PROBABILISTIC NUMERICS:

NANO-MACHINE-LEARNING

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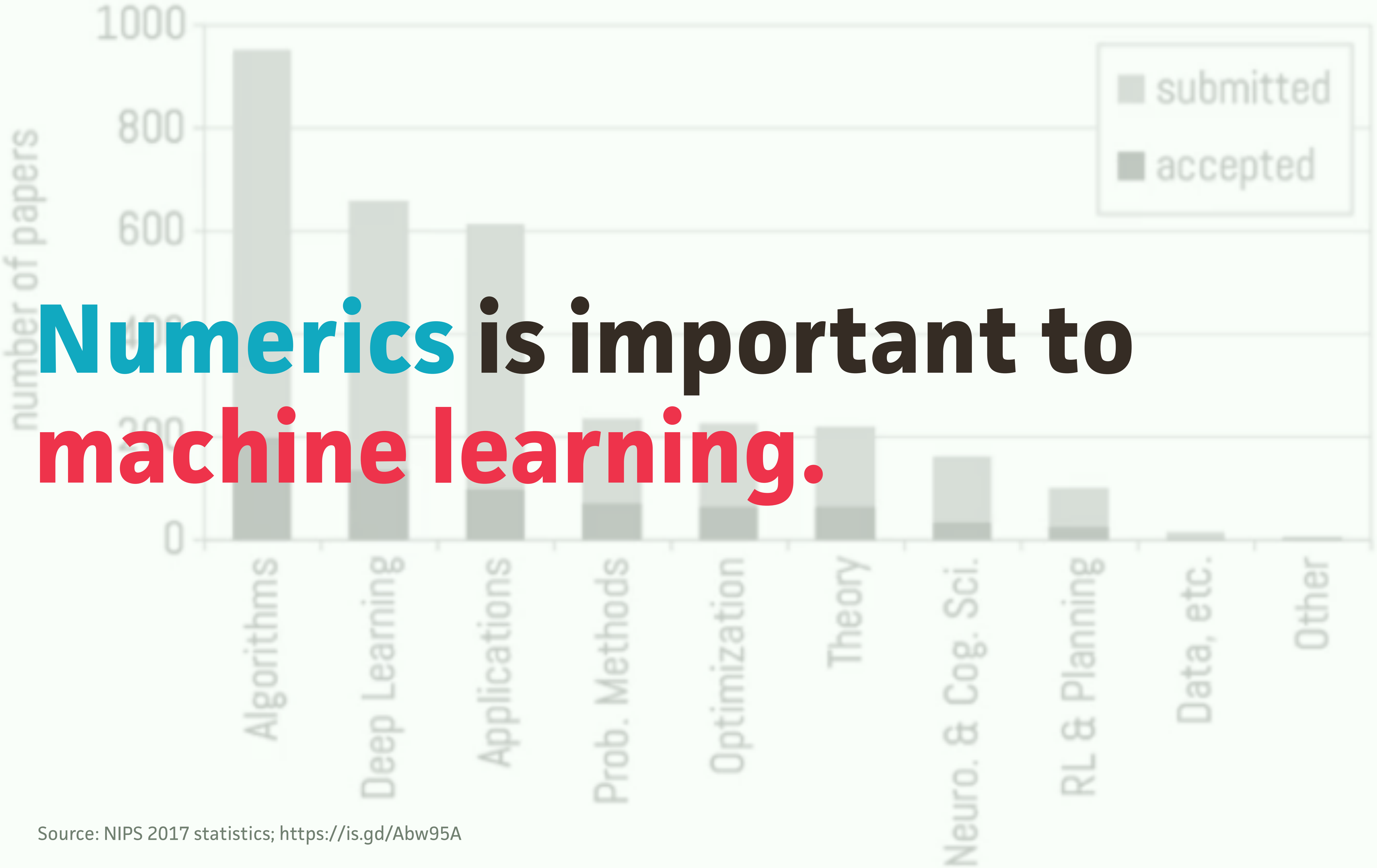
Numerics is important to machine learning.



Source: NIPS 2017 statistics; https://is.gd/Abw95A

Which numerics problems have you needed solved in the last month?

1. Linear algebra.
2. Optimisation.
3. Global optimisation.
4. Integration.
5. Ordinary differential equations.

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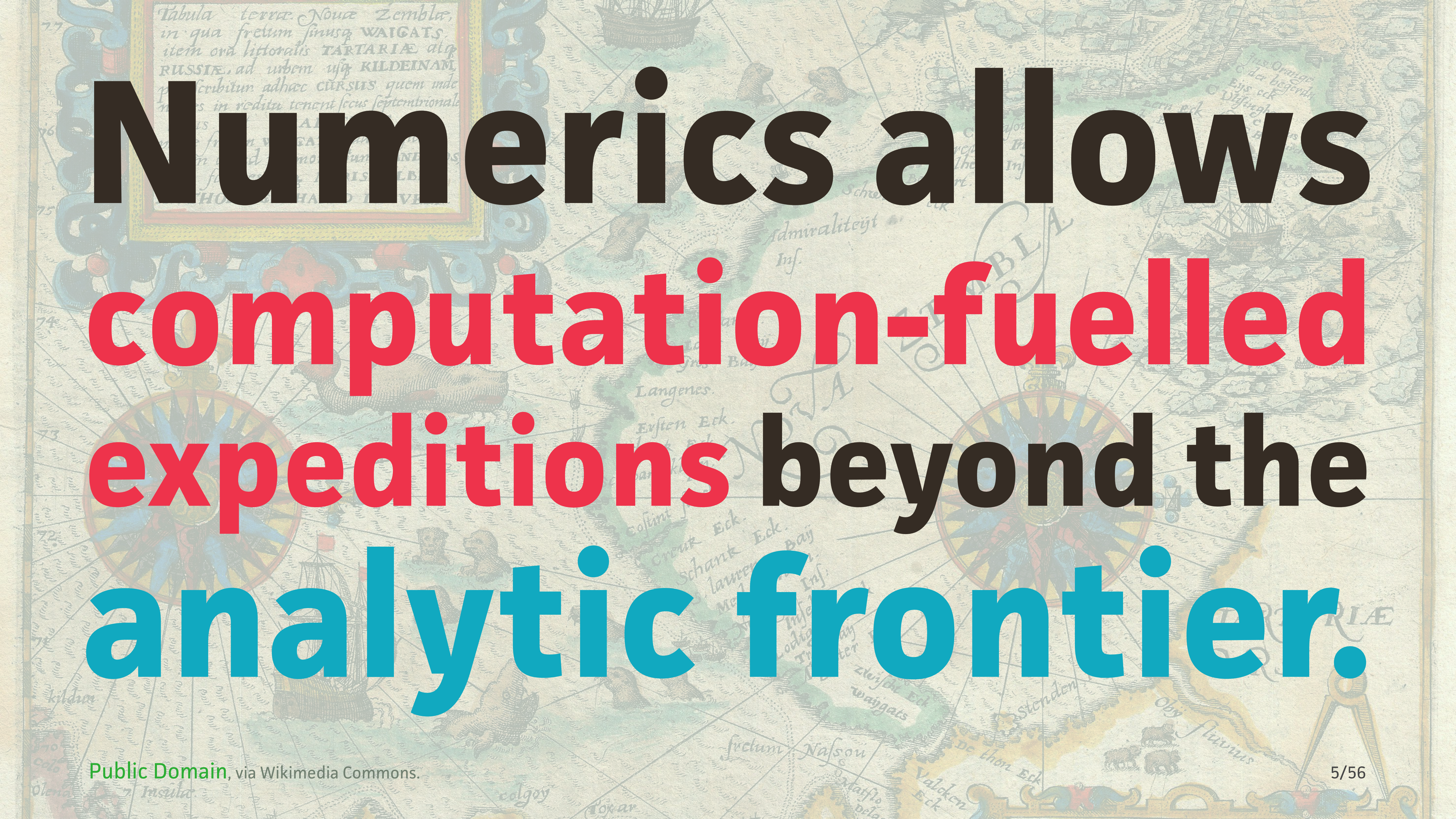

Numerics allows computation-fuelled expeditions beyond the analytic frontier.

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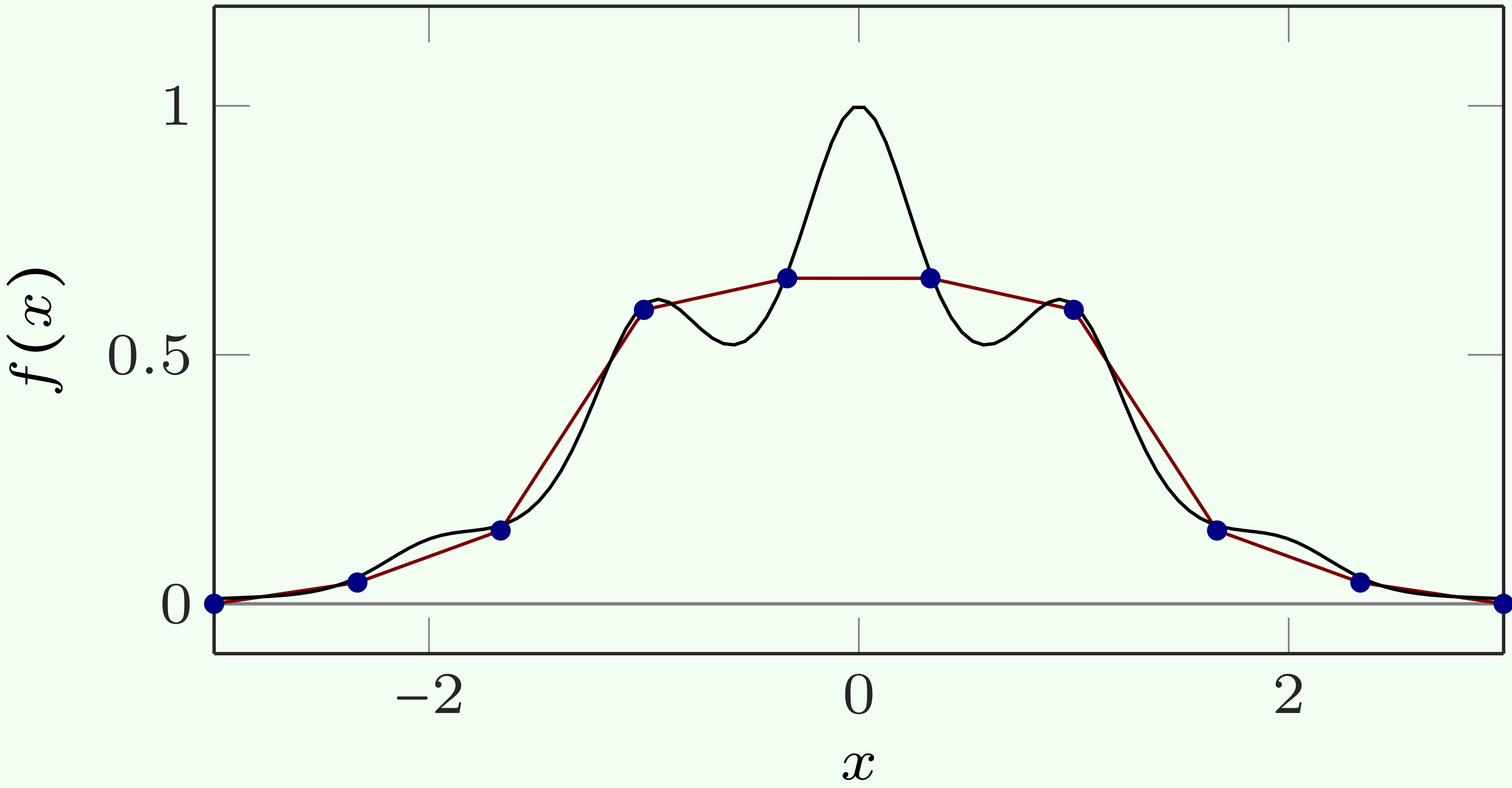
The answer to a numeric problem can only be approximated,

e.g.

$$F = \int_{-3}^{3} f(x)\mathrm{d}x$$

for

$$f(x) = \exp\left(-\left(\sin(3x)\right)^2 - x^2\right).$$



Machine learning treats algorithms as agents.

Probabilistic numerics treats numeric algorithms as agents.

As motivation:

1. numeric **error** is significant;
2. numeric methods are **generic;**
3. our numerics problems **tax our computation.**

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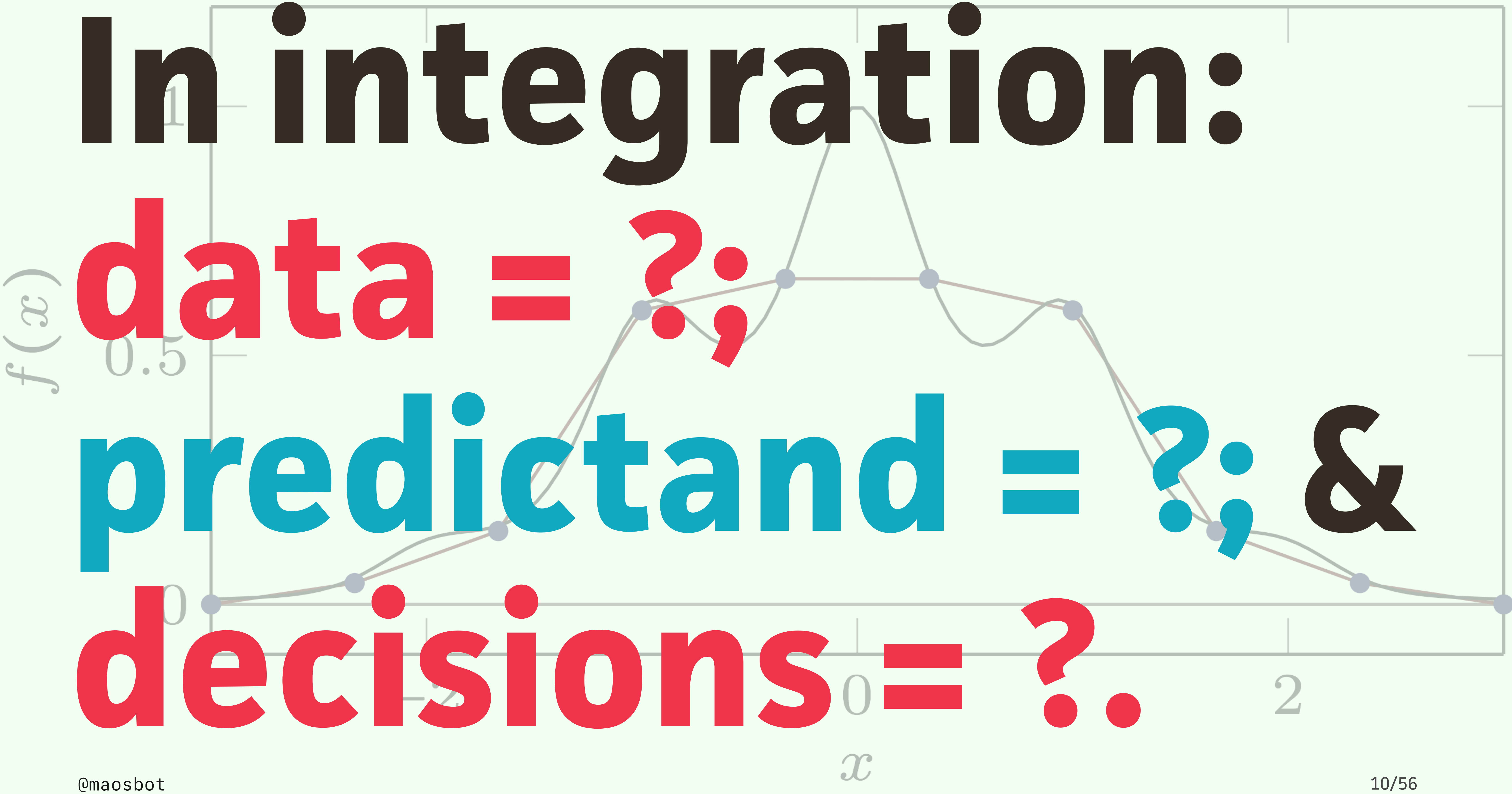
An agent receives data, predicts, & then makes decisions.

