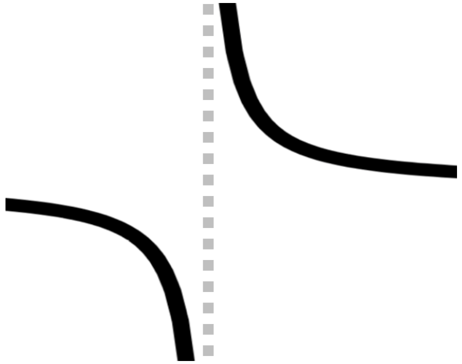
Semantics of Integrating and Differentiating Singularities

Jesse Michel, Wonyeol Lee, Hongseok Yang

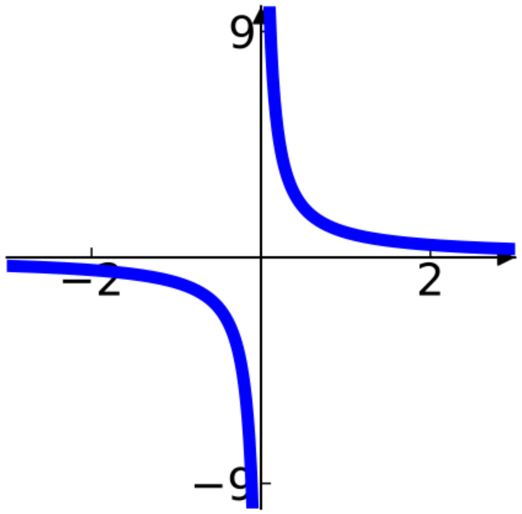
$$\frac{d}{ds}\int_a^b$$



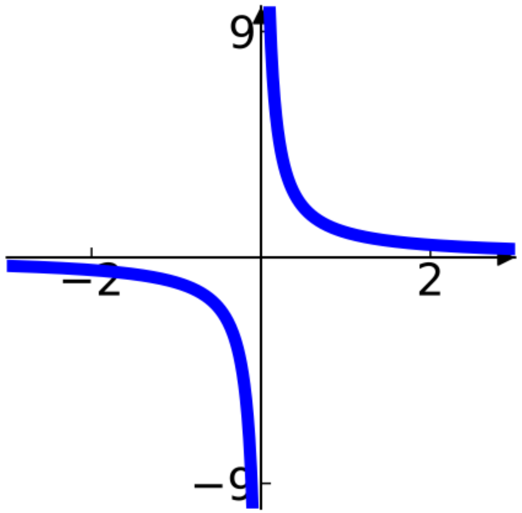
s

Singular Function

```
1/x
```



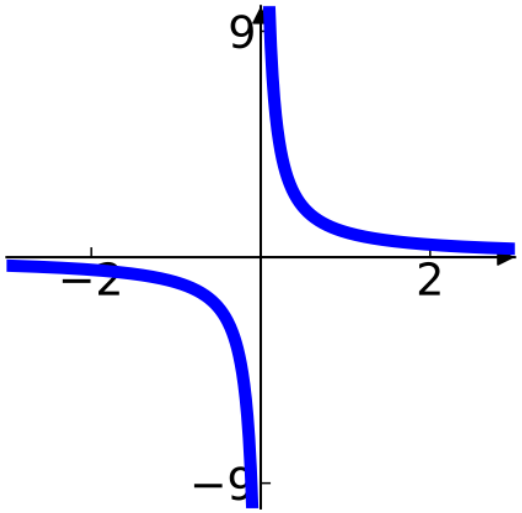
Singular Function




```
1/x
```

What happens at $x = 0$?

Singular Function

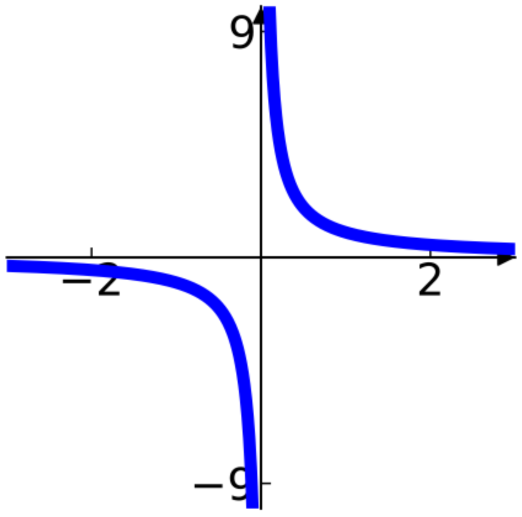



```
1/x
```

What happens at $x = 0$?

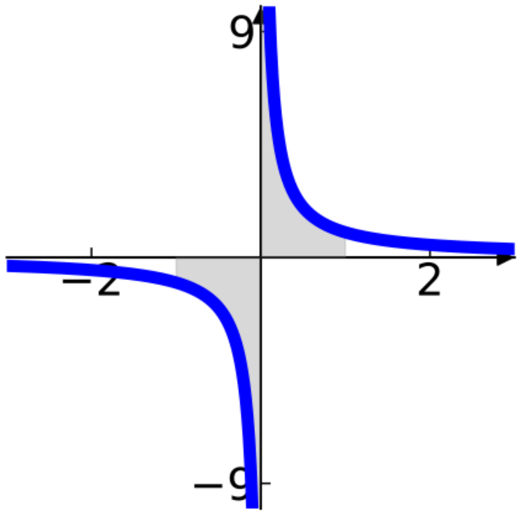
DivideByZeroError

Singular Function



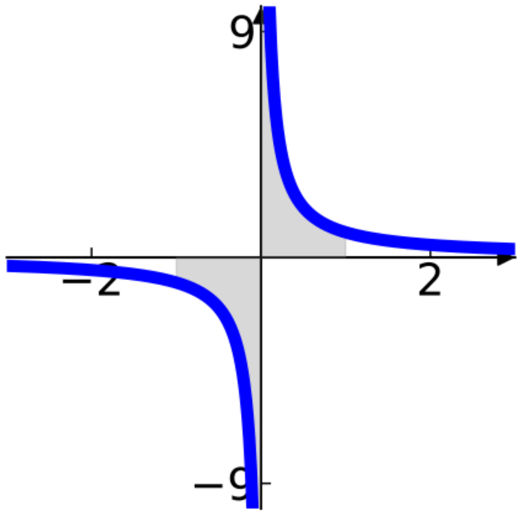
A *singular function* is a partial function such that at one or more points, the left and/or right limit diverge.

Integral of a Singular Function




```
integral (-1,1) 1/x dx
```

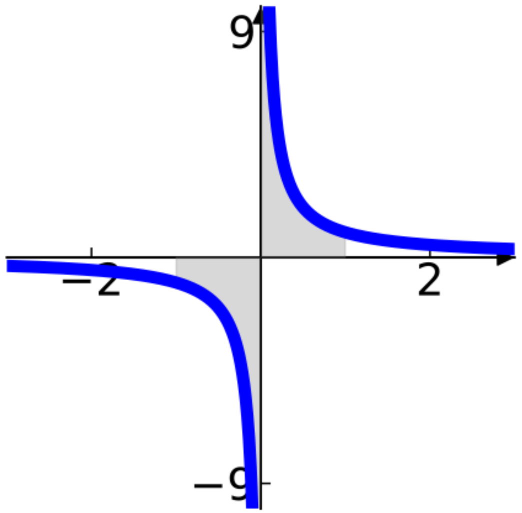
Integral of a Singular Function



integral (-1,1) 1/x dx

Is the integral, $\int_{-1}^{1} \frac{1}{x}\, dx$, well-defined?

Integral of a Singular Function

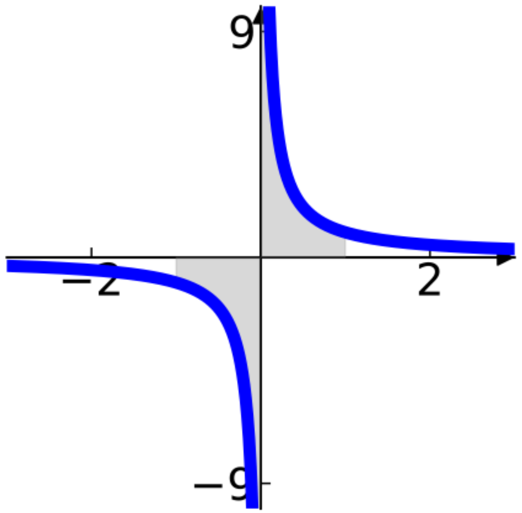



```
integral (-1,1) 1/x dx
```

Is the integral, $\int_{-1}^{1} \frac{1}{x}\,dx$, well-defined?

No!

Integral of a Singular Function



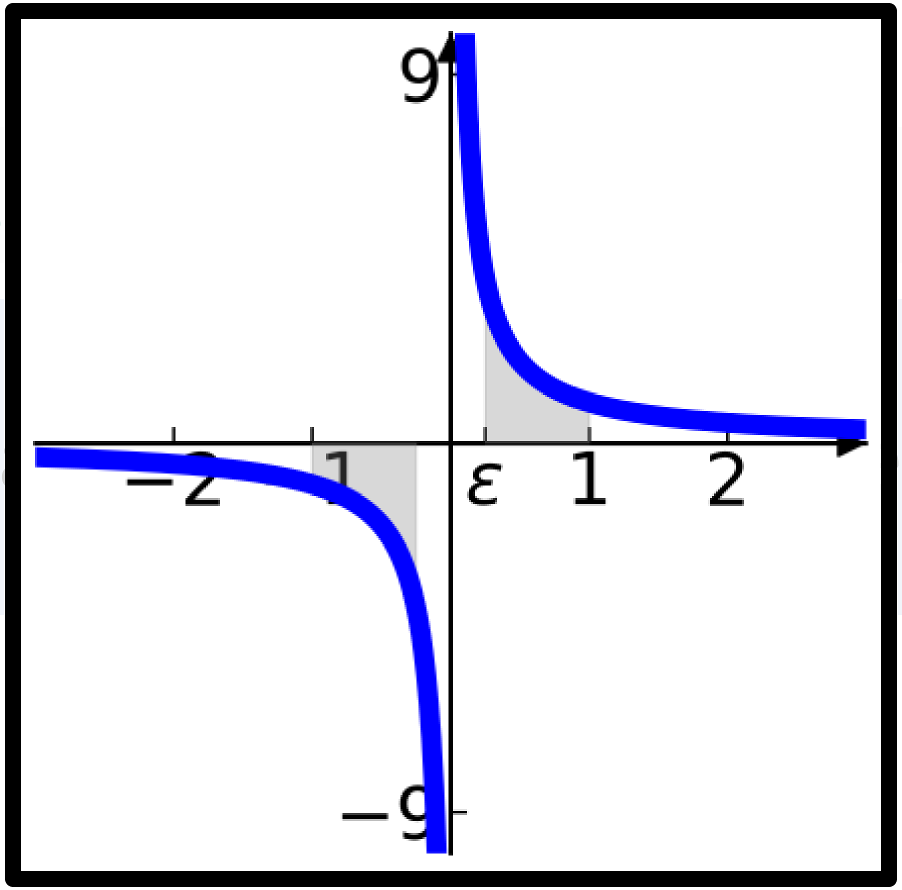

```
integral (-1,1) 1/x dx
```

Can we make a version that is well-defined?

