

Installation

We assume you have done the following: Installed [miniconda](#) and

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

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

Practical Numerical Optimization with Scipy, Estimagic and JAXopt

Scipy Conference 2022

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About Us



- Website: janosg.com
- GitHub: [janosg](https://github.com/janosg)
- Started estimagic in 2019
- Just submitted PhD thesis,
looking for jobs soon



- Website: tmensinger.com
- GitHub: [timmens](https://github.com/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. Advanced topics
5. Jax and Jaxopt

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

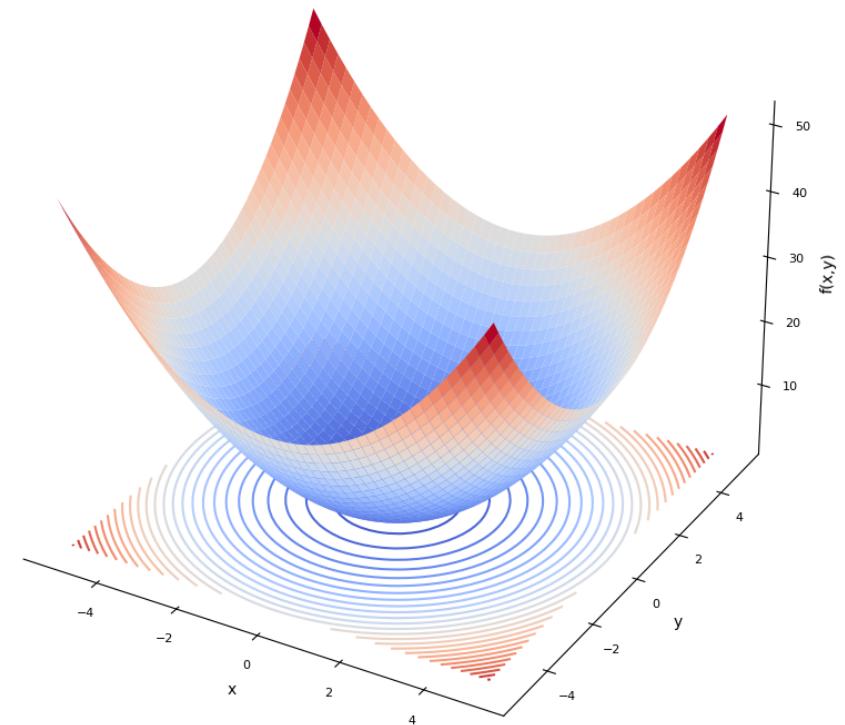
Introduction to `scipy.optimize`

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: $a^*, b^* = \operatorname{argmin} f(a, b)$
- Possible extensions:
 - Constraints
 - Bounds
- Optimum at $a^* = 0, b^* = 0$,
 $f(a^*, b^*) = 0$



Solve example problem 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 1: 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

```
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 II

```
>>> 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

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?

- 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

```
>>> 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'])
```

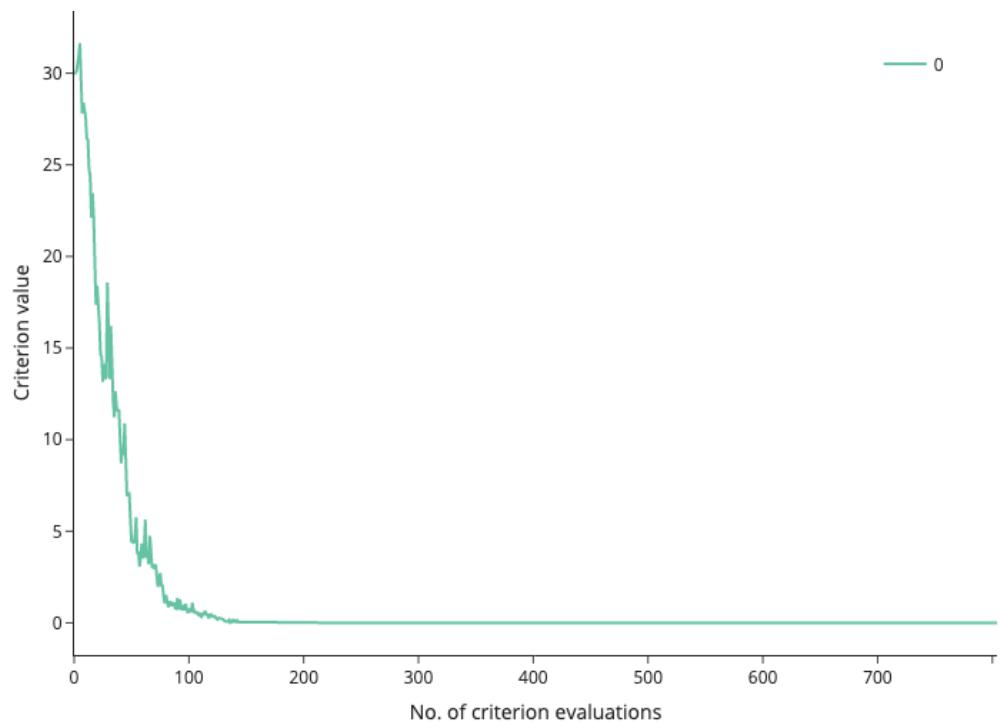
Logging and Dashboard

```
>>> 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

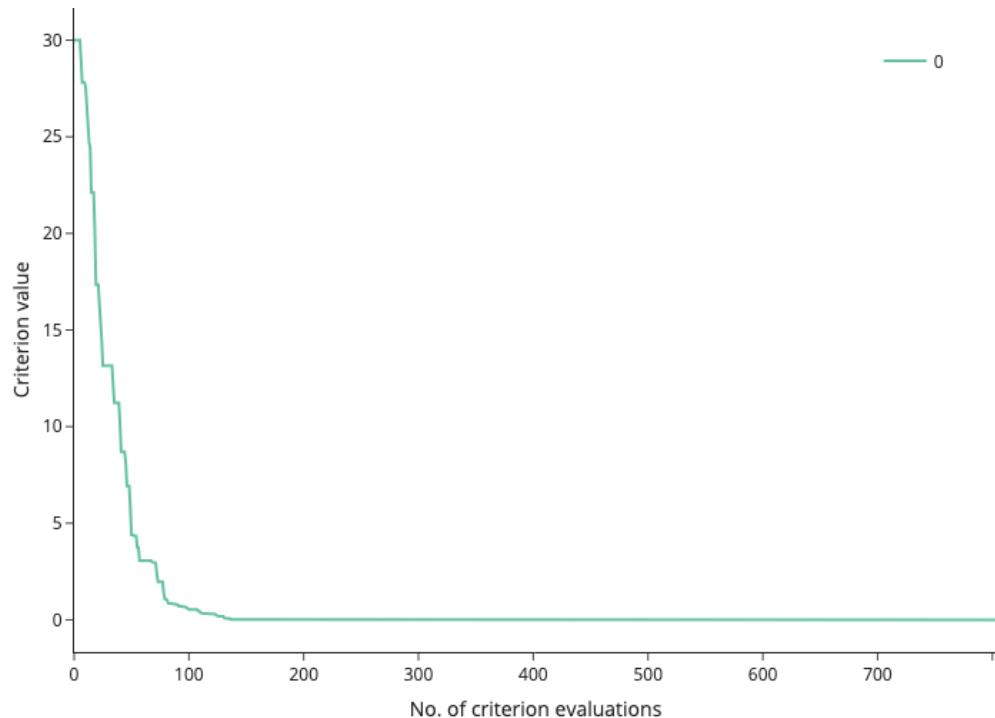
```
em.criterion_plot(res)
```



- 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)
```

