Optimal Sampling for Sorting and Selection

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- They are simple, elegant, beatiful and practical solutions to two basic problems of Computer Science: sorting and selection
- They are primary examples of the divide-and-conquer principle

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Quicksort

```
void quicksort(vector<Elem>& A, int i, int j) {
    if (i < j) {
        int p = select_pivot(A, i, j);
        swap(A[p], A[l]);
        int k;
        partition(A, i, j, k);
        // A[i..k − 1] ≤ A[k] ≤ A[k + 1..j]
        quicksort(A, i, k - 1);
        quicksort(A, k + 1, j);
} }
```

Quickselect

```
Elem quickselect(vector<Elem>& A,
                 int i, int j, int m) {
   if (i >= j) return A[i];
   int p = select_pivot(A, i, j, m);
   swap(A[p], A[l]);
   int k;
   partition(A, i, j, k);
   if (m < k)      quickselect(A, i, k - 1, m);
   else if (m > k) quickselect(A, k + 1, j, m);
   else            return A[k];
}
```

Partition

```
void partition(vector<Elem>& A,
               int i, int j, int& k) {
       int l = i; int u = j + 1; Elem pv = A[i];
       for ( ; ; ) {
          do ++l; while(A[l] < pv);
          do --u; while(A[u] > pv);
          if (l >= u) break;
          swap(A[l], A[u]);
       };
       swap(A[i], A[u]); k = u;
}
```

The Recurrences for Average Cost

- Probability that the selected pivot is the k–th of n elements: $\pi_{n,k}$
- Average number of comparisons Q_n to sort n elements:

$$Q_n = n - 1 + \sum_{k=1}^{n} \pi_{n,k} \cdot (Q_{k-1} + Q_{n-k})$$

The Recurrences for Average Cost

- Average number of comparisons $C_{n,m}$ to select the m-th out of n:

$$C_{n,m} = n - 1 + \sum_{k=m+1}^{n} \pi_{n,k} \cdot C_{k-1,m} + \sum_{k=1}^{m-1} \pi_{n,k} \cdot C_{n-k,m-k}$$

Quicksort: The Average Cost

- For the standard variant, the splitting probabilities are $\pi_{n,k} = 1/n$
- Average number of comparisons Q_n to sort n elements (Hoare, 1962):

$$Q_n = 2(n+1)H_n - 4n$$
$$= 2n \ln n + (2\gamma - 4)n + 2 \ln n + \mathcal{O}(1)$$

where $H_n = \sum_{1 \leq k \leq n} 1/k = \ln n + \mathcal{O}(1)$ is the n-th harmonic number.

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Quickselect: The Average Cost

- Average number of comparisons $C_{n,m}$ to select the m-th out of n elements (Knuth, 1971):

$$C_{n,m} = 2(n + 3 + (n+1)H_n - (n + 3 - m)H_{n+1-m} - (m + 2)H_m).$$

- This is $\Theta(n)$ for any m, $1 \le m \le n$.

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Quickselect: The Average Cost

- The expectation characteristic function

$$m_0(\alpha) = \lim_{n\to\infty, m/n\to\alpha} \frac{C_{n,m}}{n} = 2 + 2\cdot\mathcal{H}(\alpha),$$
$$\mathcal{H}(x) = -(x\ln x + (1-x)\ln(1-x)).$$

  with $0 \le \alpha \le 1$.
- The maximum is at $\alpha = 1/2$, where $m_0(1/2) = 2 + 2\ln 2 = 3.386\ldots$
- The mean value is $\overline{m_0} = 3 \implies$ the average number of comparisons to select an item of given random rank is $3n + o(n)$.

