2020

INTRODUCTION TO NUMERICAL ANALYSIS

Lecture 2-5:
Root finding & minimization

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ROOT FINDING

- Root finding is one of classical algebra problems since your high school times...
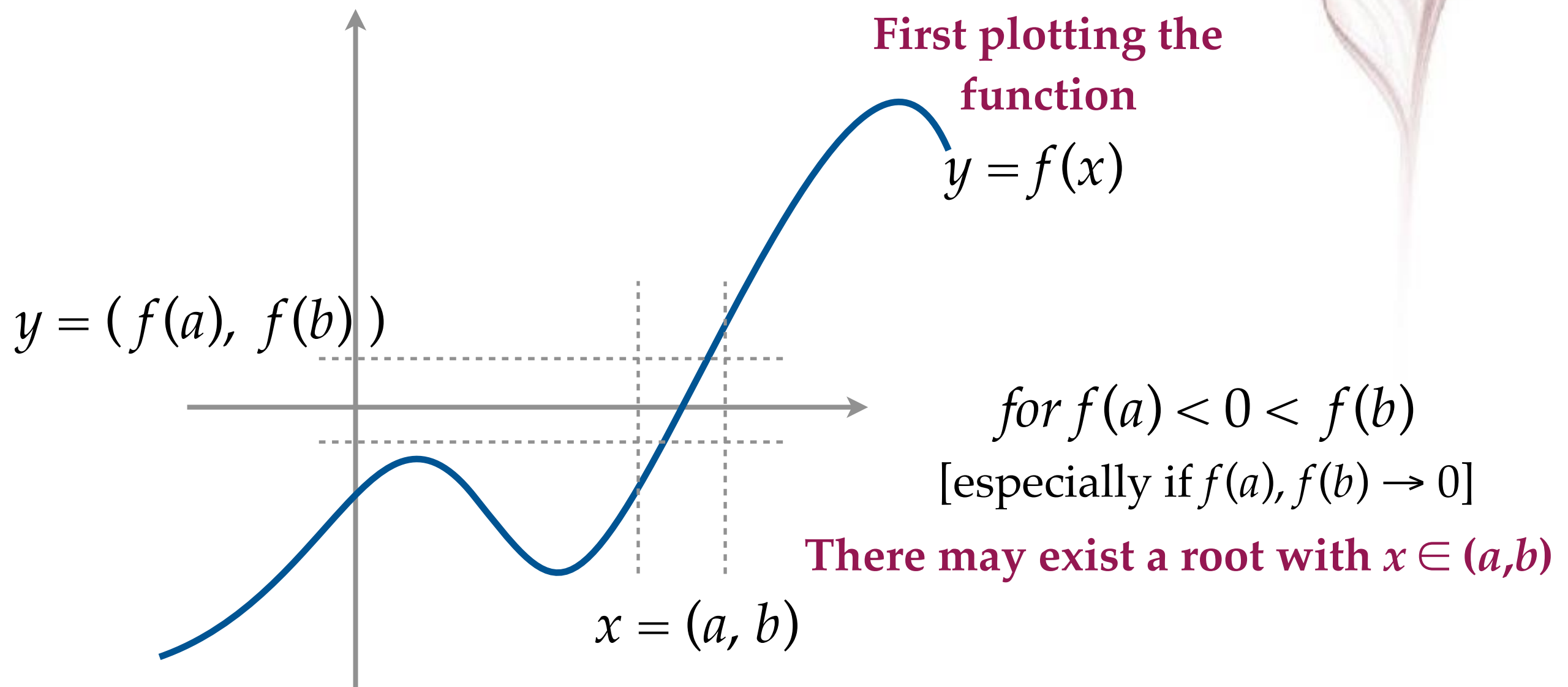
For a given function f(x),

if f(x) = 0, what's the x?

A CLASSICAL METHOD:
FIND THE ANSWER WITH YOUR EYES

- I'm not talking about peeking at other person's answer sheet...

A CLASSICAL METHOD:
FIND THE ANSWER WITH YOUR EYES

First plotting the function

$y = f(x)$

$y = (\, f(a),\ f(b)\,)$

$for\ f(a) < 0 < f(b)$

[especially if $f(a), f(b) \to 0$]

There may exist a root with $x \in (a,b)$

$x = (a,\ b)$

(Assessment: try to find an invalid example!)

LET DO SUCH A PRACTICE WITH YOUR COMPUTER

- Suppose we know that there is an solution of f(x) = 0 for x ∈(a,b), how to find the best solution by your computer?
- Surely there is an "almost" trivial algorithm: the **Bisection method**
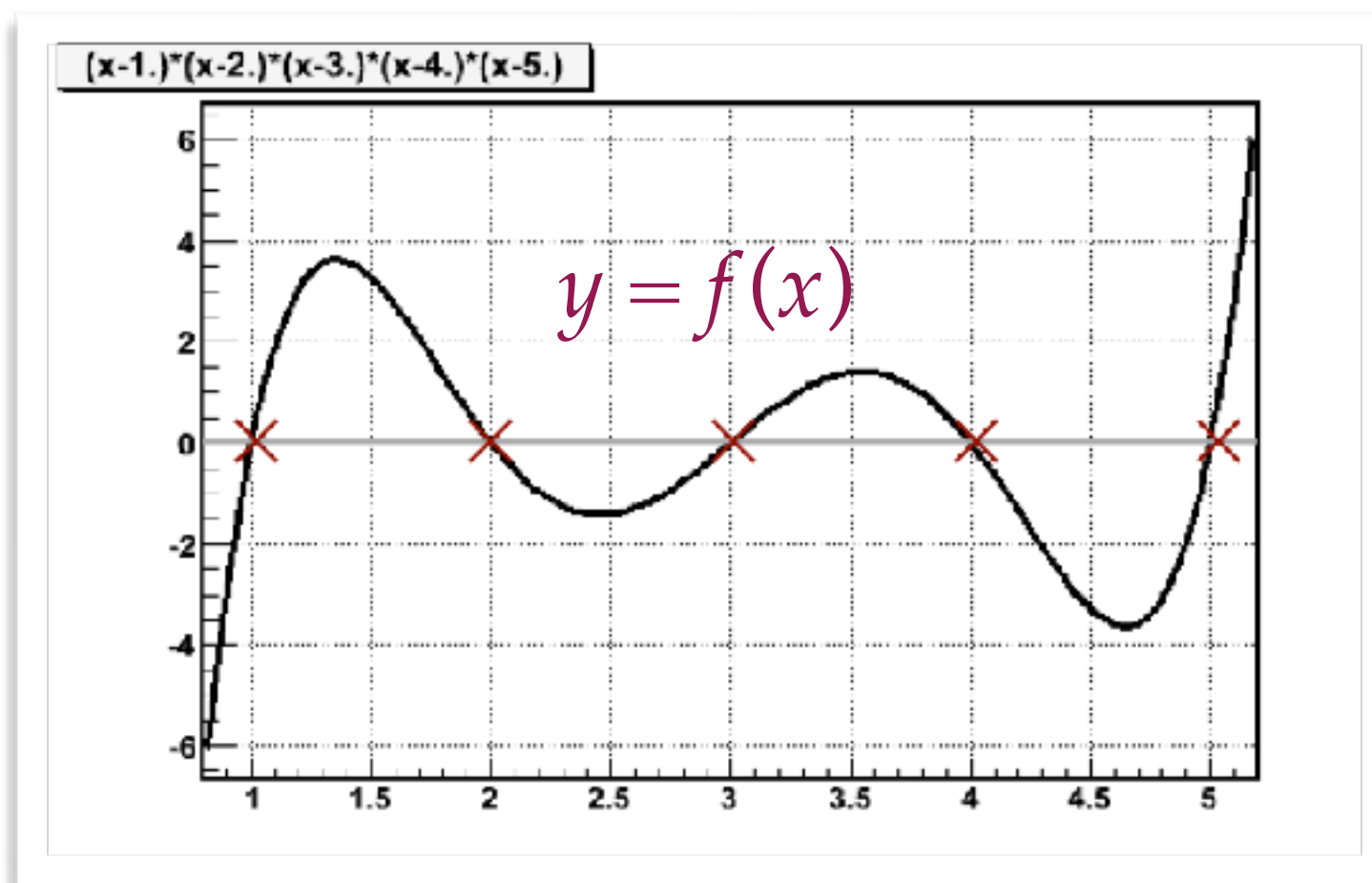
$$x = a' = \frac{a+b}{2}$$

$$x = a$$

$$x = b$$
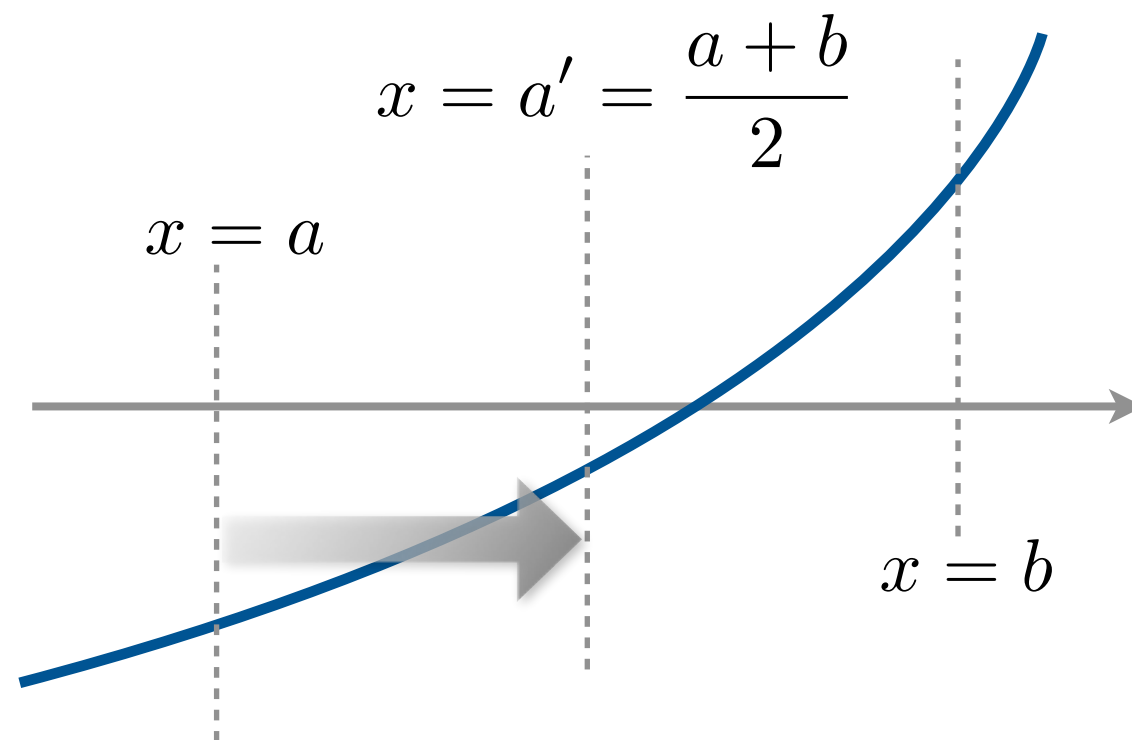
*Keep updating the boundaries with the middle point of **a** and **b**, until reaching the limited precision.*

LET'S GIVE IT A TRY!

■ Suppose that we are going to solve the following equation:

$$f(x) = (x - 1) \cdot (x - 2) \cdot (x - 3) \cdot (x - 4) \cdot (x - 5) = 0$$

$y = f(x)$

Surely we know that there are 5 explicit solutions.

A DEMO IMPLEMENTATION

- A simple implementation of the Bisection method:

```python
def f(x):
    return (x-1.)*(x-2.)*(x-3.)*(x-4.)*(x-5.)

a, b = 2.4, 3.4
fa, fb = f(a), f(b)

for step in range(50):   ⇐ Let's do maximum 50 iterations
    c = (a+b)*0.5   ⇐ Test point c – at the middle of a and b
    fc = f(c)

    print('Step: %2d, root = %.16f, diff = %.16f' % (step,c,abs(c-3.)))

    if abs(a-c)<1E-14: break   ⇐ Limited precision = $10^{-14}$

    if fc*fa>0.:
        a, fa = c, fc
    else:
        b, fb = c, fc
```

1205-example-01.py

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A DEMO IMPLEMENTATION (II)

■ Terminal output:

```
Step:   0, root = 2.8999999999999999, diff = 0.1000000000000001
Step:   1, root = 3.1499999999999999, diff = 0.1499999999999999
Step:   2, root = 3.0249999999999999, diff = 0.0249999999999999
Step:   3, root = 2.9624999999999999, diff = 0.0375000000000001
Step:   4, root = 2.9937499999999999, diff = 0.0062500000000001
Step:   5, root = 3.0093749999999999, diff = 0.0093749999999999
... ...
Step:  10, root = 3.0000976562499999, diff = 0.0000976562499999
... ...
Step:  20, root = 2.9999999046325683, diff = 0.0000000953674317
... ...
Step:  30, root = 3.0000000000931322, diff = 0.0000000000931322
... ...
Step:  40, root = 2.9999999999999090, diff = 0.0000000000000910
... ...
Step:  44, root = 2.9999999999999942, diff = 0.0000000000000058
Step:  45, root = 3.0000000000000084, diff = 0.0000000000000084
Step:  46, root = 3.0000000000000013, diff = 0.0000000000000013
```

HIGHER ORDER METHOD(S)

- Although this bisection algorithm sounds not so smart, but it must success (if the function is ***well behaved***).