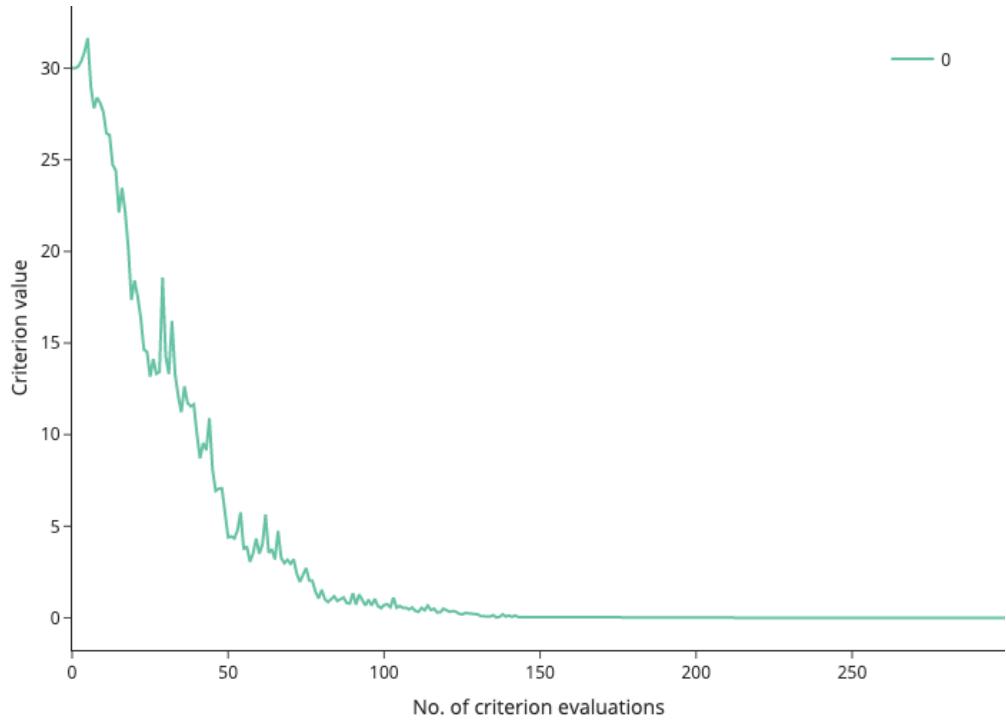


- `monotone=True` shows the current best value
- useful if there are extreme values in history

Criterion plot (3)

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

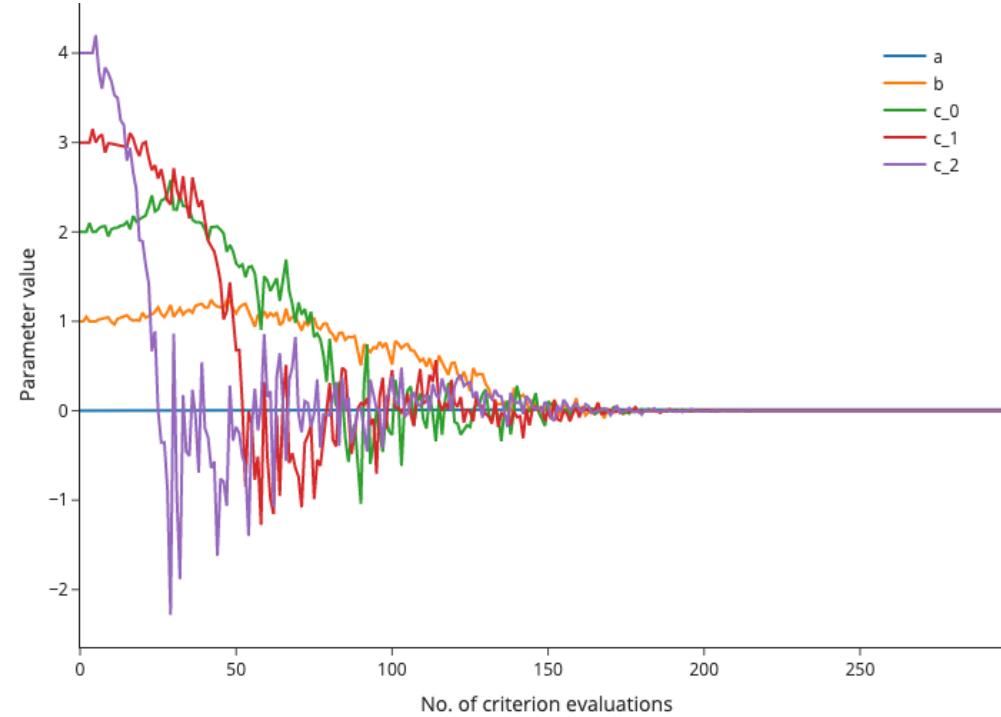
- `max_evaluations` sets upper limit of x-axis



