Title: Scientific Computation (PHYS 608) - Lecture 5

Date: Oct 30, 2009 10:30 AM

URL: http://pirsa.org/09100181

Abstract:

Terminal Shell Edit View Window Help Fri 10:49

Terminal — vim — 131

```
program convert

      real r
      integer :: i
      equivalence(i,r)

      i = Z'BA390000'
      write (*,'(f20.13,I12)')r,i
      write (*,*)r,i
      r = -52.234375
      write(*,'(Z8)')i
end program convert
~
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~
```
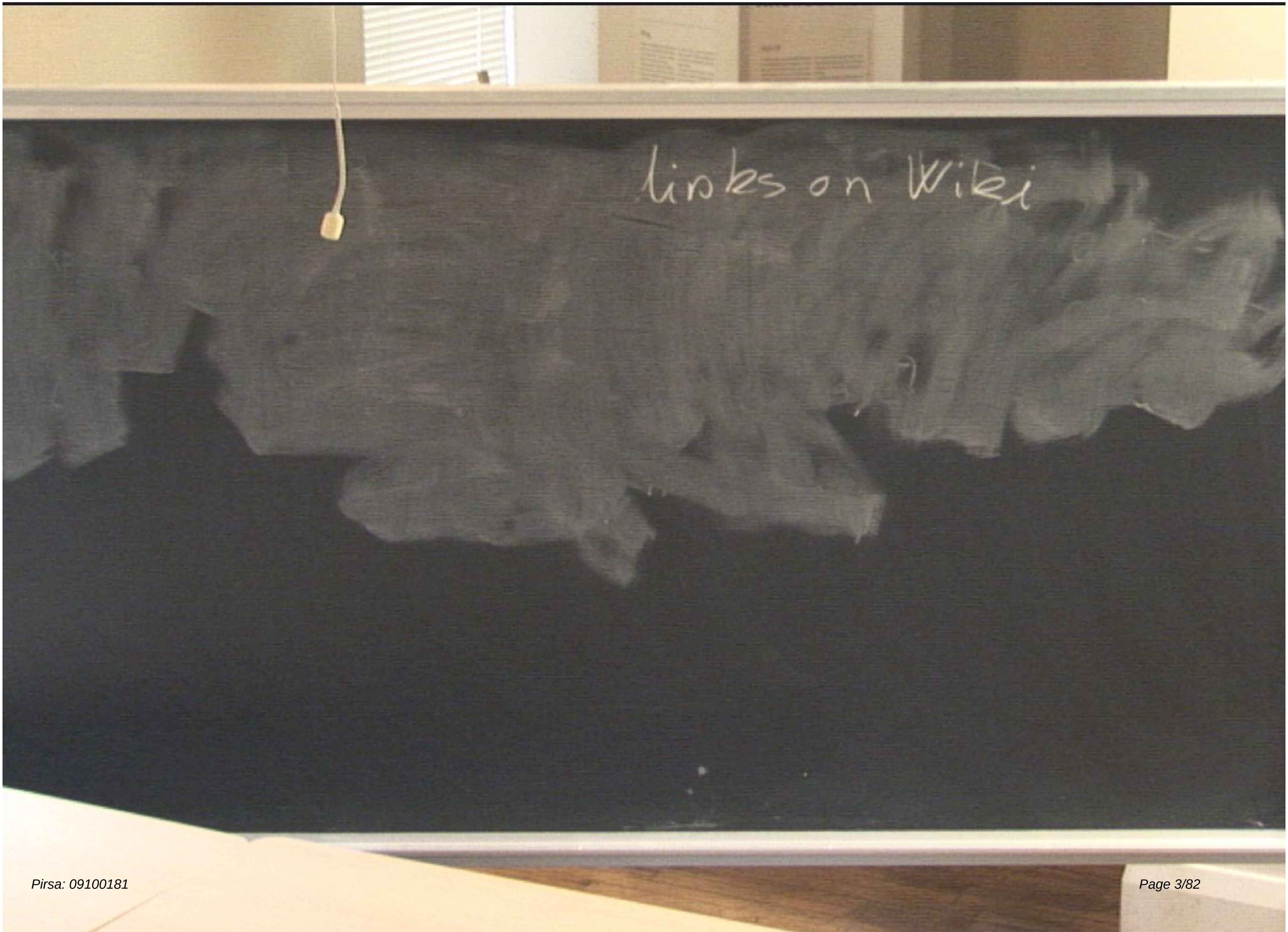
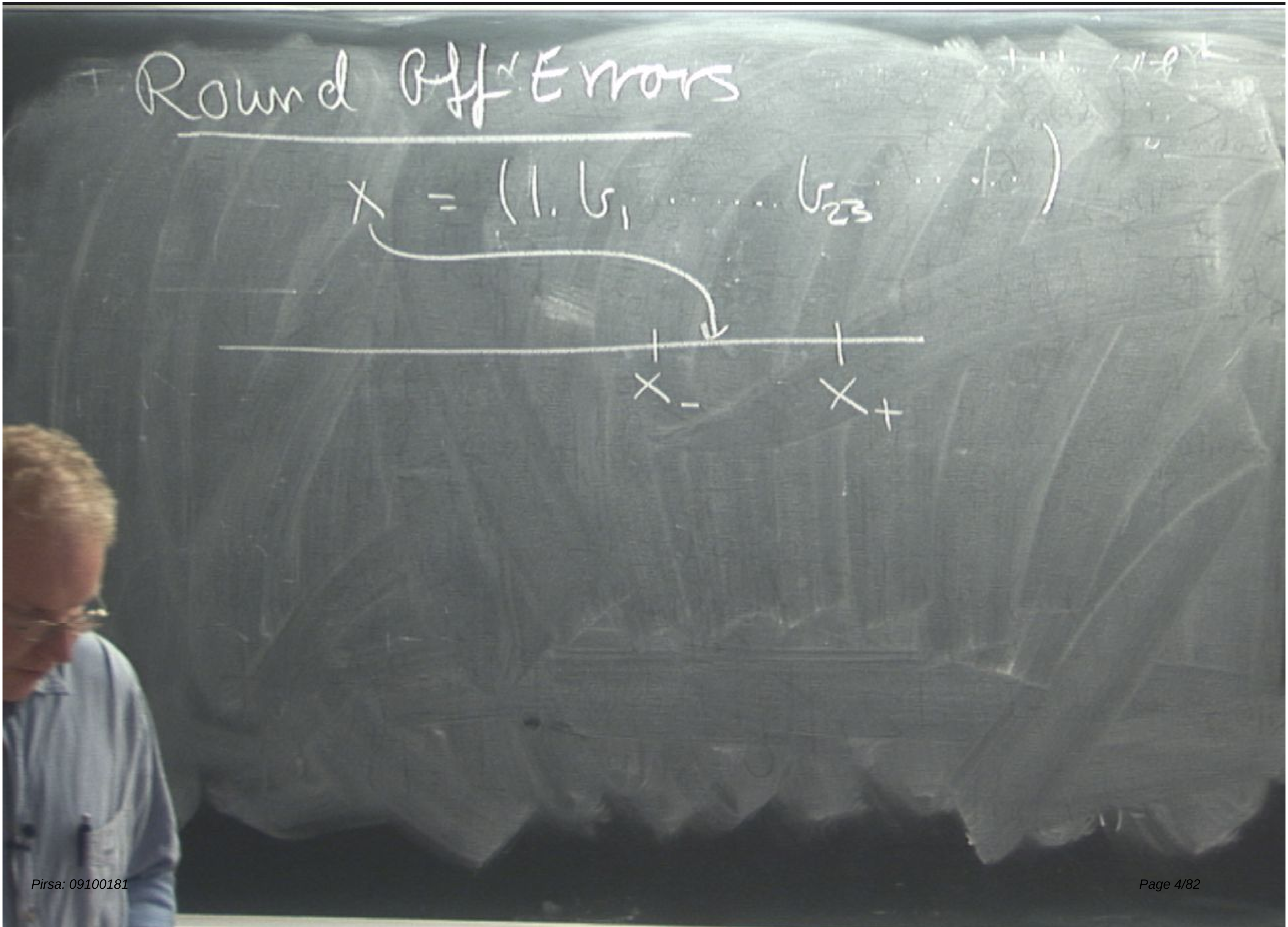
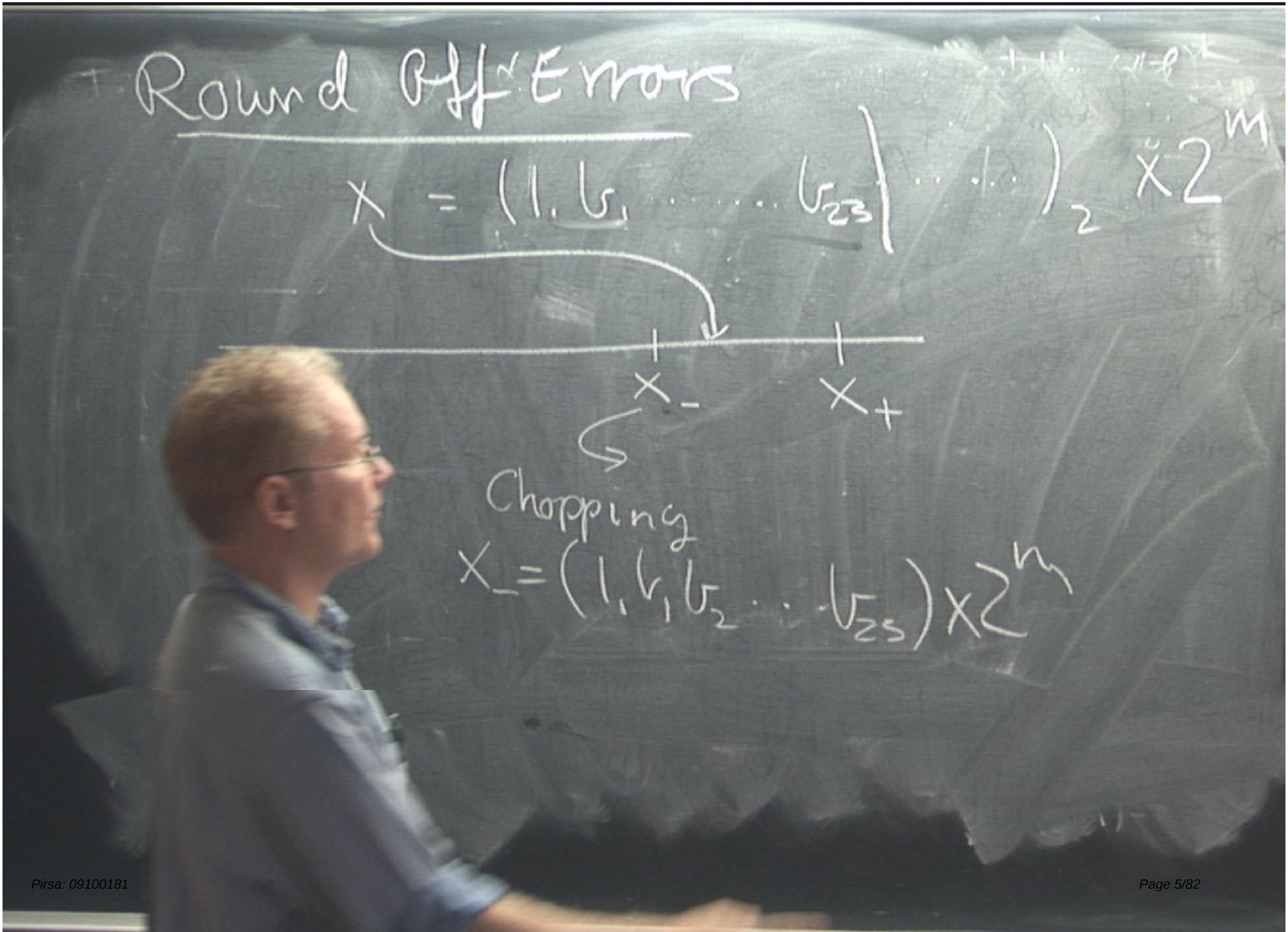
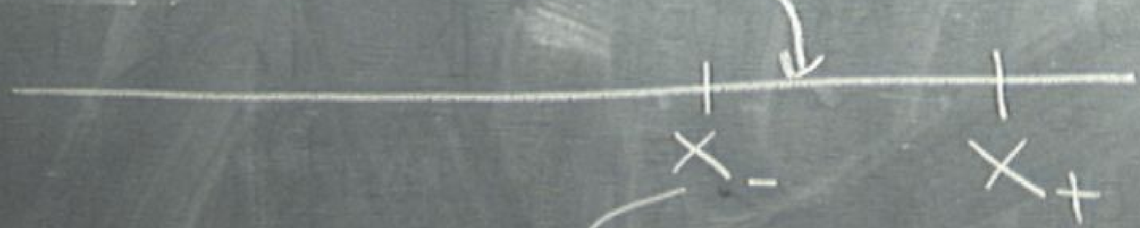


links on Wiki


Round Off Errors
x = (1. b1 .... b23 ....)
x−
x+


Round Off Errors
$x = (1.b_1 \ldots b_{23} | \ldots)_2 \times 2^m$
x_-
x_+
Chopping
$x_- = (1.b_1 b_2 \ldots b_{23}) \times 2^m$

