

Fundamental Algorithms

Chapter 2: Sorting

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Part I

Simple Sorts

The Sorting Problem

Definition

Sorting is required to order a given sequence of elements, or more precisely:

Input : a sequence of n elements a_1, a_2, \dots, a_n

Output : a permutation (reordering) a'_1, a'_2, \dots, a'_n of the input sequence, such that $a'_1 \leq a'_2 \leq \dots \leq a'_n$.

- we will assume the elements a_1, a_2, \dots, a_n to be integers (or any element/data type on which a total order \leq is defined)
- a sorting algorithm may output the permuted data or also the permuted set of indices

Insertion Sort

Idea: sorting by inserting

- successively generate ordered sequences of the first j numbers:
 $j = 1, j = 2, \dots, j = n$
- in each step, $j \rightarrow j + 1$, one additional integer has to be inserted into an already ordered sequence

Data Structures:

- an array $A[1..n]$ that contains the sequence a_1 (in $A[1]$), \dots , a_n (in $A[n]$).
- numbers are sorted **in place**:
output sequence will be stored in A itself
(hence, content of A is changed)

Insertion Sort – Implementation

```
InsertionSort(A:Array[1..n]) {  
  
  for j from 2 to n {  
    // insert A[j] into sequence A[1..j-1]  
  
    key := A[j];  
  
    i := j-1; // initialize i for while loop  
    while i>=1 and A[i]>key {  
      A[i+1] := A[i];  
      i := i-1;  
    }  
    A[i+1] := key;  
  }  
}
```

Correctness of InsertionSort

Loop invariant:

Before each iteration of the for-loop, the subarray $A[1..j-1]$ consists of all elements originally in $A[1..j-1]$, but in sorted order.

Initialization:

- loops starts with $j=2$;
hence, $A[1..j-1]$ consists of the element $A[1]$ only
- $A[1]$ contains only one element, $A[1]$, and is therefore sorted.

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Maintenance:

- assume that the while loop works correctly (or prove this using an additional loop invariant):
 - after the while loop, i contains the largest index for which $A[i]$ is smaller than the key
 - $A[i+2..j]$ contains the (sorted) elements previously stored in $A[i+1..j-1]$; also: $A[i+1]$ and all elements in $A[i+2..j]$ are \geq key
- the key value, $A[j]$, is thus correctly inserted as element $A[i+1]$ (overwrites the duplicate value $A[i+1]$)
- after execution of the loop body, $A[1..j]$ is sorted
- thus, before the next iteration ($j:=j+1$), $A[1..j-1]$ is sorted

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Before each iteration of the for-loop, the subarray $A[1..j-1]$ consists of all elements originally in $A[1..j-1]$, but in sorted order.

Termination:

- The for-loop terminates when j exceeds n (i.e., $j=n+1$)
- Thus, at termination, $A[1 .. (n+1)-1] = A[1..n]$ is sorted and contains all original elements

Insertion Sort – Number of Comparisons

```
InsertionSort(A:Array[1..n]) {
```

```
  for j from 2 to n {
```

n-1 iterations

```
    key := A[j];
```

```
    i := j-1;
```

```
    while i >= 1 and A[i] > key {
```

```
      A[i+1] := A[i];
```

```
      i := i-1;
```

```
    }
```

```
    A[i+1] := key;
```

```
  }
```

```
}
```

t_j iterations

→ t_j comparisons

$A[i] > \text{key}$

$$\Rightarrow \sum_{j=2}^n t_j \text{ comparisons}$$

Insertion Sort – Number of Comparisons (2)

- counted number of comparisons: $T_{IS} = \sum_{j=2}^n t_j$
- where t_j is the number of iterations of the while loop (which is, of course, unknown)
- good estimate for the run time, if the comparison is the most expensive operation (note: replace “ $i \geq 1$ ” by for loop)

Analysis

- what is the “best case”?
- what is the “worst case”?

