Optimization (cont.)

Lecture 14

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Method Variants

Method: CG in scipy

Scipy's optimize module implements the conjugate gradient algorithm using a variant proposed by Polak and Ribiere, this version does not use the Hessian when calculating the next step. The specific changes are:

- α_k is calculated via a line search along the direction p_k
- and the β_{k+1} calculation is replaced as follows

$$\beta_{k+1} = \frac{r_{k+1}^T \nabla^2 f(x_k)\, p_k}{p_k^T \nabla^2 f(x_k)\, p_k} \quad \Rightarrow \quad \beta_{k+1}^{PR} = \frac{\nabla f(x_{k+1})\,(\nabla f(x_{k+1}) - \nabla f(x_k))}{\nabla f(x_k)^T \nabla f(x_k)}$$

Method: Newton-CG & BFGS

These are both variants of Newton's method but do not require the Hessian (but can be used by the former if provided).

- Newton-Conjugate Gradient (Netwon-CG) algorithm uses a conjugate gradient algorithm to (approximately) invert the local Hessian
- The Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm iteratively approximates the inverse Hessian
  - Gradient is also not required and can similarly be approximated using finite differences

Method: Nelder-Mead

This is a gradient free method that uses a series of simplexes which are used to iteratively bracket the minimum.

Method Summary

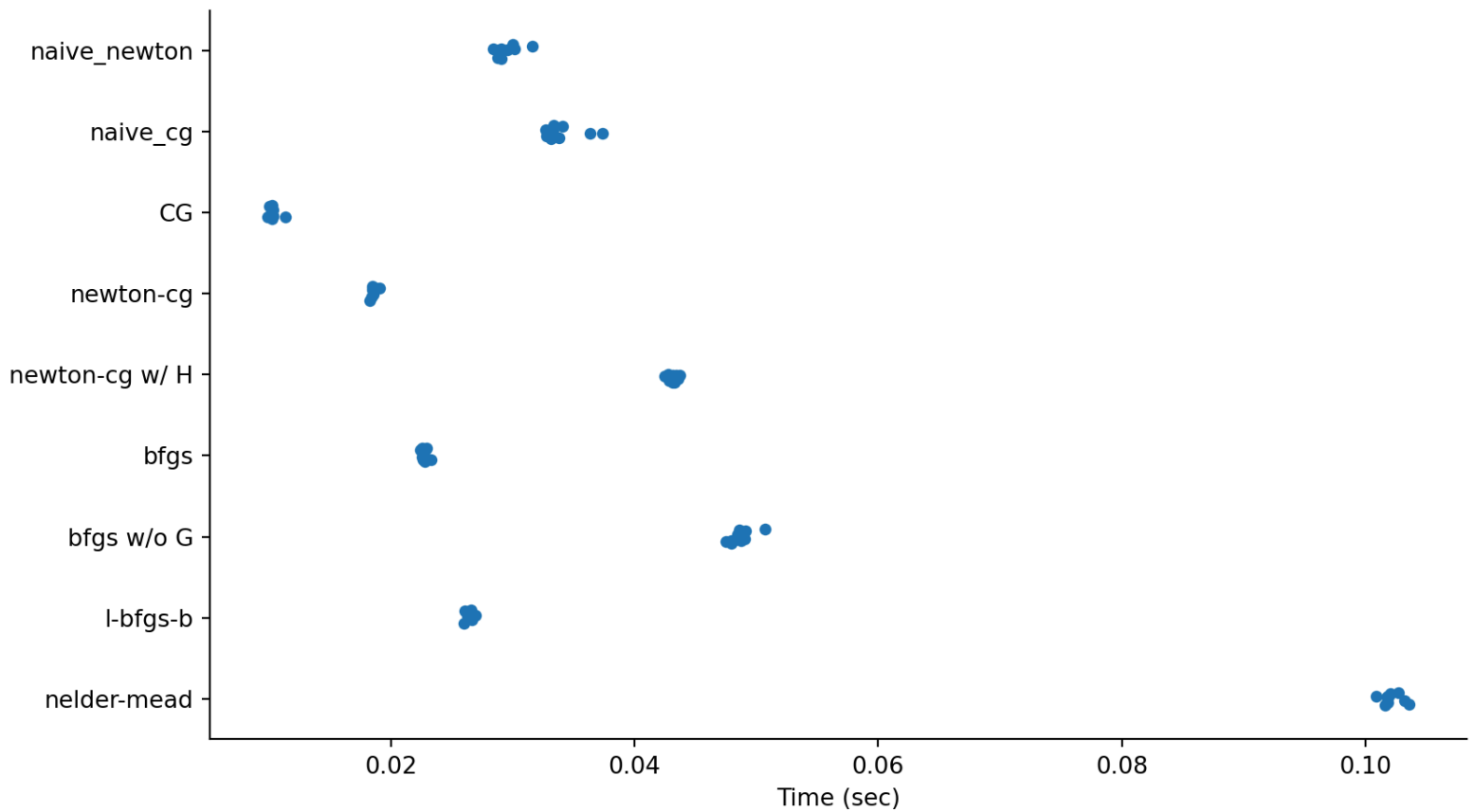
SciPy Method	Description	Gradient	Hessian
—	Gradient Descent (naive w/ backtracking)	✓	✗
—	Newton's method (naive w/ backtracking)	✓	✓
—	Conjugate Gradient (naive)	✓	✓
`"CG"`	Nonlinear Conjugate Gradient (Polak and Ribiere variation)	✓	✗
`"Newton-CG"`	Truncated Newton method (Newton w/ CG step direction)	✓	Optional
`"BFGS"`	Broyden, Fletcher, Goldfarb, and Shanno (Quasi-newton method)	Optional	✗
`"L-BFGS-B"`	Limited-memory BFGS (Quasi-newton method)	Optional	✗
`"Nelder-Mead"`	Nelder-Mead simplex reflection method	✗	✗