In integration:

data = ?;

predictand = ?; &

decisions = ?.



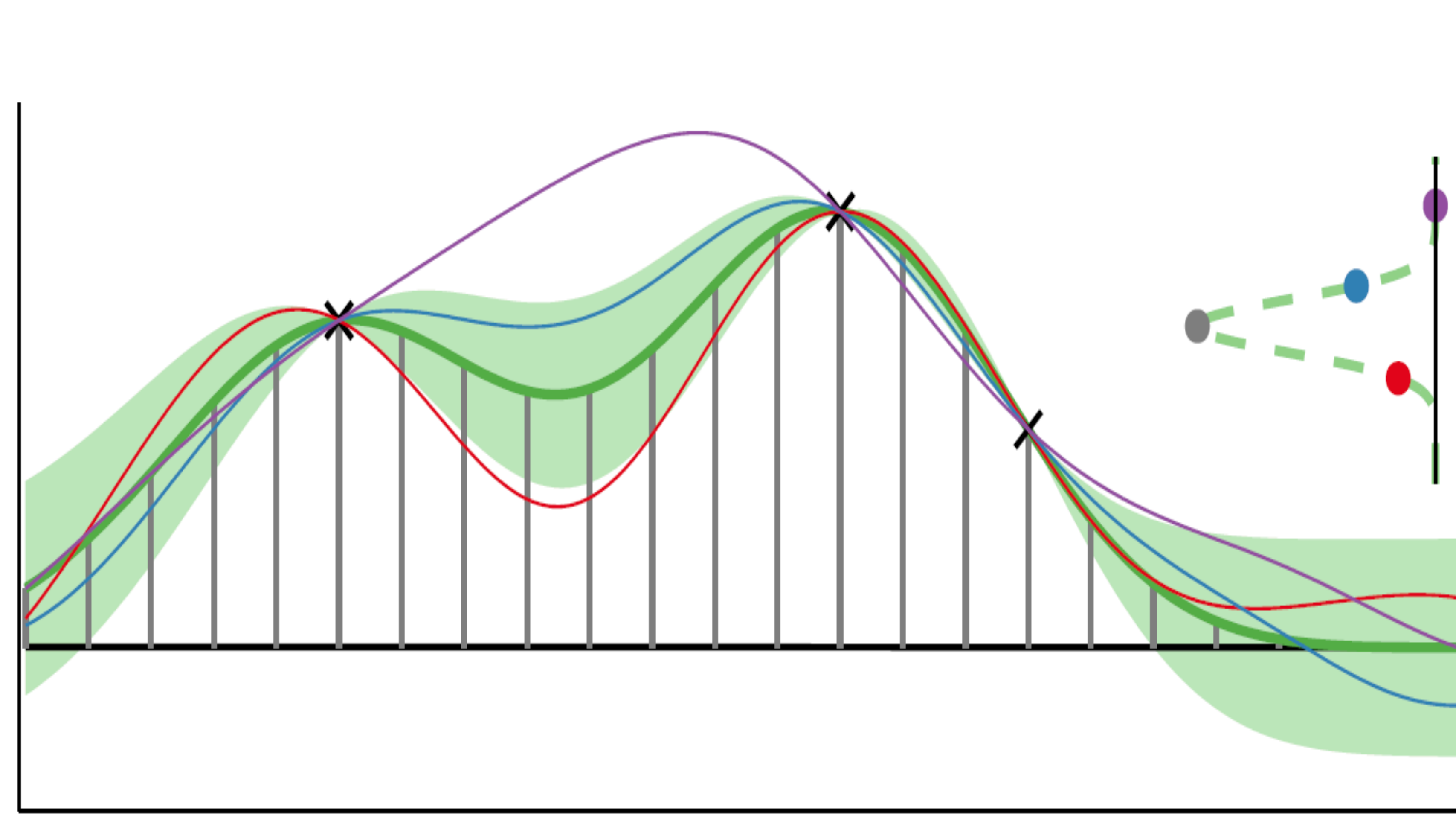
In integration:

data = evaluations;

predictand = integral; &

decisions = locations.

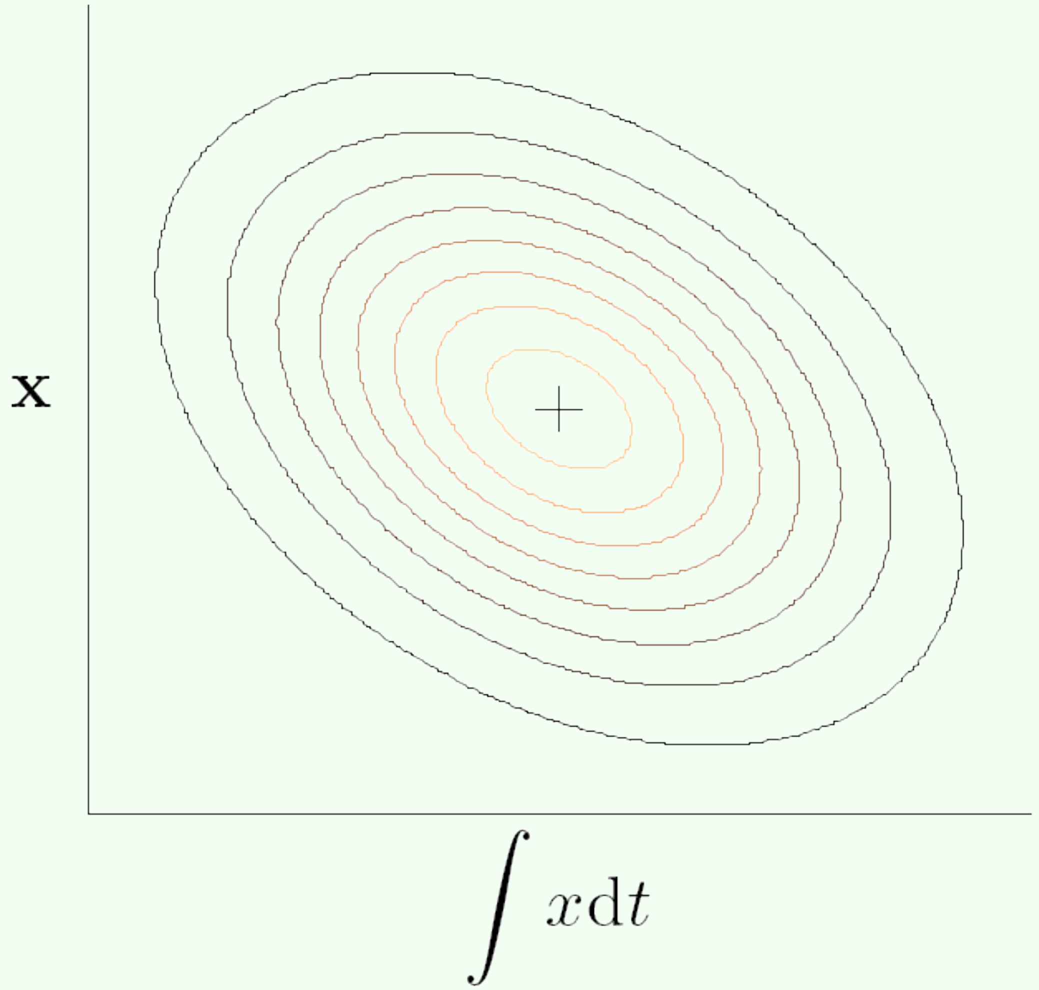
Bayesian quadrature is probabilistic numerics for integration.

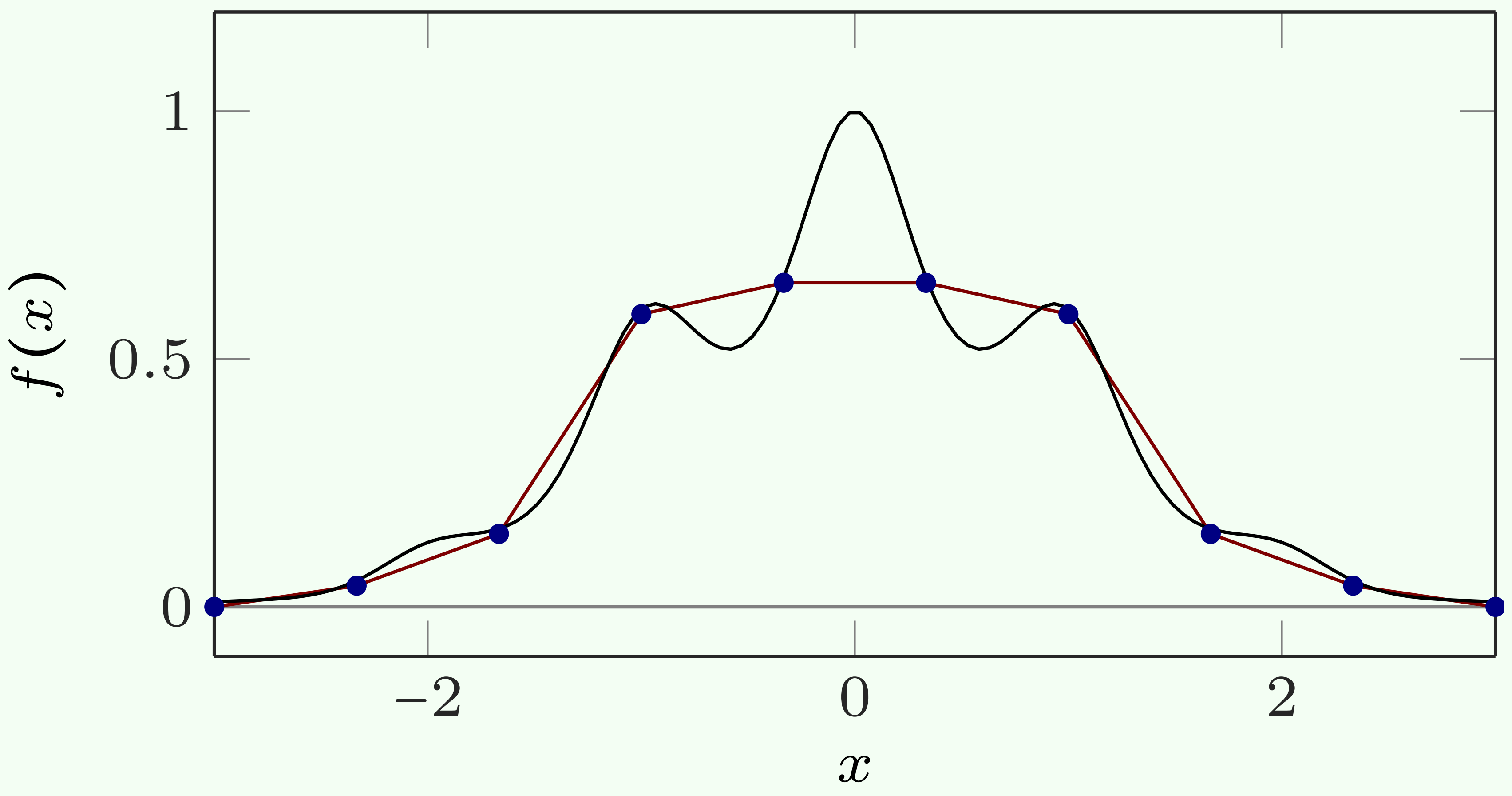


Source: D. Duvenaud.

