Introduction to Numerical Optimization

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estimagic

Installation

We assume you have done the following

- Installed miniconda or anaconda
- Executed:

```
git clone https://github.com/OpenSourceEconomics/euroscipy-estimagic.git
cd euroscipy-estimagic
conda env create -f environment.yml
conda activate euroscipy-estimagic
```

- If you haven't done so, please do so until the first practice session
- Details: https://github.com/OpenSourceEconomics/euroscipy-estimagic

About Us

- Website: janosg.com
- GitHub: janosg
- Started estimagic in 2019
- Postdoc in Econ, University of Bonn
- Open for interesting jobs

- Website: tmensinger.com
- GitHub: timmens
- estimagic core contributor
- PhD student in Econ, University of Bonn

Sections

1. Introduction to **scipy.optimize**
2. Introduction to **estimagic**
3. Choosing algorithms
4. Bounds and constraints
5. Global optimization

Structure of each topic

1. Summary of exercise you will solve
2. Some theory
3. Syntax in very simplified example
4. You solve a more difficult example in a notebook
5. Discuss one possible solution

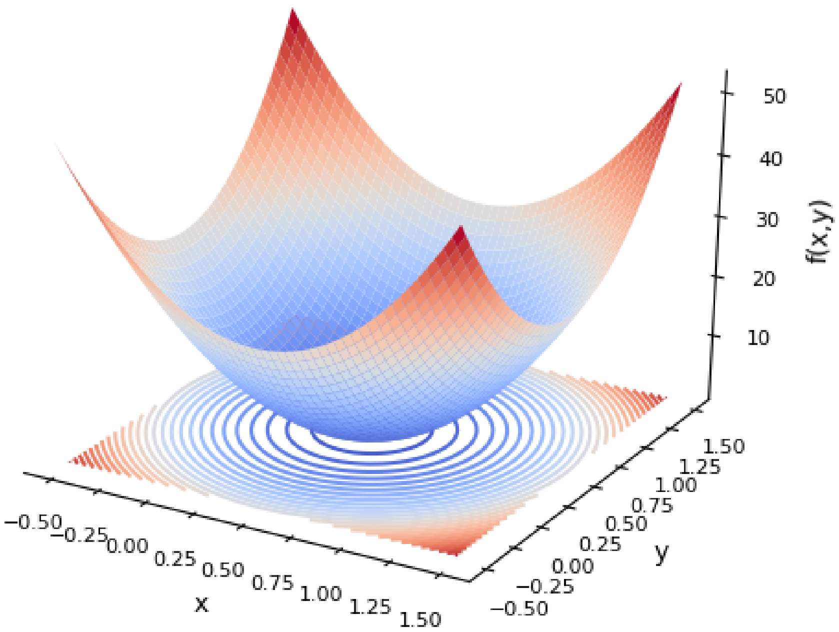
Introduction to scipy.optimize

Preview of practice session

- Translate a criterion function from math to code
- Use **scipy.optimize** to minimize the criterion function

Example problem

- **Criterion** $f(a,b) = a^2 + b^2$
- Parameters a, b
- Want: $a^*, b^* = \text{argmin} f(a,b)$
- Possible extensions:
  - Constraints
  - Bounds
- Optimum at $a^* = 0, b^* = 0$, $f(a^*, b^*) = 0$



Optimization with scipy.optimize

```
>>> import numpy as np
>>> from scipy.optimize import minimize

>>> def sphere(x):
        a, b = x
...     return a ** 2 + b ** 2

>>> x0 = np.ones(2)
>>> res = minimize(sphere, x0)
>>> res.fun
0.0
>>> res.x
array([0.0, 0.0])
```

Features of scipy.optimize

- **minimize** as unified interface to 14 local optimizers
  - some support bounds
  - some support constraints
- Parameters are 1d arrays
- Maximize by minimizing $-f(x)$
- Different interfaces for:
  - global optimization
  - nonlinear least-squares

Practice Session

First optimization with scipy.optimize (15 min)

Pros

- Very mature and reliable
- No additional dependencies
- Low overhead
- Enough algorithms for many use-cases

Cons

- Relatively few algorithms
- No parallelization
- Maximization via sign flipping
- Feedback only at end
- No feedback in case of crash
- Parameters are flat arrays

Examples from real projects I

```
>>> scipy.optimize.minimize(func, x0)
---------------------------------------------------------------------------
LinAlgError                               Traceback (most recent call last)
<ipython-input-17-7459e5b4d8d4> in <module>
----> 1 scipy.optimize.minimize(func, x0)

     95
     96 def _raise_linalgerror_singular(err, flag):
---> 97     raise LinAlgError("Singular matrix")
     98

LinAlgError: Singular matrix
```