Round Off Errors

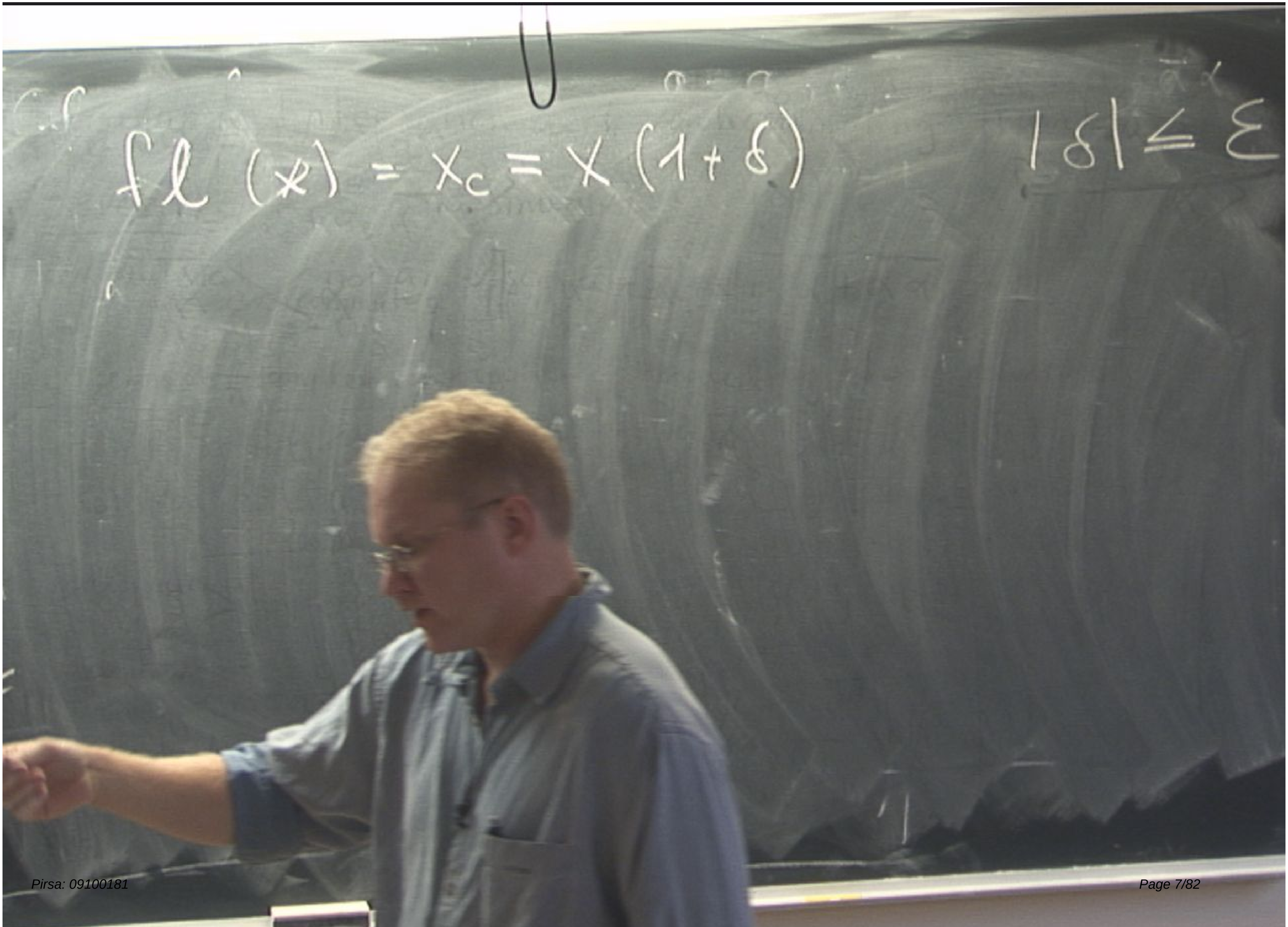
$$x = (1.b_1 \ldots\ldots b_{23} | \ldots\ldots)_2 \times 2^m$$



Chopping

$$x_- = (1.b_1 b_2 \ldots b_{23}) \times 2^m$$

$$x_+ = x_- + 2^{-23} \times 2^m$$


$fl(x) = x_c = x(1+\delta)$
$|\delta| \leq \varepsilon$

$fl(x) = x_c = x(1+\delta)$ $|\delta| \leq \varepsilon$

Real(dbl) :: x

Epsilon(x)

Round Off Errors

Subtractive Errors

$$a = b - c$$

Round Off Errors

Subtractive Errors

$$a = b - c$$

$$a_c = b_c - c_c$$

$$= b(1+\delta_b) - c(1+\delta_c)$$

$$\frac{a_c}{a} = \frac{b-c}{a} + \frac{b}{a}\delta_b - \frac{c}{a}\delta_c$$

if $b \simeq c$

$\to \infty$ $\quad b \to c$

$$\frac{a_c}{a} = 1 + \frac{b}{a}(\delta_b - \delta_c)$$

if $b \simeq c$ ∞ $b \to c$

$$\frac{a_c}{a} = 1 + \frac{b}{a}(\delta_b - \delta_c)$$

Don't subtract 2 large numbers to get a very small number

$$a = b * c$$

$$a_c = b_c * c_c$$

$$= b(1+\delta_b)\, c(1+\delta_c)$$

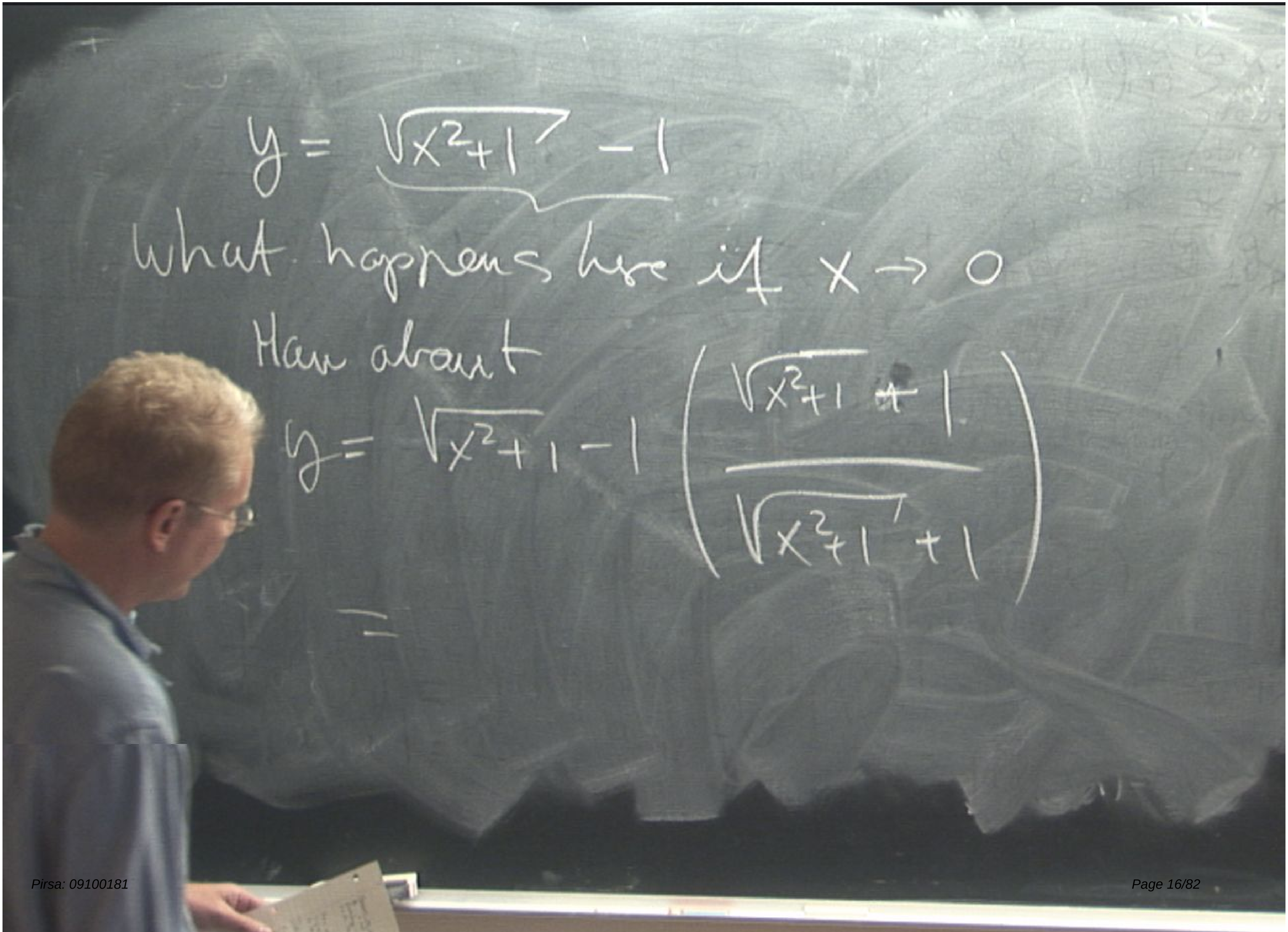
$$\Downarrow$$

$$\frac{a_c}{a} \simeq \frac{b * c}{a}\left(1+\delta_b+\delta_c\right)$$

$$y = \sqrt{x^2+1} - 1$$

$$y = \sqrt{x^2+1} - 1$$

What happens here if $x \to 0$


$y = \underbrace{\sqrt{x^2+1} - 1}$
What happens here if $x \to 0$
How about
$y = \sqrt{x^2+1} - 1 \left(\frac{\sqrt{x^2+1} + 1}{\sqrt{x^2+1} + 1} \right)$
$=$

$$y = \underbrace{\sqrt{x^2+1} - 1}$$

What happens here if $x \to 0$

How about

$$y = \sqrt{x^2+1} - 1 \left(\frac{\sqrt{x^2+1} + 1}{\sqrt{x^2+1} + 1} \right)$$

$$= \frac{x^2}{\sqrt{x^2+1} + 1}$$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