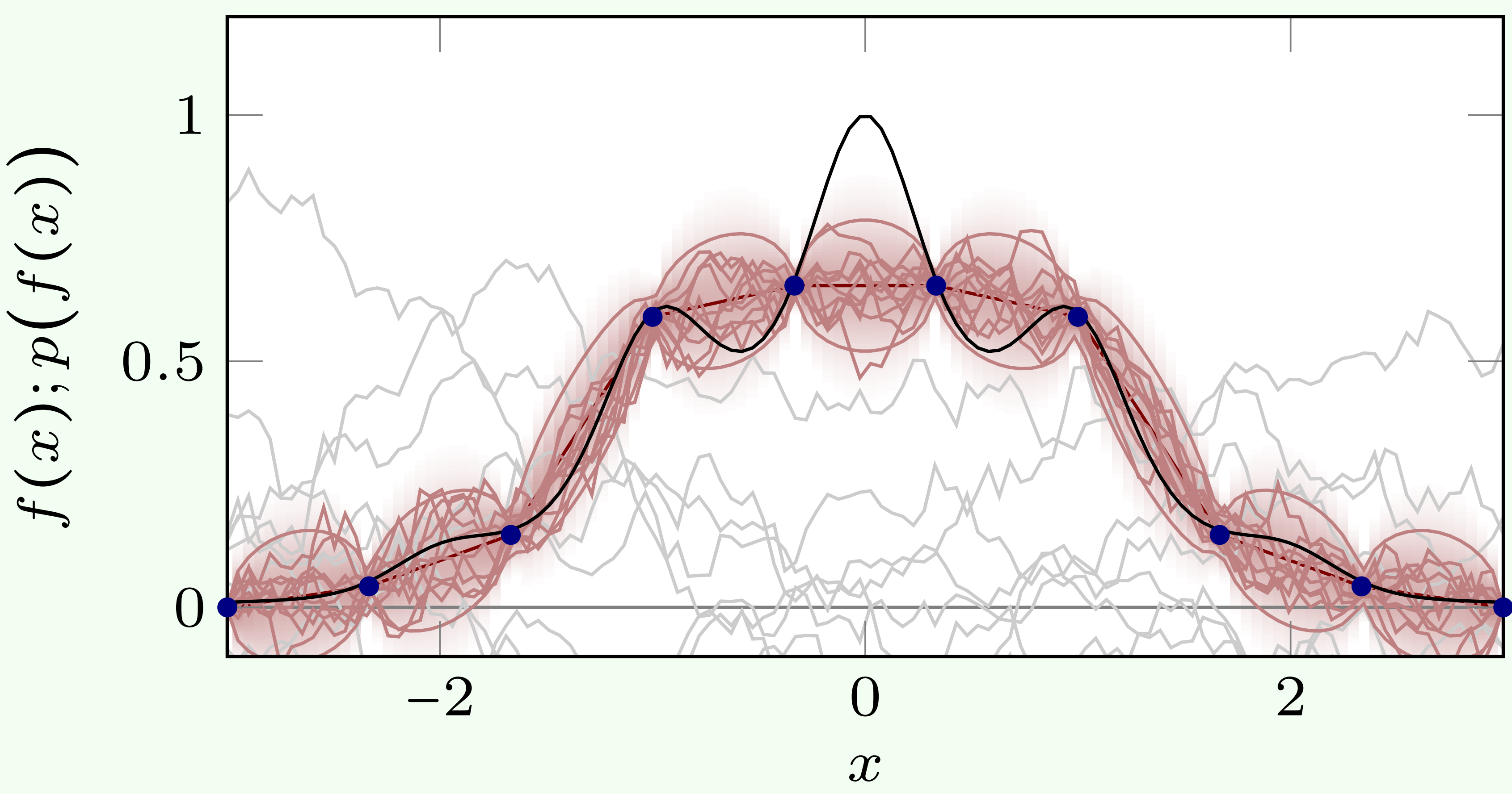
An agent is defined by its **prior** and loss function.

With a Gaussian process prior for the integrand, the integral is joint Gaussian.





$f(x)$
x
1
0.5
0
−2
0
2



$f(x); p(f(x))$
x
1
0.5
0
−2
0
2

The trapezoidal rule is the posterior mean estimate for the integral

$$F = \int_a^b f(x)\,\mathrm{d}x$$

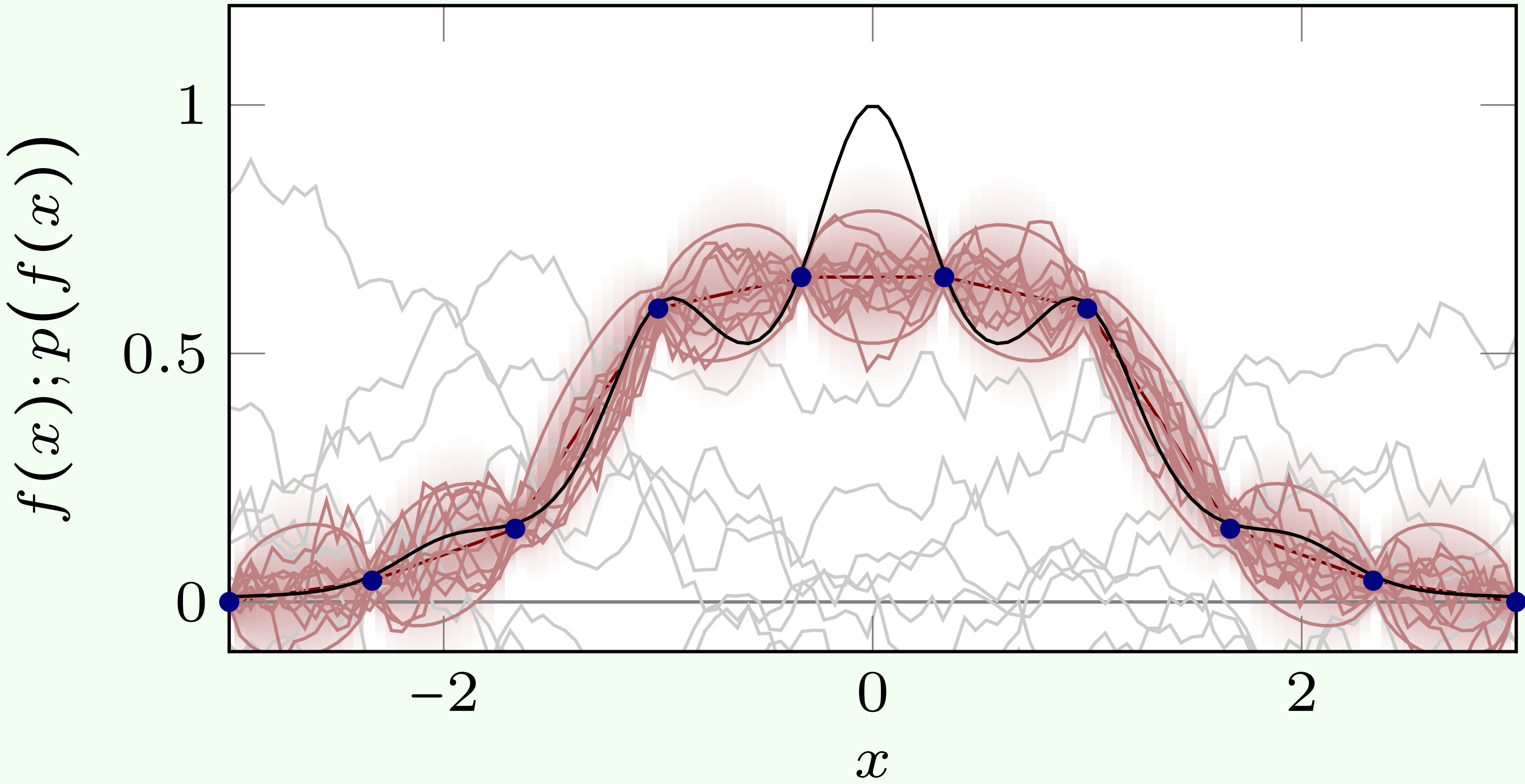
under any centered Wiener process prior

$$p(f) = \mathcal{GP}(f; 0, k)$$

with

$$k(x, x') = \theta^2 \left(\min(x, x') - \chi\right)$$

for arbitrary $\theta \in \mathfrak{R}_+$ and $\chi < a \in \mathfrak{R}$.



procedure INTEGRATE($@f, a, b, N, \theta$)

  $\delta := (b - a)/(N - 1)$ // choose step size

  $x \leftarrow a, y_1 = f(a), m \leftarrow 0, v \leftarrow 0,$ // initialise

  for $i = 2, \ldots, N$ **do**

    $x \leftarrow x + \delta$ // step

    $y_i \leftarrow f(x)$ // evaluate

    $m \leftarrow m + {}^{\delta}/2(y_{i-1} + y_i)$ // update estimate

    $v \leftarrow v + {}^{\delta^3}/12$ // update error estimate

  end for

  return $\mathbb{E}(F) = m, \mathrm{var}(F) = \theta^2 v$ // probabilistic output

end procedure

The trapezoid rule **is** Bayesian quadrature.

procedure INTEGRATE($@f, a, b, N, \theta$)

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  end for

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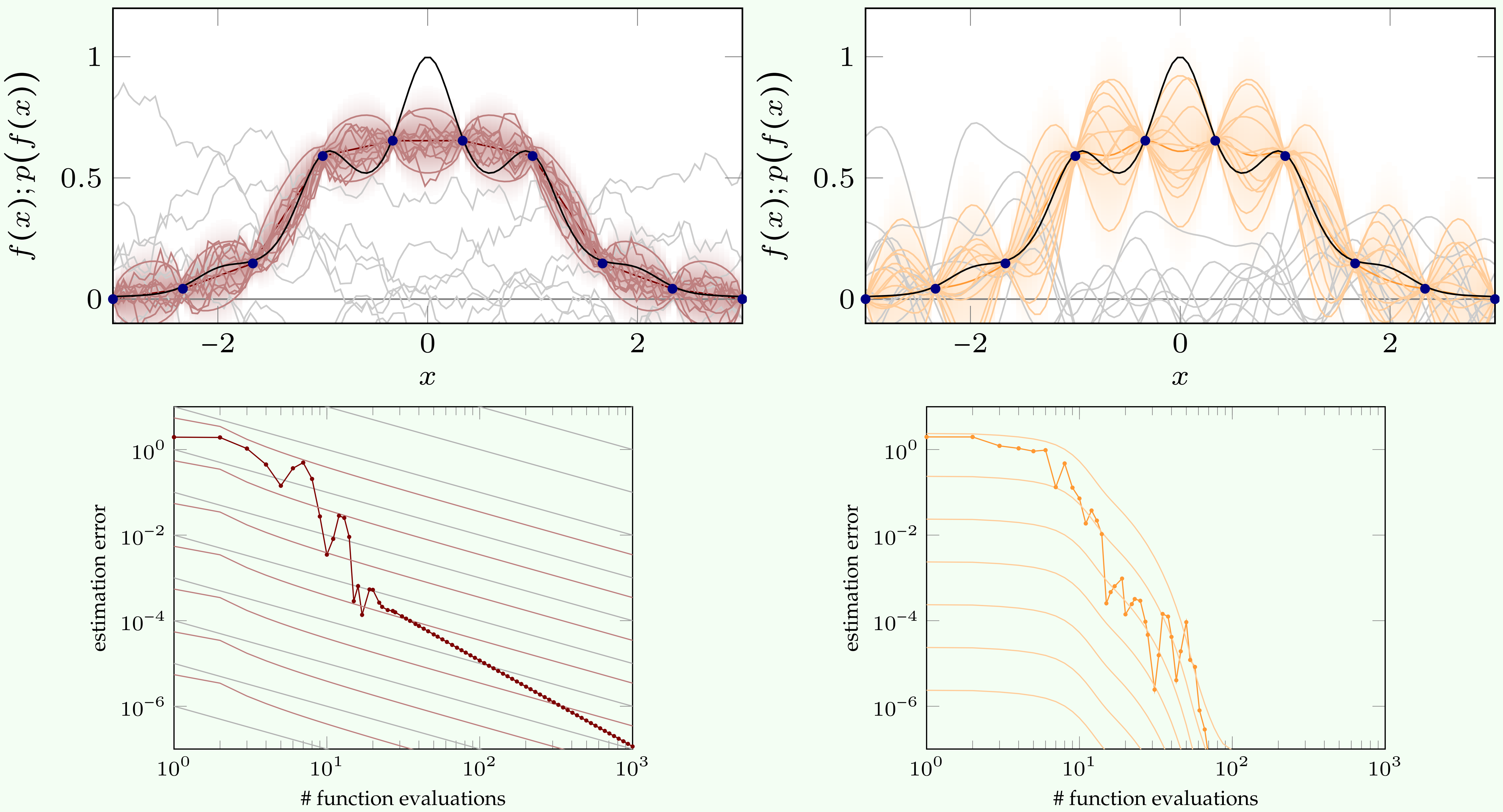
end procedure



f(x); p(f(x))
x
f(x); p(f(x))
x
estimation error
function evaluations
estimation error
function evaluations

Quiz: The convergence rate of the trapezoid rule is $\mathcal{O}(N^{-1})$: what is the rate of **Monte Carlo?**

1. $\mathcal{O}\big(\exp(-N)\big)$
2. $\mathcal{O}\left(\exp\left(-N^{-\frac{1}{2}}\right)\right)$
3. $\mathcal{O}(N^{-1})$
4. $\mathcal{O}(N^{-\frac{1}{2}})$

Quiz: The convergence rate of the trapezoid rule is $\mathcal{O}(N^{-1})$: what is the rate of Monte Carlo?

1. $\mathcal{O}\big(\exp(-N)\big)$
2. $\mathcal{O}\left(\exp\left(-N^{-\frac{1}{2}}\right)\right)$
3. $\mathcal{O}(N^{-1})$
4. $\boldsymbol{\mathcal{O}(N^{-\frac{1}{2}})}$ – **arguably the worst possible rate.**

Monte Carlo is also Bayesian quadrature.