Integral of a Singular Function

integral (-1,1) 1

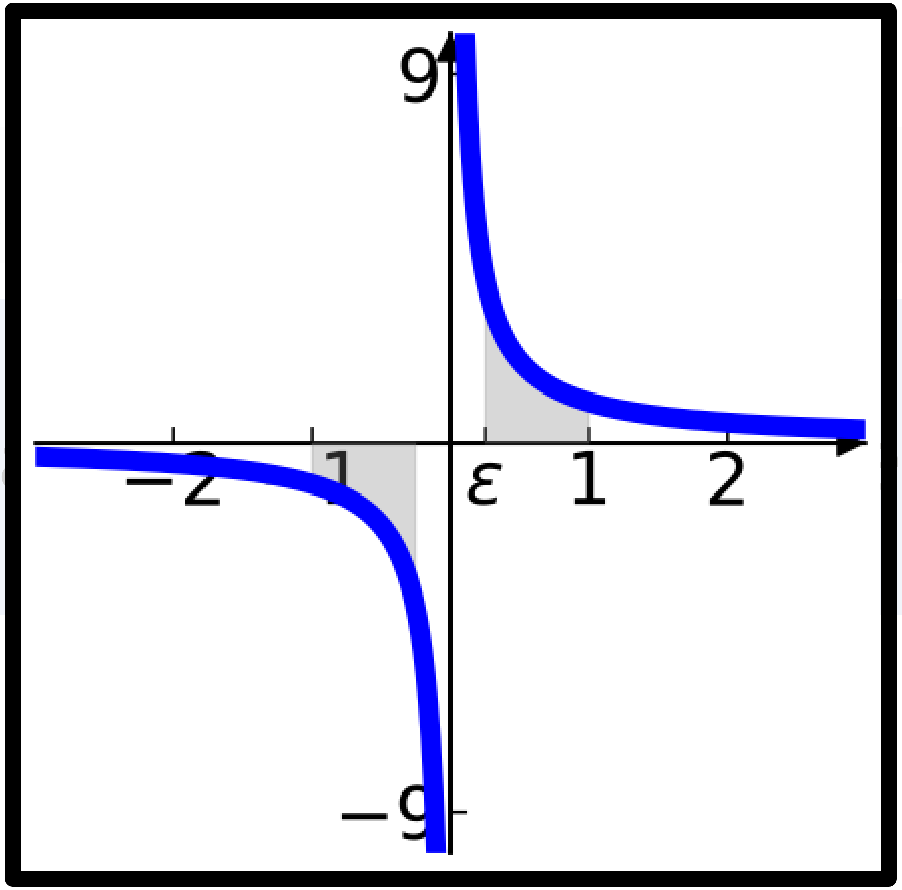
Can we m ll-defined?



Integral of a Singular Function

integral (-1,1) 1

$$\lim_{\epsilon\to 0^+}$$



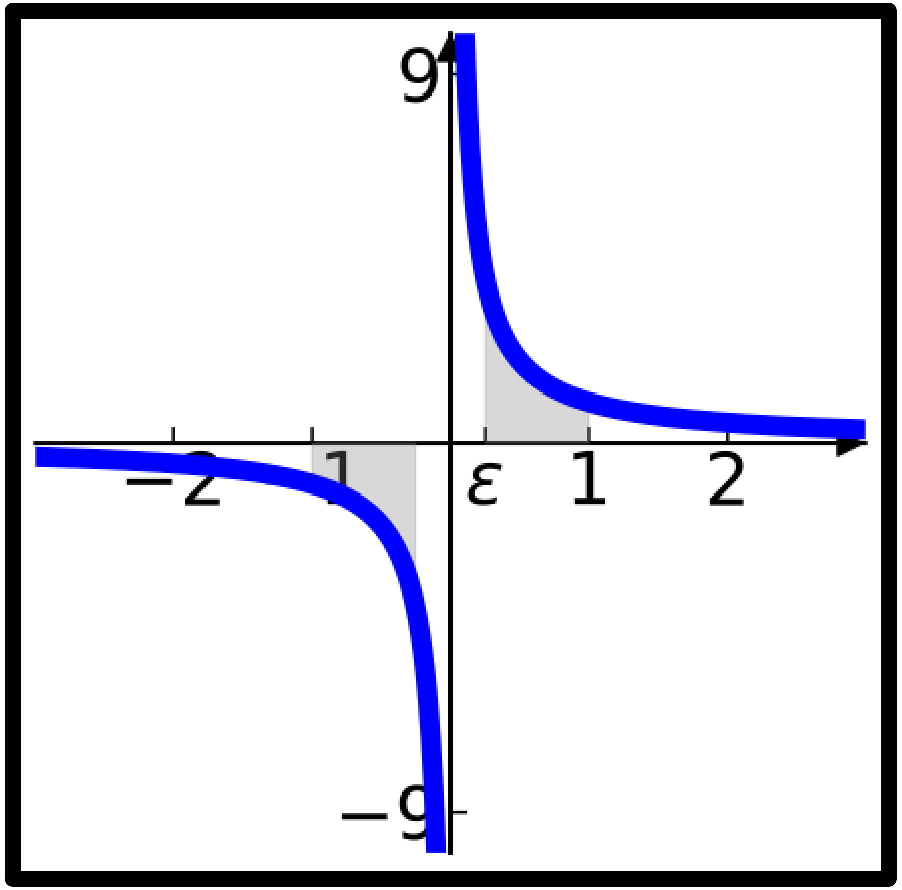
ll-define

Yes!

$$\mathcal{C}\int_{-1}^{1}\frac{1}{x}dx := \lim_{\epsilon\to 0^+}\int_{-1}^{-\epsilon}\frac{1}{x}dx + \int_{\epsilon}^{1}\frac{1}{x}dx = 0$$

Singular Integral

$$\lim_{\epsilon\to 0^+}$$

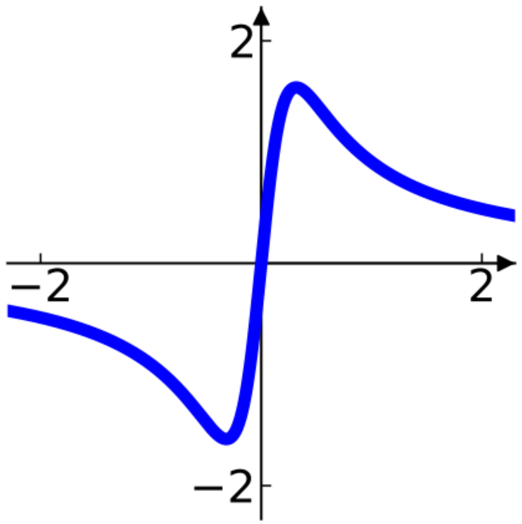


$$\mathcal{C}\int_{-1}^{1}\frac{1}{x}dx := \lim_{\epsilon\to 0^+}\int_{-1}^{-\epsilon}\frac{1}{x}dx + \int_{\epsilon}^{1}\frac{1}{x}dx = 0$$

Automatic Differentiation (AD)

