Adaptive Envelope Rejection Sampling

Applied to Log-concave Densities

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November 7, 2022

Rejection Sampling

Let f, g be densities on $\mathbb{R}$ with $\alpha f \leq g$ for $\alpha > 0$. Let $U_1, U_2, \ldots$ be i.i.d. with uniform distribution and $Y_1, Y_2 \ldots$ be i.i.d. with density g independent of the U_i's. Define the stopping time

$$\sigma = \inf\{n \geq 1 \mid U_n \leq \alpha f(Y_n)/g(Y_n)\}. \tag{1}$$

Then Y_σ has density f. The densities need not be normalized, however, if they are then $\alpha \in (0, 1]$ and $1 - \alpha$ is the probability of rejection.

Rejection Sampling

Implementation

```
rejection_sampling <- function(n,
                               density,
                               env_density,
                               env_sampler,
                               alpha,
                               seed = NULL) {
  if(!is.null(seed)) set.seed(seed)
  samples <- numeric(n)
  succes <- tries <- 0
  for(s in 1:n) {
    reject <- TRUE
    while(reject) {
      tries <- tries + 1
      u0 <- runif(1)
      y0 <- env_sampler()
      env_y0 <- env_density(y0)
      dens_y0 <- density(y0)
      if(u0 <= alpha * dens_y0 / env_y0) {
        reject <- FALSE
        samples[s] <- y0
        succes <- succes + 1
      }
    }
  }
  list(samples, (tries - succes) / tries)
}
```

Rejection Sampling

Case Study

Let f be the density with

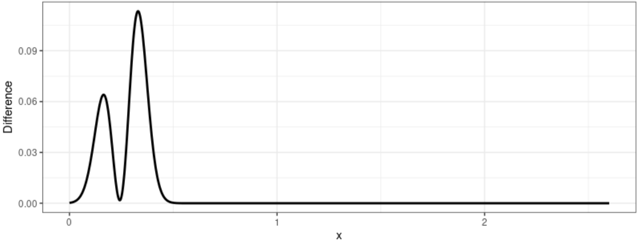
$$f(y) \propto p(y) = \prod_{i=1}^{100} \exp(y z_i x_i - e^{y x_i}). \tag{2}$$

```
poisreg <- function(x, z) {
  force(x); force(z)
  function(y) {
    expyx <- sapply(y, function(s) sum(exp(s * x)))
    exp(y * sum(x * z) - expyx)
  }
}
poisreg_derv <- function(x, z) {
  force(x)
  force(z)
  function(y) {
    expyx <- sapply(y, function(s) sum(exp(s * x)))
    x_expyx <- sapply(y, function(s) sum(x * exp(s * x)))
    xz <- sum(x * z)
    exp(y * xz - expyx) * (xz - x_expyx)
  }
}
```

Rejection Sampling

A Gaussian Envelope

The function $e^{(x-0.2423914)^2/(2\cdot 0.004079805)}$ is an envelope of p with $\alpha = 1.351351 \cdot 10^{40}$.



Adaptive Rejection Sampling

```
adap_samp <- function(n, density, density_deriv, p, zb = c(-Inf, Inf), seed = NULL) {
  if(!is.null(seed)) set.seed(seed)
  p <- sort(unique(p))
  densp <- density(p)
  a <- density_deriv(p) / densp
  b <- log(densp) - a * p
  a_diff <- a[-length(a)] - a[-1]
  check1 <- a[1] < 0 & zb[1] == -Inf
  check2 <- a[length(a)] > 0 & zb[2] == Inf
  if(check1 | check2)
    stop("Envelope is not integrable. Choose different points.")
  if(any(a == 0) | any(a_diff == 0))
    stop("Division by zero. Choose different points.")
  z <- c(zb[1], (b[-1] - b[-length(b)]) / a_diff, zb[2])
  env_quantile <- get_env_quantile(a, b, z)
  env_density <- get_env_density(a, b, z)
  samples <- numeric(n)
  succes <- tries <- 0
  for(s in 1:n) {
    reject <- TRUE
    while(reject) {
      tries <- tries + 1
      u0 <- runif(2)
      y0 <- env_quantile(u0[1])
      env_y0 <- env_density(y0)
      dens_y0 <- density(y0)
      if(u0[2] <= dens_y0 / env_y0) {
        reject <- FALSE
        succes <- succes + 1
        samples[s] <- y0
      }
    }
  }
  list(samples, (tries - succes) / tries)
}
```

