# Complexity of Machine Learning and Landscapes

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Northeastern University

ICTP - Machine Learning Landscape,
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Based on 1809.08279
with Fabian Ruehle

**see also:** 2006 work of [Douglas, Denef], 2010 work of [Cvetic, Garcia-Etxebarria, JH]

# Question 1:

## Why should string theorists care about computational complexity?

# Punchline:

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Difficulties that we run into in landscapes are not only due to exponentially large sizes, which take exponential time to process by nature of their size.

There are also due to the existence of hard problems, which take exponential time to solve because of their complexity.

Progress requires dealing with both.

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- Undecidability: decision prob —> diophantine
  —> landscape algorithmically patchy. **[Cvetic, Garcia-Etxebarria, J.H.]**

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- What is the complexity of vacua in landscapes?
- What is the complexity of vacua in the string landscape?
- What are potential complexity loopholes and what does it mean for applying ML / AI to landscapes?

# Question 2:
# What is computational complexity?

**Flow:** **Problems —> P vs. NP —> Polytime Reduction —> Hardest NP Probs —> Optimization vs. Decision —> Example**

# Problems

- a PROBLEM    F: I —> B    maps instances to outputs.

- a DECISION PROBLEM has B = {yes, no}.

- Example: a clique of an undirected graph G is a set of vertices that are all connected to one another.

  **CLIQUE:** Given an undirected graph $G$ and $n \in \mathbb{Z}$, does $G$ have an $n$-clique?

  where I = S x Z, and S the set of undirected graphs.

- an algorithm that **computes** F always returns an output.

- **polytime** algorithms return an output in time bounded by polynomial in the input size. otherwise, will say **exponential time**.

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- is there a notion of the hardest problems in NP?

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- Specifically, if polytime alg for G, then also for F.

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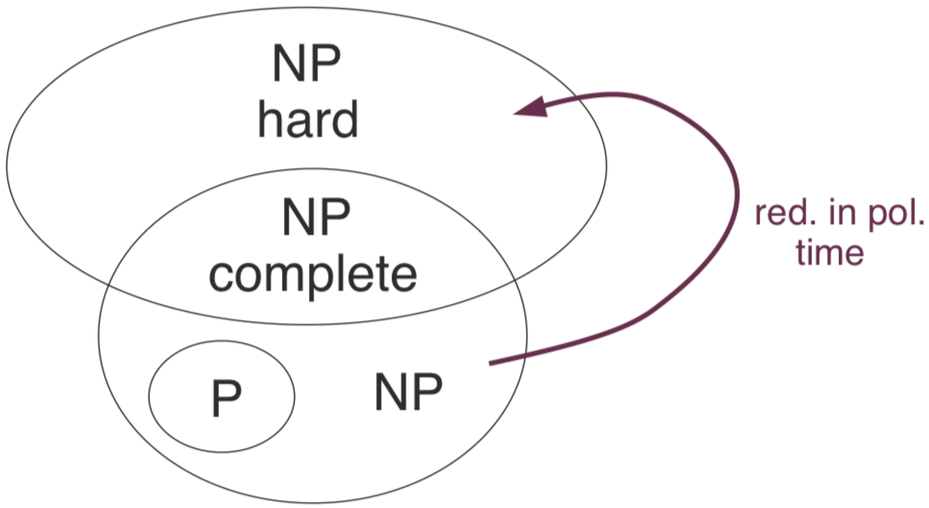


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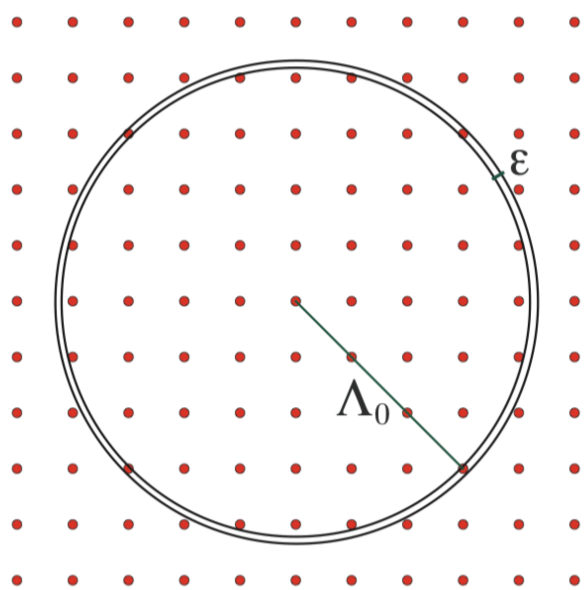

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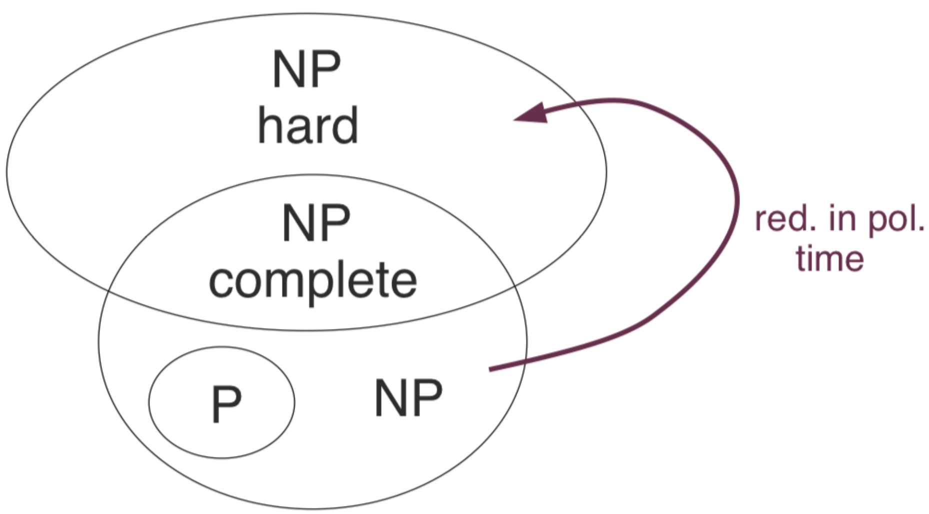


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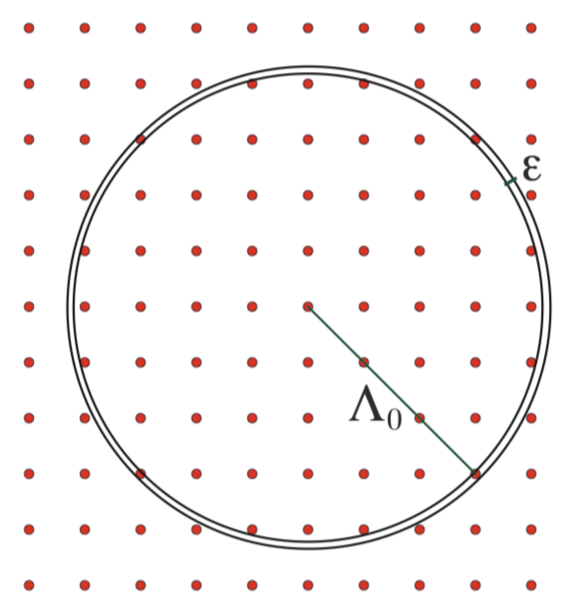

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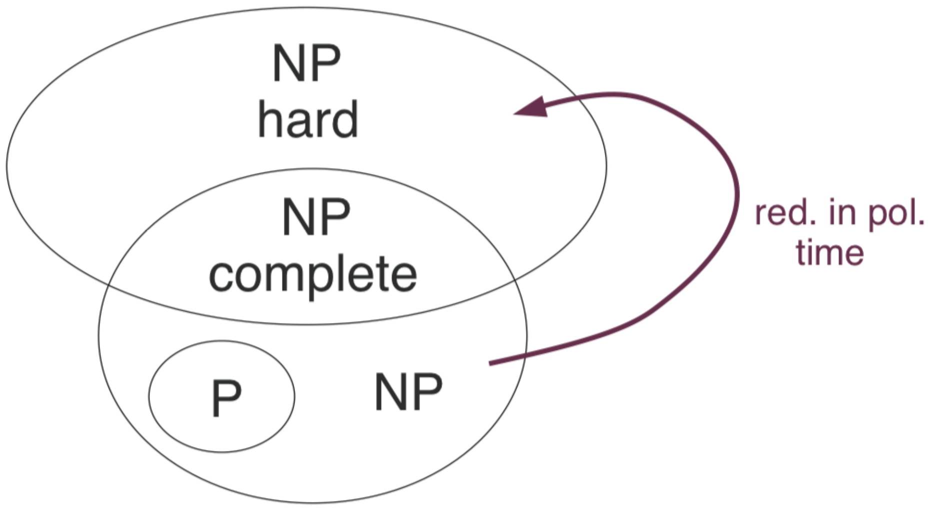