$y = x^2+0.1;$

$z = x/y$



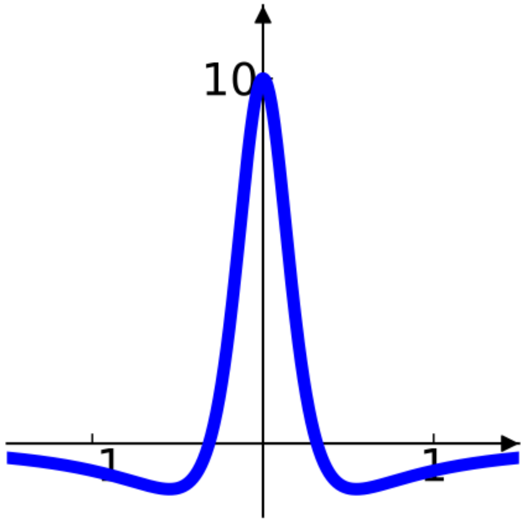
$$\frac{d}{dx}$$

$y = x^2+0.1$

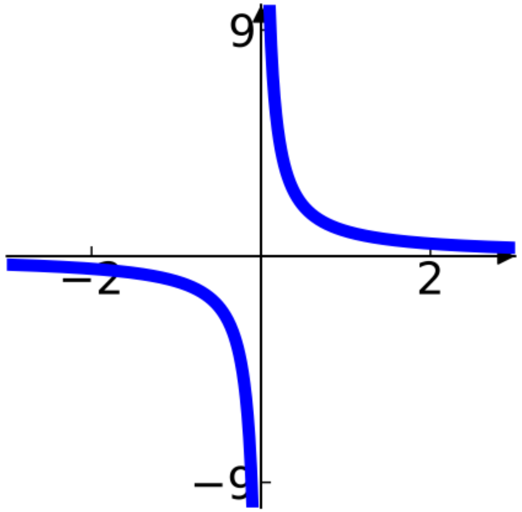
$dy = 2\cdot x$

$z = x/y$

$dz = (y - x\cdot dy)/y^2$



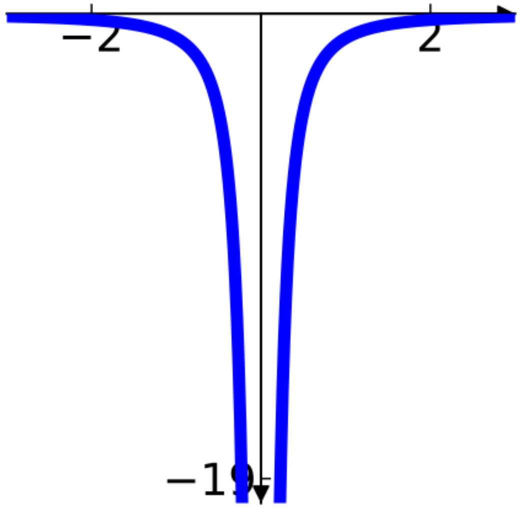
Standard AD of a Singular Function



1/x

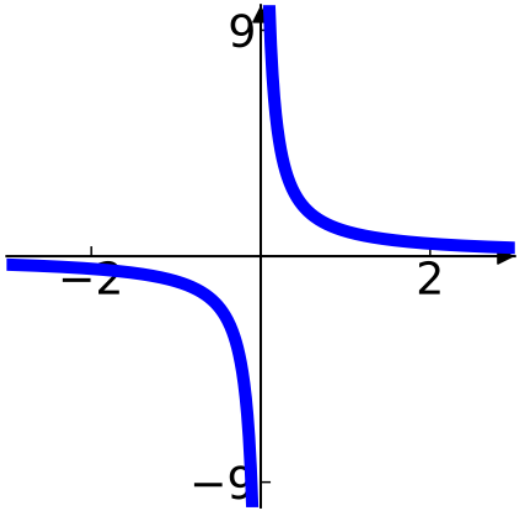
$\frac{d}{dt}$

$\frac{d}{dx}$



-1/x²

Standard AD of a Singular Function



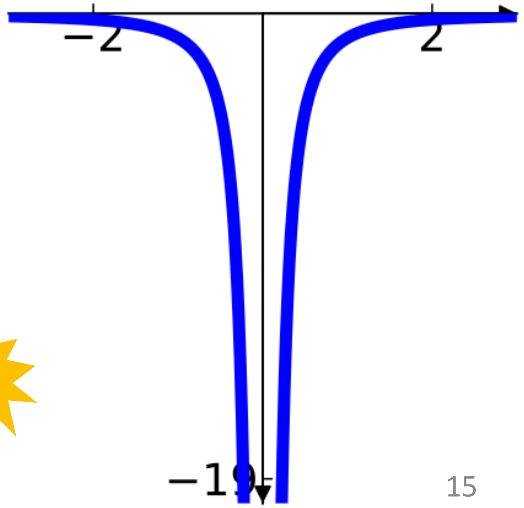

```
1/x
```

DivideByZeroError

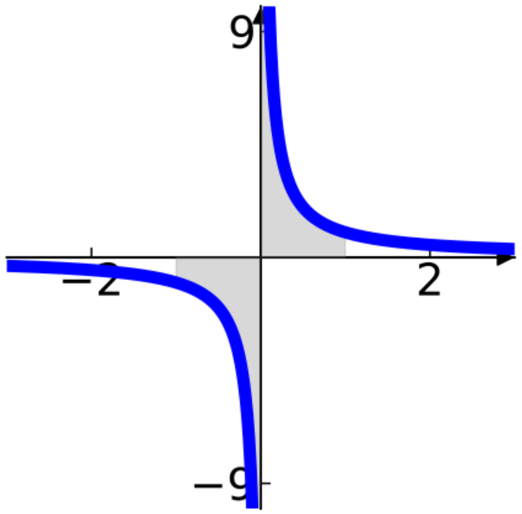
dx

```
-1/x²
```

DivideByZeroError



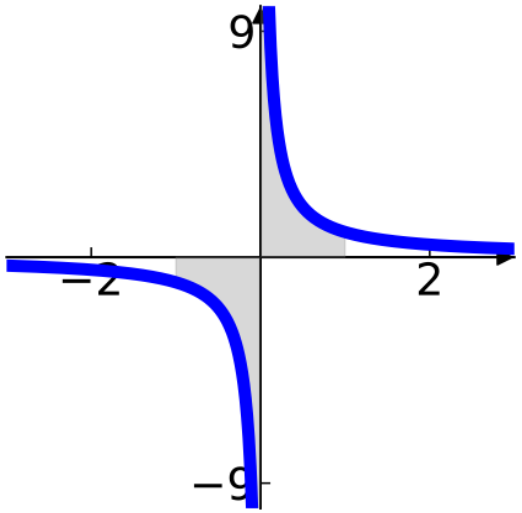
AD of a Singular Integral




```
integral (-1,1) 1/(x-s) dx
```

$$\frac{d}{ds}$$

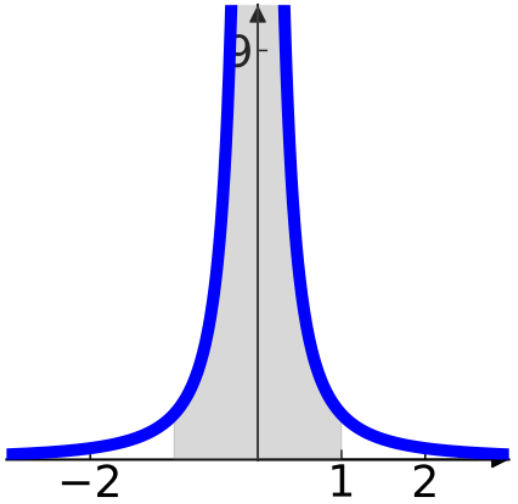
AD of a Singular Integral



integral (-1,1) 1/(x-s) dx

$$\frac{d}{ds}$$

integral (-1,1) 1/(x-s)^2 dx

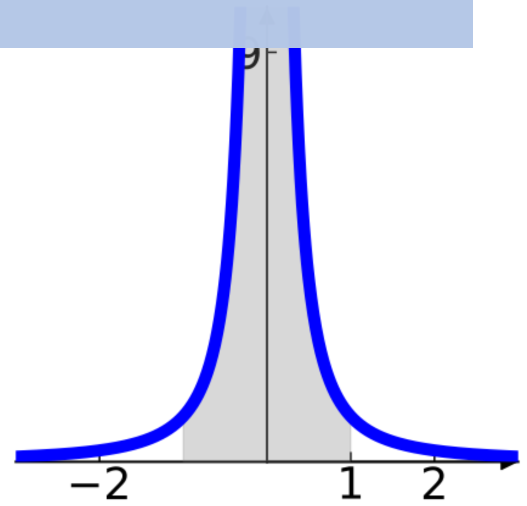


AD of a Singular Integral

integral (-1,1) 1/(x-s) dx

Is this well-defined?

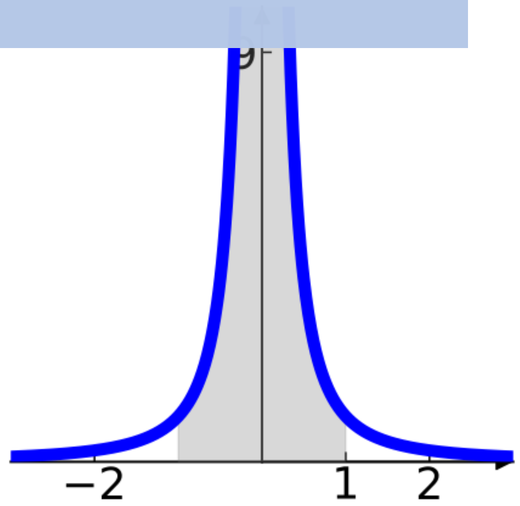
integral (-1,1) 1/(x-s)^2 dx



AD of a Singular Integral

integral (-1,1) 1/(x-s) dx

Is this well-defined?



integral (-1,1) $1/(x\text{-}s)^2$ dx

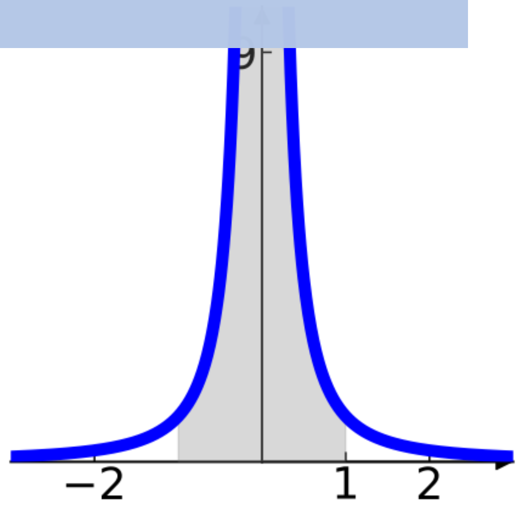
No!

AD of a Singular Integral

integral (-1,1) 1/(x-s) dx

Can we make a version that is well defined?

integral (-1,1) 1/(x-s)^2 dx



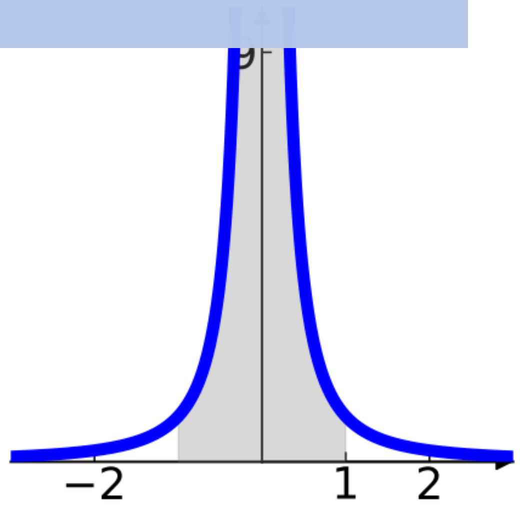
AD of a Singular Integral

Yes!

integral (-1,1) 1/(x-s) dx

Can we make a version that is well defined?

integral (-1,1) 1/(x-s)^2 dx



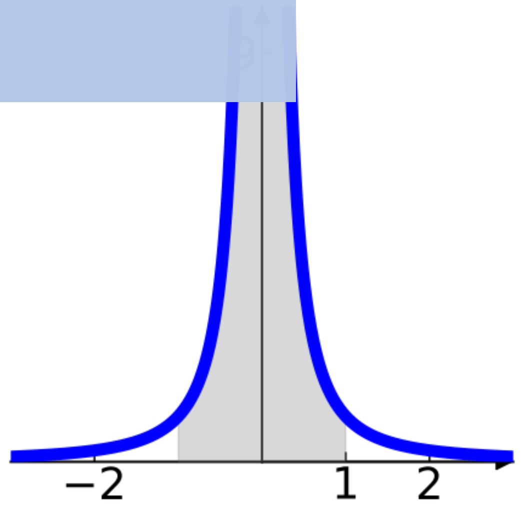
$$\mathcal{H}\int_{-1}^{1}\frac{1}{(u-s)^2}\,du=\lim_{\epsilon\to 0^+}\int_{-1}^{s-\epsilon}\frac{1}{u-s}du+\int_{s+\epsilon}^{1}\frac{1}{u-s}du-\frac{2}{\epsilon}$$

AD of a Singular Integral

integral (-1,1) 1/(x-s) dx

$$\frac{d}{ds}\mathcal{C}\int_{-1}^{1}\frac{1}{x-s}dx \neq \mathcal{C}\int_{-1}^{1}\frac{1}{(x-s)^2}dx$$

integral (-1,1) 1/(x-s)^2 dx

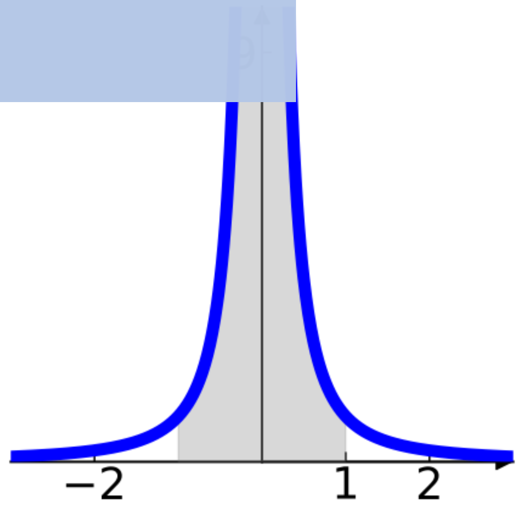


AD of a Singular Integral

integral (-1,1) 1/(x-s) dx

$$\frac{d}{ds}\mathcal{C}\int_{-1}^{1}\frac{1}{x-s}\,dx = \mathcal{H}\int_{-1}^{1}\frac{1}{(x-s)^2}\,dx$$

integral (-1,1) 1/(x-s)^2 dx



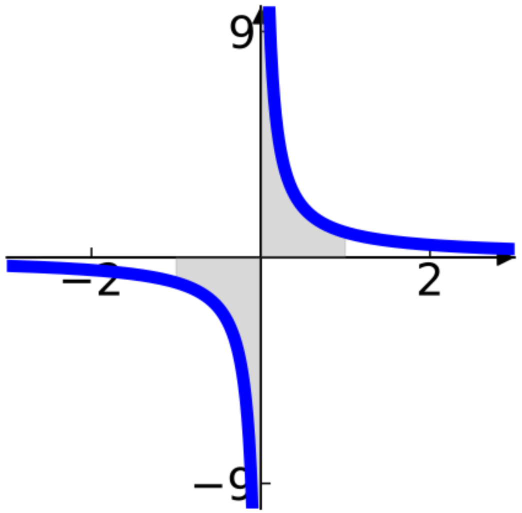
Distribution Theory: Intuition

$$f_n(x) = \frac{x}{x^2+1/n} \quad \dashrightarrow \quad \mathcal{S}\,\frac{1}{x}$$

Informally, a *distribution* is a generalized function, closed under limits and generalized derivatives.

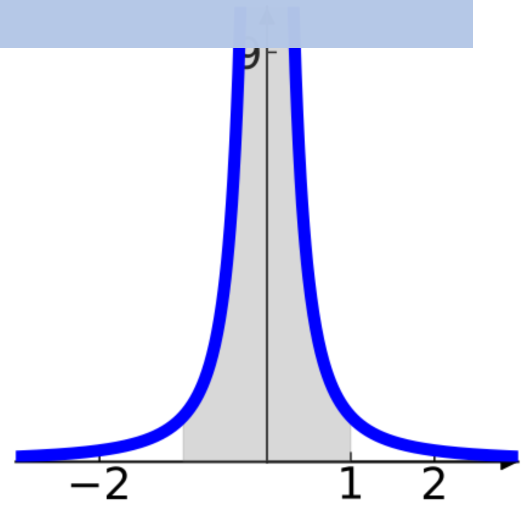
$$\frac{\mathrm{d}}{dx} f_n(x) = \frac{-x^2+1/n}{(x^2+1/n)^2} \quad \dashrightarrow \quad -\mathcal{S}\,\frac{1}{x^2}$$

AD of a Singular Integral



integral (-1,1) 1/(x-s) dx

Why does this matter?