Adaptive Rejection Sampling - Continued

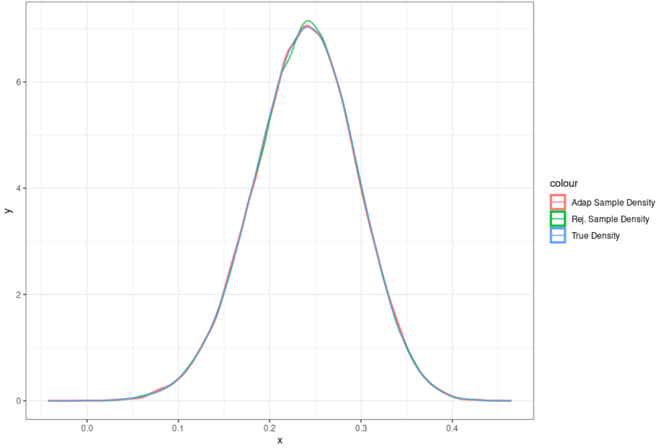
Implementation

```
get_env_quantile<- function(a, b, z) {
  force(a); force(b); force(z)
  az <- a * z[-length(z)]
  R <- exp(b) * (exp(a * z[-1]) - exp(az)) / a
  Q1 <- numeric(length(a) + 1)
  Q1[2:length(Q1)] <- cumsum(R)
  c <- Q1[length(Q1)]
  function(q) {
    ind <- c * q <= Q1
    maxi <- which.max(ind) - 1
    y <- c * q - Q1[maxi]
    log(a[maxi] * y * exp(-b[maxi]) + exp(az[maxi])) / a[maxi]
  }
}

get_env_density <- function(a, b, z) {
  force(a); force(b); force(z)
  function(x) {
    if(x > z[length(z)] | x < z[1]) return(0)
    maxi <- which.max(x <= z) - 1
    exp(a[maxi] * x + b[maxi])
  }
}
```

Comparison of the Implementations

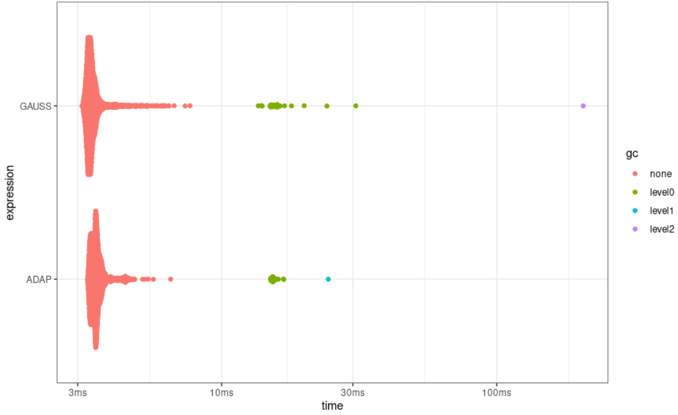
Simulating 100.000 samples with each implementation using the same seed. Using 0.15, 0.2, 0.28, 0.32 as the envelope points. The adaptive envelope had 0.09 rate of rejection and the gaussian envelope had 0.11 rate of rejection.



Comparison of the Implementations

Benchmarks Using `bench` Package

Benchmarking sampling 100 samples.



Comparison of the Implementations

Benchmarks Using bench Package

Benchmarking sampling 100 samples.

	expression	min	median	itr/s…[1]	mem_a…[2]
	<bch:expr>	<bch:tm>	<bch:tm>	<dbl>	<bch:b>
1	GAUSS	3.18ms	3.36ms	289.	794KB
2	ADAP	3.73ms	4ms	248.	480KB