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if $|b^2| \gg 4ac$

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if $|b^2| \gg 4ac$

Solution

Only 1 root will suffer subtraction

Error

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

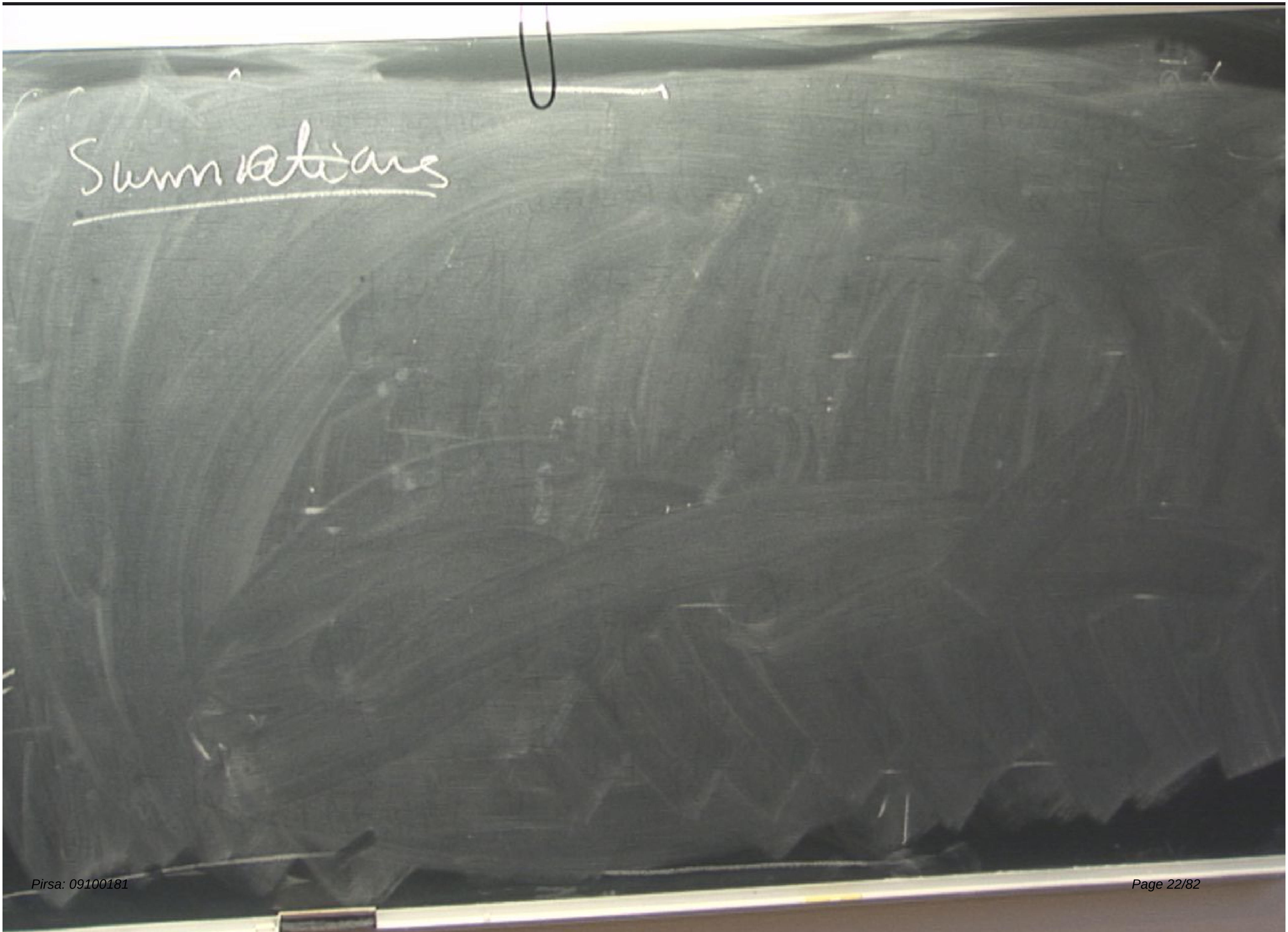
if $|b^2| \gg 4ac$

Solution

Only 1 root will suffer subtraction

Error

$x_1 x_2 = c/a$


Summations

Summations

$$\sum_{k=1}^{\infty} k^{-2} = \frac{\pi^2}{6} = 1.644934066848$$

Summations

$$\sum_{k=1}^{\infty} k^{-2} = \frac{\pi^2}{6} = 1.644934066848$$

```
sum = 0.0
do k=1, 4096
    sum = sum + 1.0 / (k*k)
```

Summations

$$\sum_{k=1}^{\infty} k^{-2} = \frac{\pi^2}{6} = 1.644\,934066848$$

```
sum = 0.0
do k=1, 4096
    sum = sum + 1.0/(k*k)
end do
```

Summations

$$\sum_{k=1}^{\infty} k^{-2} = \frac{\pi^2}{6} = 1.644934066848$$

```
Real :: sum
sum = 0.0
do k=1, 4097
    sum = sum + 1.0/(k*k)
end do
```

1.6

Summations

$$\sum_{k=1}^{\infty} k^{-2} = \frac{\pi^2}{6} = 1.644\,934\,066\,848$$

Real :: sum

sum = 0.0

do k=1, 4097

sum = sum + $\frac{1.0}{k*k}$ $\qquad O(1) + \frac{1}{k^2}$

end do

1.6

Summations

$$\sum_{k=1}^{\infty} k^{-2} = \frac{\pi^2}{6} = 1.644934066848$$

```
Real :: sum
sum = 0.0
do k=1, 4096
   sum = sum + 1.0/(k*k)
end do
```

$\nearrow 2^{12}$

1.6

$1 \cdot 2^{-24}$

LE

$O(1) + \frac{1}{k^2}$

Summations

$$\sum_{k=1}^{\infty} k^{-2} = \frac{\pi^2}{6} = 1.644934066848$$

Real :: sum

2^{12}

sum = 0.0

do k = 8096, 1, -1

sum = sum + $\frac{1.0}{k*k}$

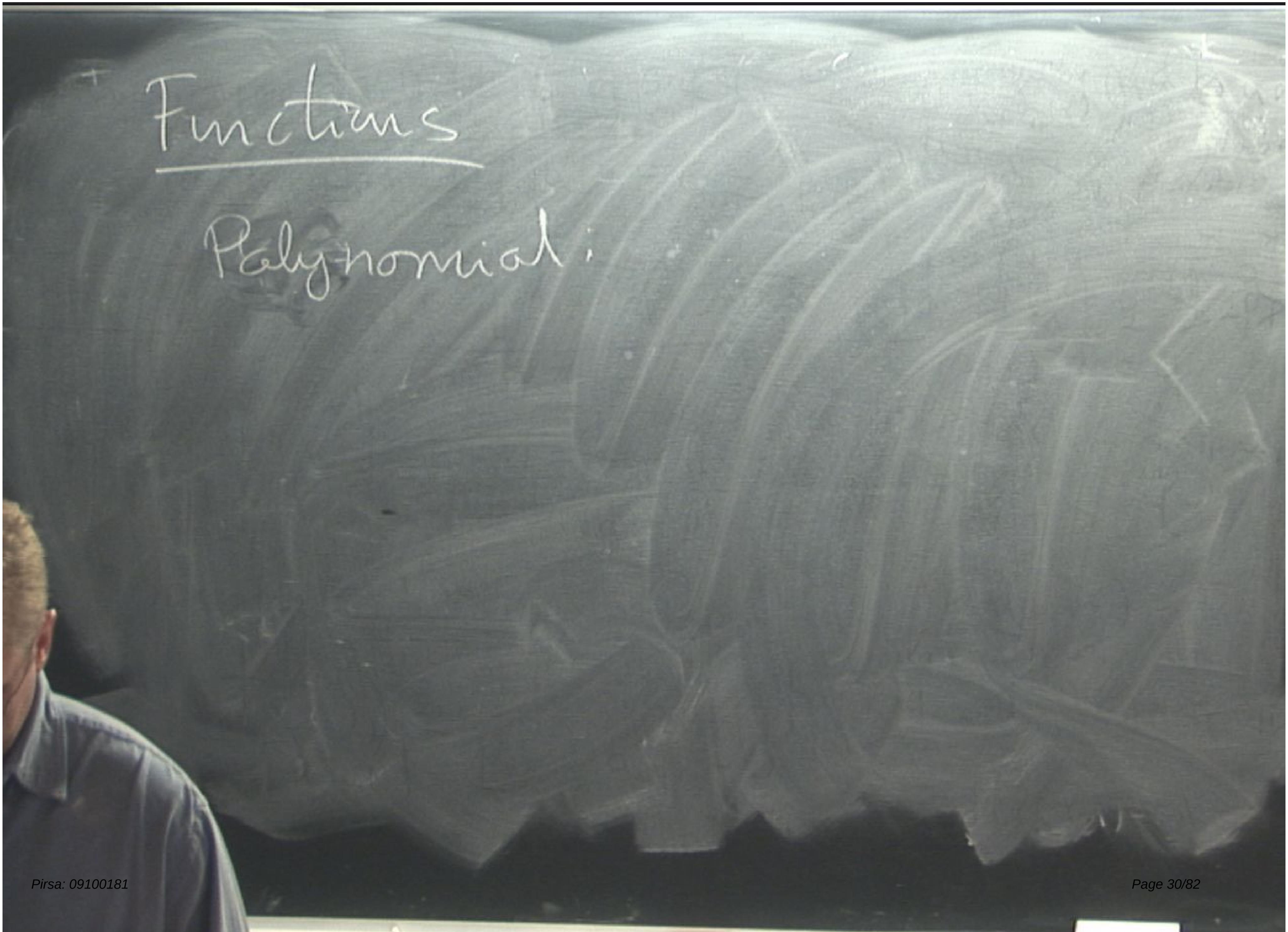
end do

1.6

2^{-24}

LE

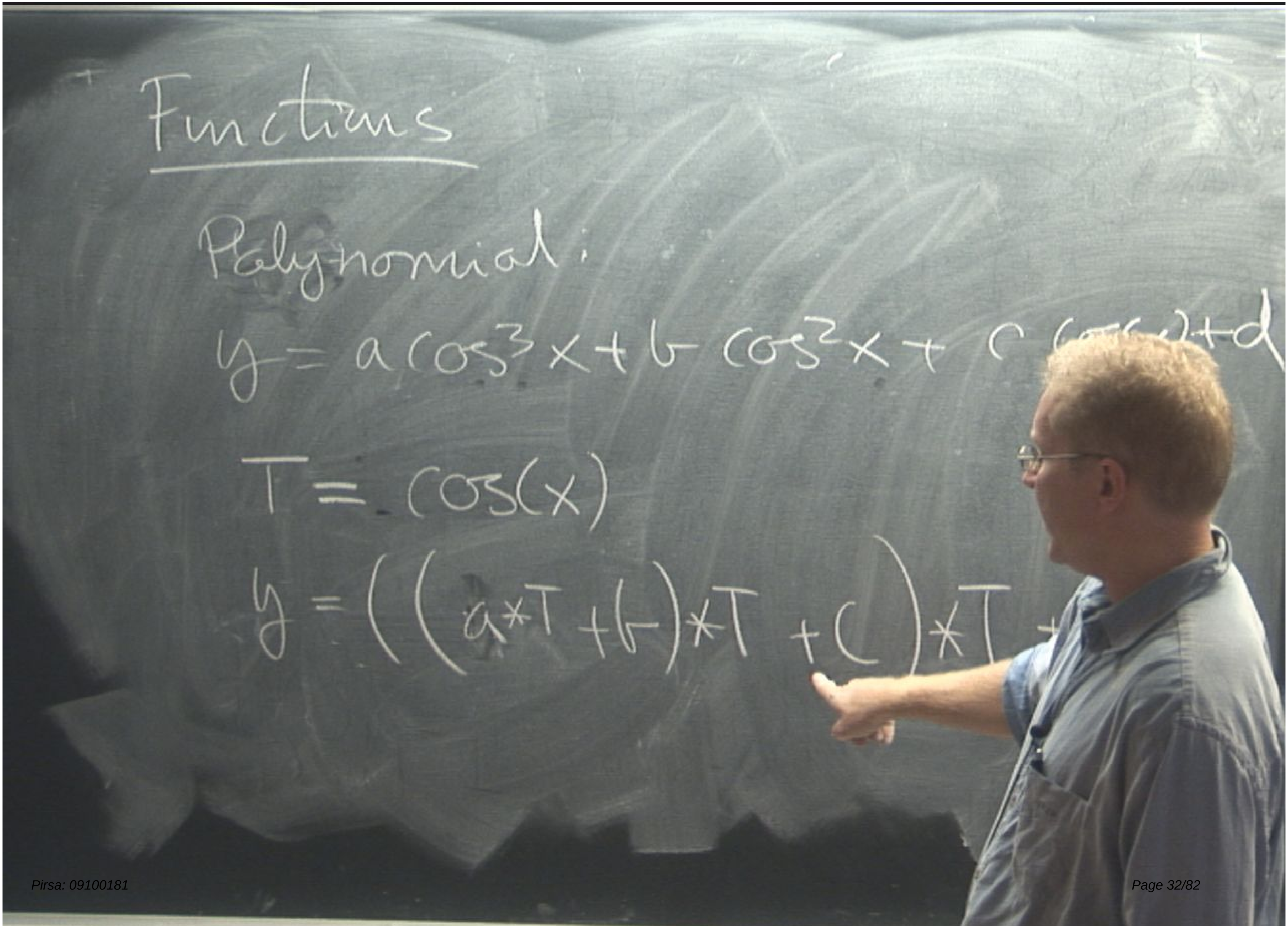
$O(1) + \frac{1}{k^2}$


Functions
Polynomial:

Functions

Polynomial:

$y = a\cos^3 x + b\cos^2 x + c\cos(x) + d$


Functions
Polynomial:
$y = a\cos^3 x + b\cos^2 x + c$
$+d$
$T = \cos(x)$
$y = ((a*T + b)*T + c)*T$

