Data Mining 2

Topic 04 : Hyperparameter Tuning

Lecture 02 : Hyperparameter Tuning

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Spring Semester, 2021

Outline

- Standard Techniques - Grid vs Random Search
- Bayesian optimisation - hyperopt and Scikit-Optimize

Recap of where we are (were from previous lecture)

- Given a pipeline / model we "can" tune each of the hyperparameters by constructing a validation curve.
- Problems . . . (manual approach is not practical anything but small problems)
  - Can have a huge (100s – 1,000s) number of parameters.
  - A sequence of 1-dimensional searches is not the same as one d-dimensional search — interplay between hyper-parameters.
- Approaches / Techniques . . .
  - Grid Search — Systematic, regular, predetermined deterministic sample of parameter space.
  - Random Search — Non-adaptive, random sample of parameter space.
  - Bayesian Search — Adaptive, random sample of parameter space.

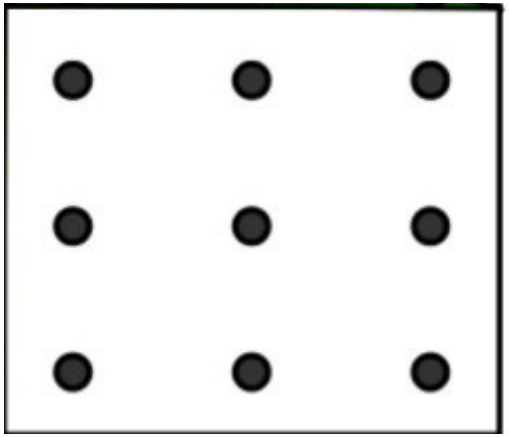
Grid Search

Validation curves are important but examining at each parameter individually is time consuming and does not take into account interactions between parameters — in effect it is a series of 1D semi-manual searches.

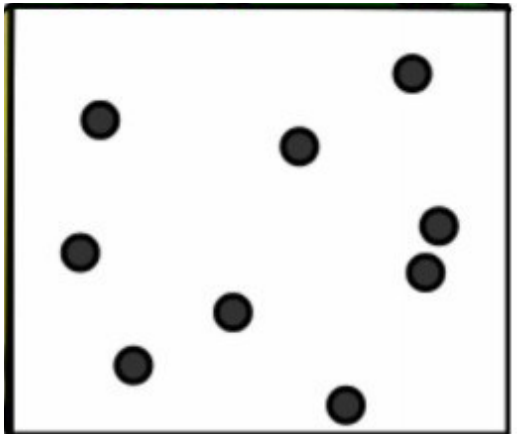
Grid Search

Try all available parameters combinations, 1 by 1, and choose the one with the best cross validation results.

Grid Search



Random Search



Grid Search (`sklearn.model_selection.GridSearchCV`)

Grid Search

Try all available parameters combinations, 1 by 1, and choose the one with the best cross validation results.

Drawbacks

- Still very slow — trying ALL combinations of ALL parameters with no modification of search based on results found to date.
- ALL combinations $\Longrightarrow$ every additional hyperparameter to vary multiplies the number of iterations you need to complete.
- It can work only with discrete values.

  If the global optimum is on `n_estimators=550`, but you are doing `GridSearchCV` from 100 to 1000 with step 100, you will never reach the optimal point.

Stratagies

- You need know / guess the approximate region of the optimum to start.
- To mitigate against drawbacks, do multiple lower dimensional grid searches, or repeat search with narrower grids and smaller step sizes.

Grid Search Example 1 I

```
from sklearn.svm import SVC
from sklearn.model_selection import GridSearchCV
pipeline = Pipeline([
    ('scl', StandardScaler()),
    ('clf', SVC(random_state=SEED))])

param_range = np.logspace(-4,4,10)
param_grid = [{
    'clf__gamma': param_range,
    'clf__C': param_range,
    'clf__kernel': ['rbf']
}]
gs = GridSearchCV(estimator=pipeline,
    return_train_score=True,
    param_grid=param_grid, scoring='accuracy', cv=10, n_jobs=-1)
```

- Switched from LogisticRegression to SVM — more hyperparameters to tweak.
- How many parameter combinations were generated/used?

