A quantum algorithm for model independent searches for new physics

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based on [arXiv:2003.02181]

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Quantum Adiabatic Optimization — D-Wave machine

- Task: Find the ground state of an Ising lattice

$$\mathcal{H} = -\sum_i h_i s_i - \sum_{i,j} J_{ij} s_i s_j \qquad s_i \in \{-1, +1\}$$

+	+	−	+	+
+	+	−	+	+
−	+	−	+	+
+	−	−	−	+
+	+	+	−	−

- 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 $\mathcal{O}\left(2^N\right)$ 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 $\mathcal{H}$.

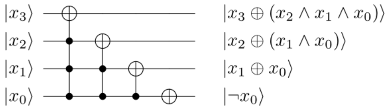
$$H(t) = \left(1 - \frac{t}{T}\right)\mathcal{H}_0 \; + \; \frac{t}{T}\mathcal{H}$$

- 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 TS to perform the hypothesis test with:
  - Function of data D
  - Inspired by H_0 and H_1
- Examples: Likelihood ratio test, χ^2 difference test

$$LR = \ln \frac{\mathcal{P}(D\ ;\ H_1)}{\mathcal{P}(D\ ;\ H_0)} \qquad \chi^2_d = \chi^2_{H_0} - \chi^2_{H_1}$$

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 TS to perform the hypothesis test with:
  - Function of data D
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- Examples: Likelihood ratio test, χ^2 difference test

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What if we don't have an alternative hypothesis?
Alternative hypothesis becomes "not H_0".

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

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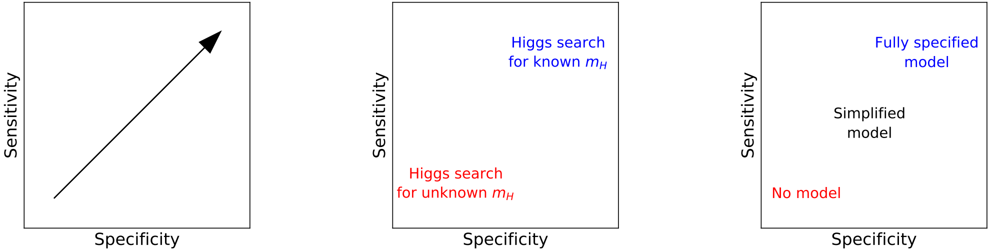
The easier it is for statistical fluctuations to mimic a given value of TS or higher.



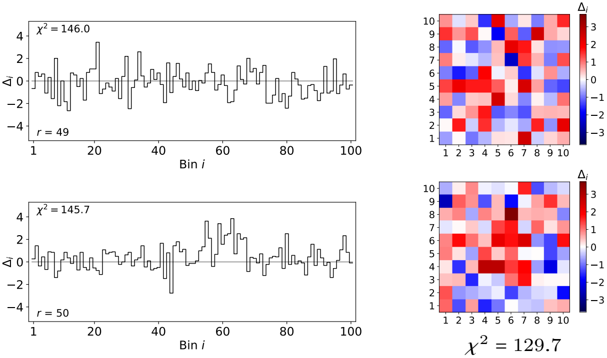
Specificity (sensitivity) takes a hit when we lose the alternative hypothesis in the design of TS.

Look-elsewhere effect in an N binned χ^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)

Δ_i-s are mutually independent, and follow a standard normal distribution under H_0.



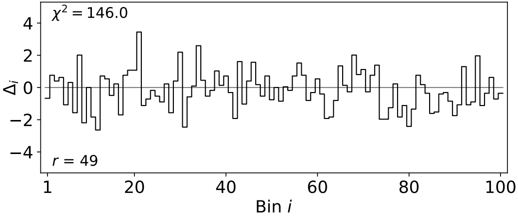
Top row: Background only
Bottom row: Background + signal

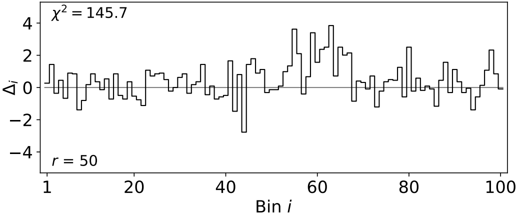
In these cases, data from the two hypotheses have the same χ^2 value.