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Variance and More

- The variance of both quicksort and quickselect is $\Theta(n^2)$ (Hennequin, 1989; Kirschenhofer & Prodinger, 1998) $\Longrightarrow$ concentration around the mean for quicksort, not for quickselect
- Higher moments are also known (e.g., Hennequin, 1989)
- Many properties about the distributions are known (e.g. Régnier, 1989, Rösler, 1991, McDiarmid & Hayward, 1996), but no closed form

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Improving Quicksort and Quickselect

- Apply general techniques: recursion removal, loop unwrapping, . . .
- Reorder recursive calls to quicksort
- Switch to a simpler algorithm for small subfiles
- Use samples to select better pivots

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Quicksort with Median-of-Three

- In quicksort with median-of-three, the pivot of each recursive stage is selected as the median of a sample of three elements (Singleton, 1969)
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Quicksort with Median-of-Three

- The splitting probabilities are

$$\pi_{n,k} = \frac{(k-1)(n-k)}{\binom{n}{3}}$$

- The average number of comparisons made by quicksort with median-of-three Q_n is (Sedgewick, 1975)

$$Q_n = \frac{12}{7} n \log n + \mathcal{O}(n),$$

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- The average number of comparisons $C_{n,m}$ made by quickselect with median-of-three is (Kirschenhofer, Martínez & Prodinger, 1997)

$$C_{n,m} = 2n + \frac{72}{35}H_n - \frac{156}{35}H_m - \frac{156}{35}H_{n+1-m} + 3m - \frac{(m-1)(m-2)}{n} + \mathcal{O}(1)$$

- To obtain this result we used the bivariate generating function

$$C(z,u) = \sum_{n\geq 0}\sum_{1\leq m\leq n} C_{n,m} z^n u^m$$

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with $0 \le \alpha \le 1$.

- For any α, $m_1(\alpha) \le m_0(\alpha)$
- The mean value is $\overline{m}_1 = 5/2$; compare to $3n + o(n)$ comparisons for standard quickselect on random ranks

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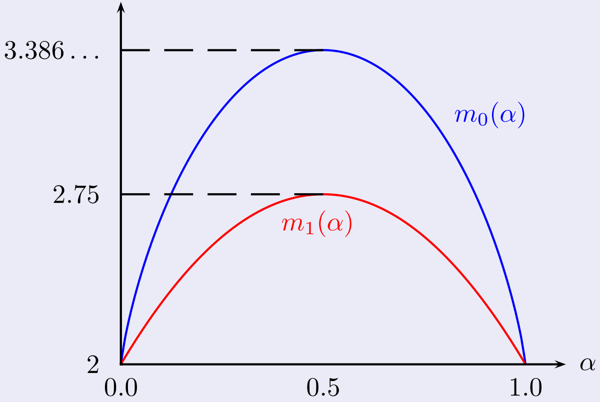
Quickselect with Median-of-Three

A plot of the standard quickselect characteristic function versus median-of-three characteristic function



Median-of-$(2t + 1)$

- The generalization to samples of size $s = (2t + 1)$ is immediate
- If $s = \Theta(1)$ then the recurrences for quicksort and quickselect are $\sim$ as for the standard case ($s = 1$)
- The splitting probabilities are:

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Quicksort with Median-of-$(2t+1)$

- Average number of comparisons $Q_n^{(t)}$ (VanEmden, 1970)

$$Q_n^{(t)} = \frac{1}{H_{2t+2} - H_{t+1}} n \log n + \mathcal{O}(n)$$

- Notice that $c_t = 1/(H_{2t+2} - H_{t+1})$ tends to $1/\ln 2$ as $t \to \infty$; this means that with large samples

$$Q_n \sim n \log_2 n$$

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- The average number of comparisons is not known; must be linear, but the coefficient $m_t(\alpha)$ remains unknown
- Average number of comparisons $C_n^{(t)}$ to select an element of random rank (Martínez & Roura, 2001):

$$C_n^{(t)} = (2 + \frac{1}{t+1})n + o(n)$$

- The variance of the number of comparisons to select an element of random rank (Martínez & Roura, 2001):