- After 5 hours and with no additional information

Examples from real projects II

```python
def parse_parameters(x):
    """Parse the parameter vector into quantities we need."""
    num_types = int(len(x[54:]) / 6) + 1
    params = {
        'delta': x[0:1],
        'level': x[1:2],
        'coeffs_common': x[2:4],
        'coeffs_a': x[4:19],
        'coeffs_b': x[19:34],
        'coeffs_edu': x[34:41],
        'coeffs_home': x[41:44],
        'type_shares': x[44:44 + (num_types - 1) * 2],
        'type_shifts': x[44 + (num_types - 1) * 2:]
    }
    return params
```

Examples from real projects III

```
cindw = pvec[23]
cindp = pvec[24]
czcap = pvec[25]
cfc = pvec[27]
crpi = pvec[27]
crr = pvec[28]
cry = pvec[29]
```

Joshua Brault
@JoshuaBrault3

Also, in the model solution (modelsol.R) the authors parameterize the fixed cost share and the Taylor rule inflation feedback parameter to the same thing. This is obviously a typo as cfc should be parameter 26 in the vector. I have no idea how this impacts their results.

dajmcdon initial commit | Latest commit 28d7874 on Mar 29, 2021 | History

1 contributor

754 lines (653 sloc) | 22.6 KB | Raw | Blame

```
gensolution <- function(pvec) {
  ## Function takes in a lengthy vector of parameters and returns matrices nearly ready for Kalman input
  stderr.ea = pvec[1]
  stderr.eb = pvec[2]
  stderr.eg = pvec[3]
  stderr.eqs = pvec[4]
  stderr.em = pvec[5]
  stderr.epinf = pvec[6]
  stderr.ew = pvec[7]
    ##
  crhoa = pvec[8]
  crhob = pvec[9]
  crhog = pvec[10]
    crhoqs = pvec[11]
    crhoms = pvec[12]
    crhopinf = pvec[13]
    crhow = pvec[14]
    cmap = pvec[15]
    cmaw = pvec[16]
    csadjcost = pvec[17]
    csigma = pvec[18]
    chabb = pvec[19]
    cprobw = pvec[20]
    csigl = pvec[21]
    cprobp = pvec[22]
    cindw = pvec[23]
    cindp = pvec[24]
    czcap = pvec[25]
    cfc = pvec[27]
    crpi = pvec[27]
    crr = pvec[28]
    cry = pvec[29]
```

Introduction to estimagic

Preview of practice session

- Translate a **scipy** optimization to **estimagic.minimize**
- Use dictionaries instead of flat arrays as parameters in the optimization
- Plot the optimization history (criterion and parameter)

What is estimagic?

estimagic

- Library for numerical optimization
- Tools for nonlinear estimation and inference
- Harmonized interface to:
  - Scipy, Nlopt, TAO, Pygmo, …
- Adds functionality and convenience

You can use it like scipy

```python
>>> import estimagic as em
>>> def sphere(x):
        a, b = x
...     return a ** 2 + b ** 2

>>> res = em.minimize(
...      criterion=sphere,
...      params=np.ones(2),
...      algorithm="scipy_lbfgsb",
... )

>>> res.params
array([ 0., 0])
```

- No default algorithm
- Options have different names

Params can be (almost) anything

```
>>> params = {"a": 0, "b": 1, "c": pd.Series([2, 3, 4])}
>>> def dict_sphere(x):
...     out = (
...         x["a"] ** 2 + x["b"] ** 2 + (x["c"] ** 2).sum()
...     )
...     return out

>>> res = em.minimize(
...     criterion=dict_sphere,
...     params=params,
...     algorithm="scipy_neldermead",
... )

>>> res.params
{'a': 0.,
 'b': 0.,
 'c': 0    0.
      1    0.
      2    0.
 dtype: float64}
```

- numpy arrays
- pd.Series, pd.DataFrame
- scalars
- (Nested) lists, dicts and tuples thereof
- Special case: DataFrame with columns **"value"**, **"lower_bound"** and **"upper_bound"**

OptimizeResult

```
>>> res
Minimize with 5 free parameters terminated successfully after 805 criterion evaluations and 507 iterations.

The value of criterion improved from 30.0 to 1.6760003634613059e-16.

The scipy_neldermead algorithm reported: Optimization terminated successfully.

Independent of the convergence criteria used by scipy_neldermead, the strength of convergence can be
assessed by the following criteria:
                             one_step     five_steps
relative_criterion_change  1.968e-15***  2.746e-15***
relative_params_change     9.834e-08*    1.525e-07*
absolute_criterion_change  1.968e-16***  2.746e-16***
absolute_params_change     9.834e-09**   1.525e-08*

(***: change ≤ 1e-10, **: change ≤ 1e-8, *: change ≤ 1e-5. Change refers to a change between accepted
steps. The first column only considers the last step. The second column considers the last five steps.)
```

Access OptimizeResult's attributes

```
>>> res.criterion
.0
>>> res.n_criterion_evaluations
805
>>> res.success
True
>>> res.message
'Optimization terminated successfully.'
>>> res.history.keys():
dict_keys(['params', 'criterion', 'runtime'])
```

