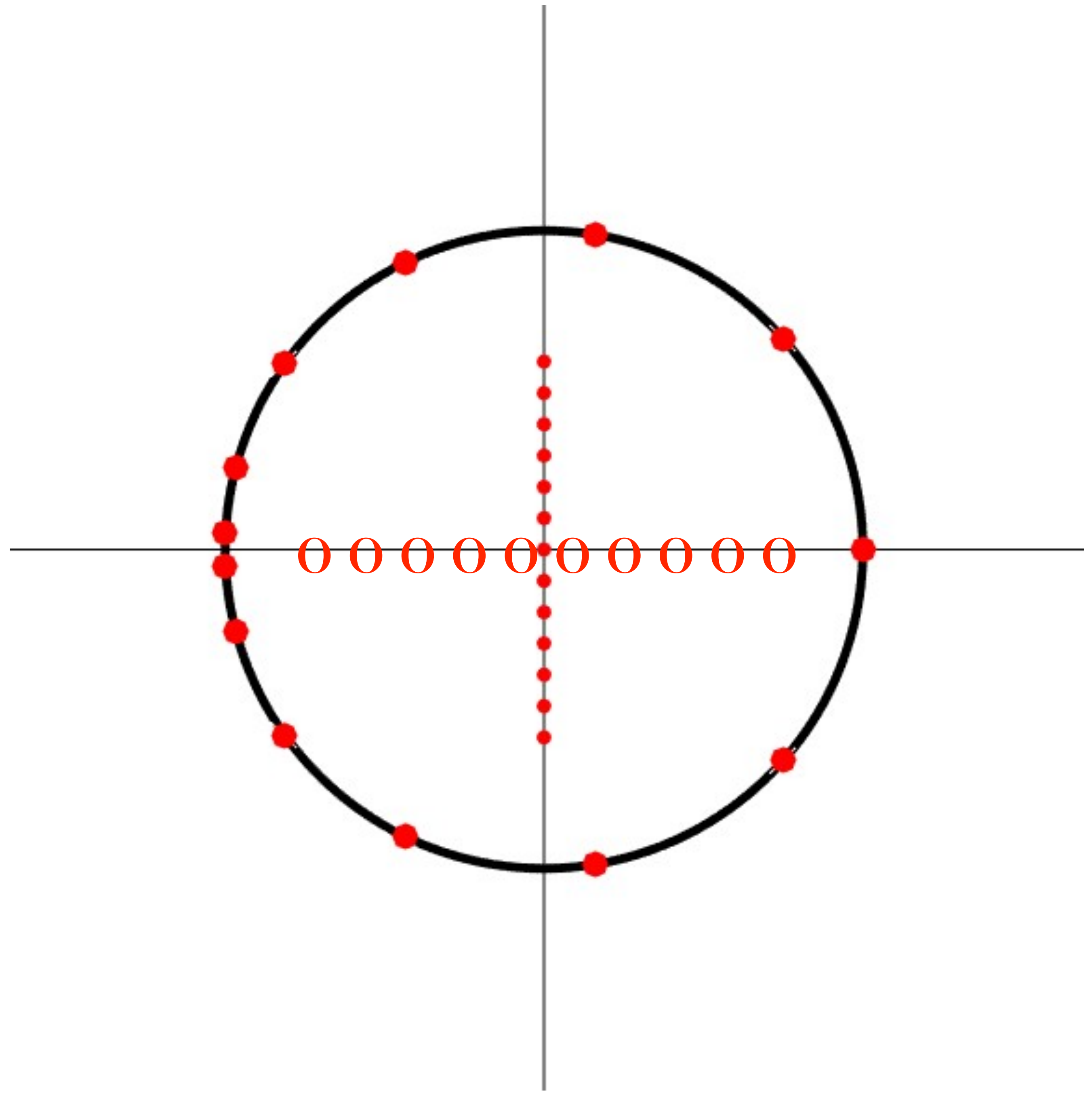
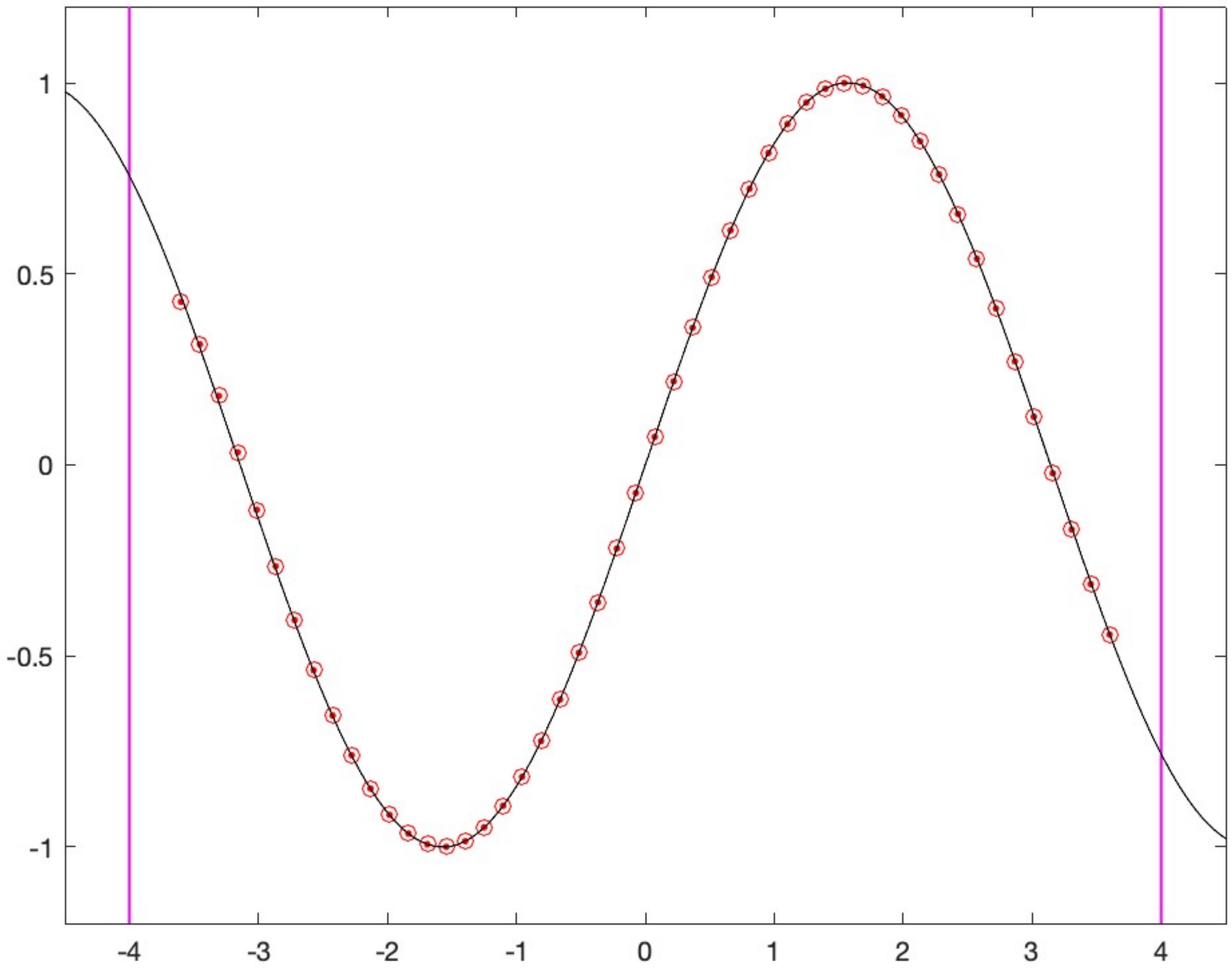
This is the cartoon to remember …