$$\mathbb{V}\left[C_n^{(t)}\right] = \frac{2t+3}{3(t+1)^2}n^2 + o(n^2)$$

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Median-of-$(2t + 1)$

- The main technique to obtain the results was the continuos master theorem (Roura, 1997); it allows to solve many recurrences of the type

$$F_n = t_n + \sum_{0 \le k < n} \omega_{n,k} F_k$$

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Median-of-$(2t+1)$

- To use the CMT one needs to find a continuous approximation of the weights $\omega_{n,k}$; we typically use $\omega(z) = \lim_{n\to\infty} n \cdot \omega_{n,z\cdot n}$
- Then one has to compute

$$\mathcal{H} = 1 - \int_0^1 \omega(z) \cdot z^a \, dz$$

where $a > -1$ is the exponent of n in t_n; we have three cases depending on $\mathcal{H} > 0$, $\mathcal{H} = 0$, $\mathcal{H} < 0$

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Adaptive Sampling for Quickselect

- Median-of-$(2t+1)$ might be a good idea for sorting: both subarrays must be recursively sorted; but it is not so natural for selection
- In proportion-from-s sampling we take an element in the sample of s elements whose rank is, in relative terms, close to the rank of the sought element (Martínez, Panario & Viola, 2004)

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- More generally, if the current relative rank is $\alpha = m/n$, we select the element of rank $r(\alpha)$ from the sample as our pivot

Example

- Standard quickselect: $s = 1, r(\alpha) = 1$
- Median-of-$(2t+1)$: $s = 2t+1, r(\alpha) = t+1$
- Proportion-from-s: $r(\alpha) \approx \alpha \cdot s$

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We are looking the fourth element ($m = 4$) out of $n = 15$ elements

9	5	10	12	3	1	11	15	7	2	8	13	6	4	14

$$\alpha = 4/15 < 1/3$$

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Adaptive Sampling for Quickselect

Theorem (Martínez, Panario & Viola, 2004)

For any adaptive sampling strategy, the expectation characteristic function $f(\alpha) = \lim_{n\to\infty, m/n\to\alpha} \frac{C_{n,m}}{n}$ satisfies

$$f(\alpha) = 1 + \frac{s!}{(r(\alpha)-1)!(s-r(\alpha))!} \times \left[\int_\alpha^1 f\left(\frac{\alpha}{x}\right) x^{r(\alpha)}(1-x)^{s-r(\alpha)}\,dx + \int_0^\alpha f\left(\frac{\alpha-x}{1-x}\right) x^{r(\alpha)-1}(1-x)^{s+1-r(\alpha)}\,dx\right]$$

Adaptive Sampling for Quickselect

Theorem (Martínez & Daligault, 2006)

The second factorial moment characteristic function $g(\alpha) = \lim_{n\to\infty, m/n\to\alpha} \frac{C_{n,m}(C_{n,m}-1)}{n^2}$ of any adaptive sampling strategy satisfies

$$g(\alpha) = 2f(\alpha) - 1 + \frac{s!}{(r(\alpha)-1)!(s-r(\alpha))!}\left[\int_\alpha^1 g(\alpha/x)x^{r(\alpha)+1}(1-x)^{s-r(\alpha)}\,dx + \int_0^\alpha g\left(\frac{\alpha-x}{1-x}\right)x^{r(\alpha)-1}(1-x)^{s+2-r(\alpha)}\,dx\right]$$