- For higher efficiency (speed), we could go for the algorithms with an idea of higher order mathematics, e.g. **Brent's Method**:

Suppose we have three points: $(x,y) = (\ a,\ f_a\ ),\ (\ b,\ f_b\ ),\ (\ c,\ f_c\ )$

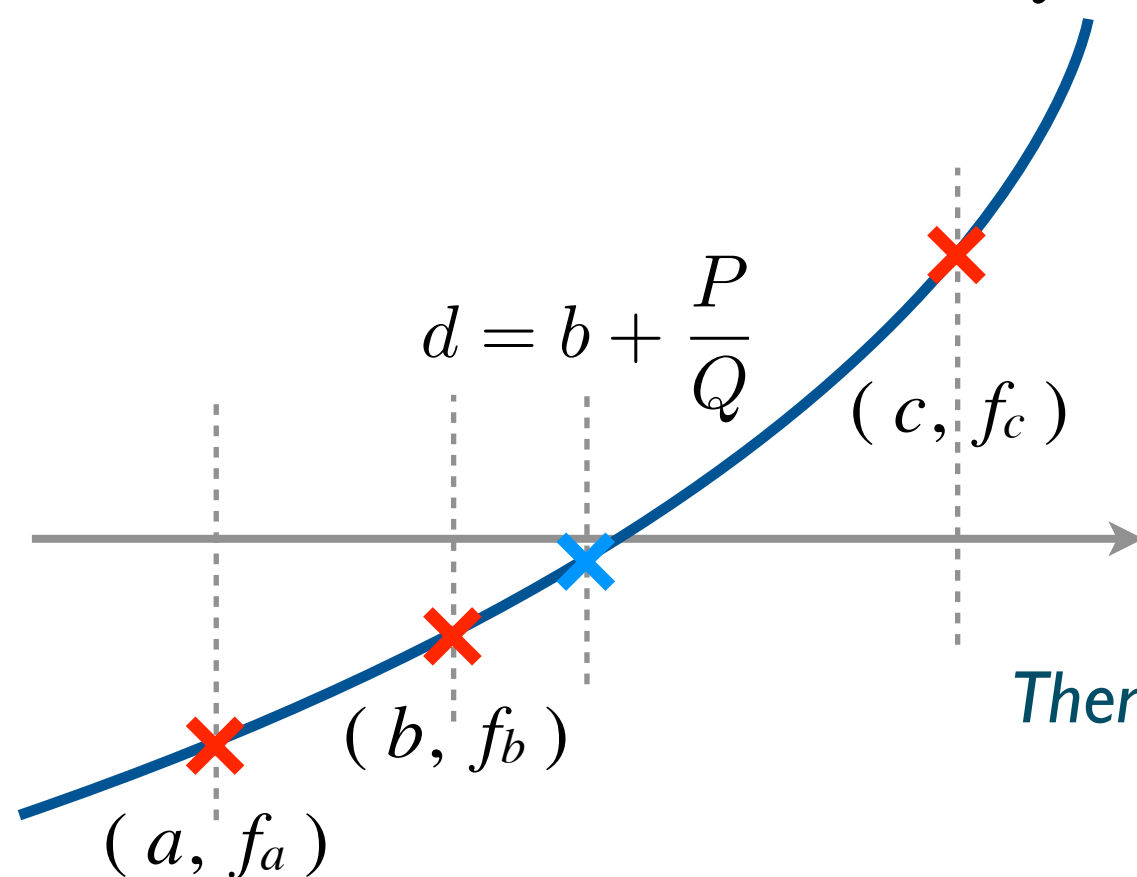Adopt Lagrange interpolation (=3 points parabola)

$$x = \frac{(y - f_a)(y - f_b)c}{(f_c - f_a)(f_c - f_b)} + \frac{(y - f_b)(y - f_c)a}{(f_a - f_b)(f_a - f_c)} + \frac{(y - f_c)(y - f_a)b}{(f_b - f_c)(f_b - f_a)}$$

The best guess of root should be located at *y = g(x) = 0*

BRENT'S METHOD

■ Suppose **x = b** is the current best guess of root, the next

best estimation is: $d = b + \dfrac{P}{Q}$

$$P = S[T(R-T)(c-b) - (1-R)(b-a)]$$

$$Q = (T-1)(R-1)(S-1)$$

$$R = \frac{f_b}{f_c}, \ \ S = \frac{f_b}{f_a}, \ \ T = \frac{f_a}{f_c}$$

$d = b + \dfrac{P}{Q}$

$(c, \ f_c)$

$(b, \ f_b)$

$(a, \ f_a)$

Then, we could pick up the best three values as the new (a,b,c) for the next iteration.

LET'S TRY IT!

```
a, b, c = 2.4, 2.5, 3.4         ⇐ Now we need 3 points to host the search
fa, fb, fc = f(a), f(b), f(c)

for step in range(50):

    R, S, T  = fb/fc, fb/fa, fa/fc
    P   = S*(T*(R-T)*(c-b)-(1.-R)*(b-a))   ⇐ Simply copy the equations here!
    Q   = (T-1.)*(R-1.)*(S-1.)

    d  = b + P/Q
    fd = f(d)

    print('Step: %2d, root = %.16f, diff = %.16f' % (step,d,abs(d-3.)))

    if abs(b-d)<1E-14: break

    if fa*fb>0.:
        a, fa = b, fb
        b, fb = d, fd       ⇐ Replace (a, b) with (b, d)
    else:
        c, fc = b, fb
        b, fb = d, fd       ⇐ Replace (c, b) with (b, d)
```

l205-example-02.py (partial)

LET'S TRY IT! (II)

■ Terminal output is like this:

```
Step:  0, root = -5.2064627478620000, diff = 8.2064627478620000
Step:  1, root =  2.9693426221720163, diff = 0.0306573778279837
Step:  2, root =  3.0066798826104528, diff = 0.0066798826104528
Step:  3, root =  2.9998524472418411, diff = 0.0001475527581589
Step:  4, root =  3.0000000378298575, diff = 0.0000000378298575
Step:  5, root =  2.9999999999999534, diff = 0.0000000000000466
Step:  6, root =  3.0000000000000000, diff = 0.0000000000000000
Step:  7, root =  3.0000000000000000, diff = 0.0000000000000000
```

■ Well, it does happen: it does **NOT** guarantee the next step will always gives a better guess of the root, especially if we approximate the function by a 2nd order parabola.

■ Alternative fix: replace the next guess by **Bisection method**, if the guess is bad/poor.

A FAIL-SAFE CODE

■ Simply fix the value of test point (`d,fd`) with
   Bisection method if the resulting values are bad:

```python
d  = b + P/Q
fd = f(d)

if (d-a)*(d-c)>0. or abs(fd)>abs(fb):
    if fa*fb>0.: d = (b+c)*0.5
    else:        d = (a+b)*0.5
    fd = f(d)

print('Step: %2d, root = %.16f, diff = %.16f' % (step,d,abs(d-3.)))
```
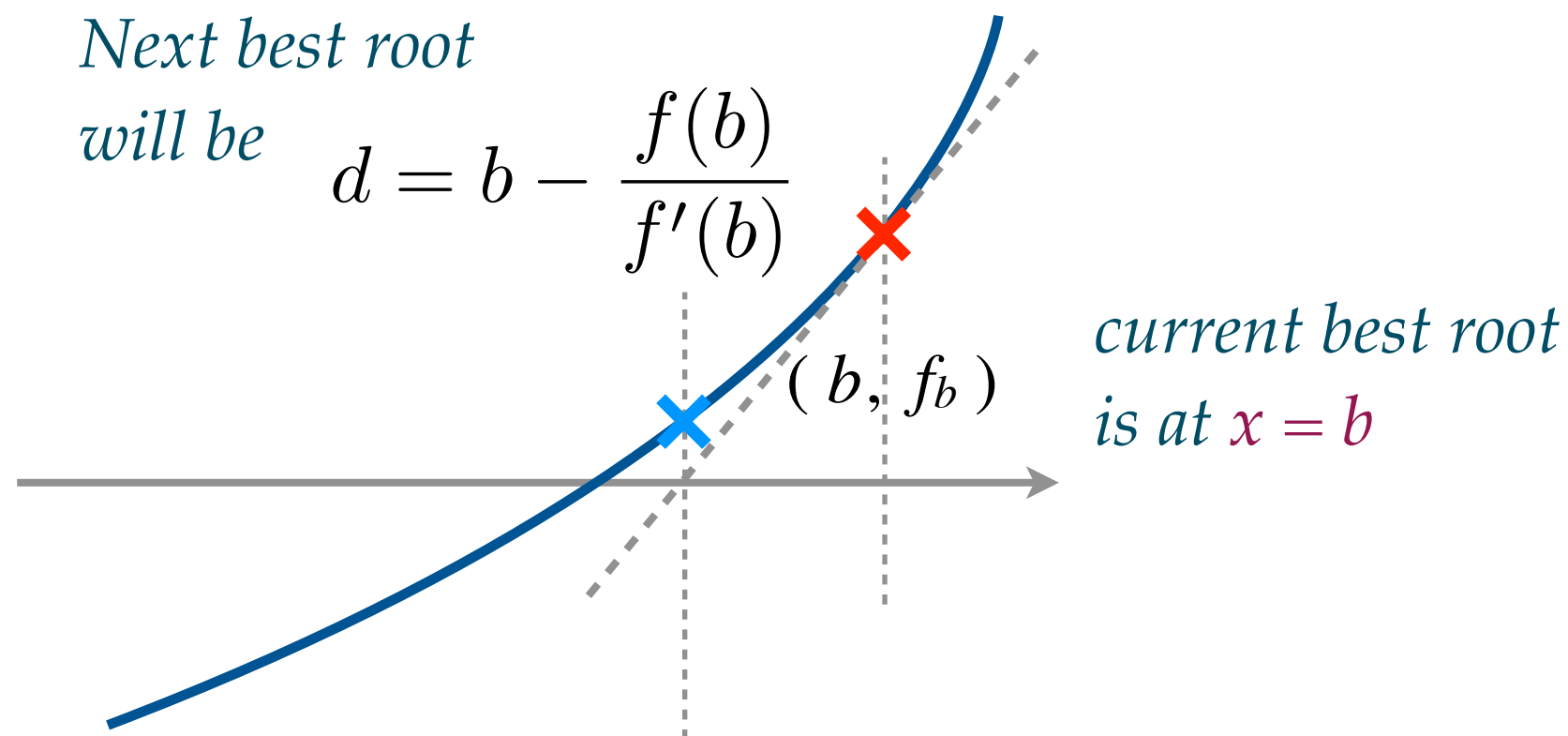
l205-example-02a.py (partial)

```
Step:  0, root = 2.9500000000000002, diff = 0.0499999999999998  ⇐ All good!
Step:  1, root = 3.0169811828014468, diff = 0.0169811828014468
Step:  2, root = 2.9993946939327074, diff = 0.0006053060672926
Step:  3, root = 3.0000006446632410, diff = 0.0000006446632410
Step:  4, root = 2.9999999999917120, diff = 0.0000000000082880
Step:  5, root = 3.0000000000000000, diff = 0.0000000000000000
Step:  6, root = 3.0000000000000000, diff = 0.0000000000000000
```

ALGORITHM WITH DERIVATIVE: NEWTON'S METHOD
(NEWTON-RAPHSON)

■ Well, where is the beloved method, which we have learned in calculus course?

$$f(x + \delta) \approx f(x) + f'(x)\delta + \frac{f''(x)}{2}\delta^2 + \ldots$$

Take out the 2nd order term

Next best root will be

$$d = b - \frac{f(b)}{f'(b)}$$

$(\, b,\, f_b \,)$

current best root is at x = b

IMPLEMENTATION: NEWTON'S METHOD

```python
def fp(x):
    return (x-2.)*(x-3.)*(x-4.)*(x-5.) + \      ⇐ Analytical solution
           (x-1.)*(x-3.)*(x-4.)*(x-5.) + \
           (x-1.)*(x-2.)*(x-4.)*(x-5.) + \
           (x-1.)*(x-2.)*(x-3.)*(x-5.) + \
           (x-1.)*(x-2.)*(x-3.)*(x-4.)

a, b, c = 2.4, 2.5, 3.4
fa, fb, fc = f(a), f(b), f(c)

for step in range(50):

    delta = -fb/fp(b)
    d   = b + delta
    fd = f(d)

    if (d-a)*(d-c)>0. or abs(fd)>abs(fb):     ⇐ Keep the protection as in the
        if fa*fb>0.: d = (b+c)*0.5                Bisection method
        else:        d = (a+b)*0.5
        fd = f(d)

    print('Step: %2d, root = %.16f, diff = %.16f' % (step,d,abs(d-3.)))
    if abs(b-d)<1E-14: break

    b, fb = d, fd
```

l205-example-03.py (partial)

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(SUPER-)FAST CONVERGING!

■ Terminal output:

```
Step:   0, root = 2.9500000000000002, diff = 0.0499999999999998
Step:   1, root = 3.0003151394705090, diff = 0.0003151394705090
Step:   2, root = 2.9999999999217564, diff = 0.0000000000782436
Step:   3, root = 3.0000000000000000, diff = 0.0000000000000000
Step:   4, root = 3.0000000000000000, diff = 0.0000000000000000
                                        ⇑ Just 3—4 steps!
```

■ **Q:** Why not to use **the numerical derivatives**?

■ **A:** As we have discussed before, it's very hard to have precise numerical solution for the derivatives. In this case the solution will be limited by the best precision of the derivative calculation. It's generally not a recommended way (but still "doable").

INTERMISSION

- With Newton's method:
  - What will happen if you remove the failed safe protection (the block of using Bisection method)?
  - Try to run the calculation with numerical derivative, how good is the solution?

```
def fp(x):        ⇐ You can try this by yourself!
    h = 1E-5
    return (f(x+h/2.)-f(x-h/2.))/h
```

l205-example-03a.py (partial)

- Try to find a not-working-so-well problem!

SOME MORE PRACTICAL EXAMPLES?

- Let's implement a function with Newton's method to calculate square-root and cubic-root. This is one of the places this method can do the work easily!

- The usual square-root function is `sqrt()`, and we can only use the `pow()` function or the `**` operator to calculate cubic-root.

- If we are looking for the square-(cubic-) root of a real number R, it's equivalent to find the root of

$$f(x) = x^2 - R \quad \text{or} \quad f(x) = x^3 - R$$

The corresponding first derivatives are

$$f'(x) = 2x \quad \text{or} \quad f'(x) = 3x^2$$

The implement the code should be very easy!

QUICK & SIMPLE CODE

Basically the implementations are the same; the only difference are the local functions `fsq()` and `fsqp()`.

```python
def squareroot(R):
    fsq = lambda x:x*x-R
    fsqp = lambda x:2.*x          ⇐ local functions

    a, b, c = 0., R*0.5, R
    fa, fb, fc = fsq(a), fsq(b), fsq(c)
    for step in range(50):
        delta = -fb/fsqp(b)
        d  = b + delta
        fd = fsq(d)

        if abs(b-d)<1E-14: return d
        b, fb = d, fd
def cubicroot(R):
    fcb = lambda x:x*x*x-R
    fcbp = lambda x:3.*x*x

    a, b, c = 0., R*0.5, R
    fa, fb, fc = fcb(a), fcb(b), fcb(c)
    for step in range(50):
        delta = -fb/fcbp(b)
        d  = b + delta
        fd = fcb(d)

        if abs(b-d)<1E-14: return d
        b, fb = d, fd
```

l205-example-04.py (partial)

LET'S TRY THE FUNCTIONS!