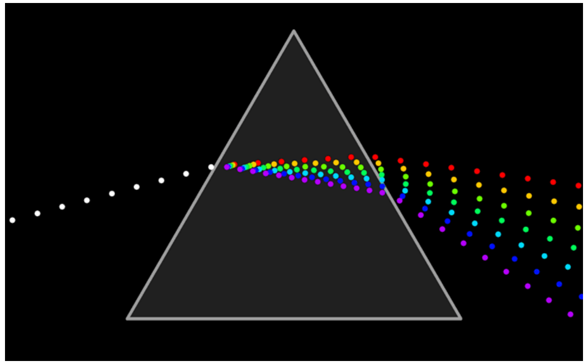


integral (-1,1) 1/(x-s)^2 dx

Singular Integrals in The Wild

Signal Processing

Hilbert Transform



Aerodynamics

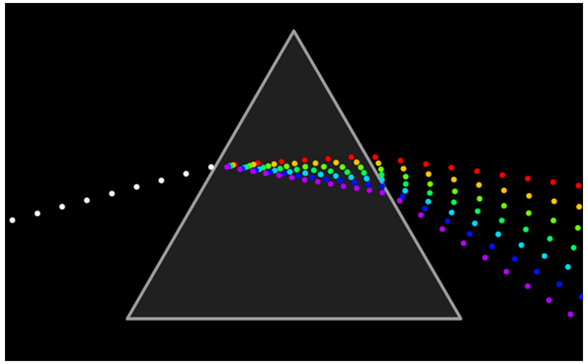
Airfoil Equation

Mechanical Engineering

Crack Problems

Singular Integrals in The Wild

Signal Processing
Hilbert Transform



Aerodynamics
Airfoil Equation

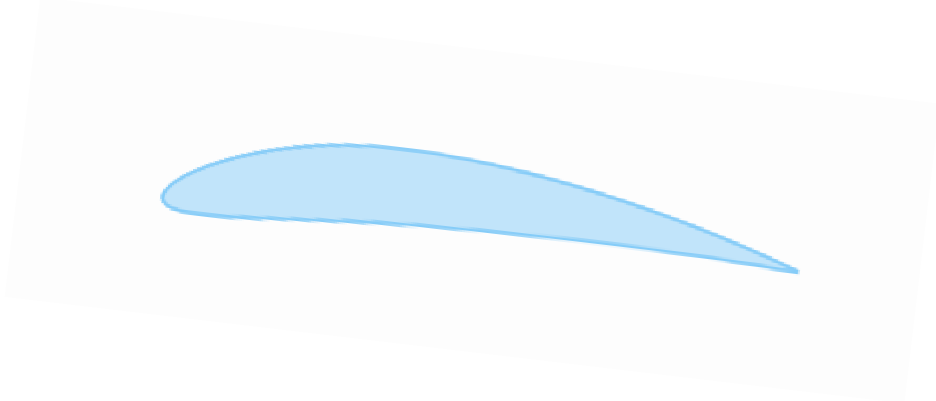
Mechanical Engineering
Crack Problems

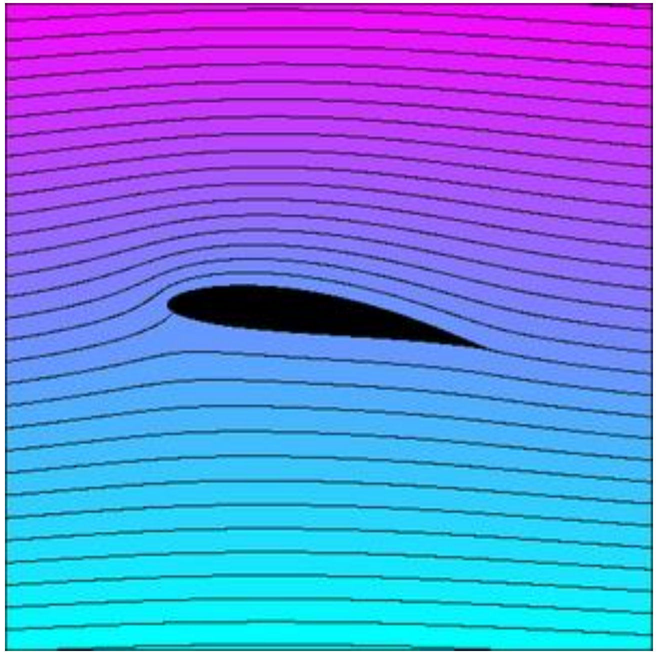
Parameters θ

$$\frac{d}{d\theta}$$

$\mathcal{L}$(Output, Target)

Aerodynamics: Airfoil Equation

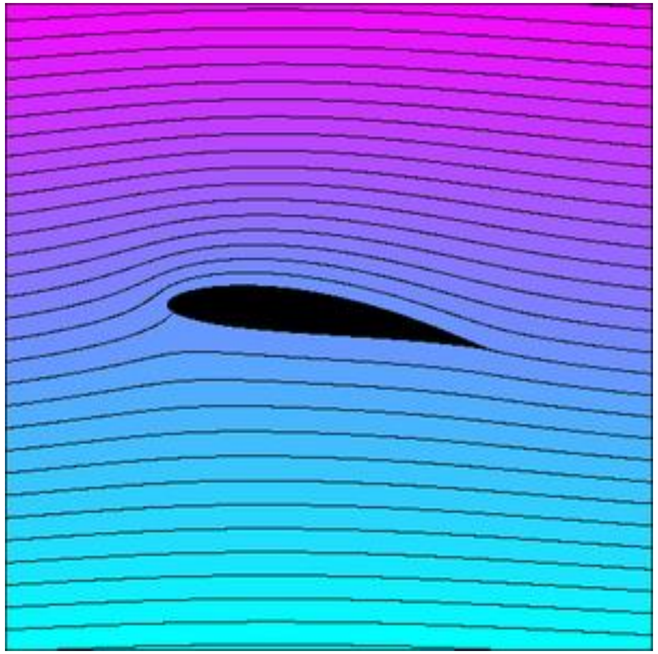




Goal: calculate the circulation density, γ

Aerodynamics: Airfoil Equation

$$-\frac{1}{2\pi}\,\mathcal{C}\int_0^c \frac{\gamma(u)}{u\ -u_0}\,du = \alpha(u_0)V_\infty \qquad \text{for } u_0 \in (0, c)$$



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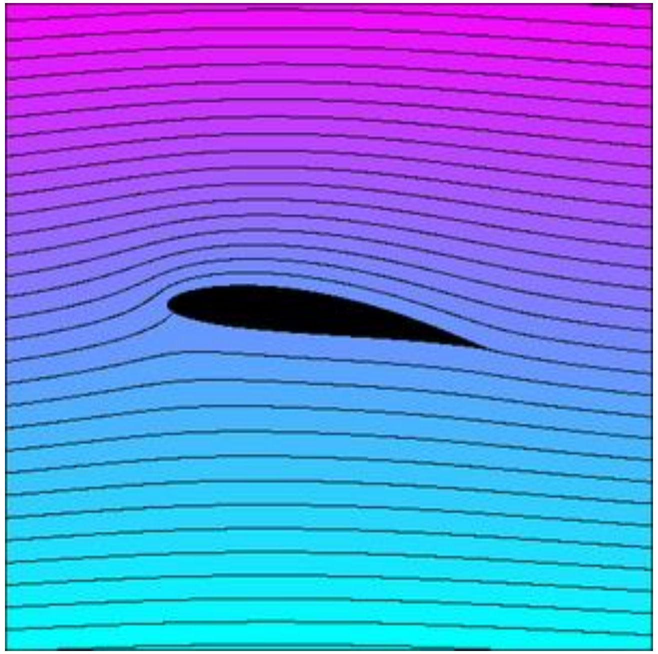


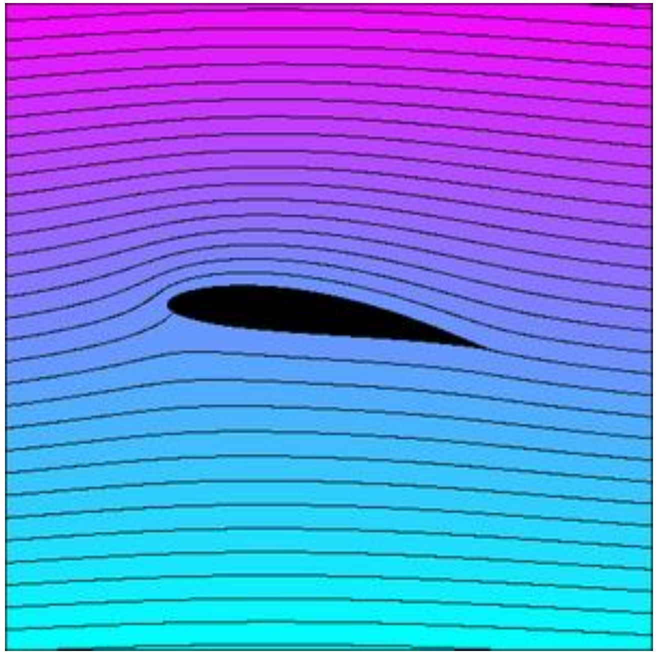
PINN: Approximate γ with a NN, $\tilde{\gamma}_\theta$

(Rassi et. al., 2021)

Goal: calculate the circulation density, γ

Aerodynamics: Airfoil Equation

$$-\frac{1}{2\pi}\,\mathcal{C}\int_0^c \frac{\gamma(u)}{u - u_0}\,du = \alpha(u_0)V_\infty \qquad \text{for } u_0 \in (0, c)$$



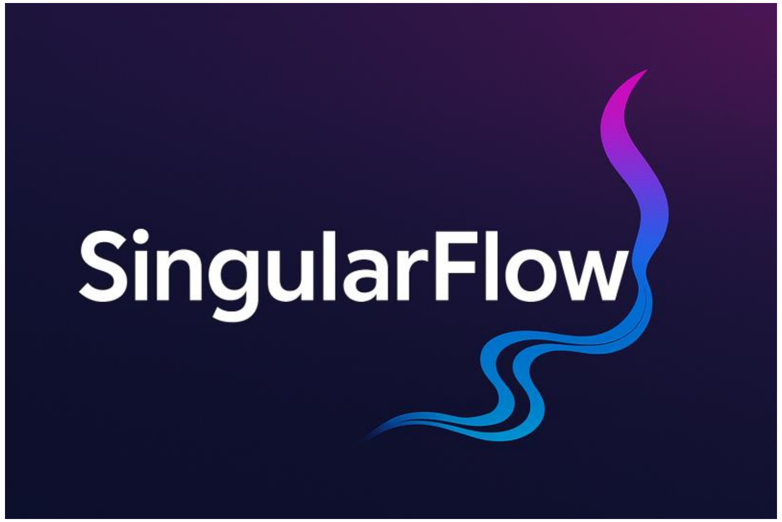
PINN: Approximate γ with a NN, $\tilde{\gamma}_\theta$