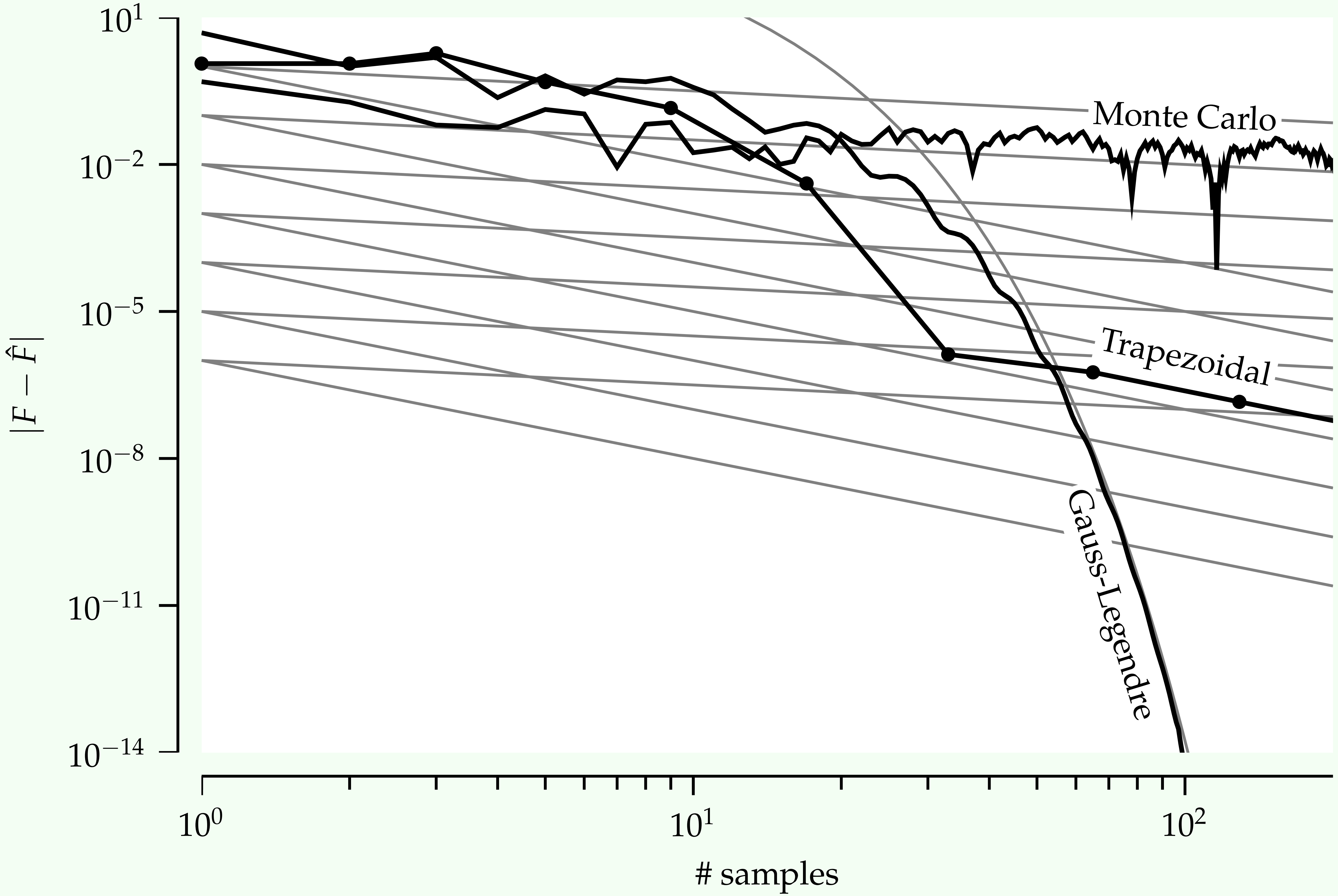
The Monte Carlo estimate

$$\int f(x)\,p(x)\,\mathrm{d}x \simeq \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

is maximum a-posteriori under the (improper) prior

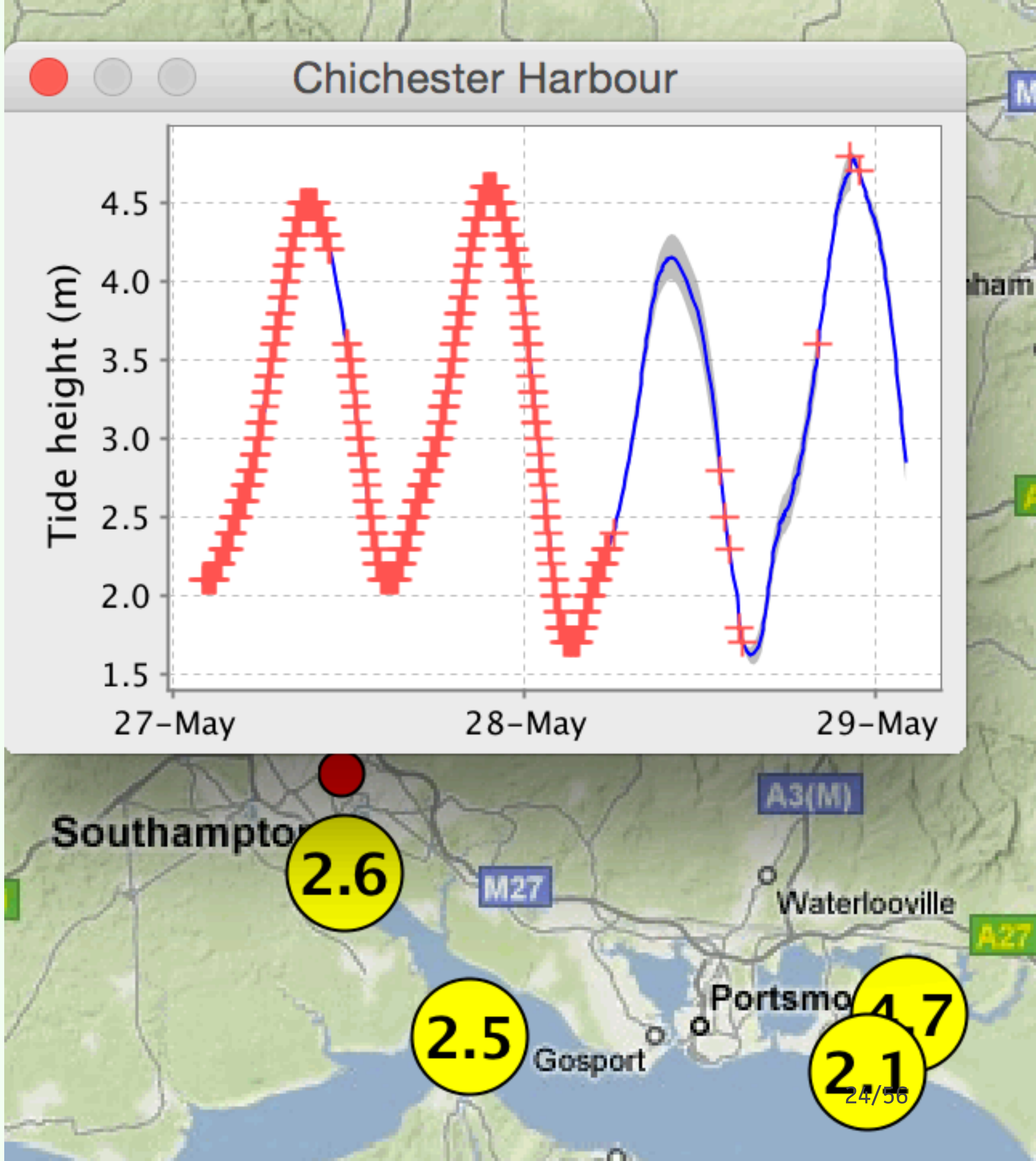
$$p(f) = \lim_{c\to 0} \mathcal{GP}\big(0, \theta^2\, \mathbb{I}(x = x') + c^{-1}\big)$$

for $\mathbb{I}$ the indicator function and with arbitrary $\theta \in \Re_+$. The corresponding posterior standard deviation estimate on the integral, $\theta\,(b-a)\big/\sqrt{N}$, matches the convergence rate of the Monte Carlo estimator.



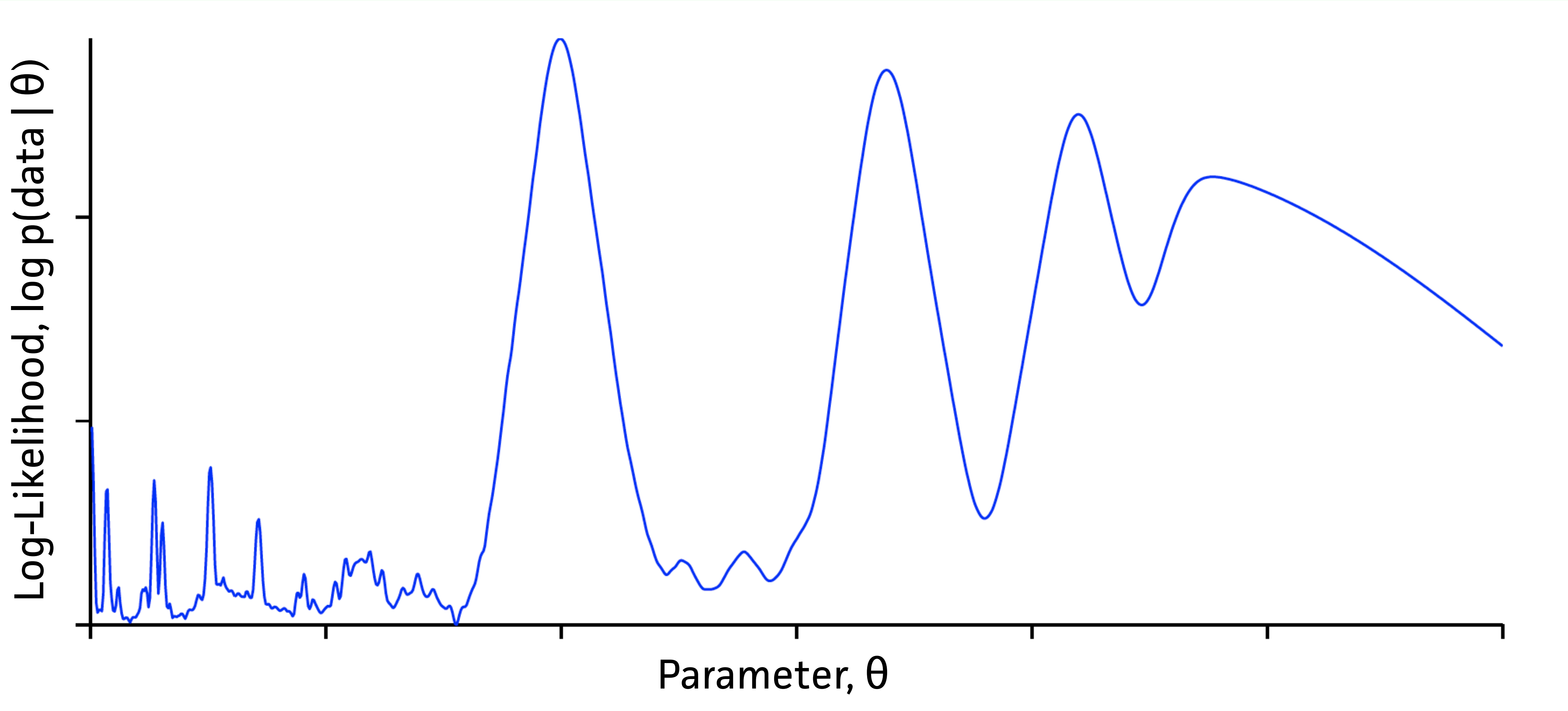
10^1
10^{-2}
10^{-5}
10^{-8}
10^{-11}
10^{-14}
$|F - \hat{F}|$
Monte Carlo
Trapezoidal
Gauss-Legendre
10^0
10^1
10^2
samples

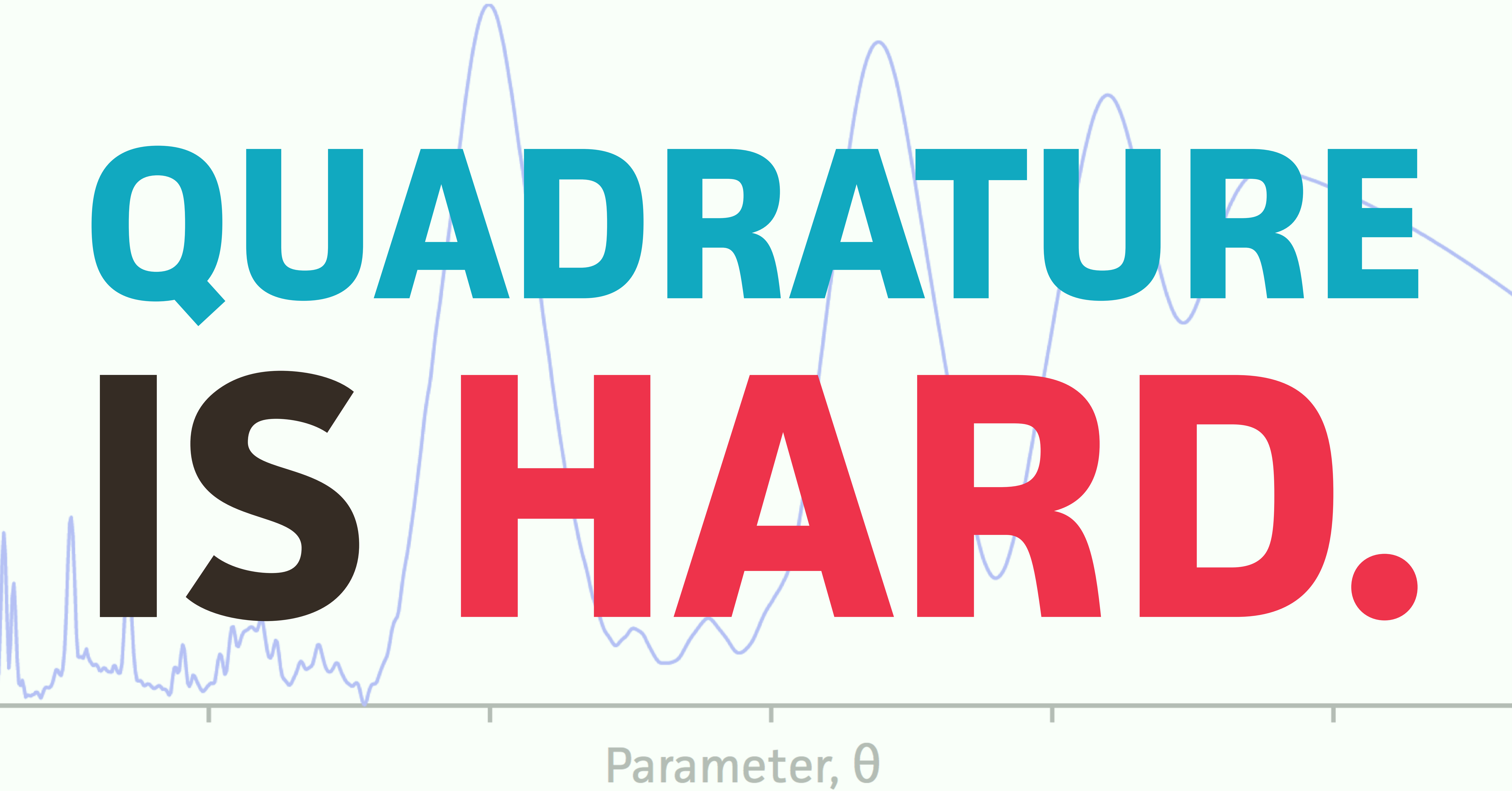
Quadrature is often required to manage model parameters.