■ This is almost a trivial task:

```python
R = 1234.

print('root = %.16f, diff = %.16f' % \
    (squareroot(R),abs(R**0.5-squareroot(R))))

print('root = %.16f, diff = %.16f' % \
    (cubicroot(R),abs(R**(1./3.)-cubicroot(R))))
```
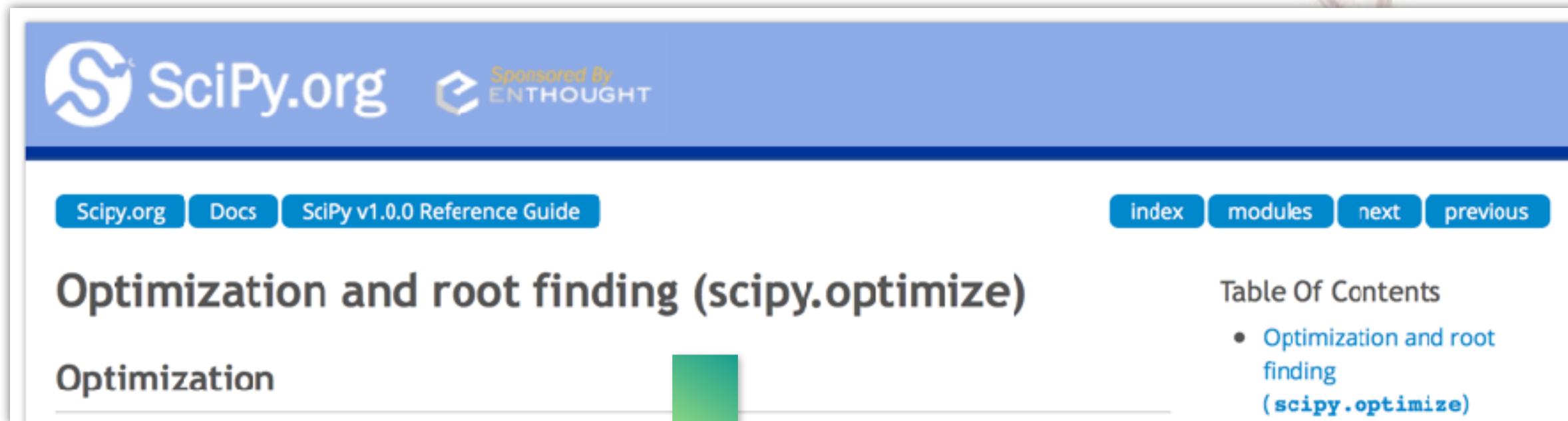
l205-example-04.py (partial)

```
root = 35.1283361405005934, diff = 0.0000000000000000
root = 10.7260146688273235, diff = 0.0000000000000000
```

Surely this code is very slow if we compare to the standard operator, but this is a very good example that almost all the math functions can be implemented in a similar way!

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USE THE FUNCTIONS FROM SCIPY

■ Everything is under **scipy.optimize**:

http://docs.scipy.org/doc/scipy/reference/optimize.html

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Optimization and root finding (scipy.optimize)

Optimization

Table Of Contents

- Optimization and root finding **(scipy.optimize)**

Root finding

Scalar functions

brentq(f, a, b[, args, xtol, rtol, maxiter, ...])   Find a root of a function in a bracketing interval using Brent's method.

brenth(f, a, b[, args, xtol, rtol, maxiter, ...])   Find root of f in [a,b].

ridder(f, a, b[, args, xtol, rtol, maxiter, ...])   Find a root of a function in an interval.

bisect(f, a, b[, args, xtol, rtol, maxiter, ...])   Find root of a function within an interval.

newton(func, x0[, fprime, args, tol, ...])   Find a zero using the Newton-Raphson or secant method.

You can see some familiar names here!

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USING THE SUPER EASY SCIPY FUNCTIONS

- Just import the **scipy.optimize** and call the corresponding method:

```python
import scipy.optimize as opt

def squareroot(R):
    fsq = lambda x:x*x-R
    fsqp = lambda x:2.*x

    return opt.newton(fsq,R*0.5,fsqp)   ⇐ Just call it!

R = 1234.

print('root = %.16f, diff = %.16f' % \
    (squareroot(R),abs(R**0.5-squareroot(R))))
```

l205-example-05.py

```
root = 35.1283361405005934, diff = 0.0000000000000000
```

MINIMIZATION OR MAXIMIZATION

- Method in calculus – **find the zero first derivative**:

$$f'(x) = 0 \quad \rightarrow \quad x = ?$$

- How about the numerical method?

- Yep, you can probably already apply what we learned from the previous section, to find the root of $f'(x) = 0$ if we know the first derivative already.

- If not, <u>this is what we are going to discuss now</u>.
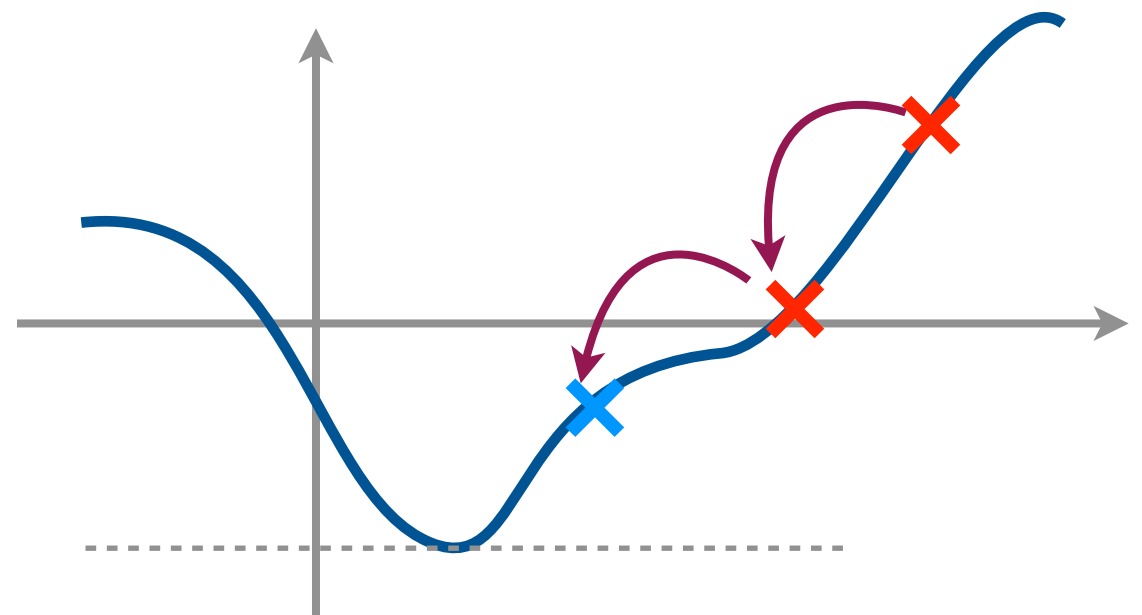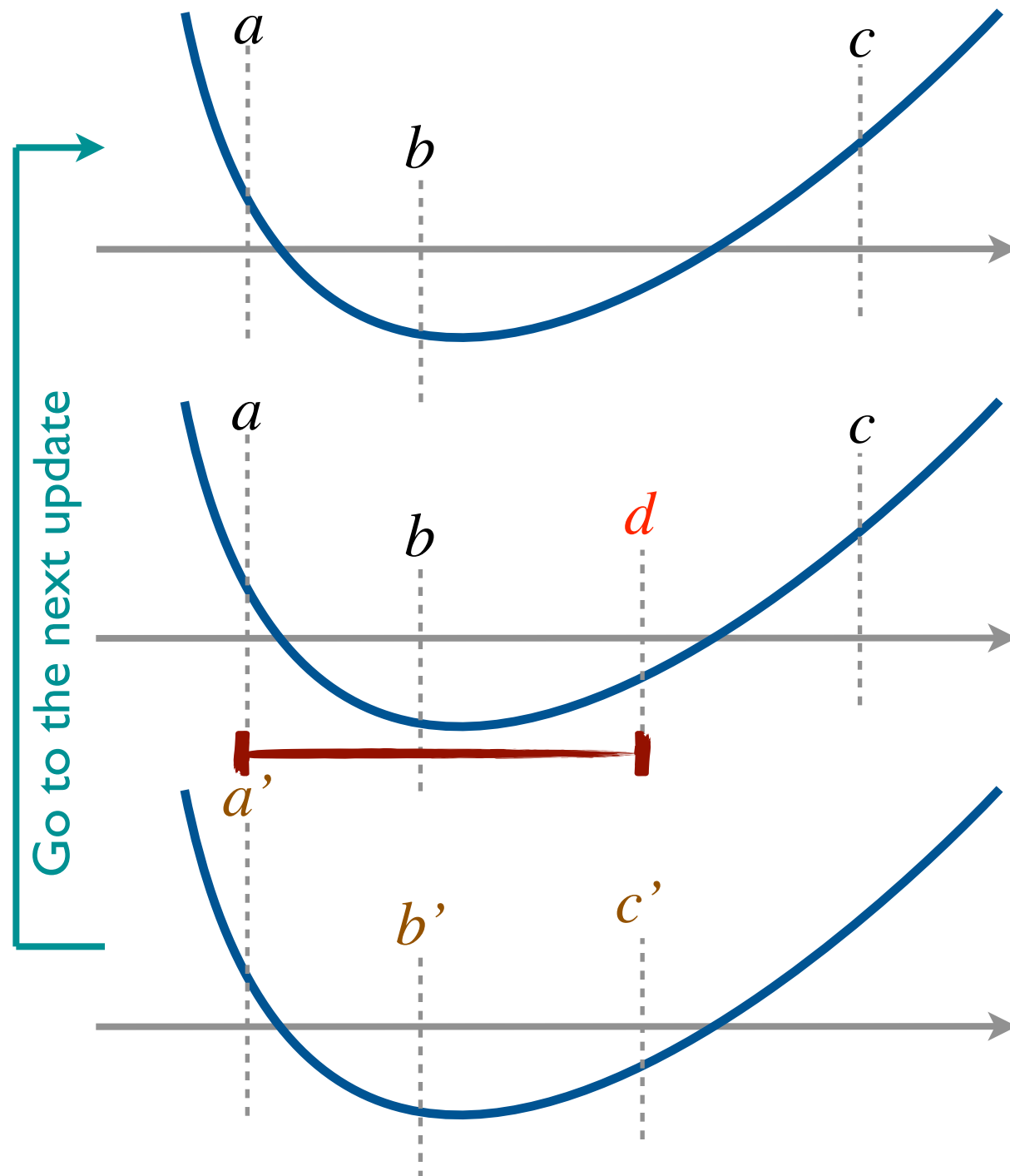
ONE DIMENSIONAL SEARCH IN A BRACKET

■ This method is very simple: if we have a bracket **(a,b,c)**, and **f(b) < f(a), f(c)**, and **b** is the current best minimum:

(a,b,c)

$x = a$

$x = c$

$x = d$

$x = b$

(a,b,d)

(b,d,c)
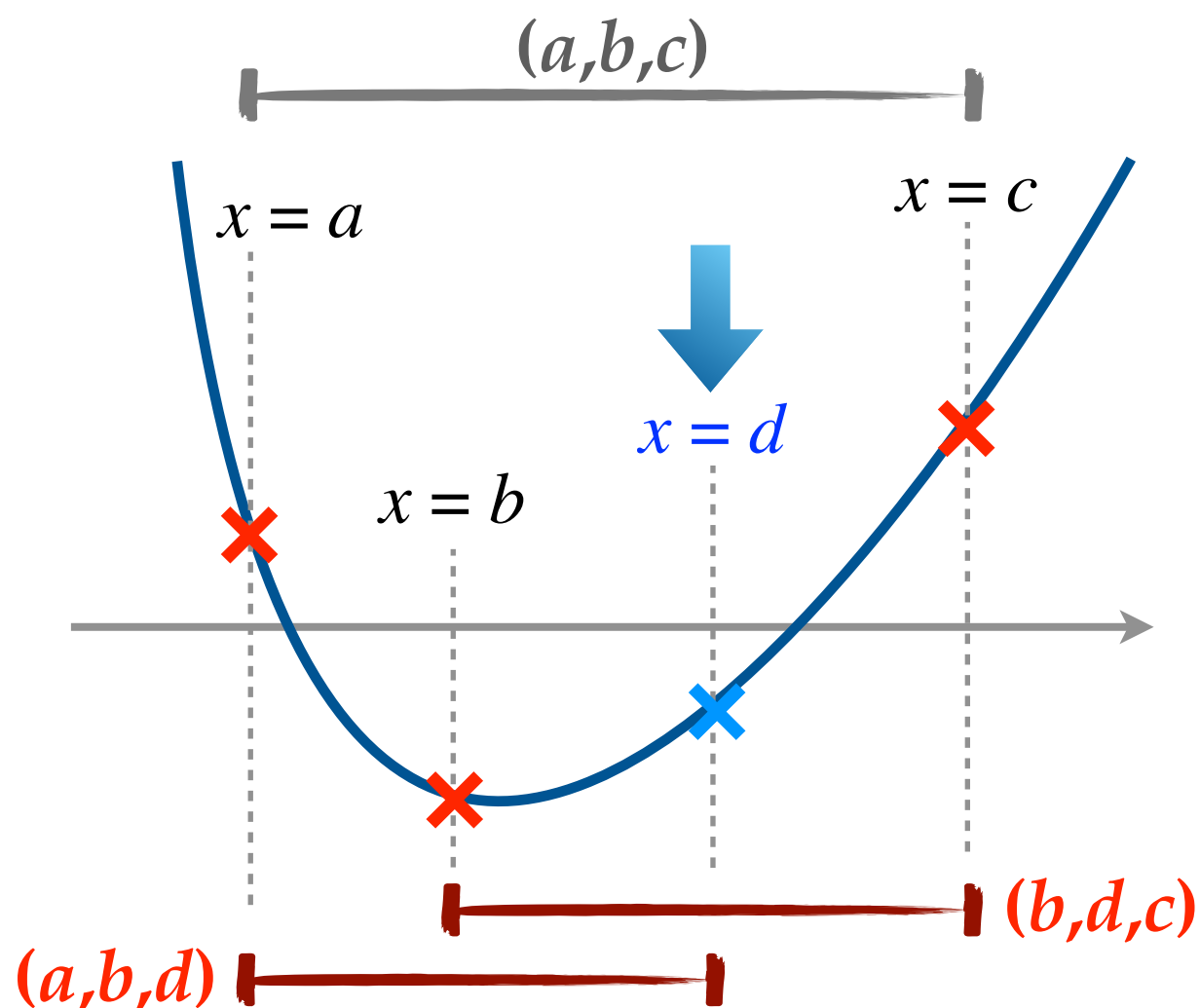
Keep updating the bracket by replacing (a,b,c) with (a,b,d) or (b,d,c) until a desired precision.

