Practical Numerical Optimization with Scipy, Estimagic and JAXopt

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About Us

- Website: janosg.com
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- Original author of estimagic
- Submitted PhD thesis, looking for interesting jobs soon

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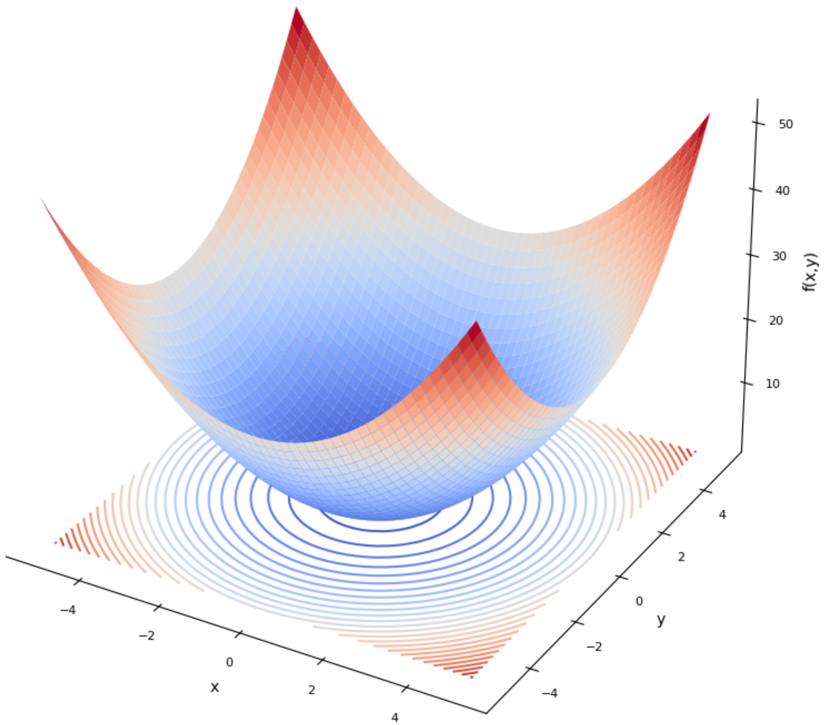
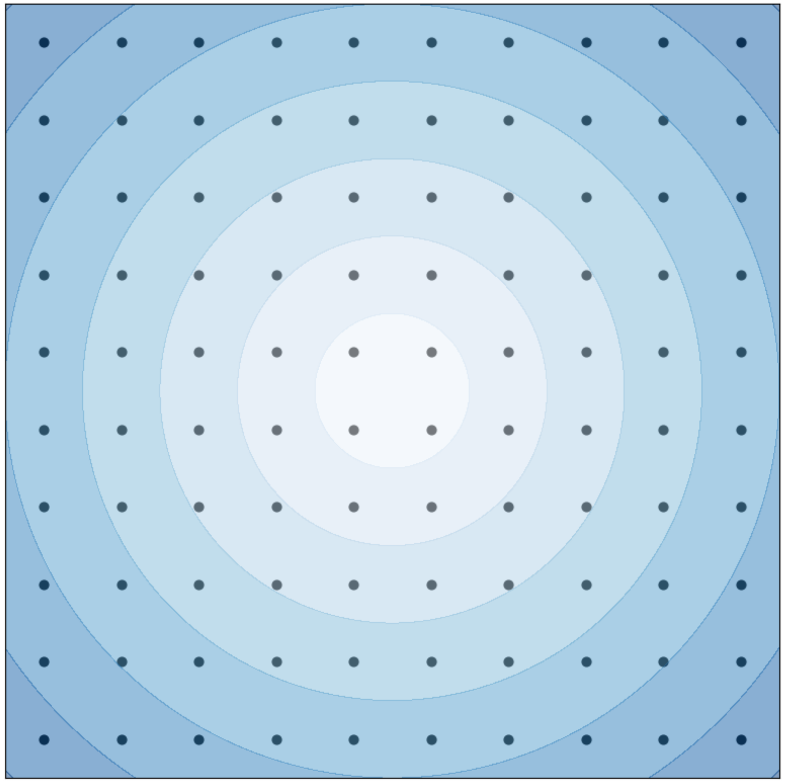
What is numerical optimization

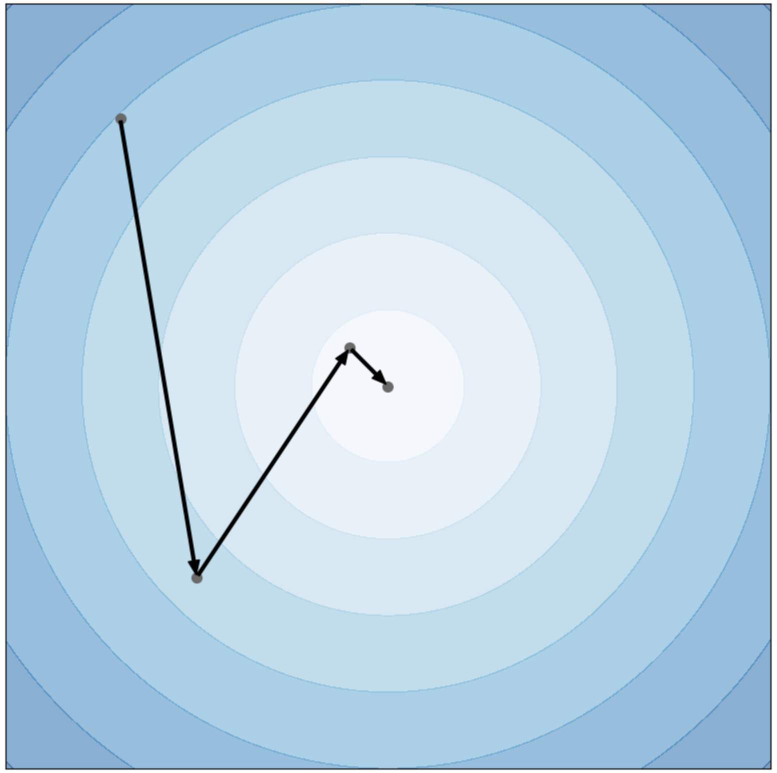
Example problem

- Parameters x_1, x_2
- Criterion $f(x_1, x_2) = x_1^2 + x_2^2$
- Want: $x_1^*, x_2^* = argmin_{x_1,x_2} f(x_1, x_2)$
- Possible extensions:
  - Constraints
  - Bounds
- Optimum at $(0, 0)$ with function value 0