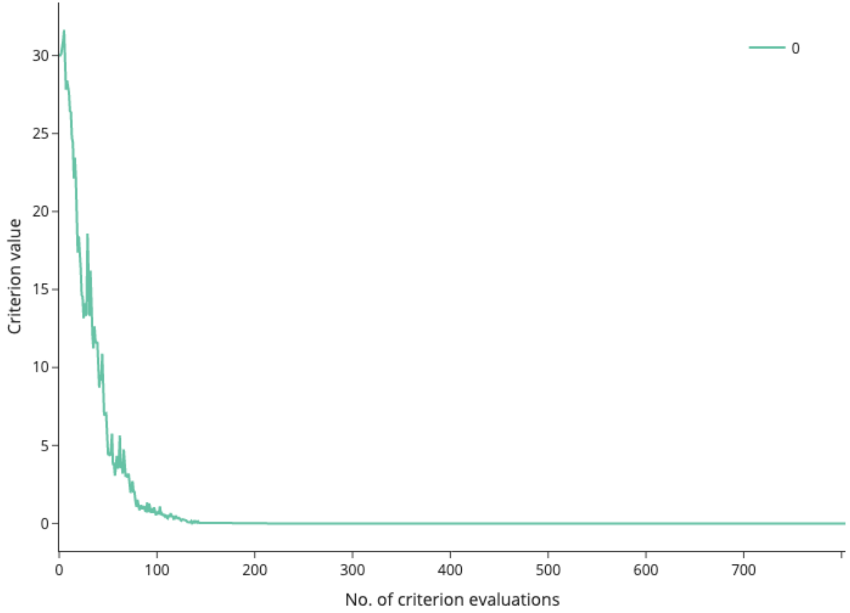
Logging and Dashboard

```
>>> res = em.minimize(
...     criterion=sphere,
...     params=np.arange(5),
...     algorithm="scipy_lbfgsb",
...     logging="my_log.db",
... )

>>> from estimagic import OptimizeLogReader

>>> reader = OptimizeLogReader("my_log.db")
>>> reader.read_history().keys()
dict_keys(['params', 'criterion', 'runtime'])

>>> reader.read_iteration(1)["params"]
array([0., 0.817, 1.635, 2.452, 3.27 ])
```

- Persistent log in sqlite database
- No data loss ever
- Can be read during optimization
- Provides data for dashboard
- No SQL knowledge needed

Criterion plot

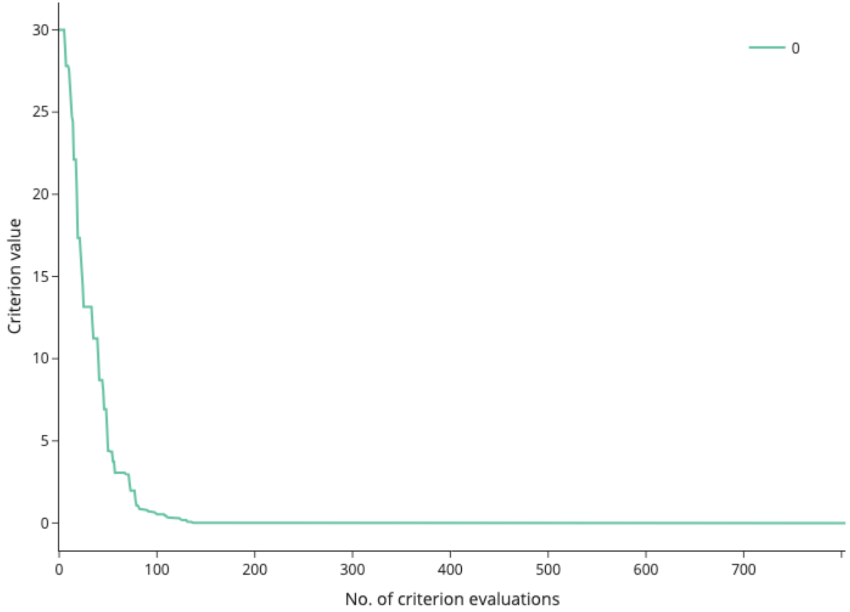
```
em.criterion_plot(res)
```



- First argument can be:
  - `OptimizeResult`
  - path to log file
  - list or dict thereof
- Dictionary keys are used for legend

Criterion plot (2)