Profiling the Implementation Using `profvis` Package

```r
adap_samp <- function(n, density, density_deriv, p, zb = c(-
Inf, Inf), seed = NULL) {
  if(!is.null(seed)) set.seed(seed)
  p <- sort(unique(p))
  densp <- density(p)
  a <- density_deriv(p) / densp
  b <- log(densp) - a * p
  a_diff <- a[-length(a)] - a[-1]
  check1 <- a[1] > 0 & a[length(a)] <0
  check2 <- a[length(a)] < 0 & is.finite( zb[1])
  check3 <- a[1] > 0 & is.finite(zb[2])
  if(!(check1 | check2 | check3))
    warning("Envelope is not integrable. Choose different
points.")
  if(any(a == 0) | any(a_diff == 0))
    stop("Divison by zero. Choose different points.")
  z <- c(zb[1], (b[-1] - b[-length(b)]) / a_diff, zb[2])
  env_quantile <- get_env_quantile(a, b, z)
  env_density <- get_env_density(a, b, z)
  samples <- numeric(n)
  succes <- tries <- 0
  for(s in 1:n) {
    reject <- TRUE
    while(reject) {
      tries <- tries + 1
      u0 <- runif(2)
      y0 <- env_quantile(u0[1])
      env_y0 <- env_density(y0)
      dens_y0 <- density(y0)
      if(u0[2] <= dens_y0 / env_y0) {
        reject <- FALSE
        succes <- succes + 1
        samples[s] <- y0
      }
```

`env_quantile <- get_env_quantile(a, b, z)`		0.4	20
`while(reject) {`		1.1	10
`u0 <- runif(2)`	-51.5	46.5	350
`y0 <- env_quantile(u0[1])`	-53.3	39.1	320
`env_y0 <- env_density(y0)`	-72.1	43.6	400
`dens_y0 <- density(y0)`	-203.7	256.3	2170
`if(u0[2] <= dens_y0 / env_y0) {`		3.0	30
`succes <- succes + 1`		1.7	10
`samples[s] <- y0`		1.0	10

Profiling the Implementation Using `profvis` Package

```
get_env_quantile<- function(a, b, z) {
  force(a); force(b); force(z)
  az <- a * z[-length(z)]
  R <- exp(b) * (exp(a * z[-1]) - exp(az)) / a
  Q1 <- numeric(length(a) + 1)
  Q1[2:length(Q1)] <- cumsum(R)
  c <- Q1[length(Q1)]
  function(q) {                                                             1.7    10
    ind <- c * q <= Q1                                                      7.1    50
    maxi <- which.max(ind) - 1                                              5.0    40
    y <- c * q - Q1[maxi]                                                   3.8    30
    log(a[maxi] * y * exp(-b[maxi]) + exp(az[maxi])) / a[maxi]     -20.1    7.7    60
  }
}

get_env_density <- function(a, b, z) {
  force(a); force(b); force(z)
  function(x) {                                                             2.2    20
    if(x > z[length(z)] | x < z[1]) return(0)                      -40.8   18.0   170
    maxi <- which.max(x <= z) - 1                                  -10.6   15.2   120
    exp(a[maxi] * x + b[maxi])                                     -20.8   14.5   120
  }
}
```

Profiling the Implementation Using `profvis` Package

```r
poisreg <- function(x, z) {
  force(x)
  force(z)
  function(y) {
    expyx <- sapply(y, function(s) sum(exp(s * x)))
    exp(y * sum(x * z) - expyx)
  }
}
```

-194.0	271.6	2180
-46.8	28.8	240

Improving the Implementation

Optimizing use of runif

```
u_samples <- runif(2 * n); k_stop <- n; k <- 1
succes <- tries <- 0
for(s in 1:n) {
  reject <- TRUE
  while(reject) {
    tries <- tries + 1
    if(k == k_stop) {
      u_samples <- runif(2 * (n - (s - 1)))
      k_stop <- n - (s - 1) + 1
      k <- 1
    }
    u0 <- u_samples[2 * (k - 1) + 1]
    u1 <- u_samples[2 * (k - 1) + 2]
    k <- k + 1
    y0 <- env_quantile(u0)
    env_y0 <- env_density(y0)
    dens_y0 <- density(y0)
    if(u1 <= dens_y0 / env_y0) {
      reject <- FALSE
      samples[s] <- y0
      succes <- succes + 1
    }
  }
}
```

Improving the Implementation

Implementation of Envelope Quantile and Density Function in RCPP

```cpp
// [[Rcpp::export]]
double RCPP_env_density(double x,
                        NumericVector a,
                        NumericVector b,
                        NumericVector z) {
  int m = z.size();
  if(x < z[0] || x > z[m - 1]) return 0;
  int maxi;
  for(maxi = 1; maxi < m; ++maxi)
    if(x <= z[maxi]) break;
  maxi -= 1;
  return std::exp(a[maxi] * x + b[maxi]);
}

// [[Rcpp::export]]
double RCPP_env_quantile(double x,
                         NumericVector a,
                         NumericVector b,
                         NumericVector z,
                         NumericVector az,
                         NumericVector Q) {
  int m = Q.size(), maxi;
  double c = Q[m - 1];
  for(maxi = 0; maxi < m; ++maxi)
    if(c * x <= Q[maxi]) break;
  maxi -= 1;
  double y = c * x - Q[maxi];
  return std::log(a[maxi] * y *
                  std::exp(-b[maxi]) + std::exp(az[maxi])) / a[maxi];
}
```