(Rassi et. al., 2021)

$$\min_\theta \sum_{i=0}^{n}\left(-\frac{1}{2\pi}\,\mathcal{C}\int_0^c \frac{\tilde{\gamma}_\theta(u)}{u - u_0^{(i)}}\,du - \alpha\left(u_0^{(i)}\right)V_\infty\right)^2$$

Goal: calculate the circulation density, γ

Story



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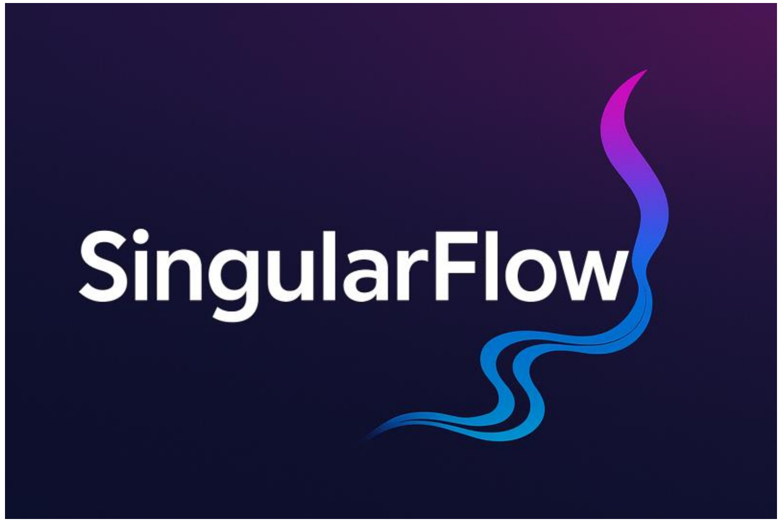
Contributions

- Identify a new problem domain
- Rigorous, accessible math formalism
- First semantics of a differentiable PL with singular integration
- Solve problems in science and engineering



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Aerodynamics: Airfoil Equation

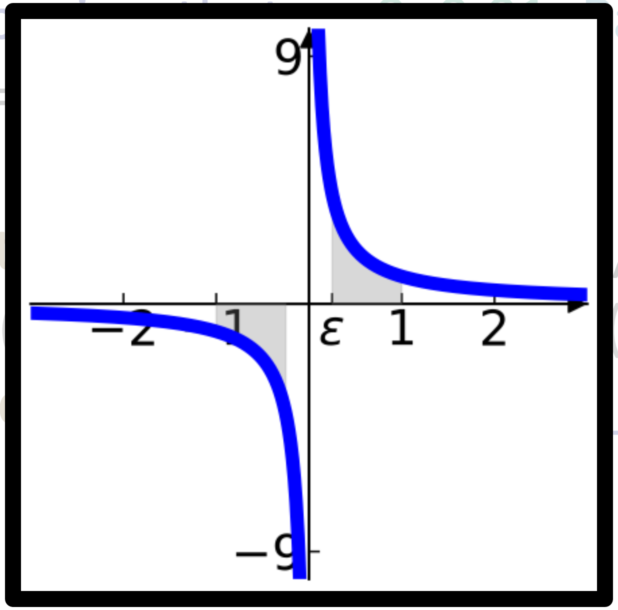
$$\min_{\theta} \sum_{i=0}^{n} \left(-\frac{1}{2\pi} \, \mathcal{C} \int_0^c \frac{\tilde{\gamma}_\theta(u)}{u \; - u_0^{(i)}} \, du - \alpha\left(u_0^{(i)}\right) V_\infty \right)^2$$

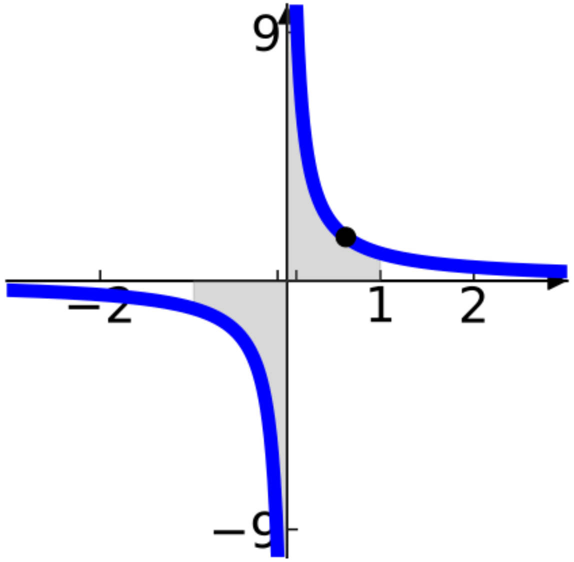
```
loss, step_size, theta = 0, 0.01, Param("theta", init())
c, V_inf = 1, 1
for uo in uos:
  est = integral (0,c) (nn(theta, u)/(u-uo)) du
  loss += (-1/(2 * pi) * est - alpha(uo) * Vinf)^2
theta -= deriv(loss, theta) * step_size
```

Aerodynamics: Airfoil Equation

How do we run the integral?

$$\lim_{\epsilon \to 0^+}$$





Aerodynamics: Airfoil Equation

How do we run the integral?

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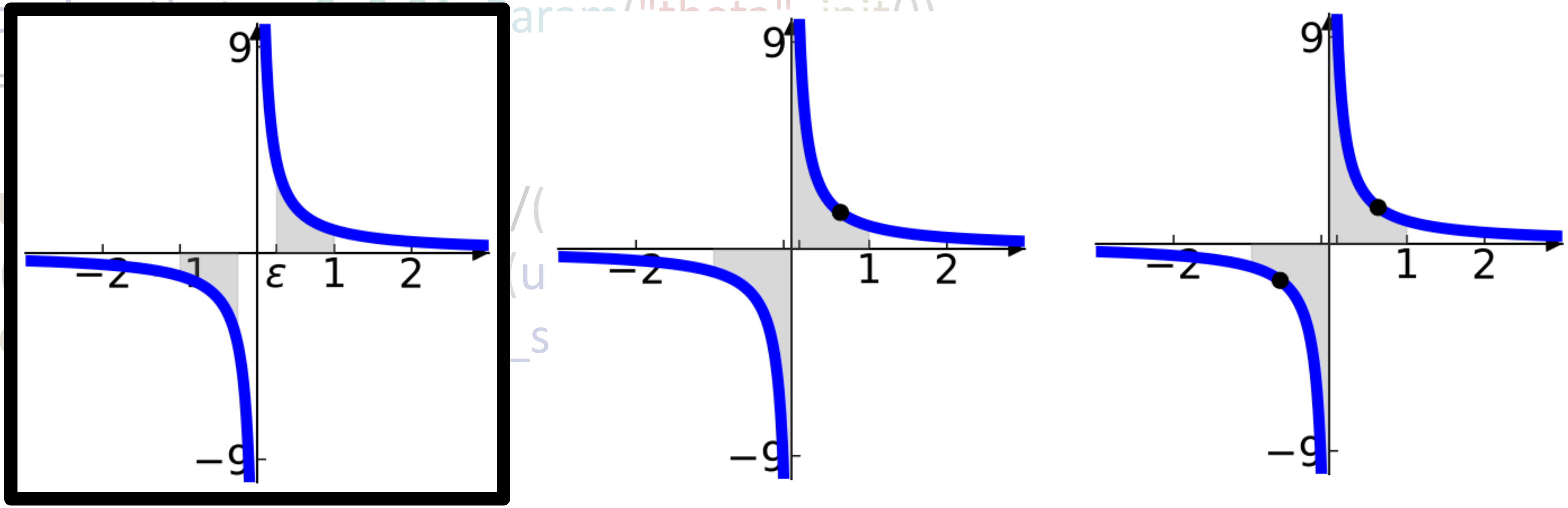
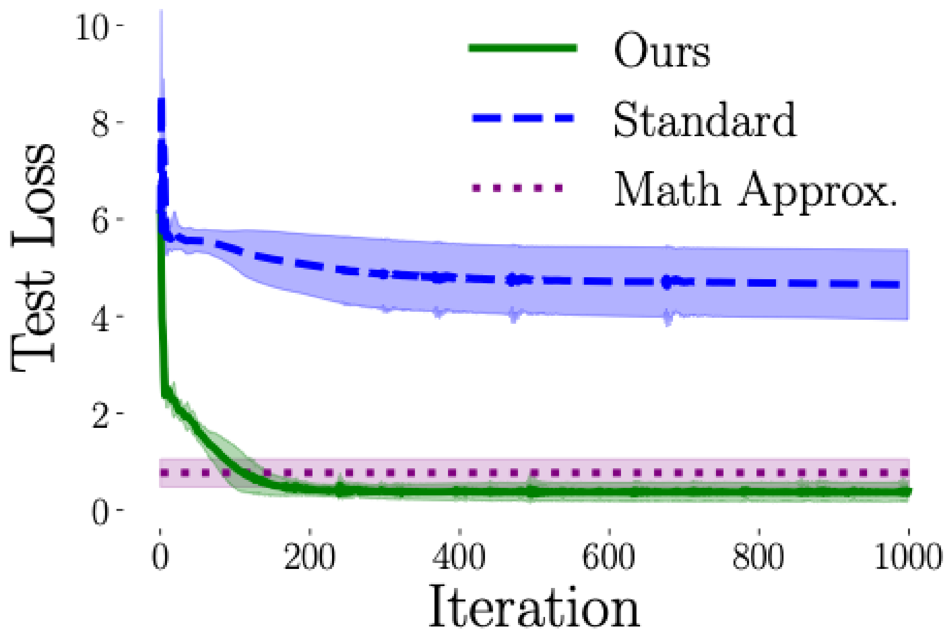


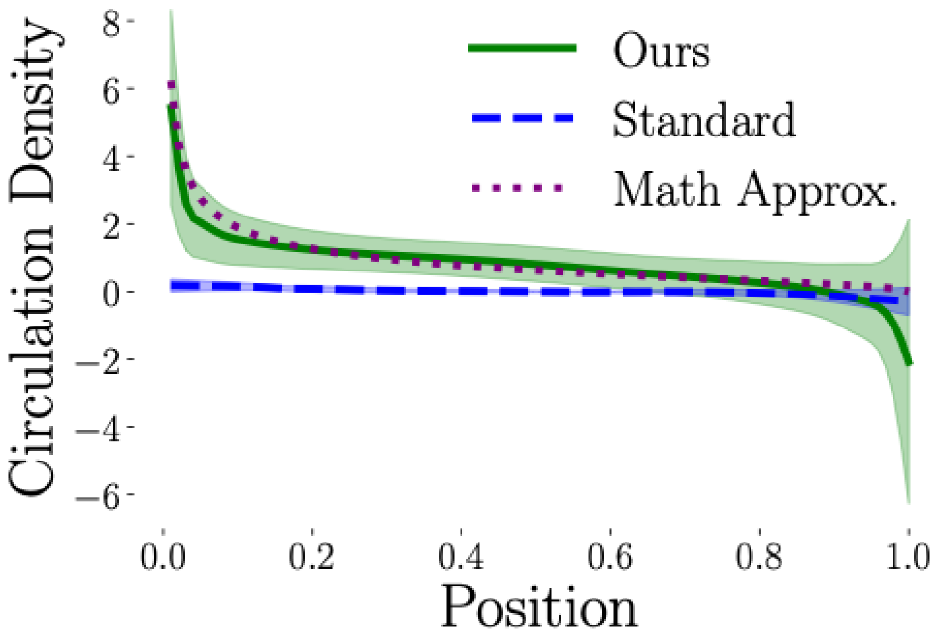
Aerodynamics: Airfoil Equation

What happens when we run the code?