Methods collection

```
def define_methods(x, f, grad, hess, tol=1e-8):
  return {
    "naive_newton":   lambda: newtons_method(x, f, grad, hess, tol=tol),
    "naive_cg":       lambda: conjugate_gradient(x, f, grad, hess, tol=tol),
    "CG":             lambda: optimize.minimize(f, x, jac=grad, method="CG", tol=t
    "newton-cg":      lambda: optimize.minimize(f, x, jac=grad, hess=None, method=
    "newton-cg w/ H": lambda: optimize.minimize(f, x, jac=grad, hess=hess, method=
    "bfgs":           lambda: optimize.minimize(f, x, jac=grad, method="BFGS", tol
    "bfgs w/o G":     lambda: optimize.minimize(f, x, method="BFGS", tol=tol),
    "l-bfgs-b":       lambda: optimize.minimize(f, x, method="L-BFGS-B", tol=tol),
    "nelder-mead":    lambda: optimize.minimize(f, x, method="Nelder-Mead", tol=to
  }
```

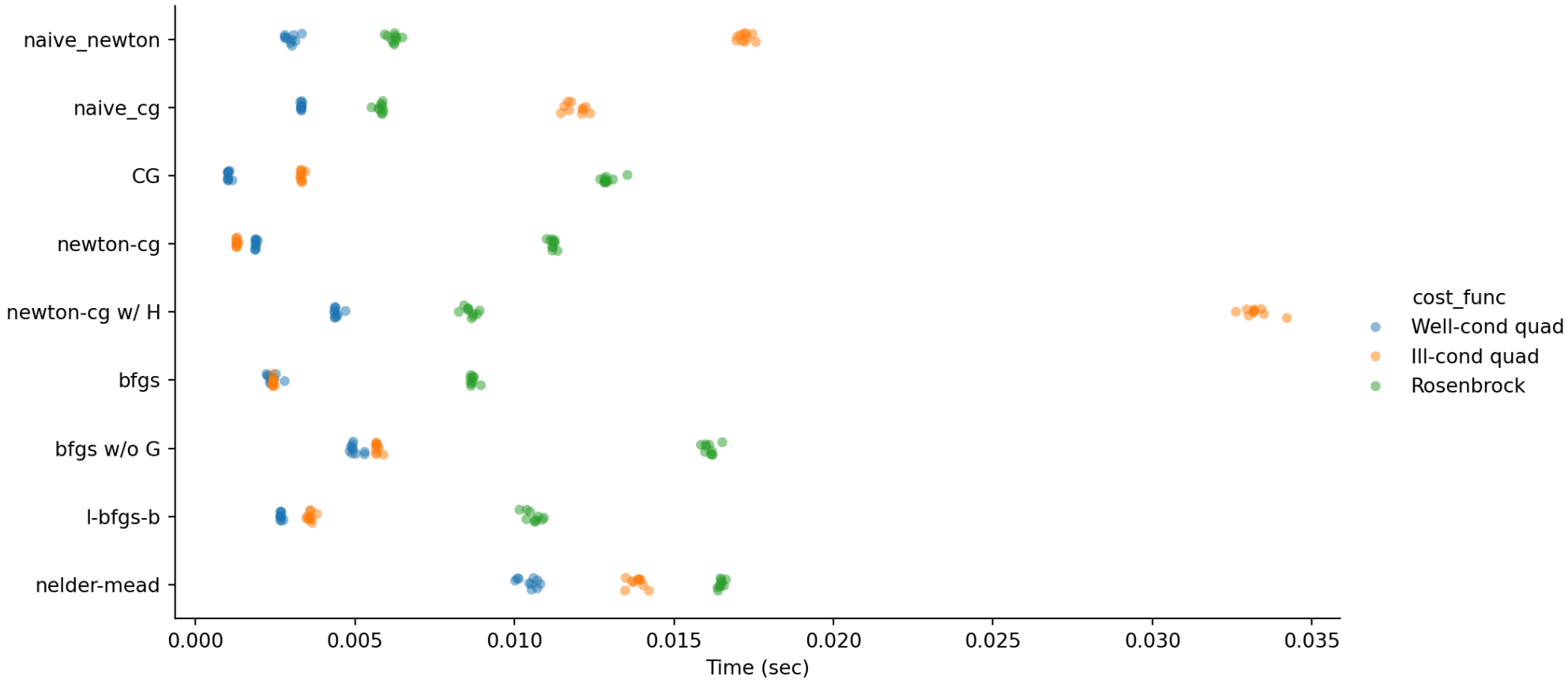
Method Timings

```
x = (1.6, 1.1)
f, grad, hess = mk_quad(0.7)
methods = define_methods(x, f, grad, hess)
df = pd.DataFrame({
  key: timeit.Timer(methods[key]).repeat(10, 100) for key in methods
})
```



