Application-Motivated Combinations of Interval and Probability Approaches, with Application to Geoinformatics, Bioinformatics, and Engineering

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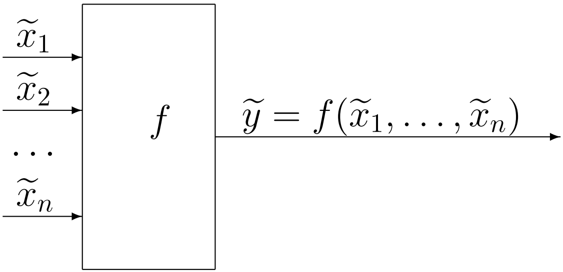
1. General Problem of Data Processing under Uncertainty

- *Indirect measurements:* way to measure y that are are difficult (or even impossible) to measure directly.
- *Idea:* $y = f(x_1, \ldots, x_n)$



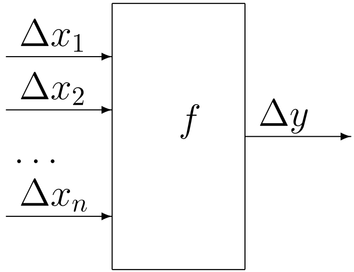
- *Problem:* measurements are never 100% accurate: $\widetilde{x}_i \neq x_i$ ($\Delta x_i \neq 0$) hence

$$\widetilde{y} = f(\widetilde{x}_1, \ldots, \widetilde{x}_n) \neq y = f(x_1, \ldots, x_n).$$

What are bounds on $\Delta y \stackrel{\text{def}}{=} \widetilde{y} - y$?

Title Page
◀◀ ▶▶
◀ ▶
Page 2 of 32
Go Back
Full Screen
Close
Quit

2. Probabilistic and Interval Uncertainty

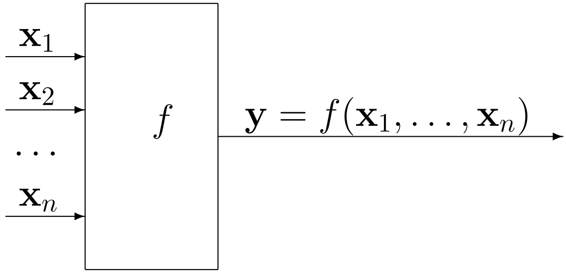


- *Traditional approach:* we know probability distribution for Δx_i (usually Gaussian).
- *Where it comes from:* calibration using standard MI.
- *Problem:* calibration is not possible in:
  - fundamental science
  - manufacturing
- *Solution:* we know upper bounds Δ_i on $|\Delta x_i|$ hence

$$x_i \in [\widetilde{x}_i - \Delta_i, \widetilde{x}_i + \Delta_i].$$

General Problem of . . .
Probabilistic and . . .
Interval . . .
Case Study: Chip Design
Combining Interval . . .
Extension of Interval . . .
Successes (cont-d)
Challenges
Case Study: . . .
Case Study: Detecting . . .
Title Page
◀◀ ▶▶
◀ ▶
Page 3 of 32
Go Back
Full Screen
Close
Quit

3. Interval Computations: A Problem



- *Given:* an algorithm $y = f(x_1, \dots, x_n)$ and n intervals $\mathbf{x}_i = [\underline{x}_i, \overline{x}_i]$.
- *Compute:* the corresponding range of y:

  $$[\underline{y}, \overline{y}] = \{f(x_1, \dots, x_n) \mid x_1 \in [\underline{x}_1, \overline{x}_1], \dots, x_n \in [\underline{x}_n, \overline{x}_n]\}.$$
- *Fact:* NP-hard even for quadratic f.
- *Challenge:* when are feasible algorithm possible?
- *Challenge:* when computing $\mathbf{y} = [\underline{y}, \overline{y}]$ is not feasible, find a good approximation $\mathbf{Y} \supseteq \mathbf{y}$.

