Algorithmic Aspects of Analysis, Prediction, and Control in Science and Engineering: Symmetry-Based Approach

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1. Need for Analysis, Prediction, and Control in Science and Engineering

- Prediction is one of the main objectives of science and engineering.
- Example: in Newton's mechanics, we want to predict the positions and velocities of different objects.
- Once we predict events, a next step is to *influence* these events, i.e., to *control* the corresponding systems.
- In this step, we should select a control that leads to the best possible result.
- To be able to predict and control a system, we need to have a good *description* of this system, so that we can:
 - use this description to *analyze* the system's behavior and
 - extract the desired prediction and control algorithms from this analysis.



2. Symmetry: a Fundamental Property of the Physical World

- One of the main objectives of science: prediction.
- Basis for prediction: we observed similar situations in the past, and we expect similar outcomes.
- In mathematical terms: similarity corresponds to symmetry, and similarity of outcomes to invariance.
- Example: we dropped the ball, it fall down.
- Symmetries: shift, rotation, etc.
- In this example, we used *geometric* symmetries, i.e., symmetries that have a direct geometric meaning.



3. Example: Discrete Geometric Symmetries

- In the above example, the corresponding symmetries form a *continuous* family.
- In some other situations, we only have a *discrete* set of geometric symmetries.
- Molecules such as benzene or cubane are invariant with respect to , e.g., rotation by 60°. molecule.

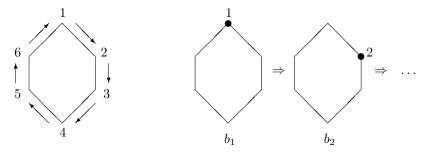


Figure 1: Benzene – rotation by 60°

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4. More General Symmetries

- Symmetries can go beyond simple geometric transformations.
- Example: the current simplified model of an atom.
- Originally motivated by an analogy with a Solar system.
- The operation has a geometric aspect: it scales down all the distances.
- However, it goes beyond a simple geometric transformation.
- In addition to changing distances, it also changes masses, velocities, replaces masses with electric charges, etc.



5. Basic Symmetries: Scaling and Shift

- To understand real-life phenomena, we must perform appropriate measurements.
- We get a numerical value of a physical quantity, which depends on the *measuring unit*.
- Scaling: if we use a new unit which is λ times smaller, numerical values are multiplied by λ : $x \to \lambda \cdot x$.
- Example: $x \text{ meters} = 100 \cdot x \text{ cm}$.
- Another possibility: change the starting point.
- Shift: if we use a new starting point which is s units before, then $x \to x + s$ (example: time).
- Together, scaling and shifts form linear transformations $x \to a \cdot x + b$.
- *Invariance*: physical formulas should not depend on the choice of a measuring unit or of a starting point.



6. Example of Using Symmetries: Pendulum

- Problem: find how period T depends on length L and on free fall acceleration g on the corresponding planet.
- Originally found using Newton's equations.
- The same dependence (modulo a constant) can be obtained only using symmetries.
- There is no fixed length, so we assume that the physics don't change if we change the unit of length.
- If we change a unit of length to a one λ times smaller, we get new numerical value $L' = \lambda \cdot L$.
- If we change a unit of time to one μ times smaller, we get a new numerical value for the period $T' = \mu \cdot T$.
- Under these transformations, the numerical value of the acceleration changes as $g \to g' = \lambda \cdot \mu^{-2} \cdot g$.



7. Pendulum Example (cont-d)

- The physics does not change by simply changing the units.
- Thus, it makes sense to require that if T = f(L, g), then T' = f(L', g').
- Substituting $T' = \mu \cdot T$, $L' = \lambda \cdot L$, and $g' = \lambda \cdot \mu^{-2} \cdot g$ into T' = f(L', g'), we get $f(\lambda \cdot L, \lambda \cdot \mu^{-2} \cdot g) = \mu \cdot f(L, g)$.
- From this formula, we can find the explicit expression for the desired function f(L, g).
- Indeed, let us select λ and μ for which $\lambda \cdot L = 1$ and $\lambda \cdot \mu^{-2} \cdot g = 1$.
- Thus, we take $\lambda = L^{-1}$ and $\mu = \sqrt{\lambda \cdot g} = \sqrt{g/L}$.
- For these values λ and μ , the above formula takes the form $f(1,1) = \mu \cdot f(L,g) = \sqrt{g/L} \cdot f(L,g)$.
- Thus, $f(L,g) = \text{const} \cdot \sqrt{L/g}$ (for the constant f(1,1)).

