Computing Standard-Deviation-to-Mean and Variance-to-Mean Ratios under Interval Uncertainty is NP-Hard

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A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

1. A Practical Problem: Checking Whether an Object Belongs to a Class

- In many practical situations, we want to check whether a new object belongs to a given class.
- In such situations, we usually have a sample of objects which are known to belong to this class.
- *Example:*
  - a biologist who is studying bats has observed several bats from a local species;
  - the question is
    - whether a newly observed bat belongs to the same species –
    - or whether the newly observed bat belongs to a different bat species.

A Practical Problem: ...
How This Problem is ...
A Standard Way to ...
Selecting the Parameter k
Case of Interval ...
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

2. How This Problem is Usually Solved

- *Problem:* checking whether an object belongs to a class.
- *To solve this problem:* we usually
  - measure one or more quantities for the objects from this class and for the new object, and
  - compare the resulting values.
- *Simplest case of a single quantity.* In this case, we have:
  - a collection of values $x_1, \ldots, x_n$ corresponding to objects from the known class, and
  - a value x corresponding to the new object.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

3. A Standard Way to Decide Whether an Object Belongs to a Class

- *Problem* (reminder): to decide whether
  - a new object with the value x
  - belongs to the class characterized by the values $x_1, \ldots, x_n$.
- *Usual solution:* check whether the value x belongs to the "k sigma" interval $[E - k \cdot \sigma, E + k \cdot \sigma]$, where:
  - $E \stackrel{\text{def}}{=} \frac{1}{n} \cdot \sum_{i=1}^{n} x_i$ is the sample mean,
  - $\sigma = \sqrt{V}$, where $V \stackrel{\text{def}}{=} \frac{1}{n} \cdot \sum_{i=1}^{n} (x_i - E)^2$ is the sample variance, and
  - the parameter k is determined by the degree of confidence with which we want to make the decision.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

4. Selecting the Parameter k

- *Problem* (reminder): to decide whether
  - a new object with the value x
  - belongs to the class characterized by the values $x_1, \ldots, x_n$.
- *Solution* (reminder): check whether the value x belongs to the "k sigma" interval $[E - k \cdot \sigma, E + k \cdot \sigma]$
- Usually, we take:
  - $k = 2$ (corresponding to confidence 0.9),
  - $k = 3$ (corresponding to 0.999), or
  - $k = 6$ (corresponding to $1 - 10^{-8}$).

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

5. Formulation of the Problem

- *Problem:* checking whether an object belongs to a class.
- *Standard approach:* an object belongs to the class if the value x belongs to the "k sigma" interval

$$[E - k \cdot \sigma, E + k \cdot \sigma], \text{ where:}$$

  - $E \stackrel{\text{def}}{=} \frac{1}{n} \cdot \sum_{i=1}^{n} x_i$ is the sample mean, and
  - $\sigma = \sqrt{V}$, where $V \stackrel{\text{def}}{=} \frac{1}{n} \cdot \sum_{i=1}^{n} (x_i - E)^2$ is the sample variance
- How confident are we about the decision
  - depends on the smallest values k^- for which $x \geq E - k^- \cdot \sigma$, and
  - on the smallest value k^+ for which $x \leq E + k^+ \cdot \sigma$.

6. How to Compute the Parameters Describing Confidence?

- The inequality $x \geq E - k^- \cdot \sigma$ is equivalent to $k^- \cdot \sigma \geq E - x$ and $k^- \geq \dfrac{E - x}{\sigma}$.
- Thus, when $x < E$, the corresponding smallest value is equal to $k^- = \dfrac{E - x}{\sigma}$.
- Similarly, the inequality $x \leq E + k^+ \cdot \sigma$ is equivalent to $k^+ \cdot \sigma \geq x - E$ and $k^+ \geq \dfrac{x - E}{\sigma}$.
- Thus, when $x > E$, the corresponding smallest value is equal to $k^+ = \dfrac{x - E}{\sigma}$.
- So, to determine the parameter describing confidence, we must compute one of the ratios

$$k^- \stackrel{\text{def}}{=} \frac{E - x}{\sigma} \text{ or } k^+ \stackrel{\text{def}}{=} \frac{x - E}{\sigma}.$$