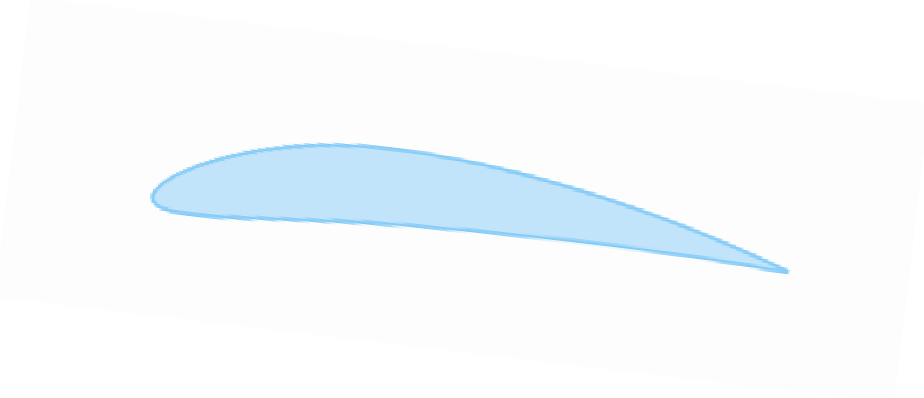
```
loss, step_size, theta = 0, 0.01, Param("theta", init())
c, V_inf = 1, 1
for uo in uos:
  est = integral (0,c) (nn(theta, u)/(u-uo)) du
  loss += (-1/(2 * pi) * est - alpha(uo) * Vinf)^2
theta -= deriv(loss, theta) * step_size
```

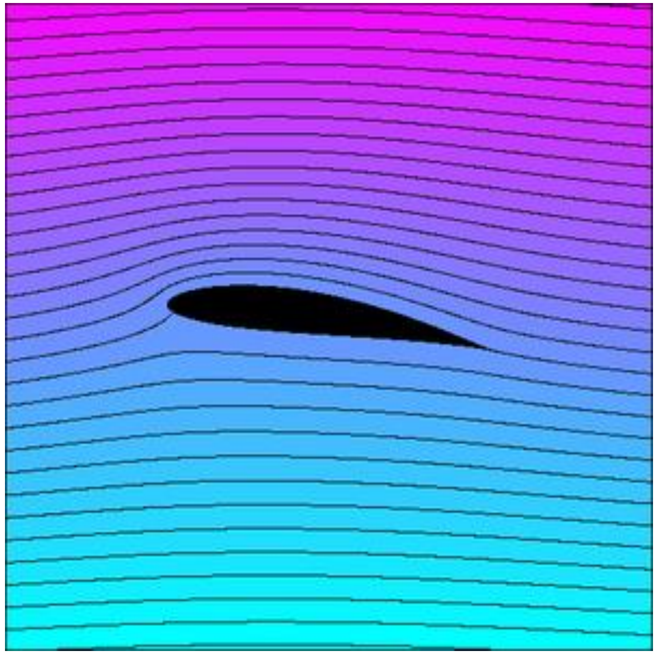
Aerodynamics: Airfoil Equation





Aerodynamics: Airfoil Equation

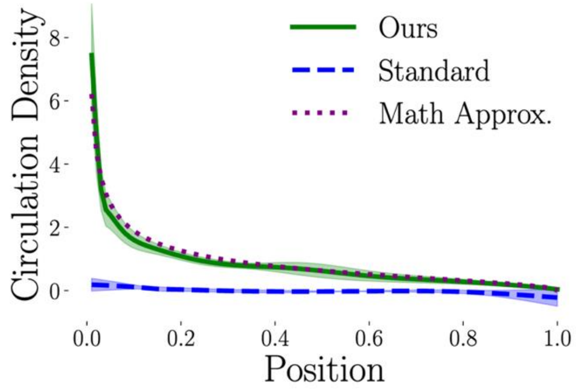




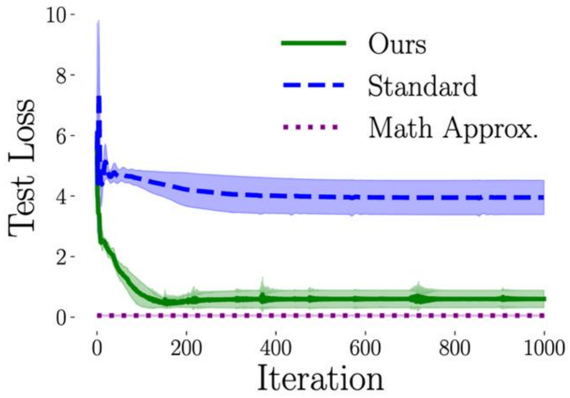
Solution: find NN params that minimize loss

Goal: calculate the circulation density, γ

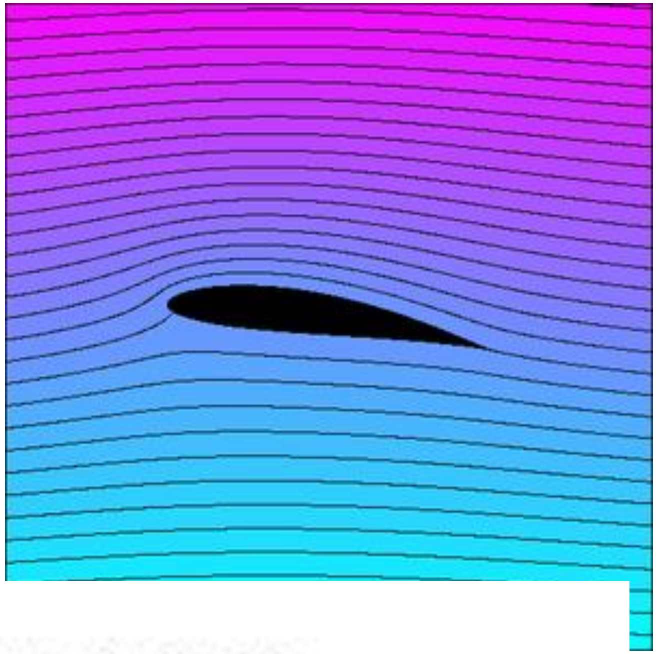
Aerodynamics: Airfoil Equation



$$-\frac{1}{2\pi}\,\mathcal{C}\int_0^c \frac{\gamma(u)}{u\ - u_0}\,du = \alpha(u_0)V_\infty$$



Aerodynamics: Airfoil Equation



AIRFOIL OPTIMIZATION BY THE METHOD OF INVERSE BOUNDARY-VALUE PROBLEMS*

A.M. ELIZAROV and E.V. FEDOROV

Goal: calculate the circulation density, γ

A Simple, Smooth Language

Expressions e ::= c | x | $h(e, \ldots, e)$
Programs $p ::= x = e \mid y = \textbf{integral}\ (a, b)\ e/(x-s)^k\ \mathbf{d}x$ | p;p

Expressions Denote Smooth Functions

Expressions $e ::= c \mid x \mid h(e, \ldots, e)$

Programs $p ::= x = e \mid y = \textbf{integral}\,(a, b)\; e/(x - s)^k\, \mathbf{d}x \mid$ p;p

Denotation $[\![e]\!]$ is a smooth map from $[\![\Gamma]\!]$ to $\mathbb{R}$

where Γ is a context and $[\![\Gamma]\!] \cong \mathbb{R}^{|\mathrm{dom}(\Gamma)|}$.

Programs are Smooth Maps

Expressions $e ::= c \;|\; x \;|\; h(e, \ldots, e)$

Programs $p ::= x = e \;|\; y = \textbf{integral}\,(a, b)\; e/(x - s)^k\, \mathbf{d}x \;|\;$ p;p

Denotation $[\![p]\!]$ is a smooth map from contexts $\mathrm{C}tx$ to contexts $\mathrm{C}tx$

$$[\![x = e]\!](\gamma) \quad = \gamma\,[x \mapsto [\![e]\!](\gamma)]$$

Programs are Smooth Maps

Expressions $e ::= c \mid x \mid h(e, \ldots, e)$

Programs $p ::= x = e \mid y = \textbf{integral}\ (a, b)\ e/(x-s)^k\ \mathbf{d}x \mid$ p;p

Denotation $[\![p]\!]$ is a smooth map from contexts Ctx to contexts Ctx

$$[\![x = e]\!](\gamma) \quad = \gamma\ [x \mapsto [\![e]\!](\gamma)]$$

$[\![\mathrm{y} = \textbf{integral}\ (a, b)\ e/(x-s)^k\ \mathbf{d}x]\!](\gamma) = \gamma\ [y \mapsto c]$, where $g(u) = [\![e]\!](\gamma[x \mapsto u])$

and $c = \begin{cases} \int_a^b \frac{g(u)}{(u-\gamma(s))^k} du & \text{if } \gamma(s) \in (-\infty, a) \cup (b, \infty) \\ \mathcal{C} \int_a^b \frac{g(u)}{u-\gamma(s)} du & \text{if } \gamma(s) \in (a, b) \text{ and } k = 1 \\ \mathcal{H} \int_a^b \frac{g(u)}{(u-\gamma(s))^k} du & \text{if } \gamma(s) \in (a, b) \text{ and } k > 1 \end{cases}$

Programs are Smooth Maps

Expr

Prog

Multiple notions of integral, where the integral of a smooth function is smooth

Denotation $[\![p]\!]$ is a smooth map from contexts Ctx to contexts Ctx

$$[\![x = e]\!](\gamma) \quad = \gamma\,[x \mapsto [\![e]\!](\gamma)]$$

$[\![\mathrm{y} = \textbf{integral}\ (a, b)\ e/(x - s)^k\ \mathbf{d}x]\!](\gamma) = \gamma\,[y \mapsto c]$, where $g(u) = [\![e]\!](\gamma[x \mapsto u])$

and
$$c = \begin{cases} \int_a^b \frac{g(u)}{(u - \gamma(s))^k} du & \text{if } \gamma(s) \in (-\infty, a) \cup (b, \infty) \\ \mathcal{C} \int_a^b \frac{g(u)}{u - \gamma(s)} du & \text{if } \gamma(s) \in (a, b) \text{ and } k = 1 \\ \mathcal{H} \int_a^b \frac{g(u)}{(u - \gamma(s))^k} du & \text{if } \gamma(s) \in (a, b) \text{ and } k > 1 \end{cases}$$

Programs are Smooth Maps

Multiple notions of integral, where the integral of a smooth function is smooth

Paper includes if-statements and finite loops

Expr…

Programs $p ::= x = e \mid y = \text{integral}\ (a, b)\ e/(x-s)^k\ \mathrm{d}x \mid p;p$

Denotation $[\![p]\!]$ is a smooth map from contexts Ctx to contexts Ctx

$$[\![x = e]\!](\gamma) \quad = \gamma\,[x \mapsto [\![e]\!](\gamma)]$$

$$[\![y = \text{integral}\ (a, b)\ e/(x-s)^k\ \mathrm{d}x]\!](\gamma) = \gamma\,[y \mapsto c], \text{ where } g(u) = [\![e]\!](\gamma[x \mapsto u])$$

$$\text{and } c = \begin{cases} \int_a^b \frac{g(u)}{(u-\gamma(s))^k} du & \text{if } \gamma(s) \in (-\infty, a) \cup (b, \infty) \\ \mathcal{C} \int_a^b \frac{g(u)}{u-\gamma(s)} du & \text{if } \gamma(s) \in (a, b) \text{ and } k = 1 \\ \mathcal{H} \int_a^b \frac{g(u)}{(u-\gamma(s))^k} du & \text{if } \gamma(s) \in (a, b) \text{ and } k > 1 \end{cases}$$

$$[\![p_1; p_2]\!](\gamma) = [\![p_1]\!]([\![p_2]\!](\gamma))$$

Denotational Semantics

Expressions $e ::= c \mid x \mid h(e, \ldots, e)$
Programs $p ::= x = e \mid y = \textbf{integral}\ (a, b)\ e/(x-s)^k\ \mathbf{d}x \mid$ p;p