We always need to keep f(b) < f(a) and f(b) < f(c) to ensure we have at least a minimum in the interval.

1D SEARCH – THE STEPS

Go to the next update

- Initial bracket **(a,b,c)**

- If **|b-c|>|a-b|**, find a new test point d in **[b,c]**

- If **f(b) < f(d)**, keep **b** as the current best estimation of the minimum point.

- Update the bracket accordingly: **c' = d**

- Go to the next update

A QUICK IMPLEMENTATION

```python
def f(x):
    return (x-0.5)*(x-0.5)*(x-10.)*(x-10.)
```
⇐ A function with 2 obvious minimal points

```python
FRAC = 0.38197
```
⇐ Magic number!
```python
a, c = 0.0, 2.0
fa, fc = f(a), f(c)
b = a+(c-a)*FRAC
fb = f(b)

for step in range(150):

    if abs(a-b)>abs(c-b): d = b+(a-b)*FRAC
    else:                 d = b+(c-b)*FRAC
    fd = f(d)
```
⇐ Insert a new testing point, between either (a,b) or (b,c)

```python
    print('Step: %2d, root = %.16f, diff = %.16f' % (step,d,abs(d-0.5)))
    if abs(b-d)<1E-14: break

    if fd<fb:
        b, d = d, b
        fb, fd = fd, fb
```
⇐ exchange **b** and **d**, keep **b** as the best solution as always

```python
    if (d-b)*(a-b)>0: a, fa = d, fd
    else:             c, fc = d, fd
```

l205-example-06.py

THE RESULTS

■ Terminal output:

```
Step:  0, root = 1.2360778381999999, diff = 0.7360778381999999
… …
Step: 10, root = 0.4946110292293492, diff = 0.0053889707706508
… …
Step: 20, root = 0.4999668808722842, diff = 0.0000331191277158
… …
Step: 30, root = 0.4999995815191064, diff = 0.0000004184808936
… …
Step: 40, root = 0.5000000029995387, diff = 0.0000000029995387
… …
Step: 50, root = 0.4999999999885979, diff = 0.0000000000114021
… …
Step: 60, root = 0.4999999999997671, diff = 0.0000000000002329
Step: 61, root = 0.4999999999999878, diff = 0.0000000000000122
Step: 62, root = 0.5000000000000400, diff = 0.0000000000000400
Step: 63, root = 0.4999999999999556, diff = 0.0000000000000444
Step: 64, root = 0.5000000000000078, diff = 0.0000000000000078
Step: 65, root = 0.5000000000000201, diff = 0.0000000000000201
Step: 66, root = 0.5000000000000001, diff = 0.0000000000000001
```

WHY 0.38197?

- A funny number used in the decision of the position of **d**? Why?

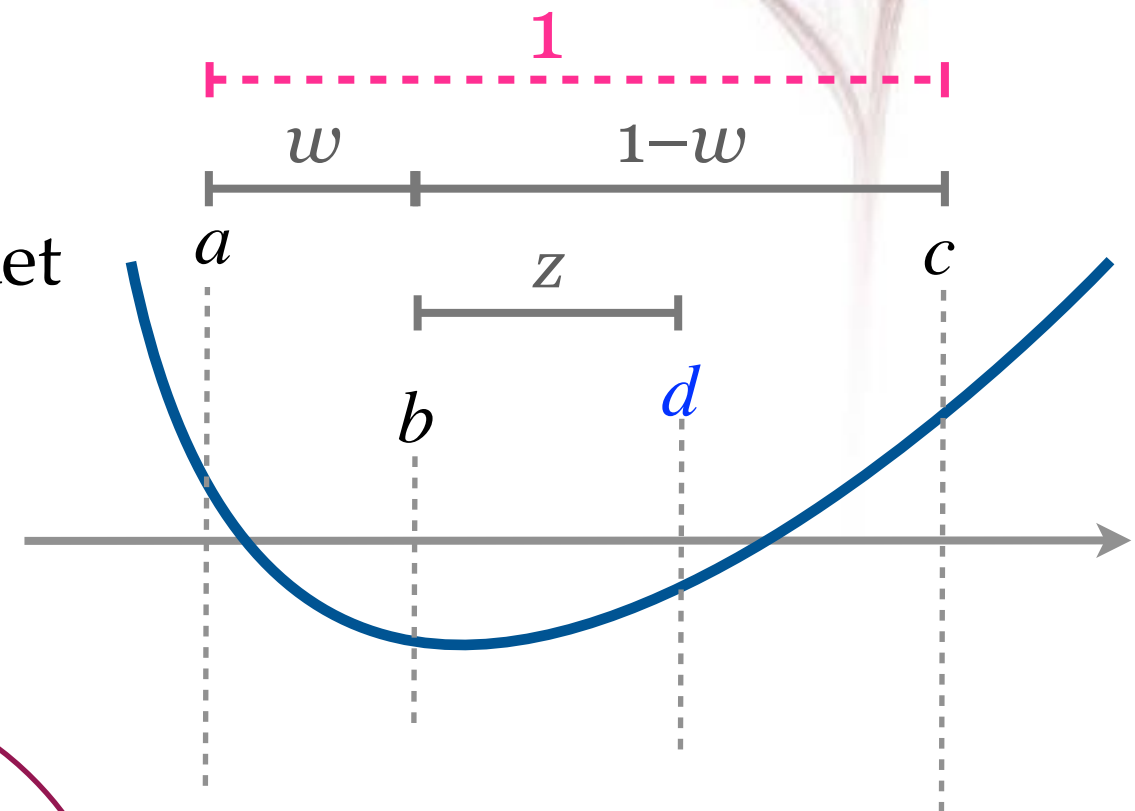- Let's look at the configuration:

- Every time, we could shrink the bracket from **1** to **(w+z)** or **(1-w)**

- In order to avoid the worst case, let's simply force them to be the same:
$$w + z = 1 - w$$

- Usually it would be the optimal if we preserve the same *"shrinking rate"*:
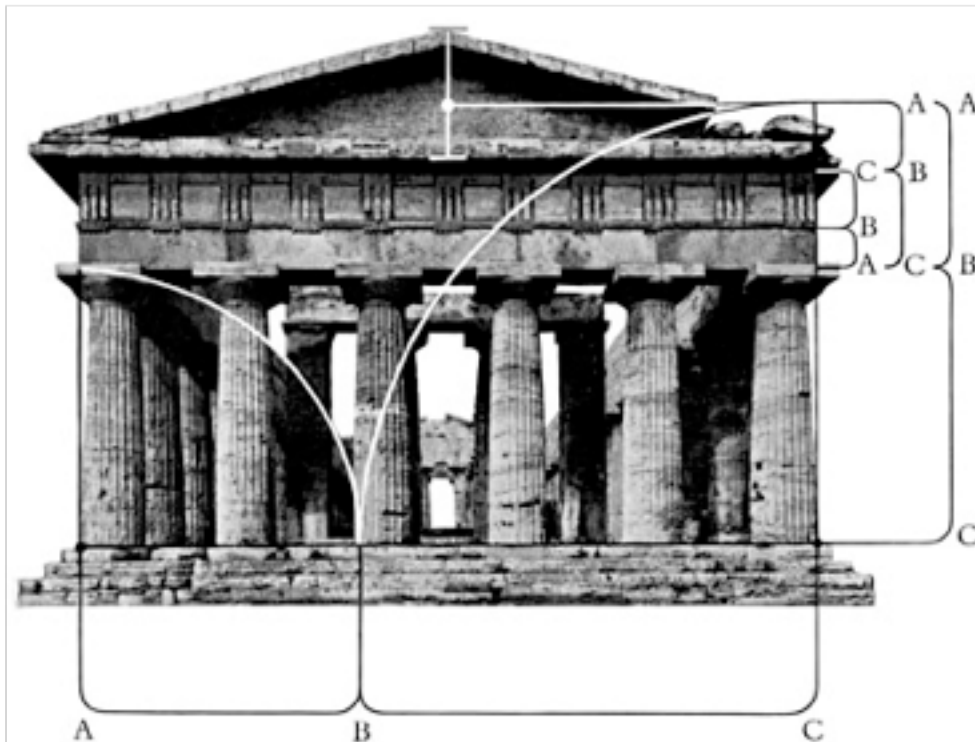$$\frac{z}{1 - w} = w$$

Then
$$w = \frac{3 - \sqrt{5}}{2} \approx 0.38197$$

WHY 0.38197? (II)

■ Actually, this is nothing but the **golden ratio**:


STATUE OF DORYPHORUS   (Spear bearer)
Copy after the bronze original by Polycletus.
(In classical times it was known as an unsurpassed representation of the perfect athletic body.)
— National Museum, Naples —

STATUE DES DORYPHORUS   (Speerträger)
Kopie nach dem Bronze-Original von Polyklet.
(War im Altertum als maßgebende Darstellung des durchgebildeten Körpers bekannt.)
— Nationalmuseum Neapel —

FRONT VIEW OF THE NEPTUNE TEMPLE IN PAESTUM
A Greek temple in Doric style of the 6th century B.C.
(The chiefstress of the gable shows the proportion of the golden mean.)

FRONTAL-ANSICHT DES NEPTUN-TEMPELS IN PAESTUM
Griechischer Tempel im dorischen Stil aus dem 6. Jh. v. Chr.
(Das Schwergewicht des Giebels weist das goldene Schnittverhältnis auf.)
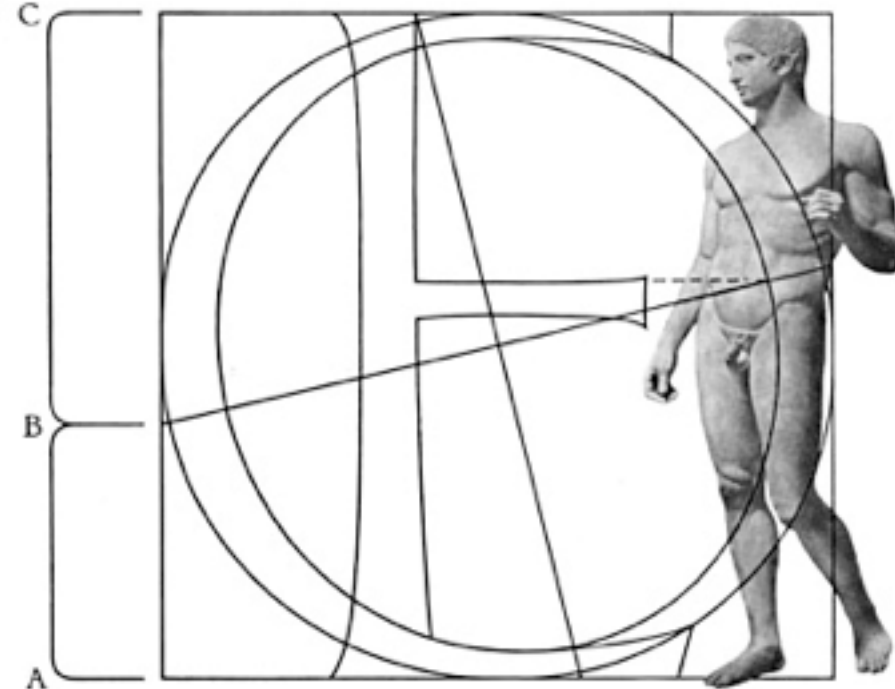
WHY 0.38197? (III)

- The nominal golden section is derived from
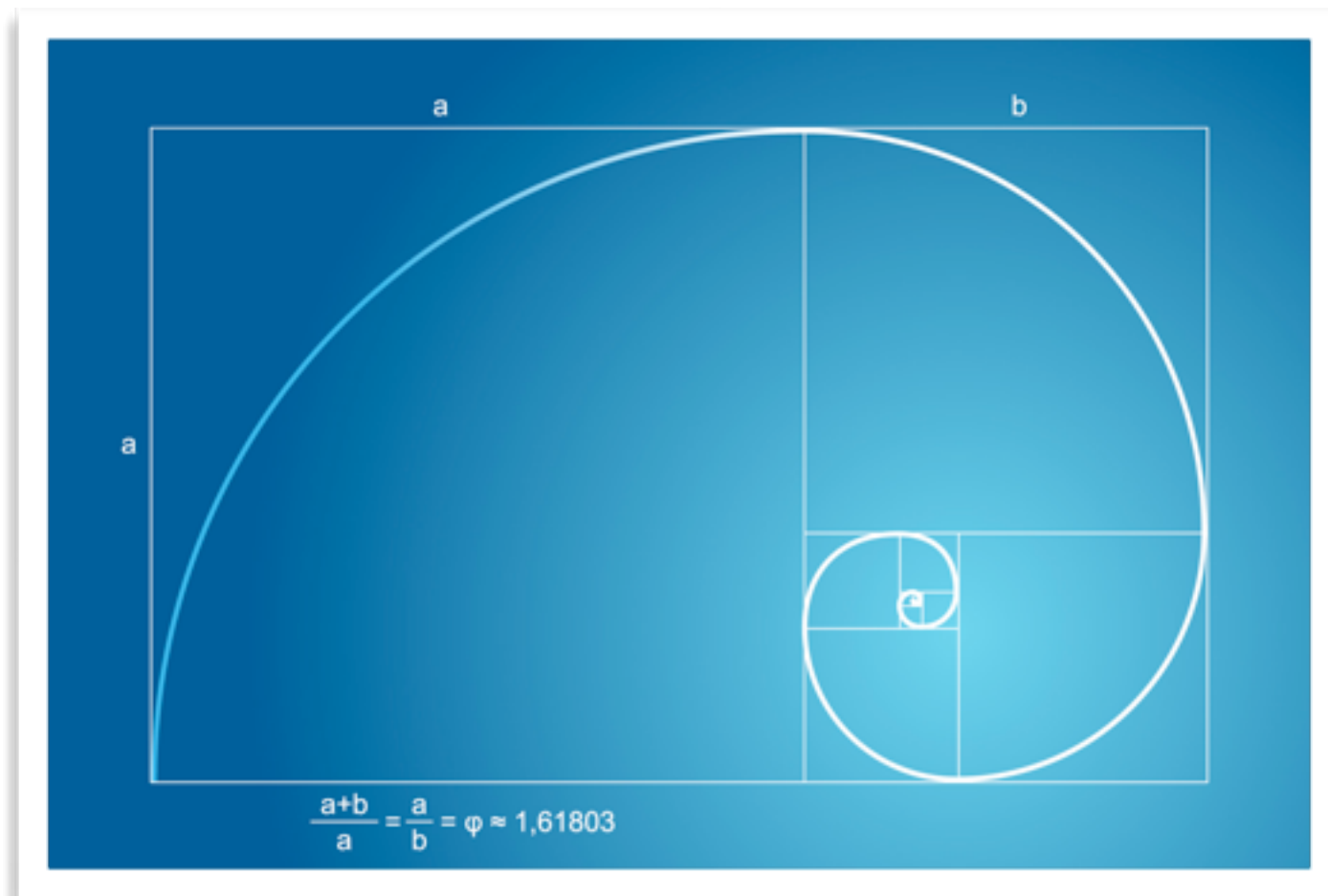
$$\phi = \frac{a+b}{a} = \frac{a}{b} \approx 1.61803$$

$$\text{And } 1 - \frac{1}{\phi} \approx 0.38197$$

So this minimum finding method is called **Golden Section Search**.

