Optimization in Python

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Optimization tools in Python

We will go over and use two tools:

1. `scipy.optimize`
2. CVXPY

See `quadratic_minimization.ipynb`

- User inputs defined in the second cell
- Enables exploration of how problem attributes affect optimization-solver performance

`scipy.optimize`

Outline

- `scipy.optimize`
- CVXPY
- Example: `quadratic_minimization.ipynb`

`scipy.optimize`

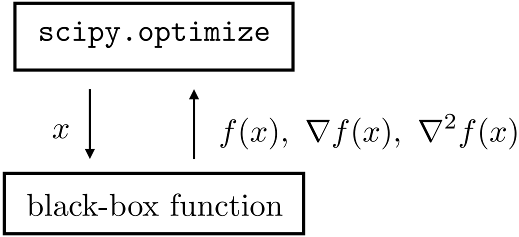
`scipy.optimize`: sub-package of SciPy, which is an open source Python library for scientific computing

- Analogous to Matlab's optimization toolbox
- Capabilities
  - Optimization
    - **Local optimization**
    - Equation minimizers
    - **Global optimization**
  - Fitting (nonlinear least squares)
  - Root finding
  - Linear Programming
  - Utilities (e.g., `check_grad` for verifying analytic gradients)

`scipy.optimize` interface

Requires the user to define a function in Python

- Can be **black box**: no closed-form mathematical expression needed!
- Only the function value $f(x)$ is required
- Can optionally provides the gradient $\nabla f(x)$ and Hessian $\nabla^2 f(x)$
- *Example*: evaluating f constitutes a run of a complicated simulation code
- **Drawback**: cannot exploit special structure underlying f



`scipy.optimize`

x

$f(x),\ \nabla f(x),\ \nabla^2 f(x)$

black-box function

`scipy.optimize`: local optimization algorithms

Unconstrained minimization

- *Derivative free*: no gradient or Hessian
    - `Nelder-Mead`: simplex
    - `Powell`: sequential minimization along each vector in a direction set
- *Gradient-based*: gradient only (no Hessian)
    - `CG`: nonlinear conjugate gradient
    - `BFGS`: quasi-Newton BFGS method
- *Gradient-based*: gradient and Hessian can be specified
    - `Newton-CG`: approximately solves Newton system using CG (truncated Newton method)
    - `dogleg`: dog-leg trust-region algorithm. Hessian must be SPD
    - `trust-ncg`: Newton conjugate gradient trust-region method

`scipy.optimize`: local optimization algorithms

Constrained minimization (all are gradient-based)

- Only bound constraints
  - `L-BFGS-B`: limited memory BFGS bound constrained optimization
  - `TNC`: truncated Newton allows for upper and lower bounds
- General constraints
  - `COBYLA`: Constrained Optimization BY Linear Approximation
  - `SLSQP`: Sequential Least SQuares Programming

`scipy.optimize`: global optimization algorithms

Global optimization (all are derivative free)

- `basinhopping`: stochastic algorithm by Wales and Doye,
  - useful when the function has many minima separated by large barriers
- `brute`: brute force minimization over a specified range
- `differential_evolution`: an evolutionary algorithm

CVXPY

Outline

`scipy.optimize`

CVXPY

Example: `quadratic_minimization.ipynb`

Modeling languages for convex optimization

- High-level language support for convex optimization has been developed recently
  1. Describe problem in high-level language
  2. Description automatically tranformed to standard form
  3. Solved by standard solver, tranformed back
- Implementations:
  - YALMIP, CVX (Matlab)
  - CVXPY (Python)
  - Convex.jl (Julia)
- Benefits:
  - Easy to perform rapid prototyping
  - Can exploit special structure because have *full mathematical description*
  - Let users focus on *what* their model should be instead of *how* to solve it
  - No algorithm tuning or babysitting
- Drawbacks:
  - Won't work if your problem isn't convex
  - Need explicit mathematical formulas for the objective and constraints
  - Thus, it *cannot handle black-box functions*

CVXPY

- **CVXPY**: “a Python-embedded **modeling language** for convex optimization problems. It allows you to **express your problem in a natural way** that follows the math, rather than in the **restrictive standard form** required by solvers.”

```
from cvxpy import *
x = Variable(n)
cost = sum_squares(A*x-b) + gamma*norm(x,1) # explicit formula!
prob = Problem(Minimize(cost,[norm(x,"inf") <=1]))
opt_val = prob.solve()
solution = x.value
```