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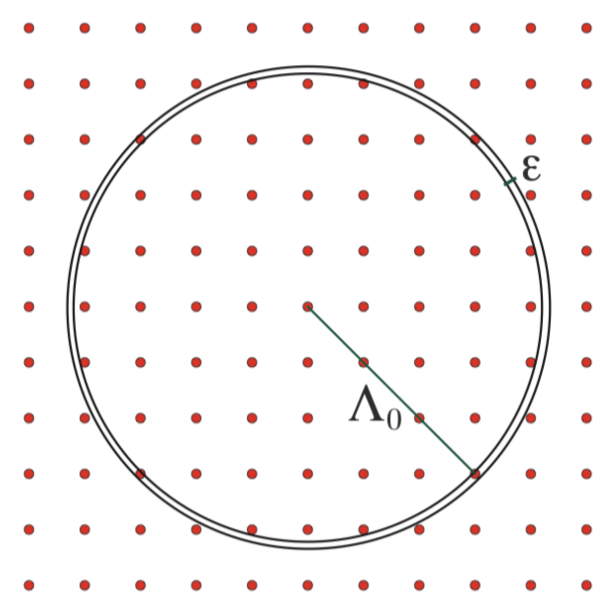

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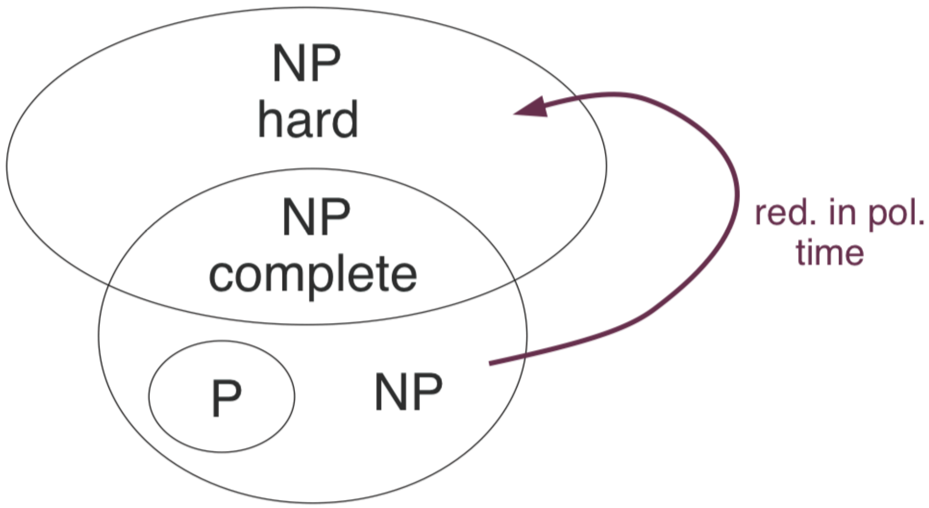


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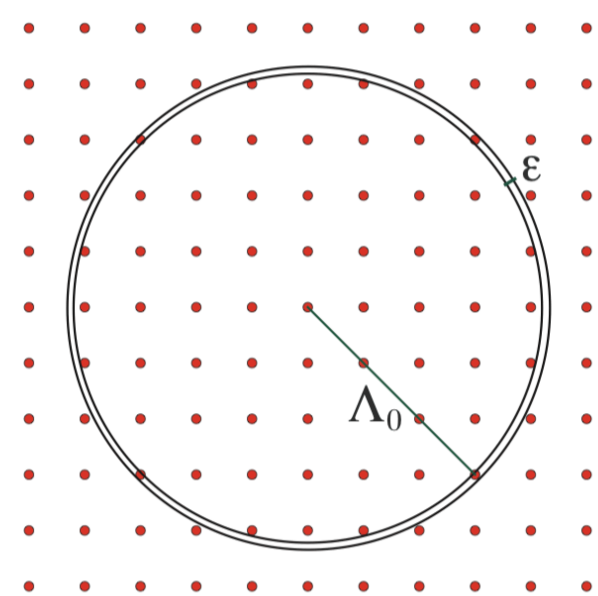

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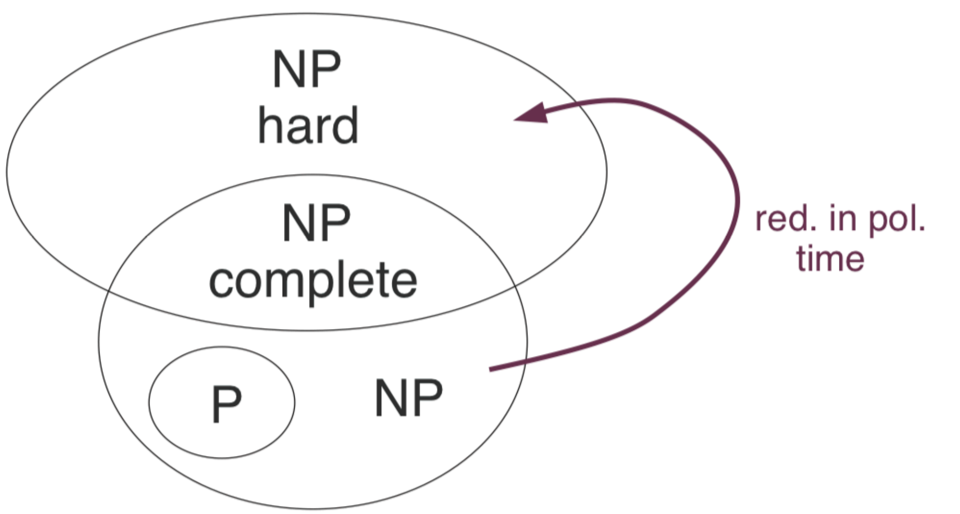


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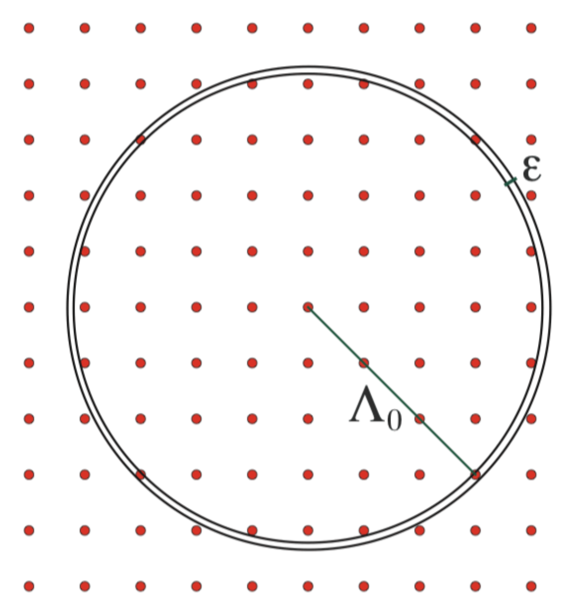

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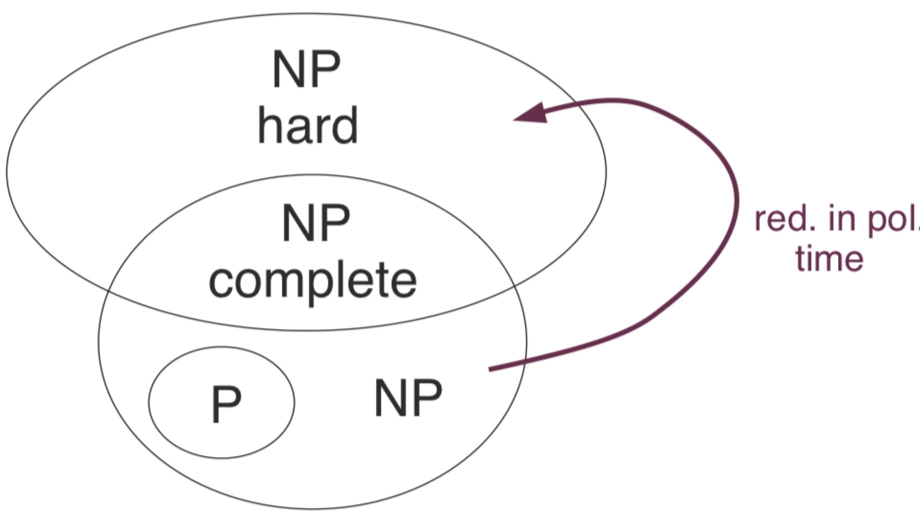


