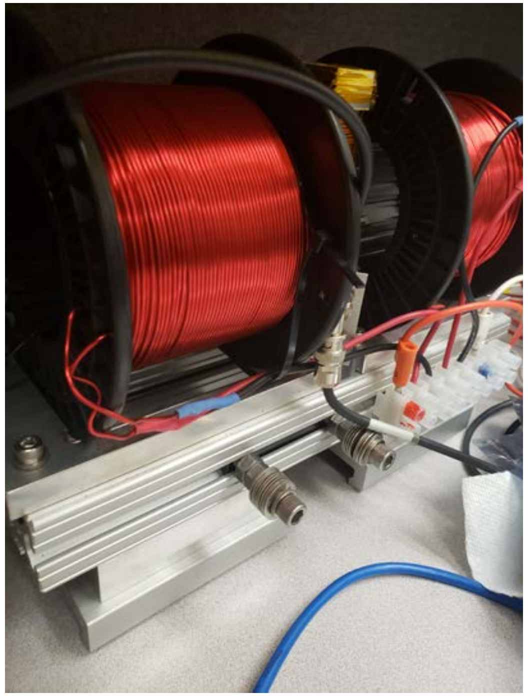
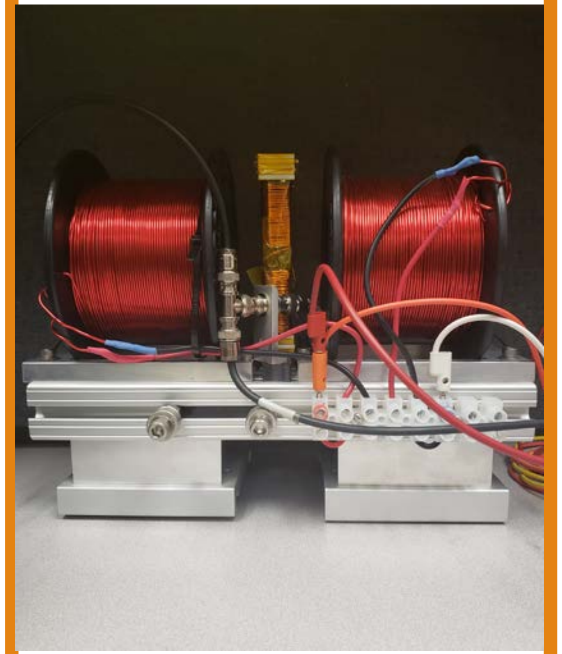




Neutron Spin Flipper Optimization using Active Learning and Fitting Algorithms

NIST Center for Neutron Research

BY: SHREYA SHETE

MENTORED BY: MARKUS BLEUEL

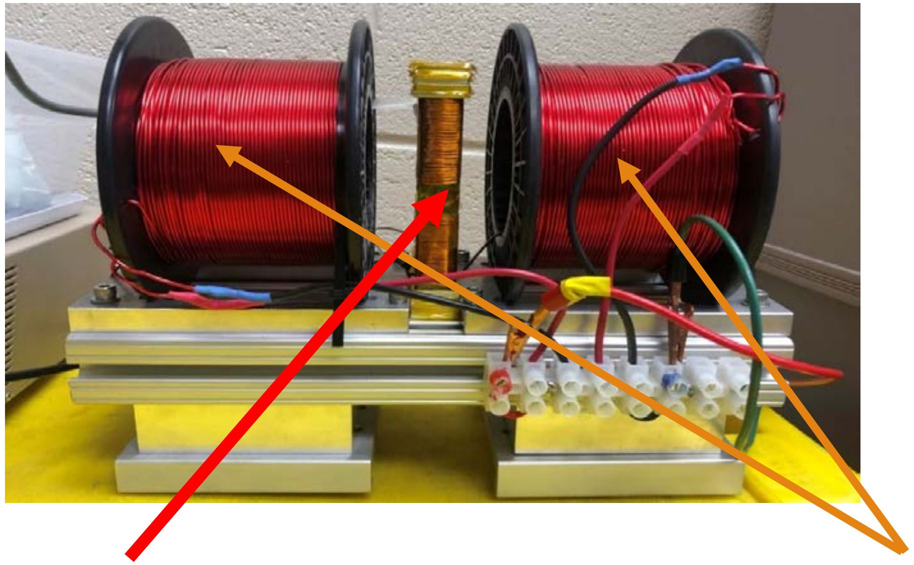
Outline

- Background
  - What is a Spin Flip and Neutron Spin Flipper?
  - Why Spin Flippers are Important
- Project Overview
  - Simulating a Neutron Spin Flipper
  - Ideal vs. Non-Ideal Spin Flips
  - Aligning a Non-Ideal Spin Flipper
- Methods
- Conclusion
- Software/Languages
- Future Steps

What is a Spin Flip and Neutron Spin Flipper?

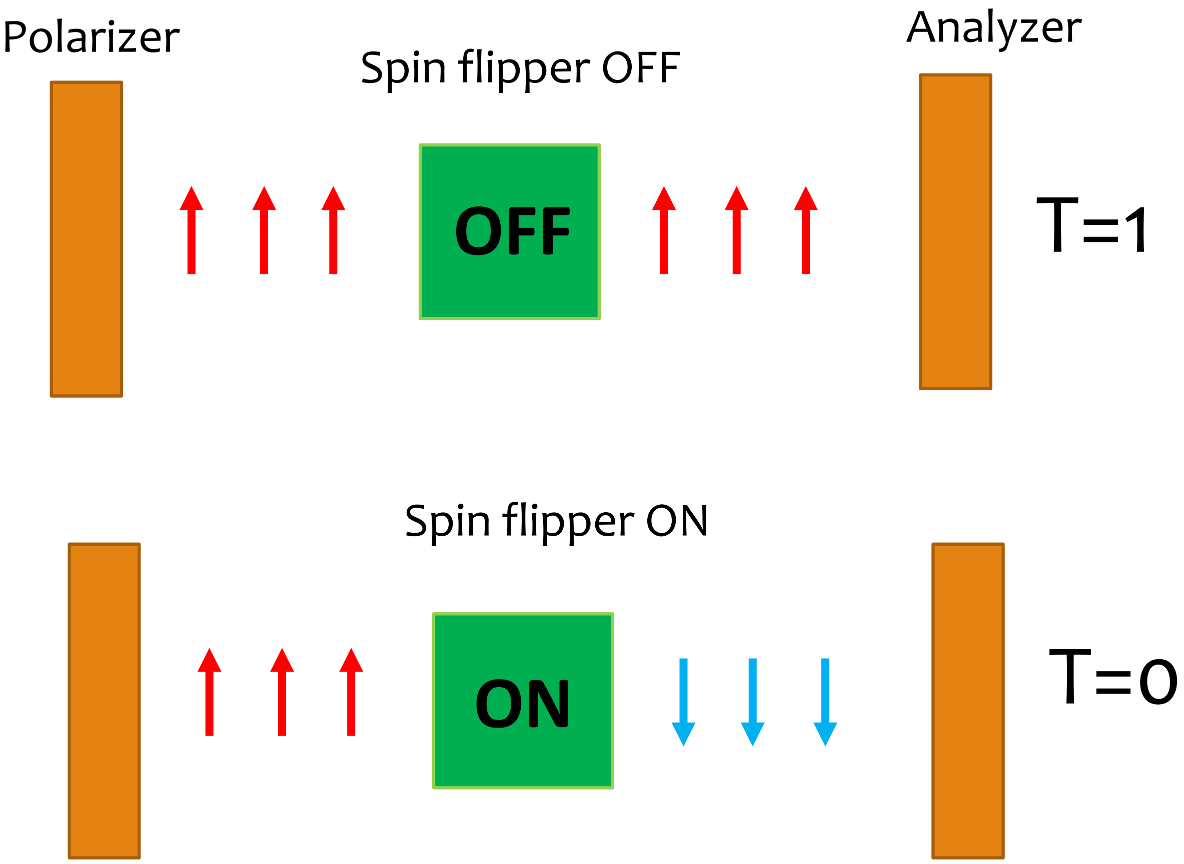
Spin Flip: a 180° rotation of the polarization vector