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

7. How to Compute the Parameters Describing Confidence (cont-d)

- *Reminder:* to determine the parameter describing confidence, we must compute one of the ratios

$$k^- \stackrel{\text{def}}{=} \frac{E - x}{\sigma} \text{ or } k^+ \stackrel{\text{def}}{=} \frac{x - E}{\sigma}.$$

- Often, reciprocal ratio are used:

$$r^- \stackrel{\text{def}}{=} \frac{1}{k^-} = \frac{\sigma}{E - x} \text{ and } r^+ \stackrel{\text{def}}{=} \frac{1}{k^+} = \frac{\sigma}{x - E}.$$

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

8. Case of Interval Uncertainty

- *Simplifying assumption:* we know the exact values $x_1, \ldots, x_n$ of the corresponding quantity.
- *In practice:* these values come from measurement, and measurements are never absolutely accurate.
- *Specifics:* the measurement results $\widetilde{x}_1, \ldots, \widetilde{x}_n$ are, in general, different from the actual (unknown) values x_i.
- *Traditional engineering techniques* assume that we know the probabilities of different values of $\Delta x_i \stackrel{\text{def}}{=} \widetilde{x}_i - x_i$.
- *In many practical situations:* we only know the upper bound Δ_i: $|\Delta x_i| \le \Delta_i$.
- *In this case:* we only know that the actual (unknown) value x_i belongs to the interval $\mathbf{x}_i \stackrel{\text{def}}{=} [\widetilde{x}_i - \Delta_i, \widetilde{x}_i + \Delta_i]$.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

9. Case of Interval Uncertainty (cont-d)

- *Reminder:* we only know that the actual (unknown) value x_i belongs to the interval $\mathbf{x}_i \stackrel{\text{def}}{=} [\widetilde{x}_i - \Delta_i, \widetilde{x}_i + \Delta_i]$.
- Different possible values $x_i \in \mathbf{x}_i$ lead, in general, to different values of the corresponding ratios $r(x_1, \ldots, x_n)$.
- Thus, it is desirable to compute the *range* of possible values of this ratio:

$$\mathbf{r} = [\underline{r}, \overline{r}] \stackrel{\text{def}}{=} \{r(x_1, \ldots, x_n) \,|\, x_1 \in \mathbf{x}_1, \ldots, x_n \in \mathbf{x}_n\}.$$

- This problem is a particular case of the main problem of *interval computation*:
  - *given:* an algorithm $f(x_1, \ldots, x_n)$ and intervals $\mathbf{x}_i$,
  - *compute:* the range

$$\mathbf{y} = [\underline{y}, \overline{y}] \stackrel{\text{def}}{=} \{f(x_1, \ldots, x_n) \,|\, x_1 \in \mathbf{x}_1, \ldots, x_n \in \mathbf{x}_n\}.$$

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

10. What is Known

- What was analyzed earlier:
  - the problem of computing the range of r, and
  - similar problems of computing ranges for the thresholds $E - k \cdot \sigma$ and $E + k \cdot \sigma$ for a given k.
- Feasible algorithms were described:
  - for computing the upper bounds for $E - k \cdot \sigma$, and
  - for computing the lower bounds for $E + k \cdot \sigma$, $\dfrac{\sigma}{E - x}$, and $\dfrac{\sigma}{x - E}$.
- For other bounds, feasible algorithms are known under certain conditions on the intervals:
  - for computing the lower bounds for $E - k \cdot \sigma$, and
  - for computing the upper bounds for $E + k \cdot \sigma$, $\dfrac{\sigma}{E - x}$, and $\dfrac{\sigma}{x - E}$.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