- `solve` method converts problem to standard form, solves and assignes `opt_val` attributes

CVXPY usage

- `cvxpy.Problem`: optimization problem
- `cvxpy.Variable`: optimiation variable
- `cvxpy.Minimize`: minimization function
- `cvxpy.Parameter`: symbolic representations of constants
  - can change the value of a constant without reconstructing the entire problem
  - can enforce to be positive or negative on construction
- Constraints simply Python lists
- Many functions implemented: see cvxpy.org website for list

Complete CVXPY example

```
import cvxpy as cvx
# Create two scalar optimization variables (CVXPY Variable)
x = cvx.Variable()
y = cvx.Variable()
# Create two constraints (Python list)
constraints = [x + y == 1, x - y >= 1]
# Form objective
obj = cvx.Minimize(cvx.square(x - y))
# Form and solve problem
prob = cvx.Problem(obj, constraints)
prob.solve()  # Returns the optimal value.
print("status:", prob.status)
print("optimal value", prob.value)
print("optimal var", x.value, y.value)
```

Ensuring convexity

- CVXPY must somehow ensure the written optimization problem is convex. How?
- **Disciplined convex programming (DCP)**
  - Defines conventions that ensure an optimization problem is convex
  - *Example*: the positive sum of two convex functions is convex
  - These rules are *sufficient* (but not necessary) for convexity
- Usage in CVXPY
  - must assess the sign and curvature of `cvxpy.Variable` and `cvx.Parameter` types:
  - `x.sign`: returns sign of `x`
  - `x.curvature`: returns the curvature of `x`

Example: `quadratic_minimization.ipynb`

Outline

`scipy.optimize`

CVXPY

Example: `quadratic_minimization.ipynb`

Explore minimization methods minimization

- Consider minimizing the quadratic function

$$f(x) = \sum_{i=1}^{n} a_i \cdot (x_i - 1)^2$$

- *Properties*: convex, smooth, minimum at $x^\star = (1, \ldots, 1)$
- Let's compare method performance for:
    1. Well-conditioned (narrow distribution of a_i) v. ill-conditioned (wide distribution of a_i)
    2. Low-dimensional (n small) v. high-dimensional (n large)

Example: `quadratic_minimization.ipynb`

`scipy.opt` function implementation

- Must define function, and optionally gradient and Hessian

```
def fun(x):
    return 0.5*sum(np.multiply(quadratic_coeff,\
               np.square(np.array(x)-np.ones(np.array(x).size))))
def fun_grad(x):
    return np.array(np.multiply(quadratic_coeff,np.array(x)\
               -np.ones(np.array(x).size)))
def fun_hess(x):
    return np.diag(quadratic_coeff)
```

- To solve, define initial guess `x0` and invoke a solver with the functions as arguments:

```
res = opt.minimize(fun,x0,method='newton-cg',jac=fun_grad,hess=fun_hess)
```

Example: `quadratic_minimization.ipynb`

CVXPY setup

Assume we have already specified:

- `dimension` (`int`): number of optimization variable n
- `quadratic_coeff` (`numpy.ndarray`): array of a_i

```
import cvxpy as cvx
x = cvx.Variable(dimension)
quadratic_coeff_cvx = cvx.Parameter(dimension,sign='Positive')
quadratic_coeff_cvx.value=quadratic_coeff
obj = cvx.Minimize(0.5*quadratic_coeff.T*cvx.square(x-1))
prob = cvx.Problem(obj)
prob.solve()
```

- Note that the objective has to be explicitly coded in CVXPY objective
- Cannot use black-box functions!

Example: `quadratic_minimization.ipynb`

Method comparison

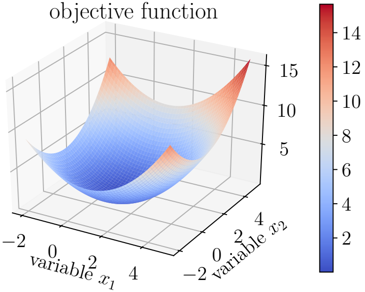
We will compare:

- Global, no gradients
  - `differential_evolution`
  - *Best performance*: non-convex, low-dimensional. Noise okay!
- Local, no gradients:
  - `Nelder-Mead`
  - `CG` with finite-difference Jacobian approximations (CGfd)
  - *Best performance*: well-conditioned, noise-free, low-dimensional
- Local, gradients:
  - `CG`
  - *Best performance*: well-conditioned, noise-free. High dimensions okay!
- Local, gradients and Hessians
  - `newton-cg`
  - `CVXPY` (requires convexity)
  - *Best performance*: noise-free. Ill-conditioning, high dimensions okay!