Grid Search Example 1 II

To perform grid search, we call the `fit` method as usual ...

```
gs = gs.fit(X_train, y_train)
print(gs.best_score_)
print(gs.best_params_)
```

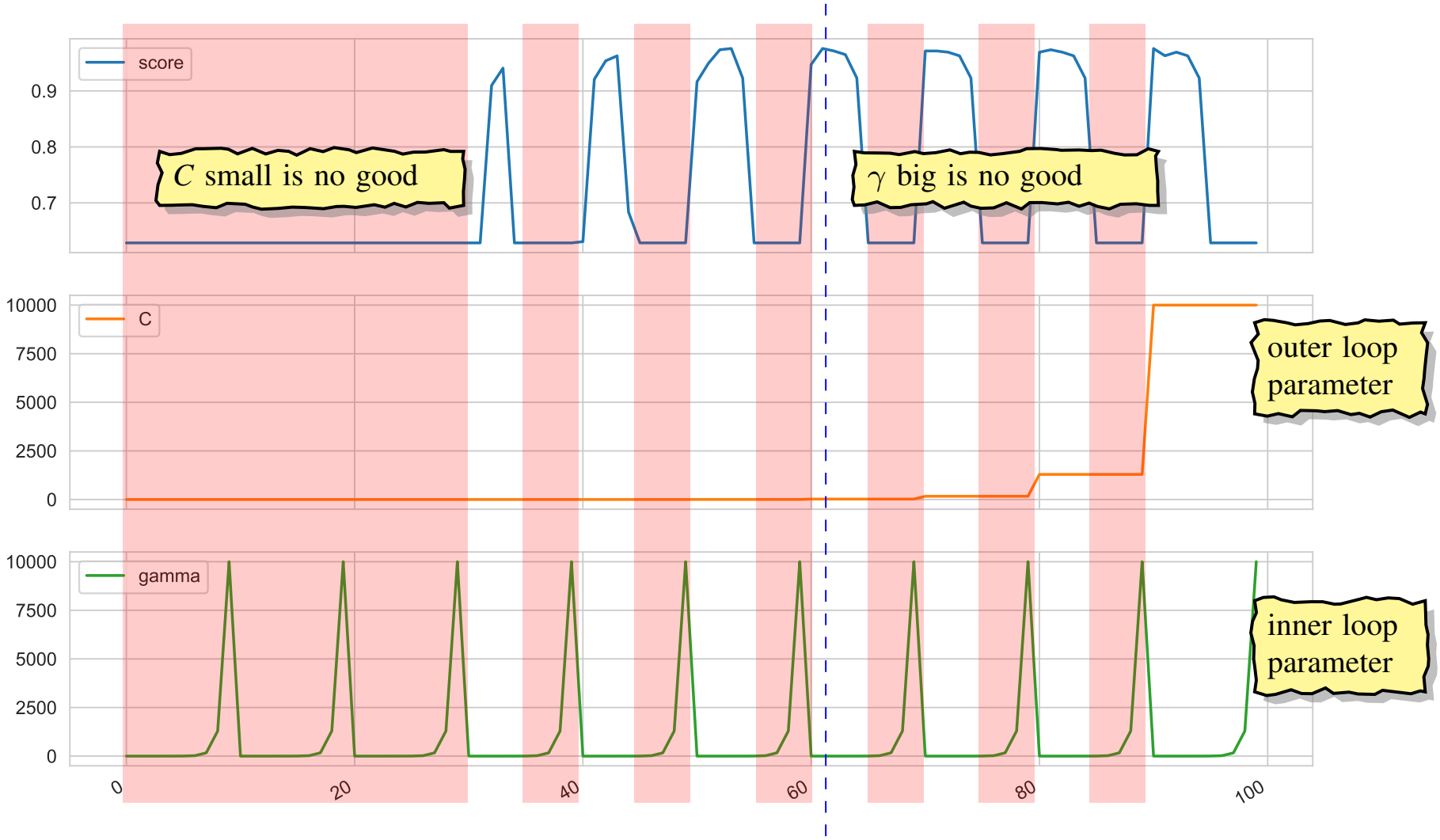
```
0.9757971014492753
{'clf__C': 2.782559402207126, 'clf__gamma': 0.046415888336127774, 'clf__kernel': 'rbf'}
```