General Problem of . . .
Probabilistic and . . .
Interval . . .
Case Study: Chip Design
Combining Interval . . .
Extension of Interval . . .
Successes (cont-d)
Challenges
Case Study: . . .
Case Study: Detecting . . .
Title Page
Page 4 of 32
Go Back
Full Screen
Close
Quit

4. Alternative Approach: Maximum Entropy

- *Situation:* in many practical applications, it is very difficult to come up with the probabilities.
- *Traditional engineering approach:* use probabilistic techniques.
- *Problem:* many different probability distributions are consistent with the same observations.
- *Solution:* select one of these distributions – e.g., the one with the largest entropy.
- *Example – single variable:* if all we know is that $x \in [\underline{x}, \overline{x}]$, then MaxEnt leads to a uniform distribution on $[\underline{x}, \overline{x}]$.
- *Example – multiple variables:* different variables are independently distributed.

5. Limitations of Maximum Entropy Approach

- *Example:* simplest algorithm $y = x_1 + \ldots + x_n$.
- *Measurement errors:* $\Delta x_i \in [-\Delta, \Delta]$.
- *Analysis:* $\Delta y = \Delta x_1 + \ldots + \Delta x_n$.
- *Worst case situation:* $\Delta y = n \cdot \Delta$.
- *Maximum Entropy approach:* due to Central Limit Theorem, Δy is $\approx$ normal, with $\sigma = \Delta \cdot \dfrac{\sqrt{n}}{\sqrt{3}}$.
- *Why this may be inadequate:* we get $\Delta \sim \sqrt{n}$, but due to correlation, it is possible that $\Delta = n \cdot \Delta \sim n \gg \sqrt{n}$.
- *Conclusion:* using a single distribution can be very misleading, especially if we want guaranteed results.
- Examples: high-risk application areas such as space exploration or nuclear engineering.

Title Page
◀◀ ▶▶
◀ ▶
Page 6 of 32
Go Back
Full Screen
Close
Quit

6. Interval Arithmetic: Foundations of Interval Techniques

- *Problem:* compute the range

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

- *Interval arithmetic:* for arithmetic operations $f(x_1, x_2)$ (and for elementary functions), we have explicit formulas for the range.

- *Examples:* when $x_1 \in \mathbf{x}_1 = [\underline{x}_1, \overline{x}_1]$ and $x_2 \in \mathbf{x}_2 = [\underline{x}_2, \overline{x}_2]$, then:
  - The range $\mathbf{x}_1 + \mathbf{x}_2$ for $x_1 + x_2$ is $[\underline{x}_1 + \underline{x}_2, \overline{x}_1 + \overline{x}_2]$.
  - The range $\mathbf{x}_1 - \mathbf{x}_2$ for $x_1 - x_2$ is $[\underline{x}_1 - \overline{x}_2, \overline{x}_1 - \underline{x}_2]$.
  - The range $\mathbf{x}_1 \cdot \mathbf{x}_2$ for $x_1 \cdot x_2$ is $[\underline{y}, \overline{y}]$, where

    $$\underline{y} = \min(\underline{x}_1 \cdot \underline{x}_2, \underline{x}_1 \cdot \overline{x}_2, \overline{x}_1 \cdot \underline{x}_2, \overline{x}_1 \cdot \overline{x}_2);$$
    $$\overline{y} = \max(\underline{x}_1 \cdot \underline{x}_2, \underline{x}_1 \cdot \overline{x}_2, \overline{x}_1 \cdot \underline{x}_2, \overline{x}_1 \cdot \overline{x}_2).$$

- The range $1/\mathbf{x}_1$ for $1/x_1$ is $[1/\overline{x}_1, 1/\underline{x}_1]$ (if $0 \notin \mathbf{x}_1$).