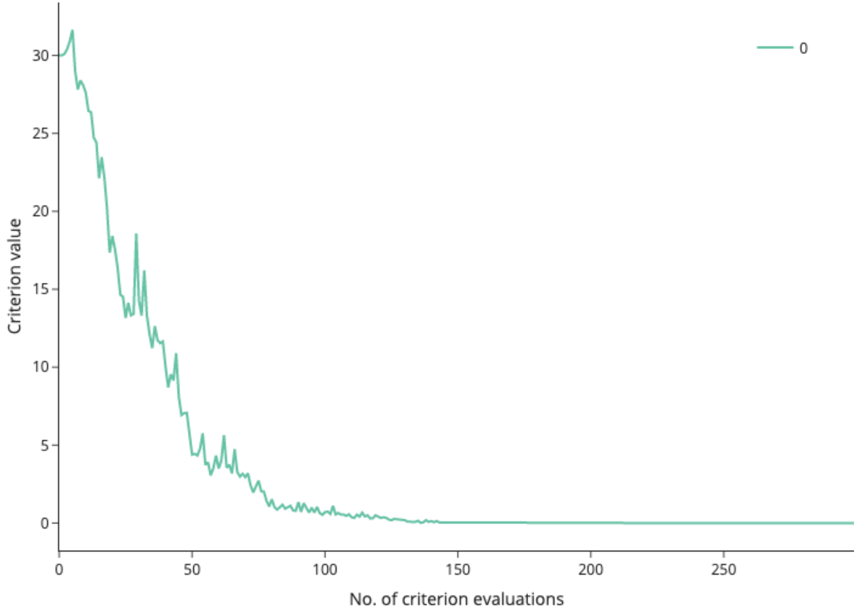
```
em.criterion_plot(res, monotone=True)
```



- **monotone=True** shows the current best value
- useful if there are extreme values in history

Criterion plot (3)

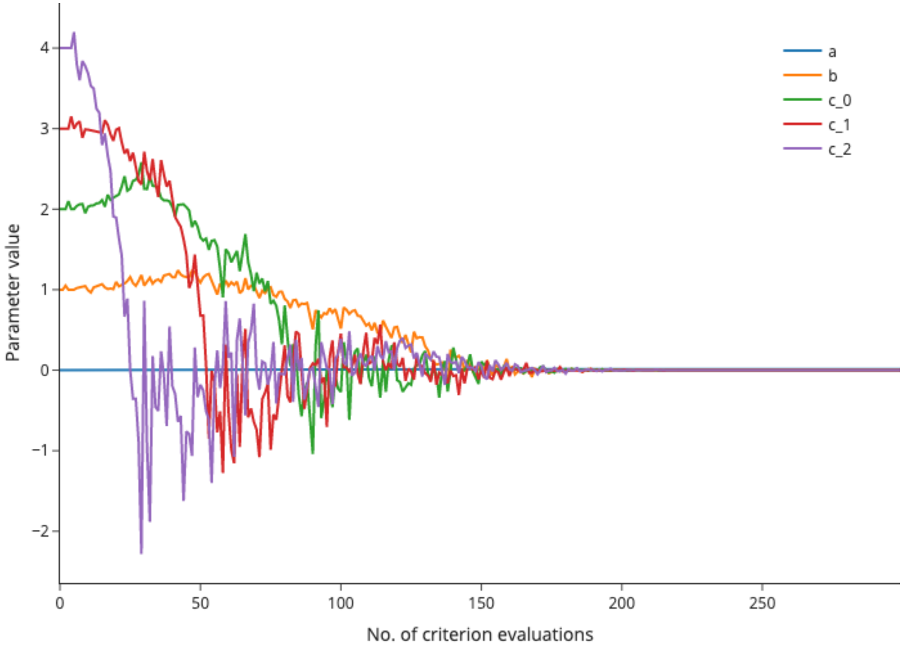
```
em.criterion_plot(res, max_evaluations=300)
```



- **max_evaluations** sets upper limit of x-axis

Params plot

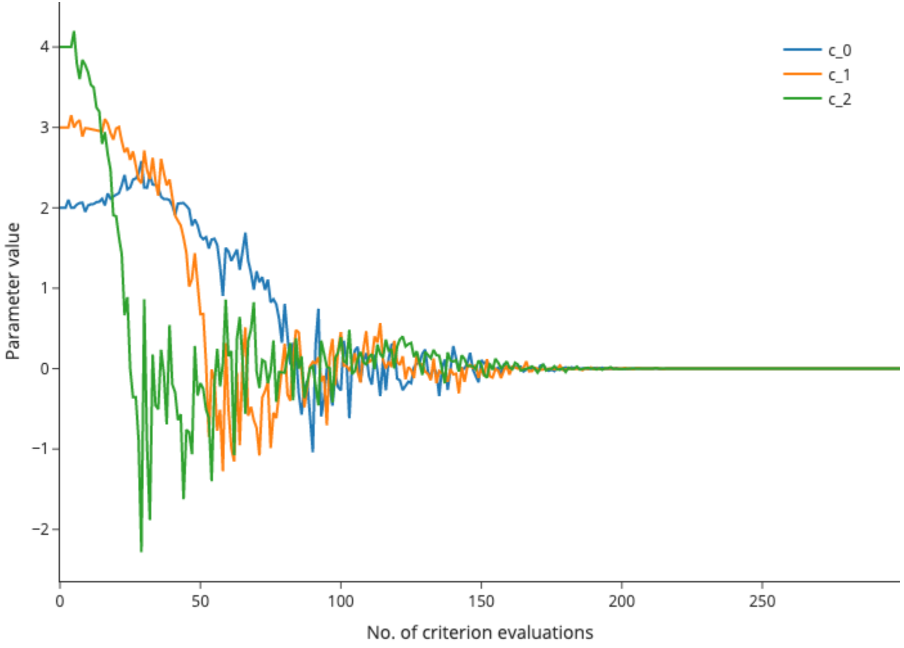
```python
# reminder: params looks like this
params = {
    "a": 0,
    "b": 1,
    "c": pd.Series([2, 3, 4])
}

em.params_plot(
    res,
    max_evaluations=300,
)
```



