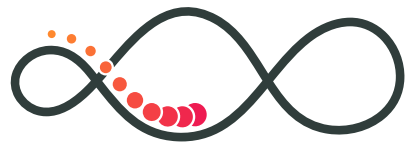
Introduction to Numerical Optimization

Janoś Gabler and Tim Mensinger, University of Bonn



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. 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

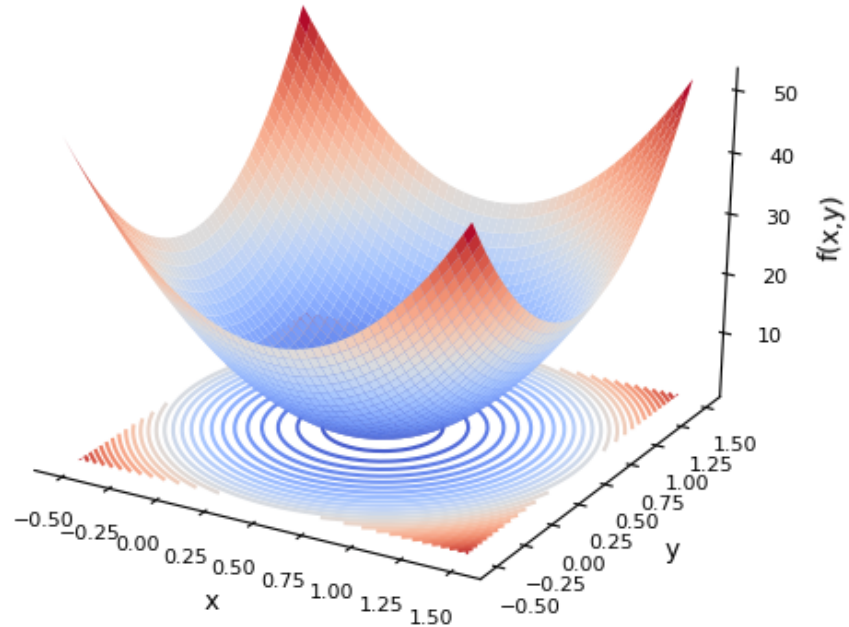
Introduction to scipy.optimize

Preview of practice session

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

Example problem

- **Criterion** $f(a, b) = a^2 + b^2$
- Parameters a, b
- Want: $a^*, b^* = \mathrm{argmin} f(a, b)$
- 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])
```

- **minimize** as unified interface to 14 local optimizers
- some support bounds or 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 (12 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

→ **In practice, you often wish for more convenience**

You hit exceptions …

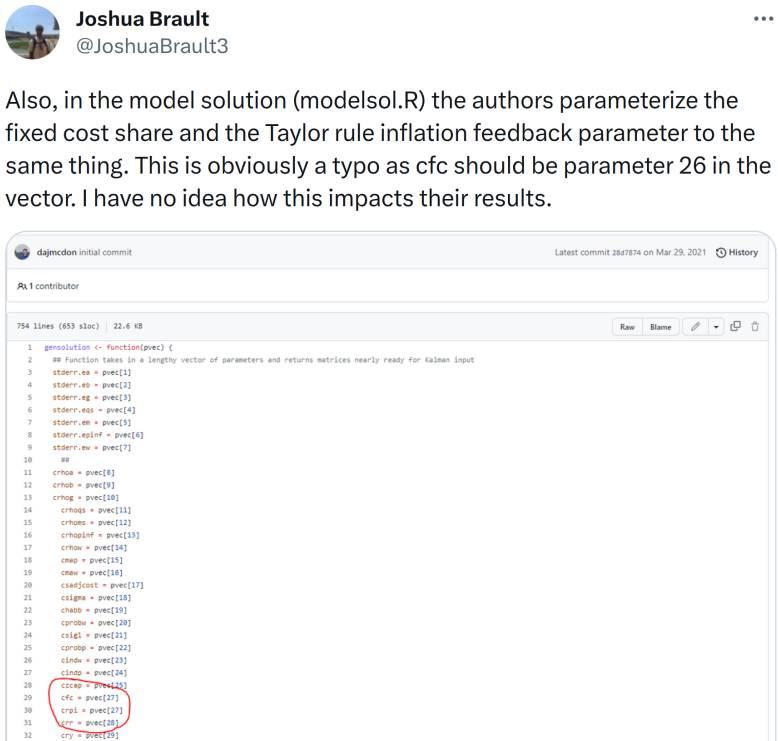
```
>>> scipy.optimize.minimize(func, x0)
---------------------------------------------------------------------------
LinAlgError                               Traceback (most recent call last)
<ipython-input-17-7459e5b4d8d4> in <module>
----> 1 scipy.optimize.minimize(func, x0)