7. Straightforward Interval Computations: Example

- *Example:* $f(x) = (x-2)\cdot(x+2)$, $x \in [1,2]$.
- How will the computer compute it?
  - $r_1 := x - 2$;
  - $r_2 := x + 2$;
  - $r_3 := r_1 \cdot r_2$.
- *Main idea:* perform the same operations, but with *intervals* instead of *numbers*:
  - $\mathbf{r}_1 := [1,2] - [2,2] = [-1,0]$;
  - $\mathbf{r}_2 := [1,2] + [2,2] = [3,4]$;
  - $\mathbf{r}_3 := [-1,0] \cdot [3,4] = [-4,0]$.
- *Actual range:* $f(\mathbf{x}) = [-3,0]$.
- *Comment:* this is just a toy example, there are more efficient ways of computing an enclosure $\mathbf{Y} \supseteq \mathbf{y}$.

8. Case Study: Chip Design

- *Chip design:* one of the main objectives is to decrease the clock cycle.
- *Current approach:* uses worst-case (interval) techniques.
- *Problem:* the probability of the worst-case values is usually very small.
- *Result:* estimates are over-conservative – unnecessary over-design and under-performance of circuits.
- *Difficulty:* we only have *partial* information about the corresponding probability distributions.
- *Objective:* produce estimates valid for all distributions which are consistent with this information.
- *What we do:* provide such estimates for the clock time.

9. Estimating Clock Cycle: a Practical Problem

- *Objective:* estimate the clock cycle on the design stage.
- The clock cycle of a chip is constrained by the maximum path delay over all the circuit paths

$$D \stackrel{\text{def}}{=} \max(D_1, \ldots, D_N).$$

- The path delay D_i along the i-th path is the sum of the delays corresponding to the gates and wires along this path.
- Each of these delays, in turn, depends on several factors such as:
  - the variation caused by the current design practices,
  - environmental design characteristics (e.g., variations in temperature and in supply voltage), etc.

10. Traditional (Interval) Approach to Estimating the Clock Cycle

- *Traditional approach:* assume that each factor takes the worst possible value.
- *Result:* time delay when all the factors are at their worst.
- *Problem:*
  - different factors are usually independent;
  - combination of worst cases is improbable.
- *Computational result:* current estimates are 30% above the observed clock time.
- *Practical result:* the clock time is set too high – chips are over-designed and under-performing.

11. Robust Statistical Methods Are Needed

- *Ideal case:* we know probability distributions.
- *Solution:* Monte-Carlo simulations.
- *In practice:* we only have *partial* information about the distributions of some of the parameters; usually:
  - the mean, and
  - some characteristic of the deviation from the mean – e.g., the interval that is guaranteed to contain possible values of this parameter.
- *Possible approach:* Monte-Carlo with several possible distributions.
- *Problem:* no guarantee that the result is a valid bound for all possible distributions.
- *Objective:* provide *robust* bounds, i.e., bounds that work for all possible distributions.

12. Towards a Mathematical Formulation of the Problem

- *General case:* each gate delay d depends on the difference $x_1, \ldots, x_n$ between the actual and the nominal values of the parameters.
- *Main assumption:* these differences are usually small.
- Each path delay D_i is the sum of gate delays.
- *Conclusion:* D_i is a linear function: $D_i = a_i + \sum\limits_{j=1}^{n} a_{ij} \cdot x_j$ for some a_i and a_{ij}.
- The desired maximum delay $D = \max\limits_i D_i$ has the form

$$D = F(x_1, \ldots, x_n) \stackrel{\text{def}}{=} \max_i \left(a_i + \sum_{j=1}^{n} a_{ij} \cdot x_j \right).$$

13. Towards a Mathematical Formulation of the Problem (cont-d)

- *Known:* maxima of linear function are exactly convex functions:

$$F(\alpha \cdot x + (1-\alpha) \cdot y) \le \alpha \cdot F(x) + (1-\alpha) \cdot F(y)$$

  for all x, y and for all $\alpha \in [0, 1]$;

- *We know:* factors x_i are independent;
  - we know distribution of some of the factors;
  - for others, we know ranges $[\underline{x}_j, \overline{x}_j]$ and means E_j.
- *Given:* a convex function $F \ge 0$ and a number $\varepsilon > 0$.
- *Objective:* find the smallest y_0 s.t. for all possible distributions, we have $y \le y_0$ with the probability $\ge 1-\varepsilon$.

