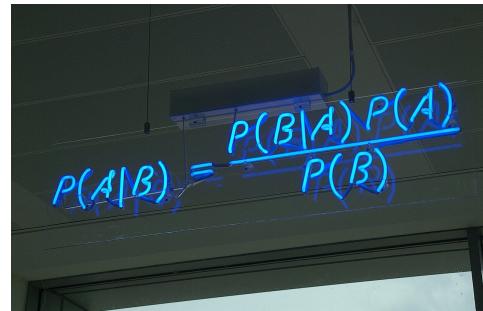




Plasma Science & Fusion Center

An introduction to Bayesian Optimization with Optuna

Enrique de Dios Zapata Cornejo



Outline

1. Optimization 101
2. Optuna
3. Hackathon (hard optimization problem)
4. Hyperparameter tuning in ML
5. Multiobjective optimization
6. Practical session

Disclaimers

1. Please, wait for questions at the end of each section
2. This not a fully Bayesian statistic tutorial
3. Gaussian processes are out of the scope of this tutorial

Optimization 101

What is optimization?

Optimization is the process of finding the solution x^* for a function $f(x)$ that maximize its output y , satisfying given constraints (optional).

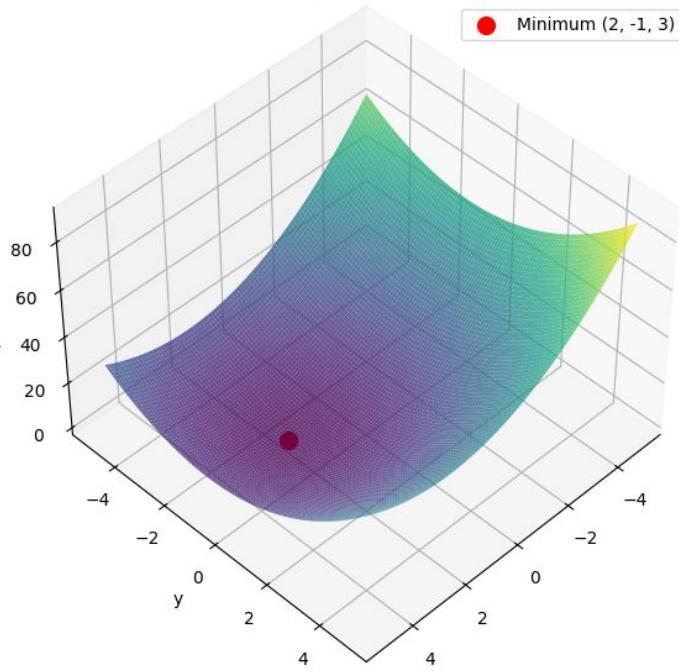
$$\mathbf{x}^* = \arg \max_{\mathbf{x} \in \chi} f(\mathbf{x})$$

χ = design space

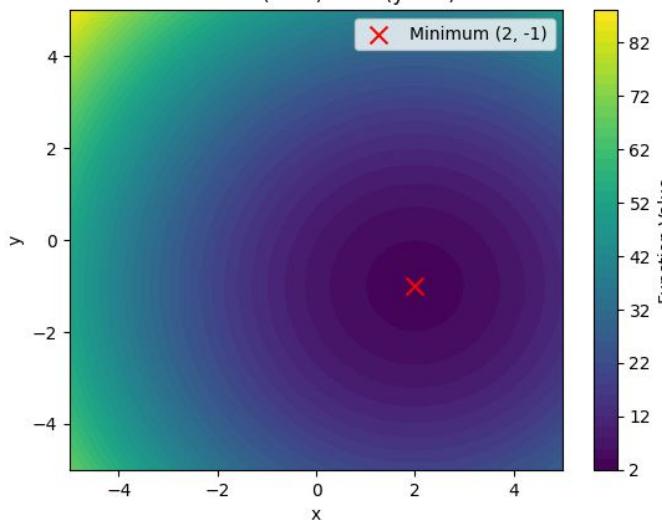
\mathbf{x}^* = optimal solution

Example 1

3D Surface Plot of $(x - 2)^2 + (y + 1)^2 + 3$



Contour Plot of $(x - 2)^2 + (y + 1)^2 + 3$



python [example1.py](#)

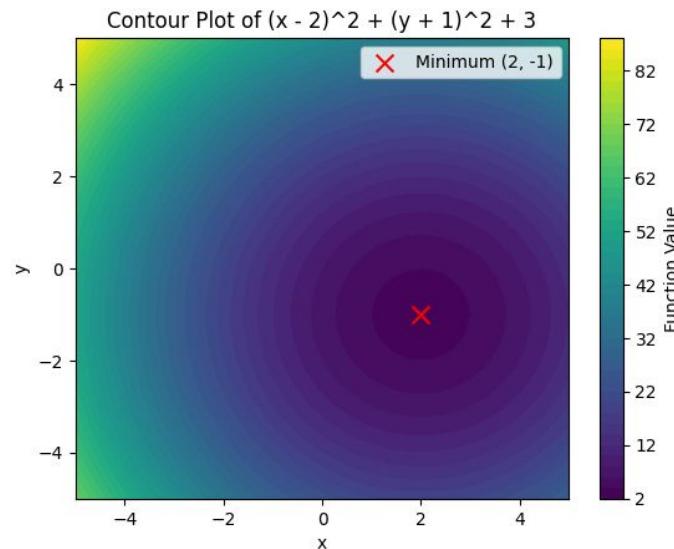
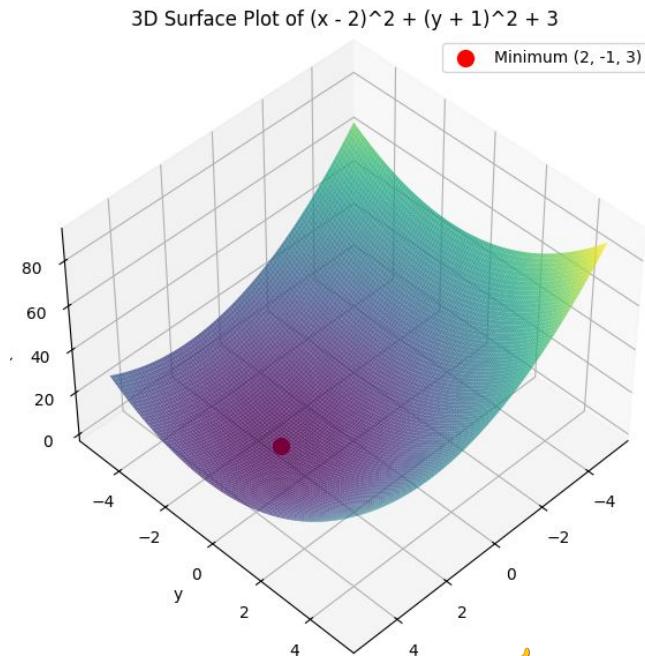
Why Bayesian optimization?

Some optimization methods.