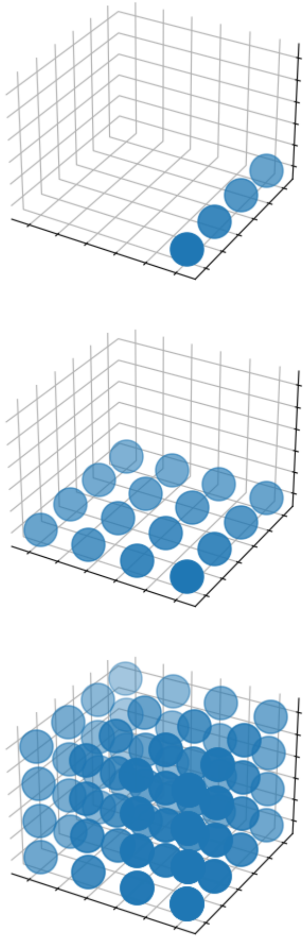


Brute force vs. smarter algorithm





Complexity of 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

In this talk

- Nonlinear optimization with continuous parameters
- Linear and nonlinear constraints
- Global optimization
- Diagnostics and strategies for difficult probles

Not Covered

- Linear programming
- Mixed integer programming
- Stochastic gradient descent

Introduction to scipy.optimize

Solve example problem with scipy.optimize

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

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

>>> x0 = np.ones(2)
>>> res = minimize(f, 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
- Maximization is done by minimizing $-f(x)$
- Different interfaces for:
    - global optimization
    - nonlinear least-squares

Practice Session 1: First optimization with scipy.optimize (15 min)

Shortcomings of scipy.optimize

- Very few algorithms
- No parallelization
- Maximization via sign flipping
- No diagnostics tools
- No feedback before optimization or in case of crash
- No built-in multistart, benchmarking, scaling, or logging
- Parameters are 1d numpy arrays

Examples from real projects I

```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 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

What is estimagic?

- Library for difficult numerical optimization
- Additional tools for nonlinear estimation
- Wraps many other optimizer libraries:
  - Scipy, Nlopt, TAO, Pygmo, ...
- Harmonized interface
- A lot of additional functionality

You can use it like scipy

```
>>> import estimagic as em

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

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

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

- No default algorithm
- Many optional arguments scipy does not have

Params can be (almost) anything

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


>>> res = em.minimize(
...     criterion=dict_sphere,
...     params={"a": 0, "b": 1, "c": pd.Series([2, 3, 4])},
...     algorithm="scipy_powell",
... )

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

- `params` can be (nested) dicts, lists, tuples or namedtuples containing numbers, arrays, Series and DataFrames.
- Special case: DataFrame with columns `"value"`, `"lower_bound"` and `"upper_bound"`

OptimizeResult is very informative

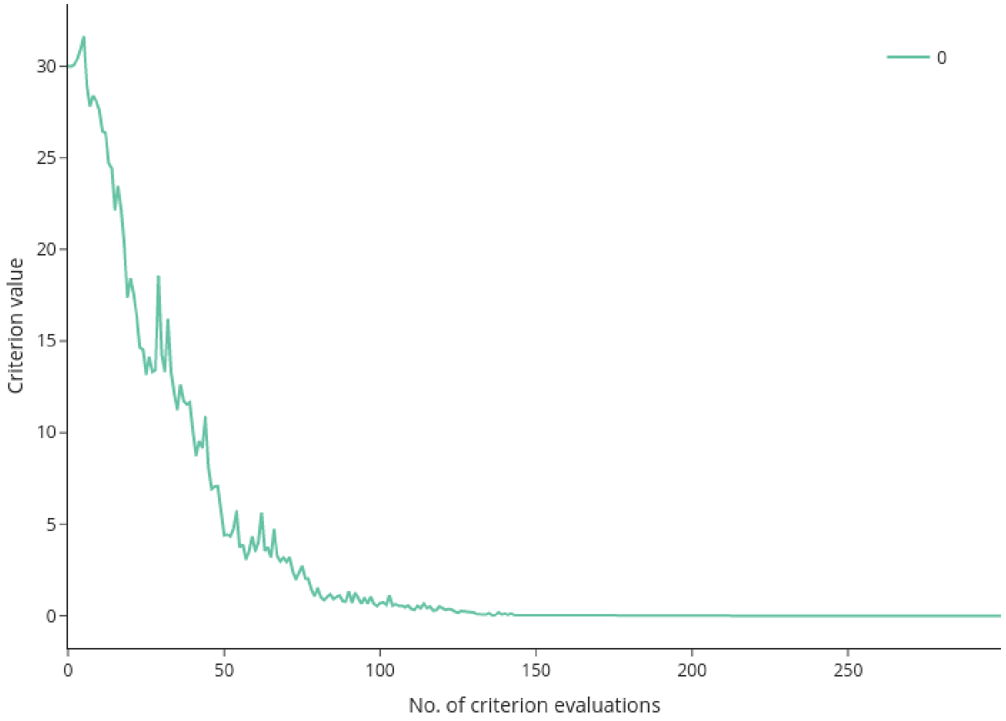
```
>>> res = em.minimize(dict_sphere, params={"a": 0, "b": 1, "c": pd.Series([2, 3, 4])}, algorithm="scipy_neldermead")
>>> res
Minimize with 5 free parameters terminated successfully after 805 criterion evaluations and 507 iterations.

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.)
```

OptimizeResult has useful 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'])
```

Criterion plot

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

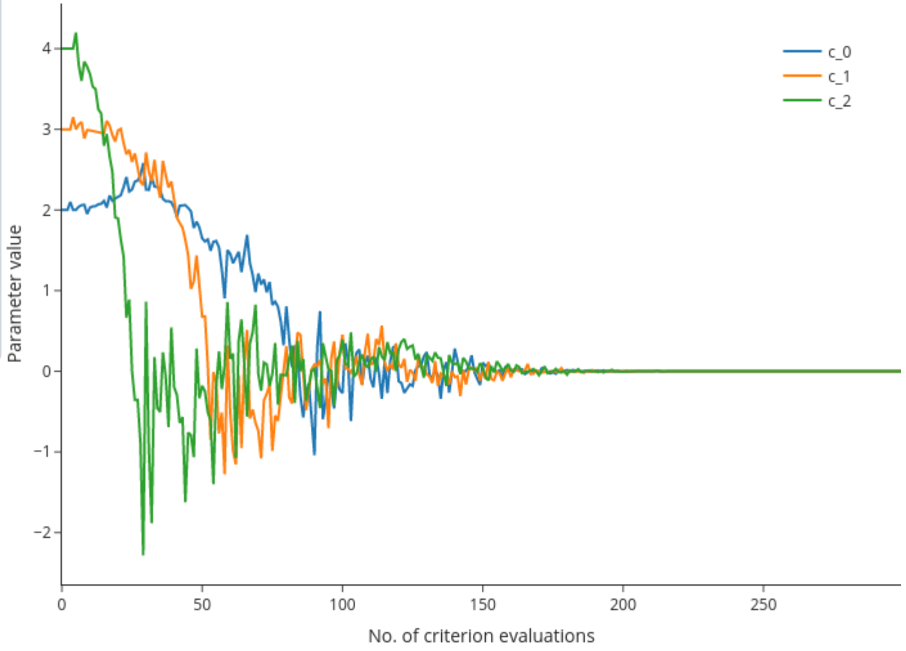


- First argument can be a `OptimizeResult` , path to log file or dictionary containing these as values
- `monotone=True` shows the current best value
- `max_evaluations` sets range of x-axis

Params plot