11. What is Known (cont-d)

- *Reminder:* for some bounds, feasible algorithms are known only under conditions on intervals:
  - for computing the lower bounds for $E - k \cdot \sigma$, and
  - for computing the upper bounds for $E + k \cdot \sigma$, $\dfrac{\sigma}{E - x}$, and $\dfrac{\sigma}{x - E}$.
- It was proven that for $E \pm k \cdot \sigma$, such conditions are necessary.
- Specifically, it was proven that the following problems are NP-hard:
  - computing the lower bound for $E - k \cdot \sigma$ and
  - computing the upper bound for $E + k \cdot \sigma$.
- This means that, unless P=NP, these problems cannot be, in general, solved in polynomial (= feasible) time.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

12. What We Do in This Talk

- *It was known:* that computing bounds for the thresholds $E - k \cdot \sigma$ and $E + k \cdot \sigma$.
- *Another problem:* computing the range **r** of the ratio
$$r = \frac{\sigma}{E - x}.$$
- *It was not known:* whether computing **r** is NP-hard.
- *In this talk:* we prove that the problem of computing **r** is NP-hard.
- *A similar problem:* computing the range **R** of a ratio
$$R \stackrel{\text{def}}{=} \frac{V}{E}.$$
- *Comment:* the ration R is used in clustering.
- *We prove:* that the problem of computing **R** is also NP-hard.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

13. Discussion

- *Known fact:*
  - to prove that a problem is NP-hard,
  - it is sufficient to prove that a particular case of this problem is NP-hard.
- We want: to prove that computing the upper bound of the ratios $\dfrac{\sigma}{E-x}$ and $\dfrac{\sigma}{x-E}$ is NP-hard.
- *It is sufficient to prove:* that computing the range of the ratio $\dfrac{\sigma}{E}$ (corr. to $x=0$) is NP-hard.
- *It is sufficient to prove:* for the case when all the intervals $[\underline{x}_i, \overline{x}_i]$ contain only non-negative values.
- *Comment:* this case is equivalent to $\underline{x}_i \geq 0$ for all i.

14. Theorem 1

The following problem is NP-hard:

- given: *a natural number* n *and* n *(rational-valued) intervals* $[\underline{x}_i, \overline{x}_i]$,
- compute: *the upper endpoint* $\overline{r}$ *of the range*

$$\mathbf{r} = [\underline{r}, \overline{r}] = \{r(x_1, \ldots, x_n) \mid x_1 \in [\underline{x}_1, \overline{x}_1], \ldots, x_n \in [\underline{x}_n, \overline{x}_n]\}$$

of the ratio $r = \dfrac{\sqrt{V}}{E}$, *where* $E = \dfrac{1}{n} \cdot \sum_{i=1}^{n} x_i$ *and*

$$V = \frac{1}{n} \cdot \sum_{i=1}^{n} (x_i - E)^2.$$

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

15. Theorem 2

The following problem is NP-hard:

- given: *a natural number n and n (rational-valued) intervals $[\underline{x}_i, \overline{x}_i]$,*
- compute: *the upper endpoint $\overline{r}$ of the range*

$$\mathbf{r} = [\underline{r}, \overline{r}] = \{r(x_1, \ldots, x_n) \,|\, x_1 \in [\underline{x}_1, \overline{x}_1], \ldots, x_n \in [\underline{x}_n, \overline{x}_n]\}$$

of the ratio $r = \dfrac{V}{E}$, *where* $E = \dfrac{1}{n} \cdot \sum\limits_{i=1}^{n} x_i$ *and*

$$V = \frac{1}{n} \cdot \sum_{i=1}^{n} (x_i - E)^2.$$

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

16. Proof of Theorem 1: Eliminating Square Root

- The expression for the ratio $r = \dfrac{\sqrt{V}}{E}$ uses a square root – to compute $\sigma = \sqrt{V}$.
- In optimization, we usually use derivatives.
- The square root function $f(x) = \sqrt{x}$ has infinite derivative when $x = 0$.
- Thus, it is desirable to avoid square roots.
- To avoid the square root problem, we can use the facts that
  - $r = \sqrt{R}$, where $R \stackrel{\text{def}}{=} \dfrac{V}{E^2}$, and
  - the function $\sqrt{x}$ is strictly increasing.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