Denotation $[\![p]\!]$ is a smooth map from contexts Ctx to contexts Ctx

$$[\![x = e]\!](\gamma) \quad = \gamma\ [x \mapsto [\![e]\!](\gamma)]$$

$[\![\mathrm{y} = \textbf{integral}\ (a, b)\ e/(x-s)^k\ \mathbf{d}x]\!](\gamma) = \gamma\ [y \mapsto c]$, where $g(u) = [\![e]\!](\gamma[x \mapsto u])$

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$[\![p_1; p_2]\!](\gamma) = [\![p_1]\!]([\![p_2]\!](\gamma))$

Operational Semantics

Expressions $e ::= c \mid x \mid h(e, \dots, e)$

Programs $p ::= x = e \mid y = \textbf{integral}\ (a, b)\ e/(x - s)^k\ \mathbf{d}x \mid$ p;p

$$\frac{(\gamma, e) \Downarrow c \quad \forall y \in \mathrm{FV}(e).\ (\gamma, D[e](y, 1)) \Downarrow c'_y}{(\gamma, \gamma', x = e) \Downarrow_o \gamma[x \mapsto c], \gamma'[x \mapsto \sum_y c'_y \cdot \gamma'(y)]}$$

Operational Semantics

Expressions $e ::= c \mid x \mid h(e, \dots, e)$

Programs $p ::= x = e \mid y = \textbf{integral}\ (a, b)\ e/(x-s)^k\ \mathbf{d}x \mid$ p;p

$$\frac{\begin{array}{l} u \leftarrow \mathcal{U}(0,1) \quad u' \leftarrow \mathcal{U}(0,1) \\ \left(\gamma, u, u', \textbf{integral}\ (a, b)\ e/(x-s)^k\ \mathbf{d}x\right) \Downarrow_h c \\ (\gamma, u, u', \textbf{integral}\ (a, b)\ e/(x-s)^k\ \mathbf{d}x) \Downarrow_h c' \\ \forall z \in \mathrm{FV}(e) \backslash \{x, s\}.\ \left(\gamma, u, u', \textbf{integral}\ (a, b)\ e/(x-s)^k\ \mathbf{d}x\right) \Downarrow_h c'_z \end{array}}{\left(\gamma, \gamma', y = \textbf{integral}\ (a, b)\ e/(x-s)^k\ \mathbf{d}x\right) \Downarrow_o \gamma[y \mapsto c], \gamma'[y \mapsto k \cdot c' \cdot \gamma'(s) + \sum_z c'_z \cdot \gamma'(y)]}$$

Operational Semantics

Separate estimates of integral and its deriv

Reuse same samples

Expressions $e ::= c \mid x \mid h(e, \ldots, e)$

Programs $p ::= \ldots \mid$ **integral** $(a, b)\ e/(x-s)^k\, \mathbf{d}x \mid$ p;p

$$\frac{\begin{array}{l} u \leftarrow \mathcal{U}(0,1) \quad u' \leftarrow \mathcal{U}(0,1) \\ \left(\gamma, u, u', \textbf{ integral}\ (a,b)\ e/(x-s)^k\, \mathbf{d}x\right) \Downarrow_h c \\ (\gamma, u, u', \textbf{ integral}\ (a,b)\ e/(x-s)^k\, \mathbf{d}x) \Downarrow_h c' \\ \forall z \in \mathrm{FV}(e) \backslash \{x, s\}.\ \left(\gamma, u, u', \textbf{ integral}\ (a,b)\ e/(x-s)^k\, \mathbf{d}x\right) \Downarrow_h c_z' \end{array}}{\left(\gamma, \gamma', y = \textbf{integral}\ (a,b)\ e/(x-s)^k\, \mathbf{d}x\right) \Downarrow_o \gamma[y \mapsto c], \gamma'[y \mapsto k \cdot c' \cdot \gamma'(s) + \sum_z c_z' \cdot \gamma'(y)]}$$

Operational Semantics

Expres

Progra

Separate estimates of integral and its deriv

Reuse same samples

$u \leftarrow \mathcal{U}(0,1) \quad u' \leftarrow \mathcal{U}(0,1)$

$(\gamma, u, u'$

$(\gamma, u, u'$

$\forall z \in \mathrm{FV}$

$$\frac{d}{ds}\mathcal{C}\int_a^b \frac{f(x)}{x-s}\,dx \neq \mathcal{C}\int_a^b \frac{f(x)}{(x-s)^2}\,dx$$

$(\gamma, \gamma', y =$

$$\frac{d}{ds}\mathcal{C}\int_a^b \frac{f(x)}{x-s}\,dx = \mathcal{H}\int_a^b \frac{f(x)}{(x-s)^2}\,dx$$

Operational Semantics

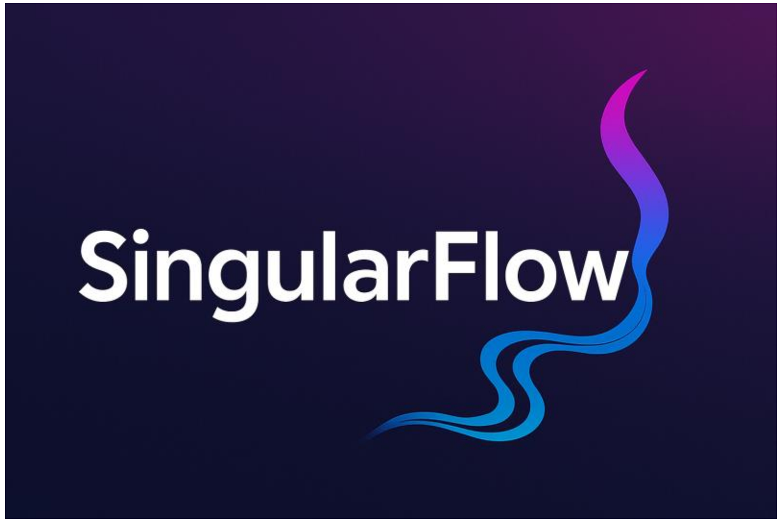
Expressions $e ::= c \mid x \mid h(e, \ldots, e)$

Programs $p ::= x = e \mid y = \textbf{integral}\,(a, b)\; e/(x - s)^k \mathrm{d}x \mid$ p;p

See the paper for the full **semantics** and a proof of **unbiasedness** and **consistency** wrt denotational semantics.

Contributions

- Identify a new problem domain
- Rigorous, accessible math formalism
- First semantics of a differentiable PL with singular integration
- Solve problems in science and engineering

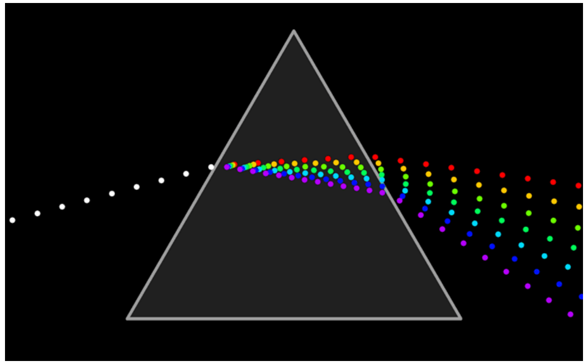


Made by OpenAI Dall-E

Singular Integrals in The Wild

Signal Processing

Hilbert Transform



Aerodynamics

Airfoil Equation

Mechanical Engineering

Crack Problems

- Core jax.custom_vjp
- Core is 100 LOC singular_integrate

Signal Processing: Hilbert Transform

$$T(s) = -\frac{1}{\pi}\mathcal{C}\int_{-1}^{1}\frac{f(u)}{u-s}du \text{ at } s = \frac{1}{2}$$

$f(u)$	Ground Truth	Ours	Standard	Mathematica
u	-0.462	$-0.46 \pm 4.1 \times 10^{-4}$	-3.6 ± 7.3	-0.46
u^2	-0.231	$-0.23 \pm 6.1 \times 10^{-4}$	-1.8 ± 3.7	-0.23
e^u	-0.291	$-0.29 \pm 9.9 \times 10^{-4}$	-11 ± 24	-0.29
ue^u	-0.894	$-0.89 \pm 5.6 \times 10^{-4}$	-6.1 ± 12	-0.89
$\sin u$	-0.409	$-0.41 \pm 3.7 \times 10^{-4}$	-3.4 ± 7.0	-0.41
$\cos u$	0.458	$0.46 \pm 1.0 \times 10^{-3}$	-5.1 ± 13	0.46

Signal Processing: Hilbert Transform

Cauchy PV is not Standard Integral

$$\fint_a^b \frac{f(x)}{x-s}\,dx \neq \int_a^b \frac{f(x)}{x-s}\,dx$$

$f(u)$	Ground Truth	Ours	Standard	Mathematica
u	-0.462	$-0.46 \pm 4.1 \times 10^{-4}$	-3.6 ± 7.3	-0.46
u^2	-0.231	$-0.23 \pm 6.1 \times 10^{-4}$	-1.8 ± 3.7	-0.23
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$\cos u$	0.458	$0.46 \pm 1.0 \times 10^{-3}$	-5.1 ± 13	0.46
		✓	✗	✓

Signal Processing: Hilbert Transform

$$\frac{d}{ds} T_1(s) = -\frac{1}{\pi} \mathcal{H} \int_{-1}^{1} \frac{f(u)}{(u-s)^2} du \text{ at } s = \frac{1}{2}$$

$f(u)$	Ground Truth	Ours	PV	Standard	Mathematica
u	0.774	$0.77 \pm 8.1 \times 10^{-4}$	-5.9×10^{2}	-4.4×10^{3}	0.77
u^2	-7.47×10^{-2}	$-7.4 \times 10^{-2} \pm 8.1 \times 10^{-4}$	-2.9×10^{2}	-2.2×10^{3}	-7.4×10^{-2}
e^u	1.52	$1.5 \pm 9.9 \times 10^{-4}$	-1.9×10^{3}	-1.5×10^{4}	-
ue^u	0.468	$0.47 \pm 1.1 \times 10^{-3}$	-9.7×10^{2}	-7.3×10^{3}	-
$\sin u$	0.816	$0.82 \pm 1.0 \times 10^{-3}$	-5.6×10^{2}	-4.2×10^{3}	0.82
$\cos u$	0.868	$0.87 \pm 3.7 \times 10^{-4}$	-1.0×10^{3}	-7.7×10^{3}	0.87
		✓	✗	✗	◐

Signal Processing: Hilbert Transform

$$\frac{d}{ds}\mathcal{C}\int_a^b \frac{f(x)}{x-s}\,dx = \mathcal{H}\int_a^b \frac{f(x)}{(x-s)^2}\,dx$$

$f(u)$	Ground Truth	Ours	PV	Standard	Mathematica
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e^u	1.52	$1.5 \pm 9.9 \times 10^{-4}$	-1.9×10^{3}	-1.5×10^{4}	-
ue^u	0.468	$0.47 \pm 1.1 \times 10^{-3}$	-9.7×10^{2}	-7.3×10^{3}	-
$\sin u$	0.816	$0.82 \pm 1.0 \times 10^{-3}$	-5.6×10^{2}	-4.2×10^{3}	0.82
$\cos u$	0.868	$0.87 \pm 3.7 \times 10^{-4}$	-1.0×10^{3}	-7.7×10^{3}	0.87
		✓	✗	✗	◐

Signal Processing: Hilbert Transform

$$\frac{d}{ds} \mathcal{C} \int_a^b \frac{f(x)}{x-s} dx \neq \mathcal{C} \int_a^b \frac{f(x)}{(x-s)^2} dx$$