Improving the Implementation

Implementation of Envelope Quantile and Density Function in RCPP

```
get_env_quantile_cpp<- function(a, b, z) {
  force(a); force(b); force(z)
  az <- a * z[-length(z)]
  R <- exp(b) * (exp(a * z[-1]) - exp(az)) / a
  Q1 <- numeric(length(a) + 1)
  Q1[2:length(Q1)] <- cumsum(R)
  c <- Q1[length(Q1)]
  function(q) {
    RCPP_env_quantile(q, a, b, z, az, Q1)
  }
}

get_env_density_cpp <- function(a, b, z) {
  force(a); force(b); force(z)
  function(x) {
    RCPP_env_density(x, a, b, z)
  }
}
```

Improving the Implementation

Benchmarking

	expression	min	median	itr/s…[1]	mem_a…[2]	g
	<bch:expr>	<bch:tm>	<bch:>	<dbl>	<bch:b>	
1	GAUSS	3.11ms	3.34ms	281.	794KB	
2	ADAP	3.28ms	3.52ms	275.	488KB	
3	ADAP_STR	2.94ms	3.16ms	313.	216KB	
4	ADAP_STR_CPP	3.64ms	3.83ms	257.	794KB	

Improving the Implementation

Partial RCPP Implementation

```
// [[Rcpp::export]]
List RCPP_adap_samp_partial(int n,
                            Function density,
                            NumericVector a,
                            NumericVector b,
                            NumericVector z) {
  int m = a.size();
  std::vector<double> Q(m + 1);
  std::vector<double> az(m);
  Q[0] = 0;
  for(int i = 1; i < m + 1; ++i) {
    az[i - 1] = a[i - 1] * z[i - 1];
    Q[i] = Q[i - 1] +
      std::exp(b[i - 1]) *
      (std::exp(a[i - 1] * z[i]) - std::exp(az[i - 1])) / a[i - 1];
  }
  NumericVector samples(n);
  int accepts = 0, tries = 0;
  for(int i = 0; i < n; ++i) {
    int reject = 1;
    while(reject == 1) {
      ++tries;
      double u0 = R::runif(0, 1);
      double u1 = R::runif(0, 1);
      double y0 = env_quantile(u0, a, b, az, Q);
      double env_y0 = env_density(y0, a, b, z);
      NumericVector dens_y0 = density(y0);
      if(u1 <= dens_y0[0] / env_y0) {
        reject = 0;
        samples[i] = y0;
        ++accepts;
      }
    }
  }
  NumericVector rate(1);
  rate[0] = ((double) tries - (double) accepts) / (double) tries;
  return List::create(samples, rate);
}
```

Improving the Implementation

Partial RCPP Implementation

```
double env_quantile(double x,
                    NumericVector &a,
                    NumericVector &b,
                    std::vector<double> &az,
                    std::vector<double> &Q) {
  int n = a.size();
  double c = Q[n];
  int maxi;
  for(maxi = 0; maxi < n + 1; ++maxi)
    if(c * x <= Q[maxi]) break;
  maxi -= 1;
  double y = c * x - Q[maxi];
  return std::log(a[maxi] * y * std::exp(-b[maxi]) +
                  std::exp(az[maxi])) / a[maxi];
}

double env_density(double x,
                   NumericVector &a,
                   NumericVector &b,
                   NumericVector &z) {
  int n = a.size();
  if(x > z[n] || x < z[0])
    return 0;
  int maxi;
  for(maxi = 0; maxi < n + 1; ++maxi)
    if(x <= z[maxi]) break;
  maxi -= 1;
  return std::exp(a[maxi] * x + b[maxi]);
}
```

