Adaptive Envelope Rejection Sampling

Applied to Log-concave Densities

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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

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

```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)
  }
}
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

The function $e^{(x-0.2423914)^2/(2\cdot0.004079805)}$ is an envelope of p with $\alpha = 1.351351 \cdot 10^{40}$.
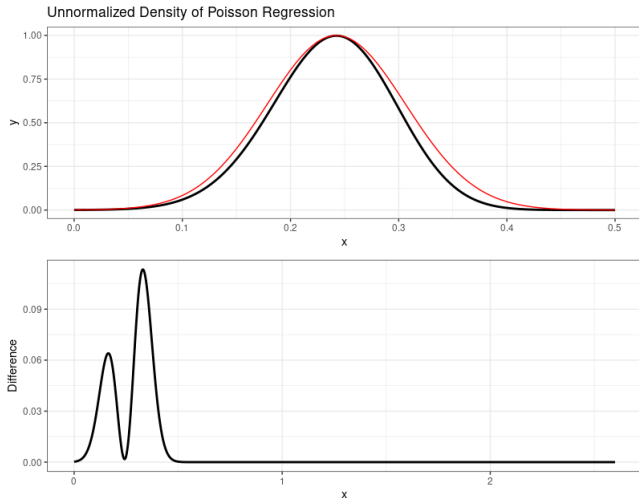
Unnormalized Density of Poisson Regression

Adaptive Rejection Sampling

```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 & 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

```r
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])
  }
}
```
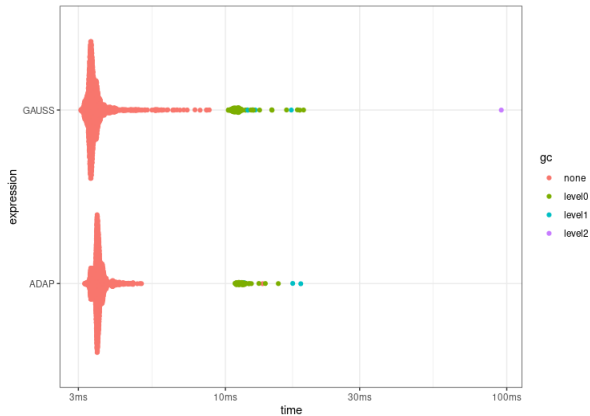
Comparison of the Implementations

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.
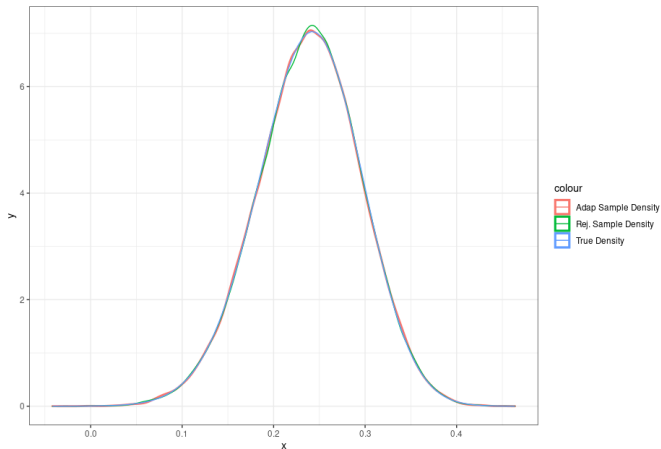
Comparison of the Implementations

Benchmarks Using `bench` Package

Benchmarking sampling 100 samples.

Benchmarking sampling 100 samples.

expression	min	median	`itr/sec`	mem_alloc
<bch:expr>	<bch:tm>	<bch:tm>	<dbl>	<bch:byt>
GAUSS	3.06ms	3.36ms	289.	928KB
ADAP	3.16ms	3.52ms	281.	937KB

Profiling the Implementation Using `profvis` Package

```
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)               0.4      20
  env_density <- get_env_density(a, b, z)
  samples <- numeric(n)
  succes <- tries <- 0
  for(s in 1:n) {
    reject <- TRUE
    while(reject) {                                       1.1      10
      tries <- tries + 1
      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
        reject <- FALSE
        succes <- succes + 1                              1.7      10
        samples[s] <- y0                                  1.0      10
      }
```
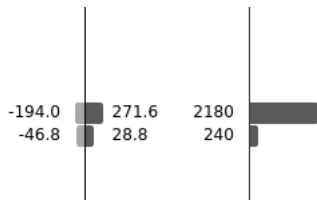
Profiling the Implementation Using `profvis` Package

```
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`

