Integration of Parametrized Integrands

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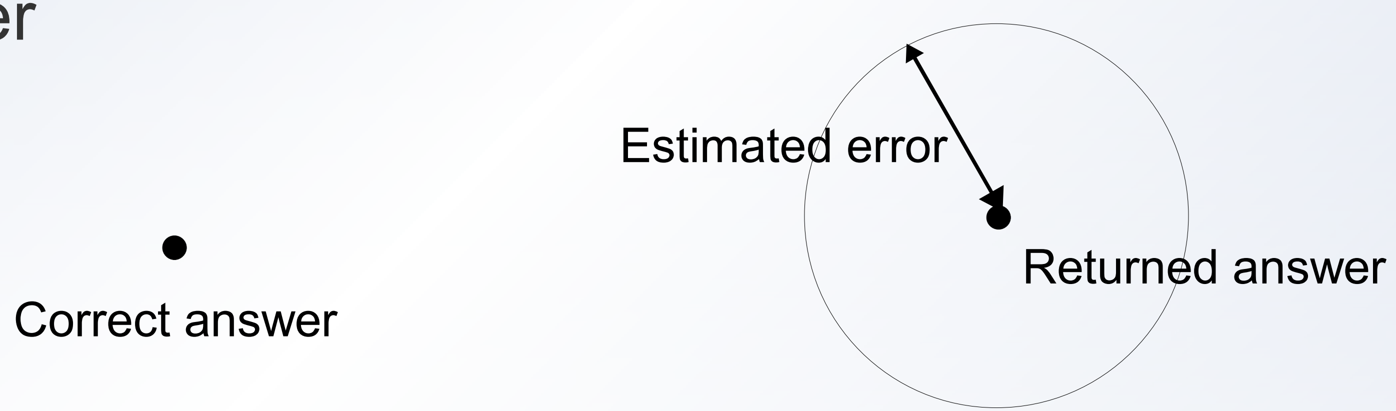
Lecture Outline

- Motivation
- Problem Statement
- Attempts using standard routines and packages
- Our approach
  - Residue Integration
  - Rational Approximation
  - Parameters handles through function composition
  - Theoretical Relative Error
- Further Speedup

Motivation

- Integration routines provided by scientific libraries and packages are widely used in computer simulations
- It is possible that such routines return answers coupled with a small error estimate that does not contain the real answer



- Here we present a case study and an alternative method employed to obtain reliable integration results

The Integral

- All integration problems in our simulation can be reduced to the following integral:

$$I(\alpha,\beta,\gamma,\delta,\xi)=\int_0^1\int_0^\infty \frac{\exp\left(-\left(\frac{u-\alpha}{\beta}\right)^2-\left(\frac{v-\gamma}{\delta}\right)^2-\frac{v}{c_0-u\,c_1}-\xi\right)}{c_0-u\,c_1}\,dv\,du$$

- We used Maple to evaluate the integral when $c_0 = 1$ and $c_1 = 0.9$ using various precisions:

```
> Digits := 16; I_(0.9138181, 0.09564921, 0.5759114, 4.1584, 1.47815);
    0.00097...
> Digits := 32; I_(0.9138181, 0.09564921, 0.5759114, 4.1584, 1.47815);
    0.00687...
> Digits := 64; I_(0.9138181, 0.09564921, 0.5759114, 4.1584, 1.47815);
    0.02194...
> Digits := 128; I_(0.9138181, 0.09564921, 0.5759114, 4.1584, 1.47815);
    0.03221...
```

Other Attempts, Packages and Libraries

- Several other numerical integration routines were explored
  - Mathematica and MatLab showed similar problems to Maple
- Both accuracy and speed are of crucial importance
  - The GNU Scientific Library offers an API to calculate integrals
    - The result reported was 0.00013 with an estimated relative error below 2.0e-8
    - GSL takes about 0.0365 seconds to produce an answer
  - The Numerical Algorithms Group library gave comparable results

