A quantum algorithm for model independent searches for new physics

Prasanth Shyamsundar
University of Florida

based on [arXiv:2003.02181]

Prof. Konstantin T. Matchev
Prasanth Shyamsundar
Dr. Jordan Smolinsky

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Quantum Adiabatic Optimization — D-Wave machine

- Task: Find the ground state of an Ising lattice

\[ H = - \sum_i h_i s_i - \sum_{i,j} J_{ij} s_i s_j \quad s_i \in \{-1, +1\} \]

- \(2^N\) possible states, where \(N\) is the number of spin sites.

- For general \(h_i\) and \(J_{ij}\), finding the exact ground state using a classical computer takes \(O(2^N)\) time. Intractable for \(N > \sim 40\)

**Adiabatic Quantum Optimization (AQO):**

- Choose a Hamiltonian \(\mathcal{H}_0\) which doesn’t commute with \(\mathcal{H}\). Initialize the system in the ground state of \(\mathcal{H}_0\).

- Adiabatically (slowly) evolve the Hamiltonian of the system from \(\mathcal{H}_0\) to \(\mathcal{H}\).

\[ H(t) = \left(1 - \frac{t}{T}\right) \mathcal{H}_0 + \frac{t}{T} \mathcal{H} \]

- System stays in the ground state of \(H(t)\). At time \(t = T\), measure the state of the system.
Quantum Adiabatic Optimization — D-Wave machine

**Takeaway:** Find an Ising Hamiltonian whose ground state describes the solution to the problem of interest. Solve using AQO.

- D-wave systems implement AQO. D-Wave 2000Q has 2048 qubits. Pegasus (2020) will have 5640 qubits.
- Approximate ground states can be found using heuristic algorithms like simulated annealing on classical computers.
- Note: AQO is different from Universal Gate Quantum Computing.
The physics problem

Search for modeled new physics in collider data

Hypothesis tests:

- Ingredients:
  1. Data $D$
  2. Null hypothesis: $H_0$ (say Standard Model)
  3. Alternative hypothesis: $H_1$ (say SM + new physics)
    
    (no free parameter in either hypothesis for simplicity)

- Test statistic $T_S$ to perform the hypothesis test with:
  - Function of data $D$
  - Inspired by $H_0$ and $H_1$

- Examples: Likelihood ratio test, $\chi^2$ difference test

$$LR = \ln \frac{P(D; H_1)}{P(D; H_0)}$$

$$\chi^2_d = \chi^2_{H_0} - \chi^2_{H_1}$$

What if we don’t have an alternative hypothesis?
Alternative hypothesis becomes “not $H_0$”.
The physics problem

Search for unmodeled new physics in collider data

Hypothesis tests

Goodness-of-fit tests:

- Ingredients:
  1. Data $D$
  2. Null hypothesis: $H_0$ (say Standard Model)
  3. Alternative hypothesis: $H_1$ (say SM + new physics) (no free parameter in either hypothesis for simplicity)

- Test statistic $T_S$ to perform the hypothesis test with:
  - Function of data $D$
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Konstantin T. Matchev, Prasanth Shyamsundar, Jordan Smolinsky [arXiv:2003.02181]
The difficulty: Look-elsewhere effect

- $p$-value depends on:
  - The data and $H_0$ (doesn’t depend on $H_1$, even when available)
  - **Test statistic** $TS$

The more types of deviations a test is sensitive to

↓

The easier it is for statistical fluctuations to mimic a given value of $TS$ or higher.

**Specificity (sensitivity) takes a hit when we lose the alternative hypothesis in the design of $TS$.**
Look-elsewhere effect in an $N$ binned $\chi^2$ test

$$\chi^2 = \sum_{i=1}^{N} \frac{(o_i - e_i)^2}{e_i} = \sum_{i=1}^{N} \Delta_i^2$$

$e_i$ is the expected count under $H_0$. $o_i$-s are Poisson distributed. $\Delta_i = \frac{o_i - e_i}{\sqrt{e_i}}$ (normalized residual)

$\Delta_i$-s are mutually independent, and follow a standard normal distribution under $H_0$.

Top row: Background only  
Bottom row: Background + signal

In these cases, data from the two hypotheses have the same $\chi^2$ value. Yet, the “eye-ball test” can distinguish between them.
Controlling the Look-elsewhere effect

► Can’t limit attention to a specific alternative hypotheses (we aren’t given one).
► Instead limit attention to “meaningful deviations”.

How are these two images different?
Can we capture the intuition in a test statistic?
Ising model to capture spatial correlations in $\Delta_i$-s

- Associate an Ising spin site with each bin in the histogram.

\[ H = -\sum_{i=1}^{N} \frac{|\Delta_i|\Delta_i}{2} \frac{s_i}{2} - \frac{1}{2} \sum_{i,j=1}^{N} w_{ij} \frac{(\Delta_i + \Delta_j)^2}{4} \frac{1 + s_i s_j}{2} \]

\[ w_{ij} = \begin{cases} 1, & \text{for nearest neighbors} \\ 0, & \text{otherwise} \end{cases} \]

- The first term tries to align spin $s_i$ with its corresponding deviation $\Delta_i$.
  - The greater the value of $\Delta_i$, the greater the reward.

- The second term tries to align spin $s_i$ with the spins $s_j$ of its neighbors.
  - The greater the value of $|\Delta_i + \Delta_j|$, the greater the reward (meaningful deviations).

- Use ground state $H_{\text{min}}$ of the system as a test statistic — the lower the ground state energy, the greater the deviation from the null hypotheses.
  - Without the second term, $H_{\text{min}} = -\chi^2/4$.
  - The pull from the second term on a spin could conflict with the pull from the first.
  - This effect makes the exact computation of the ground state intractable classically.
The new test statistic in action

1-dimensional data

- Approximate ground state discovered using simulated annealing.
- Note how some spins are anti-aligned with their deviations.
- $H_{\min}$ effectively distinguishes between signal and noise of comparable strength.

|                | $\chi^2$ | $H_{\min}$ |
|----------------|----------|------------|
| Bkg only       | 146.0    | -71.3      |
| Bkg + Sig      | 145.7    | -82.5      |
The new test statistic in action

2-dimensional data

- Approximate ground state discovered using simulated annealing.
- Note how some spins are anti-aligned with their deviations.
- $H_{\text{min}}$ effectively distinguishes between signal and noise of comparable strength.

|         | $\chi^2$ | $H_{\text{min}}$ |
|---------|----------|------------------|
| Bkg only| 129.7    | -129.6           |
| Bkg + Sig| 129.7   | -168.2           |
ROC curves and $p$-values

- The new test outperforms a number of common tests in our simulations.
Summary and outlook

Properties of a good goodness-of-fit test:

▶ Should exploit the typical differences between statistical noise and plausible real effects ✓
  – Here we leverage spatial correlations.

▶ Should work with multi-dimensional data ✓
  – New physics signals are likely to be hidden in multi-dimensional distributions.

▶ The detected deviations should be interpretable ✓
  – Extremely important in the absence of an alternative hypothesis.

New physics or background systematics?

▶ Our simulators aren’t perfect, especially parts related to non-perturbative QCD (fragmentation, hadronization), and detector response.

▶ An interpretable test can help understand and remove deficiencies in current generative models and bring down systematic uncertainties — especially important in many HL-LHC analyses expected to be bottlenecked by systematics.

Thank you! Questions?