Params plot

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

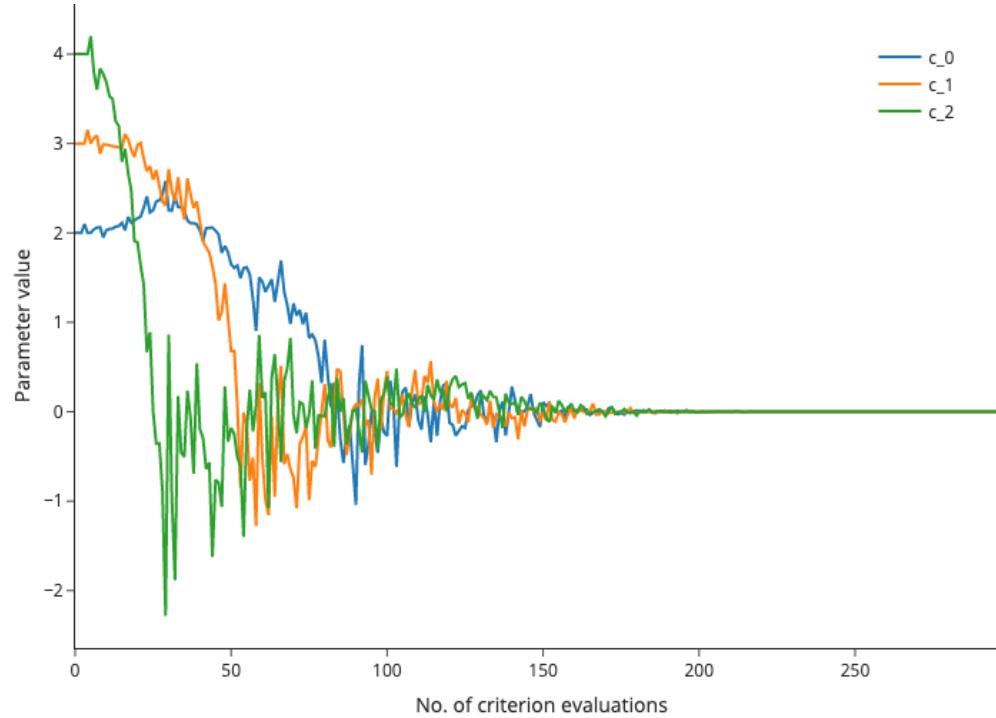
em.params_plot(
    res,
    max_evaluations=300,
)
```



- Similar options as `criterion_plot`

Params plot (2)

```
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

Previous topic

[estimagic](#)

Next topic

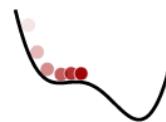
[Installation](#)

Quick search

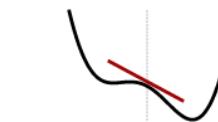
Go

Getting Started

This section contains quickstart guides for new estimagic users. It can also serve as a reference for more experienced users.



Optimization



Differentiation

Learn numerical optimization with
estimagic

Learn numerical differentiation with
estimagic



Estimation

Learn maximum likelihood and
methods of simulated moments
estimation with estimagic



Installation

Installation instructions for estimagic
and optional dependencies

Break (5 min)

Practice Session 2: Convert previous example to estimagic (15 min)

Choosing algorithms

Preview of practice session

You will get optimization problems that fail

- Figure out why they fail
- 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

- **Bound Optimization by Quadratic Approximation**
- 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 3: Play with algorithm and algo_options (20 min)

Benchmarking

Preview of practice session

- Compare different optimizers on benchmark sets
- Visualize comparison using profile and convergence plots

What is benchmarking

- Compare algorithms on functions with known optimum
- Mirror problems you actually want to solve
 - similar number of parameters
 - similar w.r.t. differentiability or noise
- Benchmark functions should be fast!

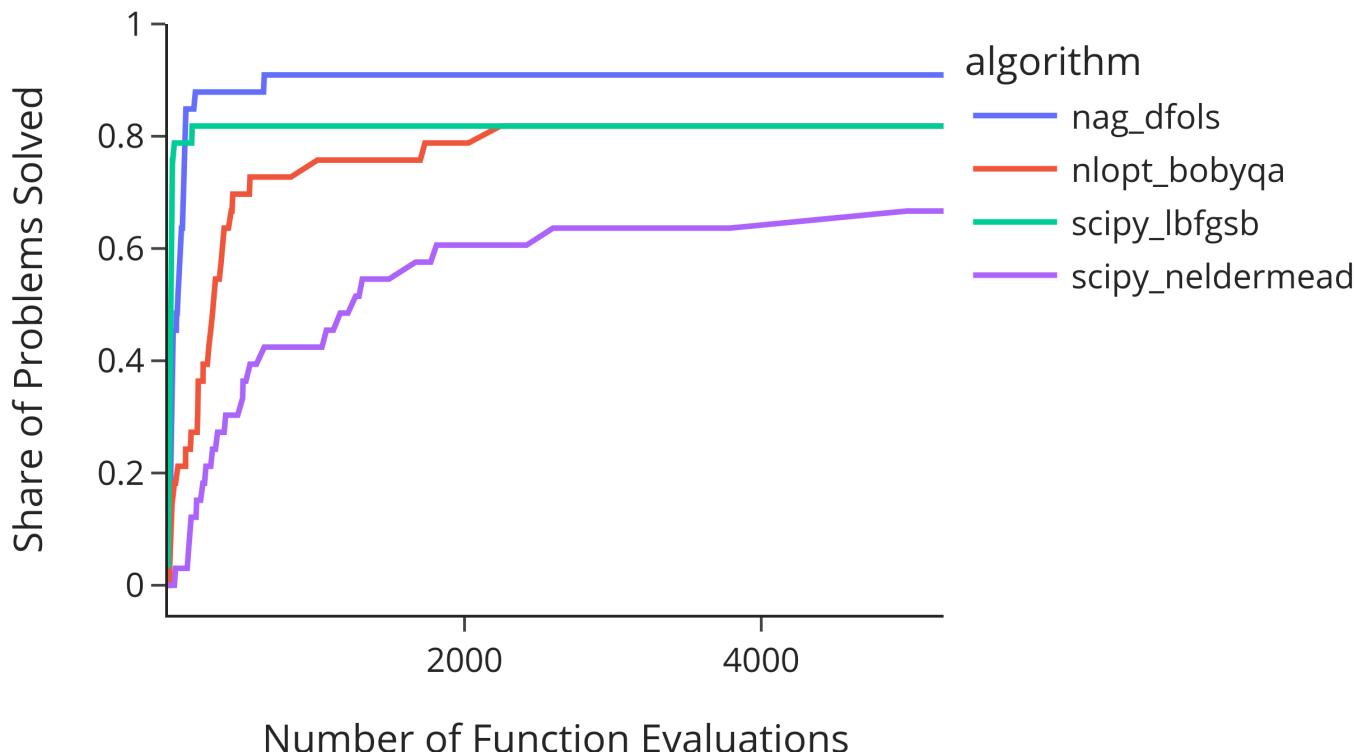
Running benchmarks in estimagic

```
problems = em.get_benchmark_problems(  
    "estimagic",  
)  
optimizers = [  
    "scipy_lbfgsb",  
    "nag_dfols",  
    "nlopt_bobyqa",  
    "scipy_neldermead",  
]  
results = em.run_benchmark(  
    problems=problems,  
    optimize_options=optimizers,  
    n_cores=4,  
    max_criterion_evaluations=1000,  
)
```