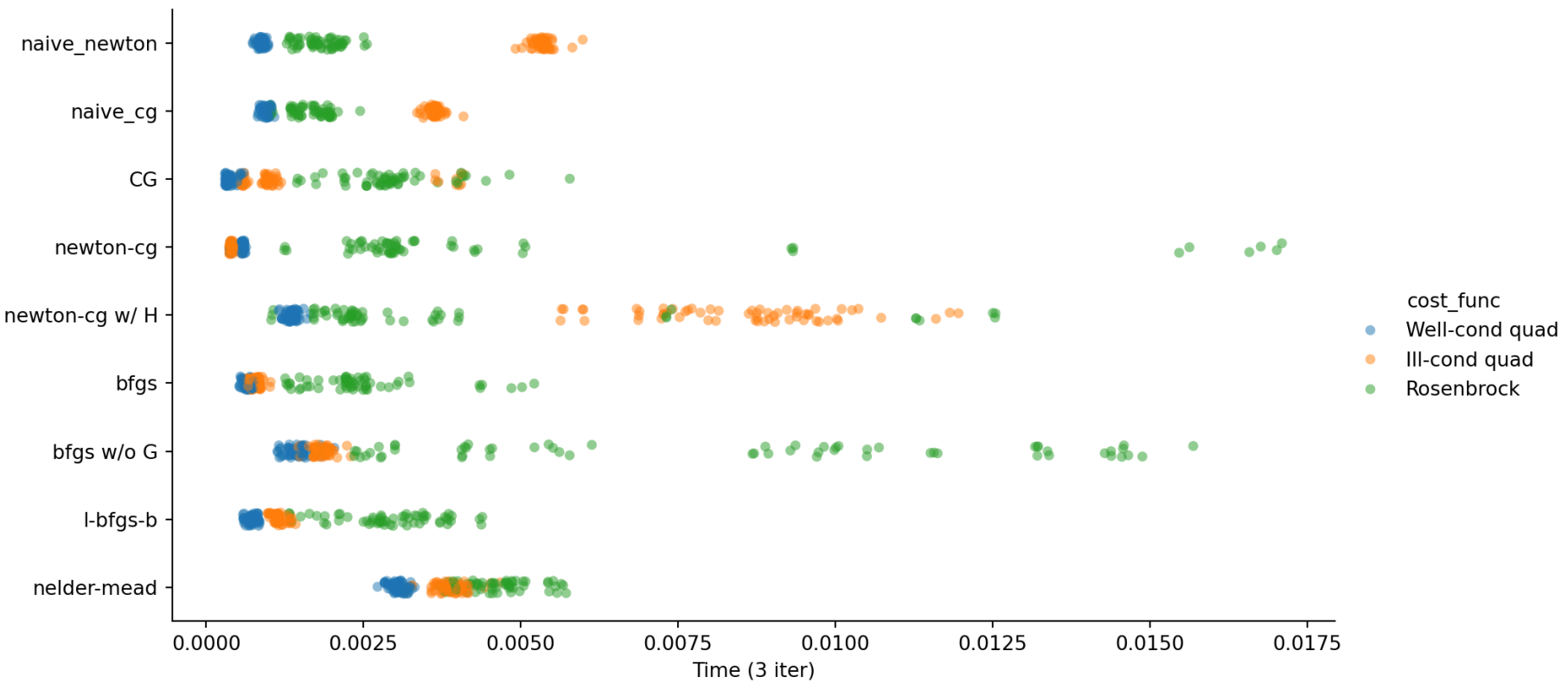
Timings across cost functions

```python
def time_cost_func(n, x, name, cost_func, *args):
  f, grad, hess = cost_func(*args)
  methods = define_methods(x, f, grad, hess)

  return ( pd.DataFrame({
      key: timeit.Timer(
        methods[key]
      ).repeat(n, n)
      for key in methods
    })
    .melt()
    .assign(cost_func = name)
  )

x = (1.6, 1.1)

time_cost_df = pd.concat([
  time_cost_func(10, x, "Well-cond quad", mk_quad, 0.7),
  time_cost_func(10, x, "Ill-cond quad", mk_quad, 0.02),
  time_cost_func(10, x, "Rosenbrock", mk_rosenbrock)
])
```


naive_newton
naive_cg
CG
newton-cg
newton-cg w/ H
bfgs
bfgs w/o G
l-bfgs-b
nelder-mead
0.000
0.005
0.010
0.015
0.020
0.025
0.030
0.035
Time (sec)
cost_func
Well-cond quad
Ill-cond quad
Rosenbrock

Random starting locations

```
pts = np.random.default_rng(seed=1234).uniform(-2,2, (20,2))

df = pd.concat([
  pd.concat([
    time_cost_func(3, x, "Well-cond quad", mk_quad, 0.7),
    time_cost_func(3, x, "Ill-cond quad", mk_quad, 0.02),
    time_cost_func(3, x, "Rosenbrock", mk_rosenbrock)
  ])
  for x in pts
])
```



Profiling - BFGS (cProfile)

```
1  import cProfile
2
3  f, grad, hess = mk_quad(0.7)
4  def run():
5    for i in range(500):