Method	Pros	Cons
Grid/Random Search	Simple	Inefficient
Gradient Descent	Fast	Needs gradients (differentiable search spaces)
Bayesian Opt	Sample-efficient	More compute upfront

Example 1: Grid search

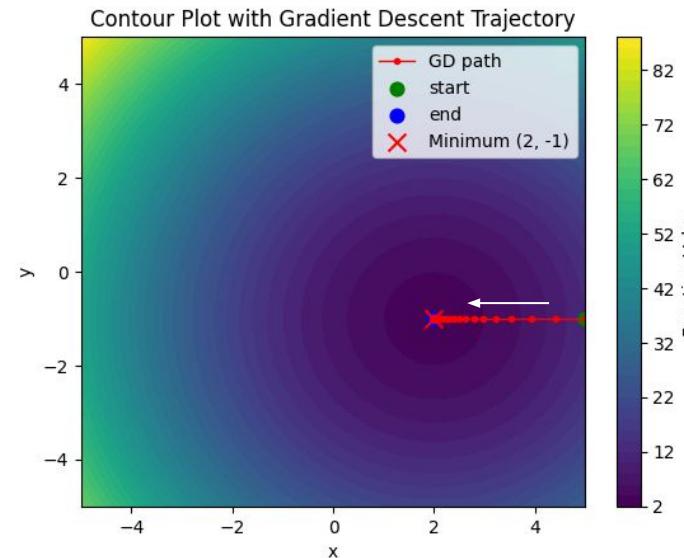
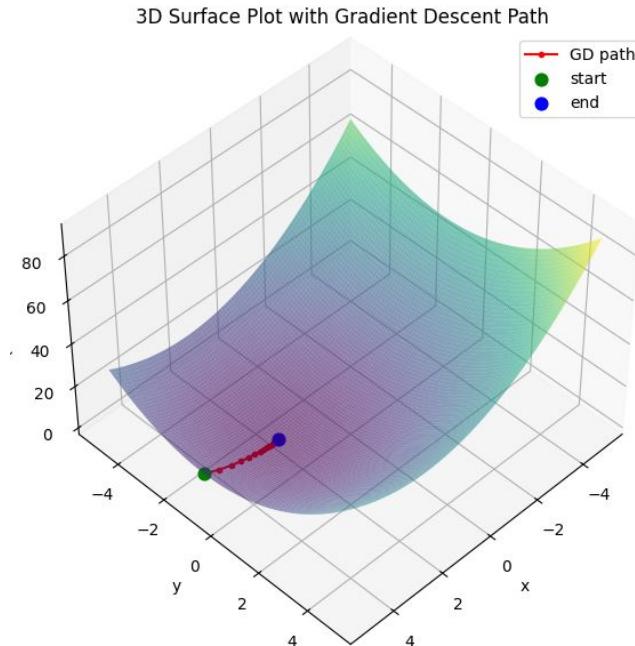
Minimum value of Z is 3.000100401203208 at $(x, y) = (1.993987975951904, -0.9919839679358722)$, with 500000 function evaluations.



python [example1.py](#)

Example 2: Gradient descent $\theta_{t+1} = \theta_t - \eta \nabla_{\theta} J(\theta_t)$

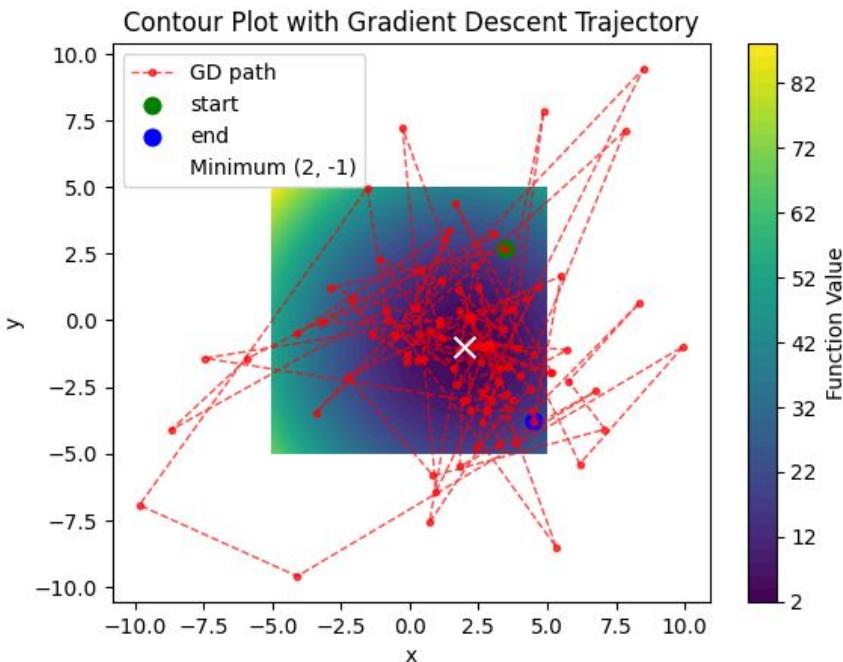
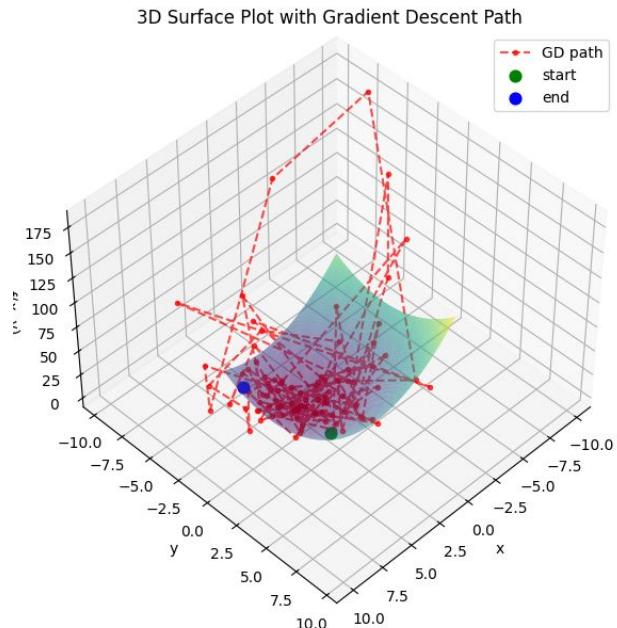
Exact value of $f(x,y)$ is 3.0 at $(x, y) = (2.0, -1.0)$ reached after 85 iterations



👉 python [example2.py](#)

Example 3: Bayesian Optimization (Spoiler!)

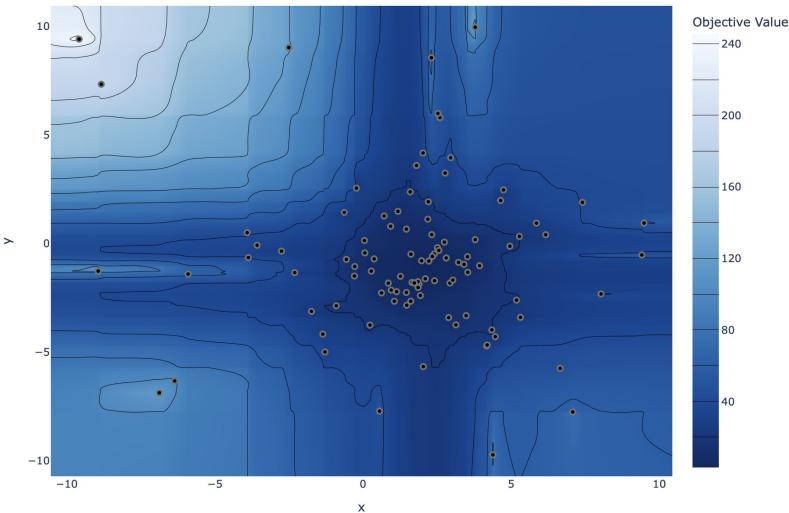
Minimum value of $f(x,y)$ is 3.0156737909138682 at $(x,y) = (1.893938637086194, -1.0665190063871524)$, with 100 trials.