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Analysis of the “best case”:

- in the best case, $t_j = 1$ for all j
- happens only, if $A[1..n]$ is already sorted

$$\Rightarrow T_{IS}(n) = \sum_{j=2}^n 1 = n - 1 \in \Theta(n)$$

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- good estimate for the run time, if the comparison is the most expensive operation (note: replace “ $i \geq 1$ ” by for loop)

Analysis of the “worst case”:

- in the worst case, $t_j = j - 1$ for all j
- happens, if $A[1..n]$ is already sorted in opposite order

$$\Rightarrow T_{IS}(n) = \sum_{j=2}^n (j - 1) = \frac{1}{2}n(n - 1) \in \Theta(n^2)$$

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- good estimate for the run time, if the comparison is the most expensive operation (note: replace “ $i \geq 1$ ” by for loop)

Analysis of the “average case”:

- best case analysis: $T_{IS}(n) \in \Theta(n)$
 - worst case analysis: $T_{IS}(n) \in \Theta(n^2)$
- ⇒ What will be the “typical” (average, expected) case?

Running Time and Complexity

“Run(ning)Time”

- the notation $T(n)$ suggest a “time”, such as run(ning) time of an algorithm, which depends on the input (size) n
- in practice: we need a precise model how long each operation of our programmes takes → very difficult on real hardware!
- we will therefore determine the number of operations that determine the run time, such as:
 - number of comparisons (sorting, e.g.)
 - number of arithmetic operations (Fibonacci, e.g.)
 - number of memory accesses

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“Complexity”

- characterises how the run time depends on the input (size), typically expressed in terms of the Θ -notation
- “algorithm xyz has linear complexity” → run time is $\Theta(n)$

Average Case Complexity

Definition (expected running time)

Let $X(n)$ be the set of all possible input sequences of length n , and let $P: X(n) \rightarrow [0, 1]$ be a probability function such that $P(x)$ is the probability that the input sequence is x .

Then, we define

$$\bar{T}(n) = \sum_{x \in X(n)} P(x)T(x)$$

as the **expected running time** of the algorithm.

Comments:

- we require an exact probability distribution (for InsertionSort, we could assume that all possible sequences have the same probability)
- we need to be able to determine $T(x)$ for any sequence x (usually much too laborious to determine)

Average Case Complexity of Insertion Sort

Heuristic estimate:

- we assume that we need $\frac{j}{2}$ steps in every iteration:

$$\Rightarrow \bar{T}_{\text{IS}}(n) \stackrel{(?)}{\approx} \sum_{j=2}^n \frac{j}{2} = \frac{1}{2} \sum_{j=2}^n j \in \Theta(n^2)$$

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- note: $\frac{j}{2}$ isn't even an integer ...
- Just considering the number of comparisons of the “average case” can lead to quite wrong results!**

in general $E(T(n)) \neq T(E(n))$

Bubble Sort

```
BubbleSort(A:Array[1..n]) {  
  for i from 1 to n do {  
    for j from n downto i+1 do {  
      if A[j] < A[j-1]  
        then exchange A[j] and A[j-1]  
    }  
  }  
}
```

Basic ideas:

- compare neighboring elements only
- exchange values if they are not in sorted order
- repeat until array is sorted (here: pessimistic loop choice)

Bubble Sort – Homework

Prove correctness of Bubble Sort:

- find invariant for i-loop
- find invariant for j-loop

Number of comparisons in Bubble Sort:

- best/worst/average case?

Part II

Mergesort and Quicksort

Mergesort

Basic Idea: **divide and conquer**

- **Divide** the problem into two (or more) subproblems:
→ split the array into two arrays of equal size
- **Conquer** the subproblems by solving them recursively:
→ sort both arrays using the sorting algorithm
- **Combine** the solutions of the subproblems:
→ merge the two sorted arrays to produce the entire sorted array

Combining Two Sorted Arrays: Merge

```
Merge (L:Array[1..p], R:Array[1..q], A:Array[1..n]) {  
  // merge the sorted arrays L and R into A (sorted)  
  // we presume that n=p+q  
  i:=1; j:=1:  
  for k from 1 to n do {  
    if i > p  
      then { A[k]:=R[j]; j:=j+1; }  
    else if j > q  
      then { A[k]:=L[i]; i:=i+1; }  
    else if L[i] < R[j]  
      then { A[k]:=L[i]; i:=i+1; }  
      else { A[k]:=R[j]; j:=j+1; }  
  }  
}
```