- CV score improved from 0.971 with default parameter values to 0.978.
- `GridSearchCV` with option `return_train_score=True`, returns results of each combination — determine effect of hyperparameters to refine grid search.

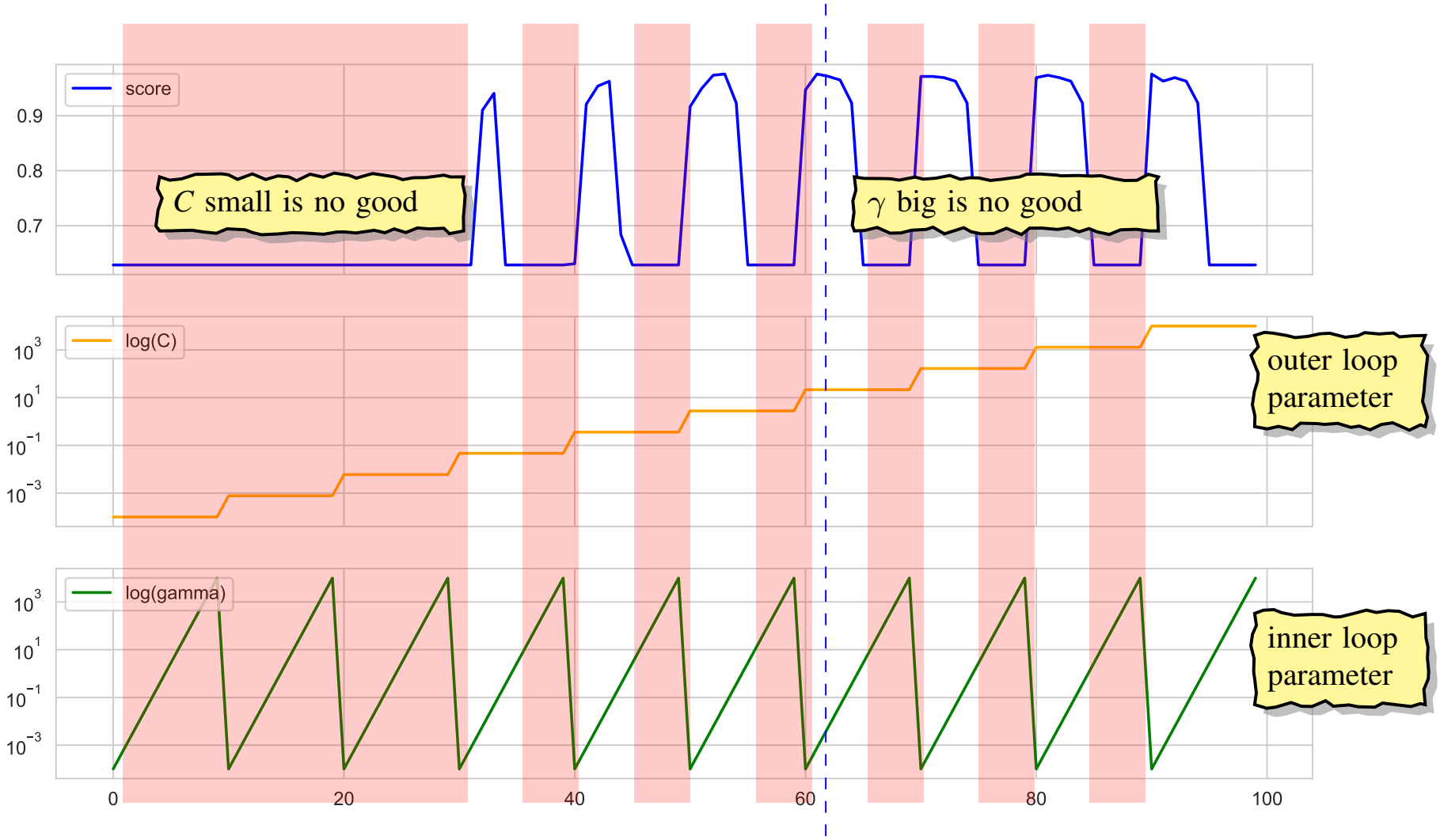
```
df_gs = pd.DataFrame(np.transpose([
    gs.cv_results_["mean_test_score"],
    gs.cv_results_["param_clf__C"].data,
    gs.cv_results_["param_clf__gamma"].data]),
    columns=['score', 'C', 'gamma'])

df_gs.plot(subplots=True,figsize=(12, 8))
plt.savefig("gs__svm__C_gamma.pdf", bbox_inches="tight")
plt.show()
```