1. Create a set of test problems:
 - dict with functions, start values and correct solutions
2. Define optimize_options
 - Optimizers to try
 - Optionally: keyword arguments for minimize
3. Get benchmark results
 - Dict with histories and solutions

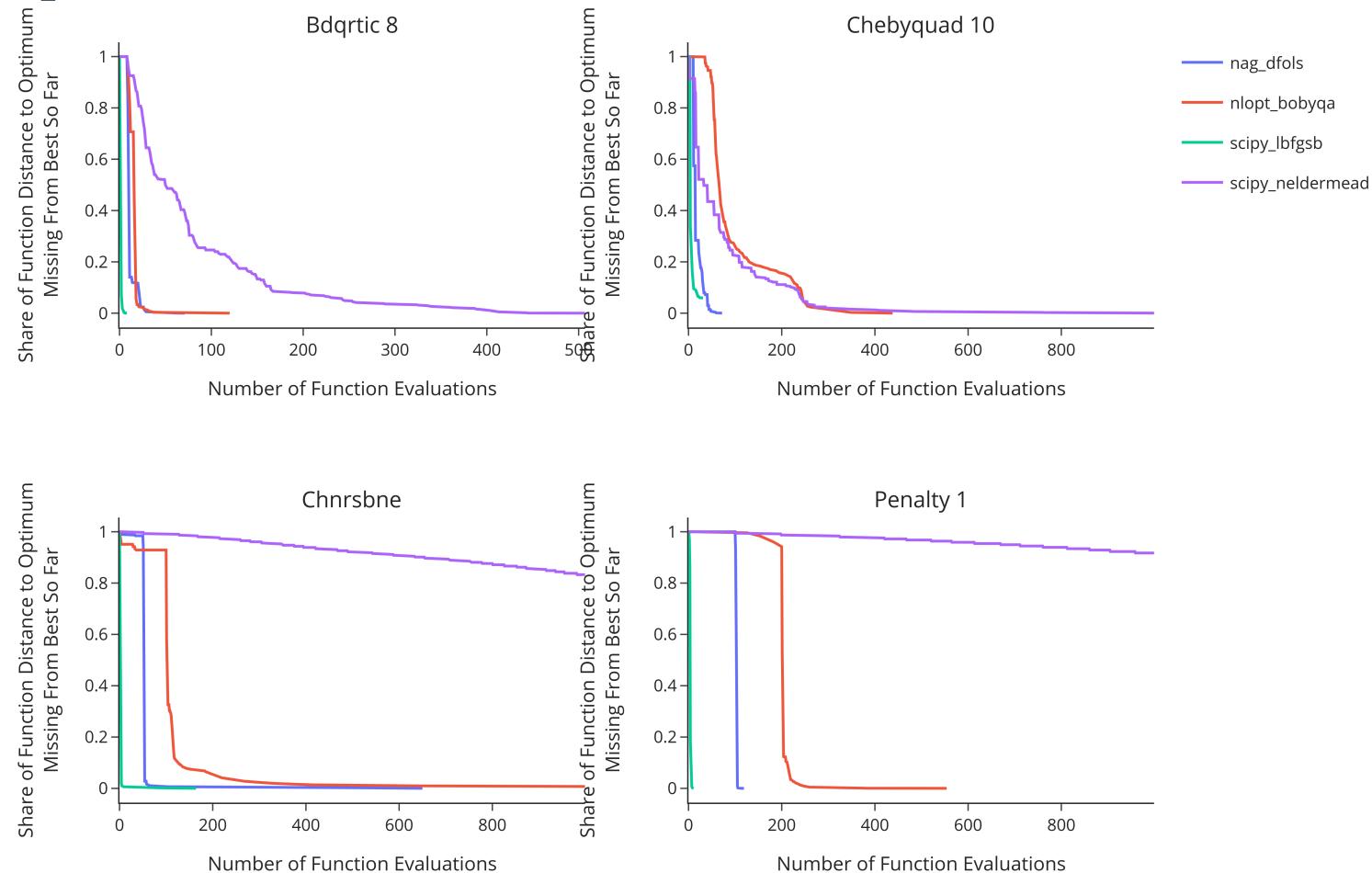
Profile plots

```
em.profile_plot(problems, results)
```



Convergence plots

```
subset = [
    "chebyquad_10",
    "chnrsbne",
    "penalty_1",
    "bdqrtic_8",
]
em.convergence_plot(
    problems,
    results,
    problem_subset=subset,
)
```



Why not look at runtime

- Benchmark functions are very fast (microseconds)
-> Runtime dominated by algorithm overhead
- Most real functions are slow (milliseconds, seconds, minutes, ...)
-> Runtime dominated by the number of evaluations
- You can do runtime plots as well

Practice Session 4: Benchmarking optimizers (15 min)

Break (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
 - $\min_x f(x) \text{ s.t. } l \leq Ax \leq u$
 - $\min_x f(x) \text{ s.t. } Ax = v$
- Nonlinear constraints:
 - $\min_x f(x) \text{ s.t. } c_1(x) = 0, c_2(x) \geq 0$
- "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_lbfgsb" 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)
 - $\min f(x) \text{ s.t. } A_1x = 0 \text{ and } A_2x \leq 0$

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 parameters 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](#)