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8. What is the Advantage of Using Symmetries?

- What is *new* is that we derived it without using any specific differential equations.
- We only used the fact that these equations do not have any fixed unit of length or fixed unit of time.
- Thus, the same formula is true not only for Newton's equations, but also for *any* alternative theory.
- Physical theories need to be experimentally confirmed.
- We do not need the whole Newton's mechanics theory to derive the pend. formula only need symmetries.
- This shows that:
 - if we have an experimental confirmation of the pendulum formula,
 - this does not necessarily mean that we have confirmed Newton's equations just the symmetries.



9. Basic Nonlinear Symmetries

- Sometimes, a system also has *nonlinear* symmetries.
- If a system is invariant under f and g, then:
 - it is invariant under their composition $f \circ g$, and
 - it is invariant under the inverse transformation f^{-1} .
- In mathematical terms, this means that symmetries form a *group*.
- In practice, at any given moment of time, we can only store and describe finitely many parameters.
- Thus, it is reasonable to restrict ourselves to *finite-dimensional* groups.
- Question (N. Wiener): describe all finite-dimensional groups that contain all linear transformations.
- Answer (for real numbers): all elements of this group are fractionally-linear $x \to (a \cdot x + b)/(c \cdot x + d)$.



10. Independence as Another Example of Symmetry

- We encounter complex systems consisting of a large number of smaller objects (or subsystems).
- Example: molecules that consist of a large number of atoms.
- The more subsystems we have, the more complex the corresponding models,
 - the more difficult their algorithmic analysis because in general,
 - we need to take into account possible interactions between different subsystems.
- Symmetry: We know that some of these subsystems are reasonably independent.
- The transformations performed on one of the subsystems does not change the state of the other.

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11. Discrete Symmetries

- In some cases, we have a discrete set of transformations under which the object is invariant.
- Example: In electromagnetism, the flas. do not change if we simply replace all pos. charges with neg. ones:
 - particles with opposite charges will continue to attract each other and
 - particles with the same charges will continue to repel each other with exactly the same force.
- Similarly, it usually does not matter whether we take, as a basis, a certain property
 - -P (such as "small") or its negation
 - $-P' \stackrel{\text{def}}{=} \neg P \text{ (such as "large")}.$
- We can easily transform the corresponding formulas into one another.



12. Symmetries and Optimization

- It is natural to require that the model be invariant with respect to the corresponding symmetries.
- In many such cases, this invariance requirement enables us to determine the model.
- Sometimes, unlikely that the corresponding model is invariant with respect to the symmetries.
- In this case, we don't restrict to a small class of possible models.
- Out of all possible models, it is necessary to select the one which is, in some reasonable sense, the best e.g.,
 - the most accurate in describing the real-life phenomena, or
 - the one which is the fastest to compute, etc.



13. Symmetries and Optimization (cont-d)

- What does the "best" mean?
- On the set of all appropriate models, there is a relation

 ≥ describing which model is better or equal in quality.
- This relation must be transitive (but we can have two models of the same quality).
- We require that this relation be final in the sense that it should define a unique best model A_{opt} , for which

$$\forall B (A_{\text{opt}} \succeq B).$$

- If none of the models is the best, then this criterion is of no use so there should exist optimal models.
- If several different models are equally best, then we can use this ambiguity to optimize something else.
- It is also reasonable to require that the relation $A \succeq B$ should be invariant relative to natural symmetries.



14. Symmetries and Optimization: Result

- Let \mathcal{A} be a set, and let G be a group of transformations defined on \mathcal{A} .
- By an optimality criterion, we mean a pre-ordering (i.e., a transitive reflexive relation) \leq on the set A.
- An optimality criterion is called *G-invariant* if

$$\forall g \in G \, \forall A, B \in \mathcal{A} \, (A \preceq B \Rightarrow g(A) \preceq g(B)).$$

• An optimality criterion is called *final* if there exists one and only one element $A_{\text{opt}} \in \mathcal{A}$ for which

$$\forall B (B \leq A_{\text{opt}}).$$

• Proposition. Let \leq be a G-invariant and final optimality criterion; then, A_{opt} is G-invariant.