Grid Search Example 1 ($C = 10$, $\gamma = 0.01$)



Grid Search Example 1 ($C = 10$, $\gamma = 0.01$) (Using log scales) III



Grid Search Example 2

GridSearch can accept a list of dictionaries so that incompatible hyperparameter combinations can still be searched. For example, different SVM kernels have different parameters:

```
pipeline = Pipeline([
    ('scl', StandardScaler()),
    ('clf', SVC(random_state=SEED))
])

from sklearn.model_selection import GridSearchCV
param_range = [0.0001, 0.001, 0.01, 0.1, 1.0, 10.0, 100.0, 1000.0]
param_grid = [
    {
        'clf__C': param_range,
        'clf__kernel': ['linear']
    },
    {
        'clf__gamma': param_range,
        'clf__C': param_range,
        'clf__kernel': ['rbf']
    }
]
```

```
0.9780676328502415
{'clf__C': 545.5594781168514, 'clf__gamma': 0.0001}
```

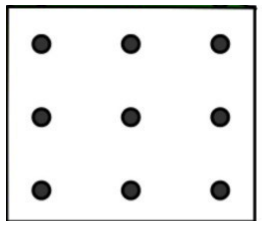
- How many hyperparameter combinations are now generated?

Random Search

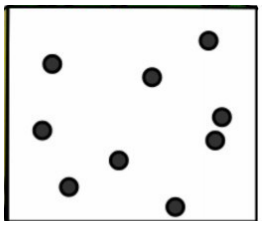
Random Search

Try random hyperparameter combinations and choose the one with the best cross validation results.

Grid Search



Random Search



Advantages

- On every step random search varies all parameters $\Rightarrow$ doesn't spend time on meaningless parameters.
- On average finds near optimal parameters much faster than Grid search.
- It is not limited by grid when optimising continuous parameters.

Disadvantages

- It may not find the global optimal parameter on a grid.
- All steps are independent. Does not use information about the results gathered to inform search.

Random Search I

```
pipeline = Pipeline([
    ('scl', StandardScaler()),
    ('clf', SVC(kernel='rbf', random_state=SEED))
])

from sklearn.model_selection import RandomizedSearchCV
from scipy.stats import randint

param_range = np.logspace(-4,4,20)

param_grid = {'clf__C': param_range,
              'clf__gamma': param_range}

rs = RandomizedSearchCV(estimator=pipeline,
    param_distributions=param_grid,
    n_iter = 100, random_state=SEED,
    return_train_score=True,
    scoring='accuracy', cv=10, n_jobs=-1)
```

- This is the same setup as used in GridSearch but doubled the number of parameter values in both C and γ, so search space is 400 points (not 100). Sampling 100 points.