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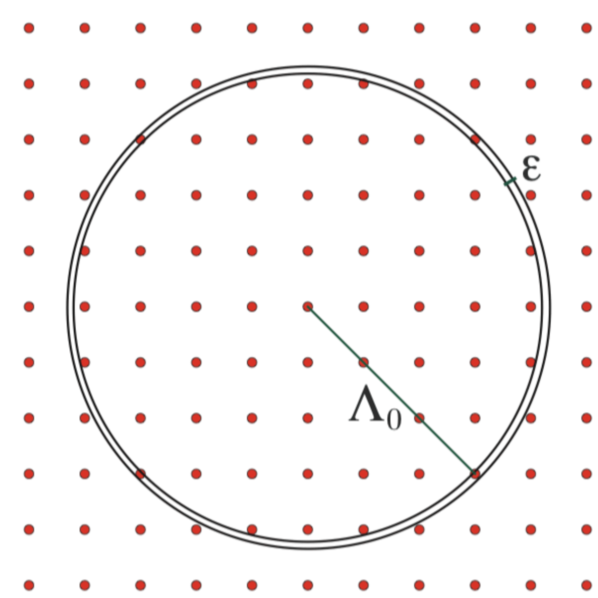

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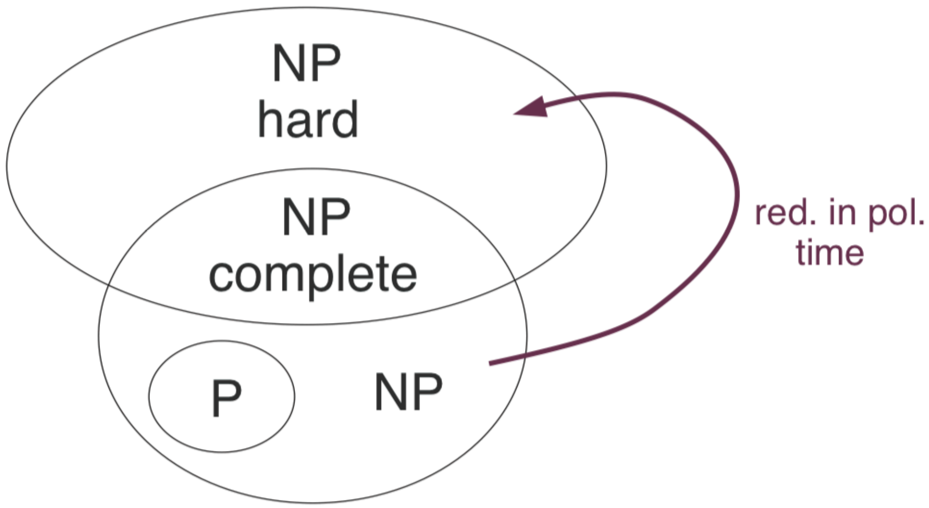


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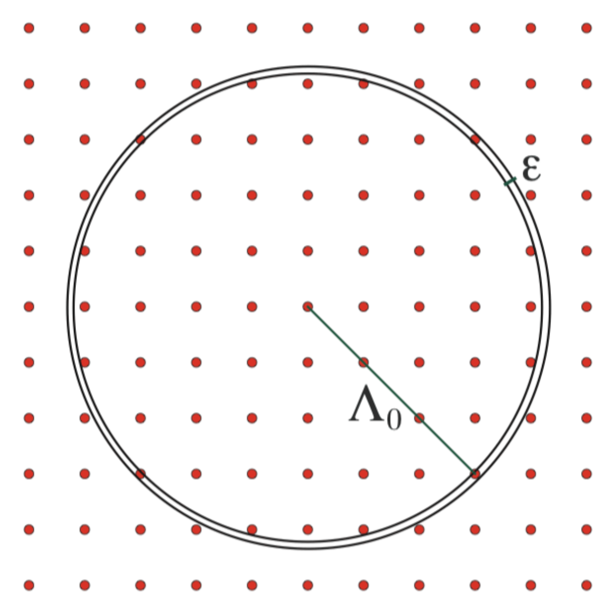

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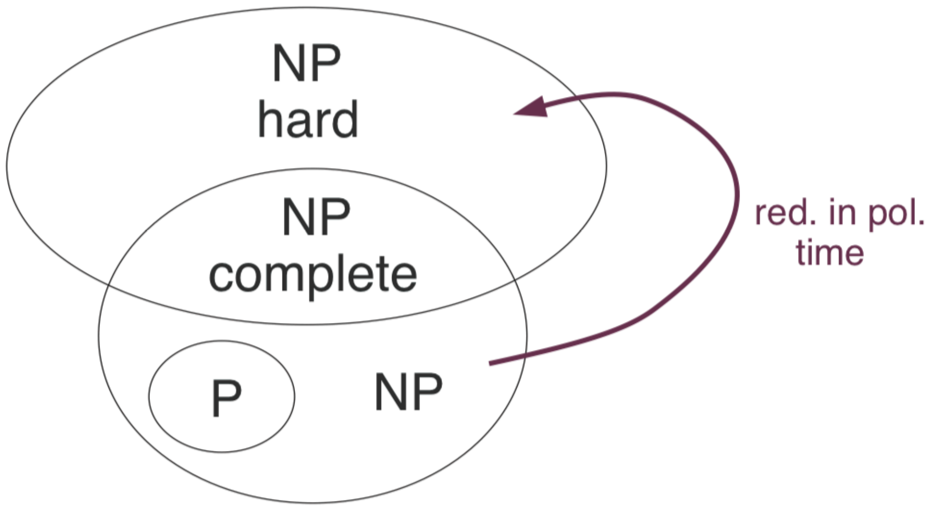
  **complexity result: [Denef, Douglas]**

  **tackle with reinforcement learning: [JH, Long, Ruehle]**

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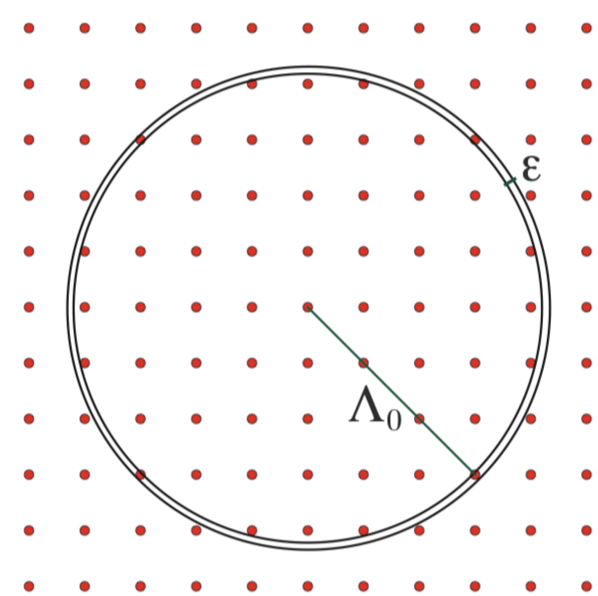

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- optimization problems O are at least as hard as associated decision problems D: solve O, implicitly solve D.

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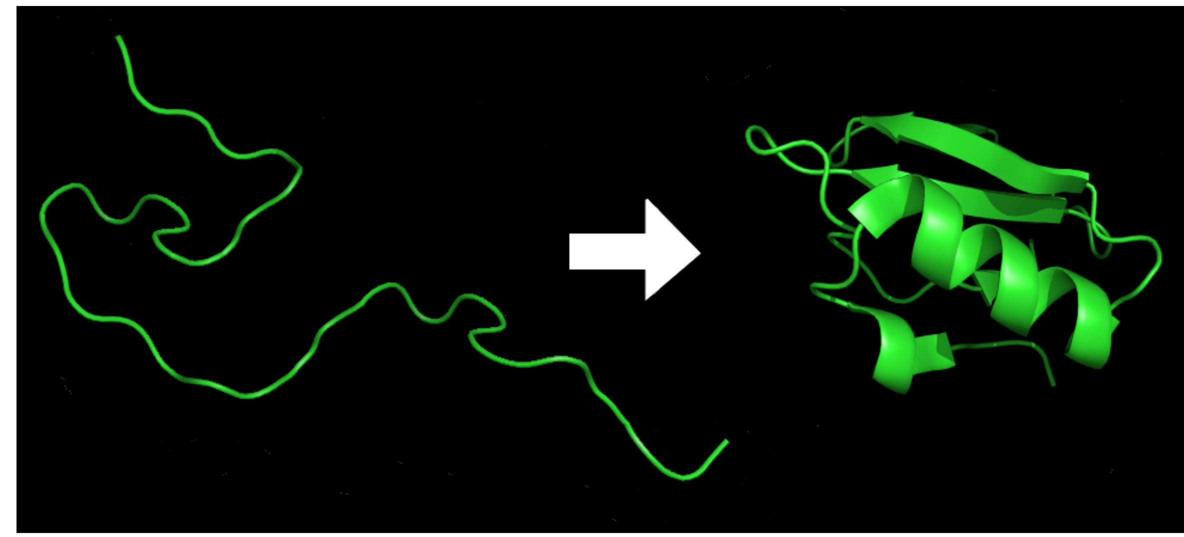
complexity result: [Unger, Moult] 1993 Early Review: chem-ph/9411008