Major drawback and alternative solution

- We hand-coded 128 and 256-point Gauss-Laguerre quadrature
- For some parameters, not even the 256-point quadrature could approximate the actual integral
  - Over 160% relative error
- Furthermore, significant additional speedup was desired
- Following is the description of our implementation to solve this problem

Integration by residues

- A well known integration technique involves contour integrals and Cauchy's residue Theorem
  - Computing the integral is thus reduced to evaluating residues
  - It requires, however, choosing contours to evaluate it
- Boas and Schoenfeld discussed in 1966 a variant of integration through residues of a function on the *Riemann Sphere*
  - No contours are thus needed to evaluate integrals

Integration (Main Theorem)

- Three integral types are discussed in the article, the second one being the one used in this approach:

Theorem 1. Let F be holomorphic in the Riemann sphere except for a finite number of singularities. Let F be holomorphic on (u,v) except for simple poles and let F be holomorphic at u and v. Then

$$P.V. \int_u^v F(t)\,dt = -(R+r)$$

where R is the sum of the residues of $F(z)\, log((z\text{-}u)/(z\text{-}v))$ for z in the Riemann sphere but not in $[u,v]$, and r is the sum of residues of $F(z)\, log((z\text{-}u)/(v\text{-}z))$ for $z \in (u,v)$

Evaluating the Integral

- After further manipulations, the integral can be reduced to

$$\int_u^v \exp\left(-\left(\frac{t-a}{b}\right)^2+(t^{-1}-d)^2\right)\left(1-\operatorname{erf}(t^{-1}-d)\right)\frac{dt}{t}$$

- However, evaluating this integral by means of Theorem 1 requires computing the residue of the (essential) singularity at infinity and zero
  - This is a difficult task!

The Residues at Infinity and Zero

- Let $F(z)$ be a complex function with, say, an essential singularity at zero with Laurent series

$$F(z) = \sum_{n=-\infty}^{\infty} a_n z^n$$

- Observe that $log((z\text{-}u)/(v\text{-}z))$ is holomorphic around zero (assuming u and v are non-zero)
  - It actually has non-zero coefficients for all terms in its series expansion

$$\log\left(\frac{z-u}{v-z}\right) = \sum_{n=0}^{\infty} b_n z^n$$

The Residues at Infinity and Zero

- Therefore, *F(z) log((z-u)/(v-z))* will have a residue at zero given by the residue of:

$$F(z)\log\left(\frac{z-u}{z-v}\right)=\left(\sum_{i=-\infty}^{\infty} a_i z^i\right)\left(\sum_{j=0}^{\infty} b_j z^j\right)$$

- Note that the residue would be an infinite series expansion resulting from the product of the two expansions

$$\sum_{k=0}^{\infty} a_{1-k} b_k$$

- Analogously if the essential singularity is at infinity

Approximation of the Integrand

- Fortunately, essential singularities can be removed by approximating the integrand using meromorphic functions
  - Meromorphic functions on the Riemann sphere are always rational functions
  - Approximations can be done over several pieces to cover the whole integration interval
    - There is a trade-off between number of poles/complexity of residues and the number of pieces that approximate the integrand
    - Neither computing many rational approximations at compile-time nor computing them at run-time is feasible

Preparing the Integrand

- First, we split the integrand into three factors:

$$\exp\left(-\left(\frac{t-a}{b}\right)^2+(t^{-1}-d)^2\right)\left(1-erf(t^{-1}-d)\right)\frac{1}{t}$$

$$\exp(-x),\ x=\left(\frac{t-a}{b}\right)^2 \qquad q(w)=\exp(w^2)(1-erf(w)),\ w=\frac{1}{t}-d \qquad \frac{1}{t}$$