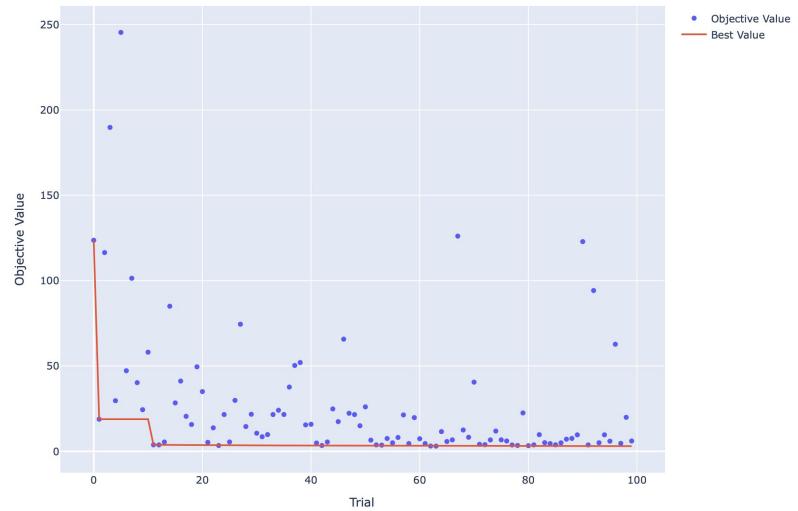
python [example3.py](#)

Example 3: Bayesian Optimization (Spoiler!)

Contour Plot



Optimization History Plot



Best parameters: {'x': 1.893938637086194, 'y': -1.0665190063871524}
 Best value: 3.0156737909138682
 Number of trials: 100 (good value after ~12 trials)

Bayesian Optimization with OPTUNA

What is Bayesian optimization?

Bayesian optimization aims to find an optimal solution by building a probability model of the objective function and use it to chose the most proximating direction.

$$P(\text{score} | \text{hyperparameters})$$

This **probabilistic model** is a *surrogate of the objective function*.

$$P(y|x)$$

Bayes theorem rules conditional probabilities

Prior $P(y)$ (the probability before the evidence is considered)

Posterior $P(y|x)$ (updated probability after the evidence is considered)

Likelihood $P(y|x)$ (probability of the evidence, given the prior belief is true)

Marginal $P(x)$ (probability of the evidence, under any circumstance)

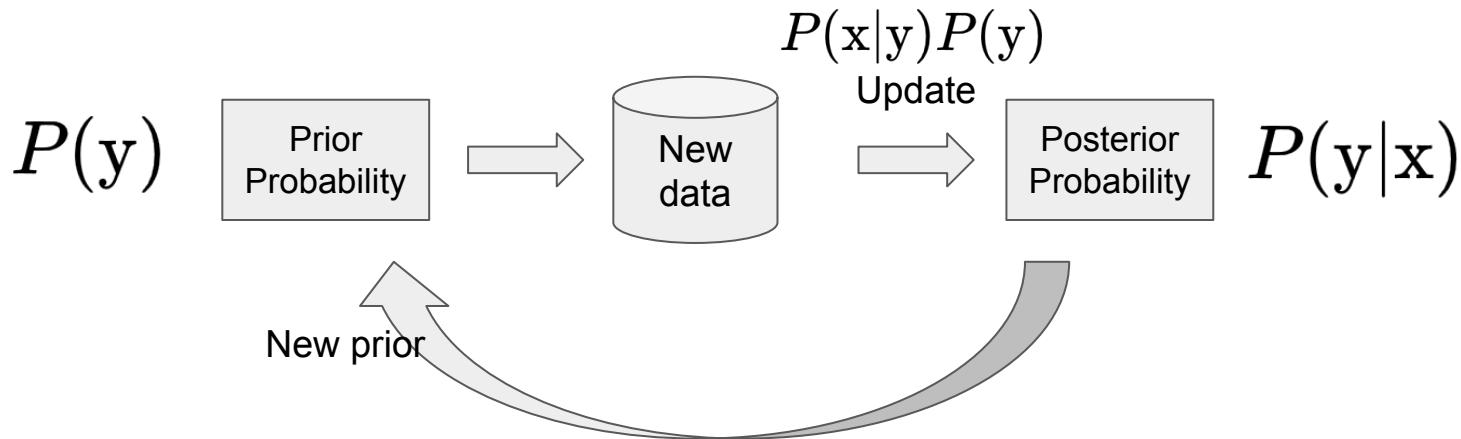
$$P(y|x) = \frac{P(x|y)P(y)}{P(x)}$$

$$P(score|parameters) = \frac{P(parameters|score)P(score)}{P(parameters)}$$

!  Often likelihood integration is intractable, then other approaches/approximations are developed.

!!  Bayesian ~ Probabilistic model

What is Bayesian optimization (BO)?



BO steps:

1. Build a surrogate probability model ! of the objective function
2. Find the hyperparameters that perform best on the surrogate (Define acquisition function !)
3. Try these hyperparameters in the true objective function
4. Update the surrogate model incorporating the new results
5. Repeat steps 2–4 until max iterations or time is reached

What is Optuna



Open-source Python lib for automated ML (hyperparam tuning, etc.)

Key Features:

- Define search space declaratively with Python (`suggest_float`, `suggest_int`, etc.)
- State of the Art algorithms with pruning (Early-stop bad trials)
- ML framework agnostic: Integrates with scikit-learn, XGBoost, PyTorch...
- Parallelization
- Visualizations: Basic plotting functions using Plotly and Matplotlib

Easy Install: `pip install optuna`

Optuna has an excellent documentation!