15. Symmetries and Optimization: Proof

- Let us prove that the model A_{opt} is indeed G-invariant, i.e., that $g(A_{\text{opt}}) = A_{\text{opt}}$ for every transf. $g \in G$.
- Indeed, let $g \in G$.
- From the optimality of A_{opt} , we conclude that for every $B \in \mathcal{A}$, we have $g^{-1}(B) \leq A_{\text{opt}}$.
- From the G-invariance of the optimality criterion, we can now conclude that $B \leq g(A_{\text{opt}})$.
- This is true for all $B \in \mathcal{A}$ and therefore, the model $g(A_{\text{opt}})$ is optimal.
- But since the criterion is final, there is only one optimal model; hence, $g(A_{\text{opt}}) = A_{\text{opt}}$.
- So, A_{opt} is indeed invariant.
- The proposition is proven.



16. Approximate Symmetries

- In many physical situations, we do not have *exact* symmetries, we only have *approximate* symmetries.
- Example: A shape of a spiral galaxy can be reasonably well described by a logarithmic spiral.
- This description is only approximate; the actual shape is slightly different.
- Actually, most symmetries are approximate.
- In some cases, the approximation is so good that we can consider the object to be fully symmetric.
- In other cases, we need to take asymmetry into account to get an accurate description of the corr. phenomena.



17. From Methods to Results

- Main algorithmic problems (reminder): analysis, prediction, and control of real-life systems.
- Up to now, we described our *methodology*: the use of symmetries.
- Let us now show the *results* of using symmetries in all algorithmic problems of sciences and engineering.
- First, we show how the symmetry-based approach can be used in the *analysis* of real-life systems.
- Then, we show how this approach can be used in the algorithmics of *prediction*.
- Finally, we show how the symmetry-based approach can be used in the algorithmics of *control*.



18. Algorithmic Aspects of Real-Life Systems Analysis: Symmetry-Based Approach

- Our main objectives are to *predict* the systems' behavior and to find the best way to *change* this behavior.
- In these tasks, we first need to *describe* the systems in precise terms.
- In Chapter 2, we show that *symmetries* can help in this description.
- Real-life systems consist of interacting *subsystems*.
- So, to describe a system, we must first describe *funda-mental* systems: molecules, elementary particles, etc.
- In Chapter 2, we focus on the description of such fundamental systems.



19. Algorithmic Aspects of Real-Life Systems Analvsis: Overview

- We start with the most natural symmetries continuous families of geom. symmetries (rotations, shifts).
- A shape of the molecule is formed by its atoms.
- We look for symmetries, i.e., for transformations that preserve the shape of a molecule.
- H_2 : invariant w.r.t. *all* rotations around its axis; we have a *continuous* family of angles from 0 to 360°.
- Benzene: only inv. w.r.t. discrete angles 60°, 120°, ...
- Except for linear molecules like H₂, a molecule cannot have a continuous family of symmetries.
- For a molecular shape to allow a continuous family of symmetries, it must contain a large number of atoms.
- Such molecules are typical in biosciences.

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20. Algorithmic Aspects of Real-Life Systems Analysis: Overview (cont-d)

- In Section 2.2, we show how, for biomolecules, the corr. symmetries naturally explain the observed shapes.
- Smaller molecules, as we have mentioned, can only have discrete symmetries.
- In Section 2.3, we show how the symmetries approach can help in describing such molecules.
- Finally, on the quantum level of elementary particles, we, in general, do not have geometric symmetries.
- Instead, we have a reasonable symmetry-related physical idea of *independence*.
- We show that this idea leads to a formal justification of quantum theory (in Feynman integral form).
- In all these cases, symmetries help.



21. Algorithmic Aspects of Real-Life Systems Analysis: Details

- Application: explaining shapes of secondary elements in protein structure.
- Protein structure is invariably connected to protein function.
- There are two important secondary structure elements: alpha-helices and beta-sheets.
- Their actual shapes can be complicated, but usually approx. by cylindrical spirals, planes and cylinders.
- Result: these geometric shapes are indeed the best approximating families for secondary structures.
- This result expands on the ideas pioneered by a renowned mathematician M. Gromov.



22. Algorithmic Aspects of Real-Life Systems Analysis: Details (cont-d)

- Application: understanding properties of molecules with variant ligands.
- Molecules can be obtained from a "template" molecule by replacing some of its atoms with *ligands*.
- Testing of all possible replacements is time-consuming.
- Avoid by testing some of the replacements and then extrapolate to others.
- D. J. Klein and co-authors proposed to use a poset extrapolation technique developed by G.-C. Rota.
- Limitation: technique originally proposed on a heuristic basis.
- No convincing justification of its applicability to chemical (or other) problems.