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 Δ_i-s

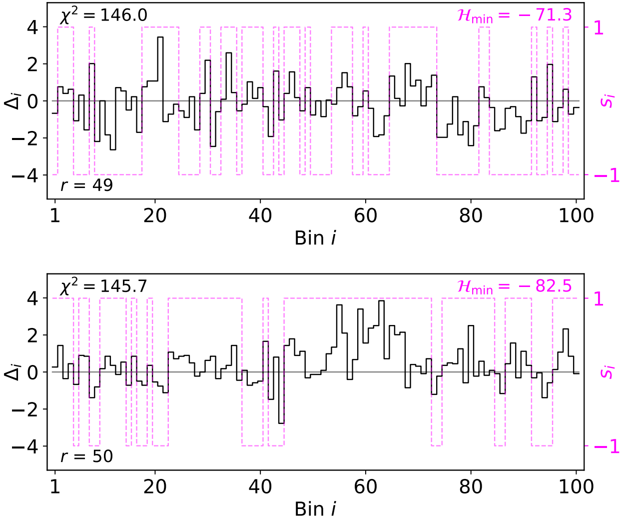
- Associate an Ising spin site with each bin in the histogram.

$$\mathcal{H} = -\sum_{i=1}^{N} \frac{|\Delta_i|\Delta_i}{2}\,\frac{s_i}{2} - \frac{1}{2}\sum_{i,j=1}^{N} w_{ij}\,\frac{(\Delta_i+\Delta_j)^2}{4}\,\frac{1+s_i s_j}{2} \qquad w_{ij} = \begin{cases} 1, & \text{for nearest neighbors} \\ 0, & \text{otherwise} \end{cases}$$

- The first term tries to align spin s_i with its corresponding deviation Δ_i.
  - The greater the value of Δ_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 $\mathcal{H}_{\text{min}}$ 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, $\mathcal{H}_{\text{min}} = -\chi^2/4$.
  - 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

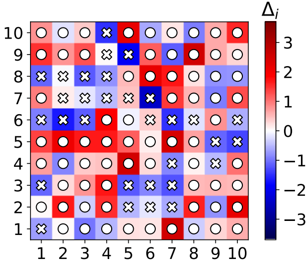


1-dimensional data

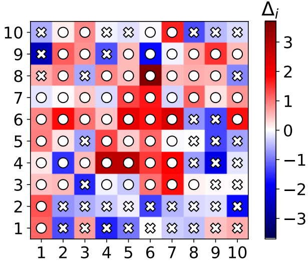
- Approximate ground state discovered using simulated annealing.
- Note how some spins are anti-aligned with their deviations.
- $\mathcal{H}_{\min}$ effectively distinguishes between signal and noise of comparable strength.

	χ^2	$\mathcal{H}_{\min}$
Bkg only	146.0	−71.3
Bkg + Sig	145.7	−82.5

The new test statistic in action



$\mathcal{H}_{\text{min}} = -129.6$



$\mathcal{H}_{\text{min}} = -168.2$

$\chi^2 = 129.7$

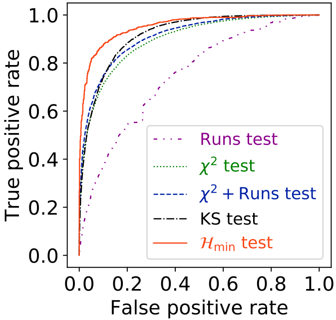
2-dimensional data

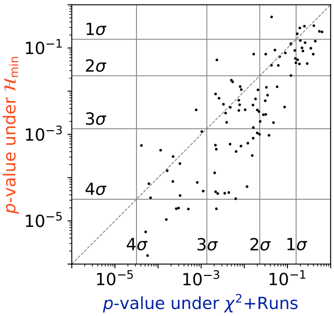
- Approximate ground state discovered using simulated annealing.
- Note how some spins are anti-aligned with their deviations.
- $\mathcal{H}_{\text{min}}$ effectively distinguishes between signal and noise of comparable strength.

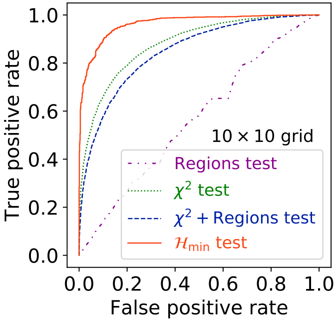
	χ^2	$\mathcal{H}_{\text{min}}$
Bkg only	129.7	−129.6
Bkg + Sig	129.7	−168.2

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?