17. Eliminating Square Root (cont-d)

- Since the function $\sqrt{x}$ is strictly increasing:
  - the smallest possible value $\underline{r}$ of r is equal to the square root of the smallest possible value of R:
  $$\underline{r} = \sqrt{\underline{R}};$$
  - the largest possible value $\overline{r}$ of r is equal to the square root of the largest possible value of R:
  $$\overline{r} = \sqrt{\overline{R}}.$$
- So:
  - the problem of computing the range of the ratio r is feasibly equivalent to
  - the problem of computing the range $[\underline{R}, \overline{R}]$ of the new ratio R.
- Thus, computing **r** is NP-hard ⇔ computing **R** is NP-hard.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

18. Proof: Part 2

- A problem is NP-hard if every problem from a certain class NP can be reduced to it.
- We will show that a known NP-hard problem $\mathcal{P}$ can be reduced to our problem $\mathcal{P}_0$. Then:
  - every problem from the class NP can be reduced to $\mathcal{P}$, and
  - $\mathcal{P}$ can be reduced to $\mathcal{P}_0$,
  - hence every problem from the class NP can also be reduced to $\mathcal{P}_0$;
  - thus, our problem $\mathcal{P}_0$ is indeed NP-hard.
- As $\mathcal{P}$, we choose a *subset sum* problem:
  - given n positive integers $s_1, \ldots, s_n$,
  - check whether there exists signs $\eta_i \in \{-1, 1\}$ for which $\sum\limits_{i=1}^{n} \eta_i \cdot s_i = 0$.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

19. Part 2 (cont-d)

- *Reminder:* we reduce the problem of computing the range $\mathbf{R} = [\underline{R}, \overline{R}]$ to the *subset sum* problem:
  - given n positive integers $s_1, \ldots, s_n$,
  - check whether there exists signs $\eta_i \in \{-1, 1\}$ for which $\sum\limits_{i=1}^{n} \eta_i \cdot s_i = 0$.
- Specifically, we will prove that for an appropriately chosen integer N:
  - such signs exist if and only if
  - for the intervals $\mathbf{x}_i = [N - s_i, N + s_i]$, the upper endpoint $\overline{R}$ is greater than or equal to

$$R_0 \stackrel{\text{def}}{=} \frac{M_0}{N^2}, \text{ where } M_0 \stackrel{\text{def}}{=} \frac{1}{n} \cdot \sum_{i=1}^{n} s_i^2.$$

A Practical Problem: ...
How This Problem is ...
A Standard Way to ...
Selecting the Parameter k
Case of Interval ...
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

20. Part 3

- *Lemma.* The ratio $R = \dfrac{V}{E^2}$ attains its maximum on the box
$$[\underline{x}_1, \overline{x}_1] \times \ldots \times [\underline{x}_n, \overline{x}_n]$$
when each of the variables x_i is equal to one of the endpoints $\underline{x}_i$ or $\overline{x}_i$.
- We will prove this statement by contradiction.
- Let us assume that for some i, the function R attains its maximum at an internal point $x_i \in (\underline{x}_i, \overline{x}_i)$.
- In this case, according to calculus, at this point,
  - the partial derivative $\dfrac{\partial R}{\partial x_i}$ should be equal to 0, and
  - the second derivative $\dfrac{\partial^2 R}{\partial x_i^2}$ should be non-positive.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

21. Part 3 (cont-d)

- Here,

$$\frac{\partial E}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{1}{n}\cdot\sum_{j=1}^{n} x_j\right) = \frac{1}{n}.$$

- Since $V = M - E^2$, where $M \stackrel{\text{def}}{=} \frac{1}{n}\cdot\sum_{j=1}^{n} x_j^2$, we have

$$\frac{\partial V}{\partial x_i} = \frac{\partial M}{\partial x_i} - \frac{\partial E^2}{\partial x_i}.$$