Prototype Neutron Spin Flipper



AC Coils
- 5 G @ 150 kHz

DC Coils
- 50 G

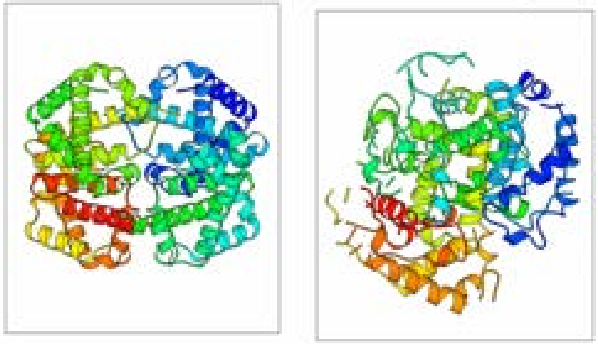


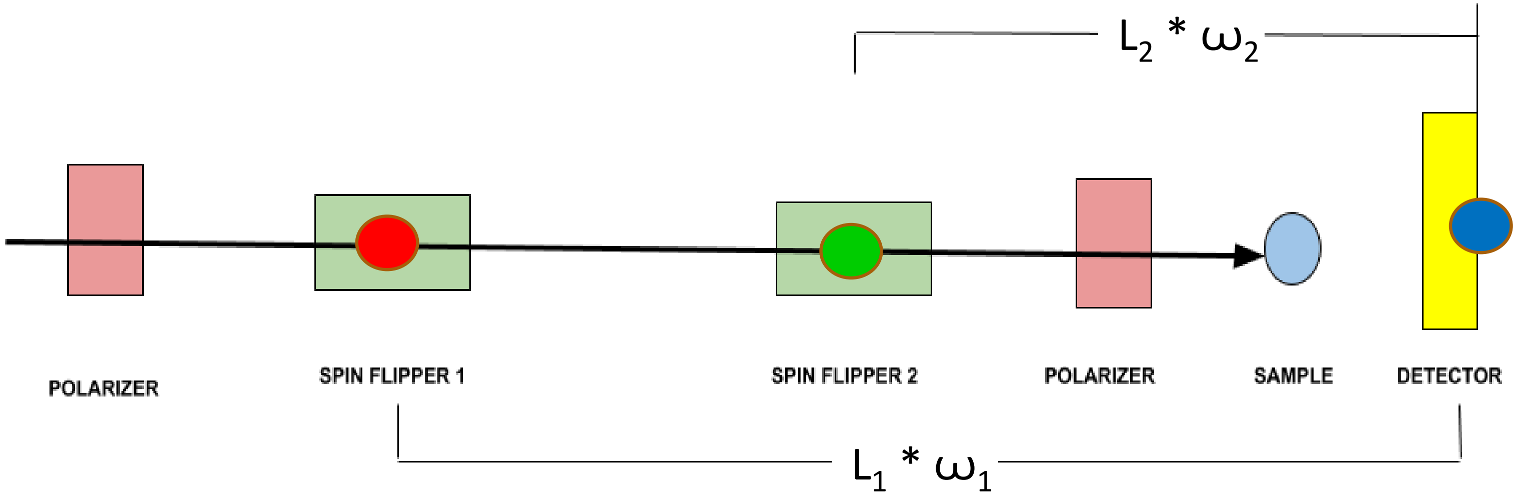
Why Neutron Spin Flippers Are Important

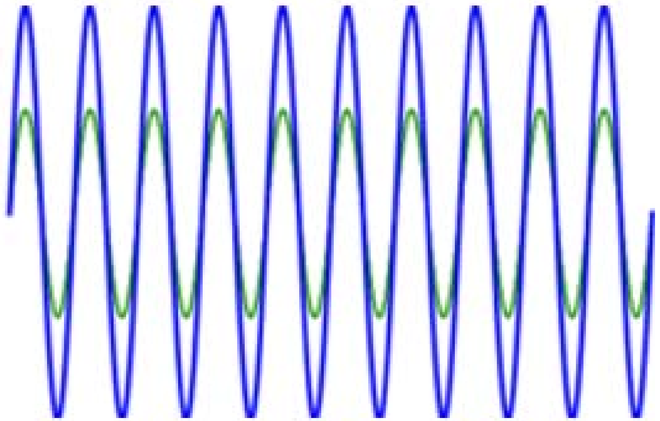
Modulated- Intensity SANS (MISANS):

- The Blue Signal is the sum of the two flipper modulations
- SANS becomes sensitive to sample dynamics when the neutron beam is modulated