14. Additional Property: Dependency is Non-Degenerate

- *Fact:* sometimes, we learn additional information about one of the factors x_j.
- *Example:* we learn that x_j actually belongs to a proper subinterval of the original interval $[\underline{x}_j, \overline{x}_j]$.
- *Consequence:* the class $\mathcal{P}$ of possible distributions is replaced with $\mathcal{P}' \subset \mathcal{P}$.
- *Result:* the new value y_0' can only decrease: $y_0' \le y_0$.
- *Fact:* if x_j is irrelevant for y, then $y_0' = y_0$.
- *Assumption:* irrelevant variables been weeded out.
- *Formalization:* if we narrow down one of the intervals $[\underline{x}_j, \overline{x}_j]$, the resulting value y_0 decreases: $y_0' < y_0$.

15. Formulation of the Problem

GIVEN:
- n, $k \le n$, $\varepsilon > 0$;
- a convex function $y = F(x_1, \ldots, x_n) \ge 0$;
- $n - k$ cdfs $F_j(x)$, $k + 1 \le j \le n$;
- intervals $\mathbf{x}_1, \ldots, \mathbf{x}_k$, values $E_1, \ldots, E_k$,

TAKE: all joint probability distributions on R^n for which:

- all x_i are independent,
- $x_j \in \mathbf{x}_j$, $E[x_j] = E_j$ for $j \le k$, and
- x_j have distribution $F_j(x)$ for $j > k$.

FIND: the smallest y_0 s.t. for all such distributions, $F(x_1, \ldots, x_n) \le y_0$ with probability $\ge 1 - \varepsilon$.

WHEN: the problem is *non-degenerate* – if we narrow down one of the intervals $\mathbf{x}_j$, y_0 decreases.

16. Main Result and How We Can Use It

- *Result:* y_0 is attained when for each j from 1 to k,
  - $x_j = \underline{x}_j$ with probability $\underline{p}_j \stackrel{\text{def}}{=} \dfrac{\overline{x}_j - E_j}{\overline{x}_j - \underline{x}_j}$, and
  - $x_j = \overline{x}_j$ with probability $\overline{p}_j \stackrel{\text{def}}{=} \dfrac{E_j - \underline{x}_j}{\overline{x}_j - \underline{x}_j}$.
- *Algorithm:*
  - simulate these distributions for x_j, $j < k$;
  - simulate known distributions for $j > k$;
  - use the simulated values $x_j^{(s)}$ to find
  $$y^{(s)} = F(x_1^{(s)}, \ldots, x_n^{(s)});$$
  - sort N values $y^{(s)}$: $y_{(1)} \le y_{(2)} \le \ldots \le y_{(N_i)}$;
  - take $y_{(N_i \cdot (1-\varepsilon))}$ as y_0.

17. Comment about Monte-Carlo Techniques

- *Traditional belief:* Monte-Carlo methods are inferior to analytical:
  - they are approximate;
  - they require large computation time;
  - simulations for *several* distributions, may mis-calculate the (desired) maximum over *all* distributions.
- *We proved:* the value corresponding to the selected distributions indeed provide the desired maximum value y_0.
- *General comment:*
  - justified Monte-Carlo methods often lead to *faster* computations than analytical techniques;
  - example: multi-D integration – where Monte-Carlo methods were originally invented.