     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

You write boilerplate code ...

```
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
```

You make mistakes …



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]
```

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

Switching packages is painful ...

0

The SciPy optimizers and NLopt have different conventions for the signature of the objective function. The documentation for the objective function in NLopt says

> The function `f` should be of the form:
>
> ```
> def f(x, grad):
>    if grad.size > 0:
> ```

etc.

So you'll need to create an objective function that accepts two arguments, `x` and `grad`. If `grad.size > 0`, the function must fill in the array with the gradient.

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answered Apr 14, 2020 at 15:20

Warren Weckesser

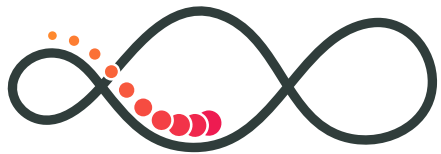
110k ● 19 ● 194 ● 214

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

- Wraps optimizers from:
  - Scipy, Nlopt, TAO, Pygmo, …
- Unified interface
- Additional functionality and convenience
- Tools for nonlinear estimation

You can use it like scipy

```
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])
```

- `minimize` works almost the same
- Supports local and global scipy algorithms
- Difference: No default algorithm

Params can be almost anything

numpy arrays

```
params = np.array([1, 2, 3])
```

pandas objects

```
params = pd.Series([1, 2], index=["a", "b"])
```

scalars

```
params = 3.14
```

lists

```
params = [1, 2, 3]
```

dicts

```
params = {"a": 1, "b": 2, "c": [3, 4]}
```

NamedTuples

```
class Params(NamedTuple):
    beta: float = 0.95
    h: np.ndarray = np.ones(3)
```

→ **You can nest these as deep as you want!**

Example: Dict of scalars and pandas Series

```
params = {"a": 0, "b": 1, "c": pd.Series([2, 3, 4])}

def dict_sphere(x):
    return x["a"] ** 2 + x["b"] ** 2 + (x["c"] ** 2).sum()

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}
```

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'])
```