Ex: Normal vs. Sickle Cell Hemoglobin







Wiki: Frequency Beating

Why Neutron Spin Flippers Are Important

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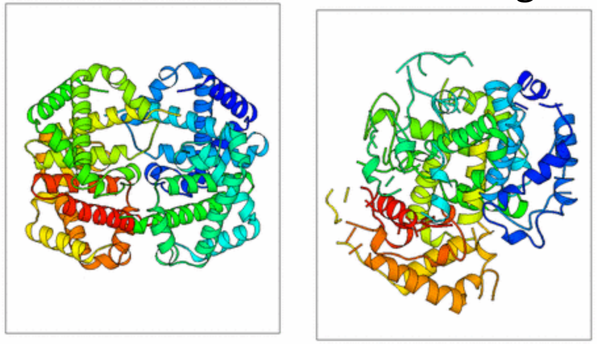
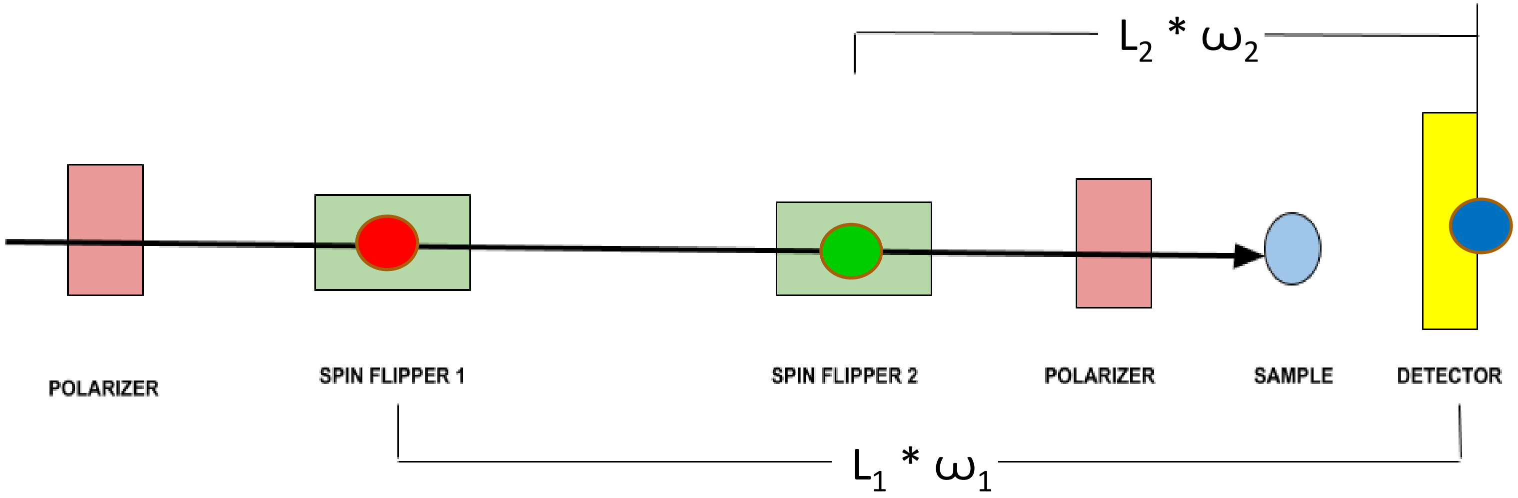
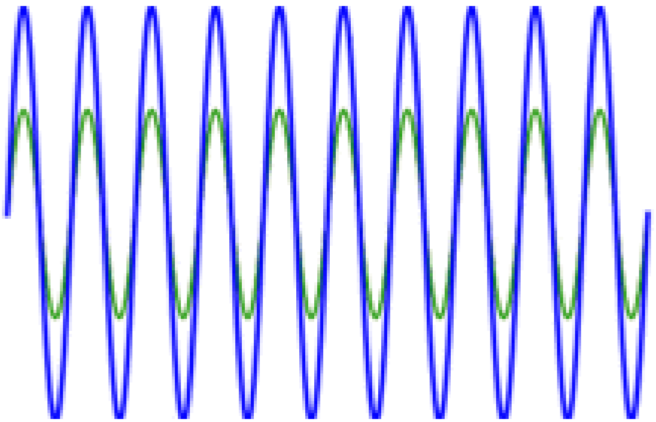






Wiki: Frequency Beating

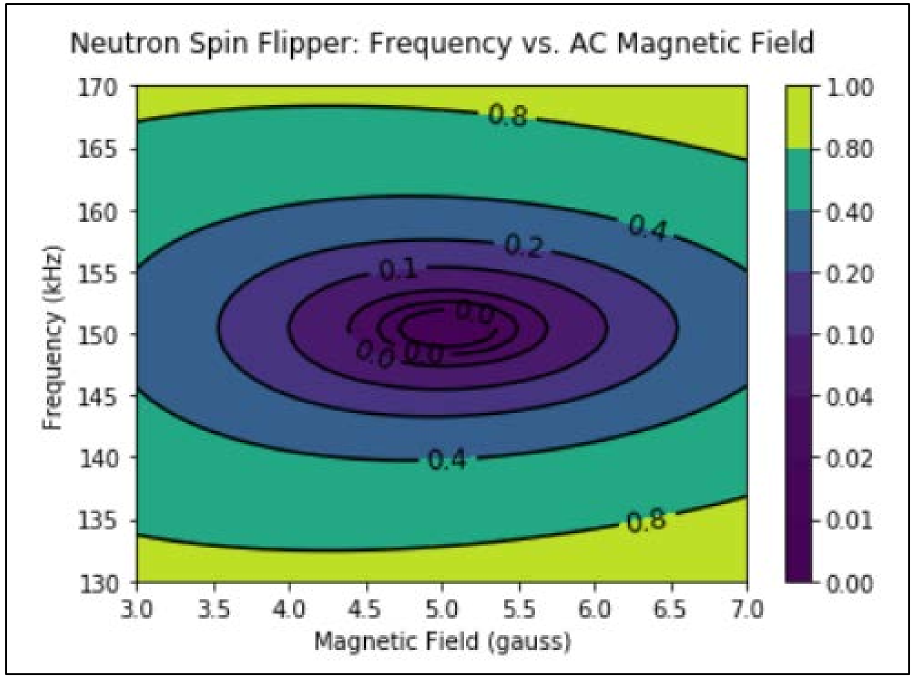
Simulating a Neutron Spin Flipper

- If neutron spin is flipped, Transmission goes to zero (T=0), which is what we measure in a real experiment