Random Search Example II

To perform grid search, we call the `fit` method as usual ...

```
rs.fit(X_train, y_train)
print(rs.best_score_)
print(rs.best_params_)
```

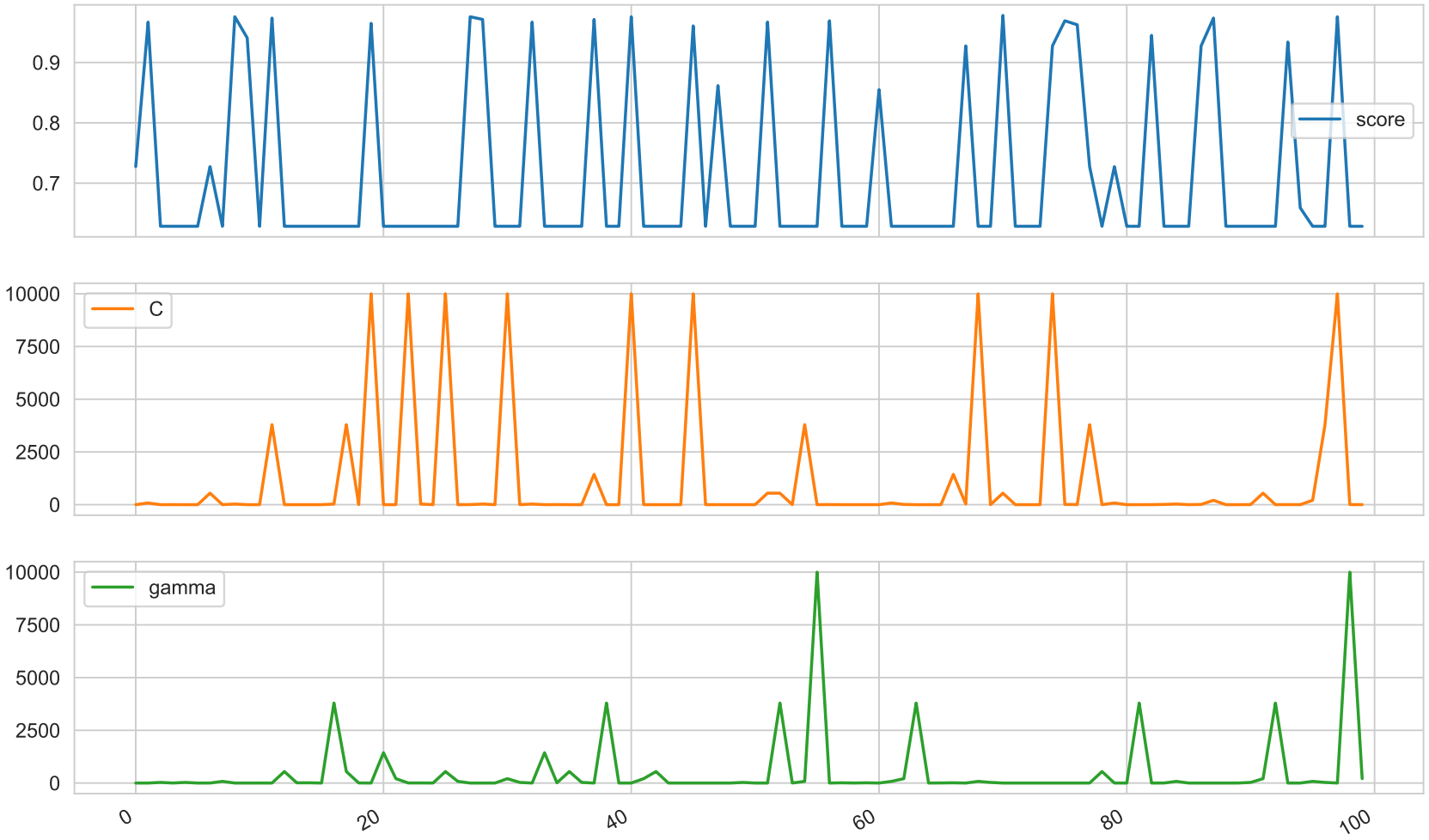
```
0.9780676328502415
{'clf__gamma': 0.0001, 'clf__C': 545.5594781168514}
```