Improving the Implementation

Partial RCPP Implementation

```
adap_samp_cpp_partial <- function(n,
                                  density,
                                  density_deriv,
                                  p,
                                  zb = c(-Inf, Inf),
                                  seed = NULL) {
  if(!is.null(seed)) set.seed(seed)
  p <- sort(unique(p))
  densp <- density(p)
  a <- density_deriv(p) / densp
  b <- log(densp) - a * p
  a_diff <- a[-length(a)] - a[-1]
  check1 <- a[1] < 0 & zb[1] == -Inf
  check2 <- a[length(a)] > 0 & zb[2] == Inf
  if(check1 | check2)
    stop("Envelope is not integrable. Choose different points.")
  if(any(a == 0) | any(a_diff == 0))
    stop("Divison by zero. Choose different points.")
  z <- c(zb[1], (b[-1] - b[-length(b)]) / a_diff, zb[2])

  RCPP_adap_samp_partial(n, density, a, b ,z)
}
```

Improving the Implementation

Benchmark

	expression	min	median	`itr/sec`	mem_al…[1]
	<bch:expr>	<bch:tm>	<bch:tm>	<dbl>	<bch:byt>
1	GAUSS	3.12ms	3.31ms	293.	794KB
2	ADAP	3.28ms	3.53ms	280.	488KB
3	ADAP_STR	2.95ms	3.16ms	314.	216KB
4	ADAP_STR_CPP	3.63ms	3.82ms	257.	784KB
5	ADAP_PARTIAL_CPP	4.46ms	4.74ms	208.	401KB

Implementing Adaptive Envelope Sampling Using R's C API

```c
#include <R.h>
#include <math.h>
#include <Rinternals.h>
#include <R_ext/Random.h> // ACCESS TO UNIF NUMBER GENERATOR

SEXP C_adap_samp(SEXP n,
                 SEXP density,
                 SEXP a,
                 SEXP b,
                 SEXP z,
                 SEXP rho) {
  int m = length(a);
  int N = INTEGER(n)[0];
  double *Q = (double *)malloc(sizeof(double) * (m + 1));
  double *az = (double *)malloc(sizeof(double) * m);
  double *a_ = REAL(a), *b_ = REAL(b), *z_ = REAL(z);

  Q[0] = 0;
  for(int i = 1; i < m + 1; ++i) {
    az[i - 1] = a_[i - 1] * z_[i - 1];
    Q[i] = Q[i - 1] +
      exp(b_[i - 1]) * (exp(a_[i - 1] * z_[i]) - exp(az[i - 1])) /
      a_[i - 1];
  }
  SEXP density_call = PROTECT(lang2(density, R_NilValue));
  SEXP samples = PROTECT(allocVector(REALSXP, N));
  double *samples_ = REAL(samples);
  int accepts = 0, tries = 0;
  GetRNGstate();
  for(int i = 0; i < N; ++i) {
    int reject = 1;
    while(reject == 1) {
      ++tries;
      double u0 = unif_rand();
      double u1 = unif_rand();
      double y0 = env_quantile(u0, a_, b_, az, Q, m);
      double env_y0 = env_density(y0, a_, b_, z_, m);
      SETCADR(density_call, PROTECT(ScalarReal(y0)));
      SEXP dens_y0 = eval(density_call, rho);
      UNPROTECT(1);
      if(u1 <= REAL(dens_y0)[0] / env_y0) {
        reject = 0;
        samples_[i] = y0;
        ++accepts;
      }
    }
  }
  PutRNGstate();
  SEXP values = PROTECT(allocVector(VECSXP, 2));
  double rate = ((double) tries - (double) accepts) / (double) tries;
  SET_VECTOR_ELT(values, 0, samples);
  SET_VECTOR_ELT(values, 1, ScalarReal(rate));
  UNPROTECT(3);
  free(Q);
  free(az);
  return values;
}
```

Implementing Adaptive Envelope Sampling Using R's C API

```
double env_quantile(double x,
                    double *a,
                    double *b,
                    double *az,
                    double *Q,
                    int n) {
  double c = Q[n];
  int maxi;
  for(maxi = 0; maxi < n + 1; ++maxi)
    if(c * x <= Q[maxi]) break;
  maxi -= 1;
  double y = c * x - Q[maxi];
  return log(a[maxi] * y * exp(-b[maxi]) + exp(az[maxi])) / a[maxi];
}

double env_density(double x,
                   double *a,
                   double *b,
                   double *z,
                   int n) {
  if(x > z[n] || x < z[0])
    return 0;
  int maxi;
  for(maxi = 0; maxi < n + 1; ++maxi)
    if(x <= z[maxi]) break;
  maxi -= 1;
  return exp(a[maxi] * x + b[maxi]);
}
```