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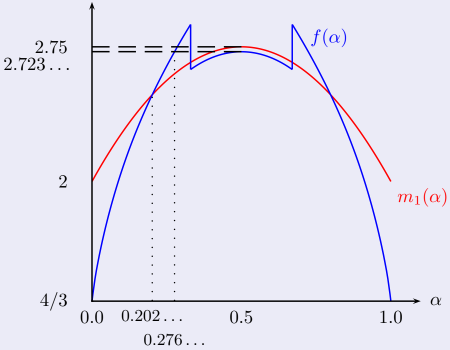
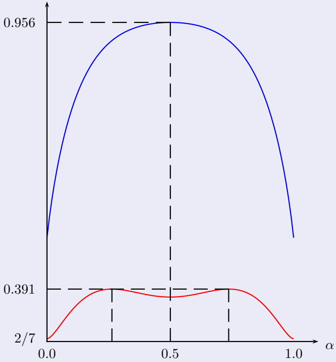
A plot of median-of-three characteristic function versus proportion-from-three $f(\alpha)$



Adaptive Sampling for Quickselect

A plot of $v(\alpha)$ for standard quickselect (Kirschenhofer & Prodinger, 1998) and for median-of-three (Martínez & Daligault, 2006)



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- With a suitable choice of the endpoints of the intervals that define $r(\alpha)$, we have shown that there exists a proportion-from-3-like strategy which makes the minimum average number of comparisons for all α (among all strategies using samples of three elements)
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Optimal Sampling for Quicksort

- We consider now samples of size $s = s(n) = 2t(n) + 1$, with $t = o(n)$ and $t \to \infty$ as $n \to \infty$, for instance $t = \log n$
- The recurrence for the average cost is now

$$Q_n = n + \Theta(s) + \sum_{k=1}^{n} \pi_{n,k} \cdot (Q_{k-1} + Q_{n-k}),$$

its important to take into account the work done to select the pivot from the sample!

Optimal Sampling for Quicksort

- We consider now samples of size $s = s(n) = 2t(n) + 1$, with $t = o(n)$ and $t \to \infty$ as $n \to \infty$, for instance $t = \log n$
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Optimal Sampling for Quicksort

- The standard techniques for fixed-size samples do not work here, the basic problem are the splitting probabilities $\pi_{n,k}$
- The CMT comes to rescue to allow us rigorously prove "handwaving" intuitive arguments ...

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Optimal Sampling for Quicksort

Theorem (Martínez & Roura, 2001)

The average number of comparisons made by quicksort with median-of-$(2t+1)$, for $t = t(n)$ satisfying $t \to \infty$ and $t/n \to 0$ when $n \to \infty$, is

$$Q_n = n \log_2 n + o(n \log n)$$

Optimal Sampling for Quicksort

Theorem (Martínez & Roura, 2001)

The average total cost (# comparisons $+ \xi \cdot$ # exchanges) of quicksort with median-of-$(2t+1)$, for $t = t(n)$ satisfying $t \to \infty$ and $t/n \to 0$ when $n \to \infty$, is

$$\hat{Q}_n = (1 + \xi/4) \cdot n \log_2 n + o(n \log n),$$

Computing the Optimal Sample Size

- The idea is to substitute the asymptotic when $t \to \infty$ into the recurrences

$$Q_n = n + \Theta(s) + \sum_{k=0}^{n-1} \pi_{n,k+1} \cdot \Big(k \log_2 k + (n-k) \log_2 (n-k) + o(k \log k + (n-k) \log(n-k))\Big),$$

- ...and compute asymptotic estimates of the right hand-side

$$Q_n = n + \beta \cdot s + \frac{n \log_2 n}{2s} + o(s),$$

where we put $\beta \cdot s + o(s)$ the (average) cost of selecting the median from the sample

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Optimal Sampling for Quicksort

Theorem (Martínez & Roura, 2001)