My comments: unfortunately I'm not able to prove this is the best ratio for a generic 1D minimum finding; but it's not a bad number in principle.

PARABOLIC INTERPOLATION: BRENT'S METHOD

- As we has shown in the previous half of this lecture, the parabolic interpolation (the Brent's method) shows a good solution of efficiency for 1D root finding.

- We are also able to do the same thing here:

Suppose we have three points: $(x,y) = (\, a,\ f_a\,), (\, b,\ f_b\,), (\, c,\ f_c\,)$

The minimum value of the function $f(x)$ is located at

$$d = b - \frac{1}{2} \cdot \frac{(b-a)^2[f_b - f_c] - (b-c)^2[f_b - f_a]}{(b-a)[f_b - f_c] - (b-c)[f_b - f_a]}$$

Current best solution

Updating term for next iteration

You may try to derive this formula by yourself!

EXAMPLE CODE

```python
FRAC = 0.38197
a, c = 0.0, 2.0          ⇐ The same initial bracket as the golden section search
fa, fc = f(a), f(c)
b = a+(c-a)*FRAC
fb = f(b)

for step in range(150):
    P = (b-a)*(b-a)*(fb-fc) - (b-c)*(b-c)*(fb-fa)
    Q = (b-a)*(fb-fc) - (b-c)*(fb-fa)      ⇐ Estimate d with the
    d = b - 0.5*P/Q                             formula given above.

    if (d-a)*(d-c)>0.:
        if abs(a-b)>abs(c-b): d = b+(a-b)*FRAC
        else:                 d = b+(c-b)*FRAC   ⇐ Fail-safe protection

    fd = f(d)
    print('Step: %2d, root = %.16f, diff = %.16f' % (step,d,abs(d-0.5)))
    if abs(b-d)<1E-14: break

    if fd<fb:
        b, d = d, b
        fb, fd = fd, fb      ⇐ keep b as the best solution as always

    if (d-b)*(a-b)>0: a, fa = d, fd
    else:             c, fc = d, fd
```

l205-example-07.py (partial)

THE OUTPUTS

- Surely the **converging speed** is much faster than the simple golden section searches:

```
Step:  0, root = 0.5645411768827963, diff = 0.0645411768827963
Step:  1, root = 0.5151073153720723, diff = 0.0151073153720723
Step:  2, root = 0.5038341068383387, diff = 0.0038341068383387
Step:  3, root = 0.5009203969723207, diff = 0.0009203969723207
Step:  4, root = 0.5002316050692824, diff = 0.0002316050692824
... ...
Step: 10, root = 0.5000000516190403, diff = 0.0000000516190403
... ...
Step: 20, root = 0.5000000000000426, diff = 0.0000000000000426
Step: 21, root = 0.5000000000000105, diff = 0.0000000000000105
Step: 22, root = 0.5000000000000026, diff = 0.0000000000000026
```

You may notice that, finding the minimum is more difficult than finding the root!

MINIMUM FINDING WITH DERIVATIVES

- This is *pretty tricky*: if you know the exact form of the **first derivative**, then a simply root finding code can already give you the maximum and minimum points.
- If we just want to apply the Newton's method, we need to know **the exact form of second derivative**.

Next best root is given by $d = b - \dfrac{f(b)}{f'(b)}$

Next best minimum/maximum is given by $d = b - \dfrac{f'(b)}{f''(b)}$

EXAMPLE CODE

```python
def fp(x):
    return 2.*(x-0.5)*(x-10.)*(x-10.)+2.*(x-0.5)*(x-0.5)*(x-10.)
def fpp(x):
    return 2.*(x-10.)*(x-10.)+8.*(x-0.5)*(x-10.)+2.*(x-0.5)*(x-0.5)

FRAC = 0.38197
a, c = 0.0, 2.0
fa, fc = f(a), f(c)      ⇐ Again, the same initial bracket!
b = a+(c-a)*FRAC
fb = f(b)

for step in range(150):
    delta = -fp(b)/fpp(b)
    d = b + delta  ⇐ update b,d according to Newton's method

    if (d-a)*(d-c)>0.:
        if abs(a-b)>abs(c-b): d = b+(a-b)*FRAC   ⇐ Fail-safe protection
        else:                 d = b+(c-b)*FRAC

    fd = f(d)
    print('Step: %2d, root = %.16f, diff = %.16f' % (step,d,abs(d-0.5)))
    if abs(b-d)<1E-14: break

    b = d
```

l205-example-08.py (partial)

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THE PERFORMANCE

■ The converging speed is **VERY GOOD**. We need only ~5 steps instead of 23 or 6x iterations. The second derivative is required!

```
Step:   0, root = 0.47471835085330082, diff = 0.0252816491469918
Step:   1, root = 0.4998006350485492, diff = 0.0001993649514508
Step:   2, root = 0.4999999874497394, diff = 0.0000000125502606
Step:   3, root = 0.4999999999999999, diff = 0.0000000000000001
Step:   4, root = 0.5000000000000000, diff = 0.0000000000000000
```

l205-example-08.py (output)

■ Alternatively, one can adopt **Brent's method** for root finding on <u>first derivate</u>: *(Well, it's not too bad at all!)*

```
Step:   0, root = 0.4358830239633310, diff = 0.0641169760366690
Step:   1, root = 0.5013516961302908, diff = 0.0013516961302908
Step:   2, root = 0.4999956151890250, diff = 0.0000043848109750
Step:   3, root = 0.5000000000658166, diff = 0.0000000000658166
Step:   4, root = 0.5000000000000000, diff = 0.0000000000000000
Step:   5, root = 0.5000000000000000, diff = 0.0000000000000000
```

l205-example-08a.py (output)

INTERMISSION

■ Try to use the SciPy implementation of Brent's method, `scipy.optimize.brentq()` to solve the same problem in l205-example-02.py and see what you get?

■ The **golden section search** – what will happen if you do not use the "golden" ratio but a whatever number, such as 0.5? Is it better or worse in terms of converging speed?

MULTIDIMENSIONAL MINIMIZATION (COMMENTS)

- If we want to find the minimum point in multi-dimensional space, it's much harder than our those 1D examples given above.

- Many numerical algorithms have been developed in order to find the minimum point for various problems.
  (or, the best algorithm could be question dependent!)

- Some named methods: **Downhill method, Conjugate gradient, Steepest Descent, Simplex method, Quasi-Newton method,** etc…

- Given the complexity of those named algorithms (*in particular many of methods require gradient calculation*), we will not discuss how to write the code by ourselves, instead — just going to use **the standard tools in SciPy** directly!

BACK TO SCIPY

- The generic minimizer **scipy.optimize.minimize()** is shown below:

http://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.minimize.html#scipy.optimize.minimize

Scipy.org | Docs | SciPy v1.0.0 Reference Guide | Optimization and root finding (`scipy.optimize`) | index | modules | next

scipy.optimize.minimize

scipy.optimize.**minimize**(*fun, x0, args=(), method=None, jac=None, hess=None, hessp=None, bounds=None, constraints=(), tol=None, callback=None, options=None*)   **[source]**

Minimization of scalar function of one or more variables.

In general, the optimization problems are of the form:

```
minimize f(x) subject to

g_i(x)  >= 0,   i = 1,...,m
h_j(x)   = 0,   j = 1,...,p
```

Let's see a super simple example for calling this tool!

where x is a vector of one or more variables. `g_i(x)` are the inequality constraints. `h_j(x)` are the equality constrains.

Optionally, the lower and upper bounds for each element in x can also be specified using the *bounds* argument.

Parameters: **fun** *: callable*

       The objective function to be minimized. Must be in the form `f(x, *args)`. The optimizing argument, `x`, is a 1-D array of points, and `args` is a tuple of any additional fixed parameters needed to completely specify the function.

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ONE LINE TO FIND THE MINIMUM

■ An example code for calling the default minimizer ("BFGS" = a quasi-Newton method by Broyden-Fletcher-Goldfarb-Shanno).

```python
import numpy as np
import scipy.optimize as opt

def f(x):                    ⇓ A 3D function with obvious minimal point of (1,2,3)
    return (x[0]-1.)**2+(x[1]-2.)**2+(x[2]-3.)**2

x_init = np.array([0.5,0.5,0.5])   ⇐ initial values

res = opt.minimize(f,x_init)

if res.success:
    print('The resulting vector:',res.x)
```

l205-example-09.py

```
The resulting vector:
[ 1.          1.99999991  3.00000009]
```

l205-example-09.py (output)
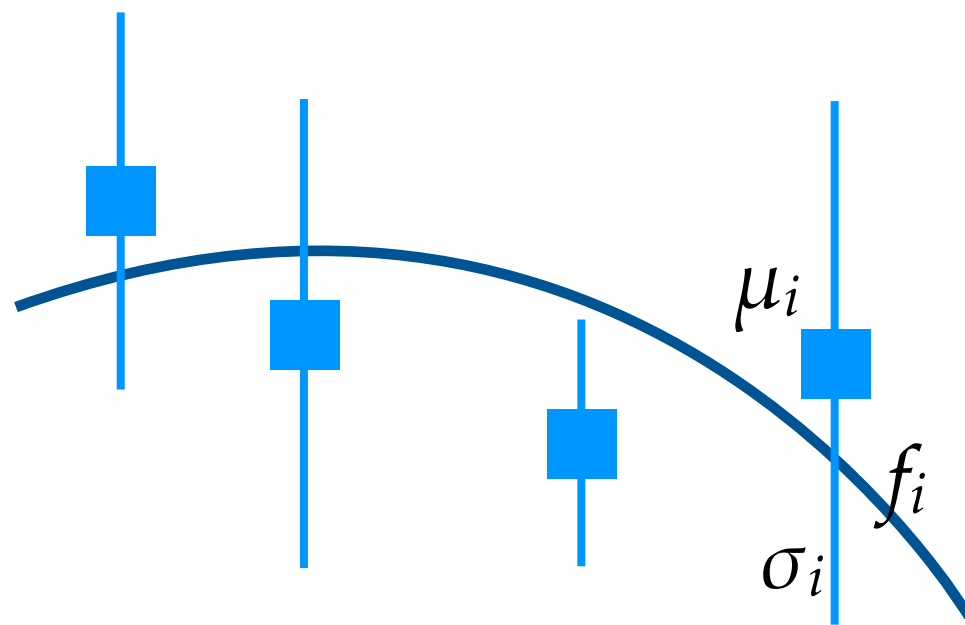
A PRACTICAL EXAMPLE: LEAST-SQUARE (χ^2) FIT

■ The best results can be obtained by minimizing a χ2 value for **N independent measurements**:

$$\chi^2 = \sum_i^N \frac{(f_i - \mu_i)^2}{\sigma_i^2}$$

f_i: expected value of the model
μ_i: i^{th} measurement
σ_i: uncertainty of ith measurement

μ_i

f_i

σ_i

Keeping updating those parameters ($\alpha,\beta,\gamma,...$) until the **best (smallest)** χ^2 value is reached.

$$f_i = f(x_i; \alpha, \beta, \gamma, \dots)$$

LET'S GET SOME REAL DATA POINTS

■ One can start with storing the data as numpy arrays and make a simple plot with error bar:

```python
import numpy as np
import matplotlib.pyplot as plt

xmin, xmax, xbinwidth = 100., 170., 2.
vx = np.linspace(xmin+xbinwidth/2,xmax-xbinwidth/2,35)   ⇐ x axis
vy = np.array(
[7,2,4,4,3,9,8,1,6,6,8,16,36,20,8,6,8,6,4,7,      ⇐ y axis: simple of
 4,10,5,6,1,4,3,4,4,6,2,6,9,5,8],dtype='float64')  counting events in bin
vyerr = vy**0.5   ⇐ assuming Poisson standard deviation

plt.plot([xmin, xmax],[0.,0.],c='black',lw=2)
plt.errorbar(vx, vy, vyerr, c='blue', fmt = 'o')
plt.grid()
plt.show()
```

l205-example-10.py

LET'S GET SOME REAL DATA POINTS (II)

- This is the output – nothing but the (in)famous **Higgs boson**.