Example: `quadratic_minimization.ipynb`

Low-dimensional, well-conditioned

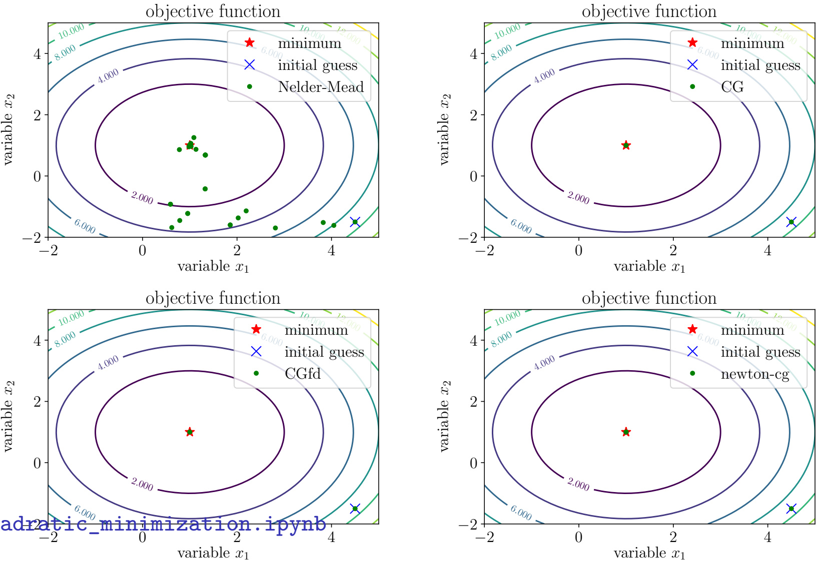
- Low-dimension: $n = 2$ optimization variables
- Well-conditioned: $a_i = 1$, $i = 1, \ldots, n$



- This is the easiest case of all!

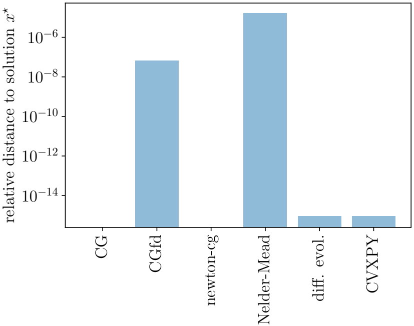
Example: `quadratic_minimization.ipynb`

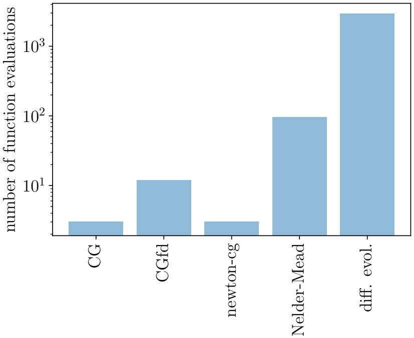
Low-dimensional, well-conditioned



Example: `quadratic_minimization.ipynb`

Low-dimensional, well-conditioned



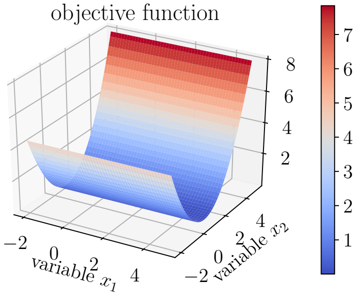


- All methods find the minimum (computed solution close to $x^\star = (1, 1)$)
- Derivative-free methods (Nelder-Mead and differential evolution) very inefficient!
- CG more expensive when finite-difference gradient approximations used