Functions

Polynomial:

$$y = a\cos^3 x + b\cos^2 x + c\cos(x) + d$$

$$T = \cos(x)$$

$$y = ((a*T + b)*T + c)*T + d$$

Functions

Polynomial:

$$y = a\cos^3 x + b\cos^2 x + c\cos(x) + d$$

$$T = \cos(x)$$

$$\boxed{y = ((a*T + b)*T + c)*T + d}$$

Taylor Series

$$f(x) \simeq f(x_0) + \sum_{n=1}^{\infty} \frac{h^n}{n!} f^{(n)}(x_0)$$

Taylor Series

$h = x - x_0$

$$f(x) \simeq f(x_0) + \sum_{n=1}^{\infty} \frac{h^n}{n!} f^{(n)}(x_0)$$

Taylor Series

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Problem / Healse

Radius of convergence

$h = x - x_0$

Taylor Series

$$f(x) \simeq f(x_0) + \sum_{n=1}^{\infty} \frac{h^n}{n!} f^{(n)}(x_0)$$

Problem / Headache

→ Radius of convergence

→ It is a polynomium

$h = x - x_0$

Taylor Series

$$f(x) \simeq f(x_0) + \sum_{n=1}^{\infty} \frac{h^n}{n!} f^{(n)}(x_0)$$

Problem/Headache

→ Radius of convergence

→ It is a polynomium
Hard to get it to diverge

$h = x - x_0$

Taylor Series

$$f(x) \simeq f(x_0) + \sum_{n=1}^{\infty} \frac{h^n}{n!} f^{(n)}(x_0)$$

Problem / Feature

→ Radius of convergence

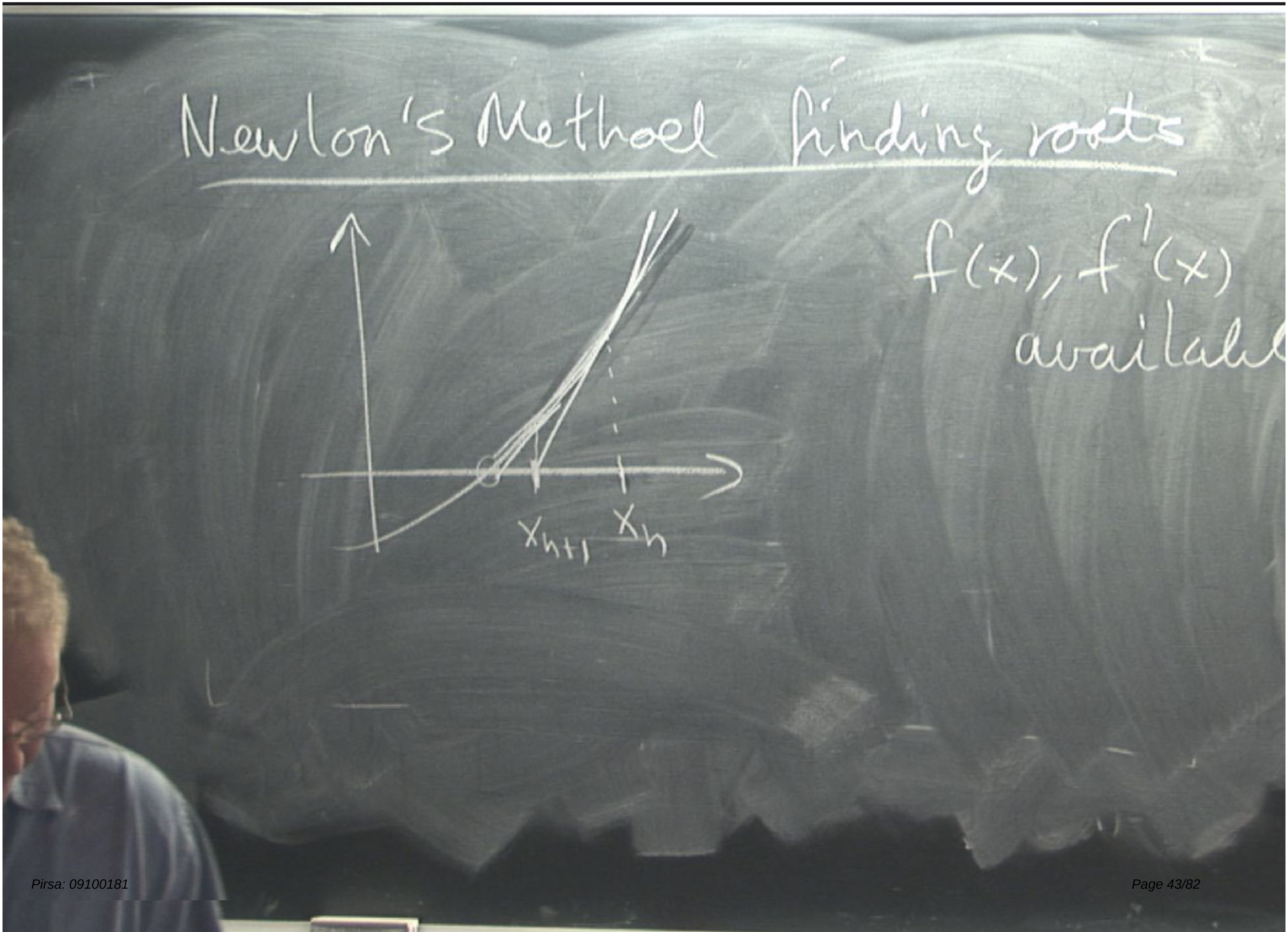
→ It is a polynomium
→ Hard to get it to diverge

Newton's Method finding roots

Newton's Method finding roots

$f(x), f'(x)$

availabl


Newton's Method finding roots
f(x), f'(x)
availabl
x_{n+1}
x_n

Newton's Method finding roots

$f(x)$, $f'(x)$
available

$\delta = x_{n+1} - x$

$$f(x+\delta) = f(x_n) + f'(x_n)\delta$$

Newton's Method finding roots

$f(x), f'(x)$ available

$\delta = x_{n+1} - x$

$$0 = f(x+\delta) \simeq f(x_n) + f'(x_n)\delta + \cancel{\ldots}$$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Newton's Method finding roots

$f(x)$, $f'(x)$ available

$\delta = x_{n+1} - x$

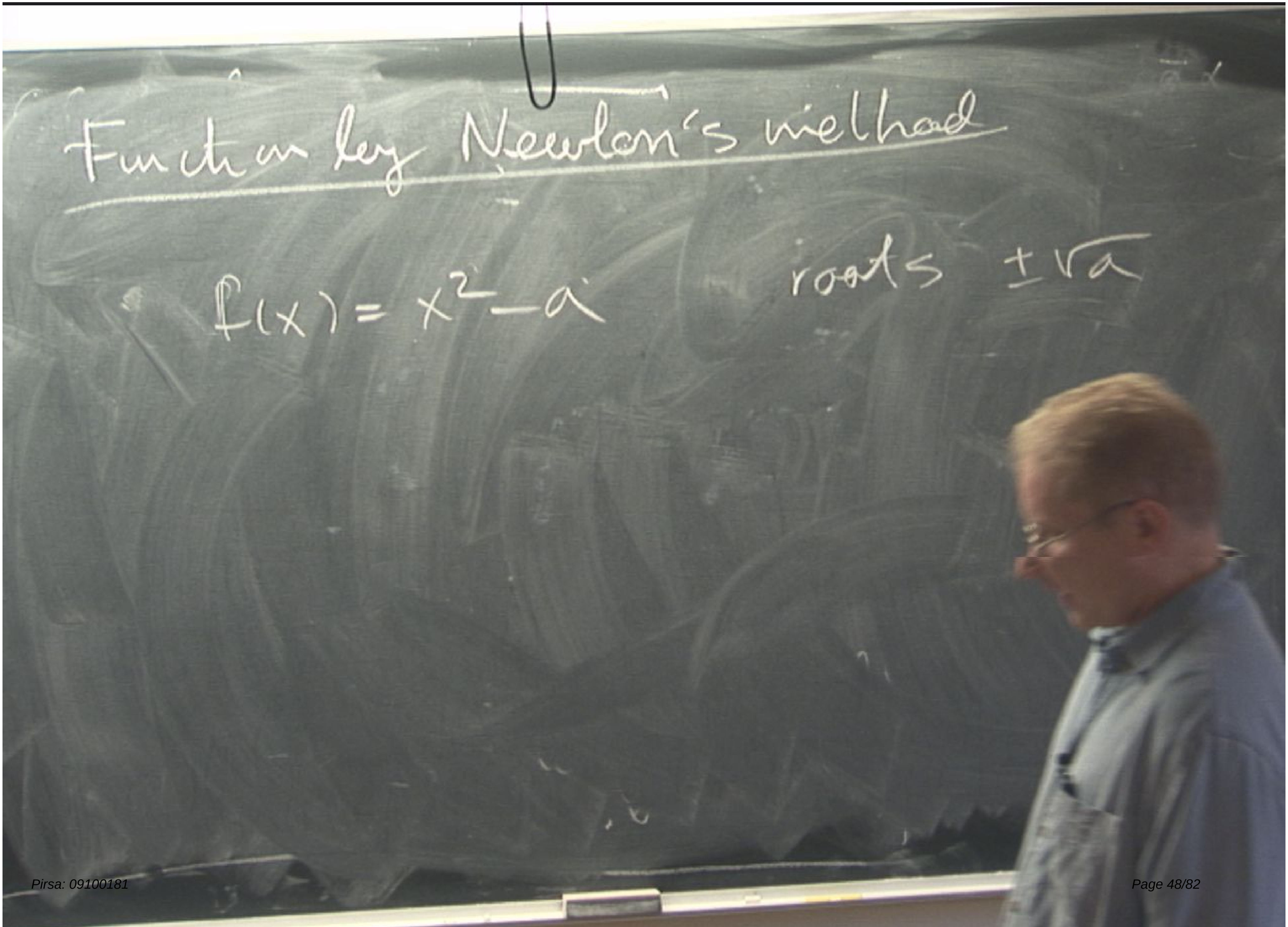
$$0 = f(x+\delta) \simeq f(x_n) + f'(x_n)\delta \cancel{+}$$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