18. Conclusions

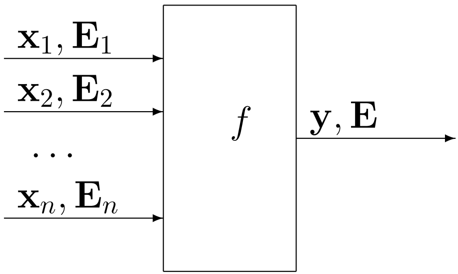
- *Problem of chip design:* decrease the clock cycle.
- *How this problem is solved now:* by using worst-case (interval) techniques.
- *Limitations of this solution:* the probability of the worst-case values is usually very small.
- *Consequence:* estimates are over-conservative, hence over-design and under-performance of circuits.
- *Objective:* find the clock time as y_0 s.t. for the actual delay y, we have $\text{Prob}(y > y_0) \le \varepsilon$ for given $\varepsilon > 0$.
- *Difficulty:* we only have *partial* information about the corresponding distributions.
- *What we have described:* a general technique that allows us, in particular, to compute y_0.

19. Combining Interval and Probabilistic Uncertainty: General Case

- *Problem:* there are many ways to represent a probability distribution.
- *Idea:* look for an objective.
- *Objective:* make decisions $E_x[u(x,a)] \to \max\limits_a$.
- *Case 1:* smooth $u(x)$.
- *Analysis:* we have $u(x) = u(x_0) + (x - x_0) \cdot u'(x_0) + \ldots$
- *Conclusion:* we must know moments to estimate $E[u]$.
- *Case of uncertainty:* interval bounds on moments.
- *Case 2:* threshold-type $u(x)$.
- *Conclusion:* we need cdf $F(x) = \mathrm{Prob}(\xi \le x)$.
- *Case of uncertainty:* p-box $[\underline{F}(x), \overline{F}(x)]$.

20. Extension of Interval Arithmetic to Probabilistic Case: Successes

- *General solution:* parse to elementary operations $+$, $-$, $\cdot$, $1/x$, max, min.
- Explicit formulas for arithmetic operations known for intervals, for p-boxes $\mathbf{F}(x) = [\underline{F}(x), \overline{F}(x)]$, for intervals $+$ 1st moments $E_i \stackrel{\text{def}}{=} E[x_i]$:



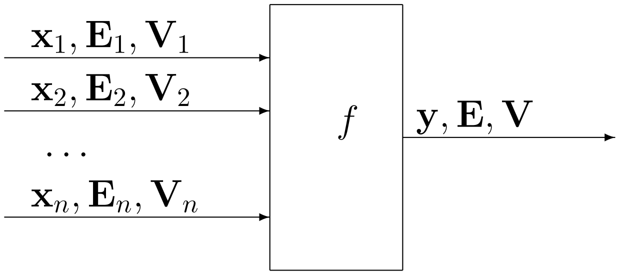
21. Successes (cont-d)

- *Easy cases:* $+$, $-$, product of independent x_i.
- *Example of a non-trivial case:* multiplication $y = x_1 \cdot x_2$, when we have no information about the correlation:
  - $\underline{E} = \max(p_1+p_2-1,0)\cdot\overline{x}_1\cdot\overline{x}_2+\min(p_1,1-p_2)\cdot\overline{x}_1\cdot\underline{x}_2+\min(1-p_1,p_2)\cdot\underline{x}_1\cdot\overline{x}_2+\max(1-p_1-p_2,0)\cdot\underline{x}_1\cdot\underline{x}_2$;
  - $\overline{E} = \min(p_1,p_2)\cdot\overline{x}_1\cdot\overline{x}_2+\max(p_1-p_2,0)\cdot\overline{x}_1\cdot\underline{x}_2+\max(p_2-p_1,0)\cdot\underline{x}_1\cdot\overline{x}_2+\min(1-p_1,1-p_2)\cdot\underline{x}_1\cdot\underline{x}_2$,

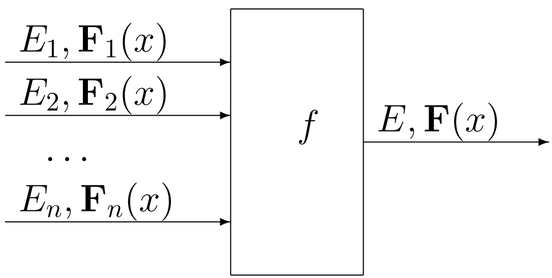
  where $p_i \stackrel{\text{def}}{=} (E_i-\underline{x}_i)/(\overline{x}_i-\underline{x}_i)$.