- Sampling half the number of points (50) in a search space 4 times larger, RandomSearch outperforms GridSearch.

```
df_rs = pd.DataFrame(np.transpose([
    rs.cv_results_["mean_test_score"],
    rs.cv_results_["param_clf__C"].data,
    rs.cv_results_["param_clf__gamma"].data]),
    columns=['score', 'C', 'gamma'])

df_rs.plot(subplots=True,figsize=(12, 8))
plt.savefig("rs__example_1.pdf", bbox_inches="tight")
plt.show()
```

Random Search Example ($C = 10000$, $\gamma = 0.0002636$) III



Every step is completely random. $\Rightarrow$ does not spent time on useless parameters, but does not use the information gathered on the first steps to improve outcomes of the latter ones.

The Problem

Both GridSearch and RandomSearch ignore information gained during the search, by using such information can searches improve?

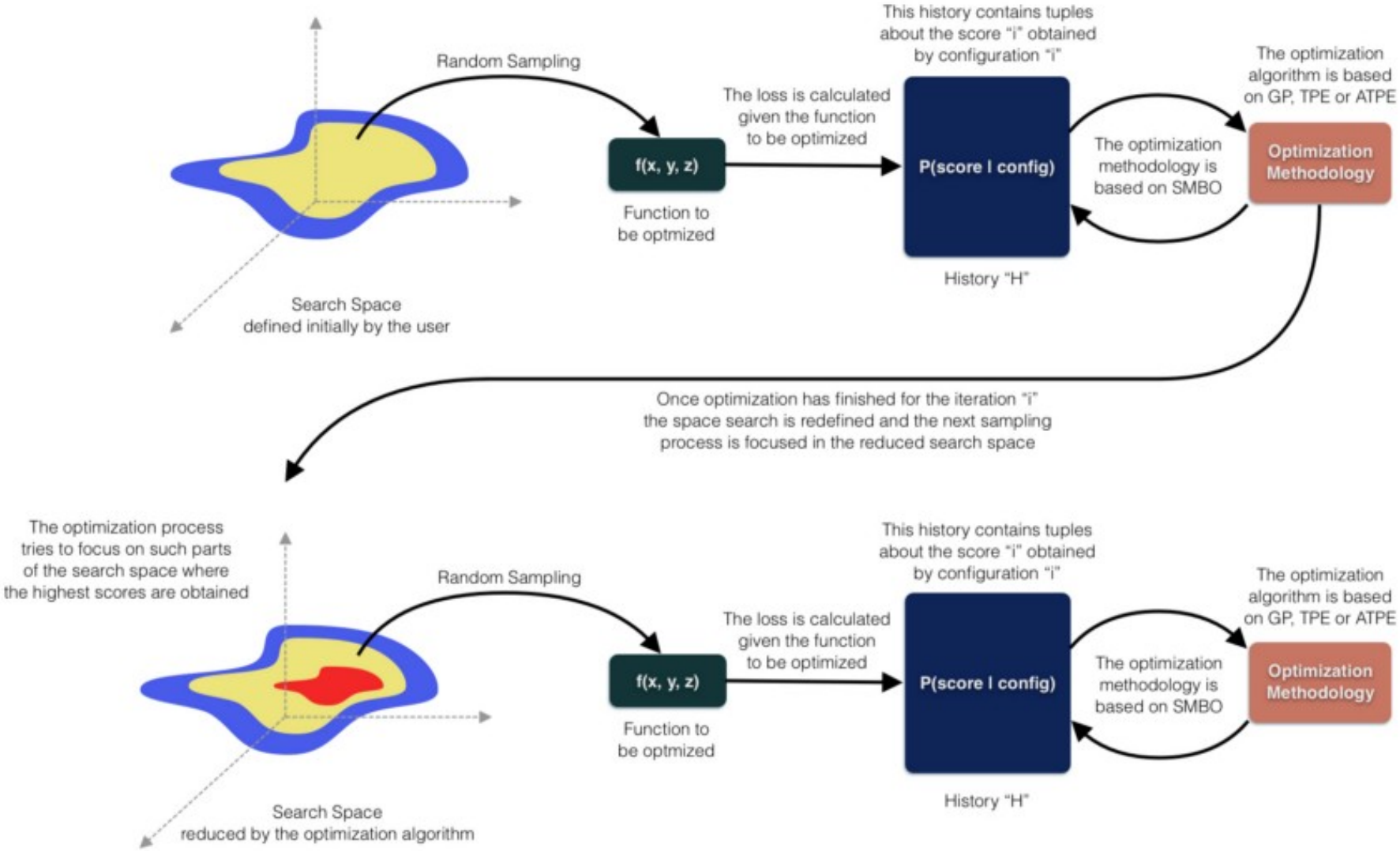
- What information would be useful?
  - Function value
  - Function derivative (gradient) — gives direction in which the function is decreasing (locally).
- Why should we do this?
  - It seems reasonable that lower function values would be clustered — so focus search near best function values found to date.
  - Making multiple decisions based on local information could locate global minimum.
- What can go wrong?
  - Multiple local minimum — can get stuck in a side valley.
    - There will be situations in which we should make decisions against current function value information — see Simulated Annealing.
  - Gradient could be flat (so no direction to go in), or worse almost flat (some algorithms become unstable), or non-existent.