converges quadratically

Function by Newton's method

$$f(x) = x^2 - a$$


Function by Newton's method
$f(x) = x^2 - a$
roots $\pm\sqrt{a}$

Function by Newton's method

$f(x) = x^2 - a$ roots $\pm\sqrt{a}$

$$x_{n+1} = x_n - \frac{x_n^2 - a}{2x_n}$$

Function by Newton's method

$$f(x) = x^2 - a \qquad \text{roots } \pm\sqrt{a}$$

$$x_{n+1} = x_n - \frac{x_n^2 - a}{2x_n}$$

$$= \frac{1}{2}\left(x_n + \frac{a}{x_n}\right)$$

Function by Newton's method

$$f(x) = x^2 - a \qquad \text{roots } \pm\sqrt{a}$$

$$x_{n+1} = x_n - \frac{x_n^2 - a}{2x_n} \qquad 4{,}000$$

$$= \frac{1}{2}\left(x_n + \frac{a}{x_n}\right)$$

Function by Newton's method

$f(x) = x^2 - a$ roots $\pm\sqrt{a}$

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Babylonians 4,000 years ago

Function by Newton's method

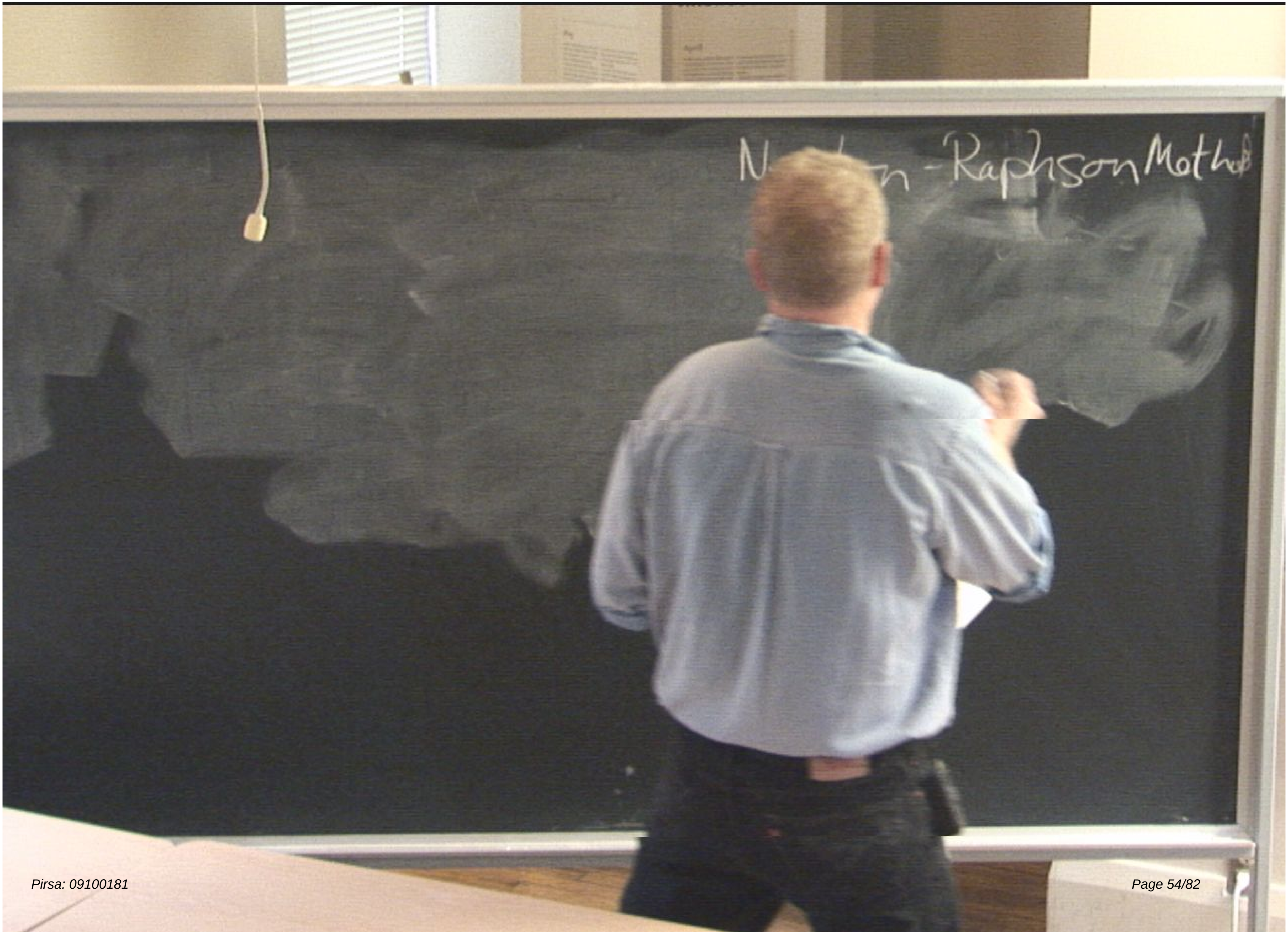
$f(x) = x^2 - a$ roots $\pm\sqrt{a}$

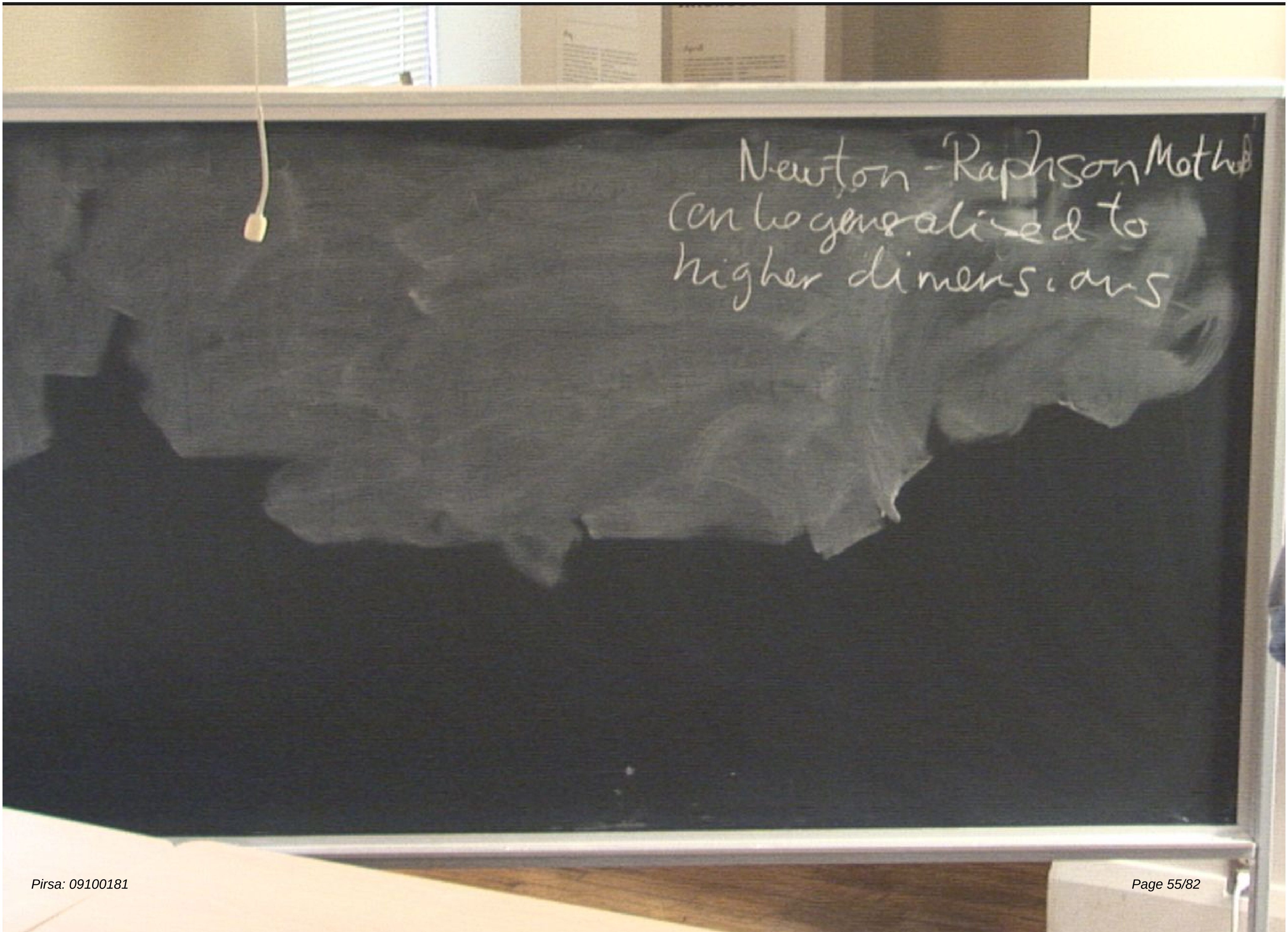