$f(u)$	Ground Truth	Ours	PV	Standard	Mathematica
u	0.774	$0.77 \pm 8.1 \times 10^{-4}$	-5.9×10^2	-4.4×10^3	0.77
u^2	-7.47×10^{-2}	$-7.4 \times 10^{-2} \pm 8.1 \times 10^{-4}$	-2.9×10^2	-2.2×10^3	-7.4×10^{-2}
e^u	1.52	$1.5 \pm 9.9 \times 10^{-4}$	-1.9×10^3	-1.5×10^4	-
ue^u	0.468	$0.47 \pm 1.1 \times 10^{-3}$	-9.7×10^2	-7.3×10^3	-
$\sin u$	0.816	$0.82 \pm 1.0 \times 10^{-3}$	-5.6×10^2	-4.2×10^3	0.82
$\cos u$	0.868	$0.87 \pm 3.7 \times 10^{-4}$	-1.0×10^3	-7.7×10^3	0.87
		✓	✗	✗	◐

Signal Processing: Hilbert Transform

$$\frac{d}{ds}\mathcal{C}\int_a^b \frac{f(x)}{x-s}\,dx \neq \int_a^b \frac{f(x)}{(x-s)^2}\,dx$$

$f(u)$	Ground Truth	Ours	PV	Standard	Mathematica
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u^2	-7.47×10^{-2}	$-7.4 \times 10^{-2} \pm 8.1 \times 10^{-4}$	-2.9×10^2	-2.2×10^3	-7.4×10^{-2}
e^u	1.52	$1.5 \pm 9.9 \times 10^{-4}$	-1.9×10^3	-1.5×10^4	-
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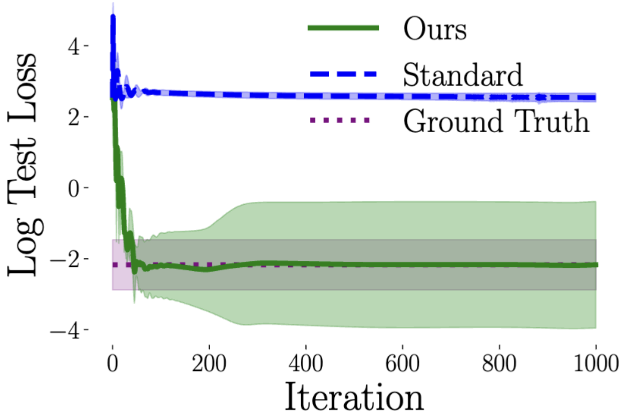
$\cos u$	0.868	$0.87 \pm 3.7 \times 10^{-4}$	-1.0×10^3	-7.7×10^3	0.87

Signal Processing: Hilbert Transform

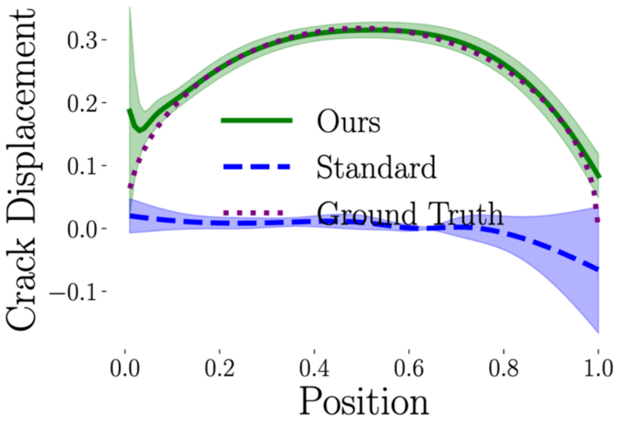
Benchmark	Standard	Ours	Standard (w. jit)	Ours (w. jit)
Finite Hilbert Transform	6.3 ± 0.22	21 ± 1.5	0.97 ± 0.47	1.2 ± 0.19
Deriv. Finite Hilbert Transform	30 ± 17	140 ± 7.1	0.96 ± 0.44	0.9 ± 0.41

Comparable speed (ms) to standard w. jit

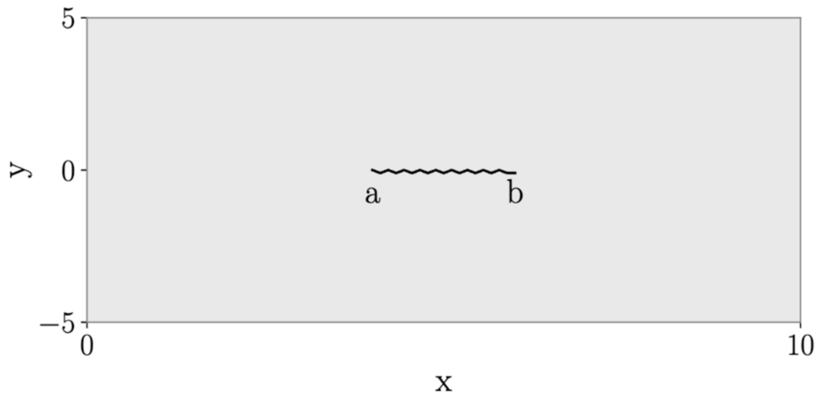
Mechanical Engineering: 1D Crack Problem

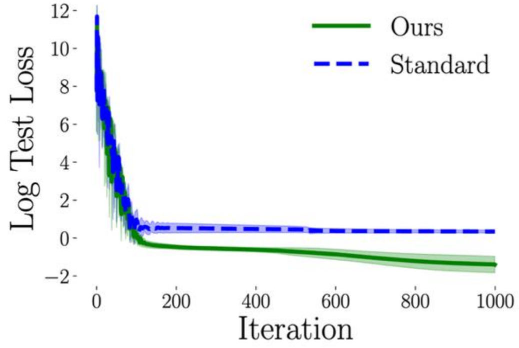


$$-\mathcal{C}\int_0^1 \frac{\sigma(t)}{t-x}\,dt + \int_0^1 \frac{\sigma(t)}{t+x}\,dt = 4x - 2\sqrt{x+x^2}$$

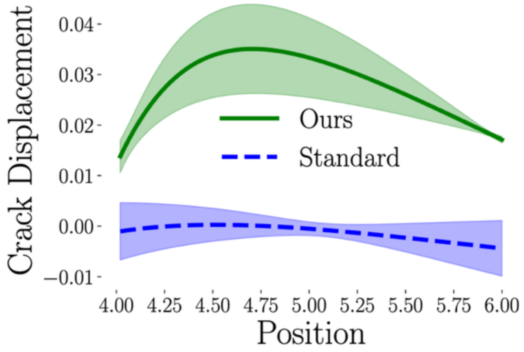


Mechanical Engineering: 2D Crack Problem





$$\mathcal{H}\int_a^b \frac{V(t)}{(t-x)^2}dt + \int_a^b V(t)K_0(t,x)dt = -\pi\frac{1+\kappa}{\mu}p(x)$$



Related Work

Math

(Cauchy, 1826)
(Hadamard, 1932)
Distribution Theory
(Gelfand and Shilov, 1964)

Semantics of PPLs

(Kozen, 1981)
(Zhou et. al., 2019)
(Lew*, Huot*, 2023)
(Lee et. al., 2023)

Numerics

Sampling PV Integrals
(Longman, 1958)

Sampling FP Integrals
(Kutt, 1975)
(Monegato, 1994 and 2009)

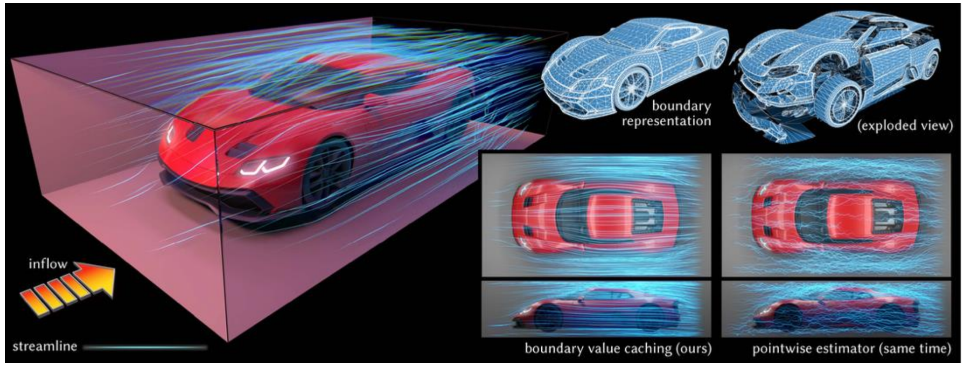
AD with Discontinuities

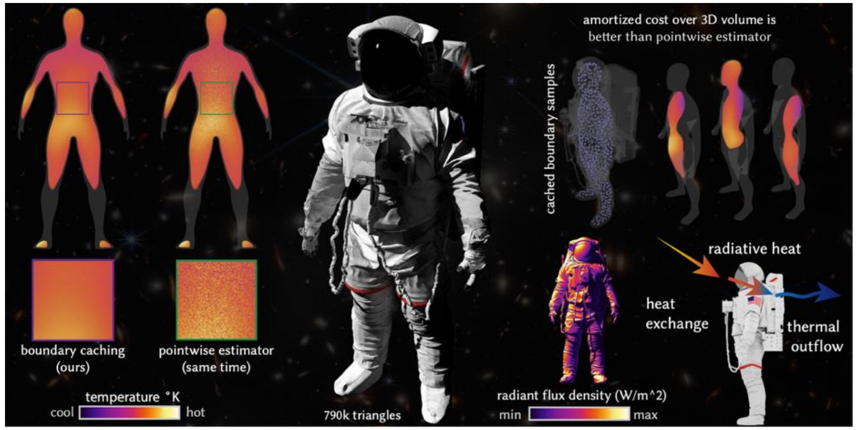
(Nilsson, 2003)
(Chaudhuri et. al., 2010)
(Sherman et. al., 2021
(Yang et. al., 2022)
(Michel et. al., 2024)

Future Work: 3D Singularities in Computer Graphics

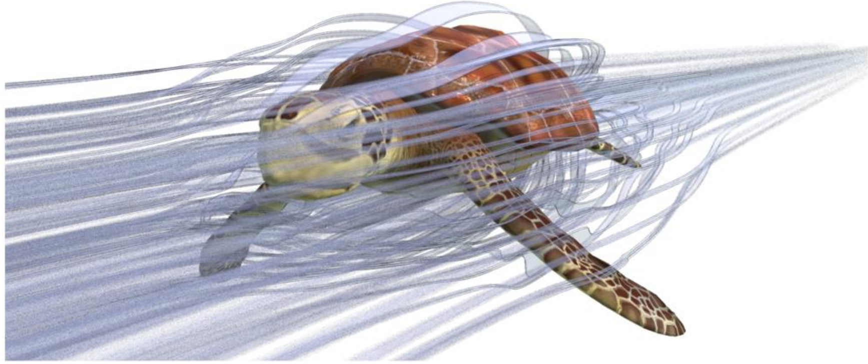
Boundary Value Caching for Walk on Spheres

(Miller*, Sawhney*, et. al., 2023)





Kelvin transformations for simulations on infinite domains.
(Nabizadeh et. al., 2021)



Future PL Work

- Multiple singularities and more general singularities
- Nested integration and multivariate integration
- More expressive control flow (e.g., while loops)
- Support for higher-order functions and recursion

Conclusion

- First language formalization for AD w/ singular integrals
- Need more language features and generality
- More applications: PDE solvers (e.g., FEniCS) and computer graphics

SingularFlow
Implementation

$$\frac{d}{ds}\int_a^b$$