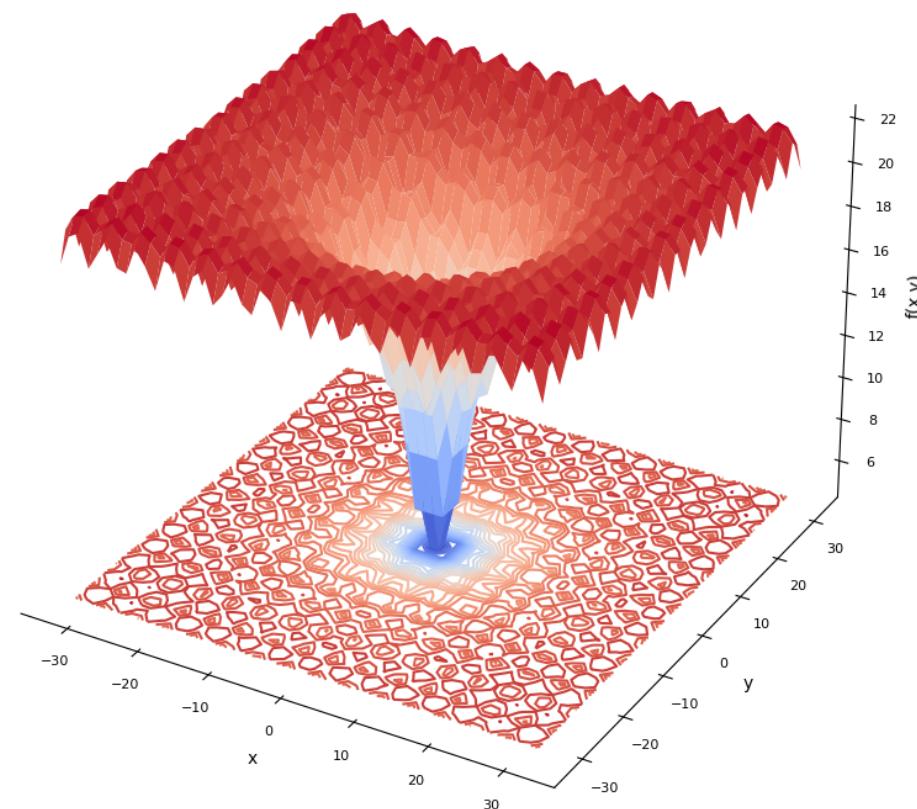
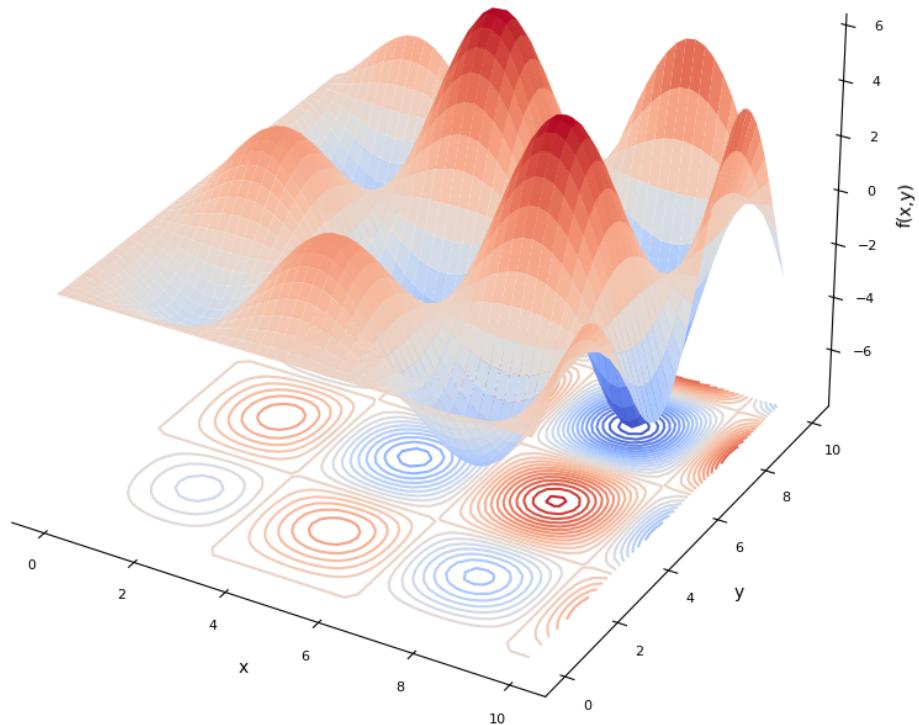
Practice Session 5: Constrained optimization (15 min)

Global optimization

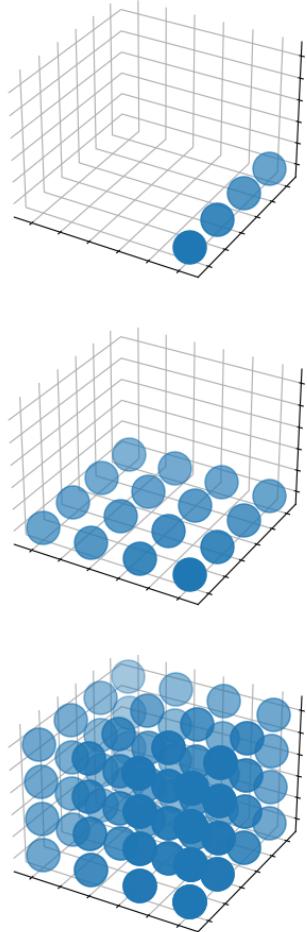
Global vs local optimization

- 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



How about brute force?



Number of Dimensions	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

Scaling

Preview of practice session

- Learn about badly scaled problems
- Visualize sensitiviy of criterion w.r.t parameters
- Use scaling to improve an optimization