Babylonians 4,000 years ago

$$x_{n+1} = x_n - \frac{x_n^2 - a}{2x_n}$$

$$= \frac{1}{2}\left(x_n + \frac{a}{x_n}\right)$$

— No radius of convergence


Raphson


Newton-Raphson Method
can be generalised to
higher dimensions

Newton-Raphson Method

can be generalised to higher dimensions

$$\vec{f}(\vec{x}) +$$

Newton-Raphson Method

can be generalised to higher dimensions

$$\vec{f}(\vec{x}) + \underline{\underline{J}} \cdot \delta\vec{x}$$

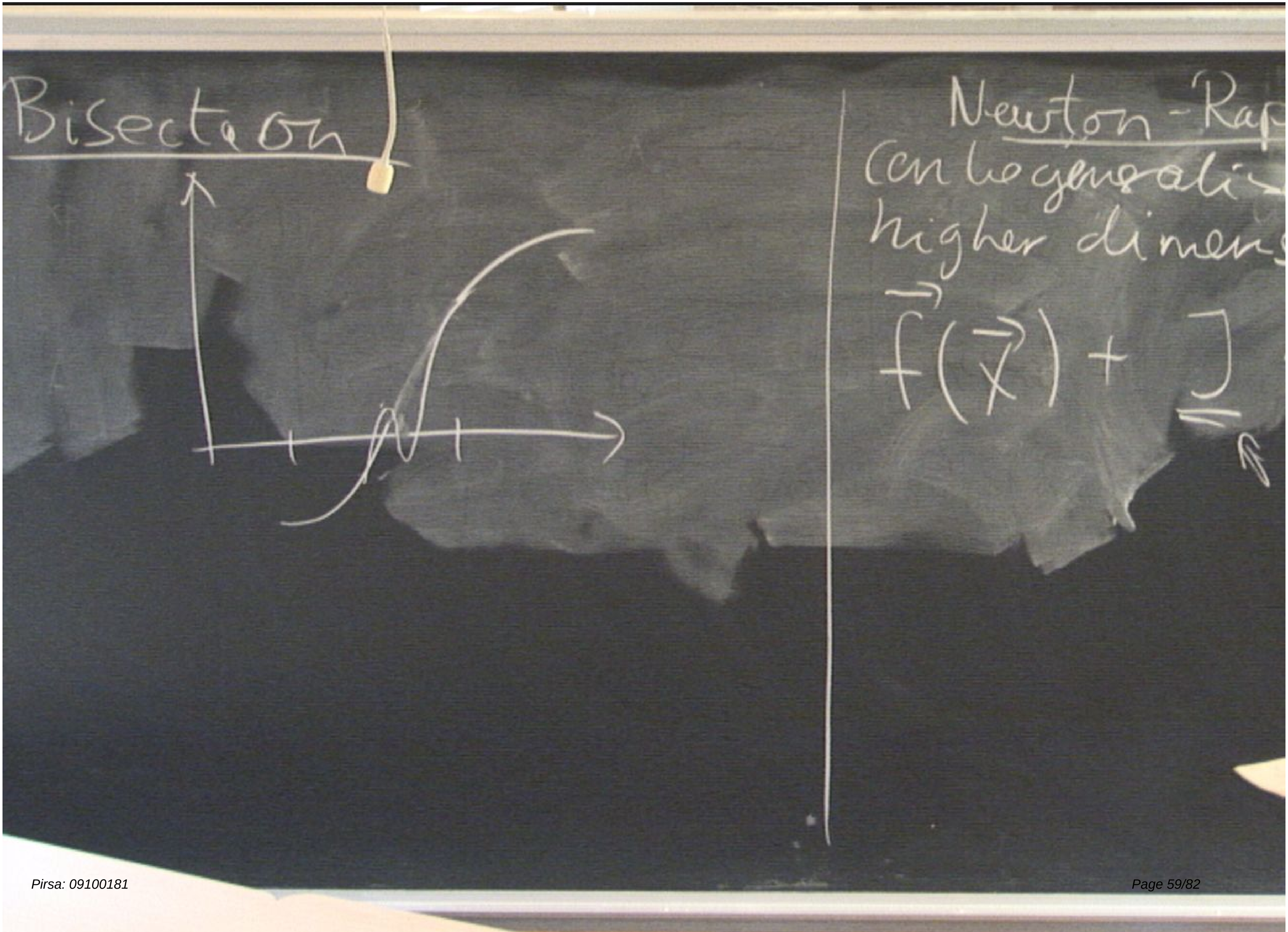
matrix

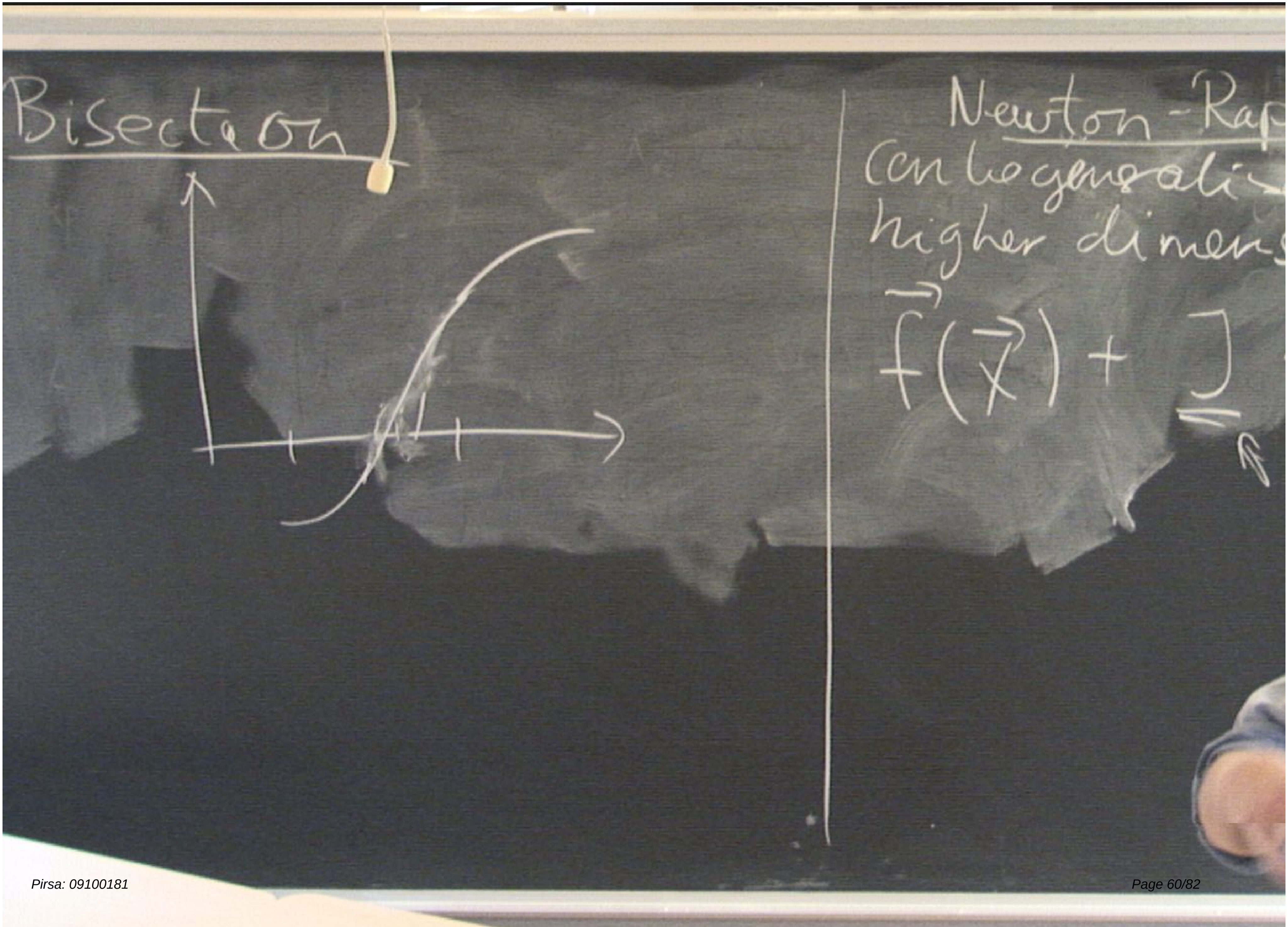
Newton-Raphson Method

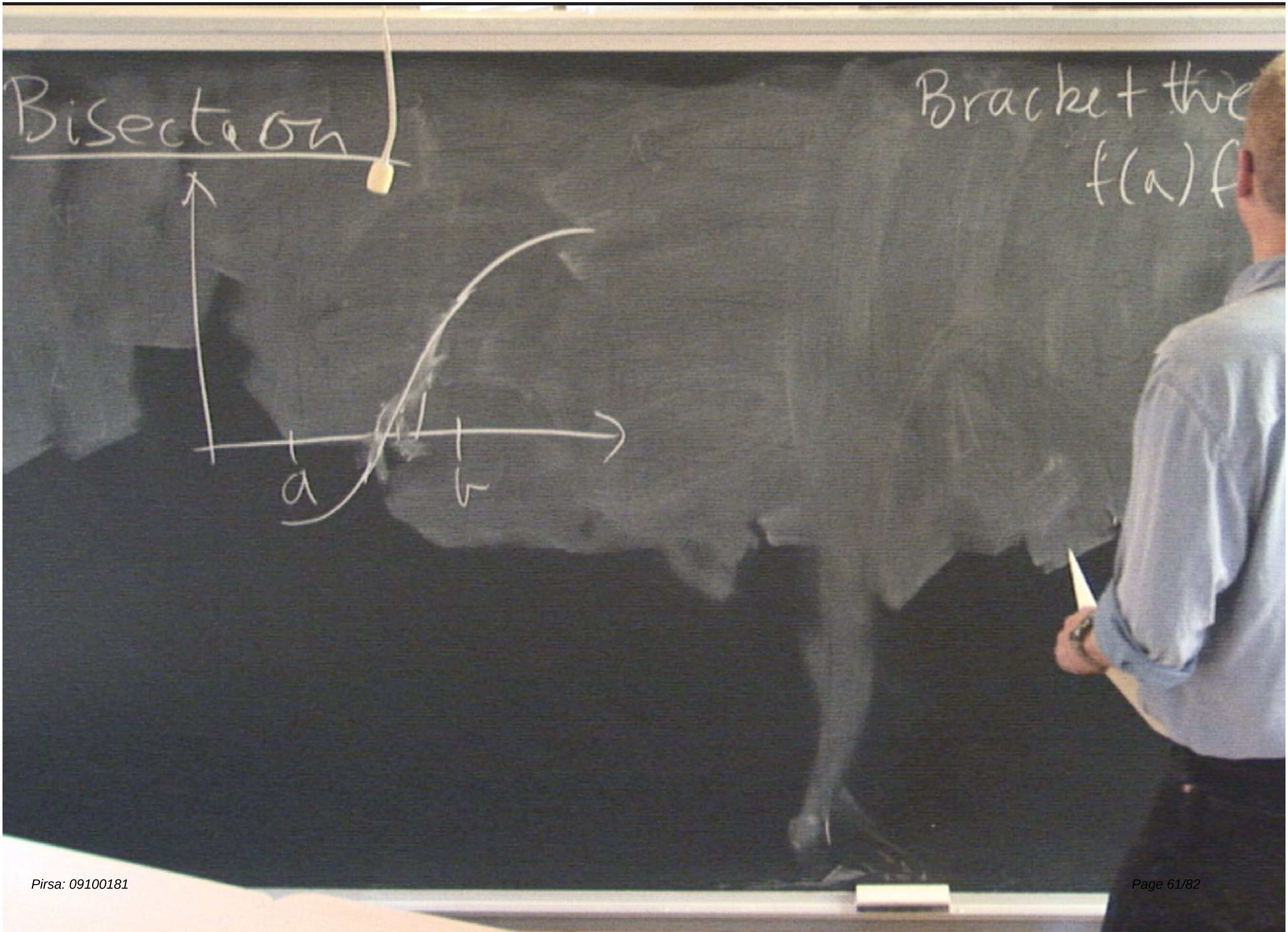
can be generalised to higher dimensions

$$\vec{f}(\vec{x}) + \underline{\underline{J}} \cdot \delta\vec{x} = 0$$

$\uparrow$ matrix

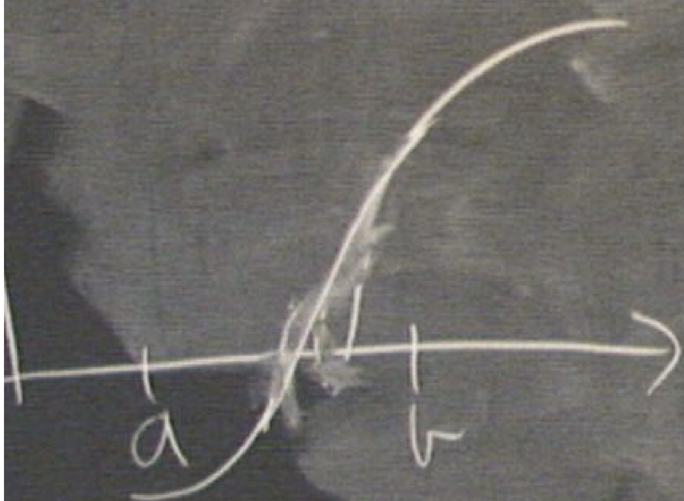

Bisection
Newton-Rap
can be generali
higher dimens
$\vec{f}(\vec{x}) + J$


Bisection
Newton-Rap
can be generali
higher dimens
$\vec{f}(\vec{x}) + \underline{J}$