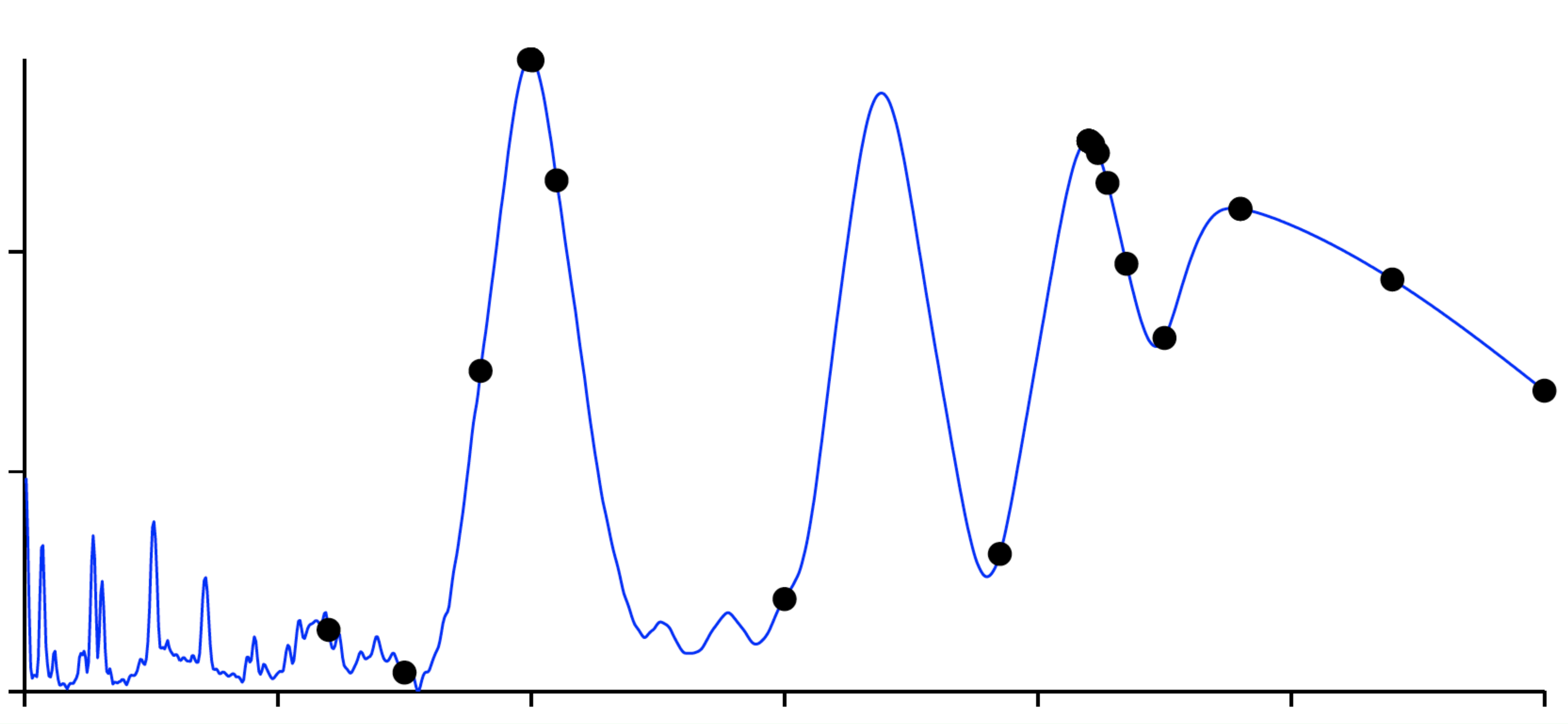
Managing parameters θ requires the **model evidence,**

$$p(\text{data}) = \int p(\text{data} \mid \theta)\, p(\theta) \mathrm{d}\theta.$$

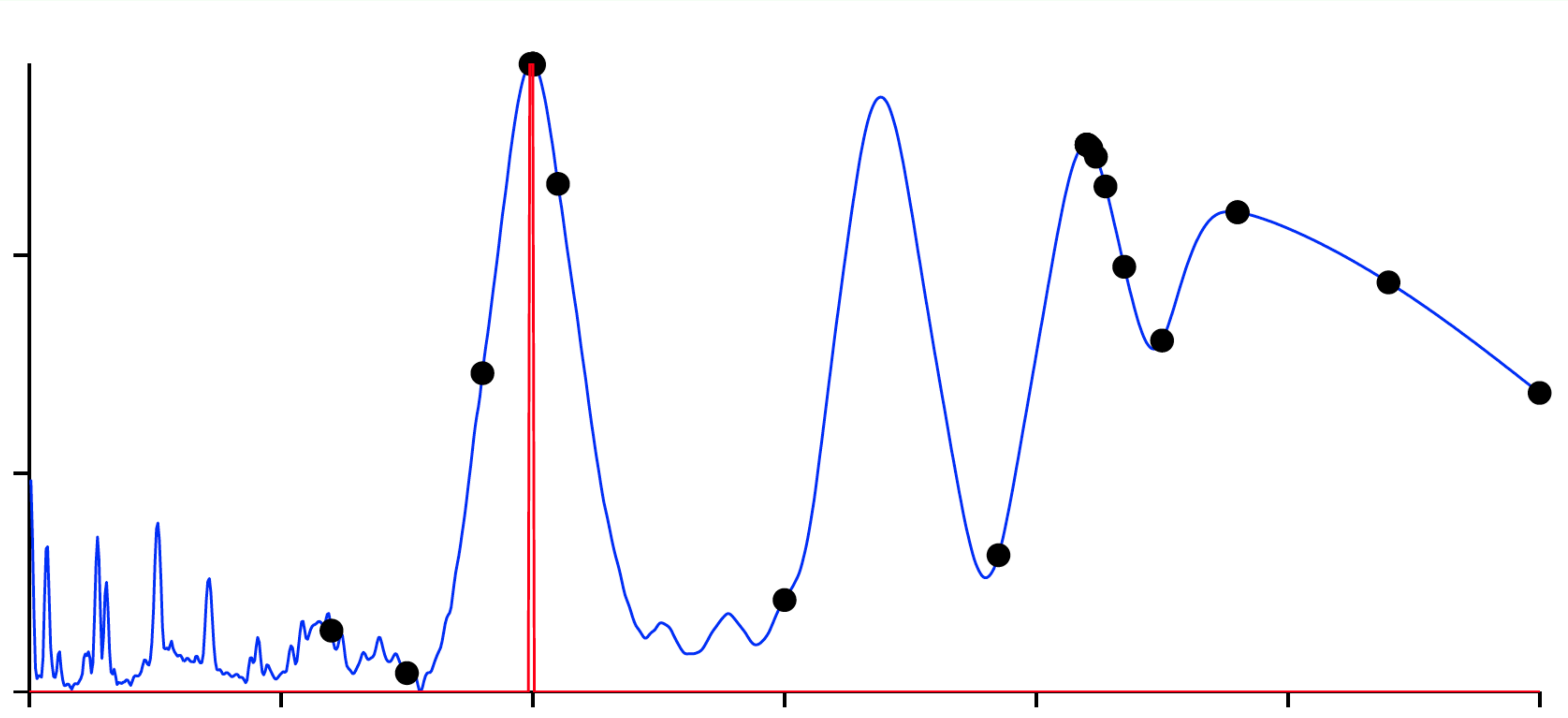



QUADRATURE
IS HARD.
Parameter, θ

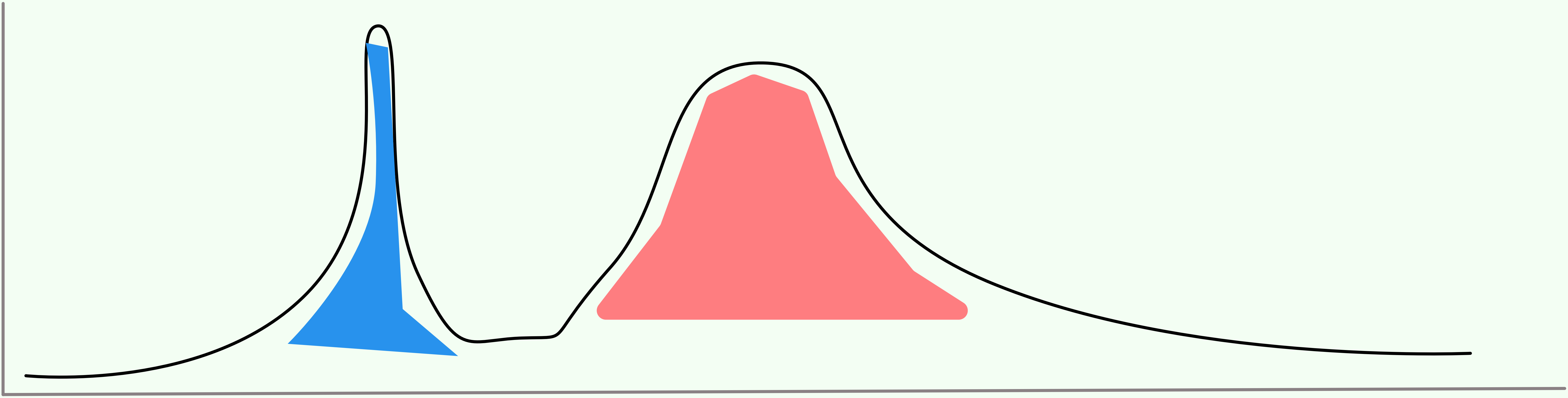
Optimisation (maximum likelihood, training) is often used in the place of quadrature.



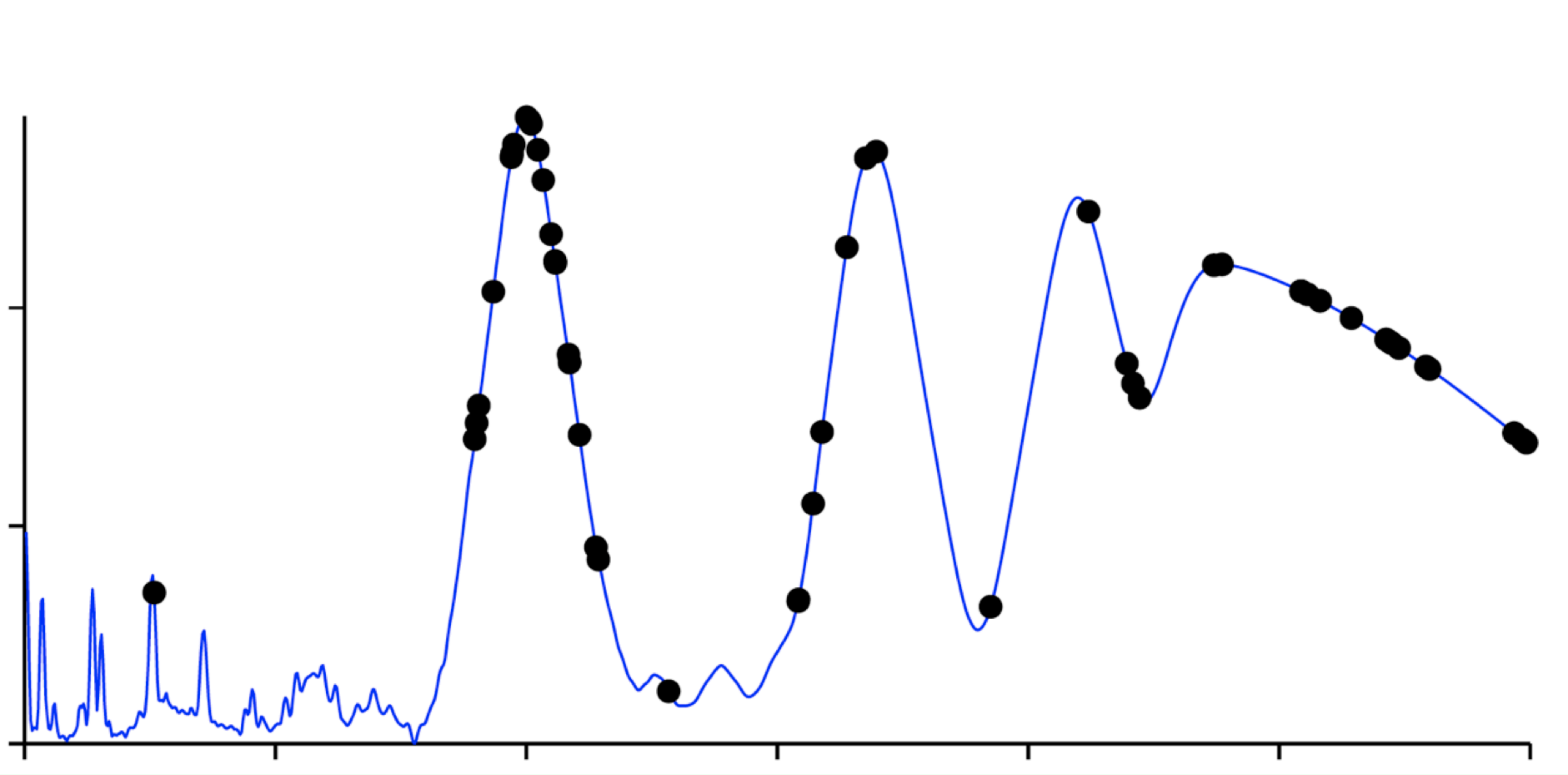
This approximates as $p(\mathrm{data}) \simeq \int p(\mathrm{data} \mid \theta)\, \delta(\theta - \theta_{\mathrm{max}})\, \mathrm{d}\theta$.



If optimising, **flat optima** are often a better representation of the integral than **narrow optima.**

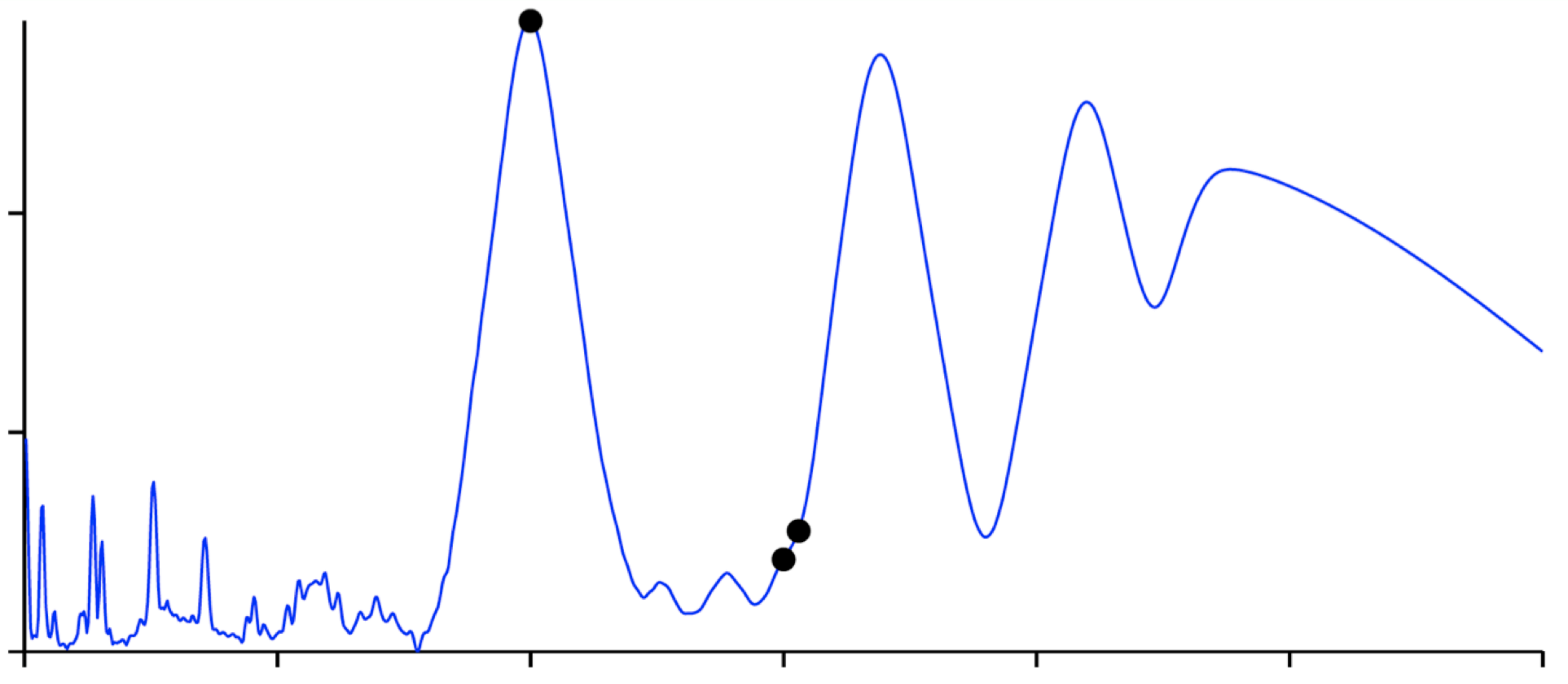


Monte Carlo has revolutionised Bayesian inference.