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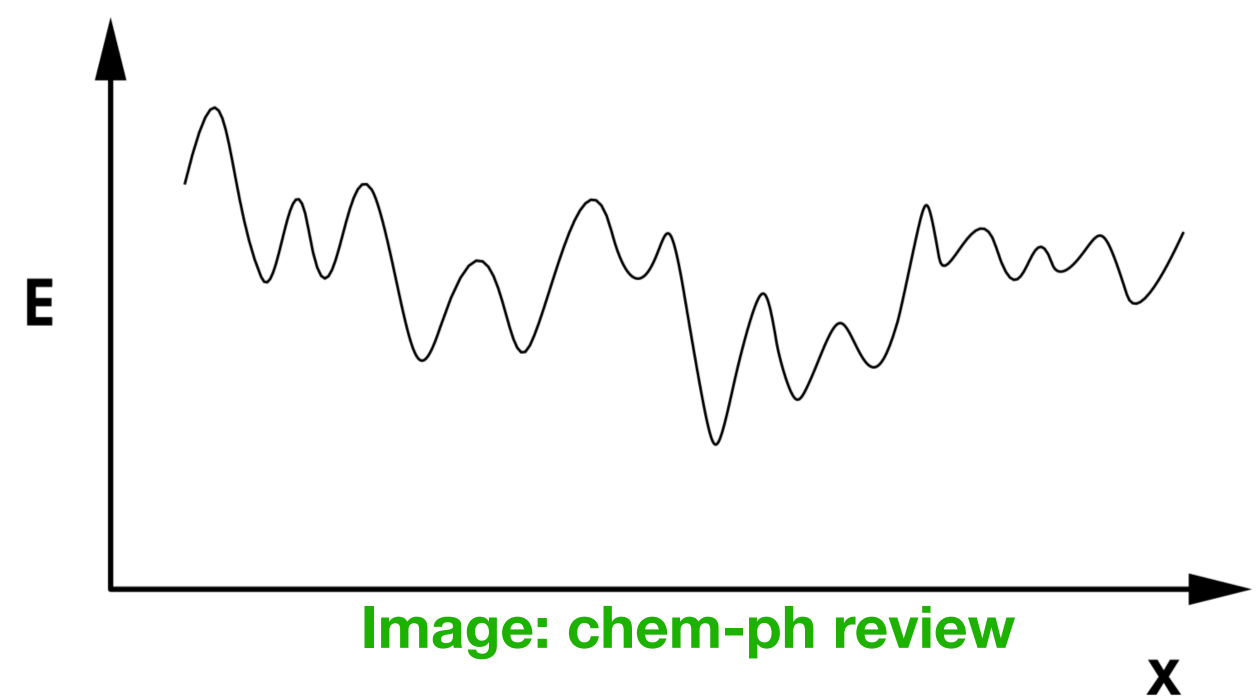


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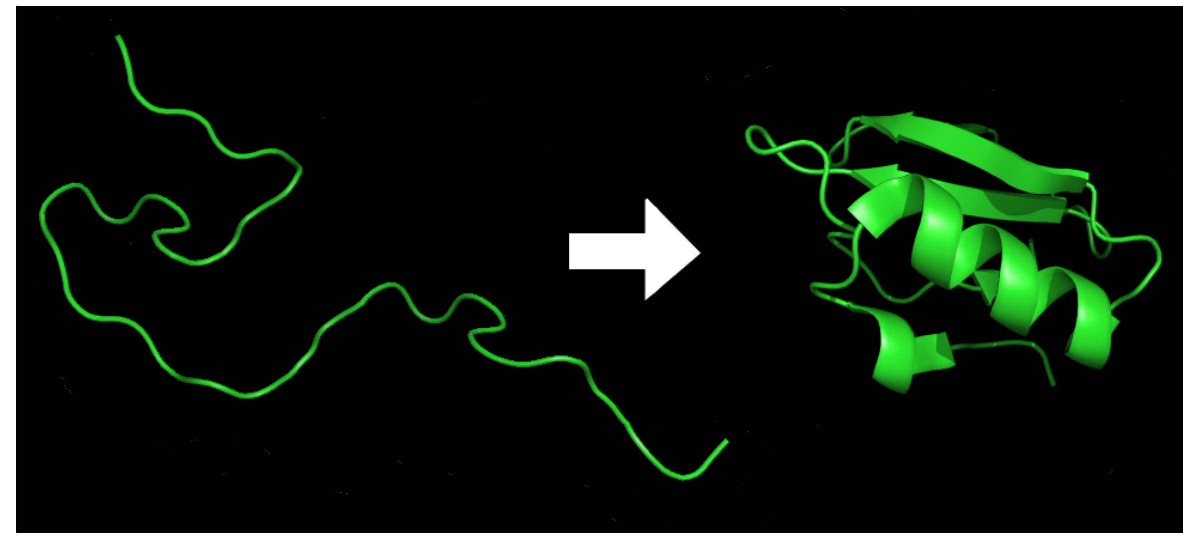

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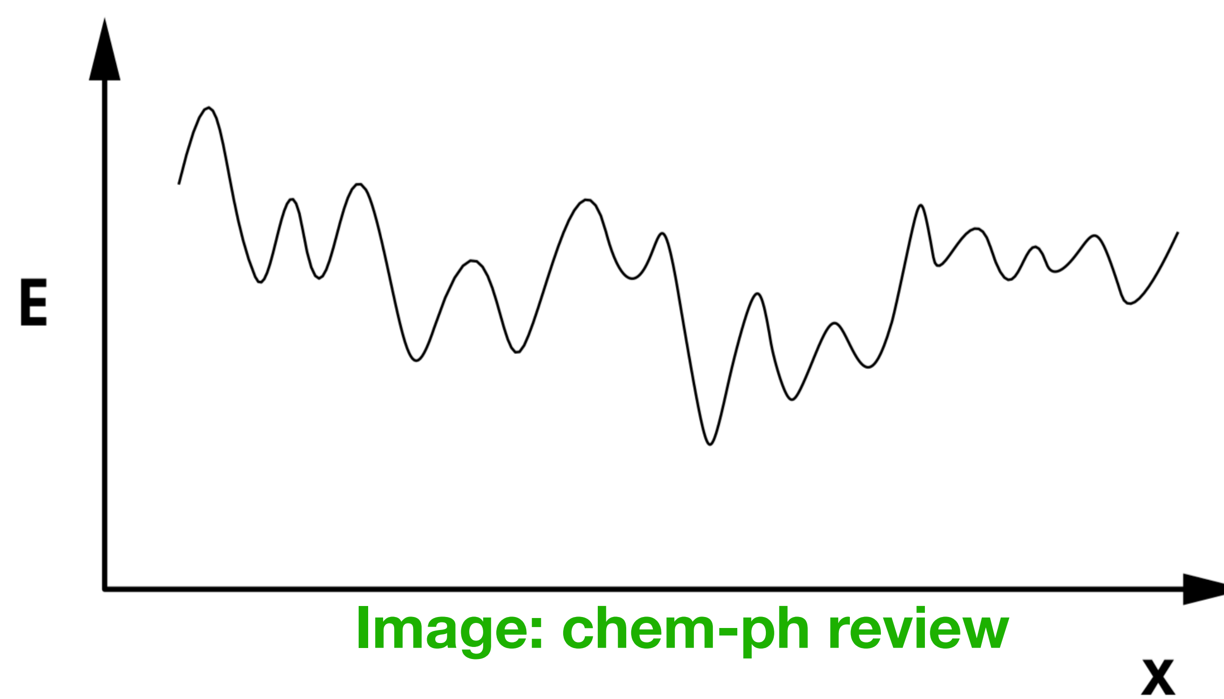