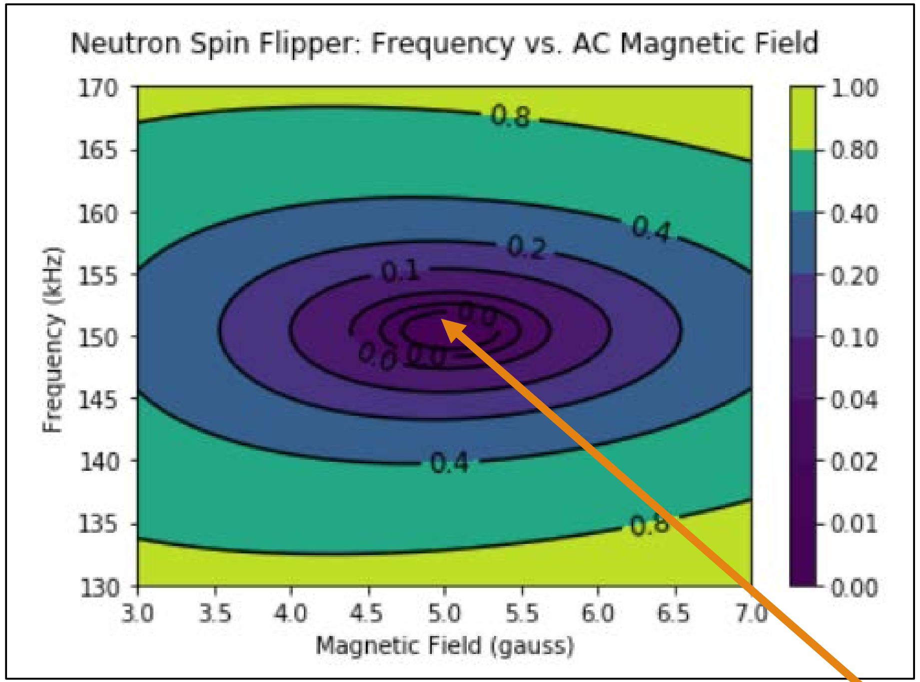
- Find a proper math function *(shown on the next slide)*
  - Ideal Test Case: When B_DC=50G, 5G@150kHz => T=0

- In reality, there are Magnetic Stray Fields that need to be accounted for *(shown on next slide)*

- The Contour Plots focus on the RF-part of the flipper
  - AC Magnetic Field on the x-axis (3-7 G)
  - Frequency of Precession on the y-axis (130-170 kHz)
  - Transmission is the z-slices/contours

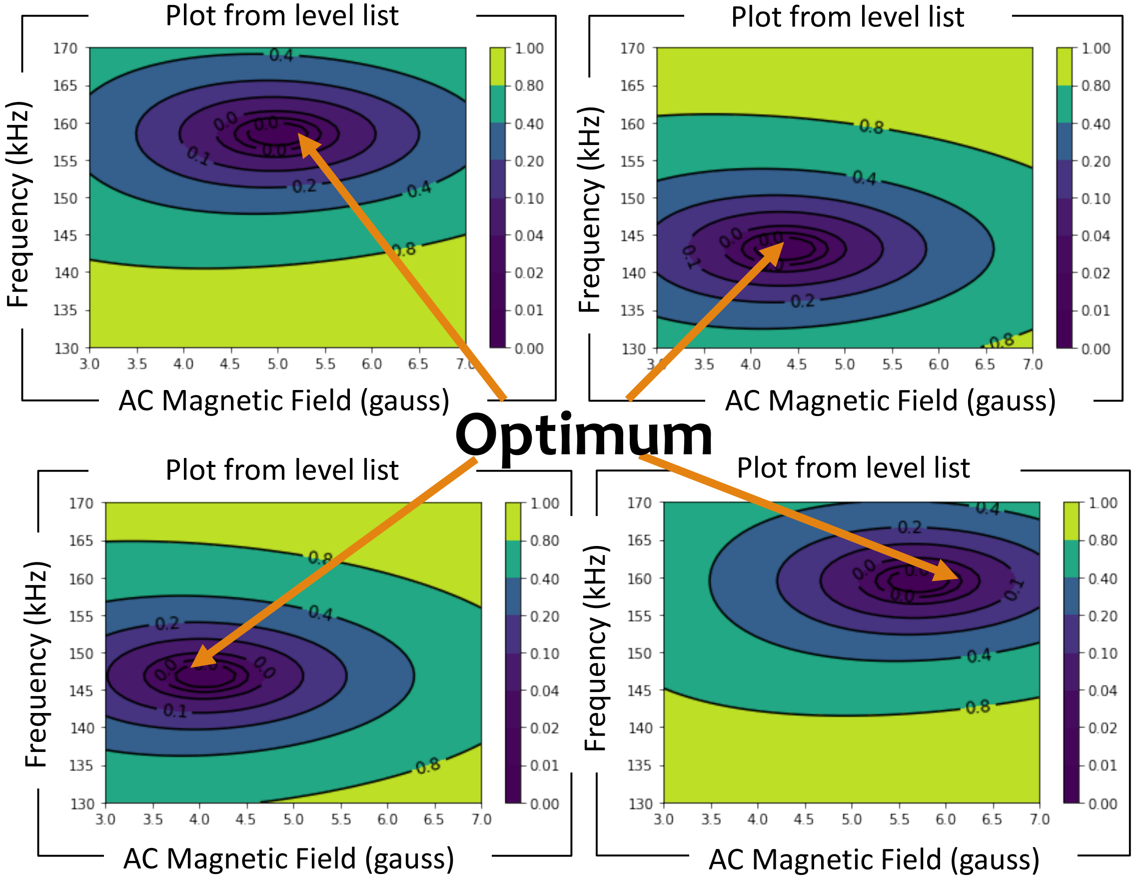


Ideal Spin Flip vs. Non-Ideal Spin Flips



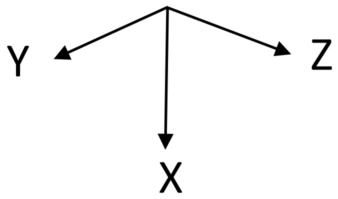
Optimum: (5, 150)

- Optimum would be at…
  - B_AC = 5 gauss
  - Frequency of Precession = 150 kHz
- Transmission=0