- Similar options as **criterion_plot**

Params plot (2)

```python
em.params_plot(
    res,
    max_evaluations=300,
    selector=lambda x: x["c"],
)
```



- **selector** is a function returning a subset of params

There is maximize

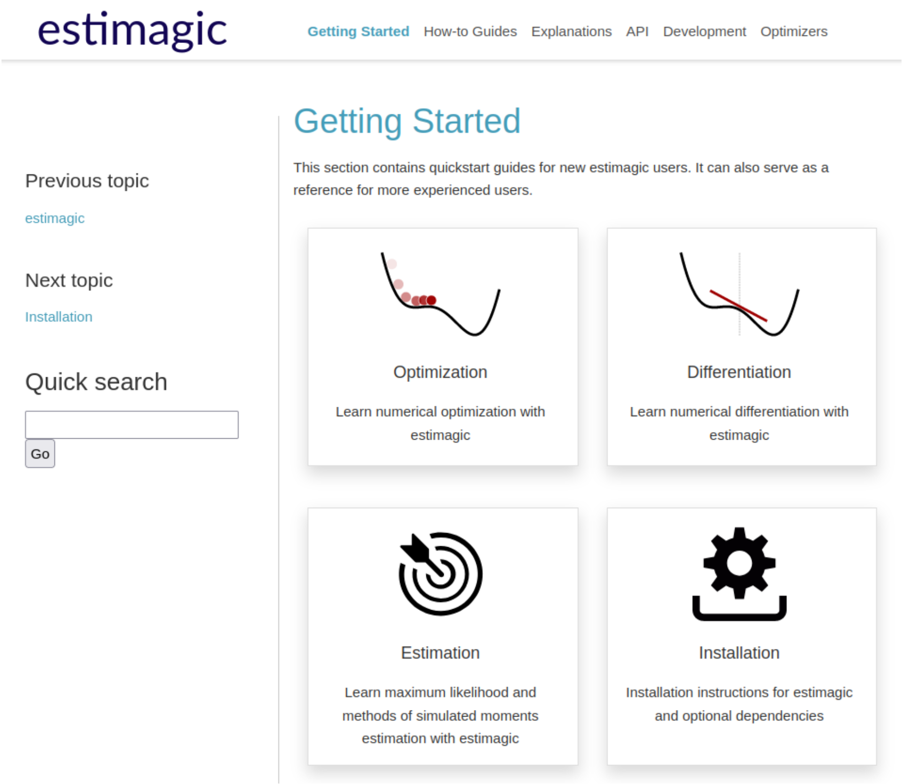
```
>>> def upside_down_sphere(params):
...     return -params @ params

>>> res = em.maximize(
...     criterion=upside_down_sphere,
...     params=np.arange(5),
...     algorithm="scipy_lbfgs",
... )
>>> res.params
array([ 0.,  0.,  0.,  0., 0.])
```

Harmonized algo_options

```
>>> algo_options = {
...     "convergence.relative_criterion_tolerance": 1e-9,
...     "stopping.max_iterations": 100_000,
...     "trustregion.initial_radius": 10.0,
... }

>>> res = em.minimize(
...     criterion=sphere,
...     params=np.arange(5),
...     algorithm="nag_pybobyqa",
...     algo_options=algo_options,
... )
>>> res.params
array([0., 0., 0., 0., 0.])
```

- The same options have the same name
- Different options have different names
  - e.g., not one **tol**
- Ignore irrelevant options

estimagic.readthedocs.io



Who is behind estimagic


Janoś Gabler


Mariam Petrosyan


Tim Mensinger


Klara Röhrl


Tobias Raabe


Annica Gehlen


Sebastian Gsell


Bahar Coskun


Aida Takhmazova


Hans-Martin von Gaudecker


Kenneth L. Judd

NUMFOCUS
OPEN CODE = BETTER SCIENCE

UNIVERSITÄT BONN

Stanford University
HOOVER INSTITUTION

Break (5 min)

Practice Session

Convert previous example to estimagic (15 min)

Choosing algorithms

Preview of practice session

You will get an optimization problem that fails

- Figure out why it fails
- Choose an algorithm that works

Relevant problem properties

- **Smoothness**: Differentiable? Kinks? Discontinuities? Stochastic?
- **Convexity**: Are there local optima?
- **Goal**: Do you need a global solution? How precise?
- **Size**: 2 parameters? 10? 100? 1000? More?
- **Constraints**: Bounds? Linear constraints? Nonlinear constraints?
- **Structure**: Nonlinear least-squares, Log-likelihood function