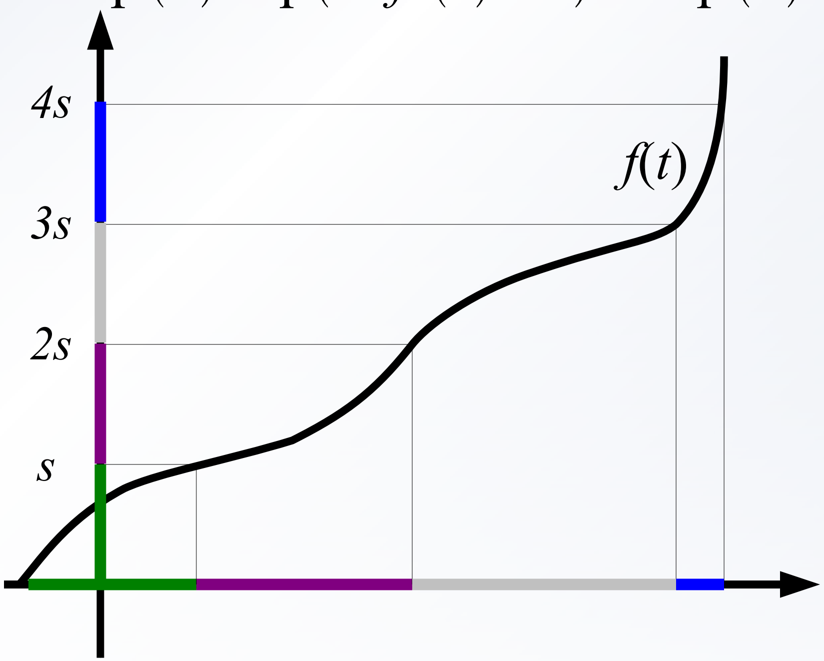
- Notice that the factors are chosen such that all the parameters are contained in a function that is composed with another function without parameters

- The parameterless functions ($\exp(-x)$ and $q(w)$) are the ones that will be approximated with rational functions

Exponential approximation

- The exponential function has an advantage when dealing with approximations of large intervals
  - One approximation can be *shifted* to cover arbitrary parts of the real line

$$\exp(-f(t)) = \exp(s)\exp(-f(t)-s) \approx \exp(s)\, rational_0(f(t)+s)$$



Approximation of $q(w)$

$$q(w) = \exp(w^2)(1 - erf(w)), \; w = \frac{1}{t} - d$$

- We can approximate $q(w)$ with only 4 rational functions:

$$2\exp(w^2), \; w \in (-\infty, -3]$$

$$rational_1(w), \; w \in [-3, 0]$$

$$rational_2(w), \; w \in [0, 10]$$

$$rational_3(w) = \frac{1}{\sqrt{\pi}\, w} - \frac{1}{2\sqrt{\pi}\, w^3}, \; w \in [10, \infty)$$

Calculating Rational Function Approximations

- $rational_3$ is composed of the first two terms in the series expansion of $q(w)$ at infinity

- All other rational functions were computed with Maple's implementation of the Remez algorithm

  - These approximations are holomorphic in $[u,v]$

  - All numerators are of degree less than or equal to that of the its denominator, thus

$$\frac{-1}{t^2} rational_k\left(\frac{1}{t}\right) t \log\left(\frac{1-tu}{1-tv}\right)$$

    is holomorphic at $t=0$ and therefore the residue at infinity is zero

Preparation to Compute the Residues

- Except for *rational*$_3$, all approximations have simple poles located off the real line and their partial fraction expansion consist of terms of the form