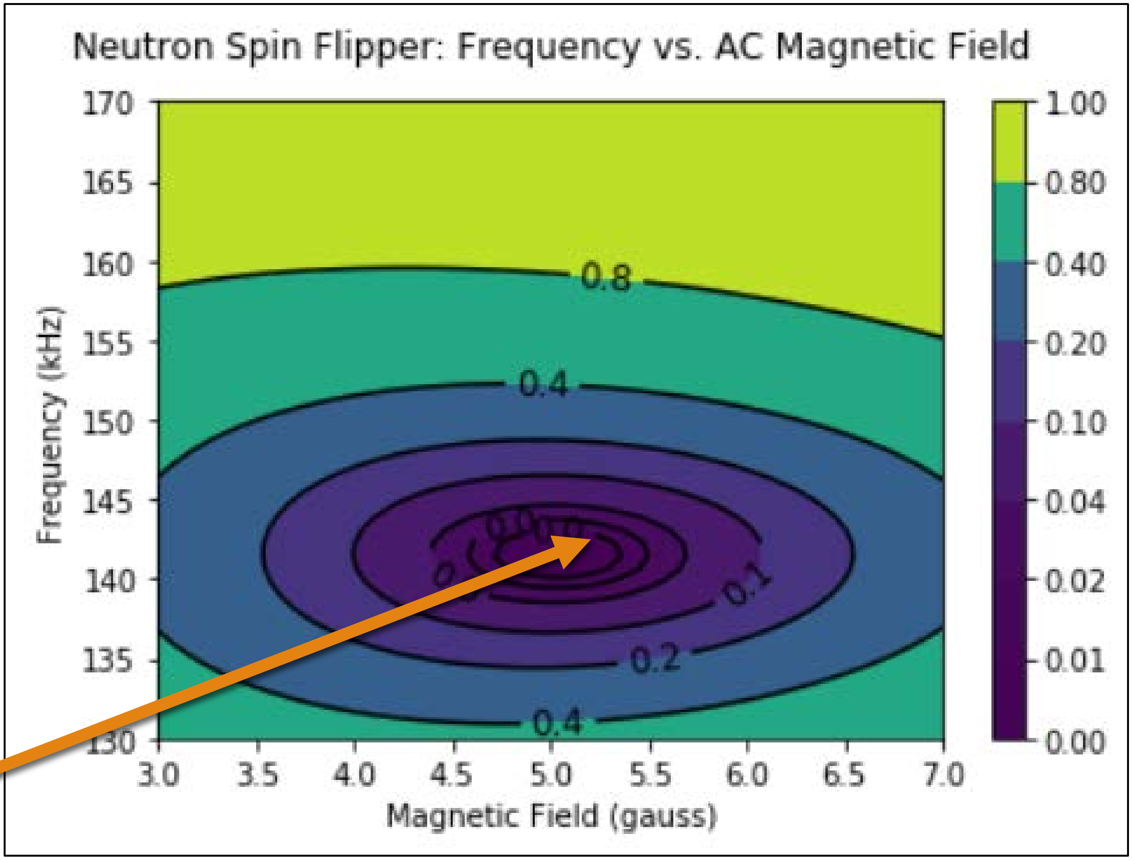


- Ideal Spin Flip Formula + Static Fields
- Optimum Shifts in Position

Aligning a Non-Ideal Spin Flipper



- Find optimum (x,y) for perfect flip with as few measurements as possible
  - X: AC Magnetic Field (gauss)
  - Y : Frequency of Precession (kHz)
  - Z: Transmission
- Test different methods and find the best way to align a flipper



Optimum (x,y)

Methods

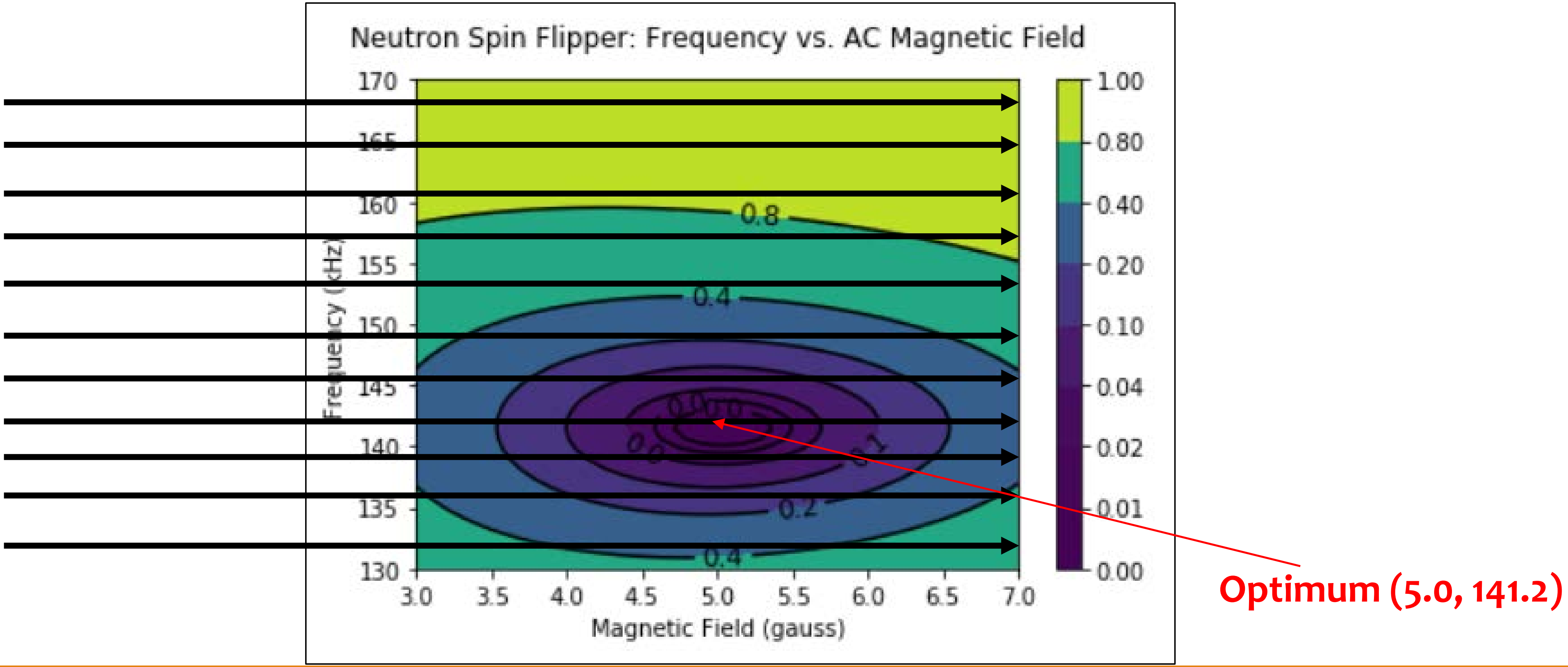
Classic Grid Search
Non-Linear Iterative Curve Fitting
Least Squares Fitting of Data Points
Bayesian Optimization

Which Method is the fastest

- In a well-known environment?
- In an unknown environment

Method 1. Classic Grid Search

Searches all of the Polarization Values in **Matrix a** to find the position of the minimum value to calculate the optimum