... but what about the CAUCHY FORMULA?!

Here we go!... **computing the sin function on the real axis**
knowing values on the imaginary axis!





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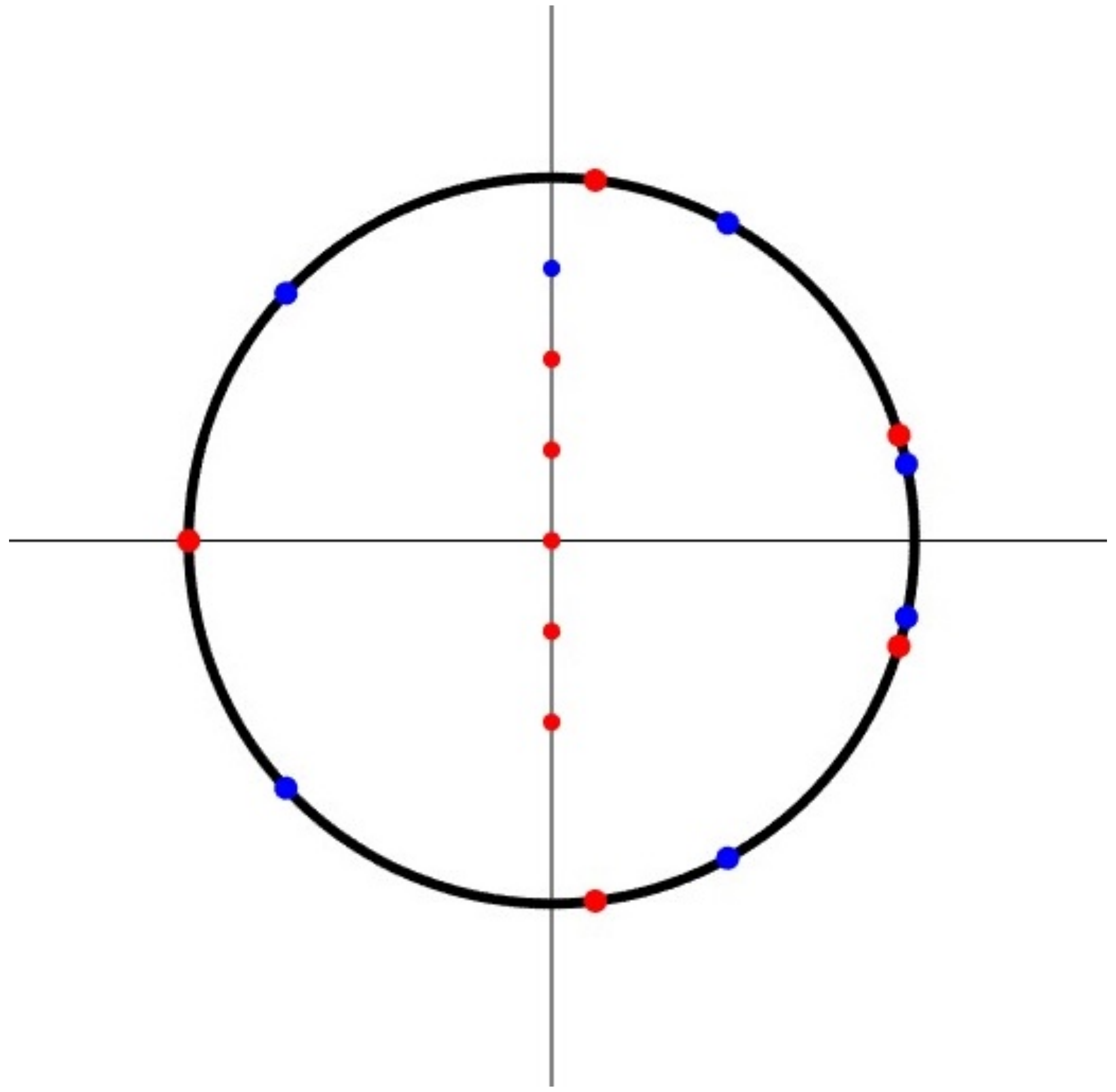
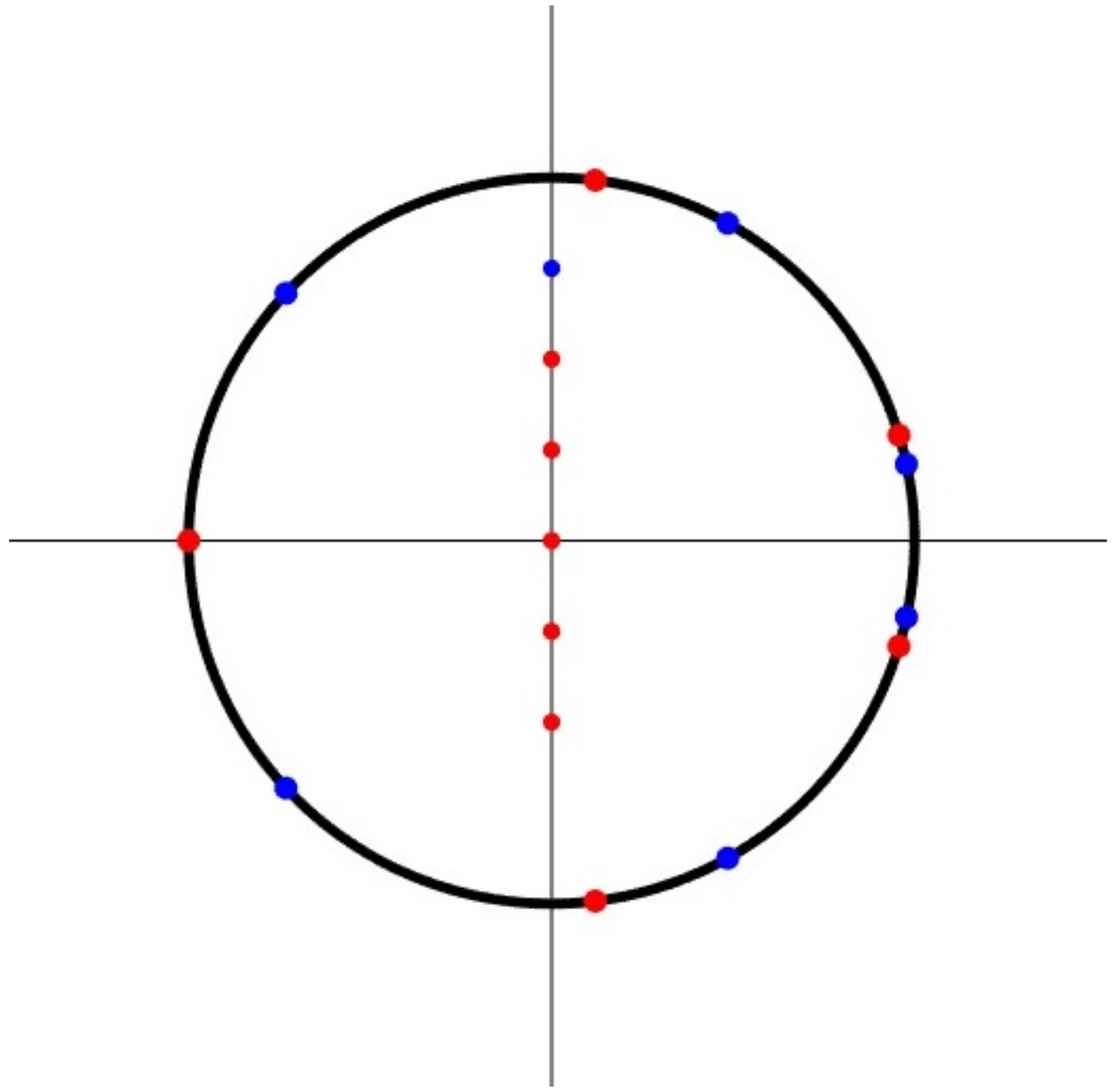
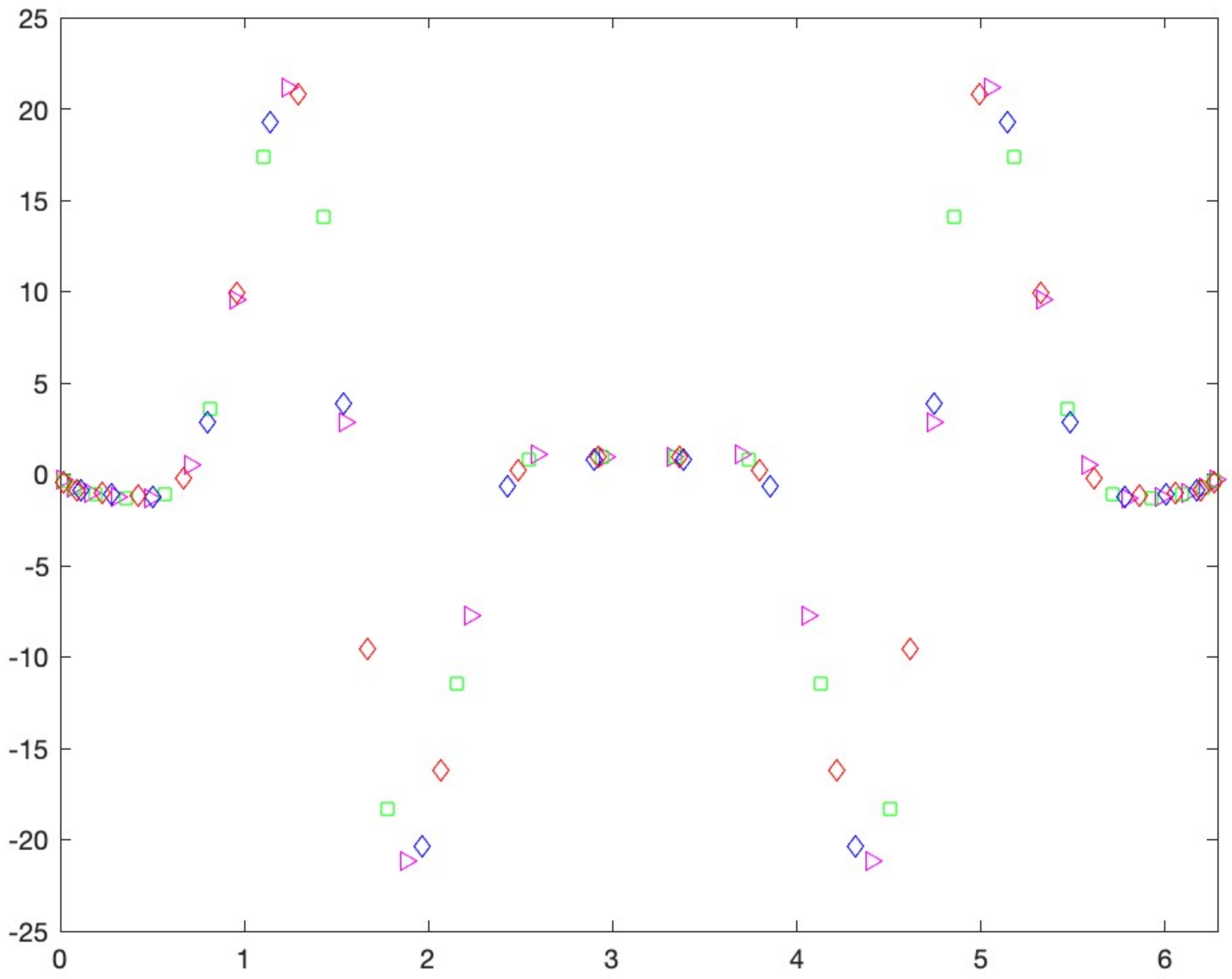


… but what about the CAUCHY FORMULA?! Can we trust this (apparently) good results?