23. Algorithmic Aspects of Real-Life Systems Analysis: Details (cont-d)

- Previously, we showed that the poset technique is equivalent to Taylor series extrapolation.
- A more familiar (and much more justified) technique.
- Results:
 - The equivalence with Taylor series extr. can be extended to the case of variant ligands.
 - This approach is also equivalent the Dempster-Shafer approach.



24. Algorithmic Aspects of Prediction: Symmetry-Based Approach

- As we have mentioned earlier, one of the main objectives of science is to predict future events.
- From this viewpoint, the first question that we need to ask is: *is it possible* to predict?
- In many cases, predictions are possible.
- In many other practical situations, what we observe is a *random* (un-predictable) sequence.
- The question of how to check whether a sequence is random is analyzed in Section 3.2.
- In this analysis, we use symmetries namely, we use scaling symmetries; see below.
- In situations when prediction is, in principle, possible, the next questions is: *how* can we predict?



25. Algorithmic Aspects of Prediction (cont-d)

- In cases when we know the corresponding equations, we can use these equations for prediction.
- In many practical situations, however, we do not know the equations.
- In such situations, we need to use general prediction and extrapolation tools, e.g., neural networks.
- In Section 3.3, we show how discrete symmetries can help improve the efficiency of neural networks.
- Once the prediction is made, the next question is *how* accurate is this prediction?
- In Section 3.4, we show how scaling symmetries can help in *quantifying* the uncertainty of the corr. model.
- In Section 3.5, we use similar symmetries to come up with an optimal way of *processing* uncertainty.



26. Algorithmic Aspects of Prediction (cont-d)

- In Sect. 3.6, on a geophysical example, we estimate the accuracy of *spatially locating* the measurement results.
- In practice, we often need to have the prediction results by a certain time.
- It is then important to perform the corresponding computations efficiently by the deadline.
- The theoretical possibility of such efficient computations is analyzed in Section 3.7.
- Overall, we show that symmetries can help with all the algorithmic aspects of prediction.



27. Example: How to Check Randomness

- A non-random sequence like 010101...can be generated by a short program.
- If a sequence is truly random, the only way to generate it is to print it bit by bit.
- The shortest length of a program that computes s is called its Kolmogorov complexity K(s).
- Thus, a sequence is random if and only if its Kolmogorov complexity is close to its length.
- The big problem is that the Kolmogorov complexity is, in general, *not* algorithmically *computable*.
- Thus, it is desirable to come up with *computable* approximations.



28. Approximating Kolmogorov Complexity

- Reminder: we need to approximate Kolmogorov complexity K(s).
- At present, most algorithms for approximating K(s):
 - use some loss-less compression technique to compress s, and
 - take the length $\widetilde{K}(s)$ of the compression as the desired approximation.
- However, this approximation has limitations: for example,
 - in contrast to K(s), where a change (one-bit) change in s cannot change K(s) much,
 - a small change in s can lead to a drastic change in $\widetilde{K}(s)$.



29. Other Applications of Kolmogorov Complexity

- Kolmogorov complexity is useful beyond checking randomness.
- E.g.: we can check how close are two DNA sequences s and s' by comparing K(ss') with K(s) + K(s'):
 - if they are *unrelated*, the only way to generate ss' is to generate s and then generate s', so:

$$K(ss') \approx K(s) + K(s');$$

- if they are *related*, we have $K(ss') \ll K(s) + K(s')$.
- By taking strings s and s' describing the same text in languages L, L', we can check how close are L and L'.



30. I-Complexity

- Limitation of K(s): a small change in $s = (s_1 s_2 \dots s_n)$ can lead to a drastic change in K(s).
- To overcome this limitation, V. Becher and P. A. Heiber proposed the following new notion of *I-complexity*.
- For each i, we find the largest $B_s[i]$ of the length ℓ of strings $s_{i-\ell+1} \dots s_i$ which are substrings of $s_1 \dots s_{i-1}$.
- For example, for aaaab, the corresponding values of $B_s(i)$ are 01230.
- We then define $I(s) \stackrel{\text{def}}{=} \sum_{i=1}^{n} f(B_s[i])$, for an appropriate decreasing function f(x).
- Specifically, it turned out that the discrete derivative of the logarithm works well: $f(x) = d\log(x+1)$, where $d\log(x) \stackrel{\text{def}}{=} \log(x+1) \log(x)$.