one of the events here
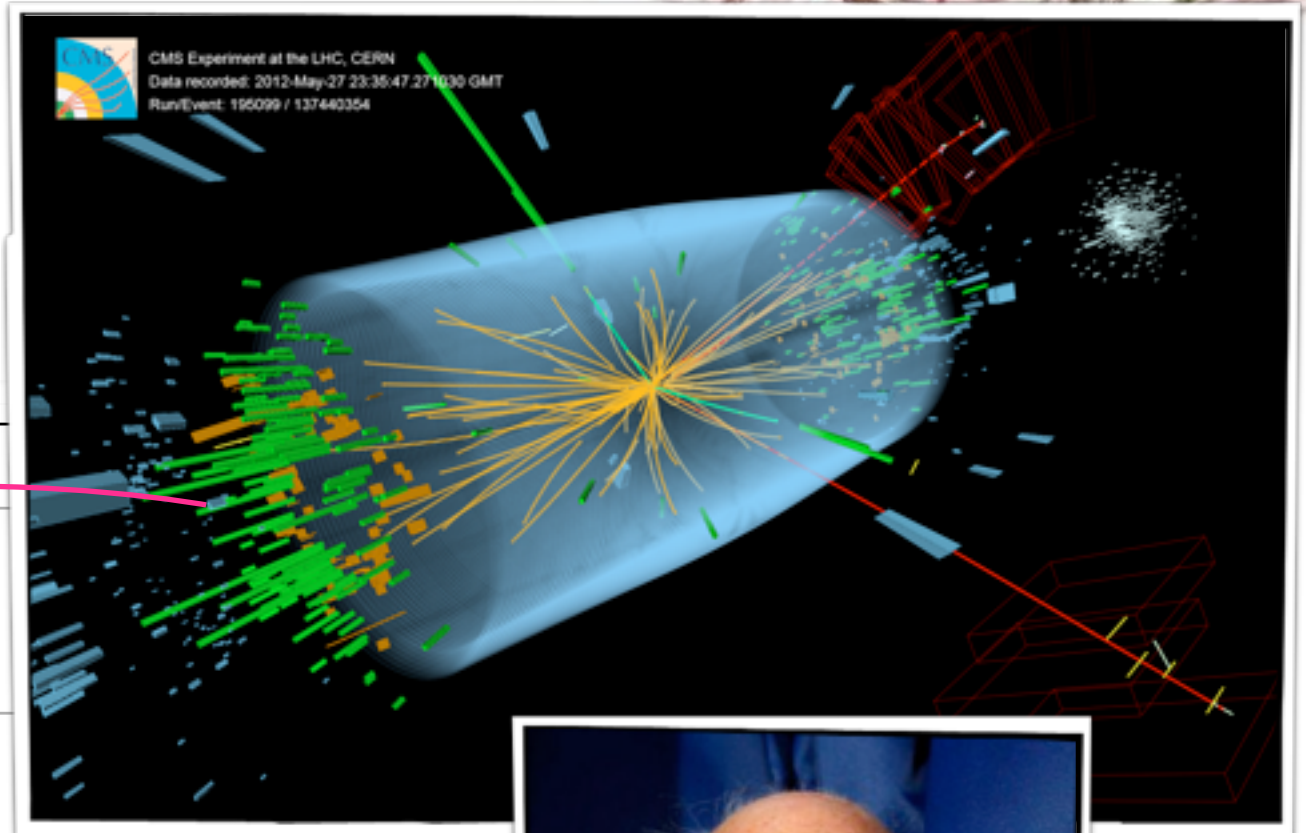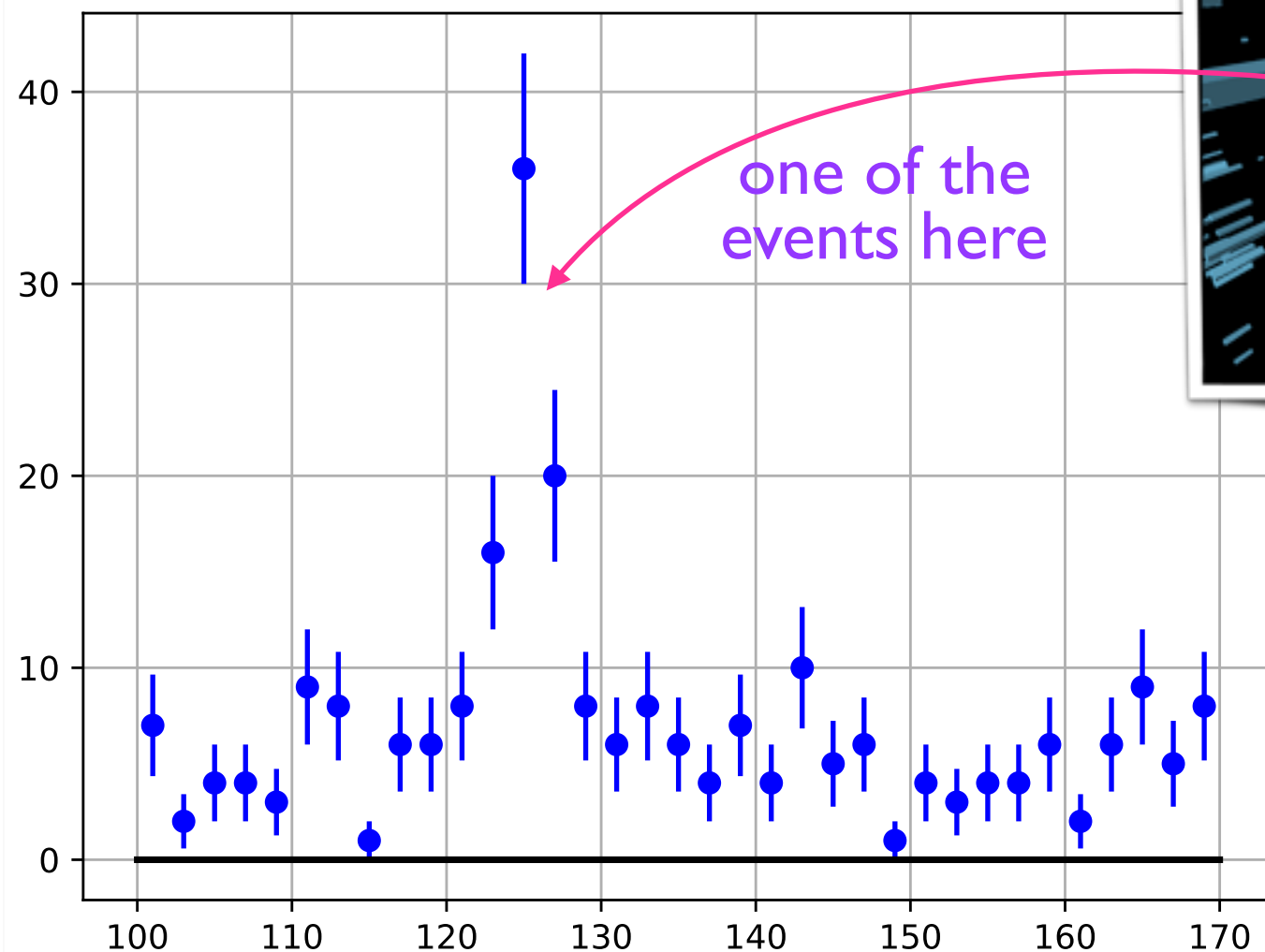
MODEL SETUP

■ In order to perform the fit, one needs to construct a model that can describe the data. Here we simple introduce a 2nd order polynomial for the background + a Gaussian signal peak.

$$f(x) = c_0 + c_1 \cdot x + c_2 \cdot x^2$$

```python
def model(x, norm, mean, sigma, c0, c1, c2):

    xp = (x-xmin)/(xmax-xmin)
    polynomial = c0 + c1*xp + c2*xp**2

    gaussian = norm*xbinwidth/(2.*np.pi)**0.5/sigma * \
               np.exp(-0.5*((x-mean)/sigma)**2)

    return polynomial + gaussian
```

1205-example-10a.py (partial)

$$g(x) = \frac{N \cdot \Delta x}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$

Δx: bin width, required for the normalization

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FITTING CORE & PLOTTING

$$\chi^2 = \sum_i^N \frac{(f_i - \mu_i)^2}{\sigma_i^2}$$

Calculate χ^2 value for a given parameter set, after skipping the single zero entry bin.

```python
def fcn(p):
    expt = model(vx,p[0],p[1],p[2],p[3],p[4],p[5])
    delta = (vy-expt)/vyerr
    return (delta**2).sum()

p_init = np.array([70.,125.,2.,4.,0.,0.])
r = opt.minimize(fcn,p_init)

if r.success:
    print('N(Higgs)  = %.1f events' % r.x[0])
    print('M(Higgs)  = %.1f GeV' % r.x[1])
    print('chi^2/ndf = %.2f' % (fcn(r.x)/(len(vy)-len(r.x))))
```

ndf = N(data points)
 −N(parameters)

partial 110-example-10a.py

```
N(Higgs)  = 69.8 events
M(Higgs)  = 125.2 GeV
chi^2/ndf = 1.57  ⇐ χ² / number of degrees of freedom ~ 1 means a good fit!
```

FITTING CORE & PLOTTING (II)

- Plotting – overlapping the fitting model on top of the data points.

- Generally you still have to judge/confirm the quality of fit by plotting.
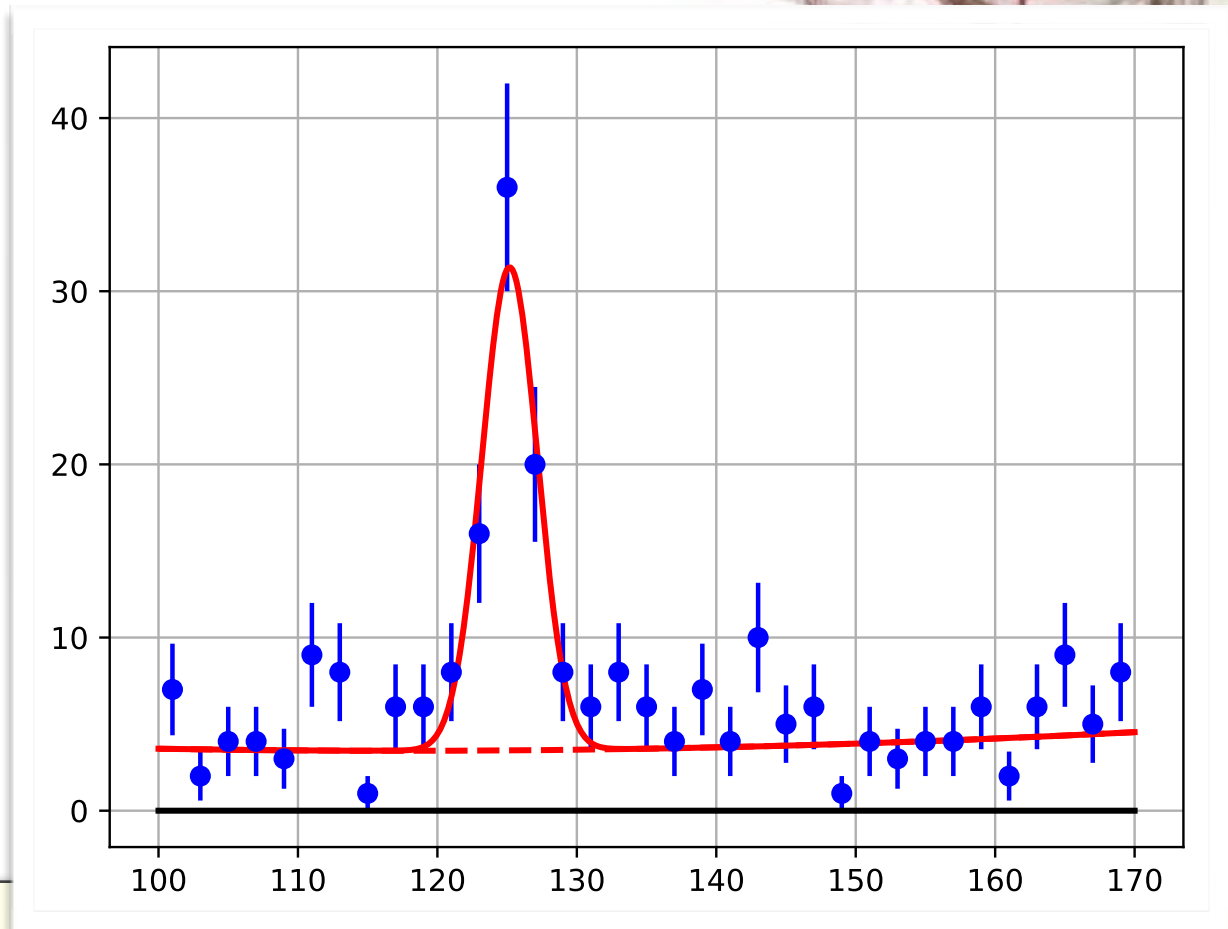

```
if r.success:
    cx = np.linspace(xmin,xmax,500)
    cy = model(cx,r.x[0],r.x[1],r.x[2],r.x[3],r.x[4],r.x[5])
    cy_bkg = model(cx,0.,r.x[1],r.x[2],r.x[3],r.x[4],r.x[5])

    plt.plot(cx, cy, c='red',lw=2)
    plt.plot(cx, cy_bkg, c='red',lw=2,ls='--')
```

⇑ background curve is obtained by setting the Gaussian norm to be 0

l205-example-10a.py (partial)

ALTERNATIVE FITTING CODE

■ Actually in scipy, there is a dedicated least-square fitting package, named curve_fit(). It also provides an estimation of fitting errors.

```python
p_init = np.array([70.,125.,2.,4.,0.,0.])
rx,rcov = opt.curve_fit(model,vx,vy,p_init,vyerr)

if np.any(rx != p_init):
    print('N(Higgs) = %.1f +- %.1f events' % (rx[0],rcov[0,0]**0.5))
    print('M(Higgs) = %.1f +- %.1f GeV' % (rx[1],rcov[1,1]**0.5))

    cx = np.linspace(xmin,xmax,500)
    cy = model(cx,rx[0],rx[1],rx[2],rx[3],rx[4],rx[5])
    cy_bkg = model(cx,0.,rx[1],rx[2],rx[3],rx[4],rx[5])
```

⇑ No needs of calculating x^2 by ourself.

⇑ square-root of the diagonal term is the uncertainty

l205-example-10b.py (partial)

```
N(Higgs) = 69.8 +- 12.4 events
M(Higgs) = 125.2 +- 0.4 GeV
```

COMMENTS

- Surely such a simple χ^2 fit is not very professional. The real fit to the Higgs mass peak is much more difficult than just few lines.

- But this is a very good demonstration in any case!