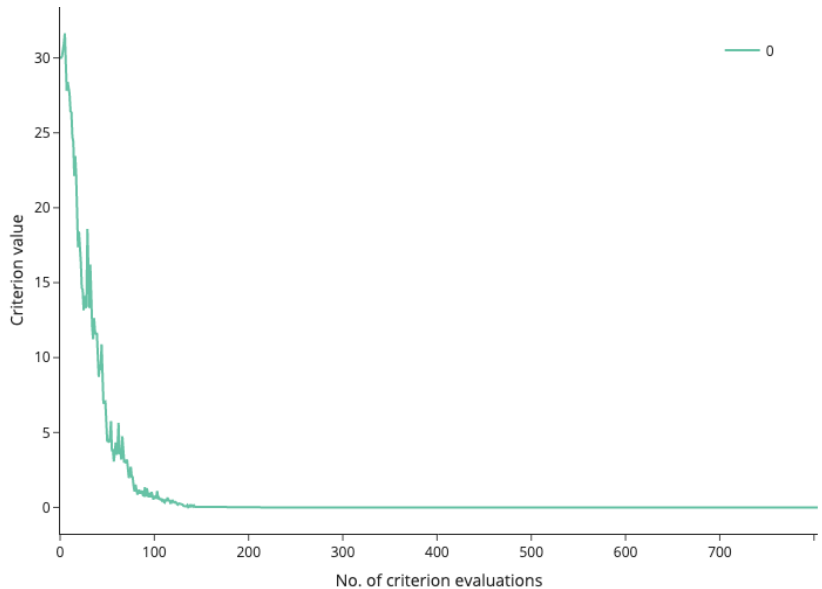
```
reader.read_iteration(1)["params"]
```

```
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

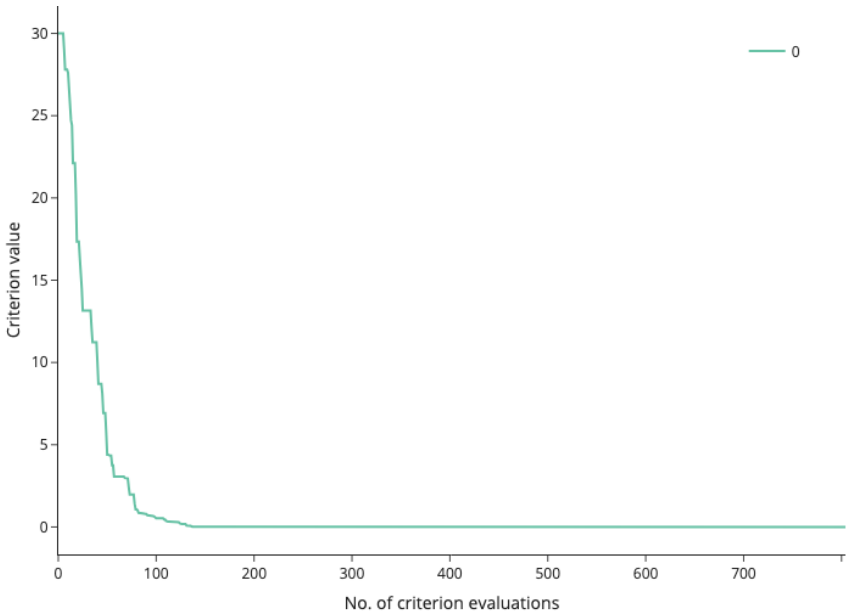
```
em.criterion_plot(res)
```



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

Criterion plot

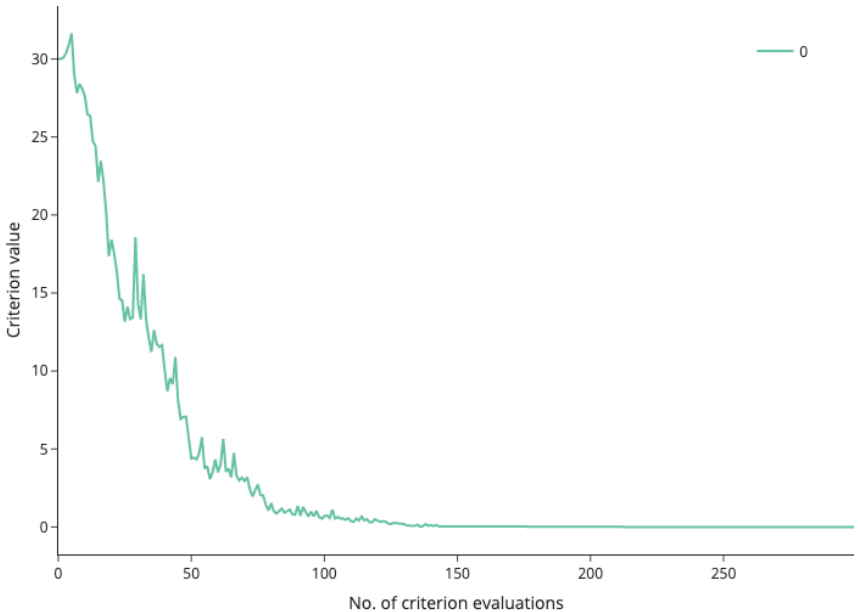
```
em.criterion_plot(res, monotone=True)