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31. Good Properties of I-Complexity

- Reminder: $I(s) = \sum_{i=1}^{n} f(B_s[i])$, where:
 - $B_s[i]$ is the the largest length ℓ of strings $s_{i-\ell+1} \dots s_i$ which are substrings of $s_1 \dots s_{i-1}$, and
 - $f(x) = \log(x+1) \log(x).$
- Similarly to K(s):
 - If s starts s', then $I(s) \leq I(s')$.
 - We have $I(0s) \approx I(s)$ and $I(1s) \approx I(s)$.
 - We have $I(ss') \leq I(s) + I(s')$.
 - Most strings have high I-complexity.
- In contrast to K(s): I-complexity can be computed in linear time.
- A natural question: why this function f(x)?

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32. Towards Precise Formulation of the Problem

- We take f(x) = F(x+1) F(x), for some F(x).
- V. Becher and P. A. Hieber selected $F(x) = \log(x)$.
- There are not much symmetries on integer values x, but we can extend F(x) to all real numbers.
- Which monotonic function F(x) from reals to reals should we choose?
- Reminder: in the continuous case, the numerical value of each quantity depends:
 - on the choice of the measuring unit and
 - on the choice of the starting point.
- By changing them, we get a new value $x' = a \cdot x + b$.
- \bullet For length x, the starting point 0 is fixed.
- So, we only have re-scaling $x \to x' = a \cdot x$ (e.g., bits vs. bytes).

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33. Our Result

- By changing a measuring unit, we get $x' = a \cdot x$.
- When we thus re-scale x, the value y = F(x) changes, to $y' = F(a \cdot x)$.
- It is reasonable to require that the value y' represent the same quantity.
- So, we require that y' differs from y by a similar rescaling:

$$y' = F(a \cdot x) = A(a) \cdot F(x) + B(a)$$
 for some $A(a)$ and $B(a)$.

• It turns out that all monotonic solutions of this equation are linearly equivalent to $\log(x)$ or to x^{α} , i.e.:

$$F(x) = \widetilde{a} \cdot \ln(x) + \widetilde{b} \text{ or } F(x) = \widetilde{a} \cdot x^{\alpha} + \widetilde{b}.$$

• So, symmetries do explain the selection of the function F(x) for I-complexity.

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34. Proof

• Reminder: for some monotonic function F(x), for every a, there exist values A(a) and B(a) for which

$$F(a \cdot x) = A(a) \cdot F(x) + B(a).$$

- *Known fact:* every monotonic function is almost everywhere differentiable.
- Let $x_0 > 0$ be a point where the function F(x) is differentiable.
- Then, for every x, by taking $a = x/x_0$, we conclude that F(x) is differentiable at this point x as well.
- For any $x_1 \neq x_2$, we have $F(a \cdot x_1) = A(a) \cdot F(x_1) + B(a)$ and $F(a \cdot x_2) = A(a) \cdot F(x_2) + B(a)$.
- We get a system of two linear equations with two unknowns A(a) and B(a).

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35. Proof (cont-d)

• We get a system of two linear equations with two unknowns A(a) and B(a):

$$F(a \cdot x_1) = A(a) \cdot F(x_1) + B(a).$$

 $F(a \cdot x_2) = A(a) \cdot F(x_2) + B(a).$

- Thus, both A(a) and B(a) are linear combinations of differentiable functions $F(a \cdot x_1)$ and $F(a \cdot x_2)$.
- Hence, both functions A(a) and B(a) are differentiable.
- So, $F(a \cdot x) = A(a) \cdot F(x) + B(a)$ for differentiable functions F(x), A(a), and B(a).
- Differentiating both sides by a, we get

$$x \cdot F'(a \cdot x) = A'(a) \cdot F(x) + B'(a).$$

• In particular, for a = 1, we get $x \cdot \frac{dF}{dx} = A \cdot F + B$, where $A \stackrel{\text{def}}{=} A'(1)$ and $B \stackrel{\text{def}}{=} B'(1)$.