Example: `quadratic_minimization.ipynb`

Low-dimensional, poorly conditioned

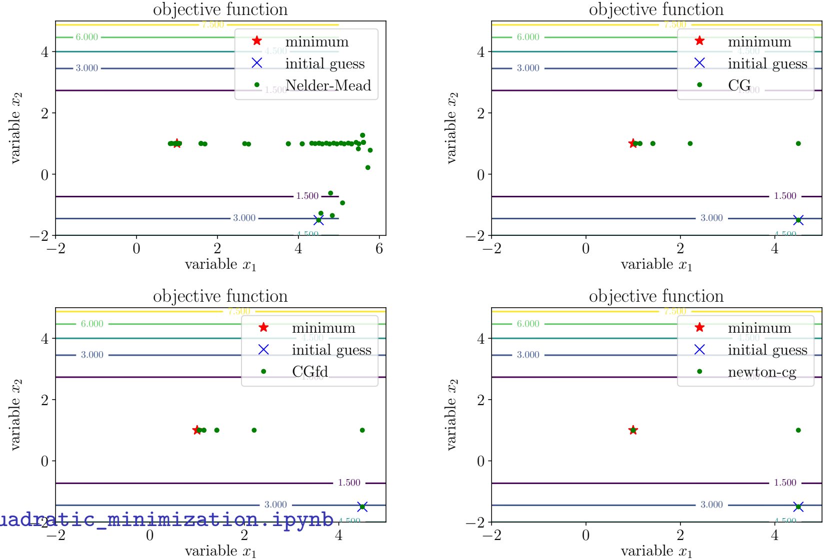
- Low-dimension: $n = 2$ optimization variables
- Poorly conditioned: $a_i = 1$ have large variance ($a_1 = 1.2 \times 10^4$, $a_2 = 1$)



- Slope is much larger in one direction relative to the other
- Hard to minimize in direction x_1 using only the gradient
- The Hessian can help in this case!

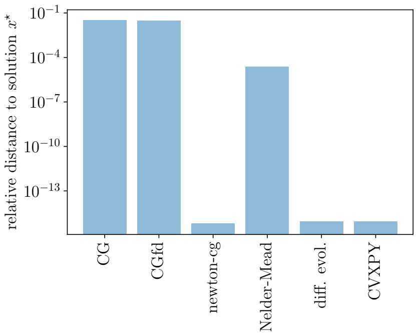
Example: `quadratic_minimization.ipynb`

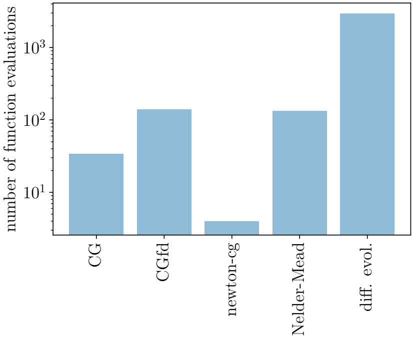
Low-dimensional, poorly conditioned



Example: `quadratic_minimization.ipynb`

Low-dimensional, poorly conditioned



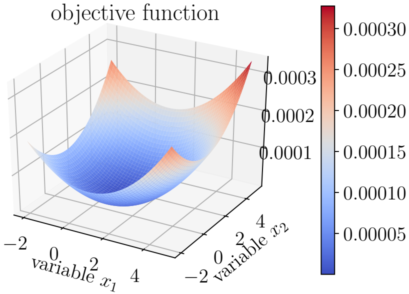


- All methods do a farily good job at finding the minimum
- `newton-cg` and `CVXPY` do the best by far (both use Hessian information)
  - Hessian information helps ‘cure’ ill conditioning!
- Derivative-free methods (Nelder-Mead and differential evolution) very inefficient

Example: `quadratic_minimization.ipynb`

High-dimensional, poorly conditioned

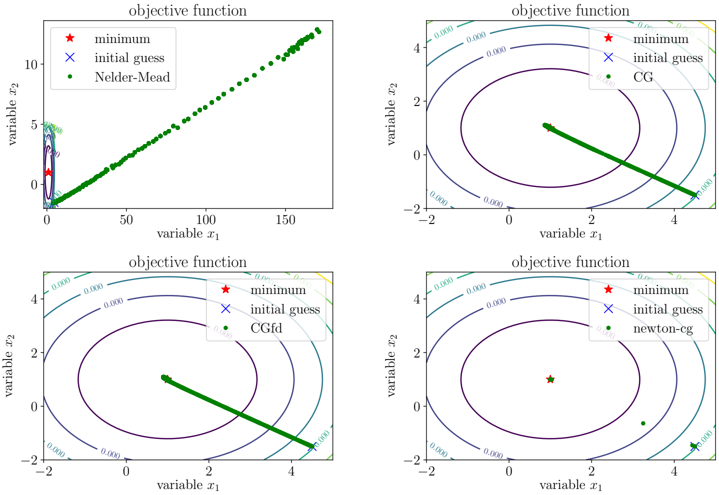
- High(er)-dimension: $n = 100$ optimization variables (not truly high dimensional)
- Poorly conditioned: $a_i = 1$ have large variance $(\max_i a_i / \min_i a_i = 3.6 \times 10^8)$