```python
params = {
    "a": 0,
    "b": 1,
    "c": pd.Series([2, 3, 4])
}
em.params_plot(
    res,
    max_evaluations=300,
    selector=lambda x: x["c"],
)
```

- Similar options as `criterion_plot`
- `selector` is a function returning a subset of params



Unified interface to (collections of) algorithms

- **Nlopt**: Local and global algorithms by Stephen Johnson (MIT)
- **Pygmo**: Global algorithms by Franceso Biscani and Dario Izzo (ESA)
- **fides**: Pure Python algorithm by Fabian Fröhlich (Harvard)
- **TAO**: Toolkit for advanced optimization (Argonne national lab)
- **Cyipopt**: Python binding by Jason Moore to **IPOPT** algorithm by Andreas Wächter (Northwestern)
- **estimagic**: Python implementations of some important algorithms
- **Will add more soon (it is quite easy)**

Constraints via reparametrizations

```python
>>> res = 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.])
```

- constraints is a list of dicts
- specify subset of parameters via `loc`, `query` or `selector`
- specify type of constraint
  - linear
  - probability
  - covariance
  - ...

Closed-form or parallel numerical derivatives

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

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

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

- Numerical derivatives are calculated if user does not provide a derivative
- Efficient parallelization on (up to) as many cores as parameters

There is maximize

```
>>> from estimagic import maximize

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

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

Built in multistart framework

```
>>> res = 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 by Fatih Guvenen and Serdar Ozkan
- Exploration phase on random sample
- Local optimizations from best points

Exploit structure of your problem

```
>>> def general_sphere(params):
...     contribs = params**2
...     out = {
...         "root_contributions": params,
...         "contributions": contribs,
...         "value": contribs.sum(),
...     }
...     return out

>>> res = minimize(
...     criterion=general_sphere,
...     params=np.arange(5),
...     algorithm="pounders",
... )
>>> res.params
array([0., 0., 0., 0., 0.])
```

- Exploit structure of the problem
- Common structures
  - least-squares: $F(x) = \sum_i f_i(x)^2$
  - sum: $F(x) = \sum_i f_i(x)$, e.g. log-likelihood
- Huge speed-ups
- Increased robustness

Logging and Dashboard

```
>>> res = minimize(
...     criterion=sphere,
...     params=np.arange(5),
...     algorithm="scipy_lbfgsb",
...     logging="my_log.db",
...     log_options={
...         "if_database_exists": "replace"
...     },
... )

>>> 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 of parameters and criterion values
- Thread safe sqlite database
- No data loss, even if computer crashes
- Can be read during optimization
- Provides data for real-time dashboard

Harmonized as much as possible but not more

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

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

- Same options have same name
- Different options have different names (e.g. not one `tol` argument)
- Ignore options that don't apply

The estimagic Team

Janos

Tim

Klara

Sebastian

Tobias

Hans-Martin

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- Collaborative Research Center Transregio 224 for funding

Break (5 min)

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

Choosing algorithms

Relevant problem properties

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

`scipy_lbfgsb`

- Limited memory BFGS
- BFGS is a method to approximate hessians from multiple gradients
- Supports bounds
- 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
- Supports bounds
- Developed by Fabian Fröhlich as a Python package
- Many advanced options to customize the optimization!
- Criterion must be differentiable
- Good solution if scipy_lbfgsb picks too extreme parameters that cause numerical overflow

`nlopt_bobyqa` , `nag_pybobyqa`

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

`scipy_neldermead`, `nlopt_neldermead`

- Popular direct search method
- `nlopt` version supports bounds
- `nlopt` version requires much fewer criterion evaluations in most benchmarks
- Never the best choice but often not the worst
- Can be very precise if run long enough