What is scaling

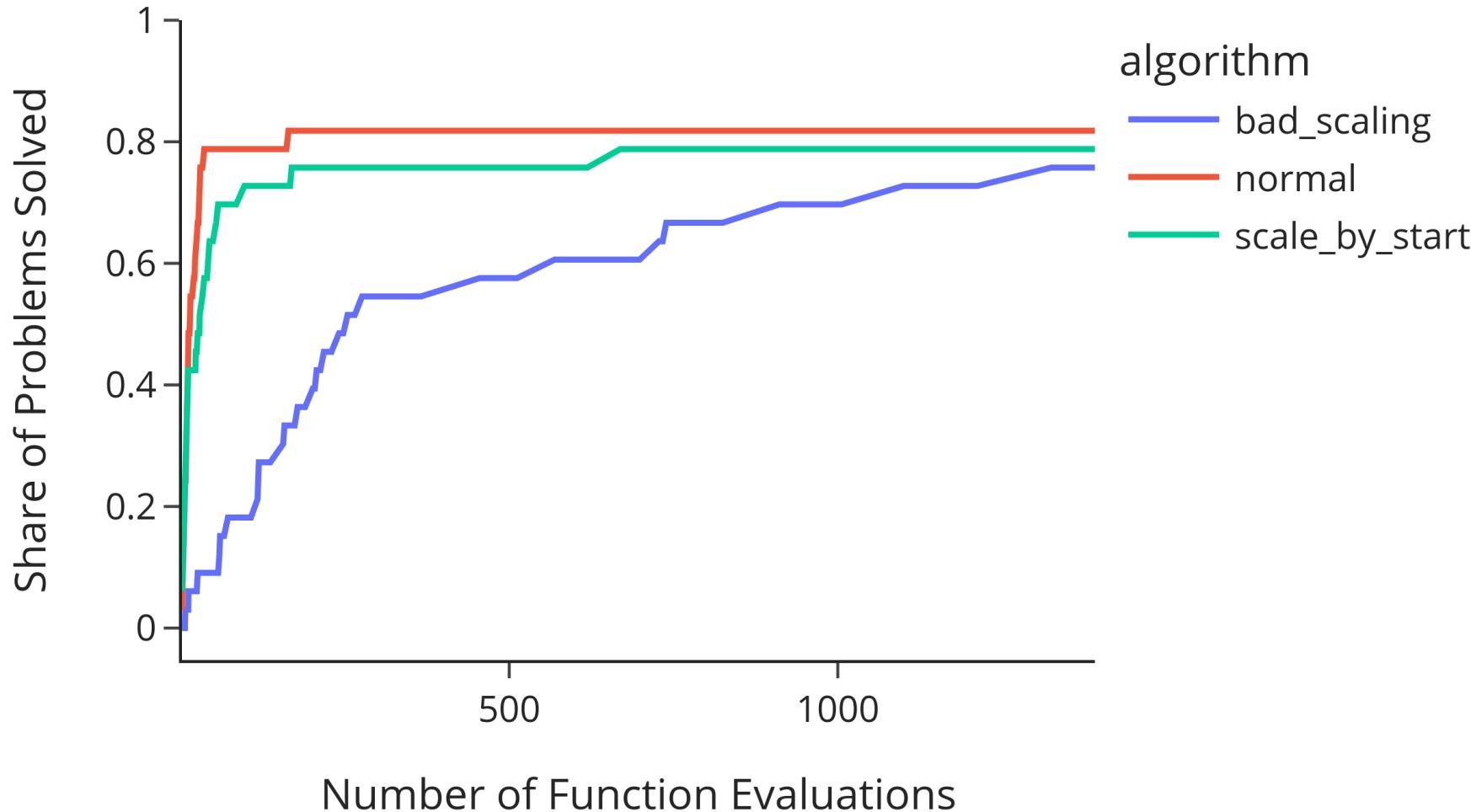
- Single most underrated topic among economists!
- Well scaled: A fixed step in any parameter dimension yields roughly comparable changes in function value
 - $f(a, b) = 0.5a^2 + 0.8b^2$
- Badly scaled: Some parameters are much more influential
 - $f(a, b) = 1000a^2 + 0.2b^2$
- Often arises when parameters have very different units

Effects of bad scaling

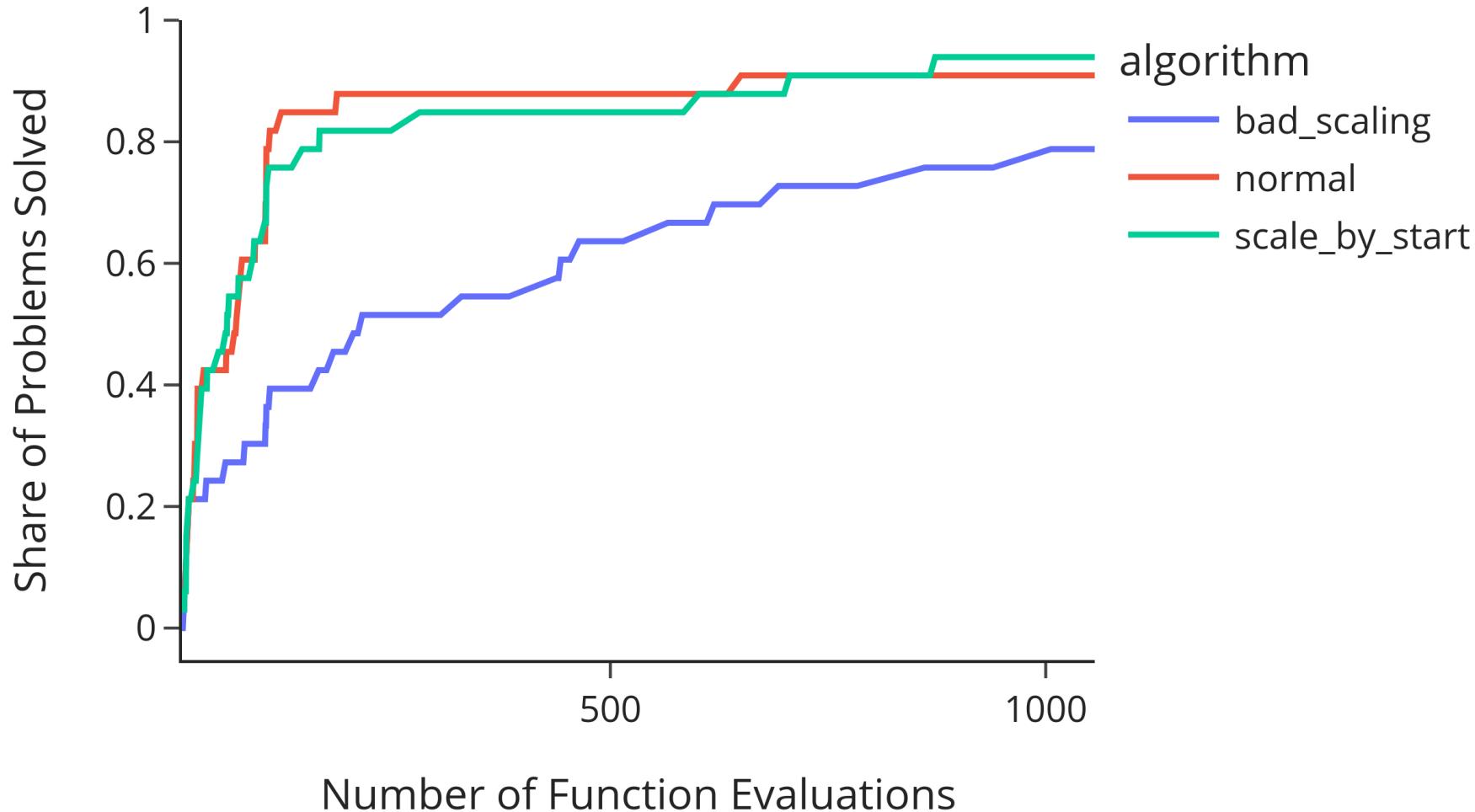
- Will try performance of optimizers on
 - Standard "estimagic" set of problems
 - badly scaled version
 - badly scaled version when `scaling=True` in `minimize`

```
problems_bad_scaling = get_benchmark_problems(  
    name="estimagic",  
    scaling=True,  
    scaling_options={"min_scale": 1, "max_scale": 1_000},  
)
```