👉 <https://optuna.readthedocs.io/en/stable/reference/index.html>

Optuna syntax

```

import numpy as np
import optuna

SEED = 42
np.random.seed(SEED)

# Define the function to optimize
def function_to_optimize(x, y):
    # Quadratic function: f(x,y) = (x-2)^2 + (y+1)^2 + 3
    # Minimum is at (2, -1) with value 3
    return (x - 2) ** 2 + (y + 1) ** 2 + 3

# Define the objective function for Optuna
def objective(trial):
    # Define parameters to optimize
    x = trial.suggest_float('x', -10.0, 10.0)
    y = trial.suggest_float('y', -10.0, 10.0)
    return function_to_optimize(x, y)

# Create study object and optimize
study = optuna.create_study(direction='minimize',
                             sampler=optuna.samplers.TPESampler(seed=SEED))
study.optimize(objective, n_trials=100)

# Print results
print(f"Best parameters: {study.best_params}")
print(f"Best value: {study.best_value}")
print(f"Number of trials: {len(study.trials)}")

```



python [example3.py](#)

} Seed

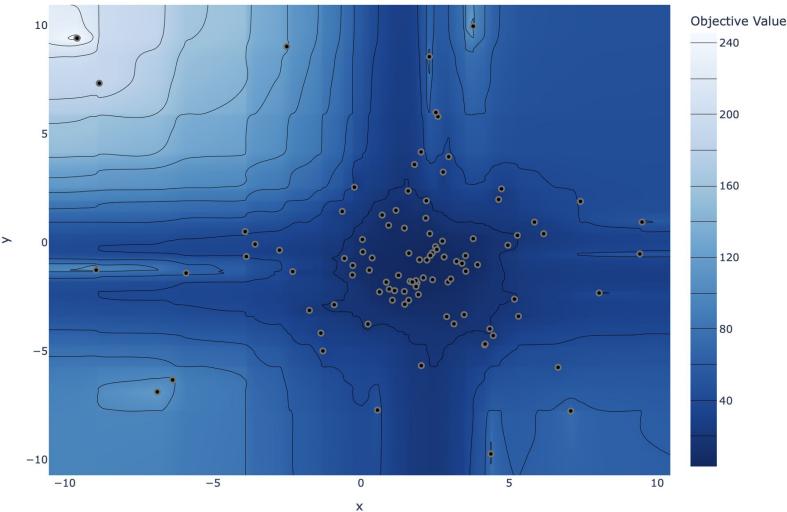
} Function to optimize
(usually a metric)

} Search space definition } Objective function
executes on each trial

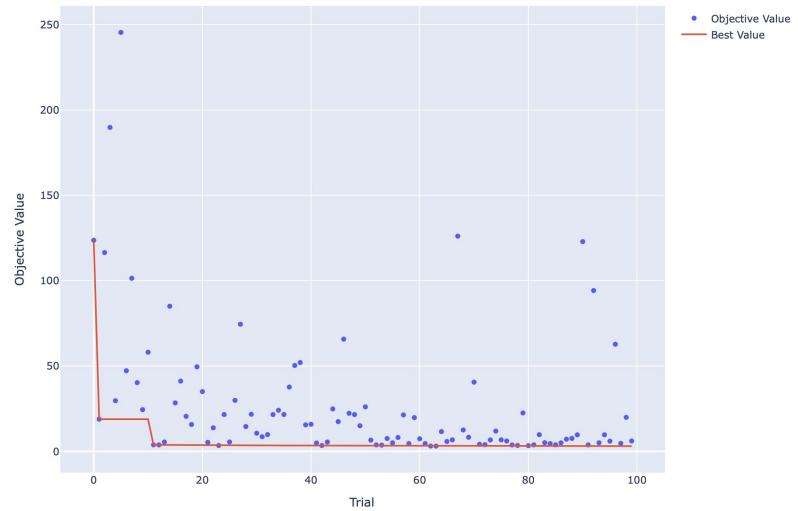
} Optimization algorithm
(sampler)

Example 3: Optuna

Contour Plot



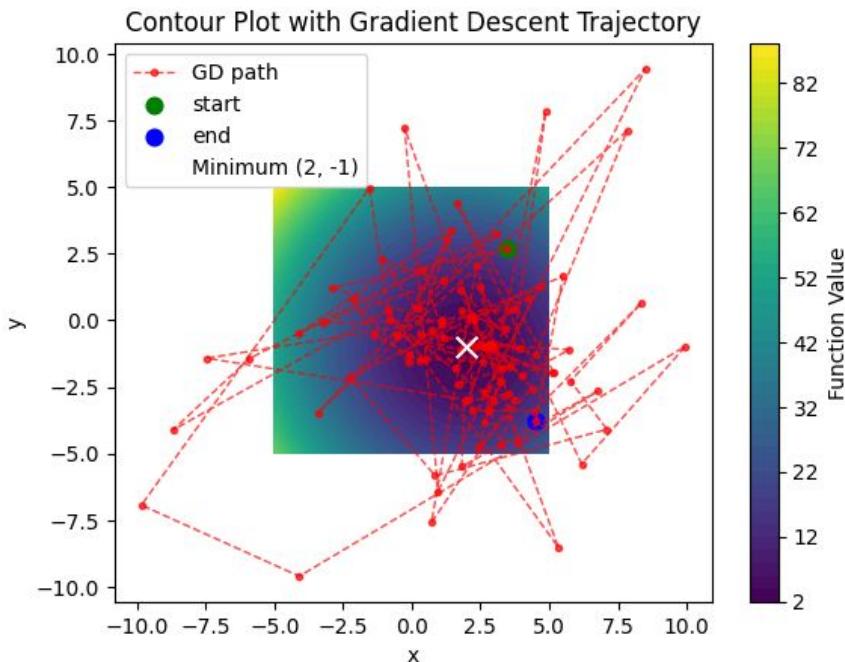
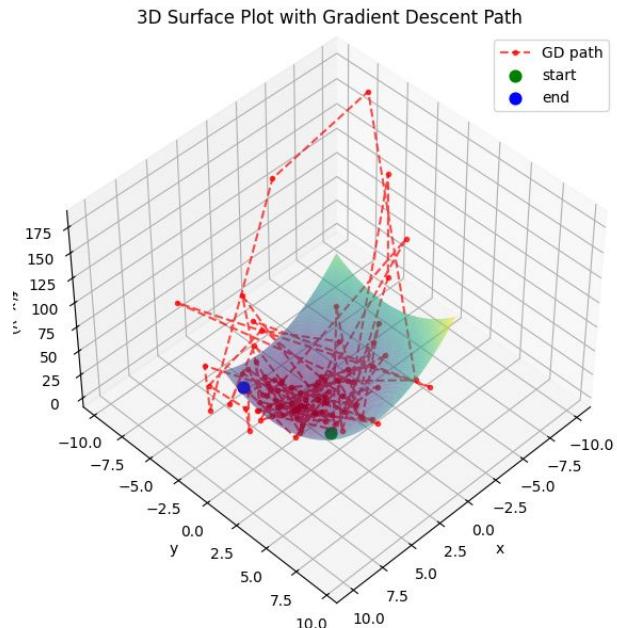
Optimization History Plot



Best parameters: {'x': 1.893938637086194, 'y': -1.0665190063871524}
 Best value: 3.0156737909138682
 Number of trials: 100 (good value after ~12 trials)

Example 3: Optuna

Minimum value of $f(x,y)$ is 3.0156737909138682 at $(x,y) = (1.893938637086194, -1.0665190063871524)$, with 100 trials.



python [example3.py](#)

Pythonic search spaces

```
import optuna

def objective(trial):
    # Categorical parameter
    optimizer = trial.suggest_categorical("optimizer", ["MomentumSGD", "Adam"])

    # Integer parameter
    num_layers = trial.suggest_int("num_layers", 1, 3)

    # Integer parameter (log)
    num_channels = trial.suggest_int("num_channels", 32, 512, log=True)

    # Integer parameter (discretized)
    num_units = trial.suggest_int("num_units", 10, 100, step=5)

    # Floating point parameter
    dropout_rate = trial.suggest_float("dropout_rate", 0.0, 1.0)

    # Floating point parameter (log)
    learning_rate = trial.suggest_float("learning_rate", 1e-5, 1e-2, log=True)

    # Floating point parameter (discretized)
    drop_path_rate = trial.suggest_float("drop_path_rate", 0.0, 1.0, step=0.1)
```