22. Challenges

- intervals + 2nd moments:



- moments + p-boxes; e.g.:



23. Case Study: Bioinformatics

- *Practical problem:* find genetic difference between cancer cells and healthy cells.
- *Ideal case:* we directly measure concentration c of the gene in cancer cells and h in healthy cells.
- *In reality:* difficult to separate.
- *Solution:* we measure $y_i \approx x_i \cdot c + (1 - x_i) \cdot h$, where x_i is the percentage of cancer cells in i-th sample.
- *Equivalent form:* $a \cdot x_i + h \approx y_i$, where $a \stackrel{\text{def}}{=} c - h$.

24. Case Study: Bioinformatics (cont-d)

- *If we know x_i exactly:* Least Squares Method $\sum\limits_{i=1}^{n}(a\cdot x_i+h-y_i)^2\to\min\limits_{a,h}$, hence $a=\dfrac{C(x,y)}{V(x)}$ and $h=E(y)-a\cdot E(x)$, where $E(x)=\dfrac{1}{n}\cdot\sum\limits_{i=1}^{n}x_i$,

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

$$C(x,y)=\frac{1}{n-1}\cdot\sum_{i=1}^{n}(x_i-E(x))\cdot(y_i-E(y)).$$

- *Interval uncertainty:* experts manually count x_i, and only provide interval bounds $\mathbf{x}_i$, e.g., $x_i\in[0.7,0.8]$.
- *Problem:* find the range of a and h corresponding to all possible values $x_i\in[\underline{x}_i,\overline{x}_i]$.

25. General Problem

- *General problem:*
  - we know intervals $\mathbf{x}_1 = [\underline{x}_1, \overline{x}_1], \ldots, \mathbf{x}_n = [\underline{x}_n, \overline{x}_n]$,
  - compute the range of $E(x) = \dfrac{1}{n}\sum\limits_{i=1}^{n} x_i$, population variance $V = \dfrac{1}{n}\sum\limits_{i=1}^{n}(x_i - E(x))^2$, etc.
- *Difficulty:* NP-hard even for variance.
- *Known:*
  - efficient algorithms for $\underline{V}$,
  - efficient algorithms for $\overline{V}$ and $C(x,y)$ for reasonable situations.
- *Bioinformatics case:* find intervals for $C(x,y)$ and for $V(x)$ and divide.

26. Case Study: Detecting Outliers

- In many application areas, it is important to detect *outliers*, i.e., unusual, abnormal values.
- In *medicine*, unusual values may indicate disease.
- In *geophysics*, abnormal values may indicate a mineral deposit (or an erroneous measurement result).
- In *structural integrity* testing, abnormal values may indicate faults in a structure.
- *Traditional engineering approach:* a new measurement result x is classified as an outlier if $x \notin [L, U]$, where

$$L \stackrel{\text{def}}{=} E - k_0 \cdot \sigma, \quad U \stackrel{\text{def}}{=} E + k_0 \cdot \sigma,$$

  and $k_0 > 1$ is pre-selected.
- *Comment:* most frequently, $k_0 = 2$, 3, or 6.