Looking at the solution of the inverse problem, we get a smooth curve showing up!

(This is the real part of the sin function at the quadrature points)

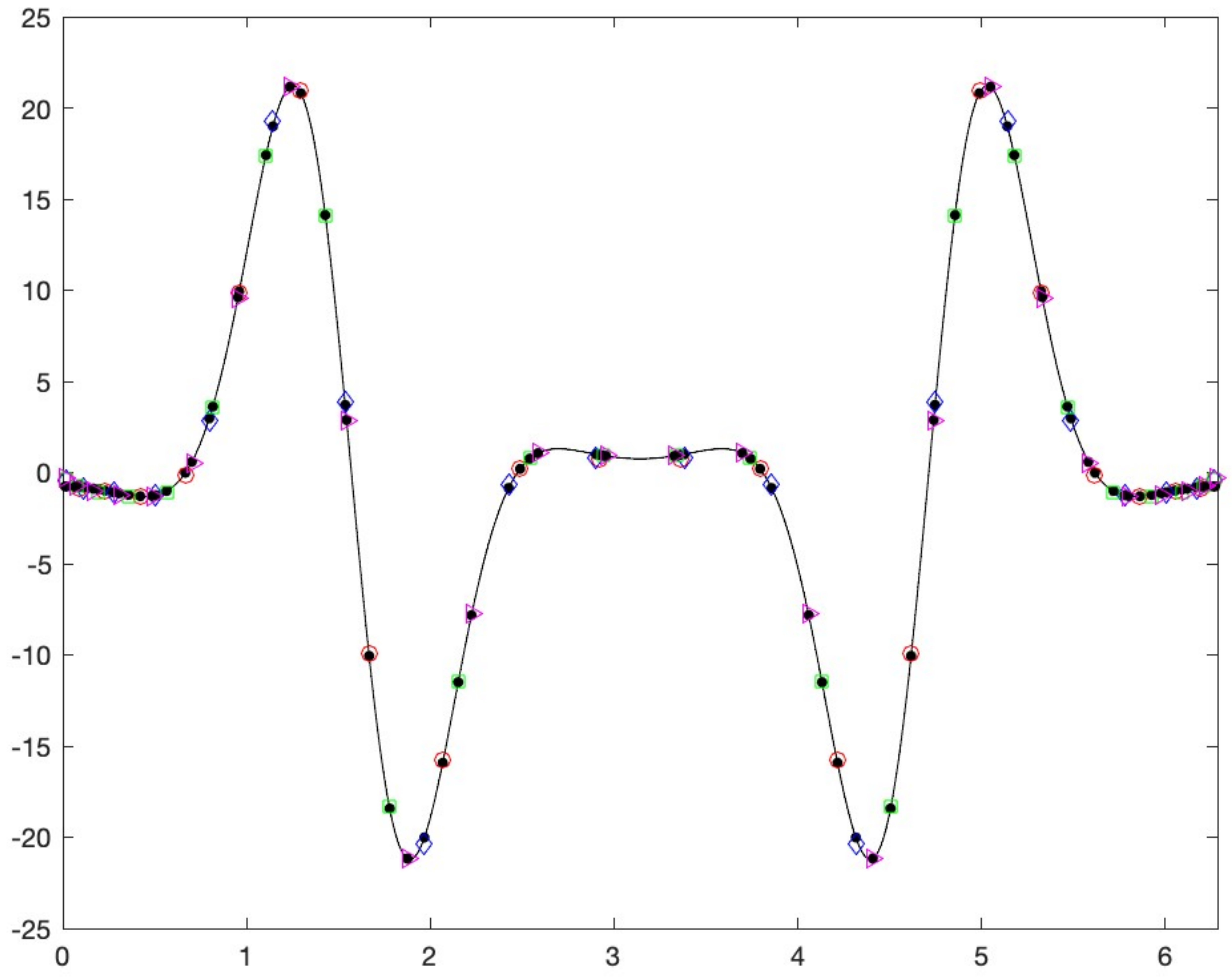




... but what about the CAUCHY FORMULA?! Can we trust this (apparently) good results? **YES!**

It is indeed what we should have found ...

(This is the real part of the sin function at the quadrature points)



I have not yet told you the entire story …

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Do you remember the great success ?

$$f(s_j) \sim \sum_k e^{-t_k(t_0\, s-1)}\, F(t_k\, t_0)\, dt$$

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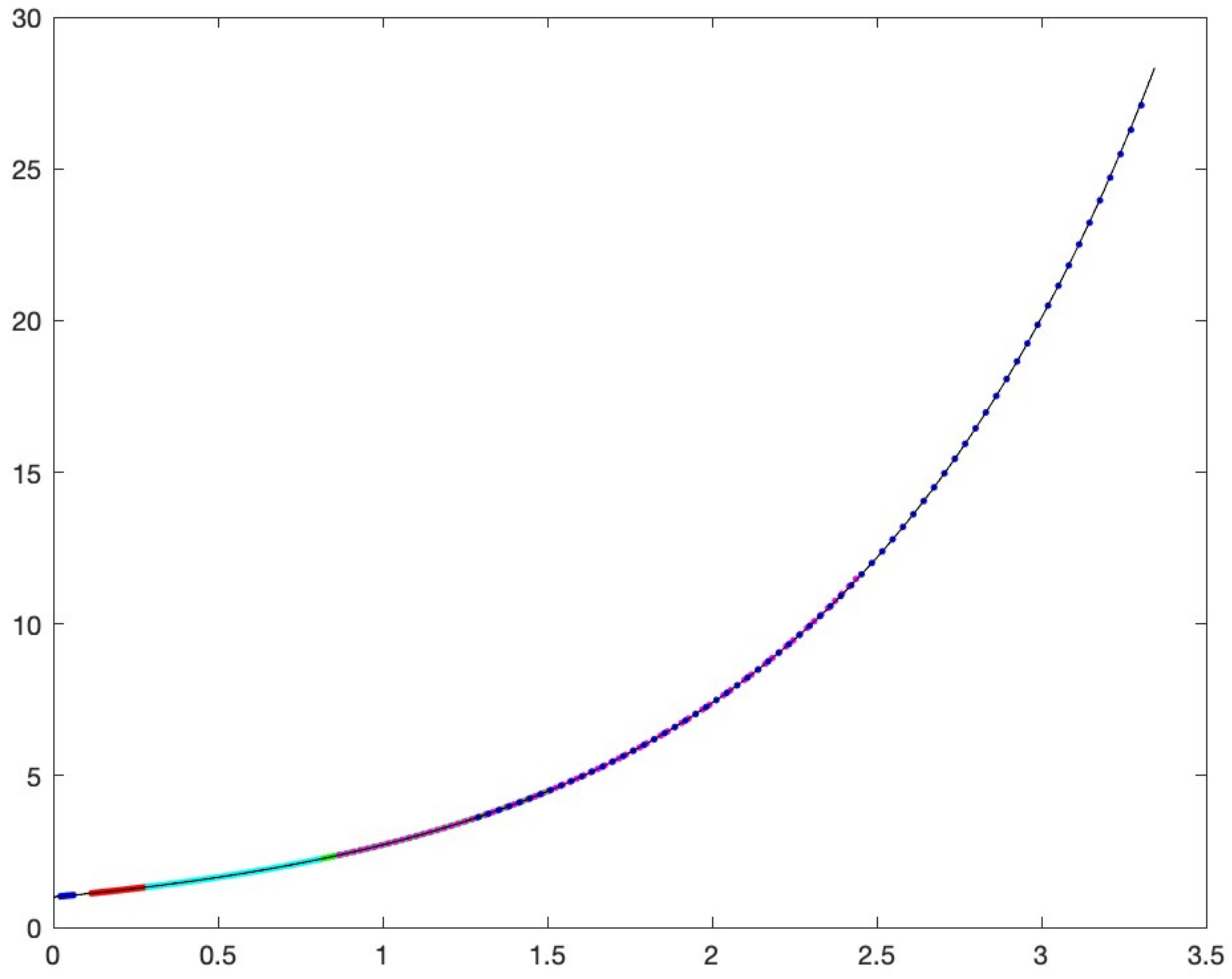