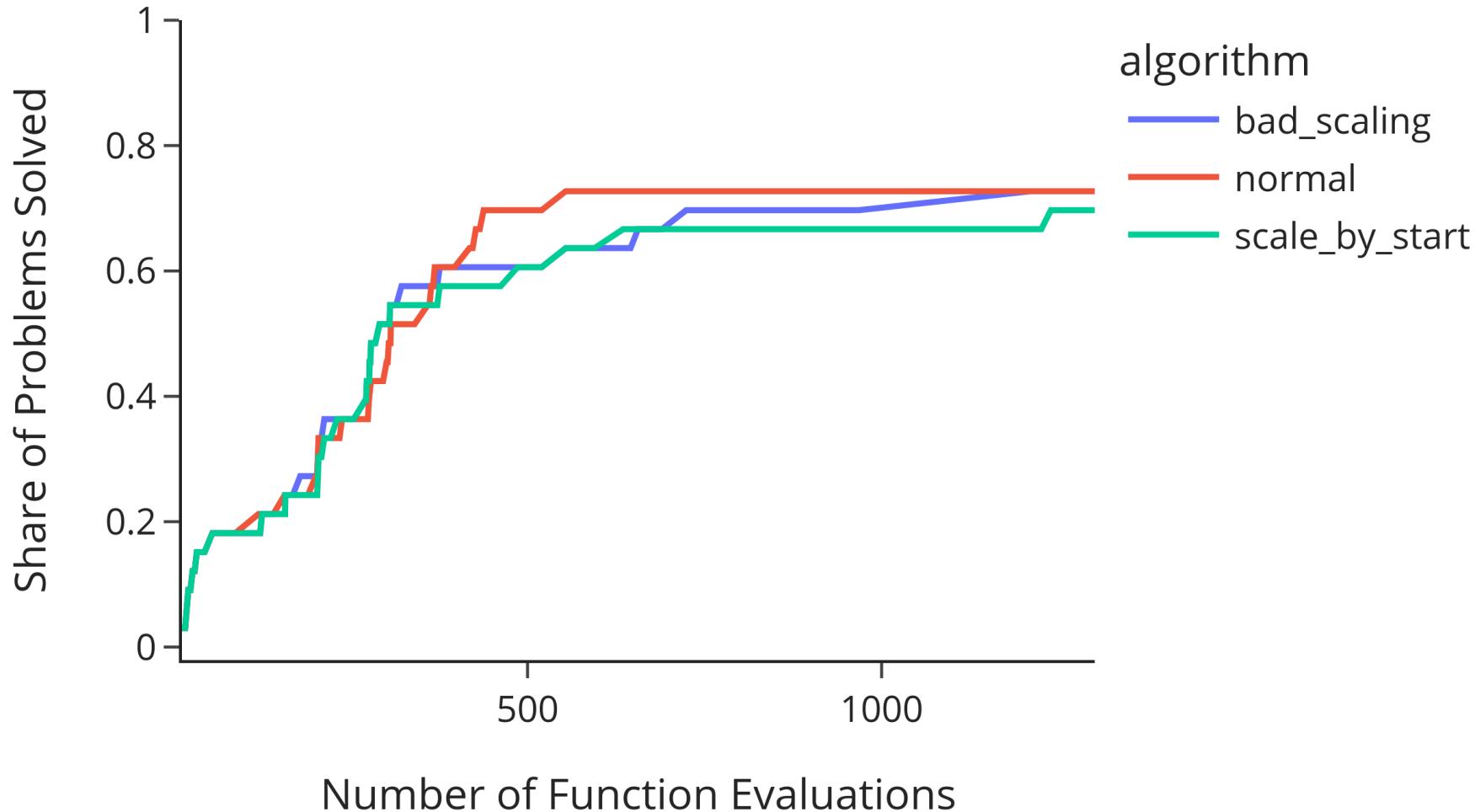
Effect of bad scaling: `scipy_lbfgsb`



Effect of bad scaling: nag_dfols



Effect of bad scaling: nlopt_bobyqa



Scaling in estimagic: By start params

```
def badly_scaled(x):
    out = (
        0.01 * np.abs(x[0])
        + np.abs(x[1])
        + (x[2] - 0.9) ** 6
    )
    return out

em.minimize(
    criterion=badly_scaled,
    params=np.array([200, 1, 1]),
    scaling=True,
)
```

- Optimizer sees x / x_{start}
- Will recover that $x[0]$ needs large steps
- Won't recover that $x[2]$ needs tiny steps

Scaling in estimagic: By bounds

```
em.minimize(  
    criterion=badly_scaled,  
    params=np.array([200, 1, 1]),  
    scaling=True,  
    lower_bounds=np.array([-200, -2, 0.8]),  
    upper_bounds=np.array([600, 2, 1]),  
    scaling=True,  
    scaling_options={"method": "bounds"},  
)
```

- Internal parameter space mapped to $[0, 1]^n$
- Will work great in this case
- Requires careful specification of bounds

Very scale sensitive

- nag_pybobyqa
- tao_pounders
- pounders
- nag_dfols
- scipy_cobyla

Somewhat scale sensitive

- scipy_lbfgsb
- fides

Not scale sensitive

- scipy_neldermead
- nlopt_neldermead
- nlopt_bobyqa
- scipy_powell
- scipy_ls_lm
- scipy_ls_trf

Practice Session 6: Scaling of optimization problems (15 min)