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36. Proof (final part)

- Reminder: $x \cdot \frac{dF}{dx} = A \cdot F + B$.
- So, $\frac{dF}{A \cdot F + b} = \frac{dx}{x}$; now, we can integrate both sides.
- When A = 0: we get $\frac{F(x)}{b} = \ln(x) + C$, so $F(x) = b \cdot \ln(x) + b \cdot C$.
- When $A \neq 0$: for $\widetilde{F} \stackrel{\text{def}}{=} F + \frac{b}{A}$, we get $\frac{dF}{A \cdot \widetilde{F}} = \frac{dx}{x}$, so $\frac{1}{A} \cdot \ln(\widetilde{F}(x)) = \ln(x) + C$, and $\ln(\widetilde{F}(x)) = A \cdot \ln(x) + A \cdot C$.
- Thus, $\widetilde{F}(x) = C_1 \cdot x^A$, where $C_1 \stackrel{\text{def}}{=} \exp(A \cdot C)$.
- Hence, $F(x) = \widetilde{F}(x) \frac{b}{A} = C_1 \cdot x^A \frac{b}{A}$.
- The theorem is proven.

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37. Algorithmic Aspects of Control: Symmetry-Based Approach

- Up to now, we concentrated on the problem of *predicting* the future events.
- Once we are able to predict future events, a natural next step is to *control* the corresponding system.
- In this step, we should select a control that leads to the *best* possible result.
- Sometimes, we know the exact equations, so we can simply use known optimization techniques.
- Often, exact equations are not known, so we have the use the knowledge of human experts.
- Many such intelligent techniques are *empirical*, their results which are far from optimal.



38. Algorithmic Aspects of Control (cont-d)

- In Chapter 4, we show that symmetry-based techniques can be very useful in improving these results.
- We will illustrate this usefulness on all level of the problem of selecting the best control.
- First, on a strategic level, we need to select the best class of strategies.
- In Sect. 4.2, we derive the best class of strategies for fuzzy control, an important class of intelligent controls.
- In the corr. derivation, we use logical symmetries the symmetry between true and false values.
- Once a class of strategies is selected, we need to select the best strategy within a given class.



39. Algorithmic Aspects of Control (cont-d)

- Once a class of strategies is selected, we need to select the best strategy within a given class:
 - in Section 4.3, we use approximate symmetries to find the best implementation of fuzzy control;
 - in Section 4.4, we show that the optimal selection of operations leads to a symmetry-based solution.
- Often, we have several strategies coming from different aspects of the problem.
- We need to combine these strategies into a single strategy that takes all the aspects into account.
- In Section 4.5, we use logical symmetries to find the best way of combining the resulting fuzzy decisions.
- Overall, we show that symmetries can help with all the algorithmic aspects of control.



40. Example: Selecting the Best Exclusive-Or Operations

- Intelligent control comes from expert statements.
- Expert statements often use logical connectives like "or".
- In natural language, "or" sometimes means "inclusive or" and sometimes means "exclusive or".
- Traditionally, intelligent control uses "inclusive or" (t-conorms).
- We want to adequately describe commonsense and expert knowledge.
- Therefore it is important to also have fuzzy "exclusive or" operations $f_{\oplus}(a,b)$.



41. Selecting Exclusive-Or Operations (cont-d)

- Reminder: it is important to have fuzzy "exclusive or" operations $f_{\oplus}(a,b)$.
- Main idea: The degrees of certainty are only approximately defined.
- It is reasonable to require that the operation be the *least sensitive* to small changes in the inputs.
- This requirement corresponds to approximate symmetry.
- Result: the least sensitive fuzzy "exclusive or" operation has the form

$$f_{\oplus}(a,b) = \min(\max(a,b), \max(1-a,1-b)).$$



42. Possible Ideas for Future Work

- In this dissertation, on numerous examples, we showed that symmetries help in science and engineering.
- The breadth and depth of these examples show that symmetry-based approach is indeed very promising.
- However, to make this approach more widely used, additional work is needed.
- Indeed, in each of our examples, the main challenge is finding the relevant symmetries.
- As of now, we have found these symmetries on a *case-by-case* basis.
- It would be great to develop a *general* methodology of finding the relevant symmetries.
- Such a general methodology would help to apply symmetrybased approach to important new practical problems.



43. Acknowledgements

- I would like to thank Dr. Vladik Kreinovich for his teachings and for pushing me with professionalism.
- I also wish to thank Dr. Luc Longpré and Dr. Larry Ellzey for their supervision, input, and expert advice.
- Thanks to Drs. Benoit Bagot, Art Duval, Yuri Gurevich, Patricia Nava, and James Salvador for their help.

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