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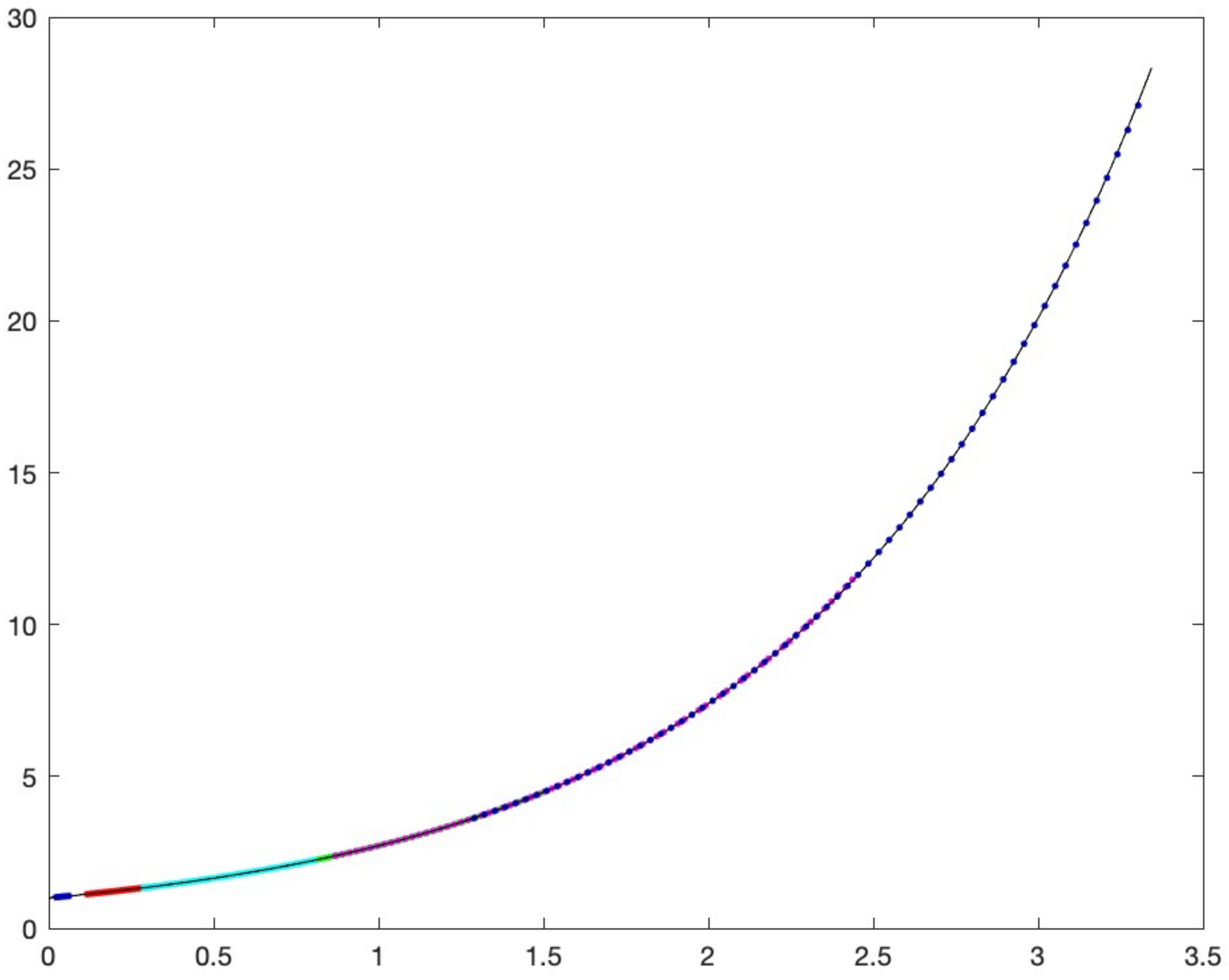
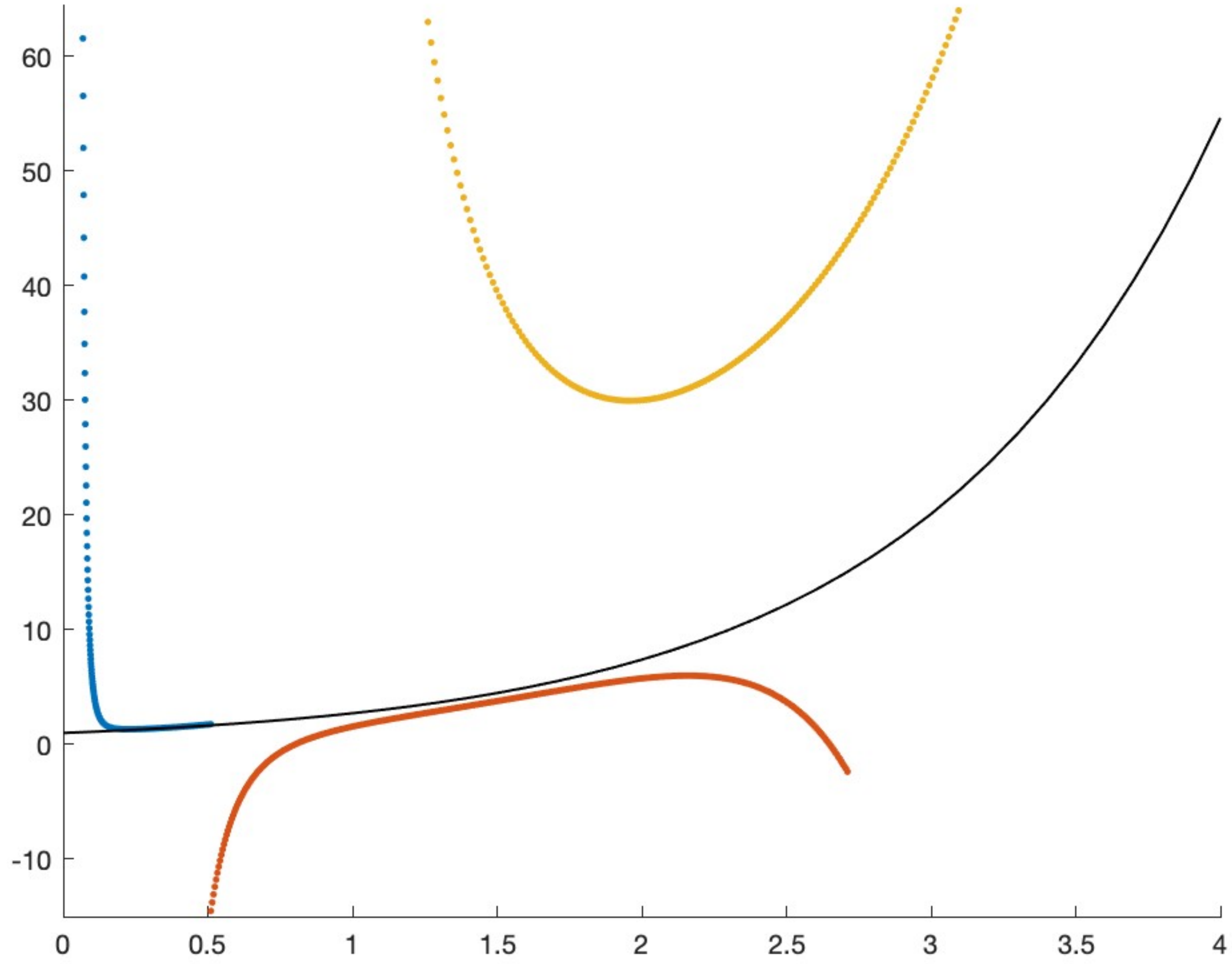
... so, what if ERRORS show up ?!?