- Here,

$$\frac{\partial E^2}{\partial x_i} = 2\cdot E\cdot\frac{\partial E}{\partial x_i} = 2\cdot E\cdot\frac{1}{n},$$

and

$$\frac{\partial M}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{1}{n}\cdot\sum_{j=1}^{n} x_j^2\right) = \frac{1}{n}\cdot 2x_i.$$

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

22. Computing the First Derivative

- So, for $V = M - E^2$, we have $\dfrac{\partial V}{\partial x_i} = \dfrac{1}{n} \cdot 2x_i - 2 \cdot E \cdot \dfrac{1}{n}$.
- Thus,

$$\frac{\partial R}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{V}{E^2}\right) = \frac{\dfrac{\partial V}{\partial x_i} \cdot E^2 - V \cdot \dfrac{\partial E^2}{\partial x_i}}{E^4} =$$

$$\frac{\left(\dfrac{1}{n} \cdot 2x_i - 2 \cdot E \cdot \dfrac{1}{n}\right) \cdot E^2 - V \cdot 2 \cdot E \cdot \dfrac{1}{n}}{E^4} = 2 \cdot \frac{x_i \cdot E - E^2 - V}{n \cdot E^3}.$$

- So, when $\dfrac{\partial R}{\partial x_i} = 0$, we get

$$x_i = \frac{E^2 + V}{E} = \frac{M}{E}.$$

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

23. Computing the Second Derivative

- We differentiate $\frac{\partial R}{\partial x_i}$ with respect to x_i.
- As a result, we get the following expression for the second derivative:

$$\frac{\partial^2 R}{\partial x_i^2} = 2 \cdot \frac{3 \cdot V + (n+3) \cdot E^2 - 4 \cdot x_i \cdot E}{n^2 \cdot E^4}.$$

- The denominator is positive.
- We assumed that the second derivative is non-positive.
- We thus conclude that

$$3 \cdot V + (n+3) \cdot E^2 - 4 \cdot x_i \cdot E =$$

$$3 \cdot M + n \cdot E^2 - 4 \cdot x_i \cdot E \le 0.$$

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

24. Proof of the Lemma

- *Reminder:* $3 \cdot M + n \cdot E^2 - 4 \cdot x_i \cdot E \le 0.$
- By definition, $E = \frac{1}{n} \cdot \sum_{j=1}^{n} x_i = \frac{1}{n} \cdot x_i + \frac{1}{n} \cdot E_i$, where we denoted $E_i \stackrel{\text{def}}{=} \sum_{j \ne i} x_j$.
- Similarly, $M = \frac{1}{n} \cdot x_i^2 + \frac{1}{n} \cdot M_i$ where $M_i \stackrel{\text{def}}{=} \sum_{j \ne i} x_j^2$.
- So, we get $3 \cdot M_i + E_i^2 - 2 \cdot x_i \cdot E_i \le 0$.
- Due to $x_i = \frac{M}{E}$, we have $x_i \cdot E = M$, hence

$$x_i \cdot \left(\frac{1}{n} \cdot x_i + \frac{1}{n} \cdot E_i\right) = \frac{1}{n} \cdot x_i^2 + \frac{1}{n} \cdot M_i.$$

- We also get $x_i \cdot E_i = M_i$, so we conclude that

$$3 \cdot M_i + E_i^2 - 2 \cdot x_i \cdot E_i = M_i + E_i^2 \le 0.$$

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

25. Proof of the Lemma

- *Reminder:* we proved that $M_i + E_i^2 \le 0$.
- However, for large enough N – specifically, for $N > \max\limits_i s_i$ – we have $x_j > 0$.
- Hence $M_i = \frac{1}{n} \cdot \sum\limits_{j \ne i} x_j^2 > 0$ and thus,

$$M_i + E_i^2 > 0.$$

- This shows that the maximum of R cannot be attained at an internal point of the interval $(\underline{x}_i, \overline{x}_i)$.
- Thus, this maximum can only be attained when $x_i = \underline{x}_i$ or $x_i = \overline{x}_i$.
- The Lemma is proven.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

26. Proof of Theorem 1

- *Statement:* $\overline{R} \geq R_0 = \dfrac{M_0}{N^2} \Leftrightarrow$ there exist signs $\eta_i \in \{-1, 1\}$ for which $\sum\limits_{i=1}^{n} \eta_i \cdot s_i = 0$.