Implementing Adaptive Envelope Sampling Using R's C API

```
adap_samp_c <- function(n, density, density_deriv, p, seed = NULL, zb = c(-Inf, Inf)) {
  if(!is.null(seed)) set.seed(seed)
  p <- sort(unique(p))
  densp <- density(p)
  a <- density_deriv(p) / densp
  b <- log(densp) - a * p
  a_diff <- a[-length(a)] - a[-1]
  check1 <- a[1] < 0 & zb[1] == -Inf
  check2 <- a[length(a)] > 0 & zb[2] == Inf
  if(check1 | check2)
    stop("Envelope is not integrable. Choose different points.")
  if(any(a == 0) | any(a_diff == 0))
    stop("Divison by zero. Choose different points.")
  z <- c(zb[1], (b[-1] - b[-length(b)]) / a_diff, zb[2])

  .Call("C_adap_samp",
        as.integer(n),
        density,
        a,
        b,
        z,
        environment())
}
```

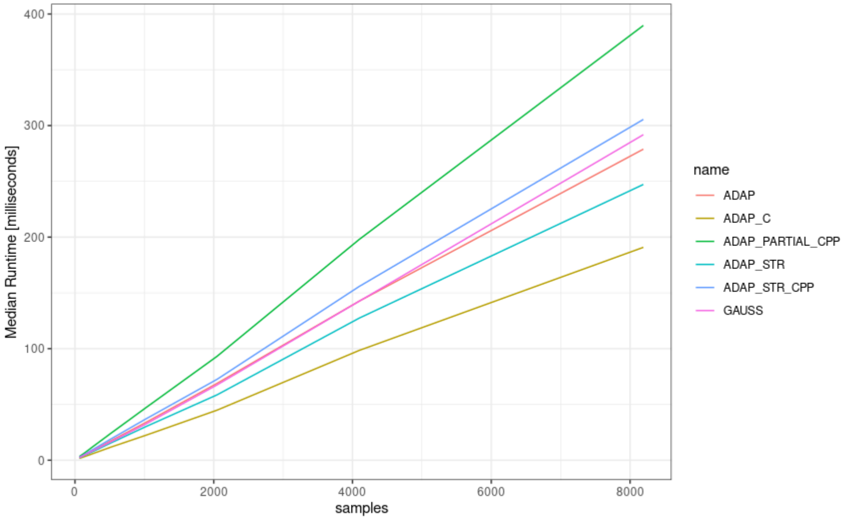
Final Benchmarks

Table

	expression	min	median	`itr/sec`	mem_al…[1]
	<bch:expr>	<bch:tm>	<bch:tm>	<dbl>	<bch:by>
1	GAUSS	3.12ms	3.32ms	293.	794KB
2	ADAP	3.28ms	3.52ms	281.	488KB
3	ADAP_STR	2.93ms	3.17ms	313.	216KB
4	ADAP_STR_CPP	3.64ms	3.82ms	257.	784KB
5	ADAP_PARTIAL_CPP	4.49ms	4.75ms	208.	206KB
6	ADAP_C	2.23ms	2.38ms	413.	407KB

Final Benchmarks

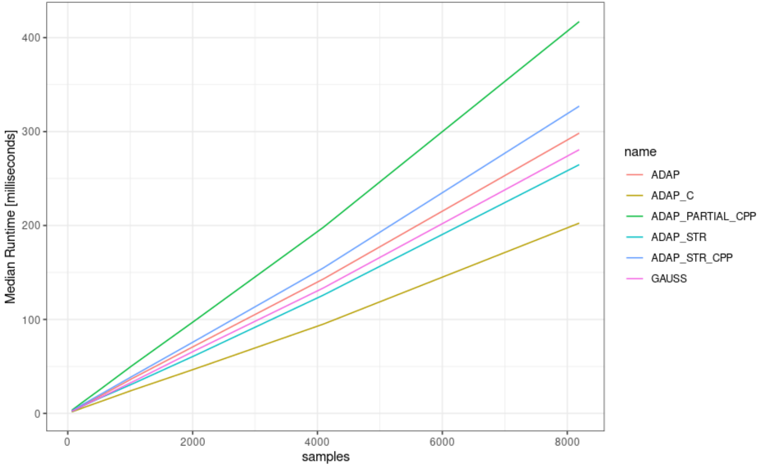
Scaling



Final Benchmarks

Scaling

Different points 0.1, 0.2, 0.3 for adaptive envelope.



Density of Samples from C Implementation