-> Properties guide selection but experimentation is important

scipy_lbfgsb

- Limited memory BFGS
- BFGS: Approximate hessians from multiple gradients
- Criterion must be differentiable
- Scales to a few thousand parameters
- Beats other BFGS implementations in many benchmarks
- Low overhead

fides

- Derivative based trust-region algorithm
- Developed by Fabian Fröhlich as a Python package
- Many advanced options to customize the optimization!
- Criterion must be differentiable
- Good solution if **scipy_lbfgsb** is too aggressive

nlopt_bobyqa, nag_pybobyqa

- **B**ound **O**ptimization **by** **Q**uadratic **A**pproximation
- Derivative free trust region algorithm
- **nlopt** has less overhead
- **nag** has options to deal with noise
- Good for non-differentiable not too noisy functions
- Slower than derivative based methods but faster than neldermead

scipy_neldermead, nlopt_neldermead

- Popular direct search method
- **scipy** does not support bounds
- **nlopt** requires fewer criterion evaluations in most benchmarks
- Almost never the best choice but sometimes not the worst

scipy_ls_lm, scipy_ls_trf

- Derivative based optimizers for nonlinear least squares
- Criterion needs structure: $F(x) = \sum_i f_i(x)^2$
- In estimagic, criterion returns a dict:

```
def sphere_ls(x):
    # x are the least squares residuals in the sphere function
    return {"root_contributions": x, "value": x @ x}
```

- **scipy_ls_lm** is better for small problems without bounds
- **scipy_ls_trf** is better for problems with many parameters

nag_dfols, pounders

- Derivative free trust region method for nonlinear least-squares
- Both beat bobyqa for least-squares problems!
- **nag_dfols** is usually the fastest
- **nag_dfols** has advanced options to deal with noise
- **pounders** can do criterion evaluations in parallel

ipopt

- Probably best open source optimizer for nonlinear constraints

Practice Session

Play with **algorithm** and **algo_options** (10 min)

Bounds and constraints

Preview of practice session

- Solve optimization problem with
  - parameter bounds
  - fixed parameters
  - linear constraints

Bounds

- Lower and upper bounds on parameters
- Also called box constraints
- Handled by most algorithms
- Need to hold for start parameters
- Guaranteed to hold during entire optimization
- Specification depends on **params** format

How to specify bounds for array params

```
>>> def sphere(x):
...     return x @ x

>>> res = em.minimize(
...     criterion=sphere,
...     params=np.arange(3) + 1,
...     lower_bounds=np.ones(3),
...     algorithm="scipy_lbfgsb",
... )
>>> res.params
array([1., 1., 1.])
```

- Specify **lower_bounds** and **upper_bounds**
- Use **np.inf** or **-np.inf** to represent no bounds

How to specify bounds for DataFrame params

```
>>> params = pd.DataFrame({
...         "value": [1, 2, 3],
...         "lower_bound": [1, 1, 1],
...         "upper_bound": [3, 3, 3],
...     },
...     index=["a", "b", "c"],
... )

>>> def criterion(p):
...     return (p["value"] ** 2).sum()

>>> em.minimize(criterion, params, algorithm="scipy_lbfgsb")
```

How to specify bounds for pytree params

```
params = {"x": np.arange(3), "intercept": 3}

def criterion(p):
    return p["x"] @ p["x"] + p["intercept"]

res = em.minimize(
    criterion,
    params=params,
    algorithm="scipy_lbfgsb",
    lower_bounds={"intercept": -2},
)
```

- Enough to specify the subset of params that actually has bounds
- We try to match your bounds with params
- Raise **InvalidBoundsError** in case of ambiguity

Constraints

- Constraints are conditions on parameters
- Linear constraints
  - $\min_x f(x) s.t. l \leq Ax \leq u$
  - $\min_x f(x) s.t. Ax = v$
- Nonlinear constraints:
  - $\min_x f(x)$ s.t. $c_1(x) = 0, c_2(x) >= 0$
- "estimagic-constraints":
  - E.g. find probabilities or covariance matrix, fix parameters, …

Example: Find valid probabilities

```
>>> res = em.minimize(
...     criterion=sphere,
...     params=np.array([0.1, 0.5, 0.4, 4, 5]),
...     algorithm="scipy_lbfgsb",
...     constraints=[{
...         "loc": [0, 1, 2],
...         "type": "probability"
...     }],
... )

>>> res.params
array([0.33334, 0.33333, 0.33333, -0., 0.])
```

- Restrict first 3 parameters to be probabilities
  - Between 0 and 1
  - Sum to 1
- But "scipy_lbfsb" is unconstrained?!

What happened

- Estimagic can implement some types of constraints via reparametrization
- Transforms a constrained problem into an unconstrained one
- Constraints must hold in start params
- Guaranteed to hold during entire optimization

Which constraints can be handled via reparametrization?