}

Categories

}

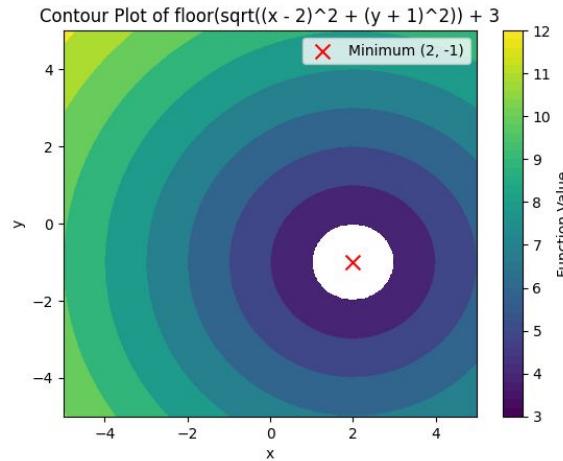
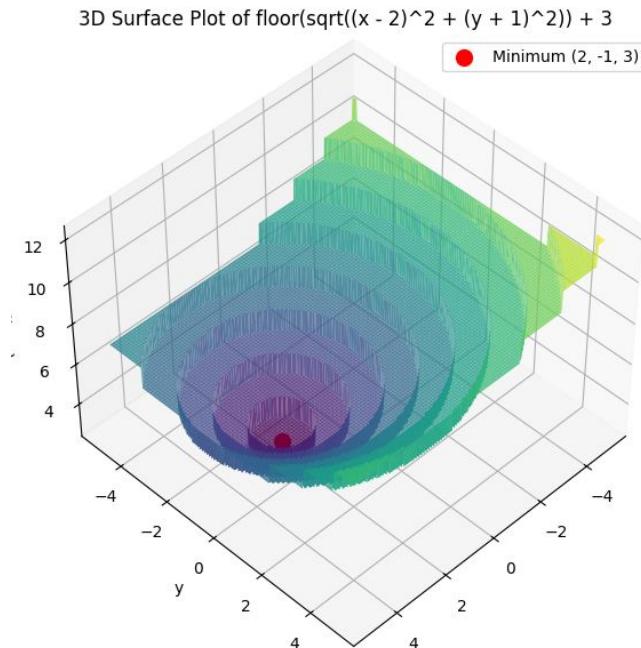
Integers

}

Floats

Why is optimization so hard?

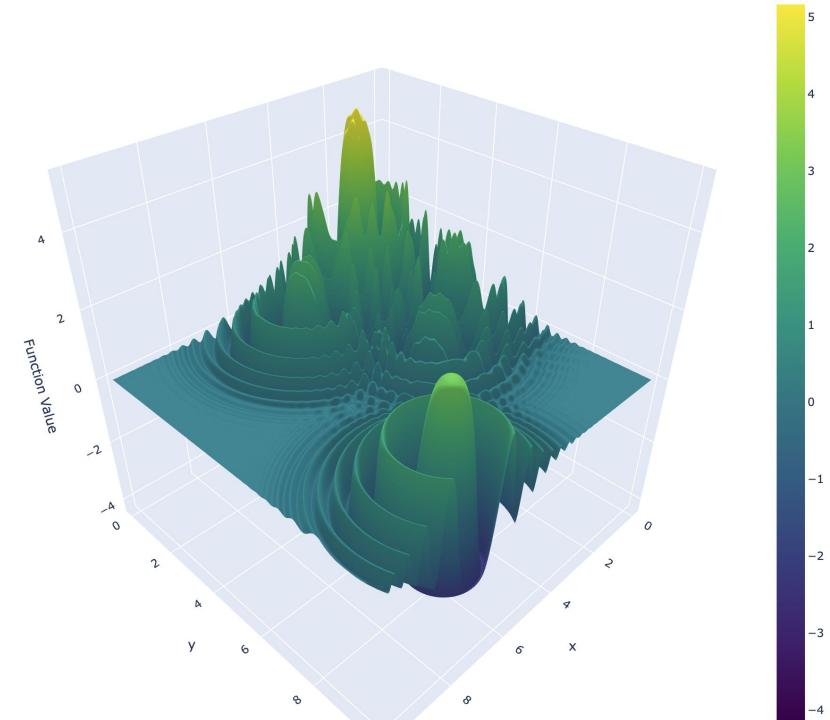
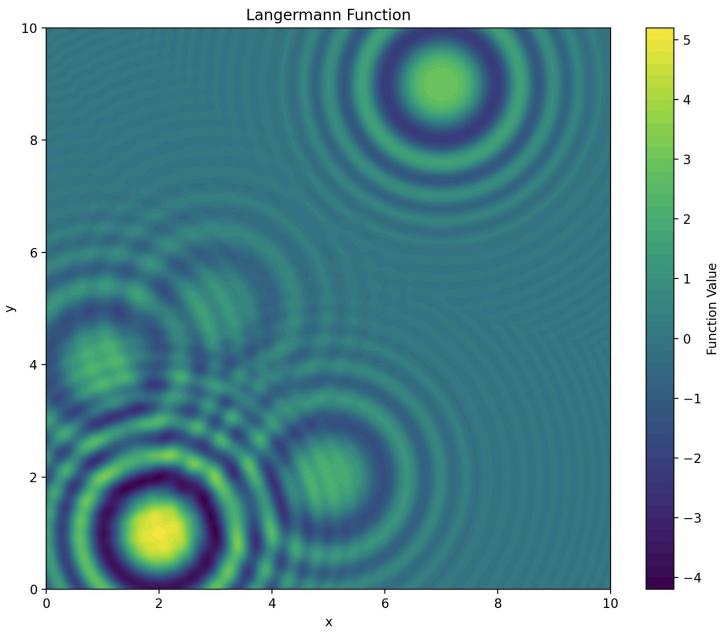
Noise and discontinuities in real data make harder to find a good solution.



python [example4.py](#)

Why is optimization so hard?

Algorithms tend to get stuck in local minima



python [example5.py](#)

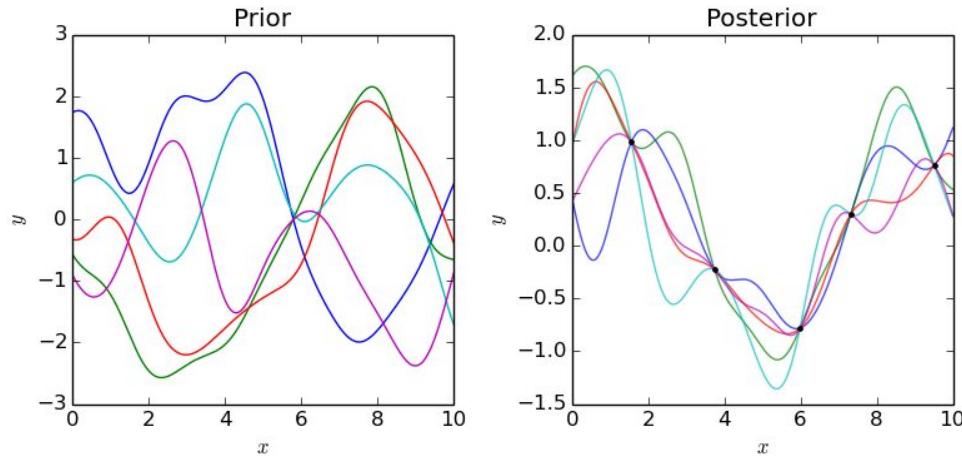
Search algorithms

Optuna provides the following sampling algorithms:

- Grid Search implemented in [GridSampler](#)
- Random Search implemented in [RandomSampler](#)
- **Tree-structured Parzen Estimator** algorithm implemented in [TPESampler \(default\)](#)
- CMA-ES based algorithm implemented in [CmaEsSampler](#)
- **Gaussian process-based algorithm** implemented in [GPSampler](#)
- Algorithm to enable partial fixed parameters implemented in [PartialFixedSampler](#)
- Nondominated Sorting Genetic Algorithm II implemented in [NSGAIISampler](#)
- A Quasi Monte Carlo sampling algorithm implemented in [QMCSampler](#)

Gaussian Processes

A Gaussian process is a probability distribution over possible functions that fit a set of points. We use it as surrogate $P(y|x)$ of the objective function $y=f(x)$.



$$P(\text{score}|\text{hyperparameters})$$

$$P(y|x)$$

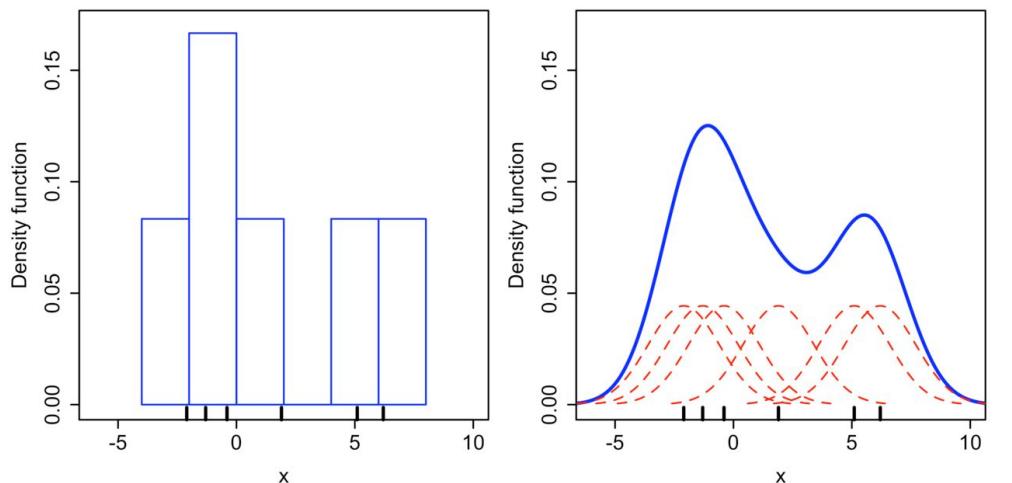


https://en.wikipedia.org/wiki/Gaussian_process

Tree Parzen Estimators

Tree ~ Decision ~ Good and Bad trials

Parzen = Kernel density estimation



$$\hat{f}_h(x) = \frac{1}{nh\sigma} \frac{1}{\sqrt{2\pi}} \sum_{i=1}^n \exp\left(\frac{-(x - x_i)^2}{2h^2\sigma^2}\right),$$



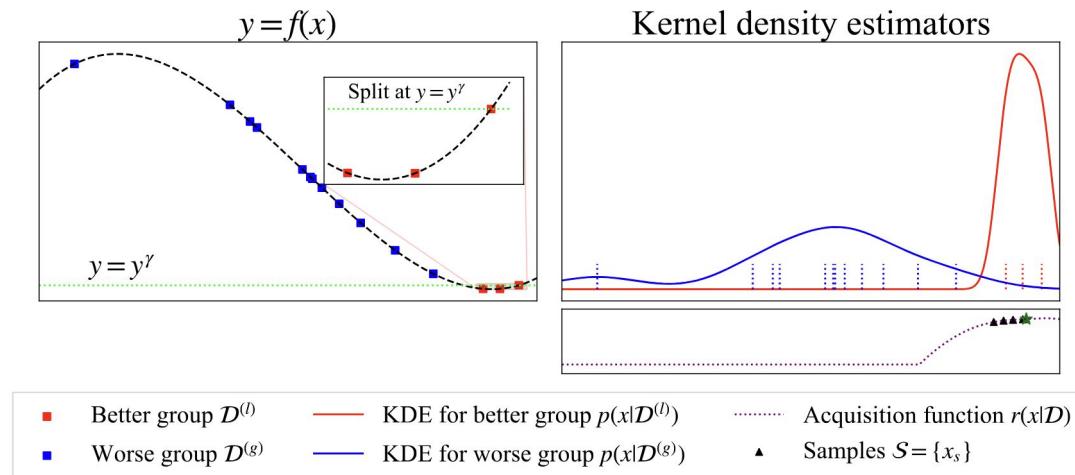
Tree Parzen Estimators

Tree = Decision tree ~ Good and Bad trials

Parzen = Kernel density estimation

It models likelihood with two distributions $P(\text{bad trial})$ and $P(\text{good trial})$

$y < y^*$ represents a lower value of the objective function than the threshold



$$P(x|y) = \begin{cases} l(x) & \text{if } y < y^* \\ g(x) & \text{if } y \geq y^* \end{cases} \quad \begin{matrix} \text{P(bad trial)} \\ \text{P(good trial)} \end{matrix}$$

Search algorithms

	TPESampler	GPSampler	CmaEsSampler	NSGAIISampler	NSGAIISampler	GridSampler
Float parameters	✓	✓	✓	▲	▲	✓
Integer parameters	✓	✓	✓	▲	▲	✓
Categorical parameters	✓	✓	▲	✓	✓	✓
Pruning	✓	▲	▲	✗ (▲ for single-objective)	✗ (▲ for single-objective)	✓
Multivariate optimization	✓	✓	✓	▲	▲	▲
Conditional search space	✓	▲	▲	▲	▲	▲
Multi-objective optimization	✓	✓	✗	✓ (▲ for single-objective)	✓ (▲ for single-objective)	✓
Batch optimization	✓	▲	✓	✓	✓	✓
Distributed optimization	✓	▲	✓	✓	✓	✓
Constrained optimization	✓	✓	✗	✓	✓	✗
Time complexity (per trial) (*)	$O(dn \log n)$	$O(n^3)$	$O(d^3)$	$O(mp^2)$ (***)	$O(mp^2)$ (***)	$O(dn)$
Recommended budgets (#trials) (**)	100–1000	-500	1000–10000	100–10000	100–10000	number of combinations

 Note

✓: Supports this feature. ▲: Works, but inefficiently. ✗: Causes an error, or has no interface.