6      optimize.minimize(fun = f, x0 = (1.6, 1.1), jac=grad, method="BFGS", tol=1e-11)
7
8  cProfile.run('run()', sort="tottime")
```

```
         503504 function calls in 0.209 seconds

   Ordered by: internal time

   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
      500    0.043    0.000    0.204    0.000 _optimize.py:1328(_minimize_bfgs)
    29000    0.019    0.000    0.019    0.000 {method 'reduce' of 'numpy.ufunc' objects}
    13000    0.011    0.000    0.033    0.000 _optimize.py:194(vecnorm)
     5000    0.009    0.000    0.021    0.000 <string>:3(f)
    18000    0.009    0.000    0.022    0.000 fromnumeric.py:69(_wrapreduction)
     5000    0.008    0.000    0.010    0.000 <string>:9(gradient)
     4500    0.008    0.000    0.097    0.000 _dcsrch.py:201(__call__)
    10000    0.007    0.000    0.018    0.000 numeric.py:2475(array_equal)
     4500    0.006    0.000    0.034    0.000 _linesearch.py:86(derphi)
    13000    0.005    0.000    0.021    0.000 fromnumeric.py:2338(sum)
     5000    0.004    0.000    0.019    0.000 _differentiable_functions.py:39(wrapped)
     9000    0.004    0.000    0.005    0.000 _dcsrch.py:269(_iterate)
     4500    0.004    0.000    0.104    0.000 _linesearch.py:100(scalar_search_wolfe1)
```