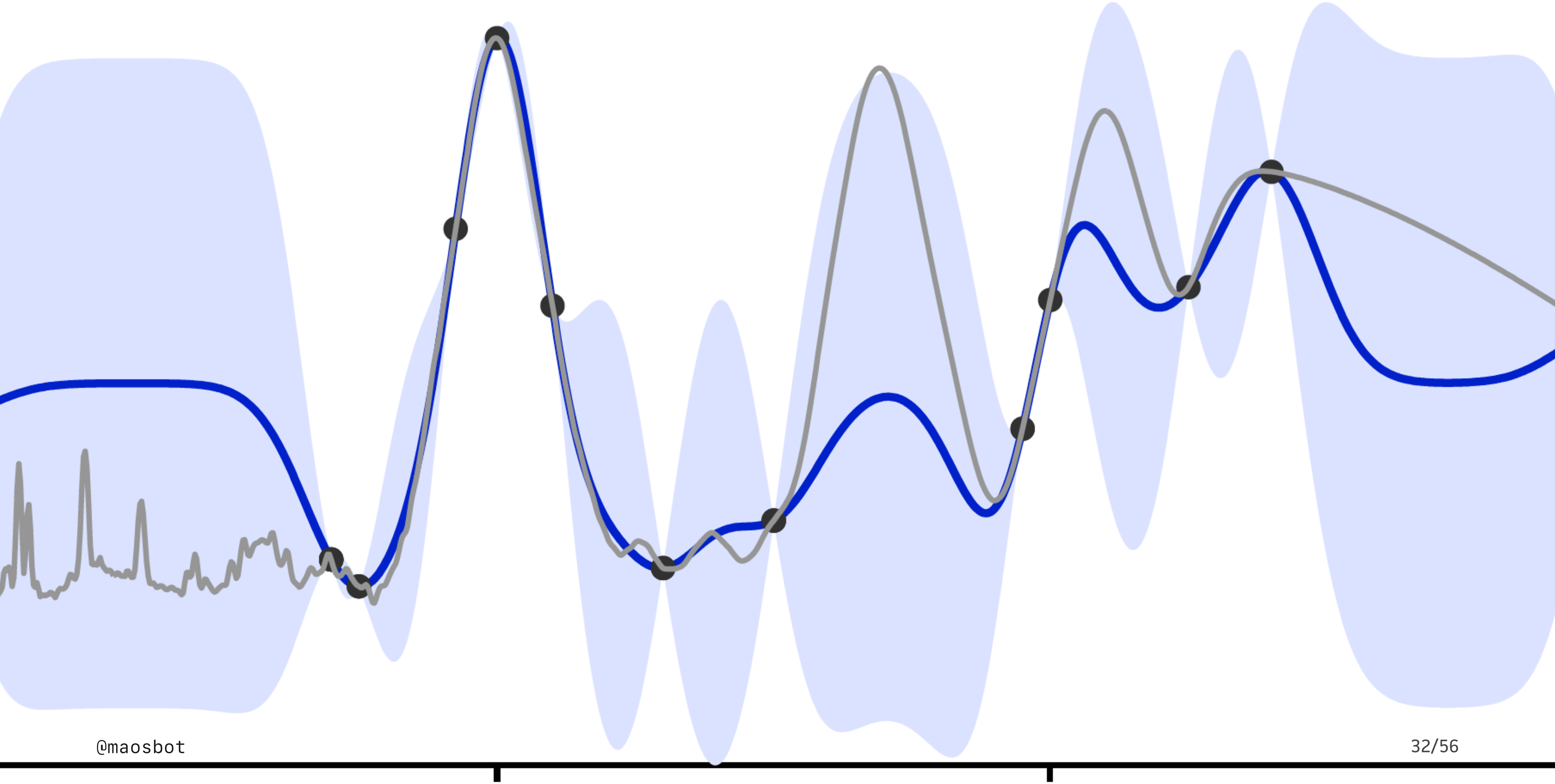


Monte Carlo estimators, $\int f(x)\,p(x)\,\mathrm{d}x \simeq \frac{1}{N}\sum_{i=1}^{N} f(x_i)$,

ignore relevant information.



O'Hagan, A. (1987). Monte Carlo is Fundamentally Unsound. Journal of the Royal Statistical Society. Series D (The Statistician).



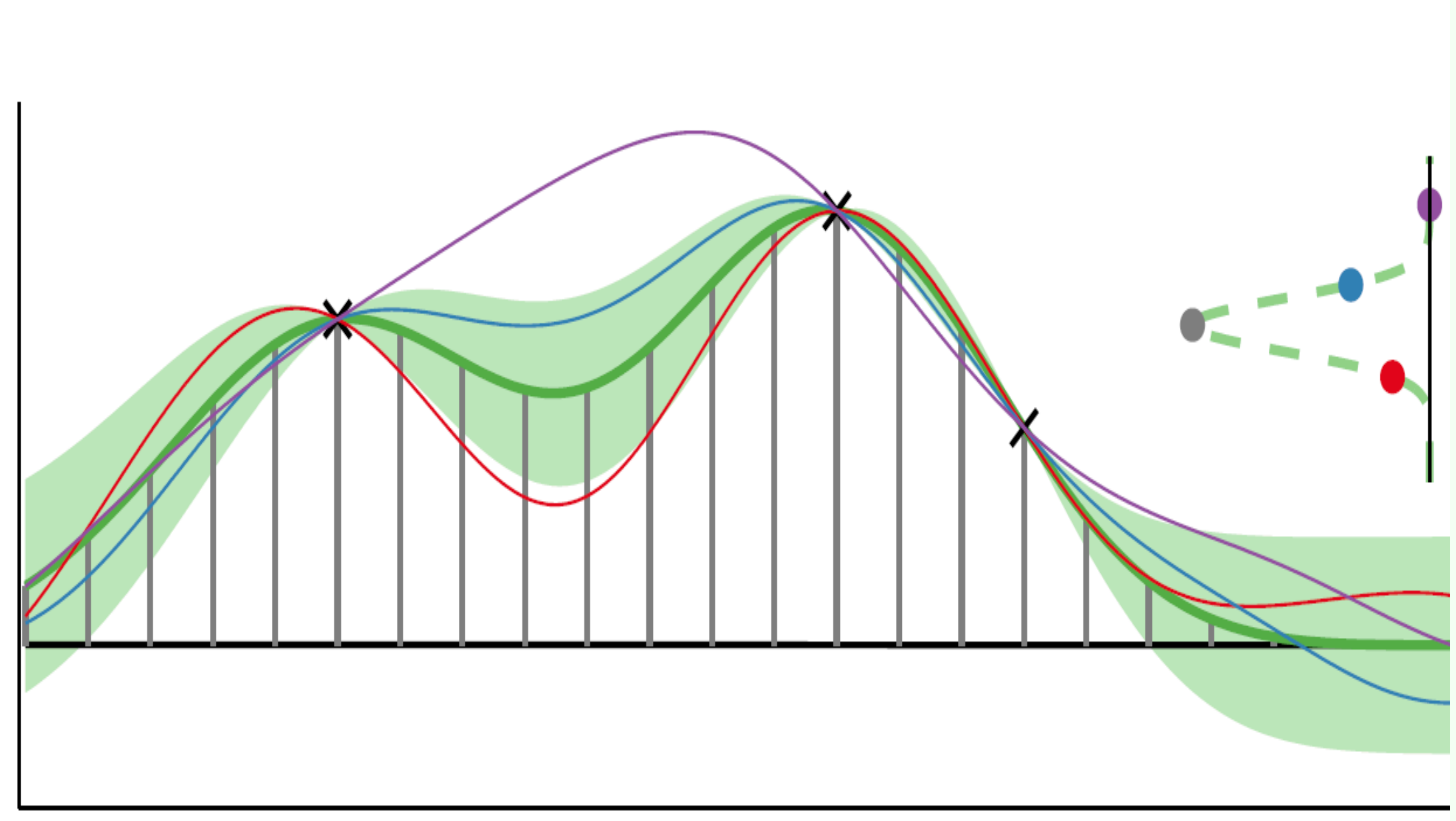
```
ea = params[]
wa = params[2:3]
secw, sesw = np.sqrt(ea)*np.cos(wa), np.sqrt(ea)*np.sin(wa)
```

We often have relevant prior knowledge: like the problem's source code.

```
bx, by = af.baseline_m(df.time, pv_base, df.px, df.py, nthr)
px, py = af.am_model_em(df.time, np.r_[pv_base, pv_1, pv_2], 2, 1
mx, my = 1e6*(bx+px), 1e6*(by+py)
```

The perfect prior is intractable.

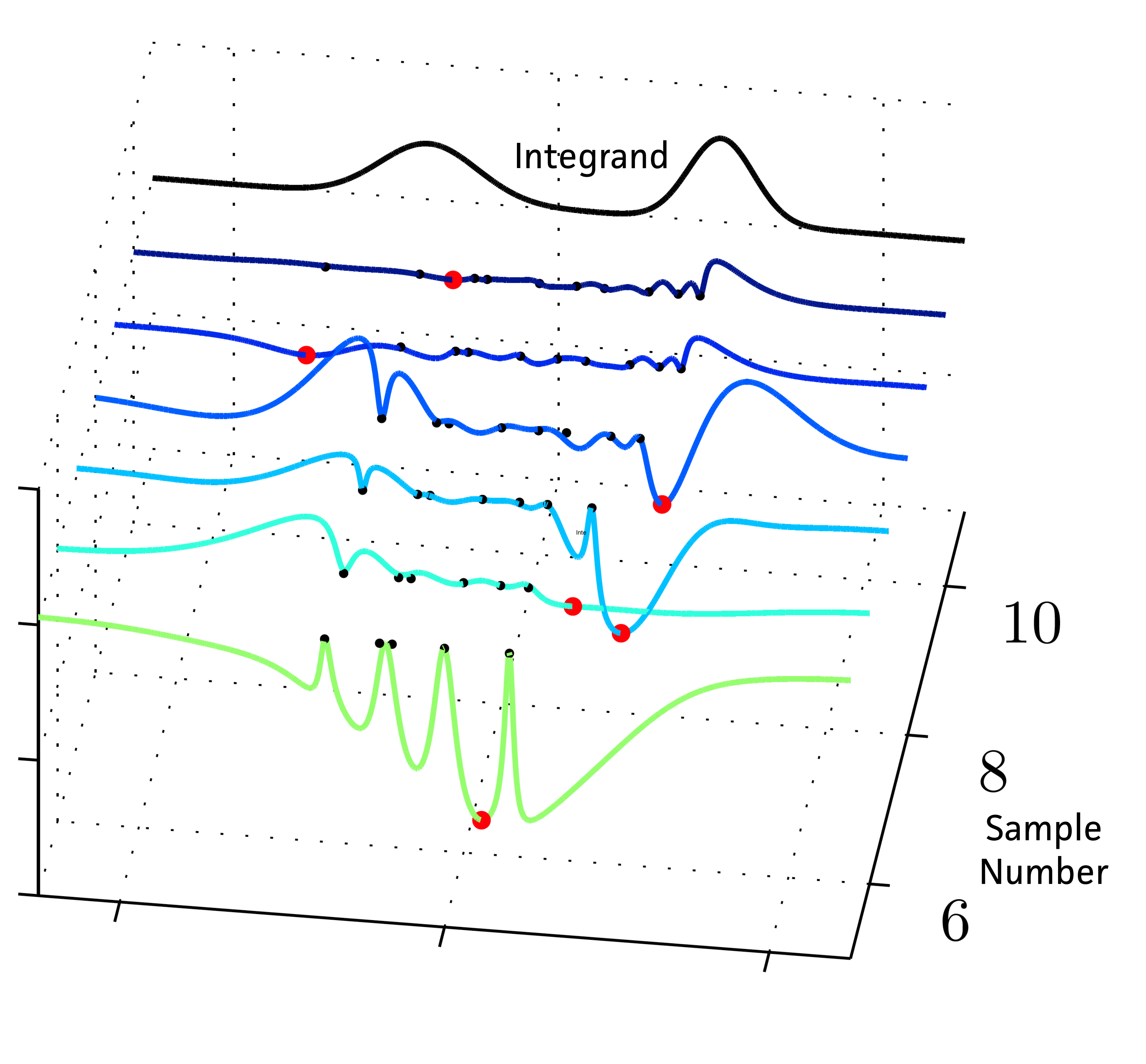
An agent is defined by its prior and loss function.