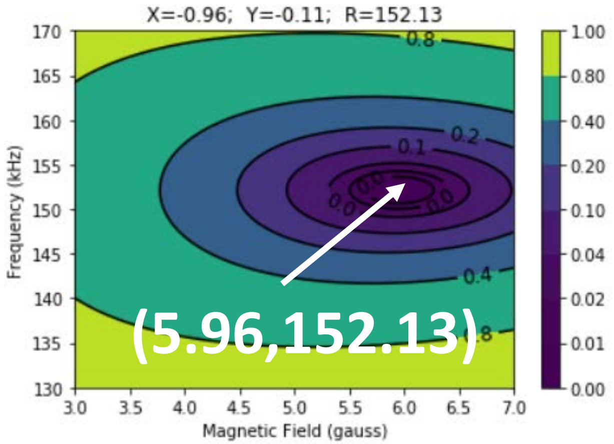
Method 2. Non-Linear Iterative Curve Fitting

1. Pick a minimization model/ method
2. Make initial guess: (5, 150) for optimum
3. Program computes model and compares to dataset to calculate fitting error
4. If fitting error > required fitting accuracy
   - Program changes parameters and repeats process until either
     - required fitting accuracy is achieved
     - max iterations is reached

Fastest

Methods	Average nfev
L-BFGS-B	26.46
Powell	148.67
Nelder-Mead	75.64
BFGS	51.72
CG	127.76
SLSQP	42.52
COBYLA	148.78
TNC	37.86
trust-constr	34.53

Slowest




```
 L-BFGS-B
Minimum: [  5.95502599 152.13439381]
 Powell
Minimum: [  5.95504358 152.13434775]
 Nelder-Mead
Minimum: [  5.95503703 152.13432826]
 BFGS
Minimum: [  5.95504949 152.13434571]
 CG
Minimum: [  5.95504067 152.13522283]
 SLSQP
Minimum: [  5.95494264 152.13512091]
 COBYLA
Minimum: [  5.95512266 152.13313905]
 TNC
Minimum: [  5.95480379 152.13559236]
 trust-constr
Minimum: [  5.95504354 152.13434661]
```

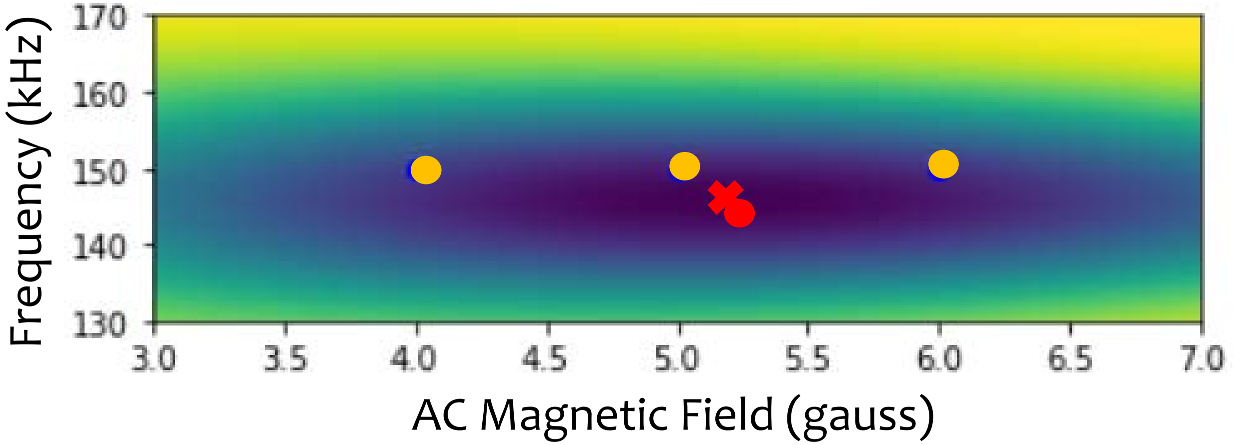
Method 3. Least Square Fitting of Data Points

Fits 4 Points to find

- BDC_X, BDC_Y, BDC_Z
  - account for the static fields/randomness in the program
  - Used to calculate the optimum

Example with 3 Points:

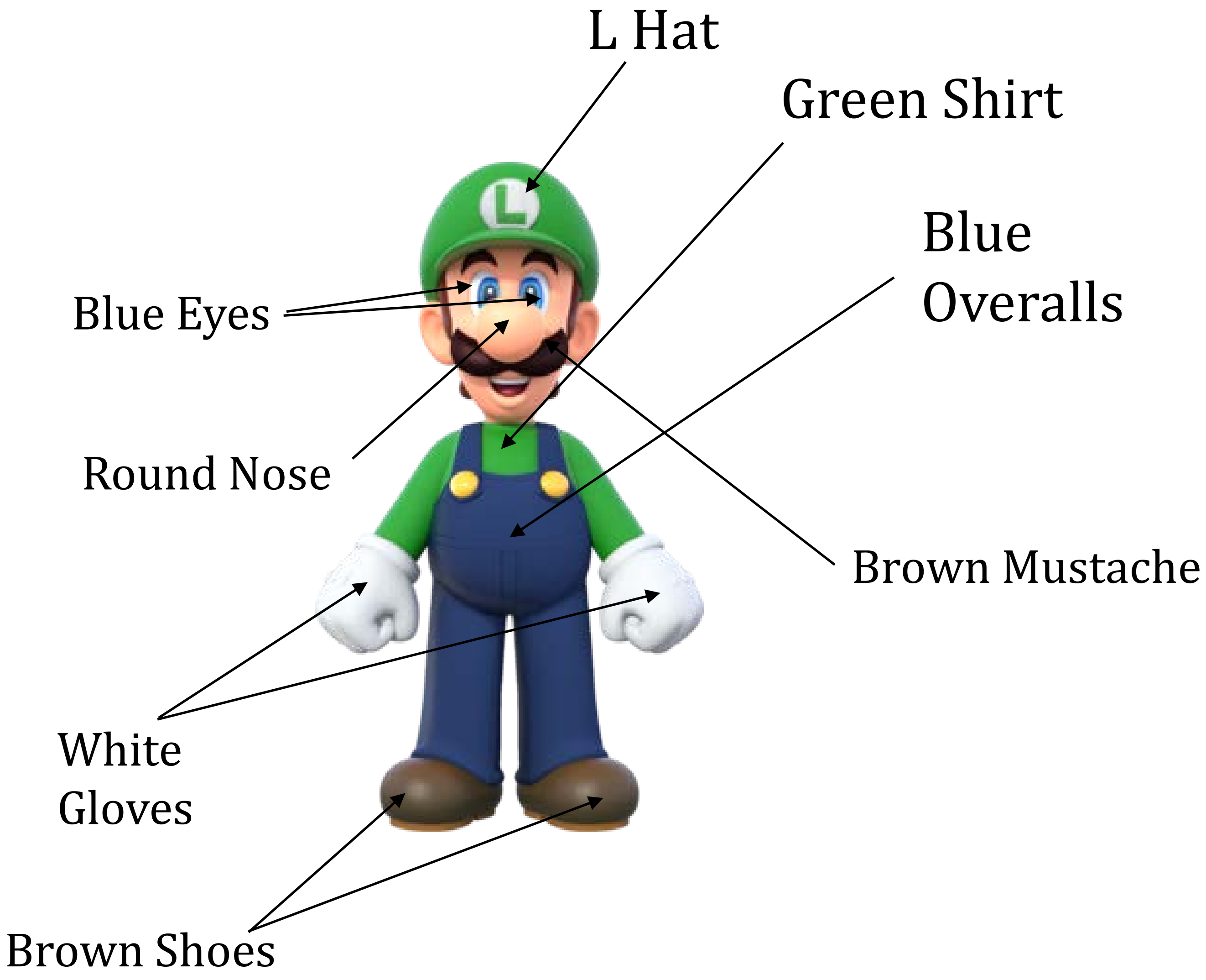
```
target -0.18825334153867512 -0.43444607927213696 145.9198948657415
result [ -0.16707025   0.          154.06600899]
min [   5.16923046 145.91928062] val 1.8543074298271733e-09
```