- Higher dimensions pose significant challenges to gradient-free methods

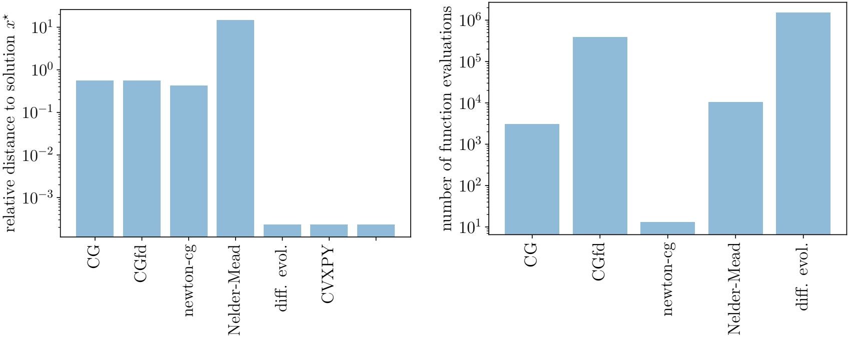
Example: `quadratic_minimization.ipynb`

High-dimensional, poorly conditioned



Example: `quadratic_minimization.ipynb`

High-dimensional, poorly conditioned



- Nelder–Mead fails to find the minimum in 10,0000 function evaluations
- Differential evolution finds the minimum, but incurs $> 10^6$ function calls!
- CG w/ finite-difference gradients is very expensive ($n + 1$ function calls per gradient)
- `newton-cg` and CVXPY do extremely well (both use Hessian information)

Example: `quadratic_minimization.ipynb`

Lessons

- Gradient information helps “cure” high-dimensionality
    - Gradients enable a good direction to be found in a high-dimensional space
    - Without gradients, many function evaluations are needed to explore the space
    - Finite-difference approximations of the Jacobian become expensive in high dimensions (require $n + 1$ function evaluations)
- Hessian information helps “cure” ill conditioning!
    - Hessians inform the optimizer of curvature; thus the optimizer deals with ill conditioning directly
    - Ill-conditioned Hessians can still pose numerical problems

Example: `quadratic_minimization.ipynb`

Let's add noise

- Let's add sinusoidal noise to the function:

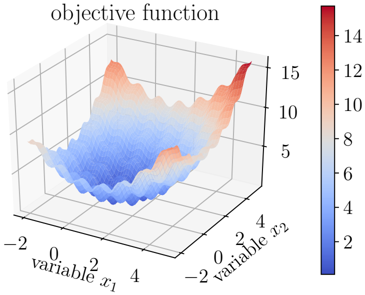
$$f(x) = \sum_{i=1}^{n} a_i \cdot (x_i - 1)^2 + b \cdot \left[n - \sum_{i=1}^{n} \cos(2\pi(x_i - 1)) \right]$$

- b controls the amount of additional noise
- For $b > 0$, the function is no longer convex!
  - Many local minima
  - Local methods may not find the global minimum!
  - CVXPY not applicable