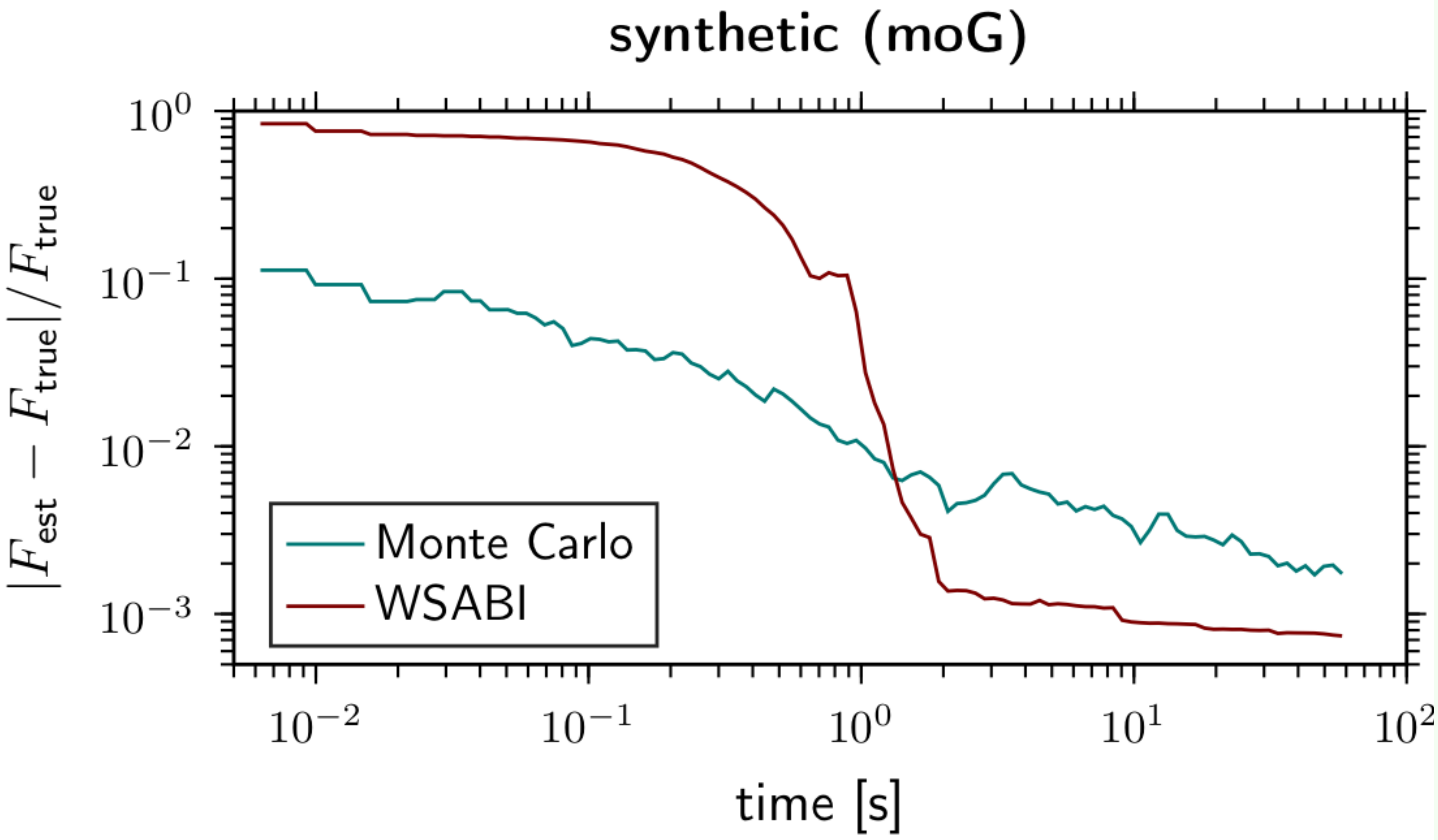
A natural **loss function** for quadrature is the **uncertainty in the integral.**

Source: D. Duvenaud.

WSABI uses a loss that is the uncertainty in the integrand.



Source: Gunter, Osborne, Garnett, Hennig, & Roberts (2014). Sampling for Inference in Probabilistic Models with Fast Bayesian Quadrature. NIPS.



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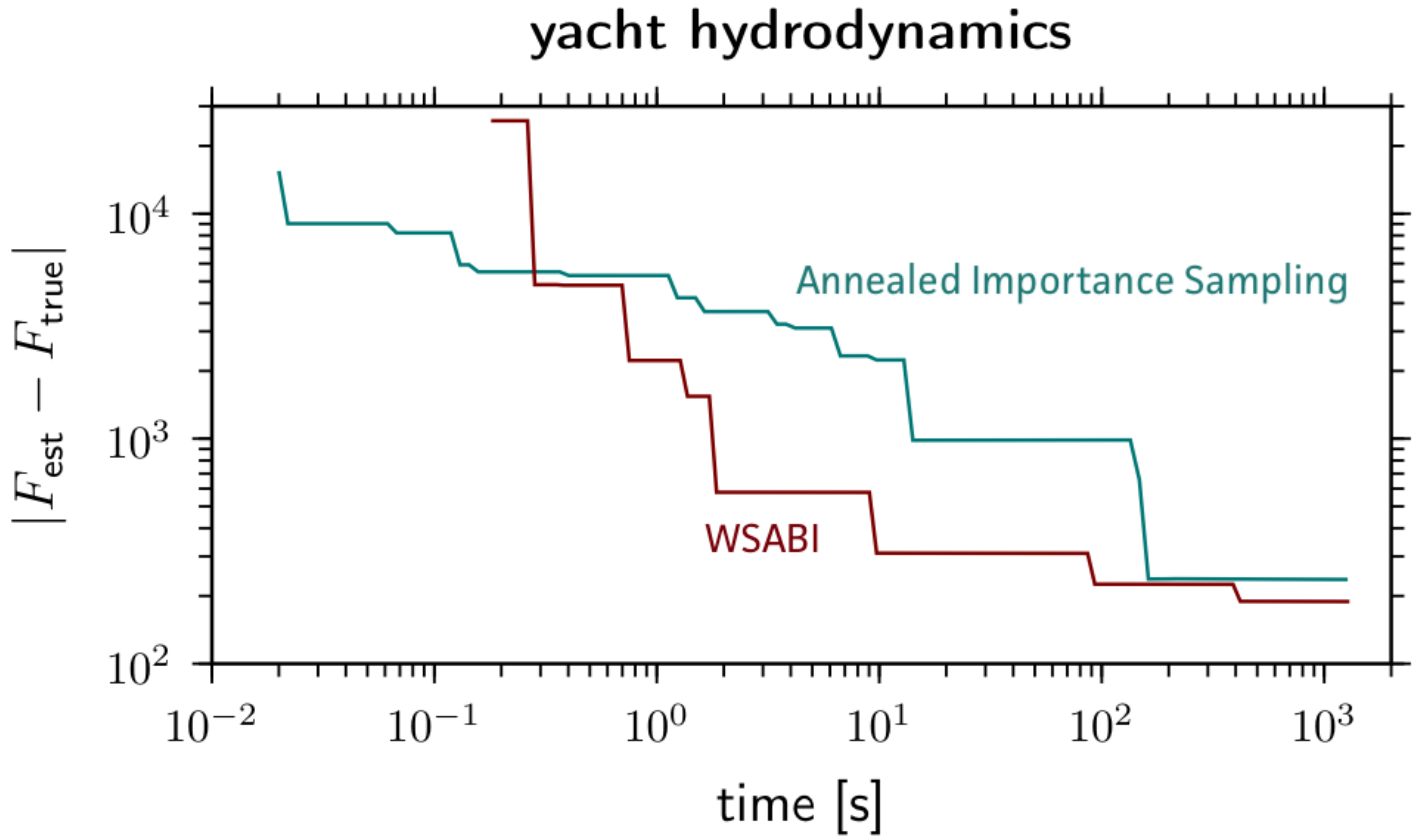

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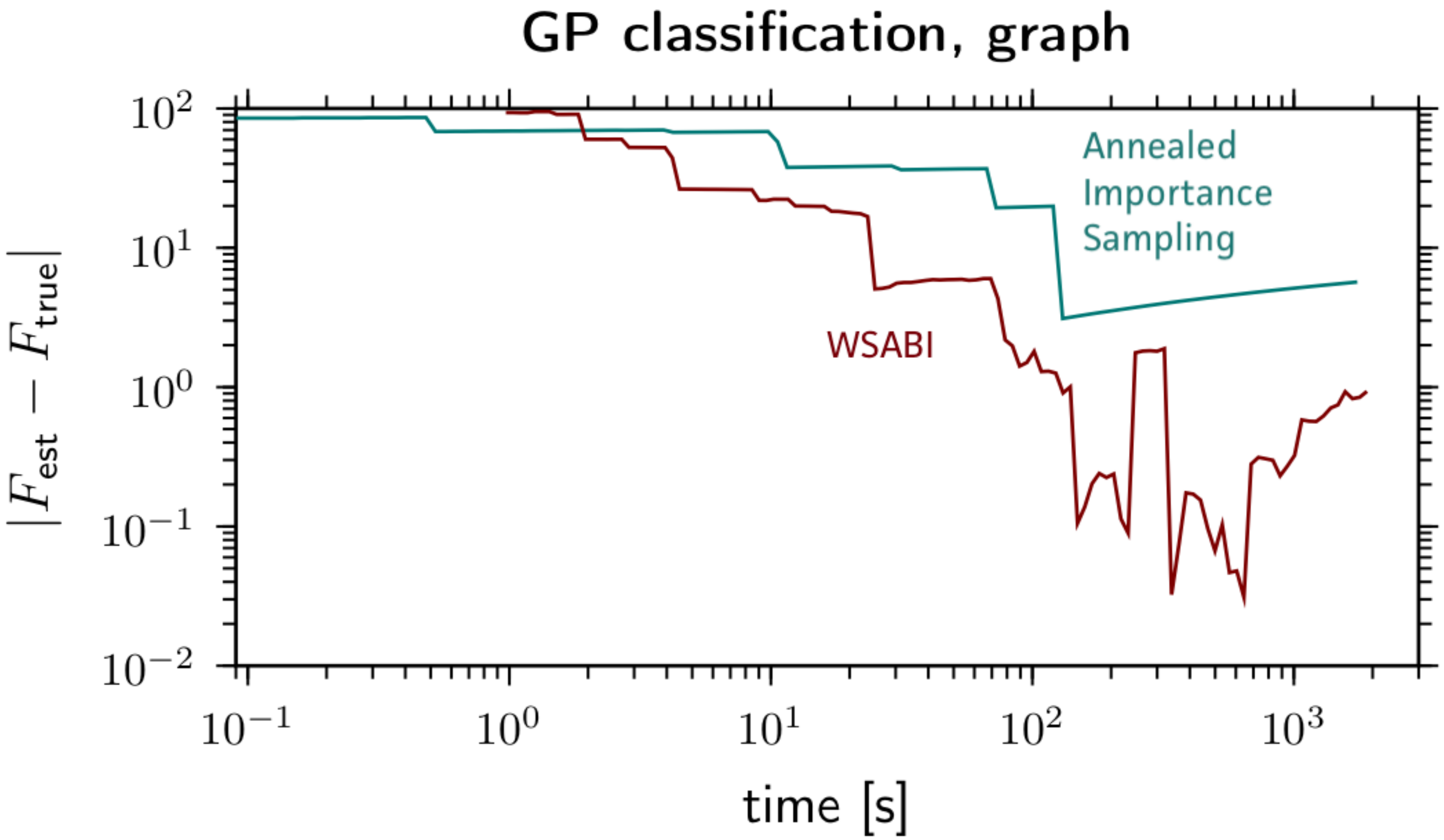

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Overhead can set you free.

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A RANDOM NUMBER IS A DECISION.

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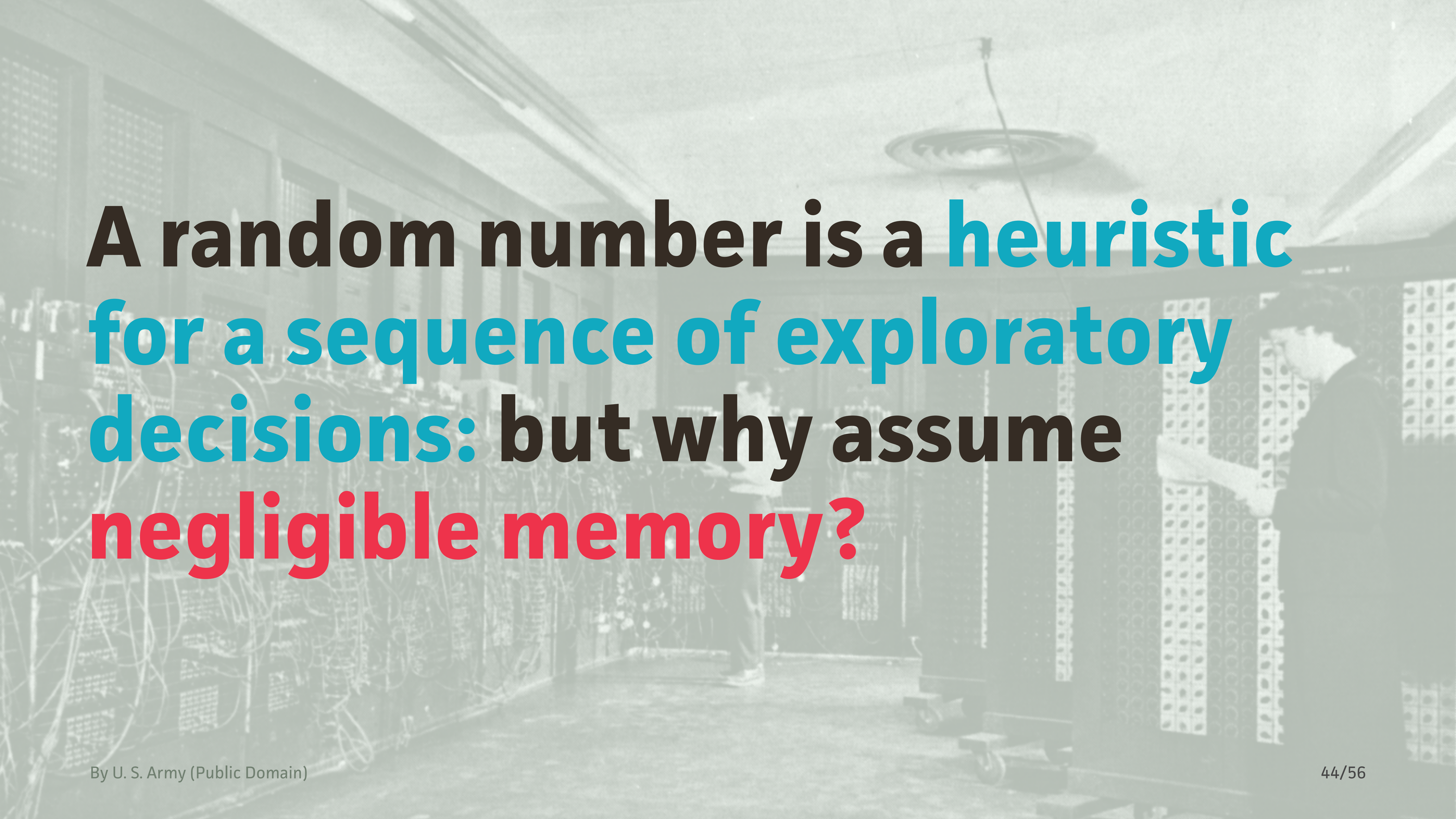
A random number assumes a completely flat expected loss.