```



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

Criterion plot

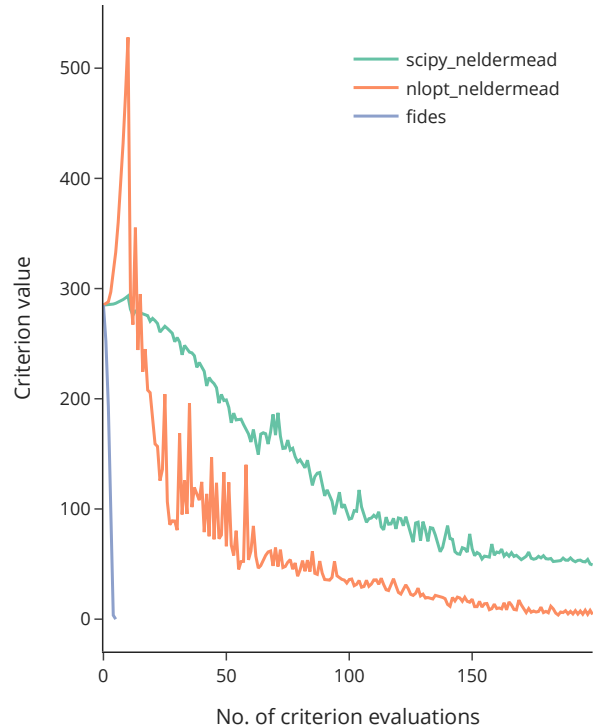
```
em.criterion_plot(res, max_evaluations=300)
```



- **max_evaluations** limits the x-axis

Criterion plot for multiple optimizations

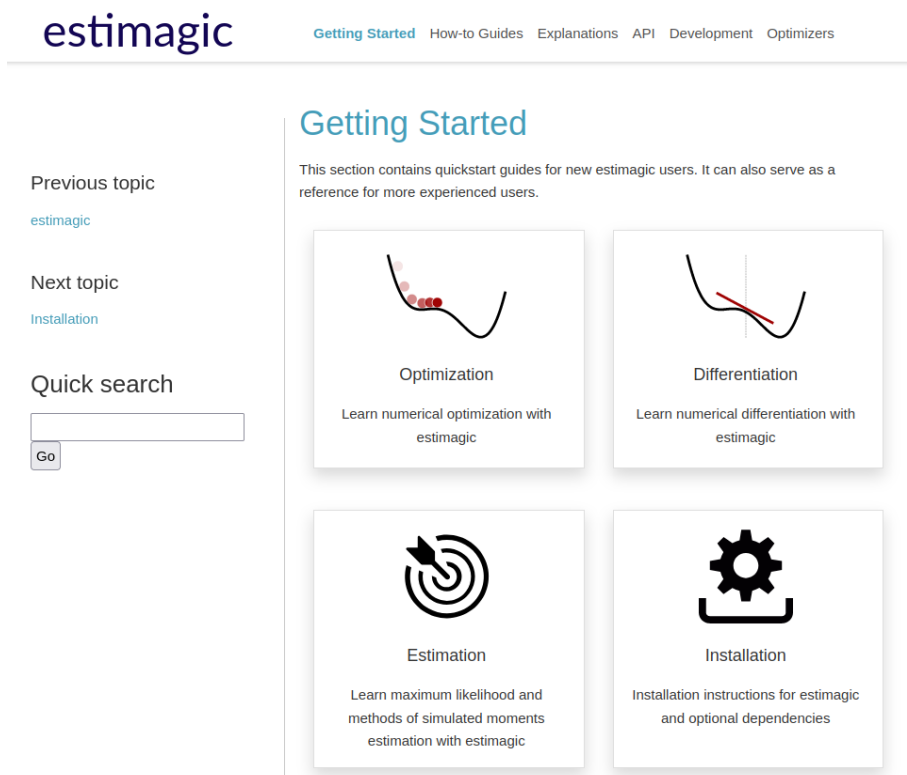
```python
def sphere(x):
    return x @ x