JAX and JAXopt

Preview of practice session(s)

- Solve an optimization problem using JAX gradients
- Solve an optimization problem using JAXopt
- Write a batched solver using JAXopt

Numerical vs automatic differentiation (oversimplified)

- **Automatic differentiation**

- Magic way to calculate precise derivatives of Python functions
- Gradient calculation takes 3 to 4 times longer than function
- Runtime is independent of number of parameters
- Code must be written in a certain way

- **Numerical differentiation**

- Finite step approximation to derivatives
- Less precise than automatic differentiation
- Runtime increases linearly with number of parameters

What is JAX

- GPU accelerated replacement for Numpy
- State of the art automatic differentiation
 - Gradients
 - Jacobians
 - Hessians
- Just in time compiler for python code
- Composable function transformations such as `vmap`

Calculating derivatives with JAX

```
>>> import jax.numpy as jnp
>>> import jax

>>> def sphere(x):
...     return jnp.sum(x ** 2)

>>> gradient = jax.grad(sphere)

>>> gradient(jnp.array([1., 1.5, 2.]))
DeviceArray([2., 3., 4.], dtype=float64)
```

Providing derivatives to estimagic

```
>>> def sphere_gradient(params):
...     return 2 * params

>>> em.minimize(
...     criterion=sphere,
...     params=np.arange(5),
...     algorithm="scipy_lbfgsb",
...     derivative=sphere_gradient,
... )

>>> em.minimize(
...     criterion=sphere,
...     params=np.arange(5),
...     algorithm="scipy_lbfgsb",
...     numdiff_options={"n_cores": 6},
... )
```

- You can provide derivatives
- Otherwise, estimagic calculates them numerically
- Parallelization on (up to) as many cores as parameters

Practice Session 7: Using JAX derivatives in estimagic (10 min)

What is JAXopt

- Library of optimizers written in JAX
- Hardware accelerated
- Batchable
- Differentiable

When to use it

- Solve many instances of same optimization problem
- Differentiate optimization w.r.t hyperparameters

Example

Economic problem:

- Many agents facing similar optimization problem
 - batchable
- Gradient of log-likelihood requires gradient of solutions
 - differentiable solutions

Simple optimization in JAXopt

```
>>> import jax
>>> import jax.numpy as jnp
>>> from jaxopt import LBFGS

>>> x0 = jnp.array([1.0, 2, 3])
>>> shift = x0.copy()

>>> def criterion(x, shift):
...     return jnp.vdot(x, x + shift)

>>> solver = LBFGS(fun=criterion)

>>> result = solver.run(init_params=x0, shift=shift)
>>> result.params
DeviceArray([-0.5, -1. , -1.5], dtype=float64)
```

- import solver
- initialize solver with criterion
- run solver with starting parameters
- pass additional arguments of criterion to run method

Vmap

```
>>> import numpy as np
>>> import scipy as sp

>>> a = np.stack([np.diag([1, 2]), np.diag([3, 4])])
>>> a[0]
array([[ 1.,  0.],
       [ 0.,  2.]))

>>> sp.linalg.inv(a[0])
array([[ 1., -0.],
       [ 0.,  0.5]])

>>> sp.linalg.inv(a)
... ValueError: expected square matrix

>>> res = [sp.linalg.inv(a[i]) for i in [0, 1]]
>>> np.stack(res)
array([[[ 1.        , -0.        ],
         [ 0.        ,  0.5       ]],
       [[ 0.33333333, -0.        ],
         [ 0.        ,  0.25      ]]])
```

- consider matrix inversion
- not defined for arrays with dimension > 2 (in `scipy`)
- loop over 2d matrices
- syntactic sugar: `np.vectorize` and the like
 - does not increase speed

Vmap in JAX

```
>>> import jax.numpy as jnp
>>> import jax.scipy as jsp
>>> from jax import vmap, jit

>>> a = jnp.array(a)

>>> jax_inv = jit(vmap(jsp.linalg.inv))

>>> jax_inv(a)
DeviceArray([[ [1.        ,  0.        ],
              [0.        ,  0.5       ],
              [[0.33333333,  0.        ],
               [0.        ,  0.25      ]]], dtype=float64)
```

- use `jax.numpy` and `jax.scipy`
- define vectorized map using `jax.vmap`
- need `jit` on the outside to compile the new function

Vectorize an optimization in JAXopt

```
>>> from jax import jit, vmap

>>> def solve(x, shift):
...     return solver.run(init_params=x, shift=shift).params

>>> batch_solve = jit(vmap(solve, in_axes=(None, 0)))
>>> shifts = jnp.array([
    [0.0, 1.0, 2.0],
    [3.0, 4.0, 5.0]
])
>>> batch_solve(x0, shifts)
DeviceArray([[ 0. , -0.5, -1. ],
            [-1.5, -2. , -2.5]], dtype=float64)
```

- import jit and vmap
- define wrapper around solve
- call vmap on wrapper
 - in_axes=(None, 0) means that we map over the 0-axis of the second argument
 - call jit at the end

Differentiate a solution in JAXopt

```
>>> from jax import jacobian

>>> jacobian(solve, argnums=1)(x0, weight)
DeviceArray([[-0.5,  0. ,  0. ],
            [ 0. , -0.5,  0. ],
            [ 0. ,  0. , -0.5]], dtype=float64)
```

- import jacobian or grad
- use argnums to specify w.r.t.
which argument we
differentiate

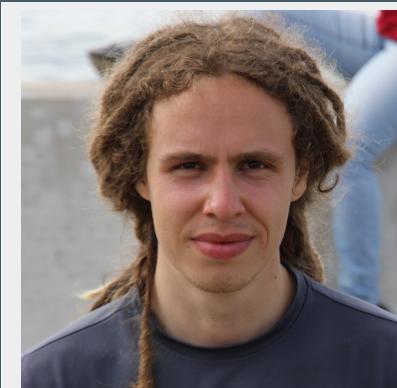
Practice Session 8: Vectorized optimization in JAXopt (15 min)

Final remarks

Tips

- Exploit least squares structure if you can
- Look at criterion and params plots
- Try multiple algorithms (based on theory) and take the best (based on experiments)
- Think about scaling
- Use multistart over genetic algorithms for well behaved functions
- Make your problem jax compatible and use automatic differentiation

The estimagic Team



Janos



Tim



Klara



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Tobias



Hans-Martin

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  on
github.com/OpenSourceEconomics/estimagic