```r
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>	
GAUSS	3.11ms	3.34ms	281.	794KB	
ADAP	3.28ms	3.52ms	275.	488KB	
ADAP_STR	2.94ms	3.16ms	313.	216KB	
ADAP_STR_CPP	3.64ms	3.83ms	257.	794KB	

Improving the Implementation

Partial RCPP Implementation

```cpp
// [[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];
  }
```

```cpp
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

```cpp
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

```r
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:by>*
GAUSS	3.12ms	3.31ms	293.	794KB
ADAP	3.28ms	3.53ms	280.	488KB
ADAP_STR	2.95ms	3.16ms	314.	216KB
ADAP_STR_CPP	3.63ms	3.82ms	257.	784KB
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];
  }
```

```c
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

```c
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

```r
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())
}
```
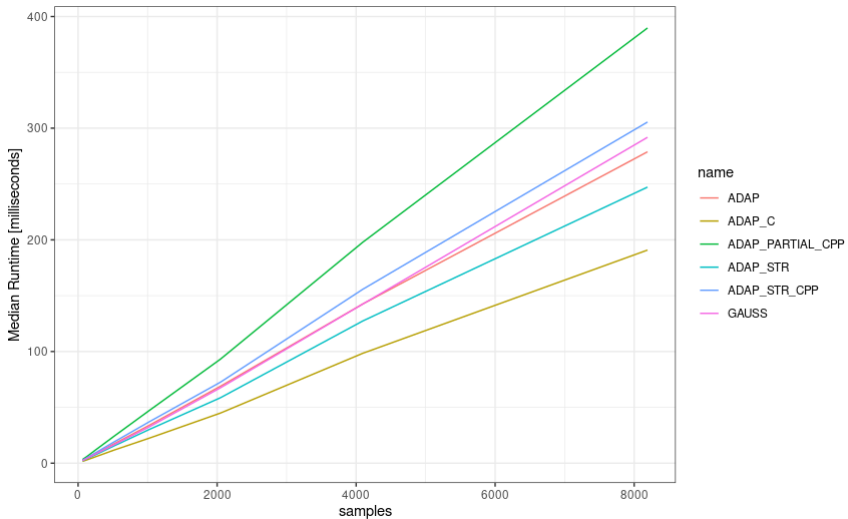
Final Benchmarks

Table

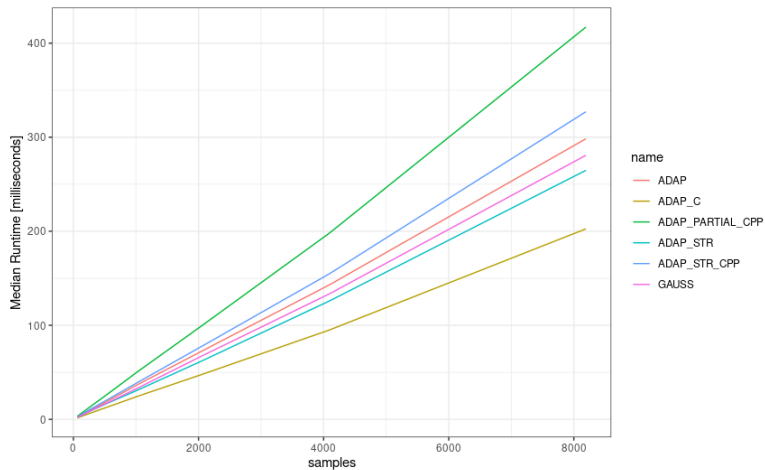|	expression	min	median	`itr/sec`	mem_al…[1]
	<bch:expr>	*<bch:tm>*	*<bch:tm>*	*<dbl>*	*<bch:by>*
1	GAUSS	3.12ms	3.32ms	293.	794KB
2	ADAP	3.28ms	3.52ms	281.	488KB
3	ADAP_STR	2.93ms	3.17ms	313.	216KB
4	ADAP_STR_CPP	3.64ms	3.82ms	257.	784KB
5	ADAP_PARTIAL_CPP	4.49ms	4.75ms	208.	206KB
6	ADAP_C	2.23ms	2.38ms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

Final Benchmarks

Scaling

Final Benchmarks

Different points 0.1, 0.2, 0.3 for adaptive envelope.

Density of Samples from C Implementation