- Fixing parameters (simple but useful)
- Finding valid covariance and correlation matrices
- Finding valid probabilities
- Linear constraints (as long as there are not too many)
    - $\min f(x)\ s.t.\ A_1 x = 0$ and $A_2 x \leq 0$

Fixing parameters

```
>>> def criterion(params):
...     offset = np.linspace(1, 0, len(params))
...     x = params - offset
...     return x @ x

unconstrained_optimum = [1, 0.8, 0.6, 0.4, 0.2, 0]

>>> res = em.minimize(
...     criterion=criterion,
...     params=np.array([2.5, 1, 1, 1, 1, -2.5]),
...     algorithm="scipy_lbfgsb",
...     constraints={"loc": [0, 5], "type": "fixed"},
... )
>>> res.params
array([ 2.5,  0.8,  0.6,  0.4,  0.2, -2.5])
```

- **loc** selects location 0 and 5 of the parameters
- **type** states that they are fixed

Linear constraints

```
>>> res = em.minimize(
...     criterion=criterion,
...     params=np.ones(6),
...     algorithm="scipy_lbfgsb",
...     constraints={
...         "loc": [0, 1, 2, 3],
...         "type": "linear",
...         "lower_bound": 0.95,
...         "weights": 0.25,
...     },
... )
>>> res.params
array([ 1.25, 1.05, 0.85, 0.65, 0.2 , -0.])
```

- Impose that average of first 4 parameters is larger than 0.95
- Weights can be scalars or same length as selected parameters
- Use "value" instead of "lower_bound" for linear equality constraint

Constraints have to hold

```
>>> em.minimize(
...     criterion=sphere,
...     params=np.array([1, 2, 3, 4, 5]),
...     algorithm="scipy_lbfgsb",
...     constraints={"loc": [0, 1, 2], "type": "probability"},
... )
```

```
InvalidParamsError: A constraint of type 'probability' is not fulfilled in params,
please make sure that it holds for the starting values. The problem arose because:
Probabilities do not sum to 1. The names of the involved parameters are: ['0', '1', '2']
The relevant constraint is:
{'loc': [0, 1, 2], 'type': 'probability', 'index': array([0, 1, 2])}.
```

Nonlinear constraints

```
>>> res = em.minimize(
...     criterion=criterion,
...     params=np.ones(6),
...     algorithm="scipy_slsqp",
...     constraints={
...         "type": "nonlinear",
...         "loc": [0, 1, 2, 3, 4],
...         "func": lambda x: np.prod(x),
...         "value": 1.0,
...     },
... )
>>> res.params
array([1.31, 1.16, 1.01, 0.87, 0.75, -0.])
```

- Restrict the product of first five params to 1
- Only work with some optimizers
- **func** can be an arbitrary python function of params that returns a number, array or pytree
- Use "lower_bound" and "upper_bound" instead of "value" for inequality constraints

Parameter selection methods

- **"loc"** can be replaced other things
- If params is a DataFrame with "value" column
  - **"query"**: An arbitrary query string that selects the relevant rows
  - **"loc"**: Will be passed to **DataFrame.loc**
- Always
  - **"selector"**: A function that takes params as argument and returns a subset of params
- More in the documentation

Practice Session

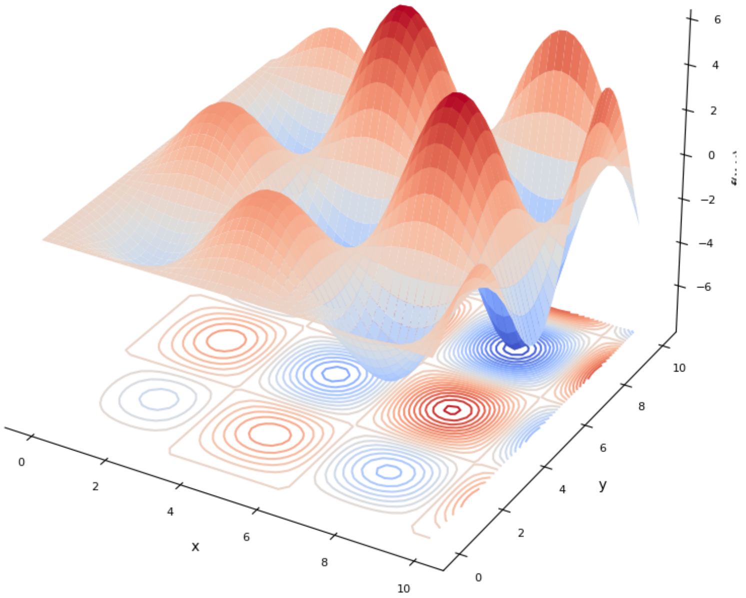
Constrained optimization (15 min)