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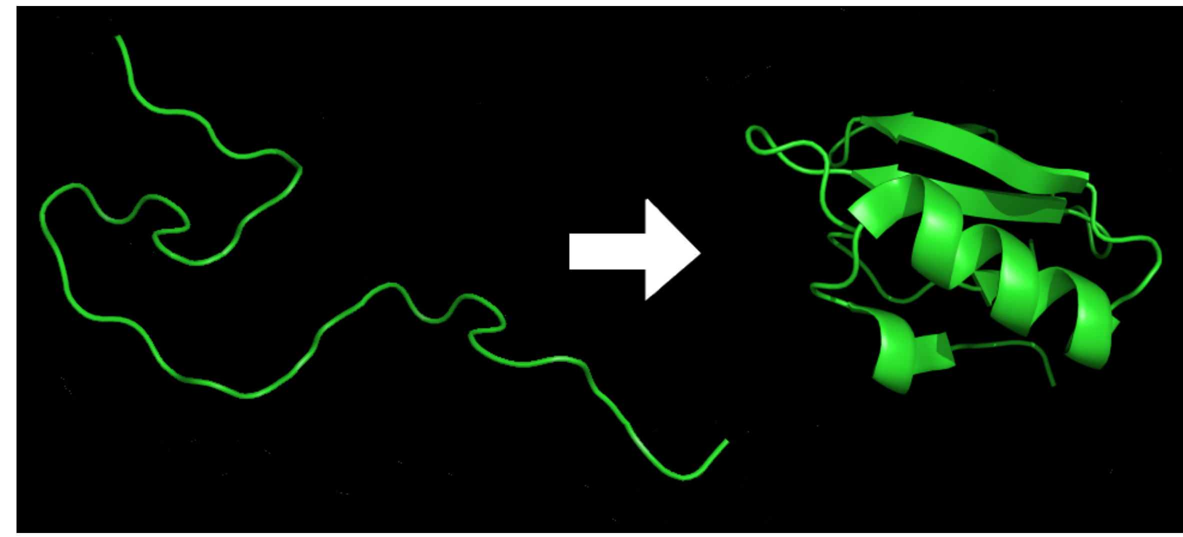

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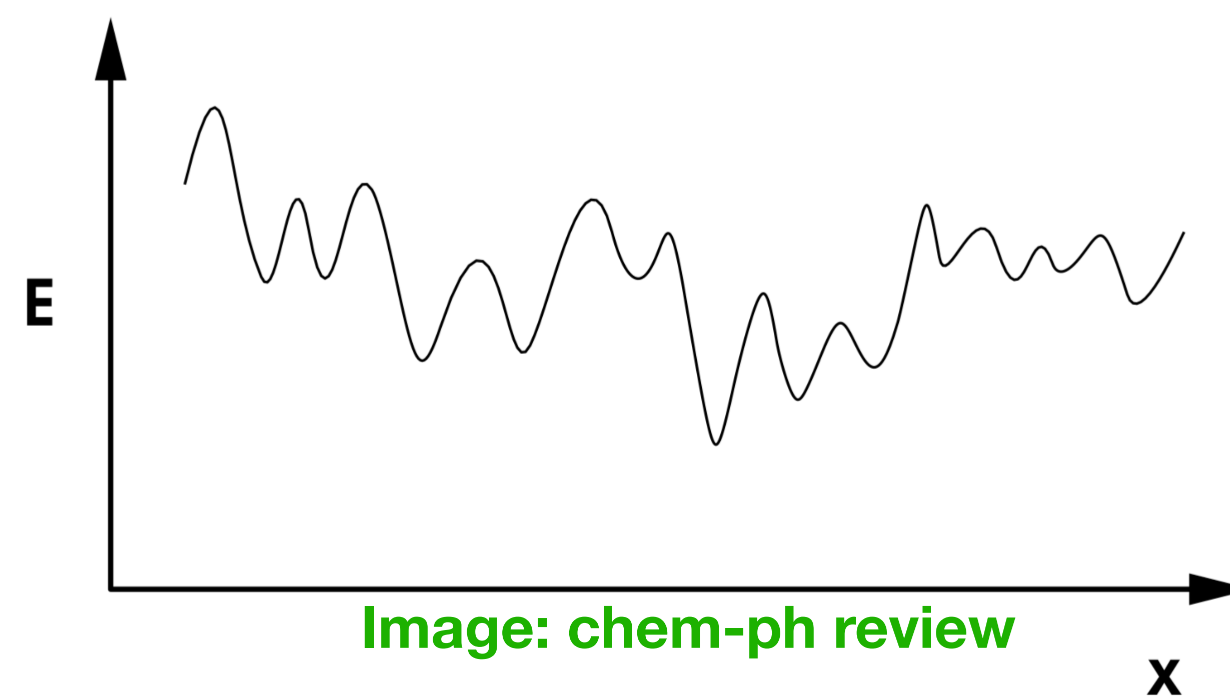


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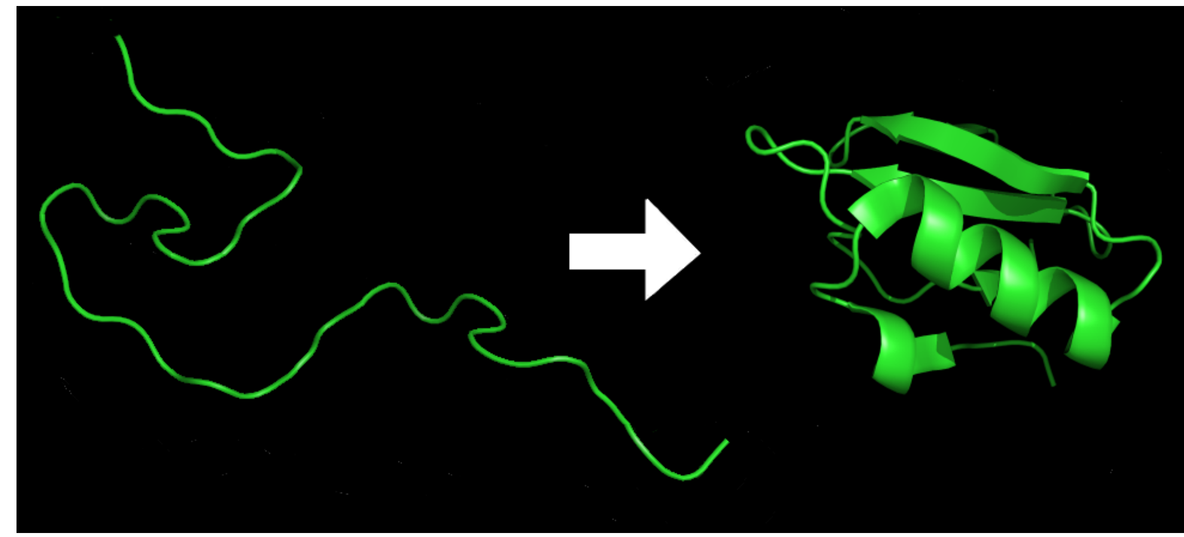

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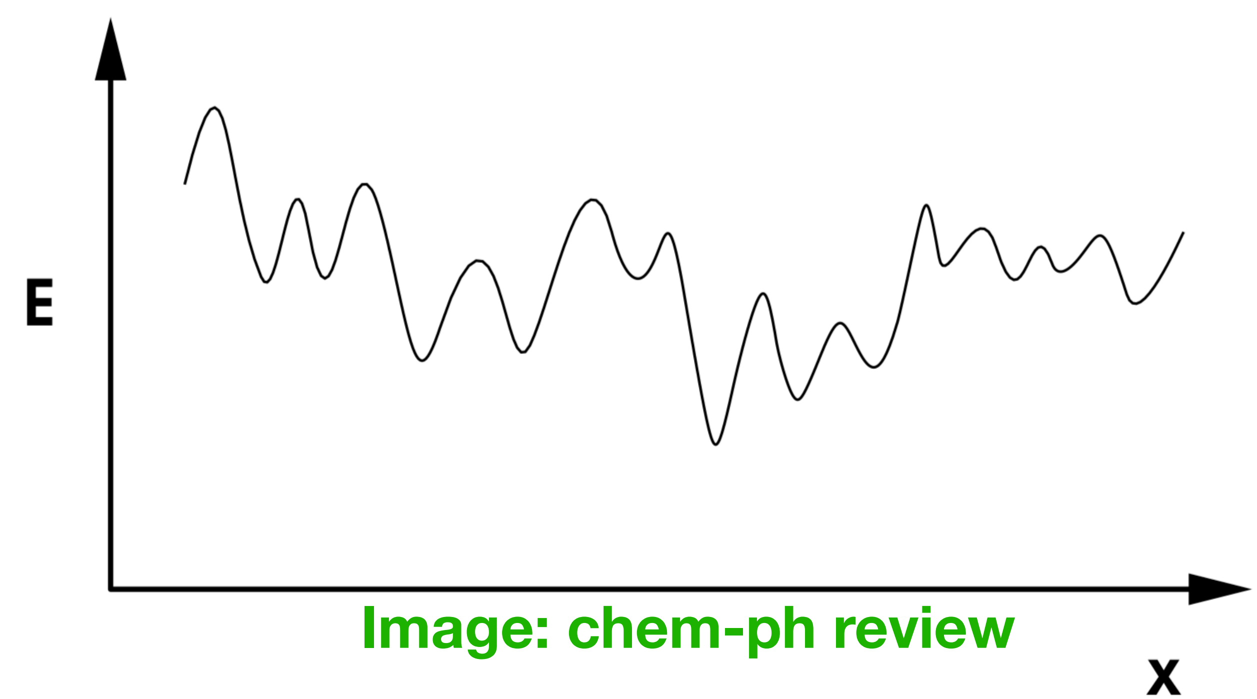