Example: `quadratic_minimization.ipynb`

Low-dimensional, well-conditioned, noisy

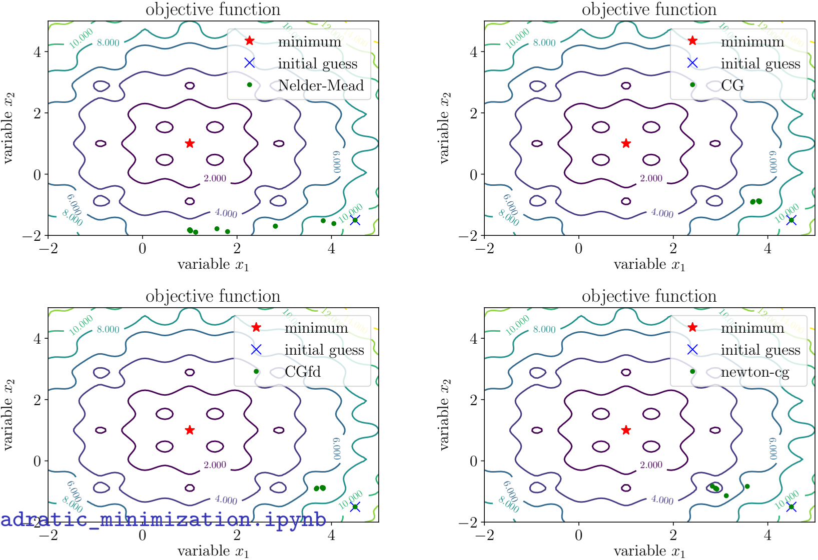
- Low-dimension: $n = 2$ optimization variables
- Well-conditioned: $a_i = 1$, $i = 1, \ldots, n$



- Many local minima in which to get “trapped”

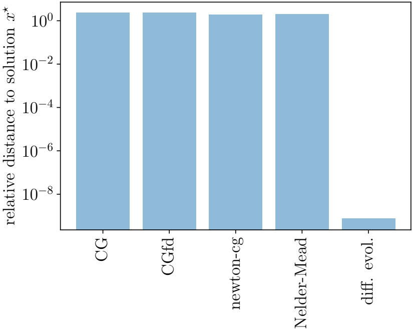
Example: `quadratic_minimization.ipynb`

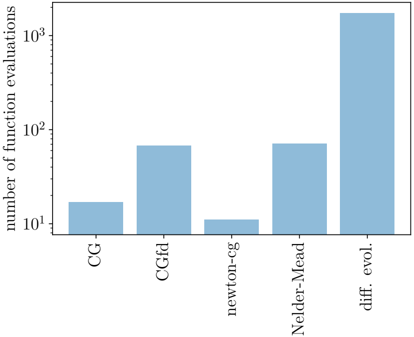
Low-dimensional, well-conditioned, noisy



Example: `quadratic_minimization.ipynb`

Low-dimensional, well-conditioned, noisy

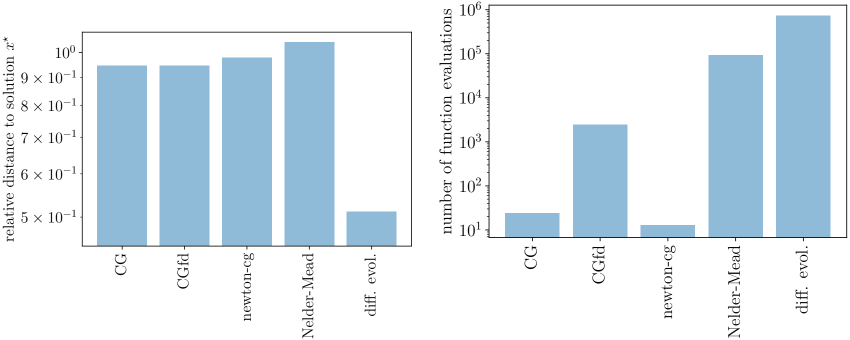




- All local methods get trapped in a local minimum
- `CVXPY` cannot be used
- differential evolution finds the closest solution,
  - However, it requires over a thousand function evaluations!

Example: `quadratic_minimization.ipynb`

High-dimensional ($n = 100$), well-conditioned, noisy



- All local methods get trapped in a local minimum (again)
- `CVXPY` cannot be used (again)
- Differential evolution comes closest to finding the solution
  - However, it requires over one million function evaluations!

Example: `quadratic_minimization.ipynb`

Lessons

Noise can make optimization very difficult!

- Makes the problem non-convex, with many local minima
- Local methods get trapped in a local minimum
- Global methods are needed, but these perform poorly in high dimensions
- Tools like CVXPY cannot be used
- **Lesson**: avoid noisy functions by any means possible (e.g., smoothing, convexification)

Example: `quadratic_minimization.ipynb`

Recap

- Global, no gradients
    - `differential_evolution`
    - *Best performance*: non-convex, low-dimensional. Noise okay!
- Local, no gradients:
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    - `CVXPY` (requires convexity)
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Example: `quadratic_minimization.ipynb`