Bayesian Optimisation

Sequential model-based optimisation (SMBO)
(also known as Bayesian optimisation) is a general technique for function optimisation that uses information from earlier function evaluations to refine the optimisation search — with the aim of minimising number of function calls.

- For sufficiently complex functions, SMBO are some of the most call-efficient (in terms of function evaluations) optimisation methods currently available.
- Compared with standard optimisation strategies such as conjugate gradient descent methods, model-based optimisation algorithms invest more time between function evaluations in order to reduce the number of function evaluations overall.
- Takes advantage of smoothness without analytic gradient.
- Supports real-valued, discrete, and conditional variables.
- Performs relatively will in high dimensions —- hundreds of variables, even with budget of just a few hundred function evaluations, i.e., number of function calls is $\mathcal{O}(\text{dimensions})$ not $\mathcal{O}(e^{\text{dimensions}})$.

Sequential model-based optimisation (in HyperOpt)



Hyperopt

Hyperopt: Distributed Asynchronous Hyper-parameter Optimisation

- Python library for optimising over awkward search spaces with real-valued, discrete, and conditional dimensions.

github.com/hyperopt/hyperopt

- Install (Anaconda) or use pip

```
conda install -cy conda-forge hyperopt
```

- Supports parallel evaluation
  - Uses MongoDB to share results of functions evaluations..

hyperopt-sklearn

- Hyperopt-based model selection algorithms in scikit-learn

github.com/hyperopt/hyperopt-sklearn

- Install using pip.

> Purpose of hyperopt is not to always to completely optimise the search space but simply to do better than people.
>
> — J Bergstra, SciPy 2013

Resources

- Tune Hyperparameters for Classification Machine Learning Algorithms
  machinelearningmastery.com/
  hyperparameters-for-classification-machine-learning-algorithms/
  List of important hyper-parameters for skilearn classifiers

- Hyperopt: A Python Library for Optimizing the Hyperparameters of Machine Learning Algorithms
  conference.scipy.org/proceedings/scipy2013/pdfs/bergstra_hyperopt.pdf
  SCIPY Conference 2013 Paper

- A Conceptual Explanation of Bayesian Hyperparameter Optimization for Machine Learning
  towardsdatascience.com/
  a-conceptual-explanation-of-bayesian-model-based-hyperparameter-optimization-for-machir
  Relatively high level comparison of hyper-parameter tuning approaches.