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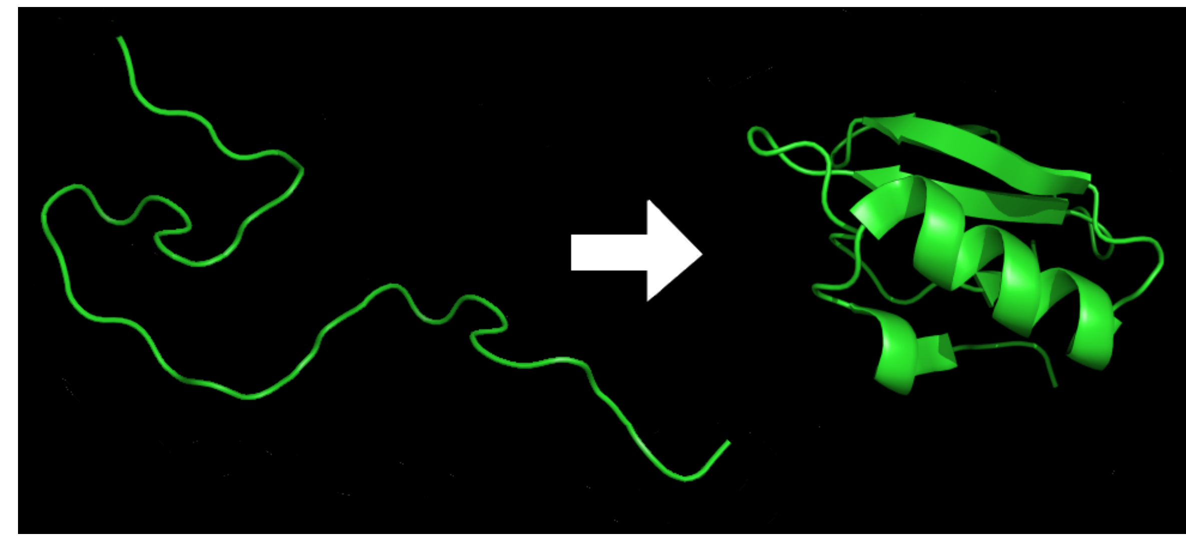

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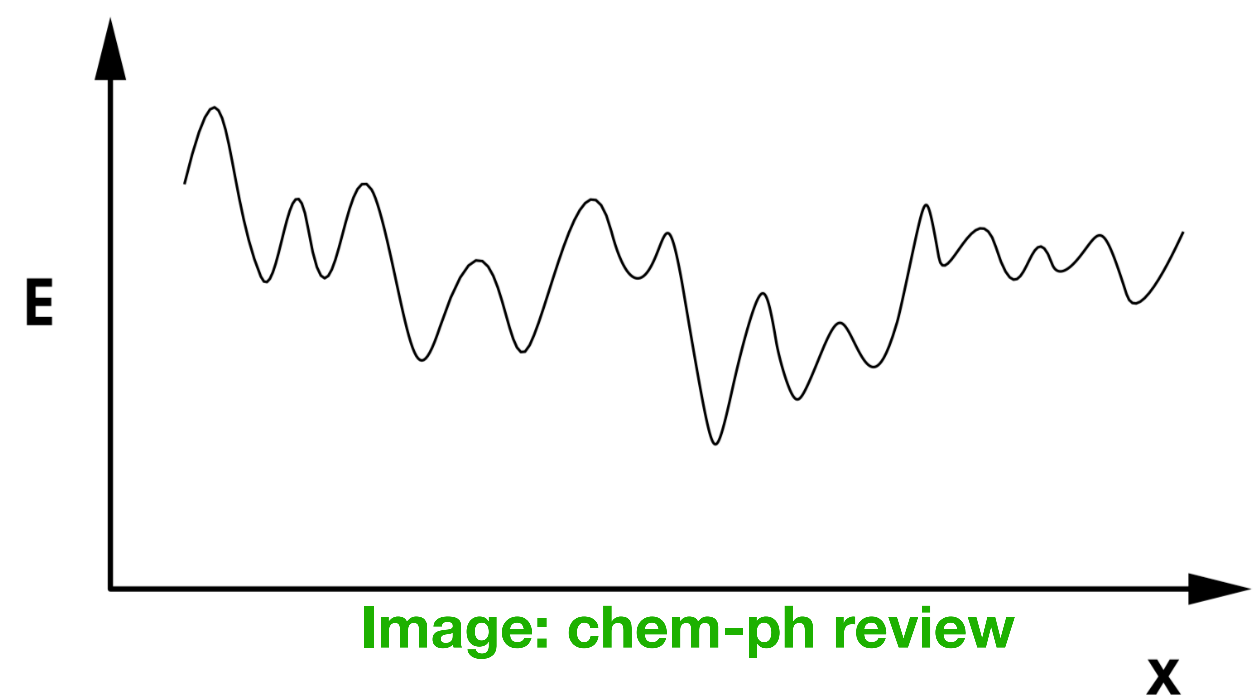


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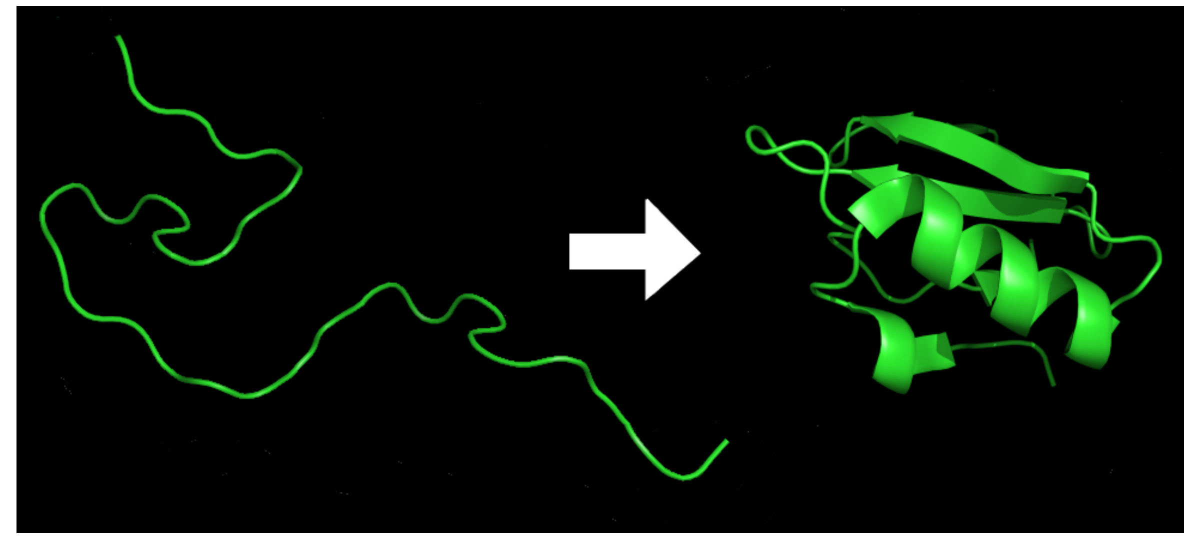
- Upshot: worst case instances are hard, but evolutionary pressure gives rise to better instances.