`scipy_ls_lm`, `scipy_ls_trf`

- Derivative based optimizers for least squares problems
- Criterion needs the structure: $F(x) = \sum_i f_i(x)^2$
- In estimagic, criterion function must return a dictionary:

```python
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 problems
- Both beat bobyqa for least-squares problems!
- `nag_dfols` is fastest and usually requires fewest criterion evaluations
- `nag_dfols` has advanced options to deal with noise
- `pounders` can do criterion evaluations in parallel

`ipopt`

- Interior point optimizer for problems with nonlinear constraints
- Probably the best open source optimizer for large constrained problems
- We wrap it via `cyipopt`
- Difficult to install on windows

Practice Session 3: Play with `algorithm` and `algo_options` (20 min)

What is benchmarking

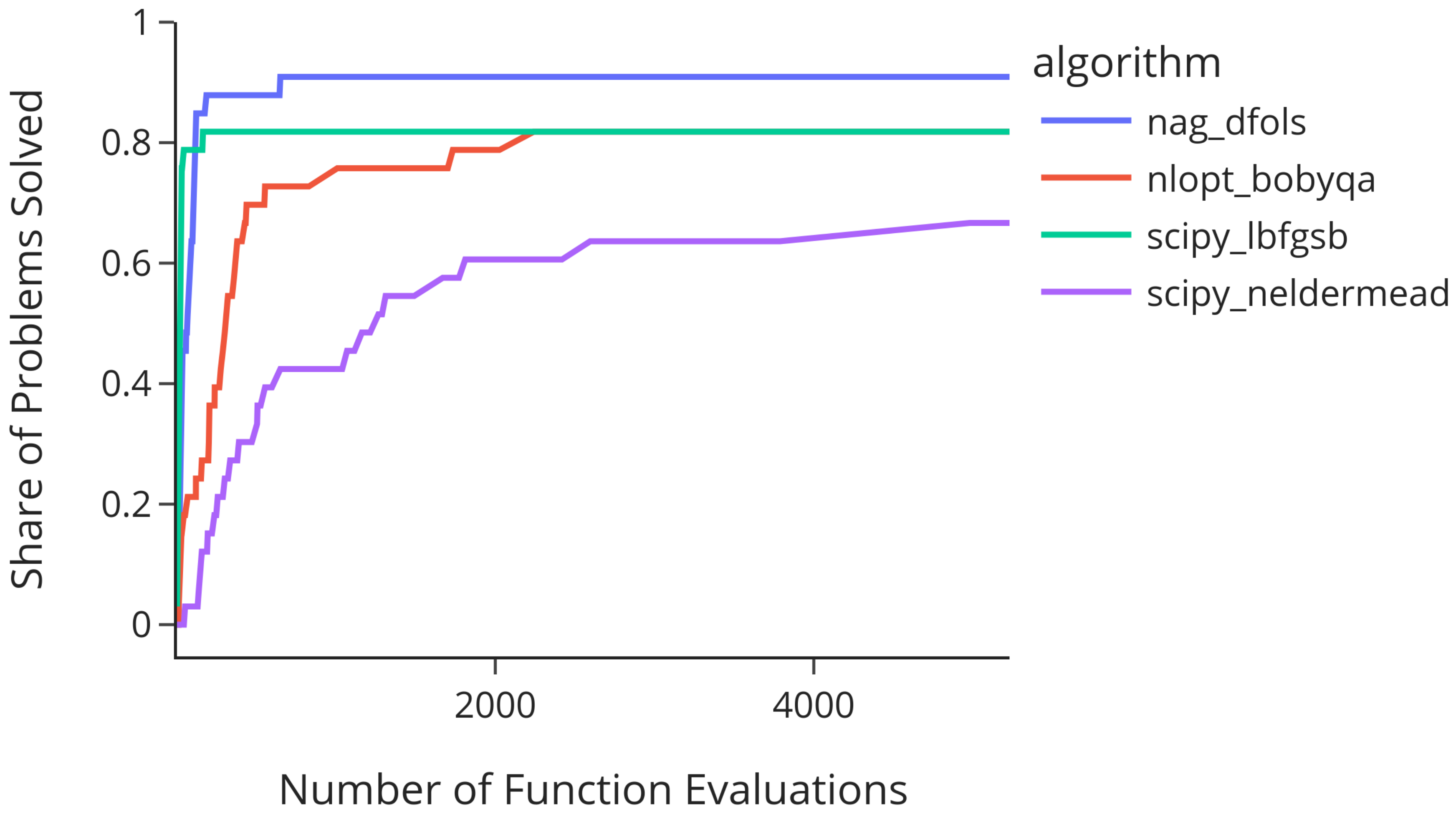
- Compare multiple algorithms on functions with known optimum
- Should mirror problems you actually want to solve
  - similar number of parameters
  - similar w.r.t. differentiability or noise
- Benchmark functions should be fast!
- Standardized benchmark sets and ways to visualize results

Running benchmarks in estimagic

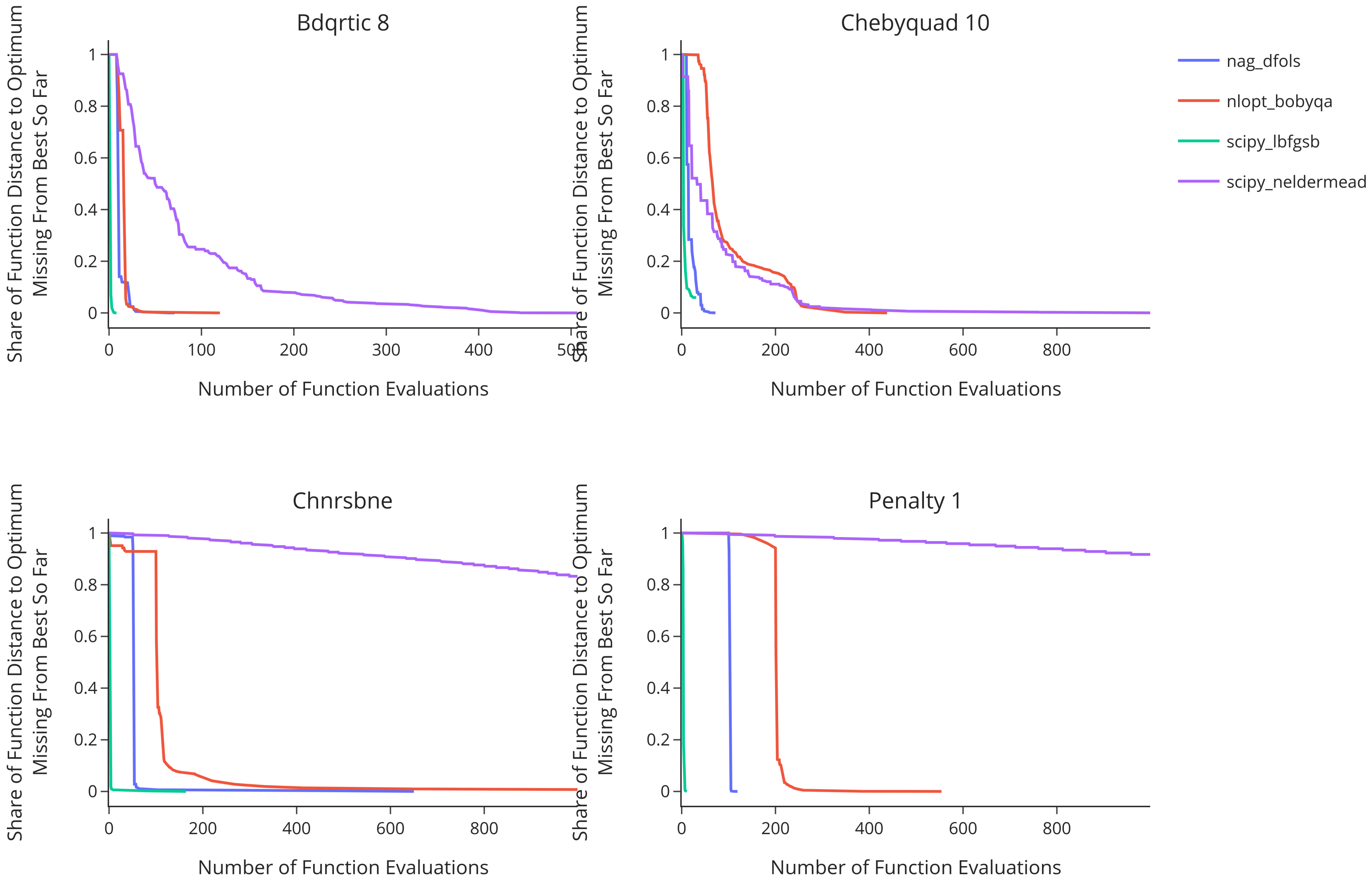
```python
problems = em.get_benchmark_problems("estimagic")
optimizers = [
    "scipy_lbfgsb",
    "nag_dfols",
    "nlopt_bobyqa",
    "scipy_neldermead",
]
results = em.run_benchmark(
    problems=problems,
    optimize_options=optimizers,
    n_cores=4,
    max_criterion_evaluations=1000,
)
```

- Multiple benchmark sets
  - more_wild
  - estimagic
  - example
- Add noise or scaling problems
- Can pass additional options to govern minimization
- Benchmarks run in parallel

Profile plots



Convergence plots



Advanced options