results = {}
for algo in ["scipy_neldermead", "nlopt_neldermead", "fides"]:
    results[algo] = em.minimize(
        sphere,
        np.arange(10),
        algorithm=algo,
    )

em.criterion_plot(results, max_evaluations=200)
```



Other features

- Parallel numerical derivatives and optimizers
- There is **maximize**
- Simple syntax for bounds and constraints
- Compatible with JAX automatic differentiation
- Sensible error handling
- Algorithms for nonlinear least-squares problems

estimagic.readthedocs.io



Practice Session

Convert previous example to estimagic (12 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

Estimagic has many optimizers

Optimization and derivatives

- The negative gradient of f is the direction of steepest descent

  $\rightarrow$ most optimizers use something gradient-like to find a search direction
- If the function is very curved, the descent direction is only valid locally

  $\rightarrow$ many optimizers use something hessian-like to determine the step size
- Below we give you a rough intuition for our go-to algorithms:
  - How do they work?
  - When should you use them

scipy_lbfgsb

- How it works:
  - Uses gradient for search direction
  - Uses approximated hessian (from gradient history) for step length
- When to use:
  - Differentiable functions with or without box constraints
  - Scales up to a few thousand parameters
  - Low overhead
  - Beats other BFGS implementations in many benchmarks

fides

- How it works:
  - Uses gradient an approximated hessian to form taylor approximation
  - Optimum of taylor approximation is next candidate
  - This is called a *trustregion method*
- When to use:
  - Same situations as L-BFGS-B
  - More customizable
  - Good solution if **scipy_lbfgsb** is too aggressive
  - Very underrated algorithm!

nlopt_bobyqa, nag_pybobyqa

- How it works:
  - Uses interpolation to form a quadratic approximation
  - Optimum of approximation is next candidate
- When to use:
  - Go to algorithm if you do not have a closed form derivative
  - **nlopt** has less overhead
  - **nag** has options to deal with noise
  - Requires well scaled problems

scipy_neldermead, nlopt_neldermead

- How it works:
  - Evaluate function on a set of points
  - Drop worst point and add new one
- When to use
  - No closed form derivative available
  - Badly scaled problems
  - Slightly noisy problems

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

→ **Always exploit least-squares structure if you can!**

nag_dfols, pounders

- Derivative free trust region methods 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

Fix a failing optimization (12 min)

Bounds

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},
)
```

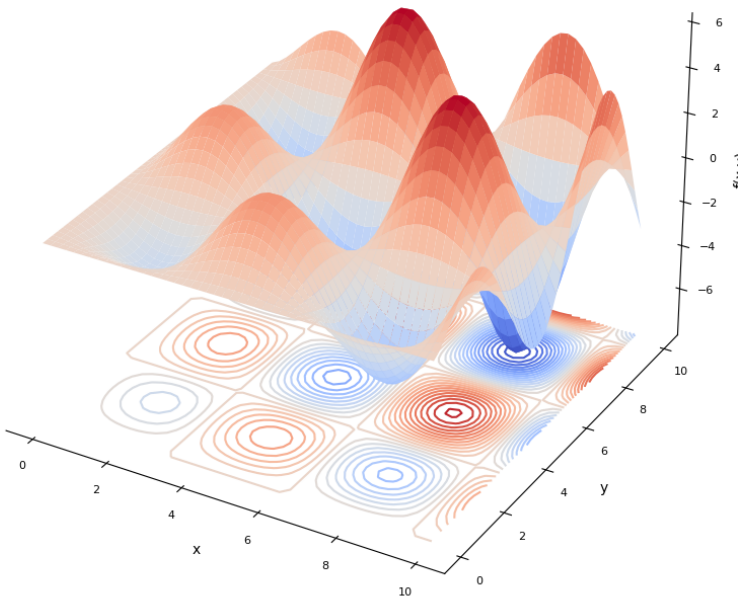
- Enough to specify the subset of params that actually has bounds
- We try to match your bounds with params
- Raise **InvalidBoundsError** in case of ambiguity