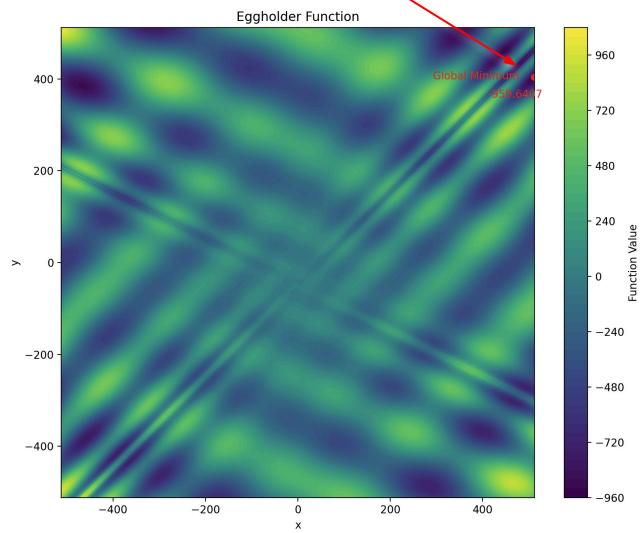
Hackathon

Eggholder function!

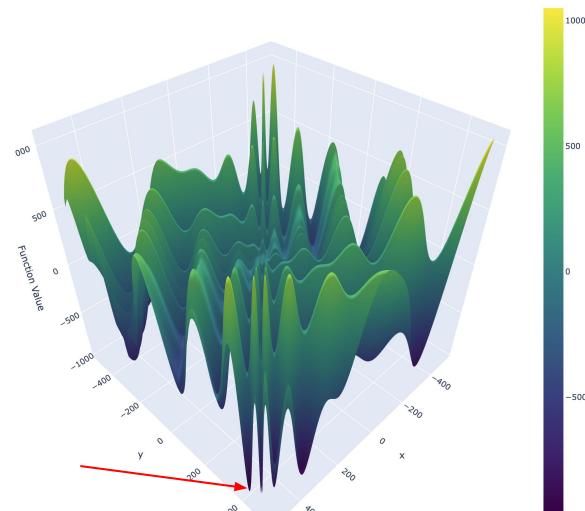
Optimization benchmark

$$f(x, y) = -(y + 47) \sin\left(\sqrt{\left|x + \frac{y}{2} + 47\right|}\right) - x \sin\left(\sqrt{|x - (y + 47)|}\right)$$

$$f(\mathbf{x}^*) = -959.6407, \text{ at } \mathbf{x}^* = (512, 404.2319)$$



Eggholder Function (3D)

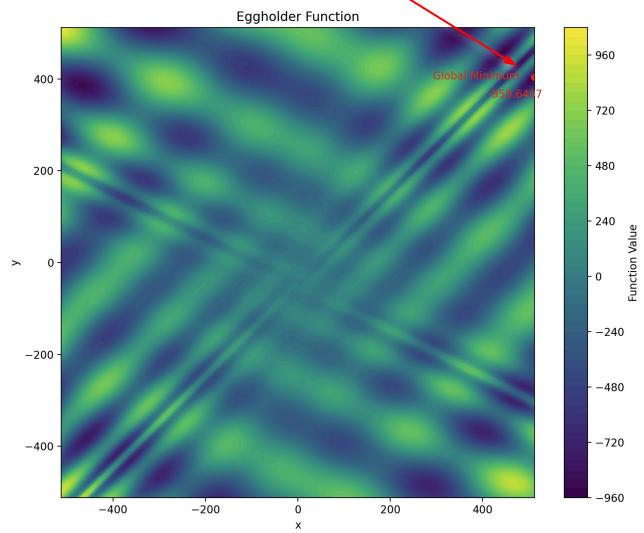


Competition

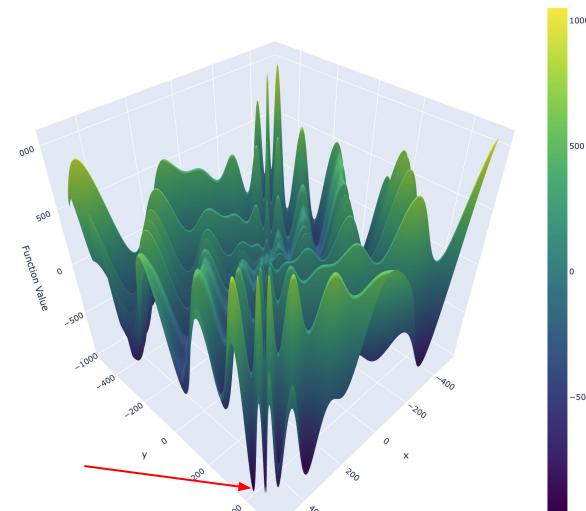
First one in publishing the closest solution (in Slack channel) will win a sweet treat!

$$f(x, y) = -(y + 47) \sin\left(\sqrt{\left|x + \frac{y}{2} + 47\right|}\right) - x \sin\left(\sqrt{|x - (y + 47)|}\right)$$

$f(\mathbf{x}^*) = -959.6407$, at $\mathbf{x}^* = (512, 404.2319)$



Eggholder Function (3D)



python [example6.py](#)

Competition snippets

First one in publishing the closest solution (in Slack channel) will win a sweet treat!

```

1 import numpy as np
2 import optuna
3
4 SEED = 42
5 np.random.seed(SEED) ←
6
7 # Define the Eggholder function
8 def eggholder(x, y):
9     return -(y + 47) * np.sin(np.sqrt(abs(x / 2 + (y + 47)))) - x * np.sin(np.sqrt(abs(x - (y + 47))))
10
11 # Define the objective function for Optuna
12 def objective(trial):
13     x = trial.suggest_int(..., ...) ←
14     y = trial.suggest_int(..., ...) ←
15     return eggholder(x, y)
16
17 # Create a study and optimize the objective function
18 # sampler = optuna.samplers.TPESampler(seed=SEED)
19 sampler = optuna.samplers.WBO # select sampler with seed=SEED
20 study = optuna.create_study(direction='minimize', sampler=sampler)
21 study.optimize(objective, n_trials=100) ←
22
23 # Get the best parameters and value
24 best_params = study.best_params
25 best_value = study.best_value
26
27 print(f"Best parameters: x = {best_params['x']}, y = {best_params['y']}")
28 print(f"Benchmark solution: x* = 512, y* = 404.2319")
29 print(f"Minimum value: {best_value}")
30 print(f"Benchmark solution: f(x*,y*)= -959.6407")
31 print(f"Difference f(x,y) with global optimum: {abs(-959.6407 - best_value)}")
```

👉 python [competition.py](#) 🤖

Needs to be reproducible!