- We will come back to this subject (statistical analysis, fitting, and modeling) again in a later lecture.
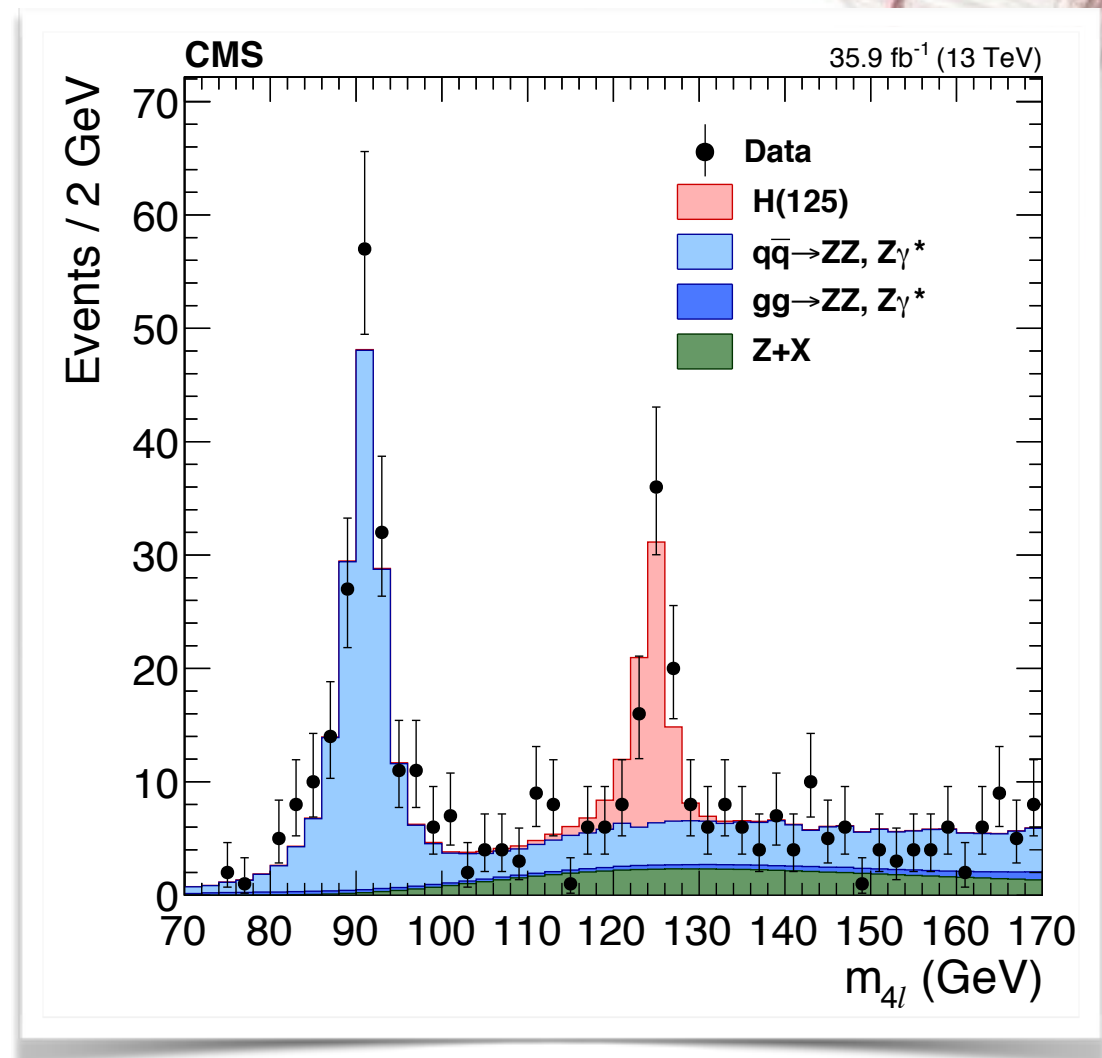
This is the real analysis plot!

IF YOUR FUNCTION IS NOT SO SMOOTH...

- The previous example works pretty well with the generic minimizer from scipy since the function fcn() is smooth, hence the *gradients can be calculated with a finite step method*.

- If the function in the minimization is not so smooth (for example, **involves event counting**), you may find the tool does not work for you out-of-box!

- In this case a different method has to be adopted. Here we are going to introduce an interesting method: **Genetic Algorithm** to resolve such a problem.

- In principle a brute-force **Grid Search** always works up to some extent, although it could be far from optimal and is very slow...

AN EXAMPLE PROBLEM

1205-example-11.py (output)
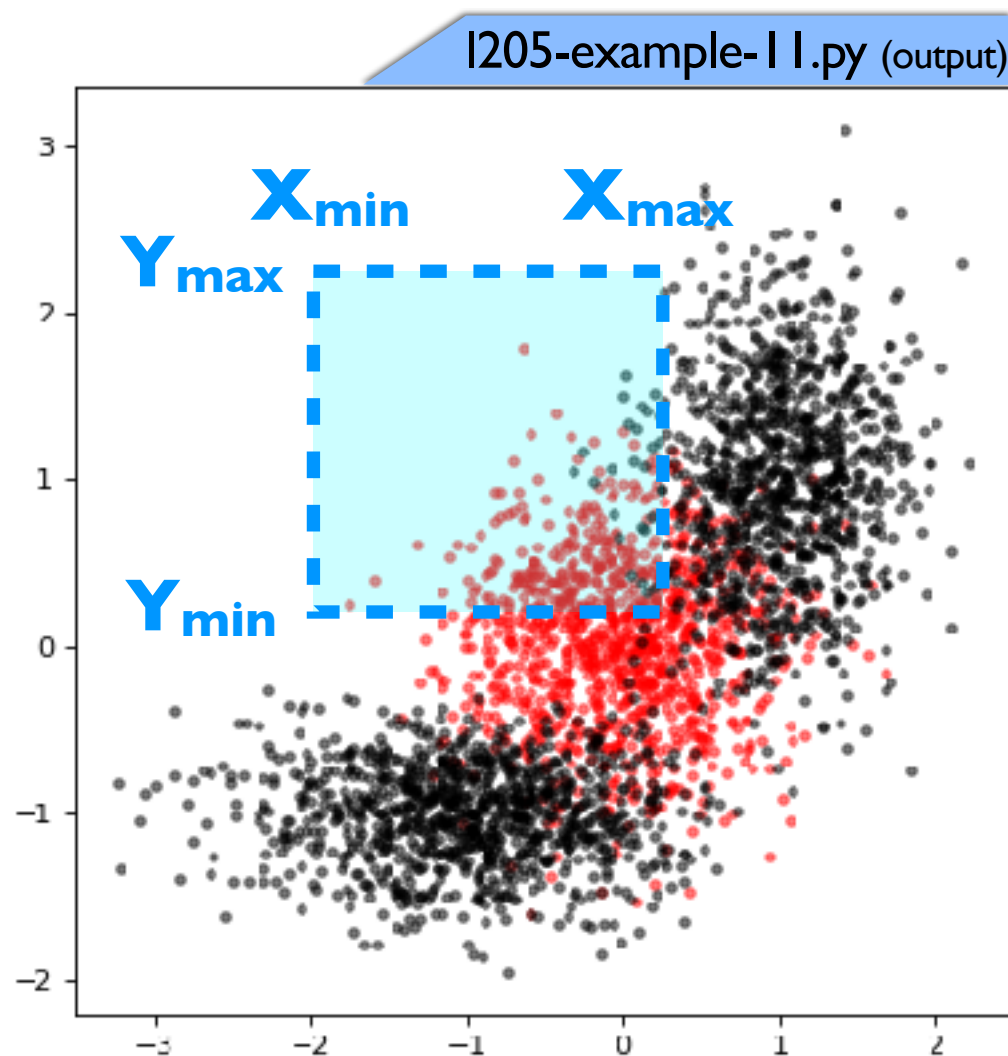
- Suppose you have a set of data, scattered as shown in the figure.

- Can you find a rectangular box which contains maximal **red dots (*signal*)**, minimal **black dots (*background*)**?

- One can define a simple counting significance by
$$\Sigma = \frac{N_{\text{sig}}}{\sqrt{N_{\text{sig}} + N_{\text{bkg}}}}$$

- So…all we need to do is to scan over all the possible values of [X$_{\text{min}}$, X$_{\text{max}}$, Y$_{\text{min}}$, Y$_{\text{max}}$], and look for latest significance value?

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SOLVE IT IN A BRUTE FORCE WAY…

- Before jump to our "fancy method", let's try to it in a simple-minded brute force **search in grid**:

  (note: scipy has a brute-search tool, you can try it too!)

```python
import numpy as np
import matplotlib.pyplot as plt

np.random.seed(123456)
sig = np.random.randn(1000,2)*0.5
bkg = np.vstack([np.random.randn(1000,2)*[0.4,0.6]+[+1.,+1.],
                 np.random.randn(1000,2)*[0.7,0.3]+[-1.,-1.]])

def fcn(x):
  nsig = ((sig[:,0]>x[0]) & (sig[:,0]<x[1]) &
          (sig[:,1]>x[2]) & (sig[:,1]<x[3])).sum()
  nbkg = ((bkg[:,0]>x[0]) & (bkg[:,0]<x[1]) &
          (bkg[:,1]>x[2]) & (bkg[:,1]<x[3])).sum()
    if nsig+nbkg<1: return 0.
    return nsig/(nsig+nbkg)**0.5
```

⇐ producing the scattered data

⇐ counting # of signal and # of background

⇑ return the significance

1205-example-11a.py (partial)

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SOLVE IT IN A BRUTE FORCE WAY…(II)

```
vec = [(a,b,c,d) for a in np.arange(-2.,2.1,0.1)
                 for b in np.arange(a,2.1,0.1)
                 for c in np.arange(-2.,2.1,0.1)
                 for d in np.arange(c,2.1,0.1)]
res = np.array([fcn(x) for x in vec])
best = res.argmax()
print('Resulting box =',vec[best],' fcn =',res[best])
```
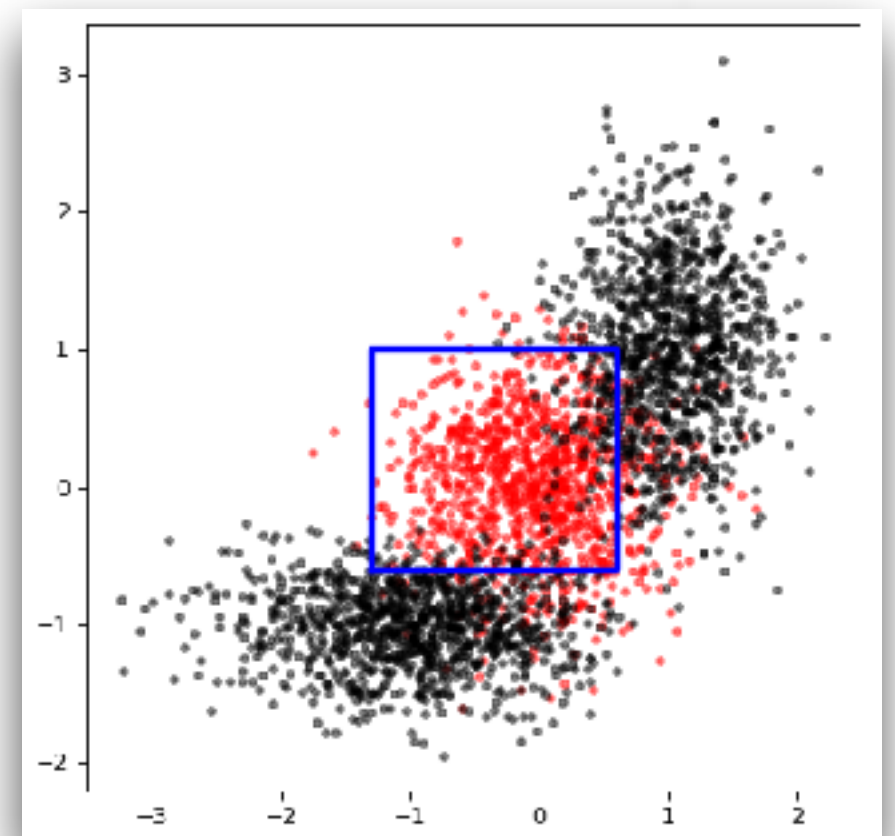
⇐ all candidate
$[X_{min}, X_{max}, Y_{min}, Y_{max}]$

l205-example-11a.py (partial)

- This is what we can obtain easily, although it may take a while:

Resulting box = (-1.3, 0.6, -0.6, 1.0)
fcn = 25.6905

Even with a step size of 0.1 (between -0.2 and +0.2), it already takes 640,000 trials in this grid search…
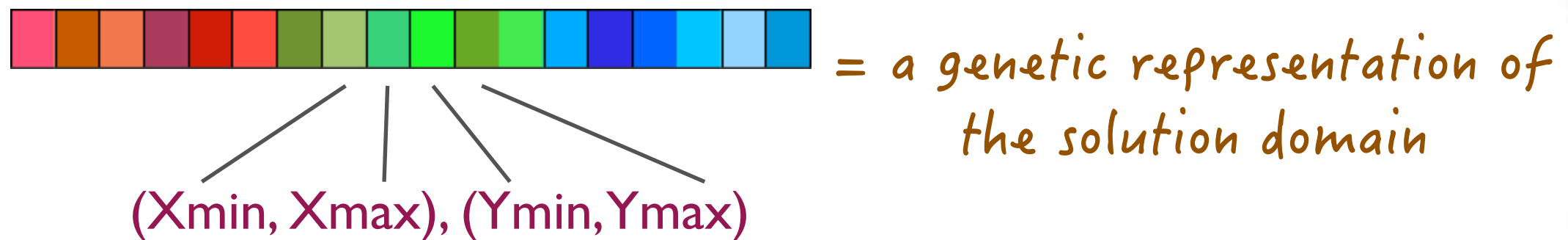
GENETIC ALGORITHM

- **Genetic algorithm (GA)** is a search technique used in computing to find exact or approximate solutions to optimization and search problems. The algorithms use the techniques inspired by evolutionary biology such as **inheritance**, **mutation**, **selection**, and **crossover**.

- GA can be used to find minimum or maximum of a function, but this function can be highly non-linear/non-smooth in a multi-dimensional space.