I have not yet told you the entire story …

… so, what if ERRORS show up ?!?

Apparently, you loose everything !



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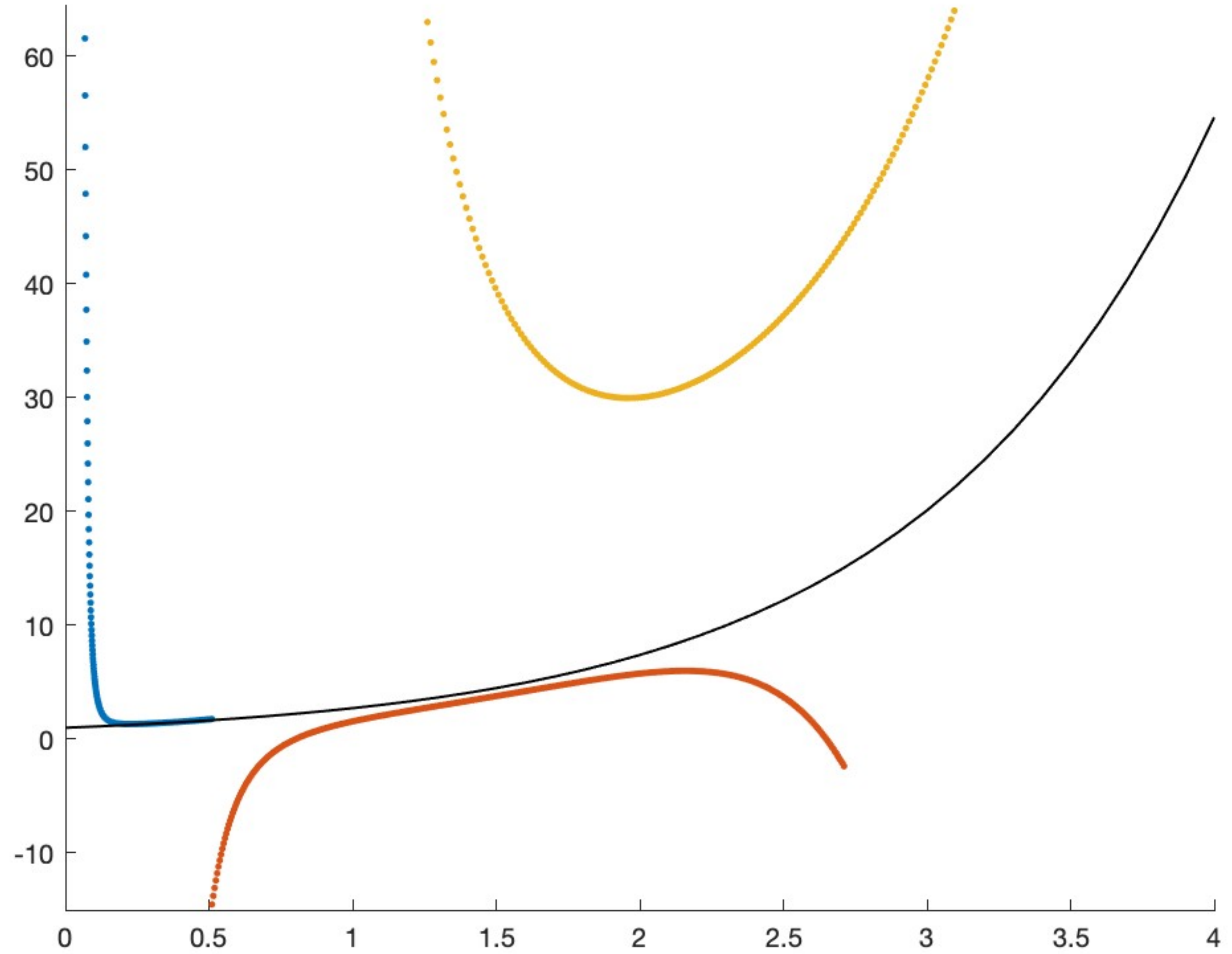
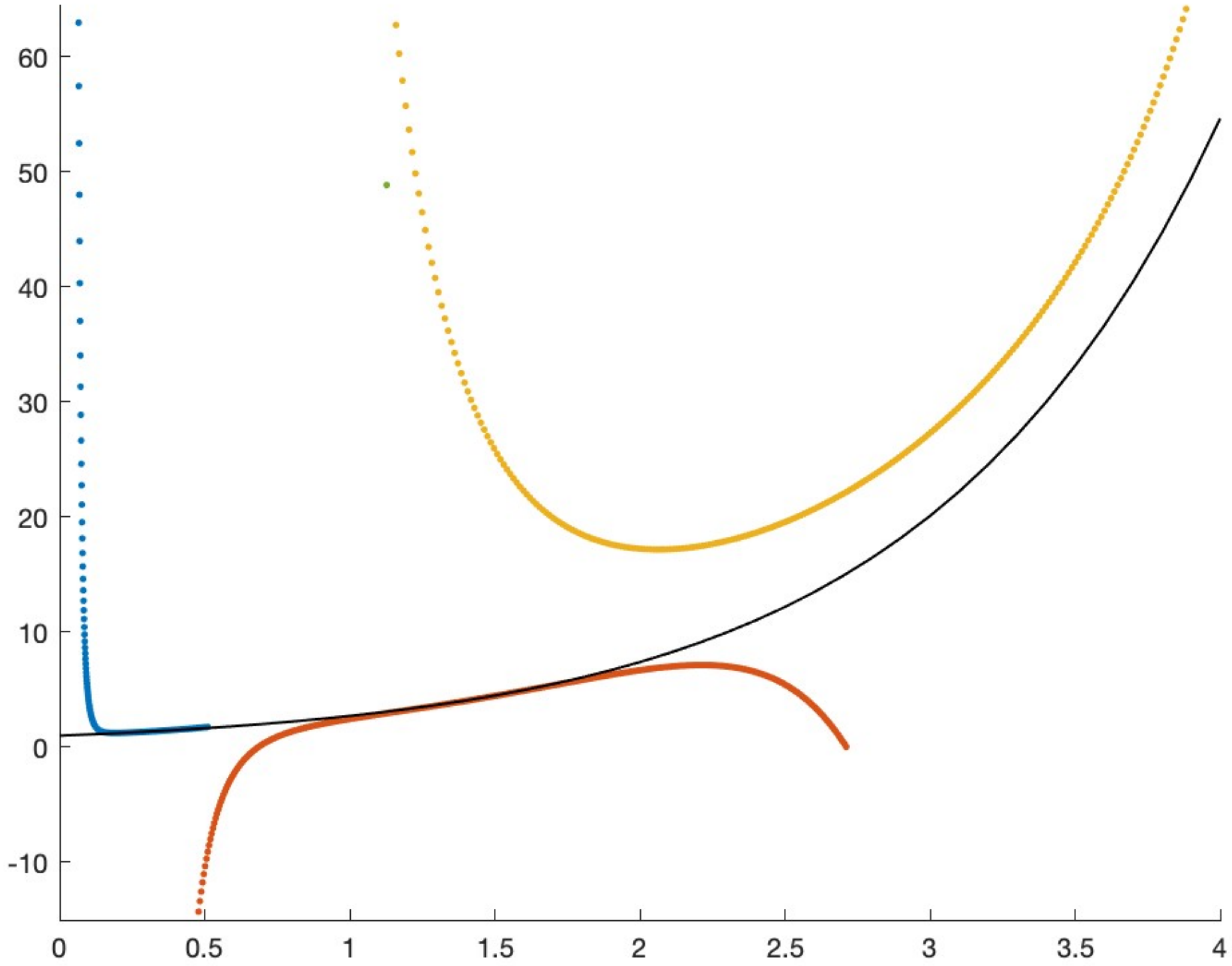


Well, that's not really the case …



The BIG ISSUE and the (dream?) project: **moving points within error-bars, the picture can change quite a lot!** This example was found by accident(!), **but one can systematically go hunting for a a smooth solution of the inverse problem…**

WORK IN PROGRESS

… and still, let's go back to the main point: the lattice QCD sign problem as an inverse problem …