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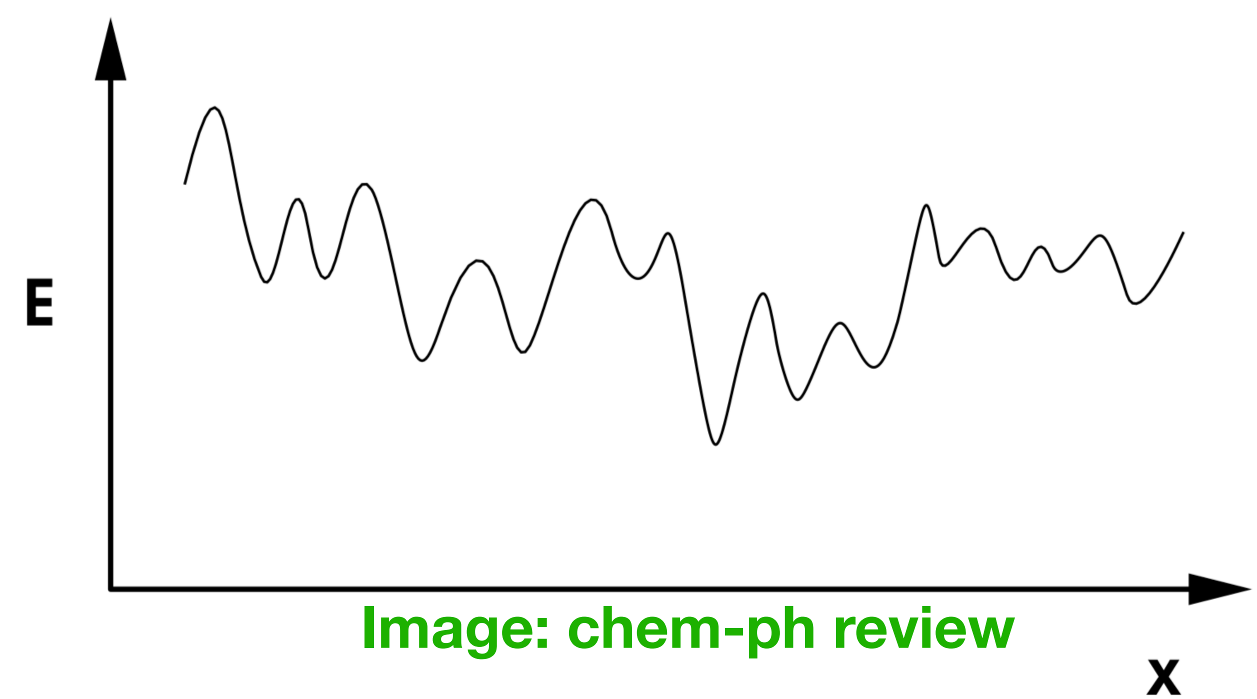


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# Question 3:

# What is the complexity of vacua in landscapes?

**Goal:** given $V(\phi)$, is it hard to find stable vacua? metastable vacua? near-vacua?

**Note: training neural nets is effectively the same problem! Complexity carries over.**

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- Maybe we tunnel to the side of a hill that is near a vacuum and inflate from there.

  Is it hard to find a near-vacuum?

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  - literal of boolean variable is the variable (x) or its negative (not x).

  - clause: an or of literals.      e.g.,  $x_1 \vee x_3 \vee \neg x_{10}$

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- **Cook-Levin theorem:** SAT is NP-complete. (see any complexity textbook).

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- Form system S of polynomial equations

  - for each boolean $x_i$, add $x_i(1-x_i)$ to S.

  - associate polynomial p(l) to each literal l via:

    $$p(l = x) = (1 - x). \qquad p(l = \neg x) = x$$

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# Are critical points hard?

- **POLYROOTS:** given a system of polynomial equations, is there a non-trivial root?
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- **Note:** S has a non-trivial root iff the CNF-formula is satisfiable. **POLYROOTS is NP-hard.**

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- h has critical points iff POLYROOTS instance has solution.
- Result: via reduction SAT —> POLYROOTS —> CRITPOINTS,

**CRITPOINTS is NP-hard.**

# Metastable Vacua

**MSVAC:** Find a local minimum of $V(\phi)$, such that $l_i \leq \phi_i \leq u_i$,

where $\phi = (\phi_1, \ldots, \phi_n) \in \mathbb{R}^n$ and $l_i, u_i \in \mathbb{R}$ are used to give so-called box constraints. Here the box constraints encode the fact that the EFT has a regime of validity that bounds the scalar fields values.

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- **special case:** only strict saddles, SGD (as in ML) finds minima in P.

# Stable Vacua

**SVAC:** Find a global minimum of $V(\phi)$, such that $l_i \leq \phi_i \leq u_i$,

- global minimum is hard because local minimum is already hard!
- difficulty of global minimization is well-known,
  e.g. global quadratic programming or protein folding.
- it was the fact that local minima is hard that we found very surprising.

# Near-Vacua

- **Definition:** $x^*$ is an **ε-approximate local minimum** of a continuous function f: U —> R if there is an open set N in U containing $x^*$ such that $f(x^*) <= f(x) + \varepsilon\, |x-x^*|$ for all x in N.

- Idea: this is a *near*-vacuum. Define associated problem:

**NEAR-VAC:** Given a scalar potential $V(\phi)$ and $\epsilon > 0$, find a point $\phi^*$ that is an $\epsilon$-vacuum.

- Fast algorithm of Vavasis: $|f(x) - f(y)| \leq M|x - y|$

**Theorem:** *Let $f : U \to \mathbb{R}$ be a $C^1$ function whose gradient satisfies a Lipschitz condition with bound $M$. Then an $\epsilon$-minimum can be found with at most $4n(M/\epsilon)^2$ function and gradient evaluations.*

- NEAR-VAC is in P.

# Question 4:

## What is the complexity of vacua in the string landscape?

**Goal:** is it hard to determine $V(\Phi)$ in string theory?

# Framing the Problem

- Hard to find both stable and metastable vacua, given V(ϕ).
- Computing V(ϕ) subject of much string research.
    - IIB: KKLT and LVS.
      **[Kachru, Kallosh, Linde, Trivedi], [Balasubranian, Berglund, Conlon, Quevedo]**
    - e.g. infinite # of M2-instantons on certain G2-manifolds.
      **[Braun, Del Zotto, JH, Larfors, Morrison, Schafer-Nameki]**
- **Q:** is it also hard to compute V(ϕ)?
- **goal:** show string V(ϕ) contributions req. solving instances of NP-complete probs.      (open up Garey and Johnson!)

# Rural Postman

Given a graph $G$, lengths $l(e) \in \mathbb{Z}^+$ for all edges $e \in E$, a subset $E' \subset E$, and a bound $B \in \mathbb{Z}^+$, we have the problem:

**RURAL POSTMAN:** Is there a circuit (closed loop) in $G$ that includes each edge in $E'$ and that has total length no more than $B$?

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**Physical Realization:** given a quiver gauge theory, does there exist a scalar GIO O that couples a fixed subset E' of fields to one another, such that dim(O) <= B?

# Integer Programming

Now we turn to INTEGER PROGRAMMING (INT-PROG). Given $(A \in \mathbb{Z}^{m\times n}, b \in \mathbb{Z}^n, c \in \mathbb{Z}^n, B \in \mathbb{Z})$,

**INT-PROG:** Is there a $y \in \mathbb{Z}^n$ such that $Ay \leq b$ and $c \cdot y \leq B$?

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**Physical Realization:** relevant for counting lattice points that satisfy hyperplane constraints, which is relevant for cohomology calculations that arise when computing matter spectra or instanton zero modes.

**Super concrete:** line bundle cohomology on toric varieties.

# Quadratic Diophantine

Finally, consider the problem QUADRATIC DIOPHANTINE EQUATION (QDE):

**QDE:** Given a quadratic diophantine equation, does it have a solution?

Though generic diophantine equations are undecidable [47] (see [11] for a study of diophantine undecidability in string theory), any single QDE is decidable [48]. However, already in the case where the QDE has the form $ax_1^2 + bx_2 = c$, it is NP-complete [49].

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**Physical Realization:** e.g., certain 3-7 instanton zero mode calculations.

**Interesting caveat:** generic diophantines are *undecidable*, due to Matiyasevich's theorem that solved Hilbert's tenth problem. (**see [Cvetic, Garcia-Etxebarria, JH]**).

# Question 5:

What are potential complexity loopholes and what does it mean for applying ML / AI to landscapes?

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    but quantum speedup isn't automatic.

  - stochastic: only strict saddles, can escape find loc min in P.
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- Accordingly: are extra classes, BPP and BQP that allow error, and also probabilistic and quantum algorithms, respectively.

# Loopholes: Special Instances and Reasonable N

- Special instances: there can be instances that are in P (nature sometimes utilizes them, e.g., ``minimal frustration” in folding).

- People solve NP-complete problems every day.

  In real-world problems (including theoretical physics) we often don’t care about asymptotic N.

  Google Brain KNAPSACK200: this is an ADK cosmological constant problem in disguise, and they use RL to solve it quickly. But 200 is a perfectly fine # moduli!