- Typical requirements:
  - A **genetic representation** of the solution domain;
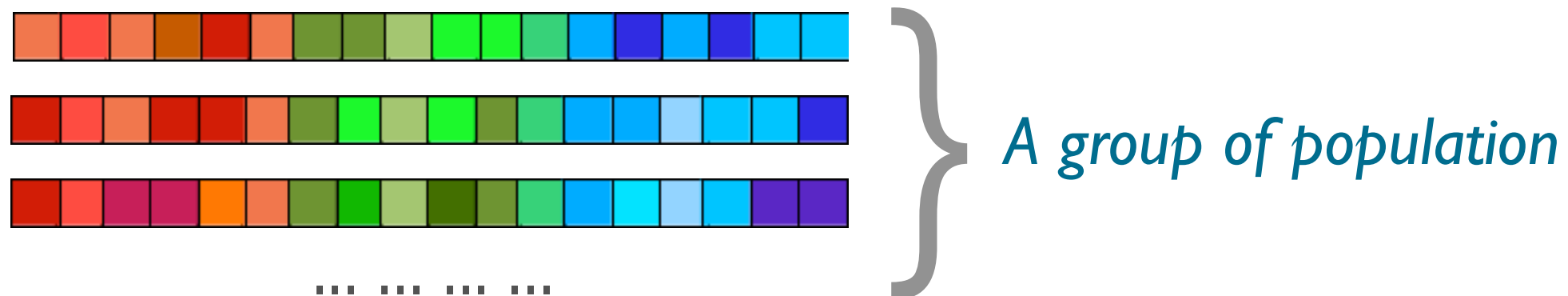 - A **fitness function** to evaluate the solution domain.
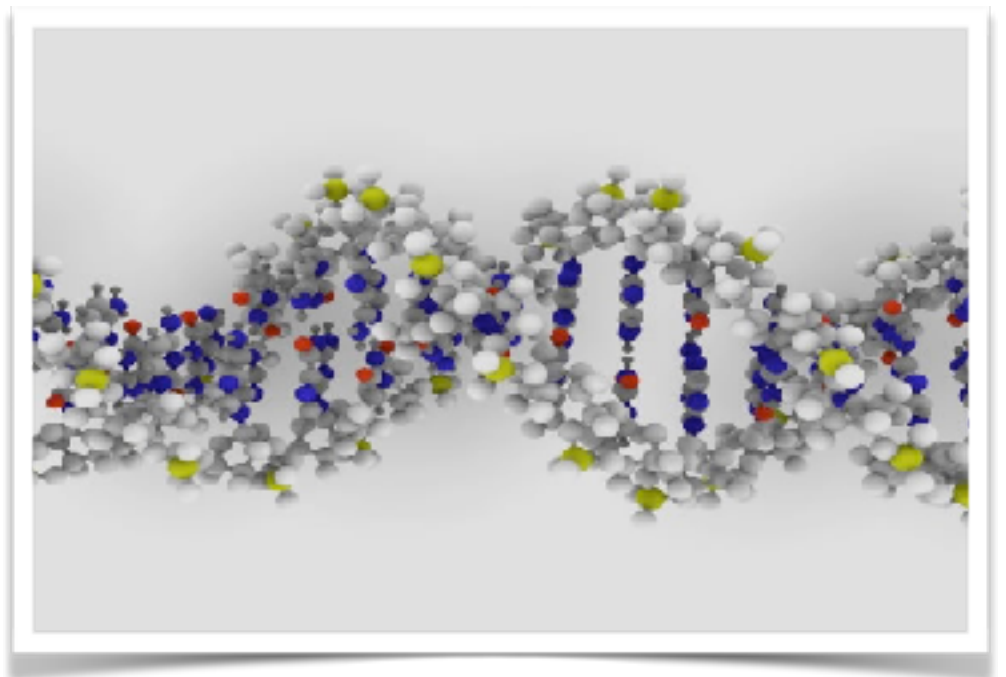
GENETIC ALGORITHM (II)

- First let's encoding the numbers (boundaries of the rectangular box) into a **chromosome** or gene:
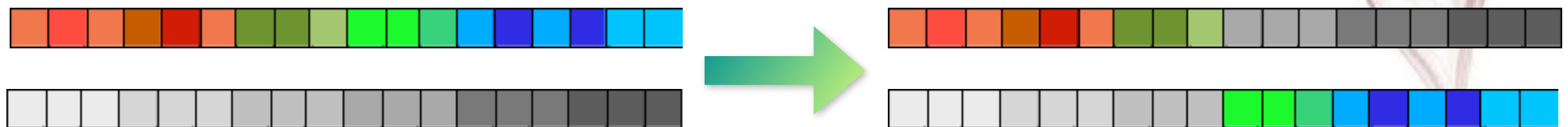

= a genetic representation of the solution domain

$(X_{min}, X_{max}), (Y_{min}, Y_{max})$

- Then generate a set of chromosomes with random numbers as the first/initial generation:

} A group of population

... ...

GENETIC ALGORITHM (III)

- Let's generate the next generations by **CROSSOVER**:

- And with **MUTATION**:

- Now we get a bigger group of population, then let's drop some of chromosomes according to their **FITNESS** and reduce the number of genes back to a constant population.
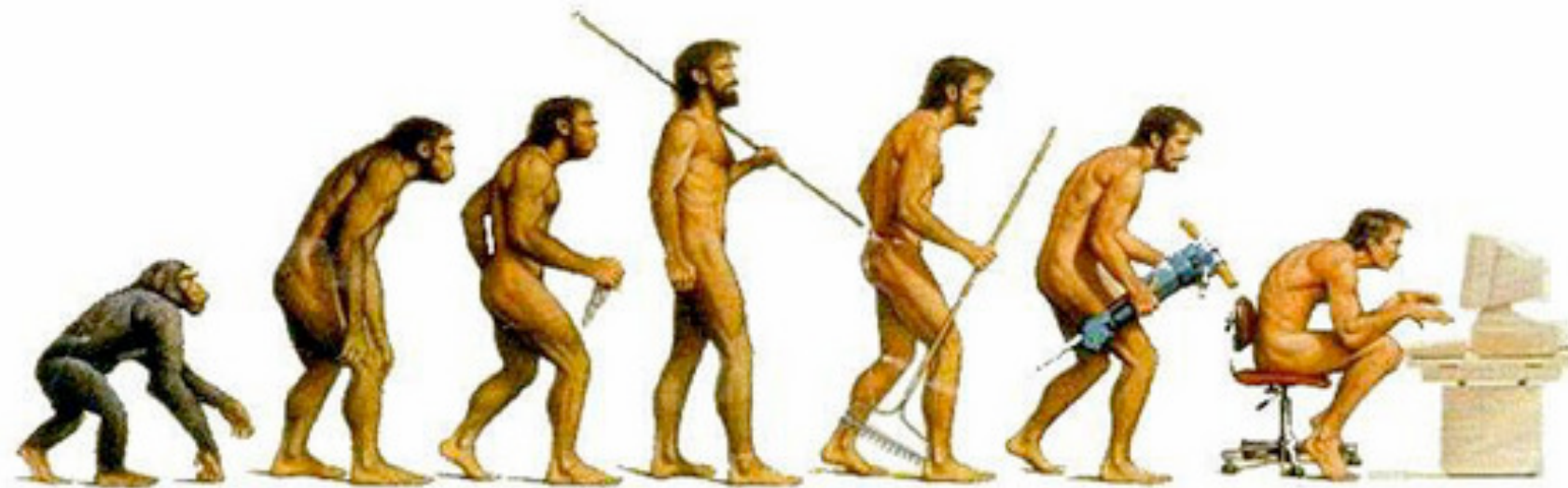
Fitness = 1.424 ✓

Fitness = 0.874 ✗

Take the counting significance as the fitness function:

$$\Sigma = \frac{N_{\text{sig}}}{\sqrt{N_{\text{sig}} + N_{\text{bkg}}}}$$

GENETIC ALGORITHM (IV)

■ The **EVOLUTION**:

What we need to do is just re-do the updating processes: <u>crossover</u>, <u>mutation</u>, and <u>kills the bad genes</u> until the population is converged at some point.


Then we just need to pick up the best chromosome as the **representation of the best solution** to our problem.

A SIMPLE IMPLEMENTATION

```python
def crossover(x,y):
    return [np.random.choice([v,w]) for v,w in zip(x,y)]
def mutation(x):
    return [v+np.random.randn()*0.2
            if np.random.rand()<0.2 else v for v in x]
```

⇐ routines for crossover & mutation

```python
population = 100
```
⇐ size of population
```python
chromo = [np.random.rand(4)*4.-2. for i in range(population)]
fitness = [fcn(x) for x in chromo]
```
⇑ initial chromosomes (all random)
```python
for gen in range(100):
    for idx in range(population):
        pick = np.random.randint(0,population,2)
        x = crossover(chromo[pick[0]],chromo[pick[1]])
```
⇐ pick up parents
```python
        x = mutation(x)
        chromo.append(x)
        fitness.append(fcn(x))

    rank = (-np.array(fitness)).argsort()[:population]
```
⇐ drop low rank ones
```python
    chromo = [chromo[i] for i in rank]
    fitness = [fitness[i] for i in rank]
    print('gen:',gen+1,'best chromo=',chromo[0],'fitness=',fitness[0])

    if np.array(fitness).std()/np.array(fitness).mean()<1E-3: break
```
⇑ stop the evolution loop if the whole population is converged.

l205-example-11b.py (partial)

RESULTS WITH GA

- It takes only O(30) generations to converge (*ie. all the chromosomes end up with very similar fitness values*).

- The code runs quick since it only takes **~3000 trials**, much more efficient comparing to the brute-force search!
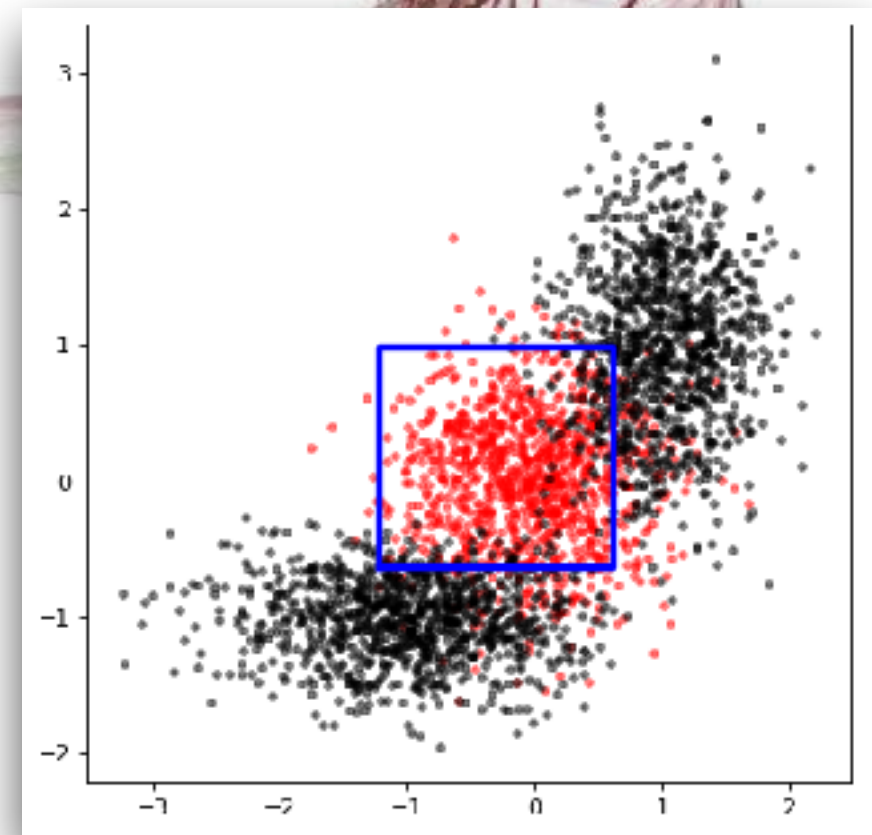
```
gen:  1 best chromo = [-1.868, 0.864, -0.780, 1.046] fitness = 24.4350
gen:  2 best chromo = [-1.452, 0.719, -0.504, 1.246] fitness = 24.8902
gen:  3 best chromo = [-1.452, 0.719, -0.504, 1.246] fitness = 24.8902
gen:  4 best chromo = [-1.173, 0.706, -0.701, 1.060] fitness = 25.3192
. . . . . .
gen: 10 best chromo = [-1.173, 0.644, -0.609, 1.060] fitness = 25.6418
. . . . . .
gen: 20 best chromo = [-1.173, 0.616, -0.628, 0.996] fitness = 25.9141
. . . . . .
gen: 27 best chromo = [-1.252, 0.613, -0.628, 0.996] fitness = 25.9289
gen: 28 best chromo = [-1.227, 0.616, -0.623, 0.996] fitness = 25.9330
```

COMMENTS

■ Again, finding minimum/maximum in multiple-dimensional space is not easy. **The best algorithm depends on the problem:**

— If the function to be minimized is smooth, take the generic minimizer (scipy or others are generally fine!);

— If the function is highly non-linear / non-smooth / broken, the grid search or GA might work better;

➡ Although the grid search will be extremely slow and not-so-precise when # of parameters goes large;

➡ GA might work better in some cases, but it does not promise to give you the best solution (*but acceptable*).

➡ There are other algorithms can do similar things, left for your own studies!

■ Training neural network is also a kind of heavy minimization over >10K parameters (dimensions), to be discussed in the later lecture.

HANDS-ON SESSION

- **Practice 1:**
  Using the root function routine (Newton's method) in SciPy, implement your own **arcsine** and **arccosine** function. Please compare your own implementations and the standard routines for the following target values:

  $\sin^{-1}(0.1)$, $\sin^{-1}(0.5)$, $\sin^{-1}(0.9)$, $\sin^{-1}(1.0)$ and
  $\cos^{-1}(0.1)$, $\cos^{-1}(0.5)$, $\cos^{-1}(0.9)$, $\cos^{-1}(1.0)$

The trick: simply find the root of $\mathbf{\sin(x) - R = 0}$ and $\mathbf{\cos(x) - R = 0}$

HANDS-ON SESSION

- **Practice 2:**
  Produce a fit to the following data points with 2nd / 3rd / 4th / 5th order polynomial, and decide which one gives you the best quality of fit, by judging the χ^2 per number of degrees of freedom?

```python
xmin, xmax, xbinwidth = 0.,1.,0.05
vx = np.linspace(0.,1.,21)
vy = np.array(
[ 0.981, 0.930, 0.900, 0.889, 0.978, 1.053, 1.000,
  0.986, 1.144, 1.188, 1.309, 1.259, 1.348, 1.435,
  1.427, 1.540, 1.426, 1.203, 0.843, 0.576, 0.060])
vyerr = np.array(
[ 0.044, 0.042, 0.037, 0.037, 0.043, 0.046, 0.038,
  0.045, 0.041, 0.041, 0.044, 0.043, 0.043, 0.041,
  0.050, 0.055, 0.052, 0.074, 0.060, 0.068, 0.082])
```

l205-practice-02.py