```python
problems = em.get_benchmark_problems(
    name="example",
    additive_noise=True,
    additive_noise_options={
        "distribution": "normal",
        "std": 0.2,
    },
    scaling=True,
    scaling_options={
        "min_scale": 0.1,
        "max_scale": 1000,
    }
)
```

- Add additive noise
- Add bad scaling
- This would be a very difficult problem set

Practice Session 4: Benchmarking optimizers (10 min)

Break (10 min)

Terminology of constraints in estimagic

- bounds: $min_x f(x)$ s.t. $l \leq x \leq u$
  - handled by most algorithms
- estimagic constraints:
  - handled by estimagic via reparametrization
- nonlinear constraints: $min_x f(x)$ s.t. $c_1(x) = 0, c_2(x) >= 0$
  - handled by some algorithms
  - can be violated during optimization

How to specify bounds

Params as numpy array

```
>>> 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.])
```

Params as DataFrame

	value	lower_bound
a	1	1
b	2	1
c	3	1
d	4	1

How to specify bounds for pytrees

```python
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

Reparametrization example

- Example:$min_x f(x_1, x_2) = \sqrt{x_2 - x_1} + x_2^2$
- Only defined if $x_1 \leq x_2$
- Not a simple bound!
- Reparametrization approach:
  - Define $\tilde{x}_2 = x_2 - x_1$ and $\tilde{f}(x_1, \tilde{x}_2) = \sqrt{\tilde{x}_2} + (x_1 + \tilde{x}_2)^2$
  - Calculate $argmin_{x_1 \in R, \tilde{x}_2 \in R^+} \tilde{f}(x_1, \tilde{x}_2)$
  - Translate solution back into x_1 and x_2

Which constraints can be handled this way?

- Fixing parameters (simple but useful)
- Find valid covariance and correlation matrices
- Find valid probabilities
- Linear constraints (as long as there are not too many)
  - $min_x f(x) s.t. A_1 x = 0, A_2 x \leq 0$
- **Guaranteed to be fulfilled during optimization**

Do not try at home

- Easy to make mistakes when implementing this
  - forget to transform start parameters
  - forget to translate back
  - forget to adjust derivative
  - confuse directions
  - use non-differentiable transformations
- **Estimagic does reparametrizations for you!**
- **Completely hides transformed x**

Fixing parameters

Linear constraints

Nonlinear constraints

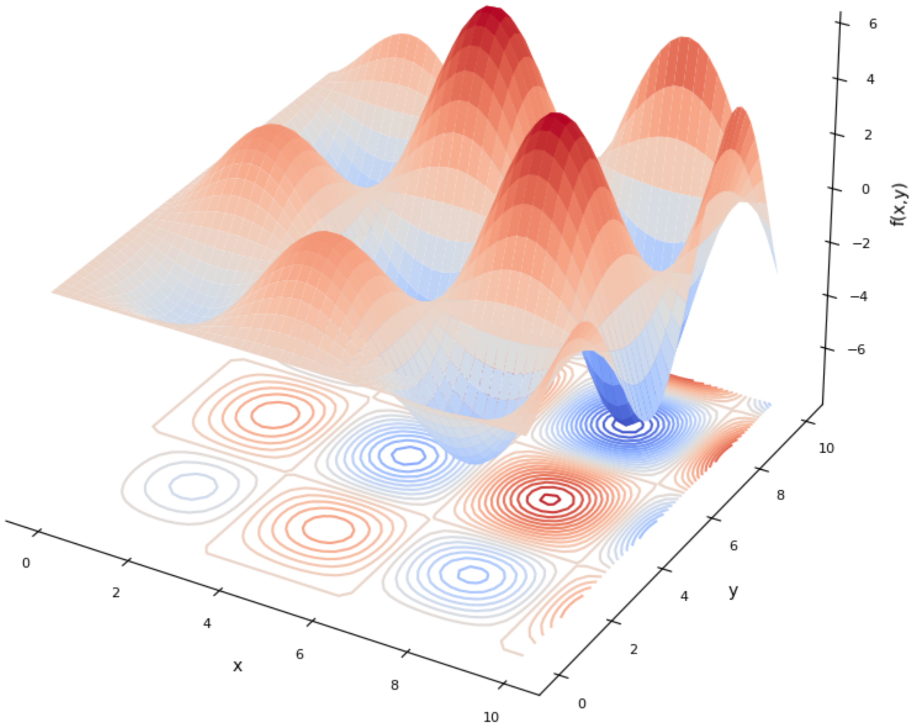
Practice Session 5: Constrained optimization (10 min)