Correctness and Run Time of Merge

Loop invariant:

Before each cycle of the for loop:

- A has the $k-1$ smallest elements of L and R already merged, (i.e. in sorted order and at indices $1, \dots, k-1$);
- $L[i]$ and $R[j]$ are the smallest elements of L and R that have not been copied to A yet (i.e. $L[1..i-1]$ and $R[1..j-1]$ have been merged to A)

Run time:

$$T_{\text{Merge}}(n) \in \Theta(n)$$

- for loop will be executed exactly n times
- each loop contains constant number of commands:
 - exactly 1 copy statement
 - exactly 1 increment statement
 - 1–3 comparisons

MergeSort

```
MergeSort(A: Array[1..n]) {  
  if n > 1 then {  
    m := floor(n/2);  
    create array L [1... m];  
    for i from 1 to m do { L[i] := A[i]; }  
  
    create array R [1... n-m];  
    for i from 1 to n-m do { R[i] := A[m+i]; }  
  
    MergeSort(L);  
    MergeSort(R);  
  
    Merge(L,R,A);  
  }  
}
```

Number of Comparisons in MergeSort

- Merge performs exactly n element copies on n elements
 - Merge performs at most $c \cdot n$ comparisons on n elements
 - MergeSort itself does not contain any comparisons between elements; all comparisons done in Merge
- ⇒ number of element-copy operations for the entire MergeSort algorithms can be specified by a recurrence (includes n copy operations for splitting the arrays):

$$C_{MS}(n) = \begin{cases} 0 & \text{if } n \leq 1 \\ C_{MS}(\lfloor \frac{n}{2} \rfloor) + C_{MS}(n - \lfloor \frac{n}{2} \rfloor) + 2n & \text{if } n \geq 2 \end{cases}$$

- ⇒ number of comparisons for the entire MergeSort algorithm:

$$T_{MS}(n) \leq \begin{cases} 0 & \text{if } n \leq 1 \\ T_{MS}(\lfloor \frac{n}{2} \rfloor) + T_{MS}(n - \lfloor \frac{n}{2} \rfloor) + cn & \text{if } n \geq 2 \end{cases}$$

Number of Comparisons in MergeSort (2)

Assume $n = 2^k$, c constant:

$$\begin{aligned} T_{\text{MS}}(2^k) &\leq T_{\text{MS}}(2^{k-1}) + T_{\text{MS}}(2^{k-1}) + c \cdot 2^k \\ &\leq 2T_{\text{MS}}(2^{k-1}) + 2^k c \end{aligned}$$

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Quicksort

Basic Idea: **divide and conquer**

- **Divide** the input array $A[p..r]$ into parts $A[p..q]$ and $A[q+1 .. r]$, such that every element in $A[q+1 .. r]$ is larger than all elements in $A[p .. q]$.
- **Conquer**: sort the two arrays $A[p..q]$ and $A[q+1 .. r]$
- **Combine**: if the divide and conquer steps are performed in place, then no further combination step is required.

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Partitioning using a **pivot element**:

- all elements that are smaller than the pivot element should go into the “smaller” partition ($A[p..q]$)
- all elements that are larger than the pivot element should go into the “larger” partition ($A[q+1..r]$)

Partitioning the Array (Hoare's Algorithm)

```
Partition (A:Array[p..r]) : Integer {  
    // x is the pivot (chosen as first element):  
    x := A[p];  
    // partitions grow towards each other  
    i := p-1; j := r+1; // (partition boundaries)  
    while true do { // i < j: partitions haven't met yet  
        // leave large elements in right partition  
        do { j:=j-1; } while A[j]>x;  
        // leave small elements in left partition  
        do { i:=i+1; } while A[i]<x;  
        // swap the two first "wrong" elements  
        if i < j  
        then exchange A[i] and A[j];  
        else return j;  
    }  
}
```

Time Complexity of Partition

How many statements are executed by the nested while loops?

Time Complexity of Partition

How many statements are executed by the nested while loops?