27. Outlier Detection Under Interval Uncertainty: A Problem

- In some practical situations, we only have intervals $\mathbf{x}_i = [\underline{x}_i, \overline{x}_i]$.
- Different $x_i \in \mathbf{x}_i$ lead to different intervals $[L, U]$.
- A *possible* outlier: outside *some* k_0-sigma interval.
- *Example:* structural integrity – not to miss a fault.
- A *guaranteed* outlier: outside *all* k_0-sigma intervals.
- *Example:* before a surgery, we want to make sure that there is a micro-calcification.
- A value x is a possible outlier if $x \notin [\overline{L}, \underline{U}]$.
- A value x is a guaranteed outlier if $x \notin [\underline{L}, \overline{U}]$.
- *Conclusion:* to detect outliers, we must know the ranges of $L = E - k_0 \cdot \sigma$ and $U = E + k_0 \cdot \sigma$.

28. Outlier Detection Under Interval Uncertainty: A Solution

- *We need:* to detect outliers, we must compute the ranges of $L = E - k_0 \cdot \sigma$ and $U = E + k_0 \cdot \sigma$.
- *We know:* how to compute the ranges $\mathbf{E}$ and $[\underline{\sigma}, \overline{\sigma}]$ for E and σ.
- *Possibility:* use interval computations to conclude that $L \in \mathbf{E} - k_0 \cdot [\underline{\sigma}, \overline{\sigma}]$ and $L \in \mathbf{E} + k_0 \cdot [\underline{\sigma}, \overline{\sigma}]$.
- *Problem:* the resulting intervals for L and U are *wider* than the actual ranges.
- *Reason:* E and σ use the same inputs $x_1, \ldots, x_n$ and are hence not independent from each other.
- *Practical consequence:* we miss some outliers.
- *Desirable:* compute *exact* ranges for L and U.
- *Application:* detecting outliers in gravity measurements.

29. Acknowledgments

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30. Proof of the Result about Chips

- Let us fix the optimal distributions for $x_2, \ldots, x_n$; then,
$$\text{Prob}(D \le y_0) = \sum_{(x_1,\ldots,x_n): D(x_1,\ldots,x_n) \le y_0} p_1(x_1) \cdot p_2(x_2) \cdot \ldots$$
- So, $\text{Prob}(D \le y_0) = \sum\limits_{i=0}^{N} c_i \cdot q_i$, where $q_i \stackrel{\text{def}}{=} p_1(v_i)$.
- Restrictions: $q_i \ge 0$, $\sum\limits_{i=0}^{N} q_i = 1$, and $\sum\limits_{i=0}^{N} q_i \cdot v_i = E_1$.
- Thus, the worst-case distribution for x_1 is a solution to the following linear programming (LP) problem:

Minimize $\sum\limits_{i=0}^{N} c_i \cdot q_i$ under the constraints $\sum\limits_{i=0}^{N} q_i = 1$ and
$$\sum_{i=0}^{N} q_i \cdot v_i = E_1,\ q_i \ge 0,\quad i = 0, 1, 2, \ldots, N.$$

31. Proof of the Result about Chips (cont-d)

- *Minimize:* $\sum\limits_{i=0}^{N} c_i \cdot q_i$ under the constraints $\sum\limits_{i=0}^{N} q_i = 1$ and $\sum\limits_{i=0}^{N} q_i \cdot v_i = E_1$, $q_i \geq 0$, $i = 0, 1, 2, \ldots, N$.
- *Known:* in LP with $N+1$ unknowns $q_0, q_1, \ldots, q_N$, $\geq N+1$ constraints are equalities.
- *In our case:* we have 2 equalities, so at least $N-1$ constraints $q_i \geq 0$ are equalities.
- Hence, no more than 2 values $q_i = p_1(v_i)$ are non-0.
- If corresponding v or v' are in $(\underline{x}_1, \overline{x}_1)$, then for $[v, v'] \subset \mathbf{x}_1$ we get the same y_0 – in contradiction to non-degeneracy.
- Thus, the worst-case distribution is located at $\underline{x}_1$ and $\overline{x}_1$.
- The condition that the mean of x_1 is E_1 leads to the desired formulas for $\underline{p}_1$ and $\overline{p}_1$.