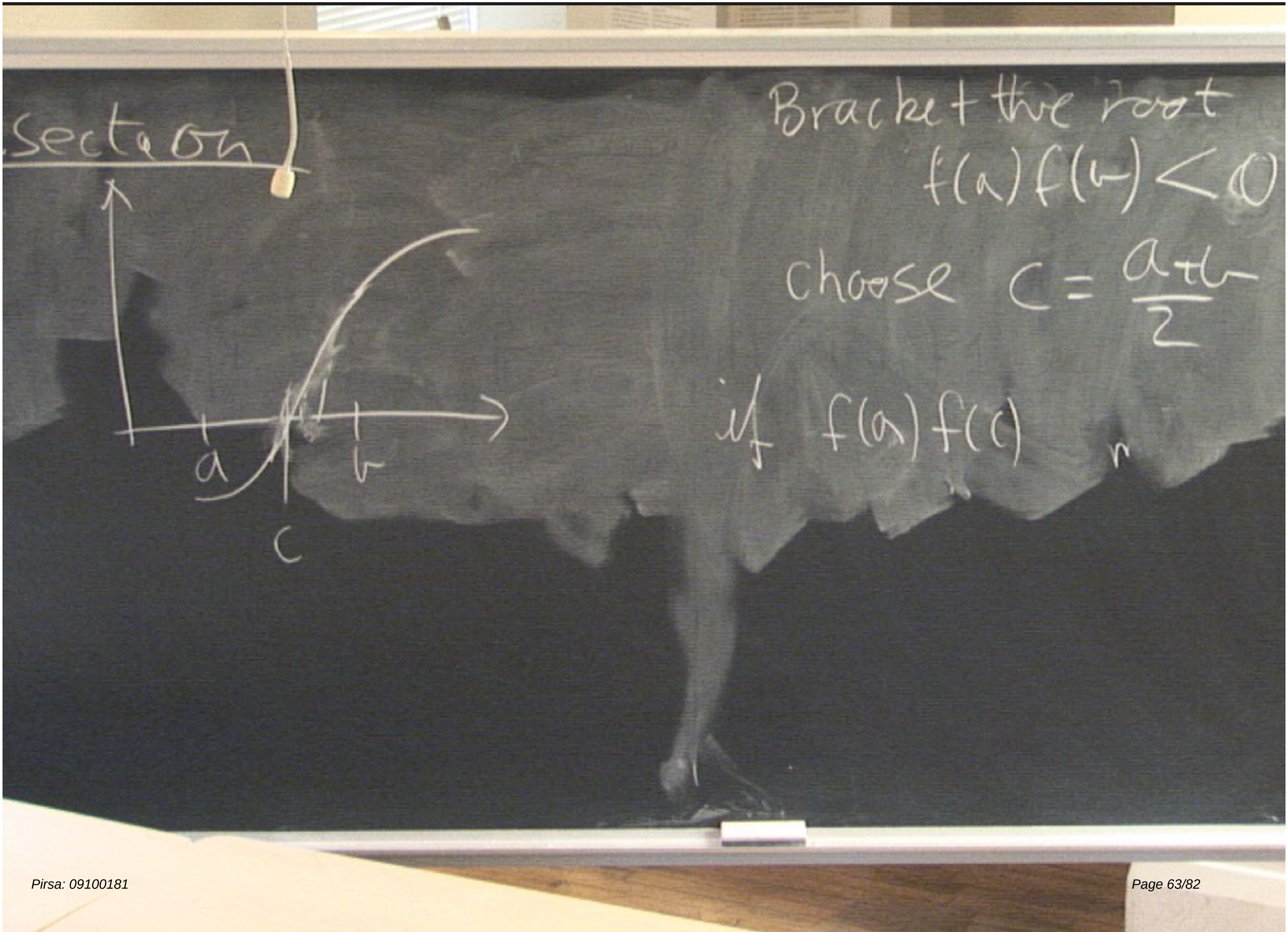

Bisection
Bracket
f(a)
a
b

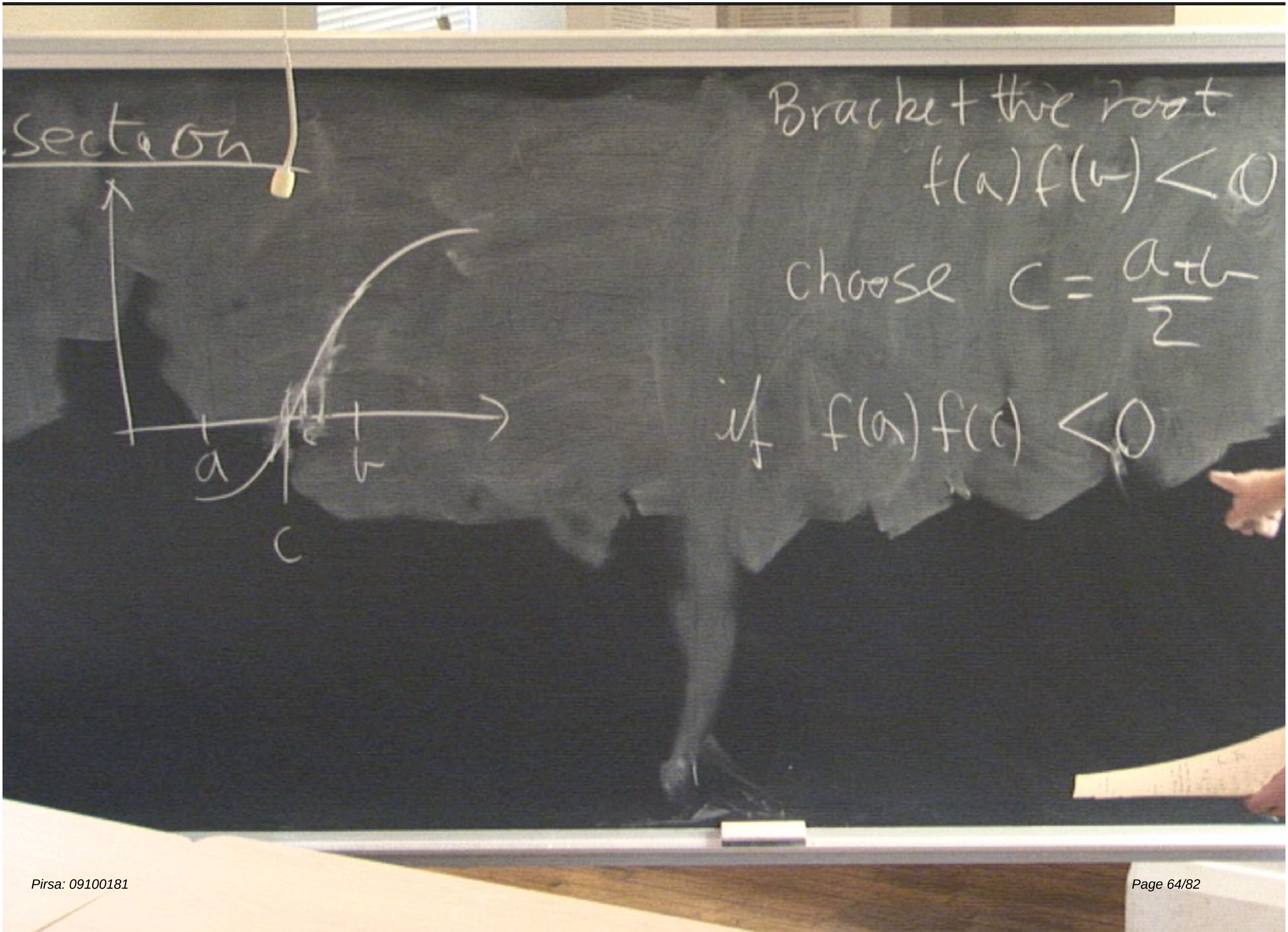
Bracket the root

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

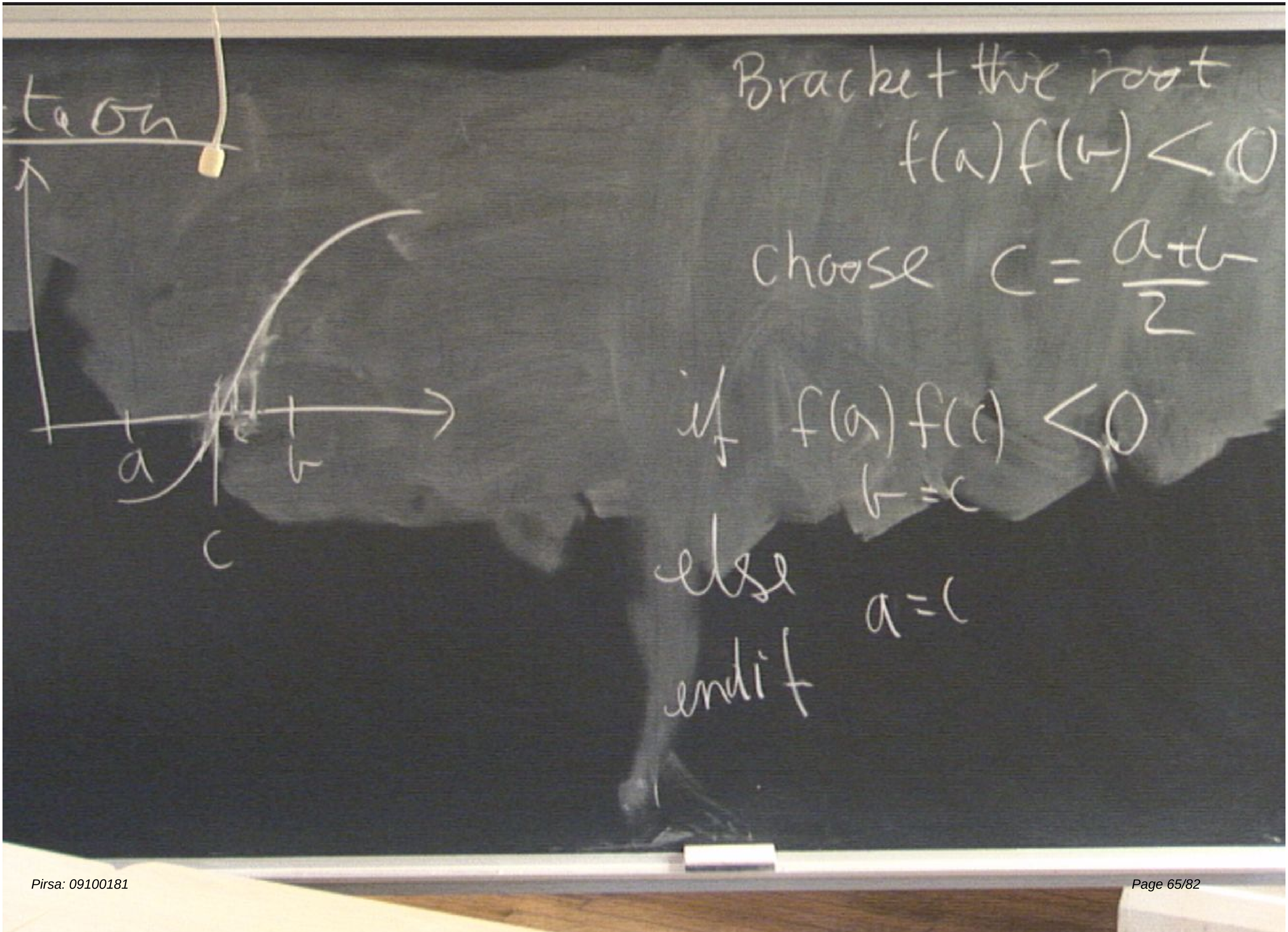


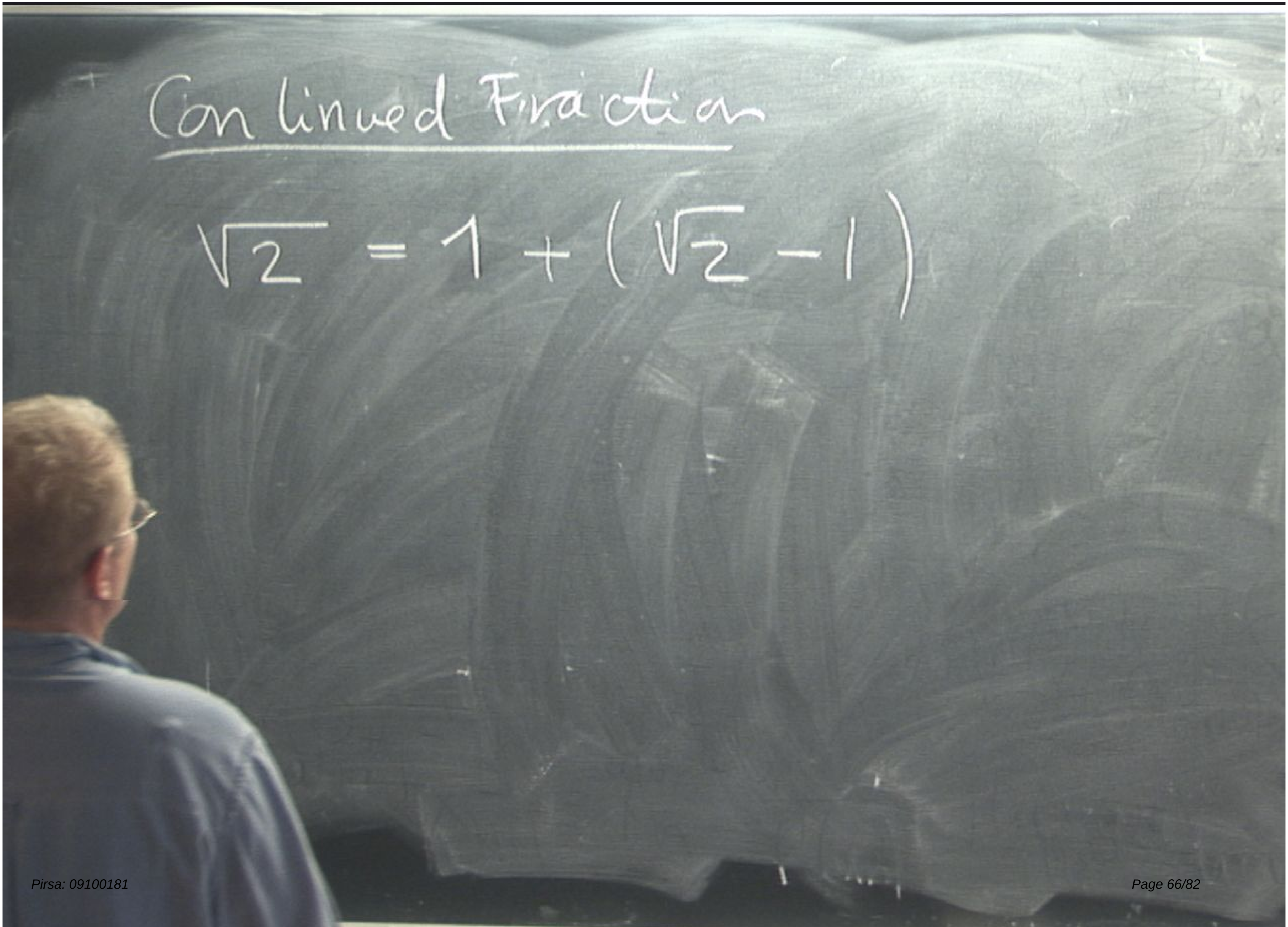
Choose $c = \frac{a+b}{2}$

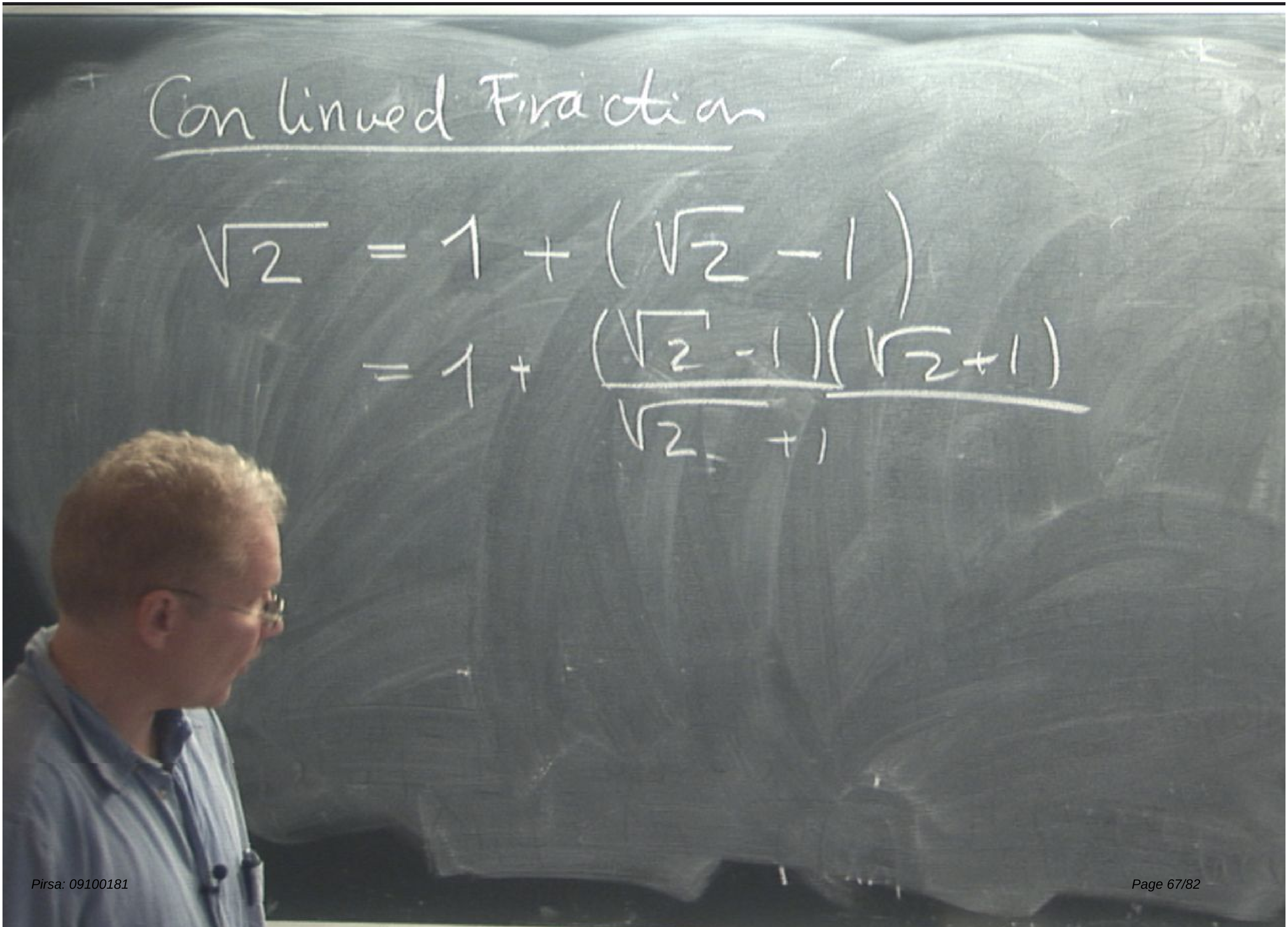

section
Bracket the root
$f(a)f(b) < 0$
choose $c = \frac{a+b}{2}$
if $f(a)f(c)$
a
b
c



section
Bracket the root
f(a) f(b) < 0
Choose c = (a+b)/2
if f(a) f(c) < 0
a
b
c


Bracket the root
f(a) f(b) < 0
choose c = (a+b)/2
if f(a) f(c) < 0
b = c
else
a = c
endif
a
b
c