  Amazon: solves traveling salesman in warehouses. But your shopping cart only ever have O(10) items! Not O(1,000,000).

# Some Implications

- Each of these loopholes gives potentials ways forward for computationally complex problems that we care about.
- As far as I can tell, there are no hard and fast rules (as we're used to with ML), one should try different possibilities and look for best results.
- Some techniques (e.g. RL, with stochasticity, ε-greedy) can immediately have some of the loopholes bult in.

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  - practical implication: one of two obstacle to large N landscapes.
  - physical implication: dynamics can be understood by complexity.

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- **What is the complexity of vacua in the string landscape?**
  - determining the scalar potential involves many hard problems.

- **What are potential complexity loopholes and what does it mean for applying ML / AI to landscapes?**
  - break assumptions. e.g., classical, exact computation.
  - nice instances exist, or real-world N. **punchline:** complexity != give up!

# Final Thought:

Most of the string landscape lives at large N, but complexity limits our ability to work in that regime, e.g., our ability to make statistical predictions.

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**This motivates a concrete ML program:**
at various moderate N, learn distributions for generating random EFTs that match string observables, study whether they can be scaled to large N, and (if so) make predictions.

See Cody's talk.

# Thanks!

# Practical Implications

**Question:** **what are the practical takeaways?**

**does this mean anything for dS swampland?**

# Practical Implications

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- **Recap 1:** given $V(\phi)$, finding either stable or metastable vacua is co-NP-hard.

  finding critical points $\phi^*$ is NP-hard.

  determining whether critical point $\phi^*$ is min is co-NP-hard only if Hessian is positive semi-def at $\phi^*$.

- **Recap 2:** determining $V(\phi)$ in string theory requires solving instances of NP-complete problems.

- **Nested hard problems.** If P != NP, difficulty of finding string vacua is exponential in # of scalar fields.

- explains absence of concrete vacua at # scalars >= 20.
  makes dS swampland not directly verifiable. but it is falsifiable.

# MSVAC Proof

- MAX-CLIQUE: does G have a clique of size >= n?
- QP: is $x^*$ a global minimum of $x^T H x + c^T x$.
- QPLOC: is $x^*$ a local minimum of same.
- Vavasis: QPLOC is co-NP-hard by red. from MAX-CLIQUE.
  But it is a boundary point that is hard.
- [JH, Ruehle]: to Vavasis' QPLOC instance, map it to BOX-QUARTLOC, which makes Vavasis' boundary point and interior point and makes that problem quartic.
- [JH, Ruehle]: MSVAC is co-NP-hard via inclusion from BOX-QUARTLOC.
- remember: co-NP-hard decision problem occurs at points with PSD Hessian.

# Dynamical Implications

**Question:** could complexity affect dynamics?

(this is more speculative, based primarily
on two papers of Douglas, Denef et al and considering
our results in light of their ideas.)

# Complexity Measure

**landscape measure: [Douglas, Denef, Greene,  Zukowski] 2017**
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  **2)** if there is an alternative to solving the hard problem, might expect that.

- what we don’t expect is to see solutions to hard instances of the hard problem.

# Implications for Proteins

- **what might this mean?**

  **1)** see simple instances

  (e.g. bioproteins evolved for simple fast folding)

  **2)** see alternative to solving hard problem.

  (e.g. synthetic proteins in genei are hard instances, don't reach ground state.)

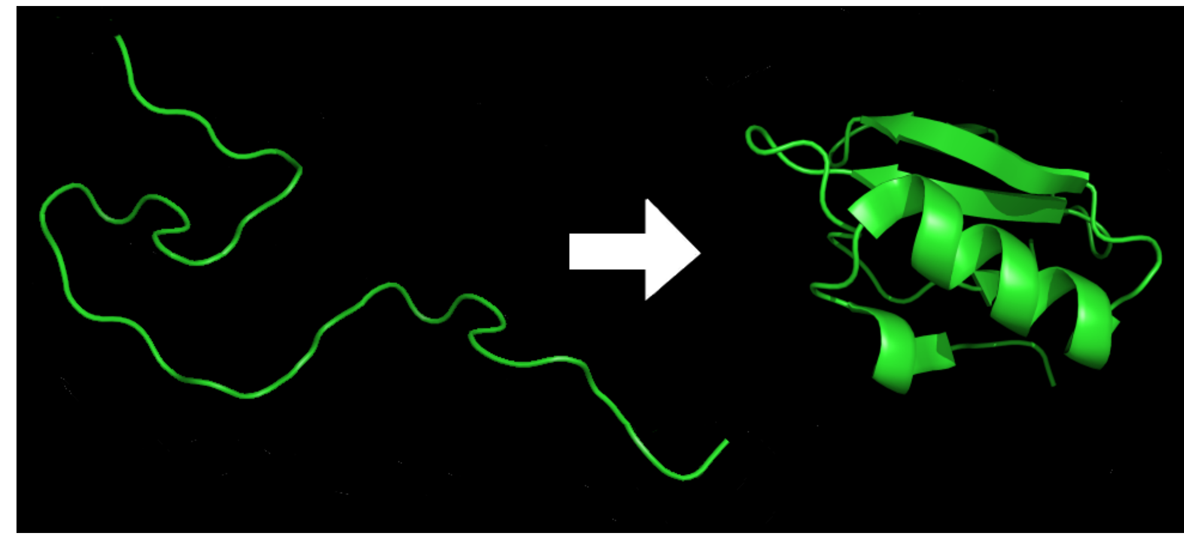

Image: Wikipedia

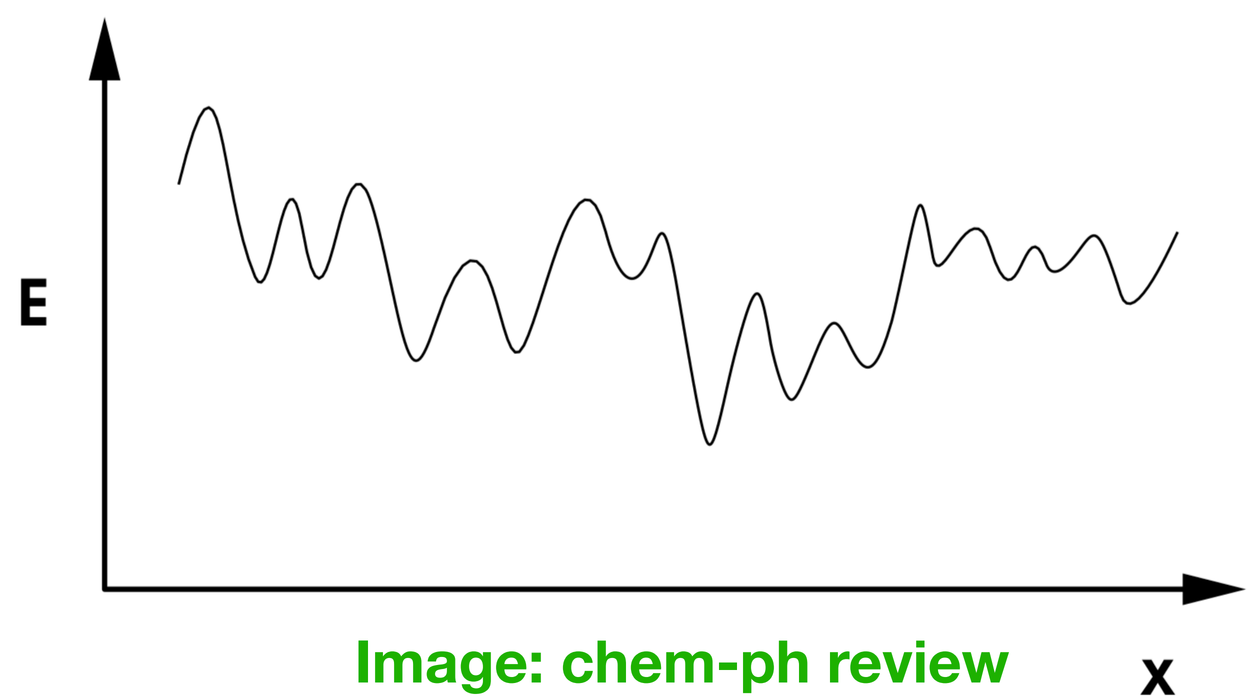


Image: chem-ph review

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- **what might this mean?**

  **1)** see simple instances.
  (e.g. find field or string theory vacua that are in P.)

  **2)** see alternative to solving hard problem.
  (in rolling solution, don't reach local minimum.)

  **3)** long lifetimes? need study of string vacuum decay distribs.