A random number is a heuristic for a sequence of exploratory decisions: but why assume negligible memory?



By U. S. Army (Public Domain)

Using random numbers makes your algorithm **unimprovable.**

Source: By Jake Archibald from London, England - Sebastian Vettel - Ferrari - Halo, CC BY 2.0. References: Henderson et al. “Deep Reinforcement Learning that Matters” (2017); Islam et al. “Reproducibility of Benchmarked Deep Reinforcement Learning Tasks for Continuous Control” (2017); Colas, Sigaud, and Oudeyer. “How Many Random Seeds? Statistical Power Analysis in Deep Reinforcement Learning Experiments” (2018); Mania, Guy, and Recht. “Simple random search provides a competitive approach to reinforcement learning” (2018).

A random number may be intended to be **unbiased**, but there are **no adversaries in numerics.**

Source: Brown, Mané, Roy, Abadi & Gilmer (2017) "Adversarial Patch".

Quiz: which of these sequences is random?

1. 6224441111111114444443333333
2. 1693993751058209749445923078
3. 7129042634726105902083360448
4. 1000111111011111111001010000

Quiz: which of these sequences is **random?**

1. 6224441111111114444443333333: seven d6 rolls with i repeats of the ith roll.
2. 1693993751058209749445923078: the 41st to 70th digits of π.
3. 7129042634726105902083360448: this sequence was generated by the von Neumann method with seed 908344.
4. 1000111111011111111001010000: digits taken from a CD-ROM published by George Marsaglia.

A finite string of random numbers is **encoding some bias!**

Recall:

1. numeric error is significant;

2. numeric methods are generic;

3. our numerics problems tax our computation.

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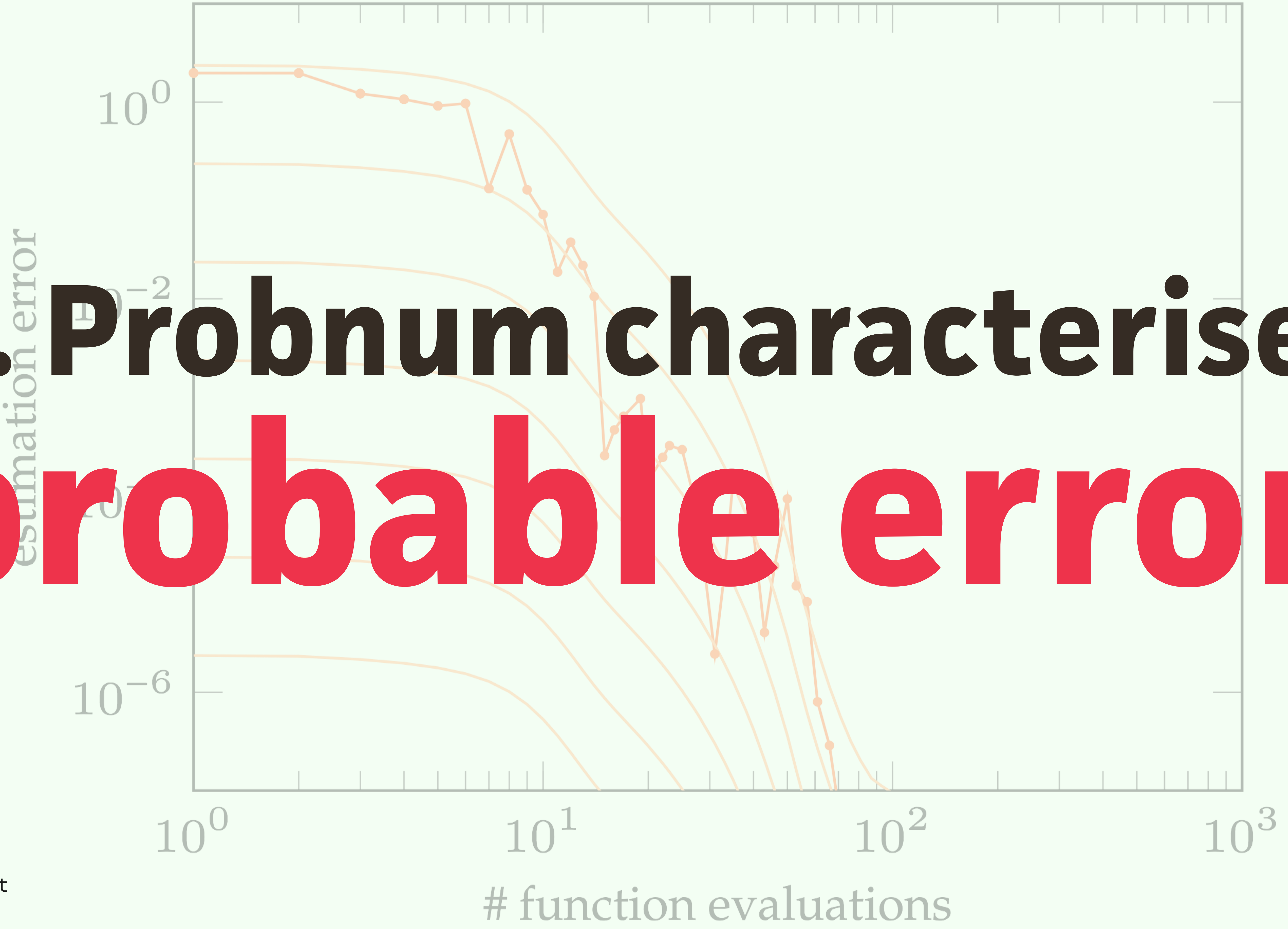
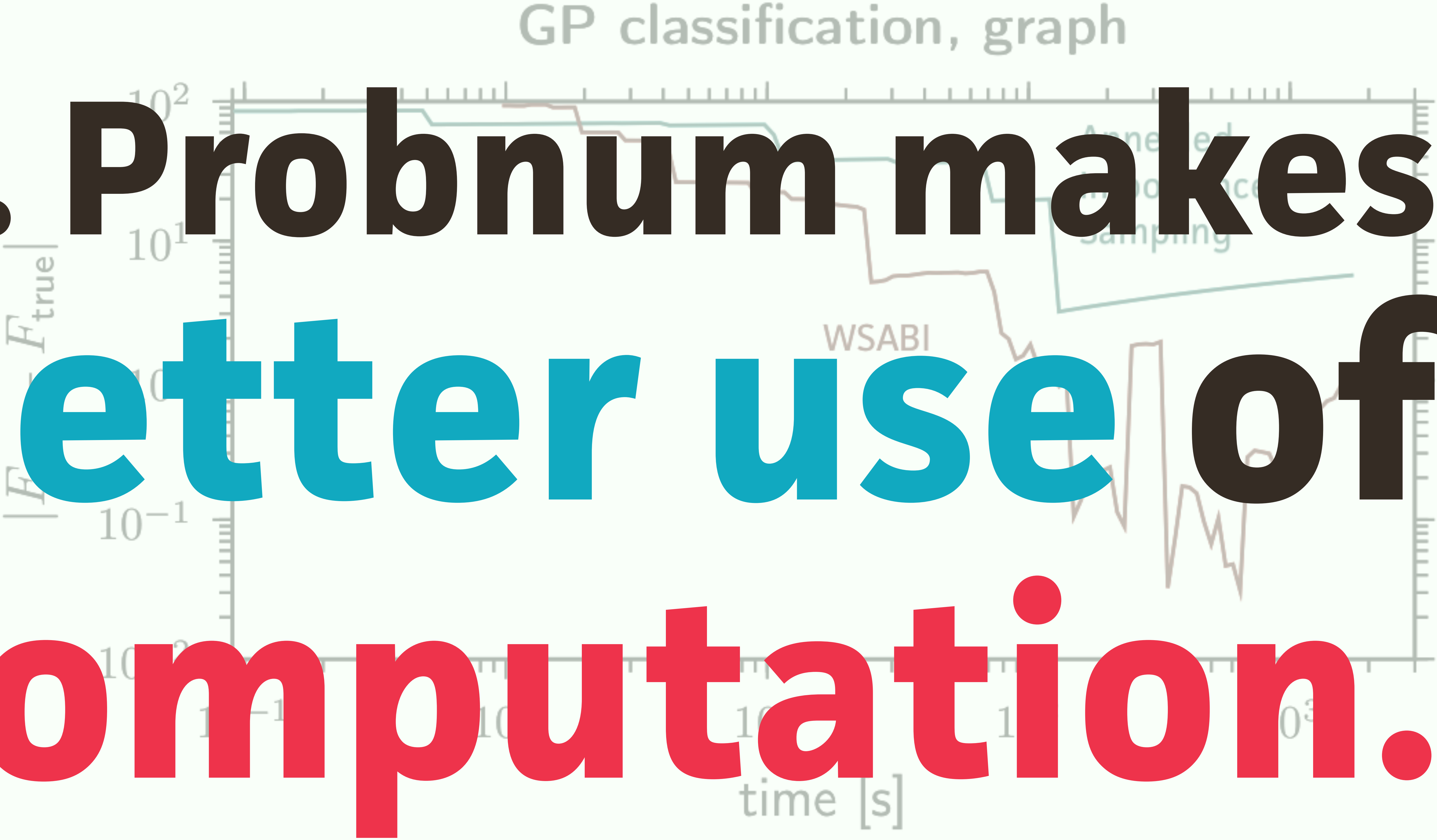
1. Probnum characterises **probable error.**



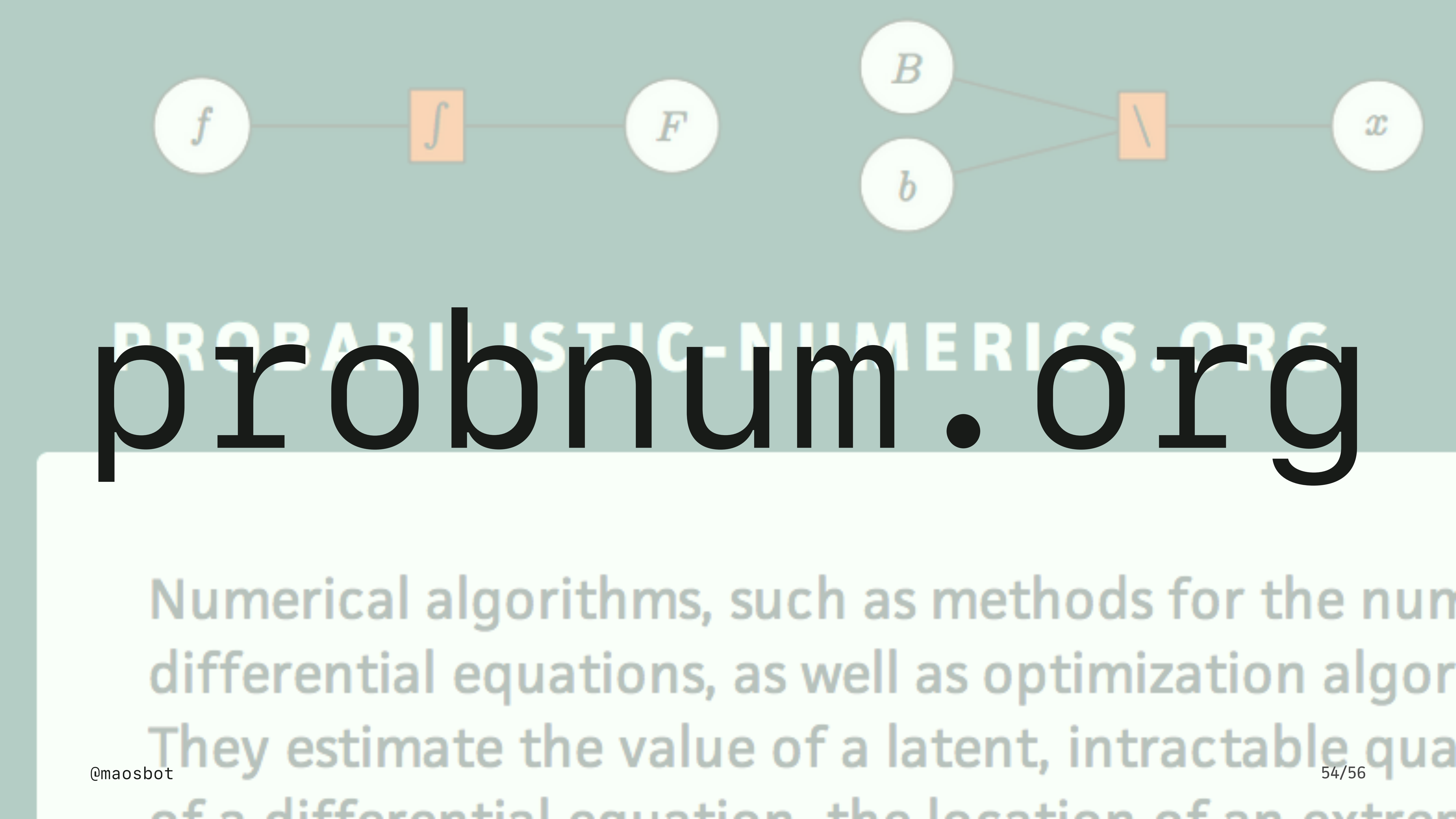
2. Probnum tailors procedures to problems.

3. Probnum makes better use of computation.



PROBABILISTIC-NUMERICS.ORG

Numerical algorithms, such as methods for the num
differential equations, as well as optimization algor
They estimate the value of a latent, intractable qua


f
F
B
b
x
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Numerical algorithms, such as methods for the num
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LITERATURE

This page collects literature on all areas of probab
not hesitate to contact us. The fastest way to get
file in /_bibliography, then either send us a pull-re

QUICK-JUMP LINKS:

- General and Foundational
- Quadrature
- Linear Algebra
- Optimization
- Ordinary Differential Equations
- Partial Differential Equations

Huge thanks to **Philipp Hennig.**