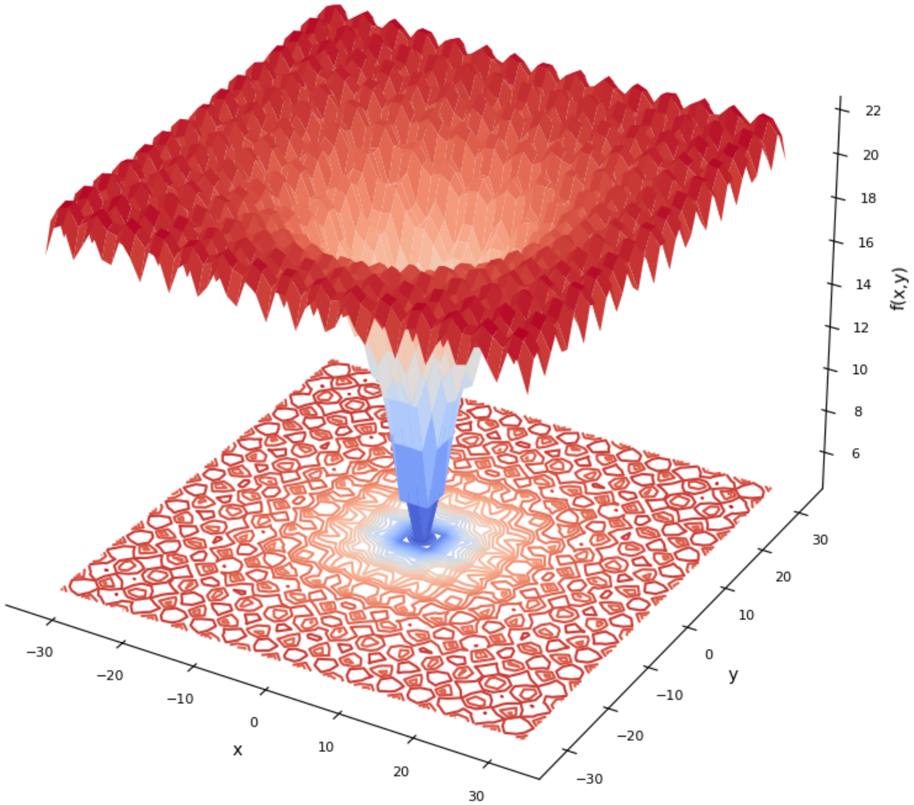
Global optimization

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
- Global and local optimization are the same for convex problems

Examples





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 (in estimagic)

- Inspired by [tiktak algorithm] by Fatih Guvenen and Serdar Ozkan
- 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 was rediscovered several times
- Use any estimagic algorithm for local optimization
- Can distinguish soft and hard bounds

How to choose

- Extremely expensive criterion (i.e. can only do a few evaluations):
  -> Bayesian optimization
- Differentiable function or least-squares structure and not too many local optima:
  -> Multistart with a 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

Advanced multistart

- Many local optima:
  - Large `"n_sample"`
  - Low `"share_optimizations"`
  - Weak convergence criteria
  - Refine result with stricter convergence criteria
- Few local optima:
  - Stick with defaults