Global optimization

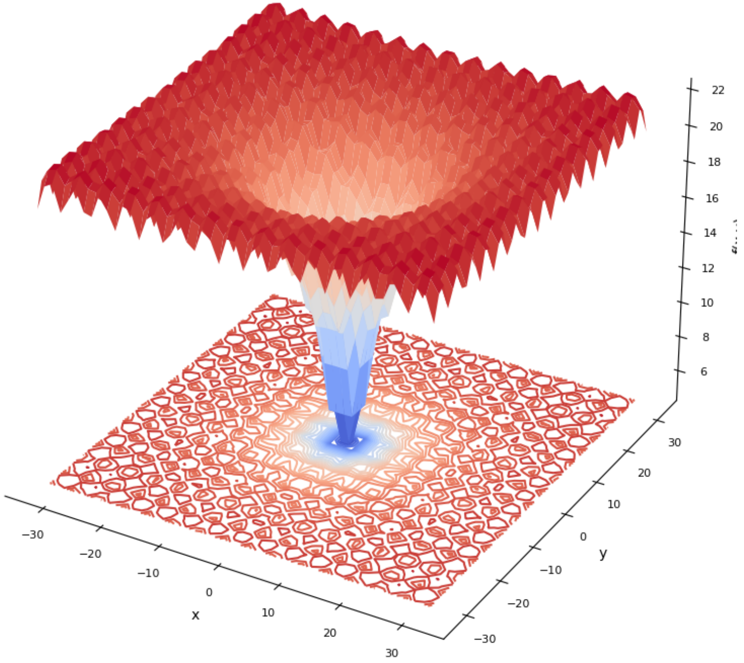
Global vs local optimization

- Local: Find any local optimum
  - All we have done so far
- Global: Find best local optimum
  - Needs bounds to be well defined
  - Extremely challenging in high dimensions
- Local = global for convex problems

Examples

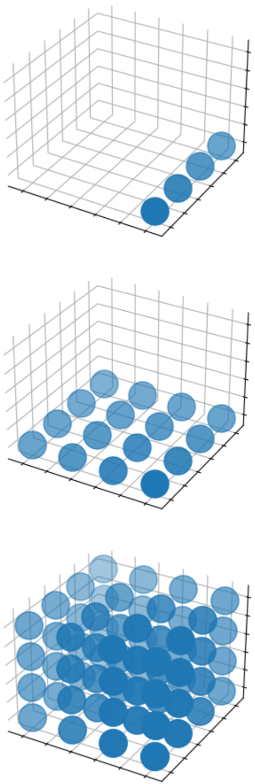


Alpine



Ackley

How about brute force?



Dimension	Runtime (1 ms per evaluation, 100 points per dimension)
1	100 ms
2	10 s
3	16 min
4	27 hours
5	16 weeks
6	30 years

Genetic algorithms

- Heuristic inspired by natural selection
- Random initial population of parameters
- In each evolution step:
    - Evaluate "fitness" of all population members
    - Replace worst by combinations of good ones
- Converge when max iterations are reached
- Examples: **"pygmo_gaco"**, **"pygmo_bee_colony"**, **"nlopt_crs2_lm"**, …

Bayesian optimization

- Evaluate criterion on grid or sample of parameters
- Build surrogate model of criterion
- In each iteration
  - Do new criterion evaluations at promising points
  - Improve surrogate model
- Converge when max iterations is reached

Multistart optimization:

- Evaluate criterion on random exploration sample
- Run local optimization from best point
- In each iteration:
  - Combine best parameter and next best exploration point
  - Run local optimization from there
- Converge if current best optimum is rediscovered several times

Multistart example

```
>>> res = em.minimize(
...     criterion=sphere,
...     params=np.arange(5),
...     algorithm="scipy_neldermead",
...     soft_lower_bounds=np.full(5, -5),
...     soft_upper_bounds=np.full(5, 15),
...     multistart=True,
...     multistart_options={
...         "convergence.max_discoveries": 5,
...         "n_samples": 1000
...     },
... )
>>> res.params
array([0., 0., 0., 0.,  0.])
```

- Turn local optimizers global
- Inspired by tiktak algorithm
- Use any optimizer
- Distinguish hard and soft bounds

How to choose

- Extremely expensive criterion (i.e. can only do a few evaluations):
  - Bayesian optimization
- Well behaved function:
  - Multistart with local optimizer tailored to function properties
- Rugged function with extremely many local optima
  - Genetic optimizer
  - Consider refining the result with local optimizer
- All are equally parallelizable

Summary

Summary

- You have solved a simple problem with scipy.optimize
- For larger problems, estimagic provides more convenience
  - `params` don't have to be flat arrays
  - Support for many more algorithms
  - `criterion_plot` and `params_plot` help you select the right algorithm
  - Logging and error handling help to deal with crashes
  - Multistart to make local optimizers global
- Many more features to explore in the documentation

How to contribute

- Make issues or provide feedback
- Improve or extend the documentation
- Suggest, wrap or implement new optimizers
- Teach estimagic to colleagues, students and friends
- Make us happy by giving us a star on
  github.com/OpenSourceEconomics/estimagic