Options search space ($x \in [-512, 512]$, $y \in [-512, 512]$):

trial.suggest_categorical()
for categorical parameters

trial.suggest_int()
for integer parameters

trial.suggest_float()
for floating point parameters

Options (try different samplers, include a seed):

<https://optuna.readthedocs.io/en/stable/reference/samplers>

Hyperparameter tuning in ML

Hyperparameter tuning in ML

```
### Optuna hyperparameter optimization
import optuna
import numpy as np
from sklearn.model_selection import cross_val_score, StratifiedKFold

SEED = 42
np.random.seed(SEED)

def objective(trial):
    scale = trial.suggest_categorical("scale", [True, False])
    n_layers = trial.suggest_int("n_layers", 1, 10)
    hidden = tuple(trial.suggest_int(f"n_units_{i}", 4, 128, log=True) for i in range(n_layers))
    activation = trial.suggest_categorical("activation", ["relu", "tanh", "logistic"])
    solver = trial.suggest_categorical("solver", ["adam", "sgd"])
    alpha = trial.suggest_float("alpha", 1e-6, 1e-2, log=True)
    learning_rate_init = trial.suggest_float("learning_rate_init", 1e-5, 1e-1, log=True)
    batch_size = trial.suggest_categorical("batch_size", [16, 32, 64])

    clf_trial = (make_pipeline(
        StandardScaler() if scale else None,
        MLPClassifier(
            hidden_layer_sizes=hidden,
            activation=activation,
            solver=solver,
            alpha=alpha,
            learning_rate_init=learning_rate_init,
            batch_size=batch_size,
            max_iter=2000,
            early_stopping=True,
            random_state=SEED
        )
    ))

    score = np.mean(cross_val_score(clf_trial, X_train, y_train, cv=3, scoring='accuracy'))
    return score

sampler = optuna.samplers.TPESampler(seed=SEED)
study = optuna.create_study(direction="maximize", sampler=sampler)
study.optimize(objective, n_trials=500)
```

Decide preprocessing options

Decide architecture
and training options

👉 python [example7.py](#) 🤖

👉 Visit https://optuna.org/#code_examples to check your ML

library

Model selection

```
def objective(trial):

    classifier_name = trial.suggest_categorical(
        "classifier",
        [
            "SVC",
            "NaiveBayes",
        ],
    )

    scale = trial.suggest_categorical("scale", [True, False])
    if classifier_name == "SVC":
        svc_c = trial.suggest_float("svc_c", 1e-10, 1e10, log=True)
        classifier_obj = sklearn.svm.SVC(C=svc_c, gamma="auto")

    elif classifier_name == "NaiveBayes":
        classifier_obj = sklearn.naive_bayes.GaussianNB()

    clf_pipeline = make_pipeline(StandardScaler() if scale else None, classifier_obj)

    score = cross_val_score(clf_pipeline, X_train, y_train, n_jobs=-1, cv=3)
    accuracy = score.mean()
    return accuracy
```

Suggest model type
as category



python example8.py



Multiobjective optimization

Multiobjective optimization

```

def objective(trial):
    # Suggest feature subset
    feature_mask = []
    for i in range(X.shape[1]):
        feature_mask.append(trial.suggest_categorical(f"feature_{i}", [True, False]))
    X_selected = X_train[:, feature_mask]
    number_of_features = sum(feature_mask)
    if X_selected.shape[1] == 0:
        return 0.0, number_of_features

    # Train and evaluate model
    clf = GaussianNB()
    score = cross_val_score(clf, X_selected, y_train, cv=5, scoring="accuracy")
    return score.mean(), number_of_features

# Create study (single-objective maximizing the combined metric)
sampler = optuna.samplers.TPESampler(seed=SEED)
study = optuna.create_study(directions=["maximize", "minimize"], sampler=sampler)

# Enqueue the first trial with ALL features selected
all_features_params = {f"feature_{i}": True for i in range(X.shape[1])}
study.enqueue_trial(all_features_params)

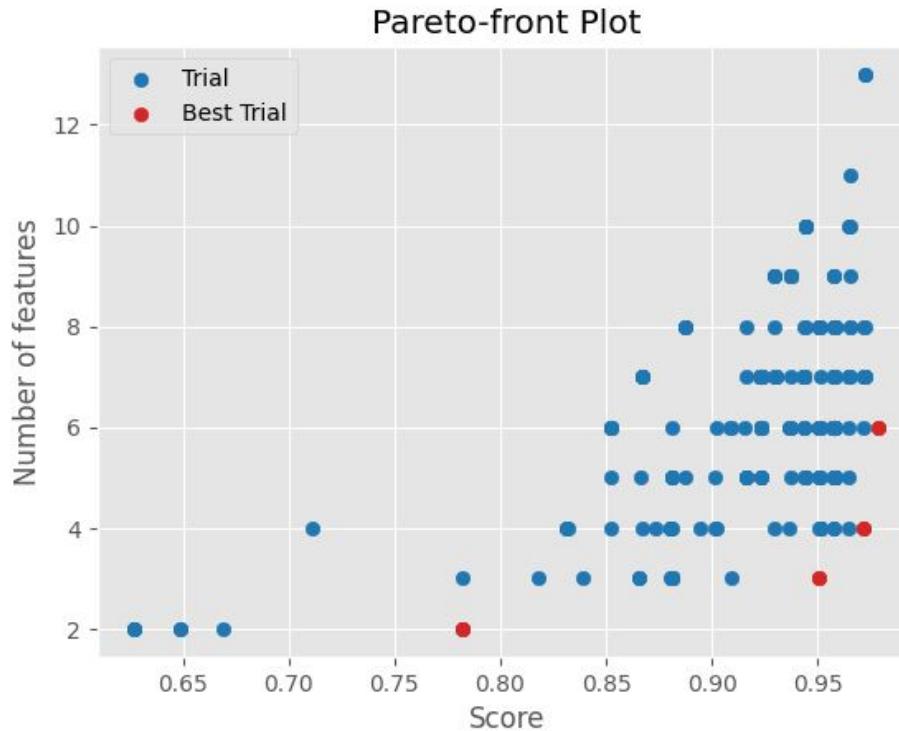
# Now optimize (this will run the enqueued trial first, then 99 more)
study.optimize(objective, n_trials=300)

```

Mask a feature subset

Important to try all features!!

Pareto front



Practical session

Practical session

1 Use BO to get a PERFECT! accuracy score in IRIS dataset. Try different models!

👉 https://scikit-learn.org/stable/supervised_learning.html

👉 python practical_session.py


To conclude...

More advanced features...

Parallelization (Problem with reproducibility)

Early stopping “Pruners”

Human-in-the-loop to validate trials using dashboard

Save models during optimization

Add constraints to the optimization

Save and resume studies

Ignore duplicate samples

Handle exceptions/errors during trials

References

Webpapers & papers

[A Conceptual Explanation of Bayesian Hyperparameter Optimization for Machine Learning](#). Will Koehrsen. Medium. 2018

1. Algorithms for Hyper-Parameter Optimization [[Link](#)]
2. Making a Science of Model Search:
Hyperparameter Optimization in Hundreds of Dimensions for Vision Architectures [[Link](#)]
3. Bayesian Optimization Primer [[Link](#)]
4. Taking the Human Out of the Loop: A Review of Bayesian Optimization [[Link](#)]

Optimization benchmarks

<https://www.sfu.ca/~ssurjano/egg.html>

OPTUNA

<https://optuna.readthedocs.io/en/stable/index.html>

<https://optuna.readthedocs.io/en/stable/tutorial/index.html>

Gaussian Processes

<https://distill.pub/2019/visual-exploration-gaussian-processes/>

<https://thegradient.pub/gaussian-process-not-quite-for-dummies/>

TPEs

https://en.wikipedia.org/wiki/Kernel_density_estimation

<https://arxiv.org/abs/2304.11127>

Multiobjective optimization

<https://medium.com/optuna/optuna-v4-5-81e78d8e077a>