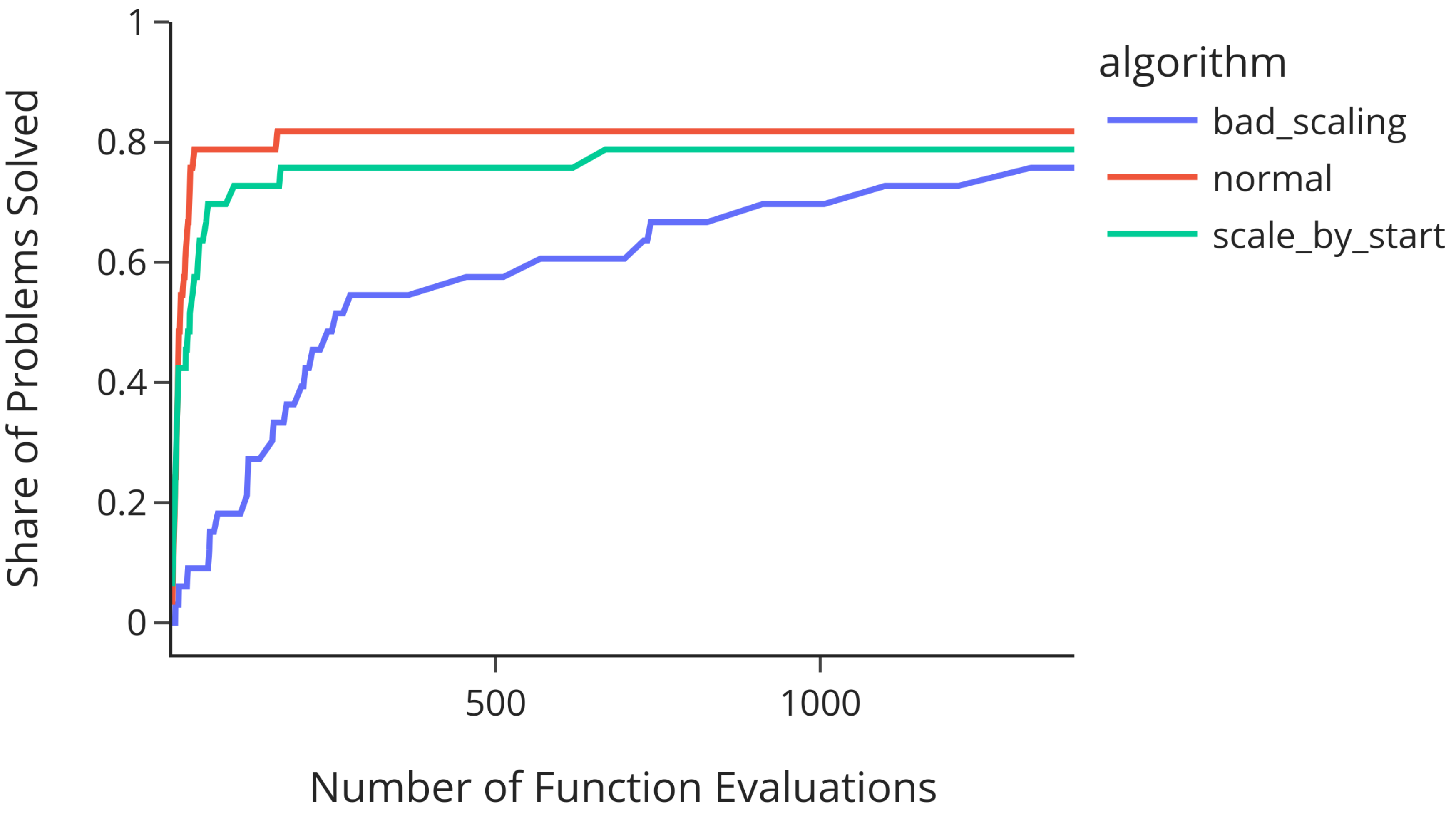
Benchmark results

Scaling

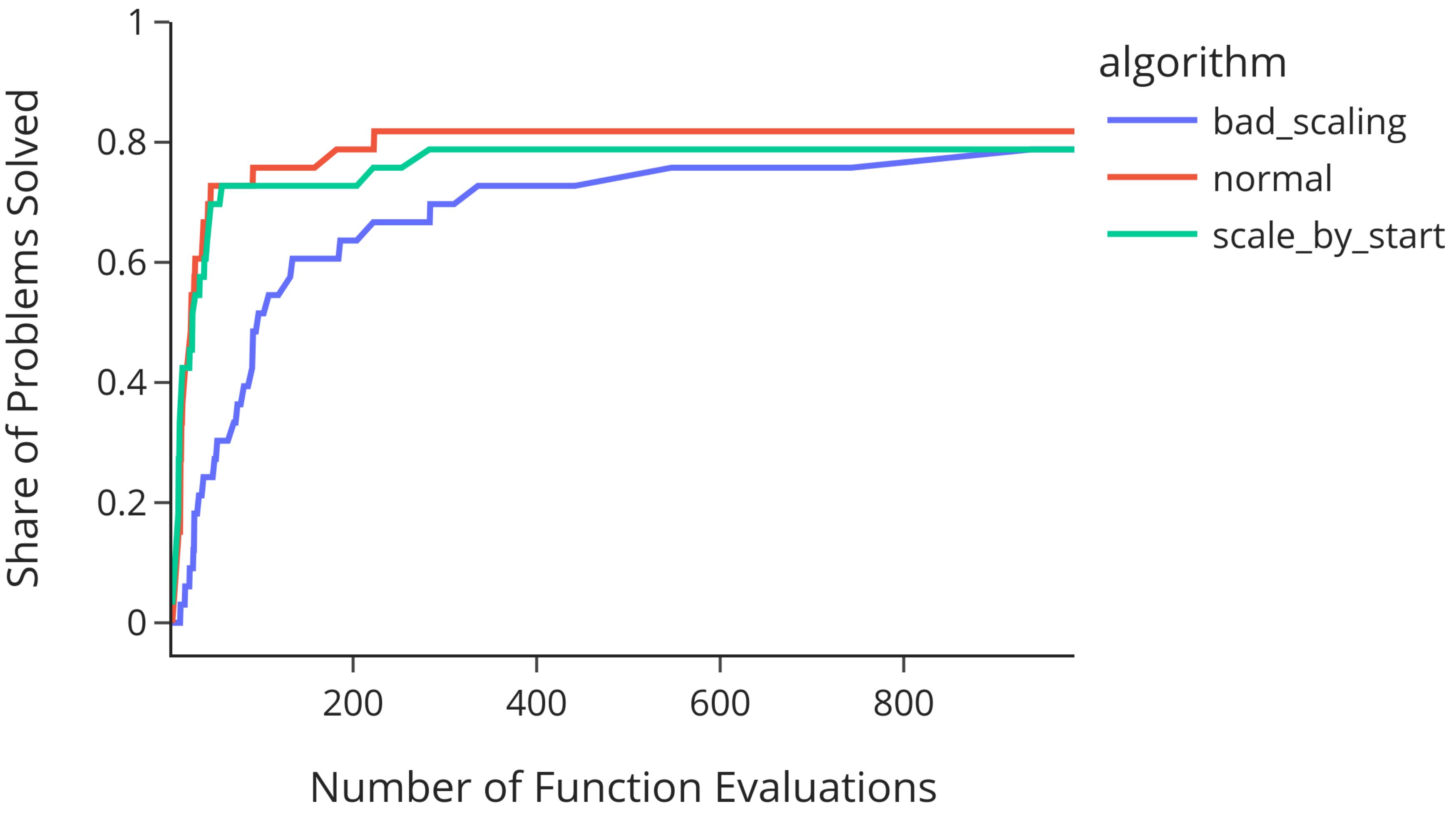
What is scaling

- Single most underrated topic among economists who do optimization!
- Well scaled: A fixed step in any parameter dimension yields roughly comparable changes in function value
  - $f(x_1, x_2) = 0.5x_1 + 0.8x_2$
- Badly scaled: Some parameters are much more influential
  - $f(x_1, x_2) = 1000x_1 + 0.2x_2$
  - $f(x_1, x_2) = e^{x_1} + \sqrt{x_2}$
- Often arises when parameters have very different units