Active Learning

- Reduces uncertainty in the model to reach optimum
- Very adaptive

Example: Classifying the Animated Figure



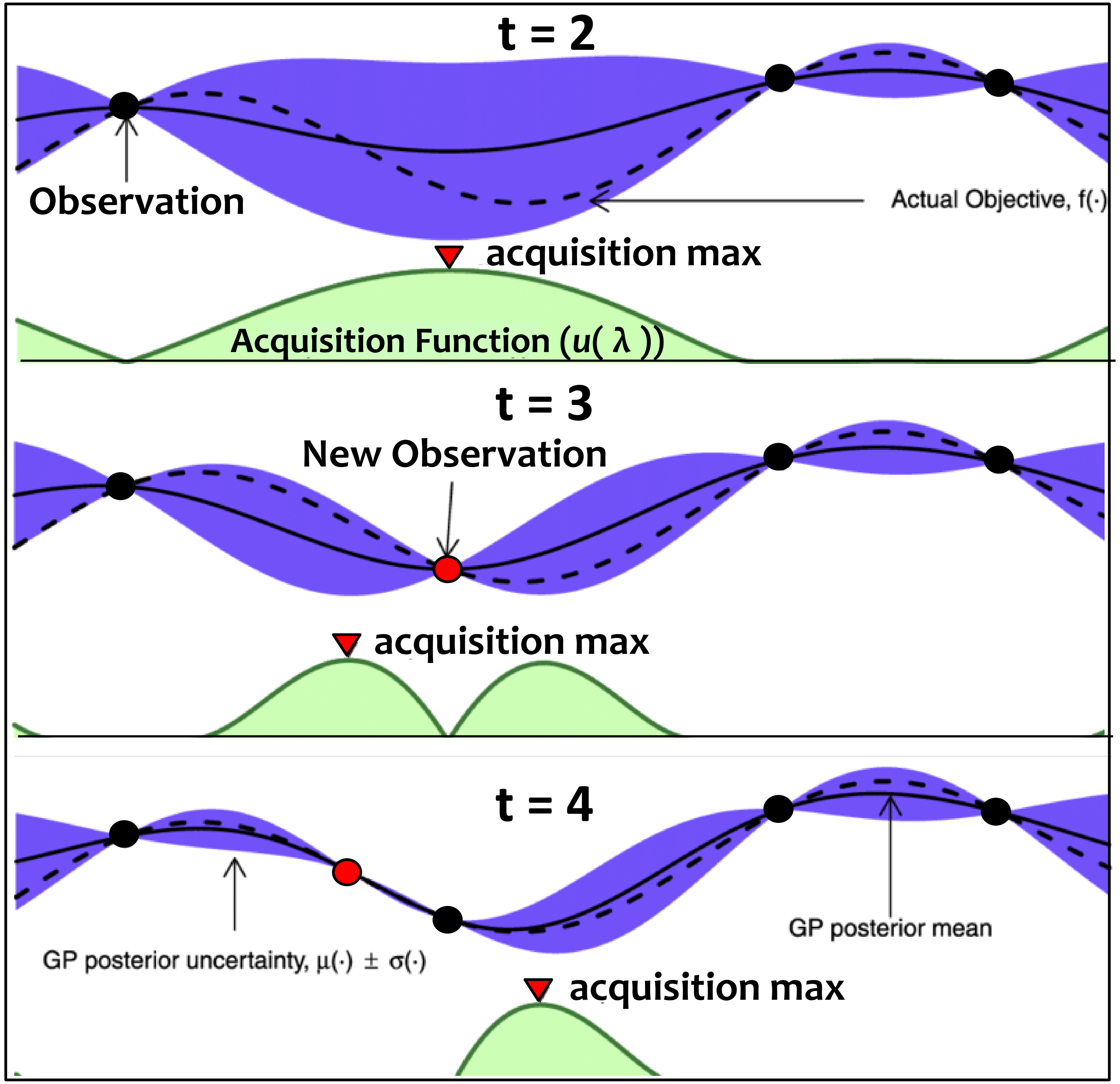
Bayesian Optimization:

Successfully Updating the Gaussian Process

1. Find acquisition max—($\max_{\lambda}(u(\lambda))$)
   - good expected value
   - high uncertainty
   - $\max_{\lambda}(u(\lambda)) = \lambda_{next}$