Profiling - BFGS (pyinstrument)

```
from pyinstrument import Profiler

f, grad, hess = mk_quad(0.7)

profiler = Profiler(interval=0.00001)

profiler.start()
opt = optimize.minimize(fun = f, x0 = (1.6, 1.1), jac=grad, method="BFGS", tol=1e-11)
p = profiler.stop()

profiler.write_html("Lec14_bfgs_quad.html")
```

Profiling - Nelder-Mead

```
from pyinstrument import Profiler

f, grad, hess = mk_quad(0.7)

profiler = Profiler(interval=0.00001)

profiler.start()
opt = optimize.minimize(fun = f, x0 = (1.6, 1.1), method="Nelder-Mead", tol=1e-11)
p = profiler.stop()

profiler.write_html("Lec14_nm_quad.html")
```

`optimize.minimize()` output

```
f, grad, hess = mk_quad(0.7)
```

```
optimize.minimize(
  fun = f, x0 = (1.6, 1.1),
  jac=grad, method="BFGS"
)
```

```
  message: Optimization terminated
successfully.
  success: True
   status: 0
      fun: 1.2739256453439323e-11
        x: [-5.318e-07 -8.843e-06]
      nit: 6
      jac: [-3.510e-07 -2.860e-06]
 hess_inv: [[ 1.515e+00 -3.438e-03]
            [-3.438e-03  3.035e+00]]
     nfev: 7
     njev: 7
```

```
optimize.minimize(
  fun = f, x0 = (1.6, 1.1),
  jac=grad, hess=hess, method="Newton-CG"
)
```

```
message: Optimization terminated successfully.
success: True
 status: 0
    fun: 2.3418652989289317e-12
      x: [ 0.000e+00  3.806e-06]
    nit: 11
    jac: [ 0.000e+00  4.102e-06]
   nfev: 12
   njev: 12
   nhev: 11
```

`optimize.minimize()` output (cont.)

```python
optimize.minimize(
  fun = f, x0 = (1.6, 1.1),
  jac=grad, method="CG"
)
```

```
message: Optimization terminated successfully.
success: True
 status: 0
    fun: 1.4450021261144105e-32
      x: [-1.943e-16 -1.110e-16]
    nit: 2
    jac: [-1.282e-16 -3.590e-17]
   nfev: 5
   njev: 5
```

```python
optimize.minimize(
  fun = f, x0 = (1.6, 1.1),
  jac=grad, method="Nelder-Mead"
)
```