- monitor increments/decrements of i and j
- after $n := r - p$ increments/decrements, i and j have the same value

⇒ $\Theta(n)$ comparisons with the pivot

⇒ $O(n)$ element exchanges

Hence: $T_{\text{Part}}(n) \in \Theta(n)$

Implementation of QuickSort

```
QuickSort (A:Array[p..r])
{
  if p>=r then return;
  // only proceed, if A has at least 2 elements:
  q := Partition (A);
  QuickSort (A[p..q]);
  QuickSort (A[q+1..r]);
}
```

Homework:

- prove correctness of Partition
- prove correctness of QuickSort

Time Complexity of QuickSort

Best Case:

- assume that all partitions are split exactly into two halves:

$$T_{\text{QS}}^{\text{best}}(n) = 2T_{\text{QS}}^{\text{best}}\left(\frac{n}{2}\right) + \Theta(n)$$

- analogous to MergeSort:

$$T_{\text{QS}}^{\text{best}}(n) \in \Theta(n \log n)$$

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Worst Case:

- Partition will always produce one partition with only 1 element:

$$\begin{aligned} T_{\text{QS}}^{\text{worst}}(n) &= T_{\text{QS}}^{\text{worst}}(n-1) + T_{\text{QS}}^{\text{worst}}(1) + \Theta(n) \\ &= T_{\text{QS}}^{\text{worst}}(n-1) + \Theta(n) = T_{\text{QS}}^{\text{worst}}(n-2) + \Theta(n-1) + \Theta(n) \\ &= \dots = \Theta(1) + \dots + \Theta(n-1) + \Theta(n) \in \Theta(n^2) \end{aligned}$$

Time Complexity of QuickSort – Special Cases?

What happens if:

- A is already sorted?

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What happens if:

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→ partition sizes always 1 and $n-1 \Rightarrow \Theta(n^2)$

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- partition sizes are always $n(1 - a)$ and na with $0 < a < 1$?

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Questions:

- What happens in the “usual” case?
- Can we force the best case?

Randomized QuickSort

```
RandPartition ( A: Array [p..r] ): Integer {  
    // choose random integer i between p and r  
    i := rand(p,r);  
    // make A[i] the (new) Pivot element:  
    exchange A[i] and A[p];  
    // call Partition with new pivot element  
    q := Partition (A);  
    return q;  
}
```

```
RandQuickSort ( A:Array [p..r] ) {  
    if p >= r then return;  
    q := RandPartition(A);  
    RandQuickSort (A[p...q]);  
    RandQuickSort (A[q+1 ..r]);  
}
```


Time Complexity of RandQuickSort

Best/Worst-case complexity?

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Best/Worst-case complexity?

- RandQuickSort may still produce the worst (or best) partition in each step
- worst case: $\Theta(n^2)$
- best case: $\Theta(n \log n)$

Time Complexity of RandQuickSort

Best/Worst-case complexity?

- RandQuickSort may still produce the worst (or best) partition in each step
- worst case: $\Theta(n^2)$
- best case: $\Theta(n \log n)$

However:

- it is not determined which input sequence (sorted order, reverse order) will lead to worst case behavior (or best case behavior);
- any input sequence might lead to the worst case or the best case, depending on the random choice of pivot elements.

Thus: only the **average-case complexity** is of interest!

Average Case Complexity of RandQuickSort

Assumptions:

- we compute $\bar{T}_{\text{RQS}}(A)$,
i.e., the expected run time of RandQuickSort for a given input A
- $\text{rand}(p, r)$ will return uniformly distributed random numbers
(all pivot elements have the same probability)
- all elements of A have different size: $A[i] \neq A[j]$

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Basic Idea:

- only count number of comparisons between elements of A
- let z_i be the i -th smallest element in A
- define

$$X_{ij} = \begin{cases} 1 & z_i \text{ is compared to } z_j \\ 0 & \text{otherwise} \end{cases}$$

- random variable $T_{\text{RQS}}(A) = \sum_{i < j} X_{ij}$

Average Case Complexity of RandQuickSort

Expected Number of Comparisons:

$$\bar{T}_{\text{RQS}}(A) = E \left[\sum_{i < j} X_{ij} \right]$$

Average Case Complexity of RandQuickSort

Expected Number of Comparisons:

$$\begin{aligned}\bar{T}_{\text{RQS}}(A) &= E \left[\sum_{i < j} X_{ij} \right] \\ &= \sum_{i < j} E [X_{ij}]\end{aligned}$$