$\Leftarrow$ If such signs exist, then we take $x_i = N + \eta_i \cdot s_i$; then:

  - $E = N$, $x_i - E = \pm s_i$, and
  - $V = \dfrac{1}{n} \cdot \sum\limits_{i=1}^{n} (x_i - E)^2 = \dfrac{1}{n} \cdot \sum\limits_{i=1}^{n} s_i^2 = M_0$, and
  - $R = \dfrac{V}{E^2} = \dfrac{M_0}{N^2} = R_0$.

- The largest possible value $\overline{R}$ must therefore be larger than or equal to this value.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

27. Proof of Theorem 1 (cont-d)

- Vice versa, assume that $\overline{R} \ge R_0$.
- Let x_i be the values for which the ratio R attains its maximum value $\overline{R}$.
- Due to the Lemma, this maximum is attained when $x_i = N + t_i$ with $t_i = \eta_i \cdot s_i$ an $\eta_i \in \{-1, 1\}$; then:
  - $E = N + e$, where $e \stackrel{\text{def}}{=} \dfrac{1}{n} \cdot \displaystyle\sum_{i=1}^{n} t_i$, and
  - $V(x_1, \ldots, x_n) = V(t_1, \ldots, t_n) = \dfrac{1}{n} \cdot \displaystyle\sum_{i=1}^{n} t_i^2 - e^2$.
- Since $t_i = \pm s_i$, we have $t_i^2 = s_i^2$ and thus, $\dfrac{1}{n} \cdot \displaystyle\sum_{i=1}^{n} t_i^2 = \dfrac{1}{n} \cdot \displaystyle\sum_{i=1}^{n} s_i^2 = M_0$ and $V = M_0 - e^2$; thus, $\overline{R} = \dfrac{M_0 - e^2}{(N + e)^2}$.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

28. Proof of Theorem 1 (cont-d)

- *Reminder:* $\overline{R} = \dfrac{M_0 - e^2}{(N+e)^2} \geq R_0$.
- Multiplying both sides by the denominator, we get

$$e^2 \cdot (N^2 + M_0) + 2 \cdot M_0 \cdot N \cdot e \leq 0.$$

- If $e > 0$, then the left-hand side is positive and cannot be ≤ 0, so $e \leq 0$.
- If $e < 0$, then this inequality leads to

$$|e|^2 \cdot (N^2 + M_0) - 2 \cdot M_0 \cdot N \cdot |e| \leq 0$$

and

$$|e| \leq \frac{2 \cdot M_0 \cdot N}{N^2 + M_0}.$$

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

29. Proof of Theorem 1 (final part)

- *Reminder:* $|e| \le \dfrac{2 \cdot M_0 \cdot N}{N^2 + M_0}$.
- Since $\dfrac{2 \cdot M_0 \cdot N}{N^2 + M_0} \to 0$ as $N \to \infty$, for sufficiently large N, we get $|e| \ge \dfrac{1}{n} > \dfrac{2 \cdot M_0 \cdot N}{N^2 + M_0}$.
- However, by definition, all the values s_i, and all the values $t_i = \pm s_i$, and the sum $n \cdot e = \sum\limits_{i=1}^{n} t_i$ are integers.
- So $|n \cdot e| \ge 1$ and $|e| \ge \dfrac{1}{n}$.
- Thus, the inequality $|e| \le \dfrac{2 \cdot M_0 \cdot N}{N^2 + M_0}$ is impossible.
- This shows that e cannot be negative, hence $e = 0$, and thus, $n \cdot e = \sum\limits_{i=1}^{n} \eta_i \cdot s_i = 0$. The theorem is proven.

A Practical Problem: . . .
How This Problem is . . .
A Standard Way to . . .
Selecting the Parameter k
Case of Interval . . .
What is Known
What We Do in This Talk
Theorem 1
Theorem 2

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A Practical Problem: . . .
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