Continued Fraction
$\sqrt{2} = 1 + (\sqrt{2} - 1)$


Continued Fraction
$\sqrt{2} = 1 + (\sqrt{2} - 1)$
$= 1 + \frac{(\sqrt{2} - 1)(\sqrt{2} + 1)}{\sqrt{2} + 1}$

Continued Fraction

$$\sqrt{2} = 1 + (\sqrt{2} - 1)$$

$$= 1 + \frac{(\sqrt{2}-1)(\sqrt{2}+1)}{\sqrt{2}+1}$$

$$= 1 + \frac{1}{2+(\sqrt{2}-1)}$$

Continued Fraction

$$\sqrt{2} = 1 + (\sqrt{2} - 1)$$

$$= 1 + \frac{(\sqrt{2}-1)(\sqrt{2}+1)}{\sqrt{2}+1}$$

$$= 1 + \frac{1}{2 + (\sqrt{2}-1)}$$

$$= 1 + \cfrac{1}{2 + \cfrac{1}{2 + \cfrac{1}{2 + \cfrac{1}{2 + \cdots}}}}$$

Continued Fraction

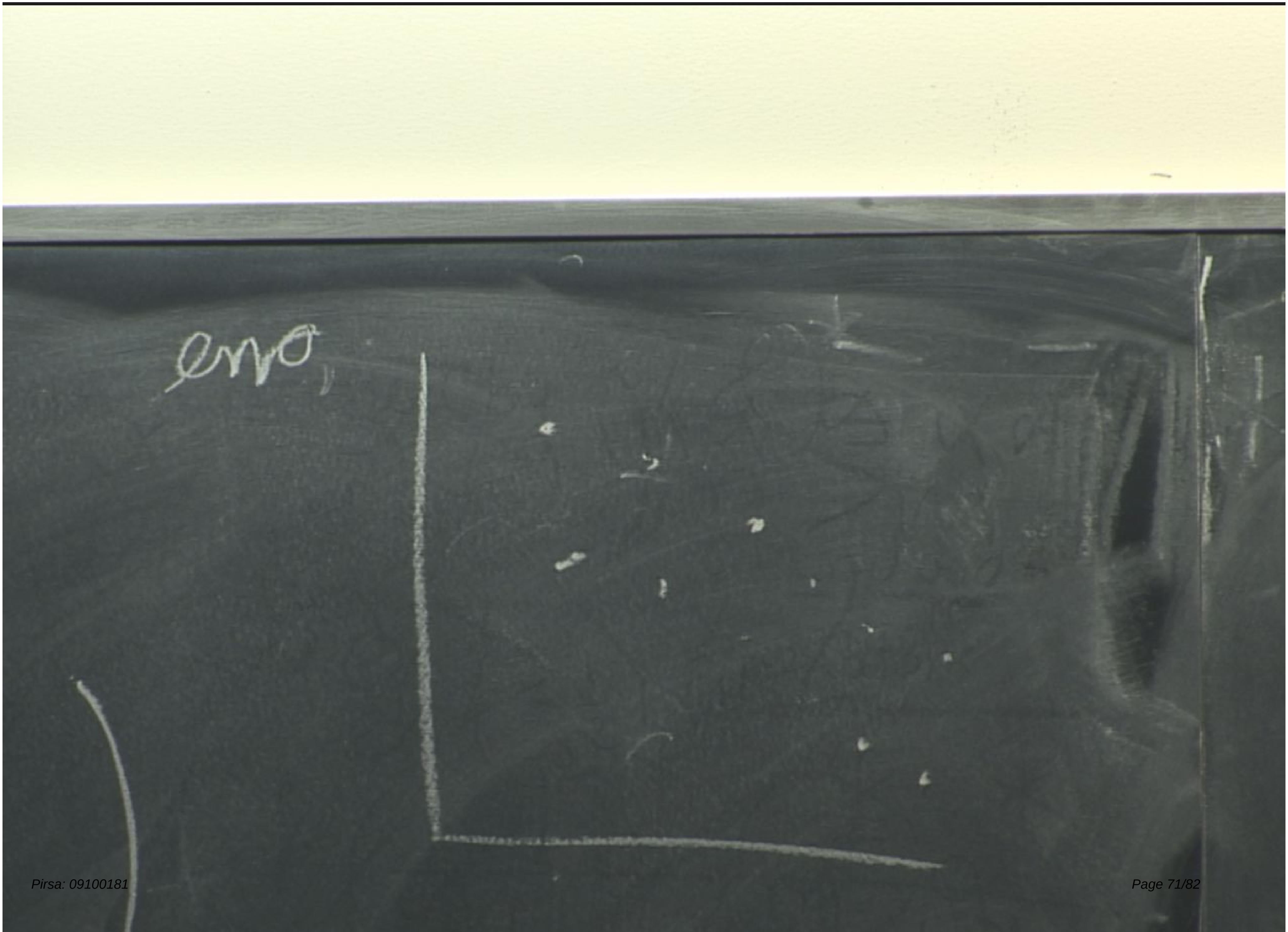
$$\sqrt{2} = 1 + (\sqrt{2} - 1)$$

$$= 1 + \frac{(\sqrt{2}-1)(\sqrt{2}+1)}{\sqrt{2}+1}$$

$$= 1 + \frac{1}{2 + (\sqrt{2} - 1)}$$

$$\left.= 1 + \cfrac{1}{2 + \cfrac{1}{2 + \cfrac{1}{2 + \cfrac{1}{2 + \cdots}}}}\right\}$$

continued fraction



How to evaluate

$$f(x) = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3}}}$$

How to evaluate

$$f(x) = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3}}}$$

We truncate

How to evaluate

$$f(x) = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3}}} \ldots$$

We truncate

$$f(x) = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2}} = \frac{b_0 b_1 b_2 + a_2 b_0 + a_1 b_2}{b_1 b_2 + a_2}$$

How to evaluate

$$f(x) = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3 \cdots}}}$$

We truncate

$$f(x) = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2}} = \frac{b_0 b_1 b_2 + a_2 b_0 + a_1 b_2}{b_1 b_2 + a_2}$$

$$= \frac{A_2}{B_2}$$

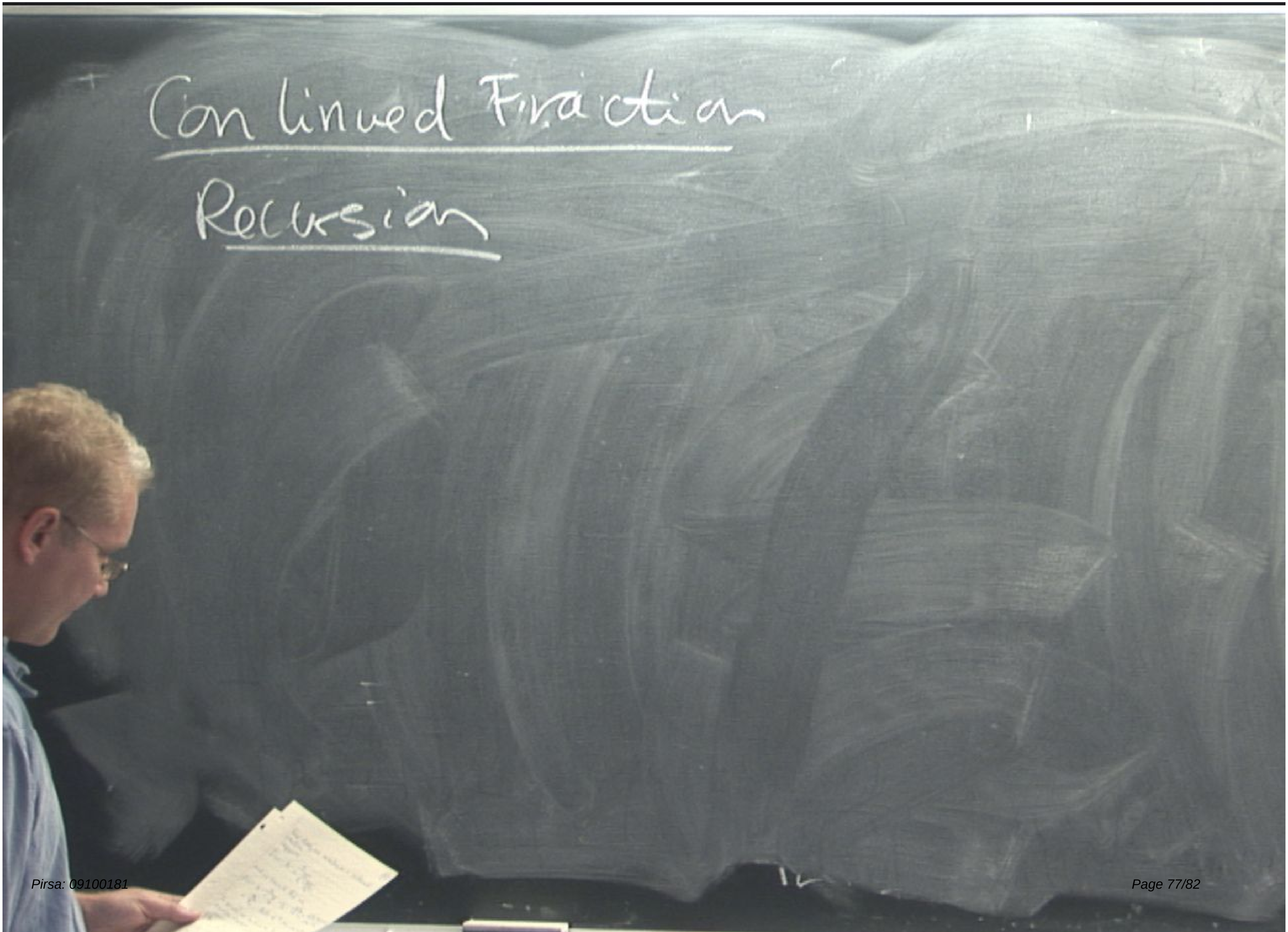
How to evaluate

$$f(x) = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3}}}$$

We truncate

$$f(x) = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2}} = \frac{b_0 b_1 b_2 + a_2 b_0 + a_1 b_2}{b_1 b_2 + a_2}$$

$$= \frac{A_2}{B_2} = \text{rational polynom}$$


Continued Fraction
Recursion

Continued Fraction

Recursion

$$A_{-1} = 1 \quad B_{-1} = 0$$

$$A_0 = b_0 \quad B_0 = 1$$

$$A_j$$

Continued Fraction

Recursion

$$A_{-1} = 1 \qquad B_{-1} = 0$$

$$A_0 = b_0 \qquad B_0 = 1$$

$$A_j = b_j A_{j-1} + a_j A_{j-2}$$

$$B_j = b_j B_{j-1} + a_j B_{j-2}$$

Continued Fraction

Recursion

$$\boxed{\begin{aligned} &A_{-1} = 1 \qquad B_{-1} = 0 \\ &A_0 = b_0 \qquad B_0 = 1 \\ &A_j = b_j A_{j-1} + a_j A_{j-2} \\ &B_j = b_j B_{j-1} + a_j B_{j-2} \end{aligned}}$$

Continued Fraction

Recursion

$$\boxed{\begin{aligned} &A_{-1} = 1 \quad B_{-1} = 0 \\ &A_0 = b_0 \quad B_0 = 1 \\ &A_j = b_j A_{j-1} + a_j A_{j-2} \\ &B_j = b_j B_{j-1} + a_j B_{j-2} \end{aligned}}$$

Check $A_2 = b_2 A_1 + a_2 A_0 = b_2(b_1 b_0 + a_1) + ($

$B_2 = b_2 B_1 + a_2 B_0 = b_2 b_1 + a_2$

Continued Fraction

Recursion

$$\boxed{\begin{aligned} A_{-1} &= 1 & B_{-1} &= 0 \\ A_0 &= b_0 & B_0 &= 1 \\ A_j &= b_j A_{j-1} + a_j A_{j-2} \\ B_j &= b_j B_{j-1} + a_j B_{j-2} \end{aligned}}$$

Check

$$A_2 = b_2 A_1 + a_2 A_0 = b_2(b_1 b_0 + a_1) + a_2 b_0$$

$$B_2 = b_2 B_1 + a_2 B_0 = b_2 b_1 + a_2$$