Average Case Complexity of RandQuickSort

Expected Number of Comparisons:

$$\begin{aligned}\bar{T}_{\text{RQS}}(A) &= E \left[\sum_{i < j} X_{ij} \right] \\ &= \sum_{i < j} E [X_{ij}] \\ &= \sum_{i < j} \Pr [z_i \text{ is compared to } z_j]\end{aligned}$$

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- suppose an element between z_i and z_j is chosen as pivot **before** z_i or z_j are chosen as pivots; then z_i and z_j are never compared

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- suppose an element between z_i and z_j is chosen as pivot **before** z_i or z_j are chosen as pivots; then z_i and z_j are never compared
- if either z_i or z_j is chosen as the first pivot in the range z_i, \dots, z_j , then z_i will be compared to z_j

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- if either z_i or z_j is chosen as the first pivot in the range z_i, \dots, z_j , then z_i will be compared to z_j
- this happens with probability

$$\frac{2}{j - i + 1}$$

Average Case Complexity of RandQuickSort

Expected Number of Comparisons:

$$\bar{T}_{\text{RQS}}(A) = \sum_{i=1}^{n-1} \sum_{j=i+1}^n \frac{1}{j-i+1}$$

Average Case Complexity of RandQuickSort

Expected Number of Comparisons:

$$\begin{aligned}\bar{T}_{\text{RQS}}(A) &= \sum_{i=1}^{n-1} \sum_{j=i+1}^n \frac{1}{j-i+1} \\ &= \sum_{i=1}^{n-1} \sum_{k=2}^{n-i+1} \frac{1}{k}\end{aligned}$$

Average Case Complexity of RandQuickSort

Expected Number of Comparisons:

$$\begin{aligned}\bar{T}_{\text{RQS}}(A) &= \sum_{i=1}^{n-1} \sum_{j=i+1}^n \frac{1}{j-i+1} \\ &= \sum_{i=1}^{n-1} \sum_{k=2}^{n-i+1} \frac{1}{k} \\ &\leq 2 \sum_{i=1}^n \sum_{k=1}^n \frac{1}{k}\end{aligned}$$

Average Case Complexity of RandQuickSort

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Part III

Outlook: Optimality of Comparison Sorts

Are Mergesort and Quicksort optimal?

Definition

Comparison sorts are sorting algorithms that use only comparisons (i.e. tests as \leq , $=$, $>$, ...) to determine the relative order of the elements.

Examples:

- InsertSort, BubbleSort
- MergeSort, (Randomised) Quicksort

Question:

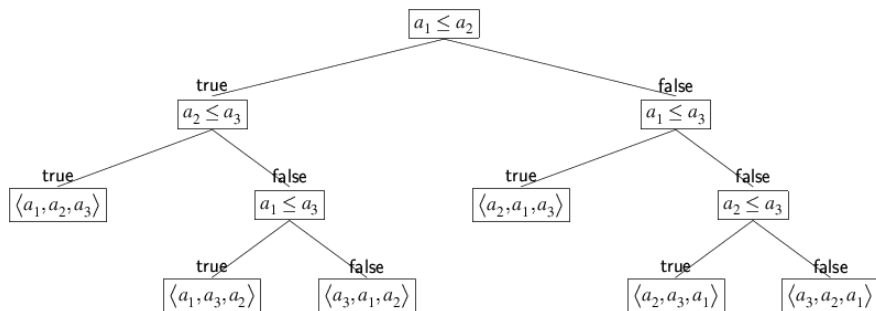
Is $T(n) \in \Theta(n \log n)$ the best we can get (in the worst/average case)?

Decision Trees

Definition

A **decision tree** is a binary tree in which each internal node is annotated by a comparison of two elements.

The leaves of the decision tree are annotated by the respective permutations that will put an input sequence into sorted order.



Decision Trees – Properties

Each comparison sort can be represented by a decision tree:

- a path through the tree represents a sequence of comparisons
- sequence of comparisons depends on results of comparisons
- can be pretty complicated for Mergesort, Quicksort, . . .