Global optimization

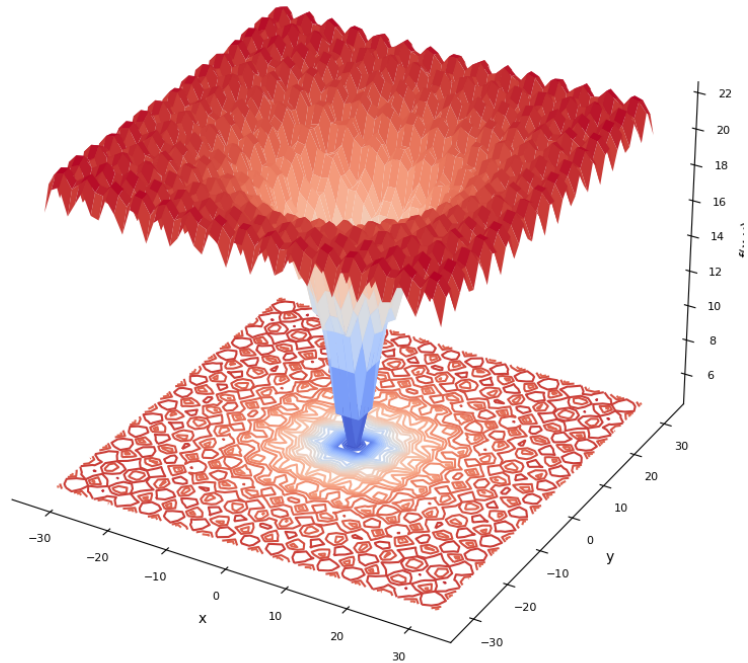
Global vs local optimization

- 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

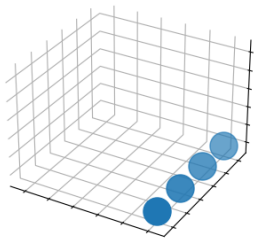


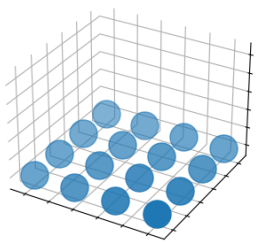
Alpine

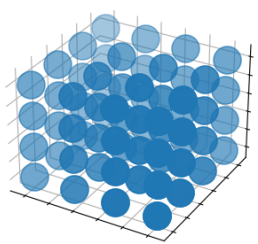


Ackley

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

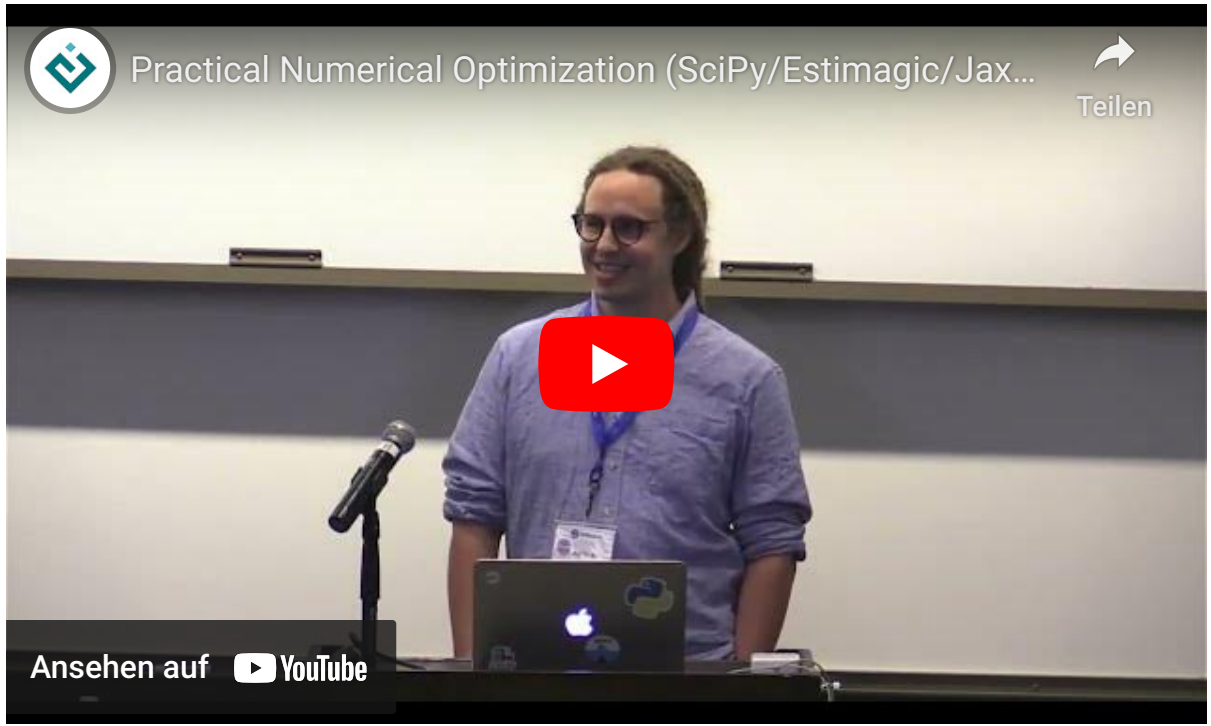
- Extremely expensive criterion (i.e. can only do a few evaluations):
  - Bayesian optimization
- Well behaved function:
  - Multistart with local optimizer tailored to function properties
- Rugged function with extremely many local optima
  - Genetic optimizer
  - Consider refining the result with local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

In-depth estimagic tutorial



The team 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

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OPEN CODE = BETTER SCIENCE

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Stanford University

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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