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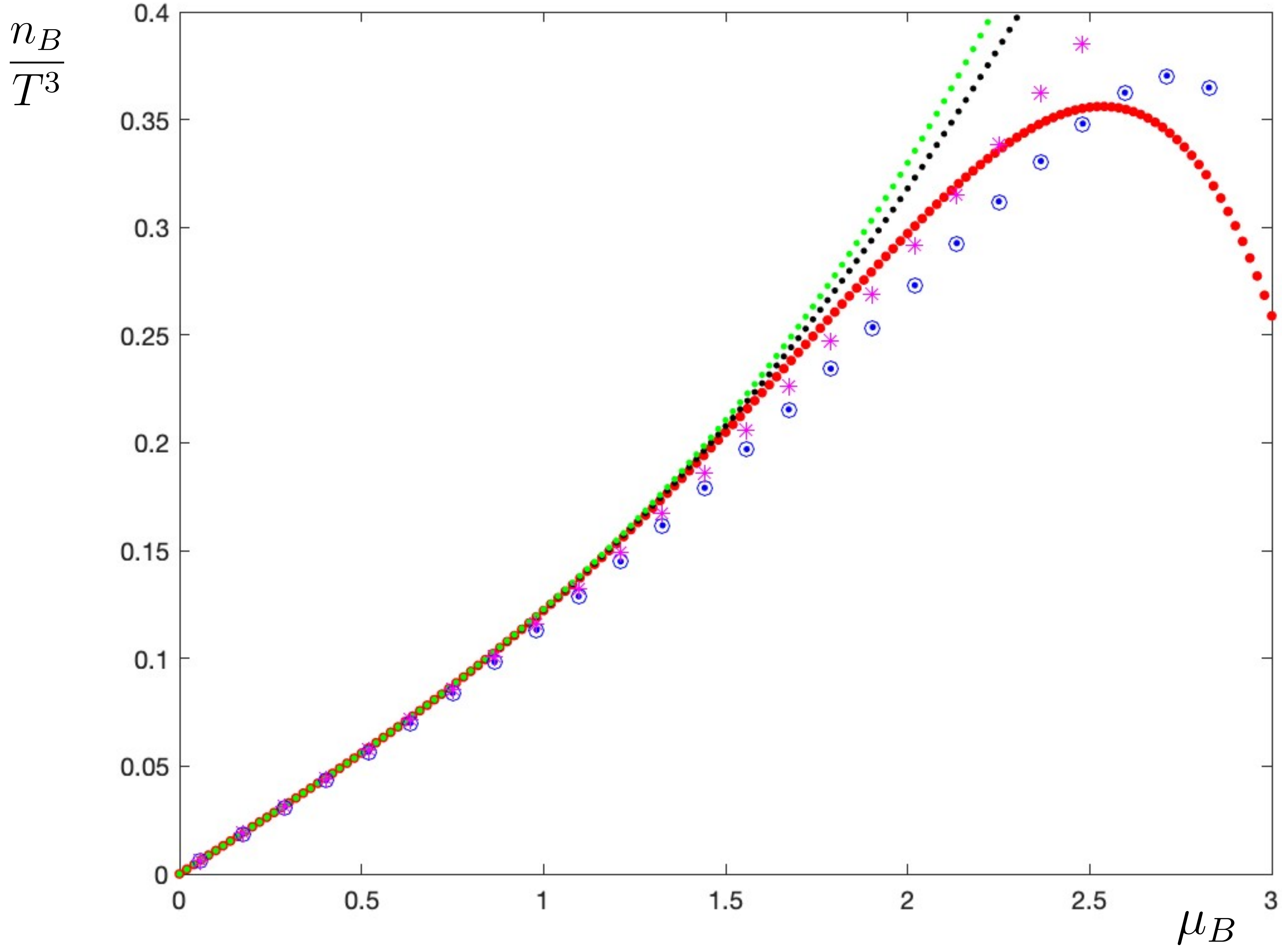
$T = 157.5\ (\sim 155)$ MeV



(VERY!) **Preliminary results from the Cauchy formula inverse problem**:

DOTS are results coming from Taylor coefficients computations (at different orders)

other symbols come from the Cauchy formula
(still quite sizeable systematic effects, i.e. sensitivity to the input we provided, but this is very preliminary

... the dream project still under its way!)