A decision tree can be used as a comparison sort:

- if every possible permutation is annotated to at least one leaf of the tree!
- if (as a result) the decision tree has at least $n!$ (distinct) leaves.

A Lower Complexity Bound for Comparison Sorts

- A binary tree of height h (h the length of the longest path) has at most 2^h leaves.
- To sort n elements, the decision tree needs $n!$ leaves.

Theorem

Any decision tree that sorts n elements has height $\Omega(n \log n)$.

Proof:

- h comparisons in the worst case are equivalent to a decision tree of height h
- with h comparisons, we can sort n elements (at best), if

$$n! \leq 2^h \quad \Leftrightarrow \quad h \geq \log(n!) \in \Omega(n \log n)$$

- because:

$$h \geq \log(n!) \geq \log\left(n^{n/2}\right) = \frac{n}{2} \log n$$

Optimality of Mergesort and Quicksort

Corollaries:

- MergeSort is an optimal comparison sort in the worst/average case
- QuickSort is an optimal comparison sort in the average case

Consequences and Alternatives:

- comparison sorts can be faster than MergeSort, but only by a constant factor
- comparison sorts can not be asymptotically faster
- sorting algorithms might be faster, if they can exploit additional information on the size of elements
- examples: **BucketSort**, CountingSort, RadixSort

Part IV

Bucket Sort – Sorting Beyond “Comparison Only”

Bucket Sort

Basic Ideas and Assumptions:

- pre-sort numbers in buckets that contain all numbers within a certain interval
- hope (assume) that input elements are evenly distributed and thus uniformly distributed to buckets
- sort buckets and concatenate them

Requires “Buckets”:

- can hold arbitrary numbers of elements
- can insert elements efficiently: in $O(1)$ time
- can concatenate buckets efficiently: in $O(1)$ time
- remark: linked lists will do

Implementation of BucketSort

```
BucketSort (A: Array[1..n]) {  
  
    Create Array B[0..n-1] of Buckets;  
    // assume all Buckets B[i] are empty at first  
  
    for i from 1 to n do {  
        insert A[i] into Bucket B[floor(n * A[i ])];  
    }  
  
    for i from 0 to n-1 do {  
        sort Bucket B[i] ;  
    }  
  
    concatenate Buckets B[0], B[1], ..., B[n-1] into A  
}
```

Number of Operations of BucketSort

Operations:

- n operations to distribute n elements to buckets
- plus effort to sort all buckets

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Best Case:

- if each bucket gets 1 element, then $\Theta(n)$ operations are required

Worst Case:

- if one bucket gets all elements, then $T(n)$ is determined by the sorting algorithm for the buckets

Bucketsort – Average Case Analysis

- probability that bucket i contains k elements:

$$P(n_i = k) = \binom{n}{k} \left(\frac{1}{n}\right)^k \left(1 - \frac{1}{n}\right)^{n-k}$$

- expected mean and variance for such a distribution:

$$E[n_i] = n \cdot \frac{1}{n} = 1 \quad \text{Var}[n_i] = n \cdot \frac{1}{n} \left(1 - \frac{1}{n}\right) = \left(1 - \frac{1}{n}\right)$$

- InsertionSort for buckets $\Rightarrow \leq cn^2 \in O(n_i^2)$ operations per bucket
- expected operations to sort one bucket:

$$\bar{T}(n_i) \leq \sum_{k=0}^{n-1} P(n_i = k) \cdot ck^2 = cE[n_i^2]$$

Bucketsort – Average Case Analysis (2)

- theorem from statistics:

$$E[X^2] = E[X]^2 + \text{Var}(X)$$

- expected operations to sort one bucket:

$$\bar{T}(n_i) \leq cE[n_i^2] = c(E[n_i]^2 + \text{Var}[n_i]) = c\left(1^2 + 1 - \frac{1}{n}\right) \in \Theta(1)$$

- expected operations to sort all buckets:

$$\bar{T}(n) = \sum_{i=0}^{n-1} \bar{T}(n_i) \leq c \sum_{i=0}^{n-1} \left(2 - \frac{1}{n}\right) \in \Theta(n)$$

(note: expected value of the sum is the sum of expected values)