$$\frac{\xi}{z-\zeta}$$

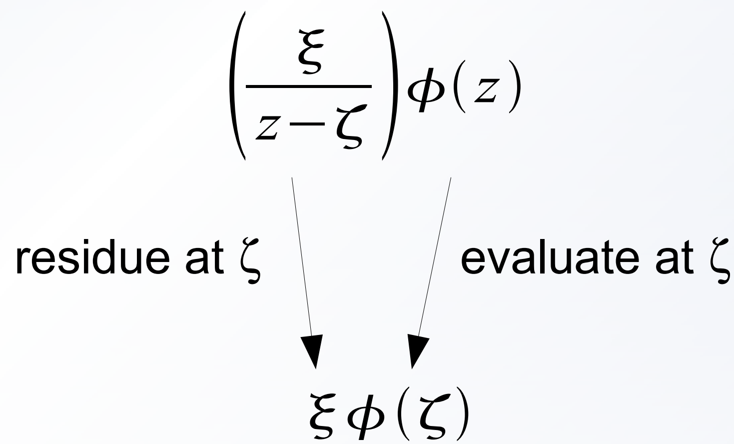
- This is because in our case, the numerator have degree strictly of smaller degree than its denominator

- Following are two lemmas that would help us compute residues of complicated function from simpler ones

Product of Factors Lemma

Lemma 2. Let ψ have a simple pole at ζ with residue ξ. If ϕ is holomorphic at ζ, then the residue of $\psi(z)\phi(z)$ at $z = \zeta$ is $\xi\phi(\zeta)$

- This effectively allows us to compute the residue of a product of two functions by calculating the residue of one of them, and then multiplying by the value of the other function evaluated at the singularity



Composition Lemma

Lemma 3. Let ζ be a point of the Riemann sphere where either $\phi'(\zeta) \neq 0$ or else ϕ has a simple pole. Let $w = \phi(\zeta)$ and let ψ either be holomorphic at w or have an isolated singularity there. If φ is a local inverse of ϕ in a neighborhood of w, then the residue of $\psi(\phi(z))$ at $z = \zeta$ is equal to the residue of $\psi(z)\varphi'(z)$ at $z = w$

- This effectively allows us to compute the residue of a composition of two functions by calculating the derivative of the inverse of the inner-most function. For example

$$\phi(z)=\frac{1}{z}-d\,,\ \psi(t)=\frac{x}{t-y}\,,\ w=y\,,\ \zeta=\frac{1}{y+d}\,,\ \frac{1}{\phi'(\zeta)}=-\zeta^2$$

residue of ψ at y

derivative of inverse at ζ

$$residue(\psi(\phi(z)),z=\zeta)=x(-(y+d)^{-2})$$

Computing the Residues

- Four cases are explored:

$$rational_3(t^{-1}-d)/t\frac{\xi}{((t-a)/b)^2+s-\zeta}\log\left(\frac{t-u'}{t-v'}\right)$$

  - At $t = 1/d$. A symbolical computation of the residue was obtained with Maple

$$rational_k(t^{-1}-d)/t\frac{\xi}{((t-a)/b)^2+s-\zeta}\log\left(\frac{t-u'}{t-v'}\right)$$

  - At $t=a\pm b\sqrt{\zeta-s}$. When k is either 1 or 2

$$rational_0(((t-a)/b)^2+s)/t\frac{\xi}{t^{-1}-d-\zeta}\log\left(\frac{t-u'}{t-v'}\right)$$

  - At $t = 1/(d+\zeta)$. The last two cases are solved using Lemma 2 and 3

Theoretical Relative Error

- Let A be an approximation to the positive integrand F with relative error over $[u,v]$

$$e = \|1 - A/F\|_\infty$$

- Then, the relative error between the integral of A and that of F is

$$\left|1 - \frac{\int A}{\int F}\right| = \left|\frac{\int F(1 - A/F)}{\int F}\right| \leqslant \frac{\int F|1 - A/F|}{\int F} \leqslant \|1 - A/F\|_\infty = e$$

- All our approximations have a relative error less than 0.1%.

Further Speedup

- To further speed up the computation, a version of *lazy evaluation* is implemented:
  - It is possible to estimate the sub-intervals that will have the highest contribution to the integral. Those are evaluated first
  - Computation stops when rest of sub-intervals are estimated to contribute less than 0.1% of the result computed so far
  - Typical time to evaluate the original integration problem is 0.000048 seconds compared to 0.0365 seconds taken by the GNU Scientific library

Acknowledgments

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QUESTIONS?