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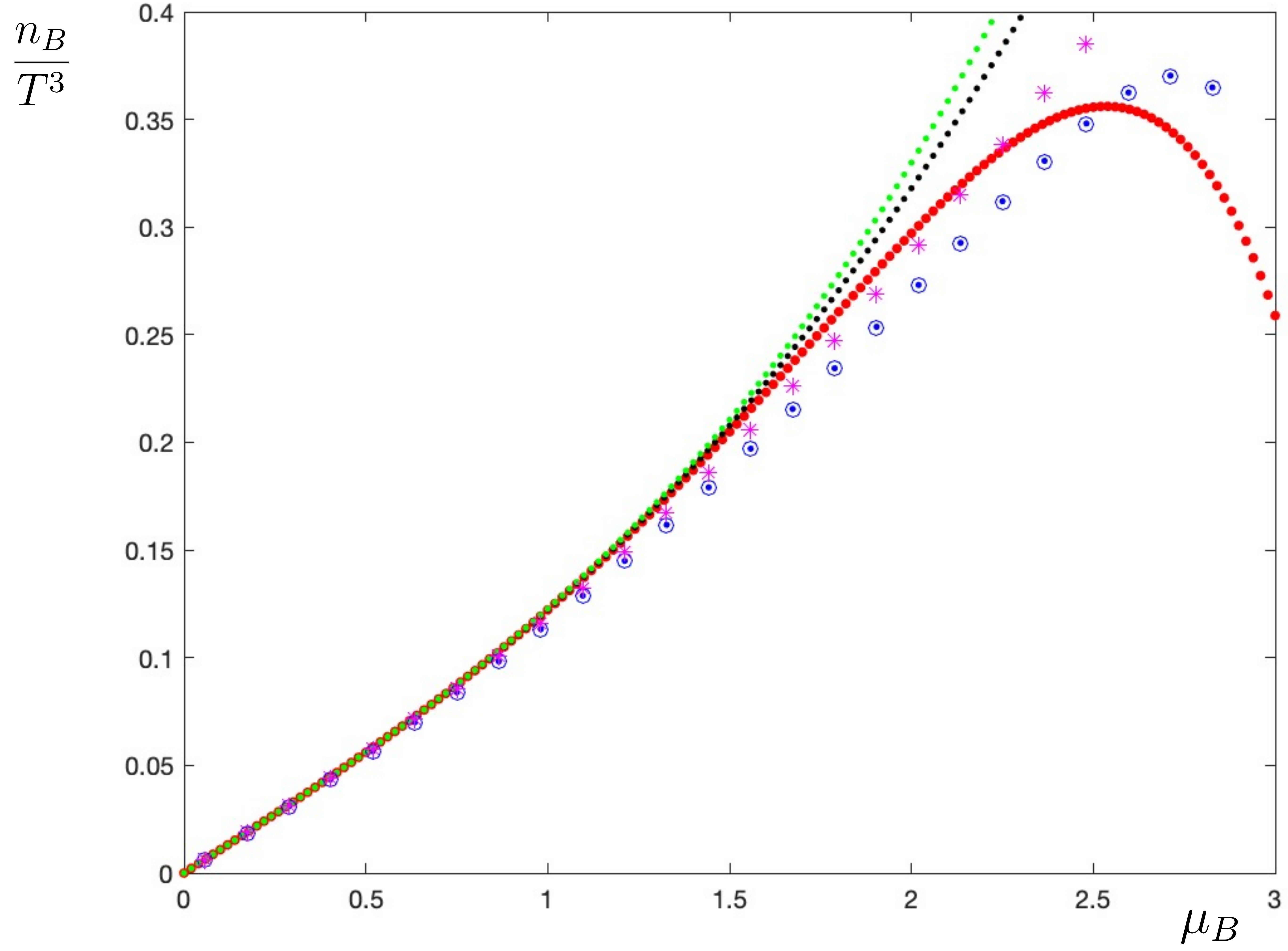

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STAY TUNED!

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- Working on (inverse) Cauchy formula for **Lattice QCD sign problem**
- …but also on **(anti)Laplace transforms** (spectral functions and all that…)
- In the end, many applications in (general) **inverse problems** …
- … which also means **interpolation and extrapolation** problems