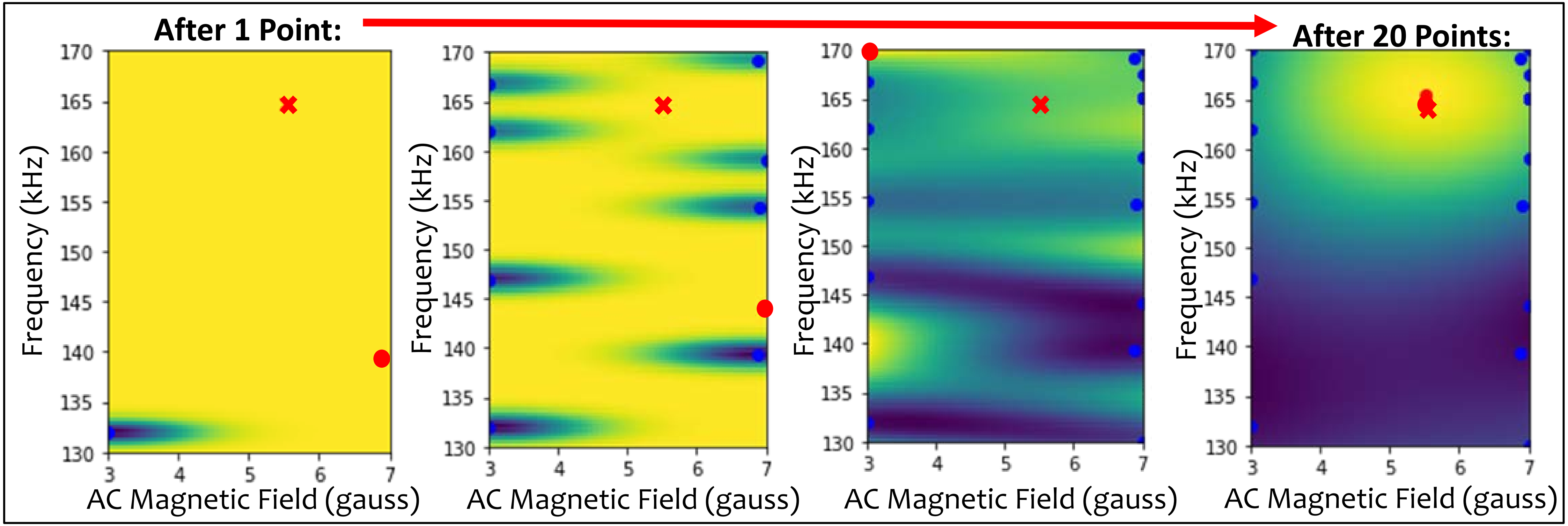
2. Use new observation (λ_{next}) to update *Gaussian Process*

3. Repeat …



Method 4. Bayesian Optimization/ Active Learning

- ✖ Optimum Point
- ● Current Point We're Measuring
- ● Previously Measured Point



Comparing Methods

Methods from Slowest to Fastest	Points Measured
Classic Grid Search	100
Non-Linear Iterative Curve Fitting	26
Bayesian Optimization	20
Least Square Fitting of Data Points	3-4

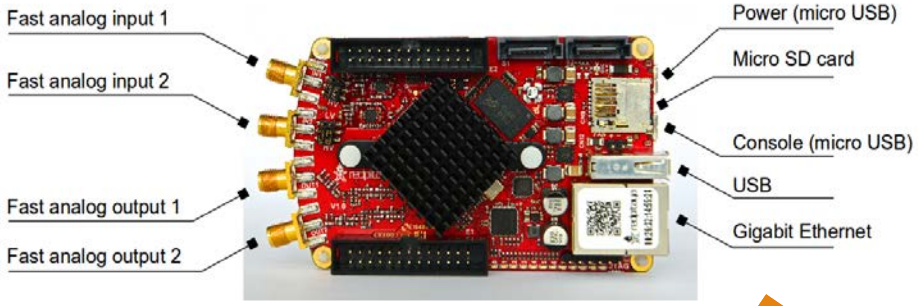
	Uses Model Function	No Model Function
Adaptive	Non-Linear Iterative Curve Fitting	Bayesian Optimization
Non-Adaptive	Least Squares Fitting of Data Points	Classic Grid Search

Conclusion

- All Methods are successful
- Classic Grid Search Method is extremely slow and inefficient.
- Bayesian Optimization and Fitting Algorithms are modern tools for such a project because they are still fast while obtaining accurate results for the optimum.
- **Which Method is the Fastest?**
  - In well-known environment: Least Square Fitting of Data Points
  - In unknown environment: Bayesian Optimization

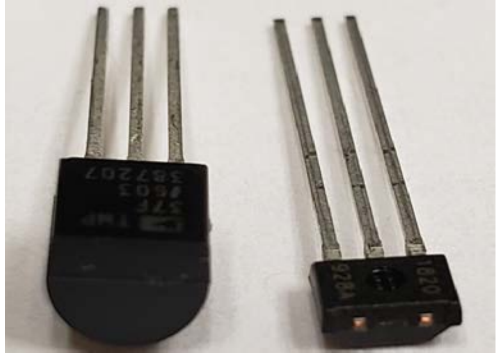
Future Steps

Use the Red Pitaya STEMLab and Magnetic Field & Temperature Sensors to monitor stability of the setup to decide when to optimize



The Red Pitaya STEMLab

- Measurement Device
- Controls Both Flippers in all aspects



Temperature Sensor

Magnetic Field Sensor

Sensor Extension Module

Software/ Languages

Interactive window for application

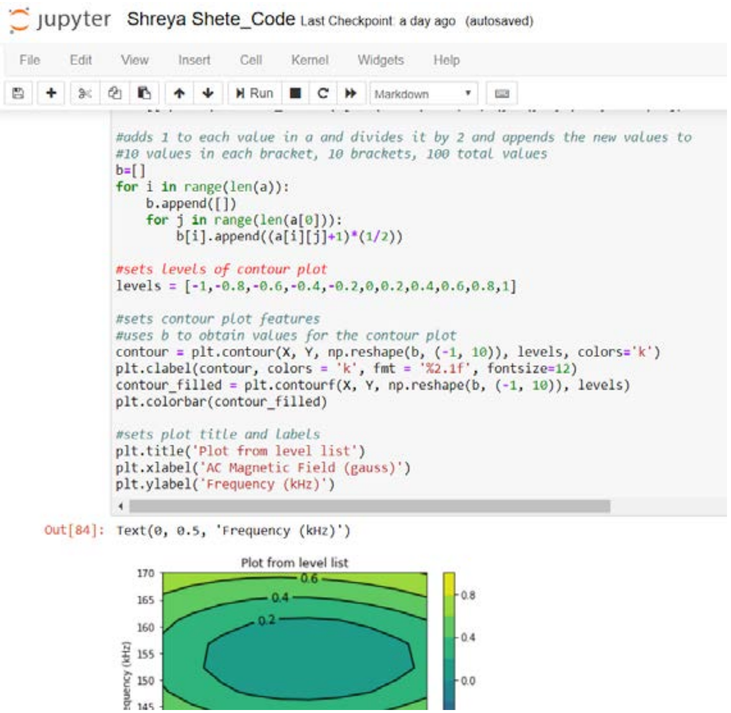
- *Python Anaconda in Jupyter Notebook*

Python Libraries for Data Graphics

- *Holoviews & Bokeh*

Python Libraries for Optimization and Machine Learning

- *SciPy & GPy (Gaussian Processes)*



Acknowledgements

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