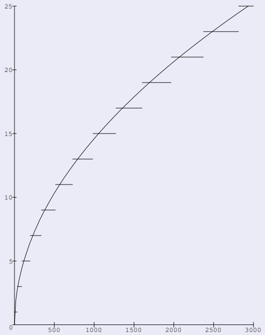
Let $s^* = 2t^* + 1$ denote the optimal sample size that minimizes the average number of comparisons made by quicksort. Then

$$t^* = \sqrt{\frac{1}{\beta}\left(\frac{4 - \xi(2\ln 2 - 1)}{8\ln 2}\right)} \cdot \sqrt{n} + o\left(\sqrt{n}\right)$$

if $\xi < \tau = 4/(2\ln 2 - 1) \approx 10.3548$

Optimal Sample Sizes for Quicksort

Optimal sample size vs. exact values



Expensive Exchanges and Optimal Sampling

- If exchanges are expensive ($\xi \geq \tau$), pick the $(\psi \cdot s)$–th element of a sample of size $\Theta(\sqrt{n})$, not the median
- If the position of the pivot is close to either end of the array, then very few exchanges are necessary on that stage, but a poor partition leads to more recursive steps. This trade-off is relevant if exchanges are very expensive
- We found an explicit formula for ψ as a function of ξ

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Optimal Sampling for Quickselect

Theorem (Martínez & Roura, 2001)

The average total cost (# comparisons $+ \xi \cdot$ # exchanges) of quickselect with median-of-$(2t+1)$ to select an element of random rank, for $t = t(n)$ satisfying $t \to \infty$ and $t/n \to 0$ when $n \to \infty$, is

$$\hat{C}_n = 2(1 + \xi/4) \cdot n + o(n \log n),$$

Optimal Sampling for Quickselect

Theorem (Martínez & Roura, 2001)

Let $s^* = 2t^* + 1$ denote the optimal sample size that minimizes the average total cost of quickselect. Then

$$t^* = \frac{1}{2\sqrt{\beta}} \cdot \sqrt{n} + o\left(\sqrt{n}\right)$$

Optimal Sampling for Quickselect

- Solving the integral equations for the expectation and second factorial moment characteristic function is difficult, but we can analyse what happens when $s \to \infty$
- For instance, if we use median-of-$(2t+1)$ sampling then $m_t(\alpha) = 2$ when $t \to \infty$; this is not optimal

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Optimal Sampling for Quickselect

Theorem (Martínez, Panario & Viola, 2004)

Proportion-from-s sampling with $s \to \infty$ achieves optimal expected performance:

$$f(\alpha) = 1 + \min(\alpha, 1 - \alpha)$$

Optimal Sampling for Quickselect

Theorem (Martínez & Daligault, 2006)

The variance of proportion-from-s sampling with $s \to \infty$ is subquadratic. Since

$$g(\alpha) = (1 + \min(\alpha, 1-\alpha))^2 = f^2(\alpha),$$

we have

$$\lim_{n\to\infty, m/n\to\alpha} \frac{\mathbb{V}[C_{n,m}]}{n^2} = g(\alpha) - f^2(\alpha) = 0$$

Optimal Sampling for Quickselect

- The two results above hold for biased proportion-from-s strategies
- The rank $r(\alpha)$ must be close to $\alpha \cdot s$ . . . but no too close!
- We want our selected pivot to be close to the sought element, but at the proper side; e.g., if $\alpha < 1/2$ the pivot should be slightly to the right of the sought element, not to the left
- Solution: take $r(\alpha) > \alpha \cdot s + 1 - \alpha$ if $\alpha < 1/2$ and symmetrically if $\alpha > 1/2$

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Optimal Sampling for Quickselect

- We can plug the asymptotic estimate $C_{n,m} = n + \min(m, n-m) + o(n)$ back into quickselect's recurrence to determine the optimal size of samples
- But it is difficult to obtain precise asymptotics, we only obtained order of magnitude

$$C_{n,m} = n + \beta \cdot s + \min(m, n-m) + \mathcal{O}\left(\frac{n}{s}\right),$$

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Optimal Sampling for Quickselect

Theorem (Martínez & Daligault, 2006)

Biased proportion-from-s sampling with $s = \Theta(\sqrt{n})$ minimizes both the expectation and variance of the number of comparisons; in particular, the variance is $\Theta(n^{3/2})$.

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