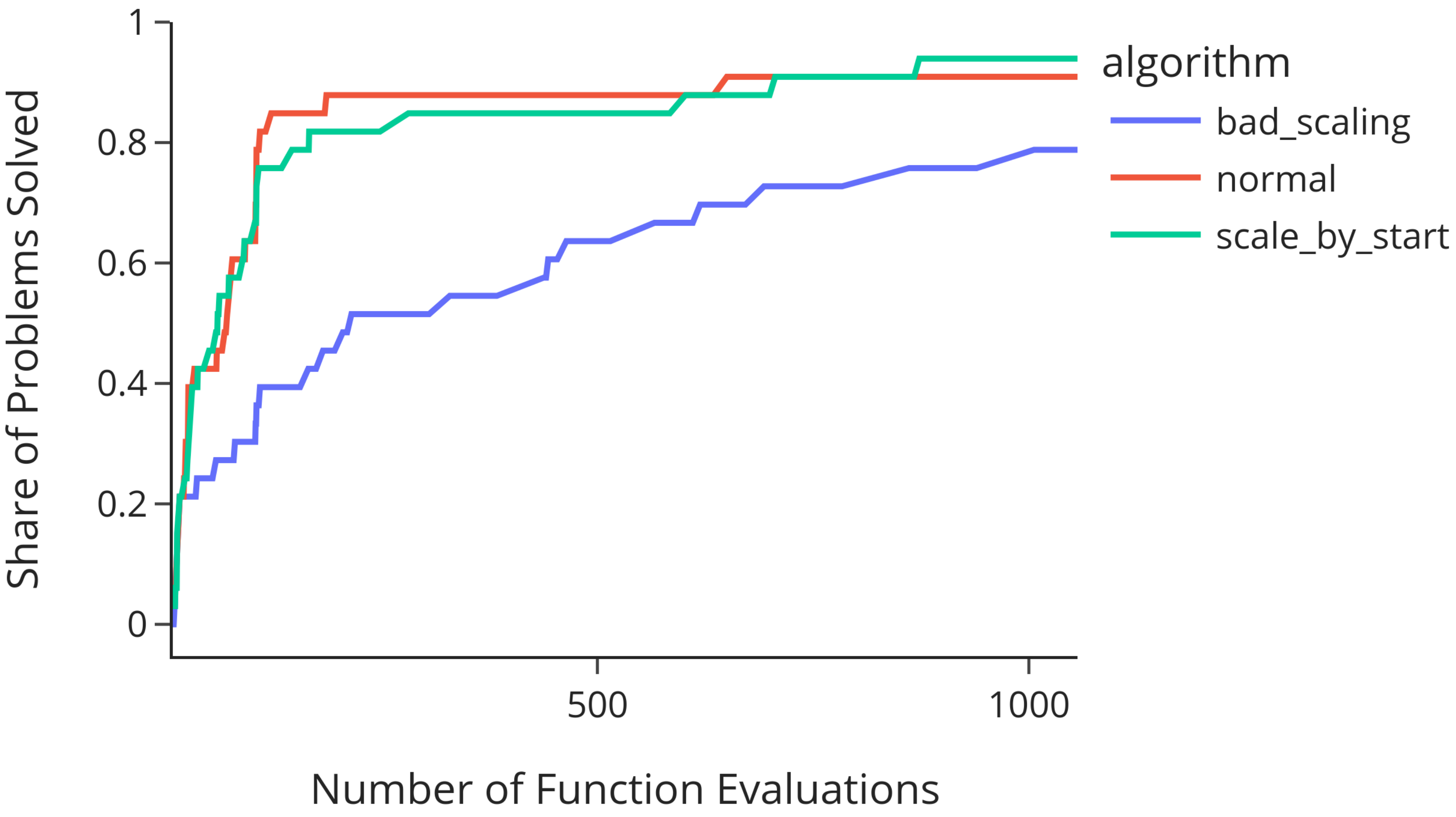
Effect of bad scaling: `scipy_lbfgsb`



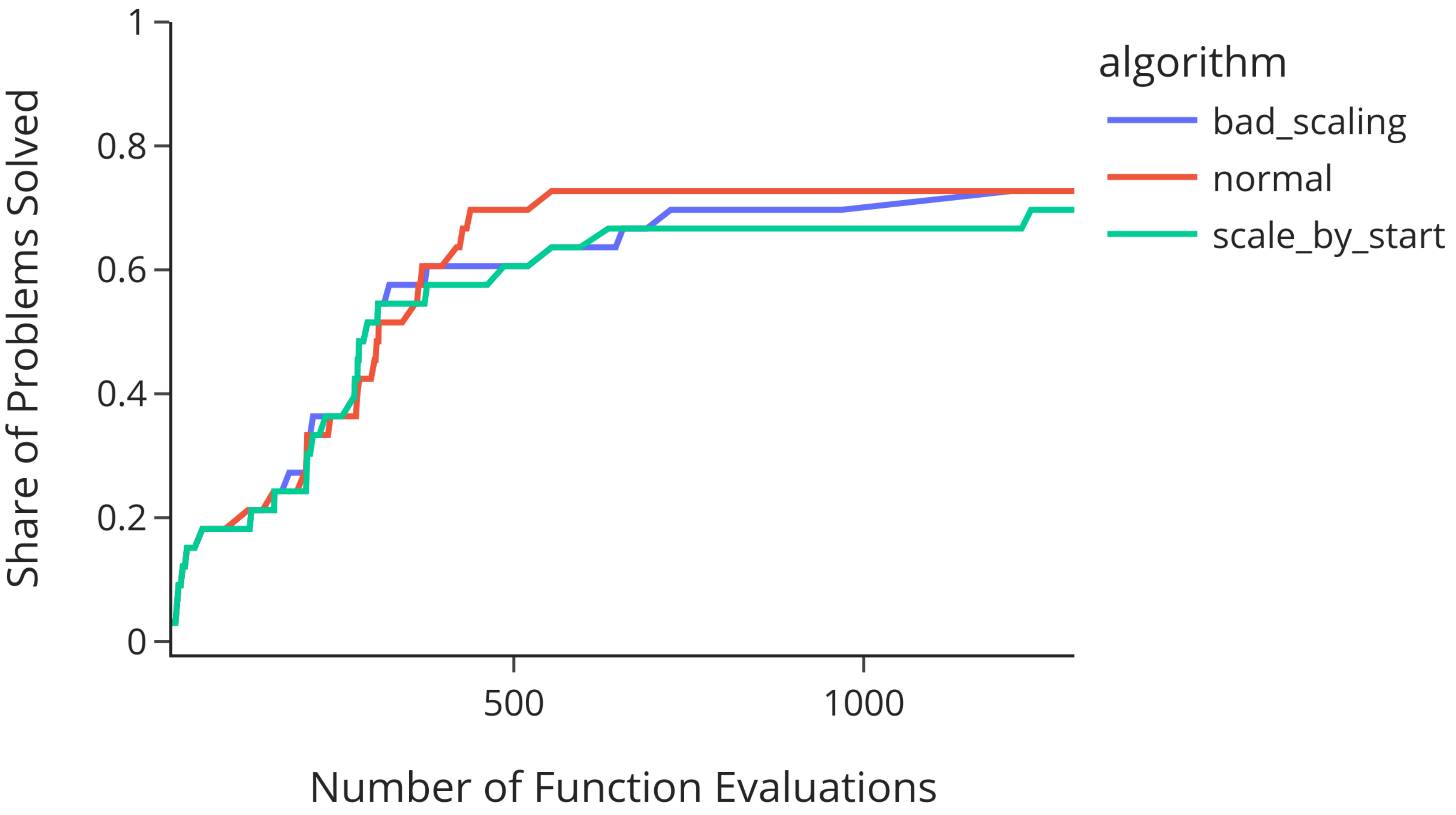
Effect of bad scaling: `fides`



Effect of bad scaling: `nag_dfols`



Effect of bad scaling: `nlopt_bobyqa`



Scaling in estimagic: By start params

```python
def badly_scaled(x):
    return 0.01 * x[0] + x[1] + x[2] ** 6

em.minimize(
    criterion=badly_scaled,
    params=np.array([200, 1, 1]),
    scaling=True,
    # pick default method explicitly
    scaling_options={
        "method": "start_values",
    }
)
```

- Optimizer sees x / x_start
- Works without bounds
- 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, 0, 0.9]),
    upper_bounds=np.array([500, 2, 1.1]),
    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 (10 min)

Features we left out

- Error handling
- Dashboard
- Log reading
- Nonlinear constraints
- Advanced parameter selection for constraints

Documentation of estimagic

- estimagic.readthedocs.io
- **Getting started**: Short tutorials
- **How to guides**: Explanations and examples for each argument of `maximize` and `minimize`
- **API Reference**: Interface of all public functions
- **Explanations**: Background information, tips and tricks, best practices

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

Numerical dervatives vs. automatic differentiation

What is JAX

Calculating derivatives with JAX

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

- Simple optimization problems
  - But many
- Robustness to hyper-parameters

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. , -0.5, -1. ], dtype=float64)
```

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

Vmap in JAX

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)))
>>> weights = jnp.array([
        [0.0, 1.0, 2.0],
        [3.0, 4.0, 5.0]
    ])

>>> batch_solve(x0, weights)
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)

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

>>> solve(x0, weight + 1)
DeviceArray([-0.5, -1. , -1.5], dtype=float64)
```

- import `jacobian` or `grad`
- use `argnums` to specify by which argument we differentiate

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

Summary