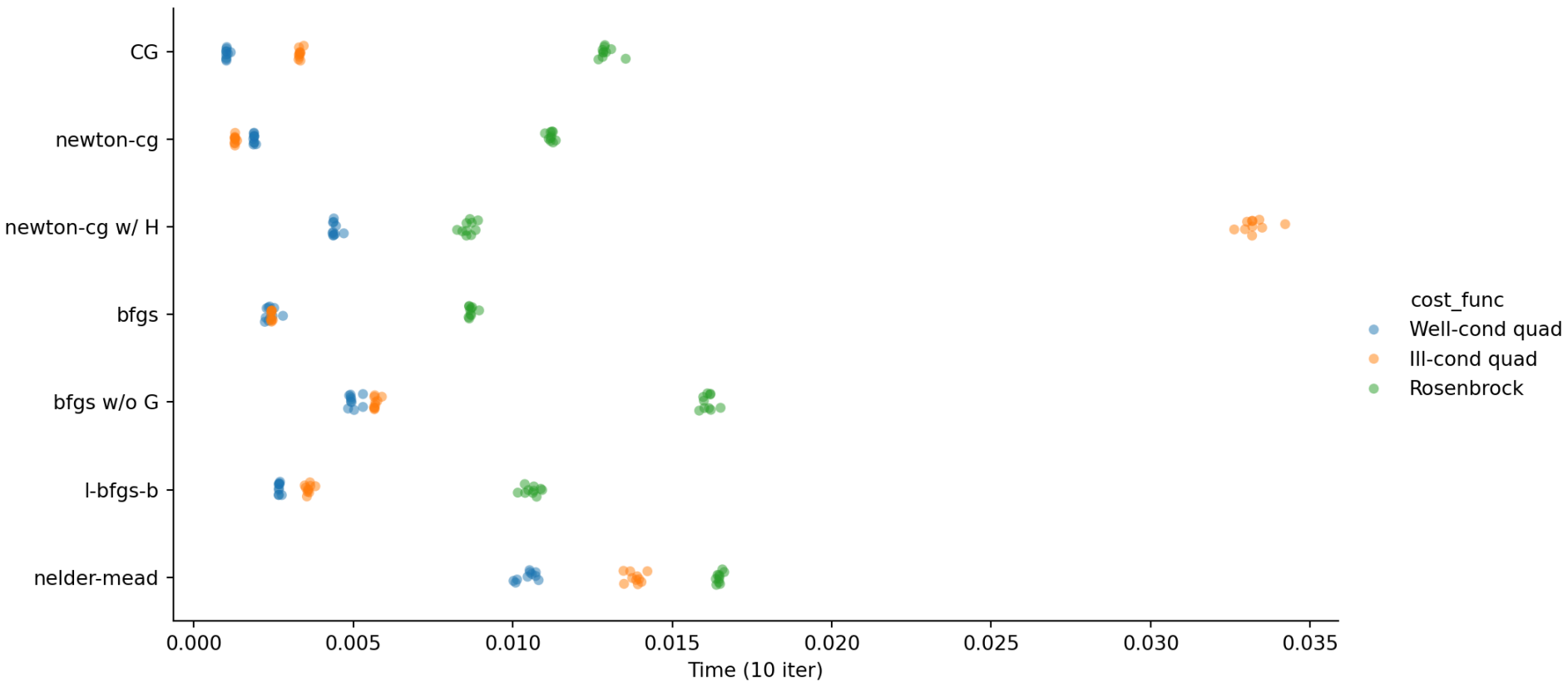
```
      message: Optimization terminated
successfully.
      success: True
       status: 0
          fun: 2.3077013477040082e-10
            x: [ 1.088e-05  3.443e-05]
          nit: 46
         nfev: 89
 final_simplex: (array([[ 1.088e-05,  3.443e-
05],
                       [ 1.882e-05, -3.825e-
05],
                       [-3.966e-05, -3.147e-
05]]), array([ 2.308e-10,  3.534e-10,  6.791e-
10]))
```

Collect

```python
def run_collect(name, x0, cost_func, *args,
  f, grad, hess = cost_func(*args)
  methods = define_methods(x0, f, grad, hess

  res = []
  for method in methods:
    if method in skip: continue

    x = methods[method]()
    time = timeit.Timer(methods[method]).rep

    d = {
      "name":    name,
      "method":  method,
      "nit":     x["nit"],
      "nfev":    x["nfev"],
      "njev":    x.get("njev"),
      "nhev":    x.get("nhev"),
      "success": x["success"],
      "time":    [time]
    }
    res.append( pd.DataFrame(d, index=[1])

  return pd.concat(res)
```

```python
df = pd.concat([
  run_collect(
    name, (1.6, 1.1),
    cost_func,
    arg,
    skip=['naive_newton', 'naive_cg']
  )
  for name, cost_func, arg in zip(
    ("Well-cond quad", "Ill-cond quad", "Ros
    (mk_quad, mk_quad, mk_rosenbrock),
    (0.7, 0.02, None)
  )
])
```

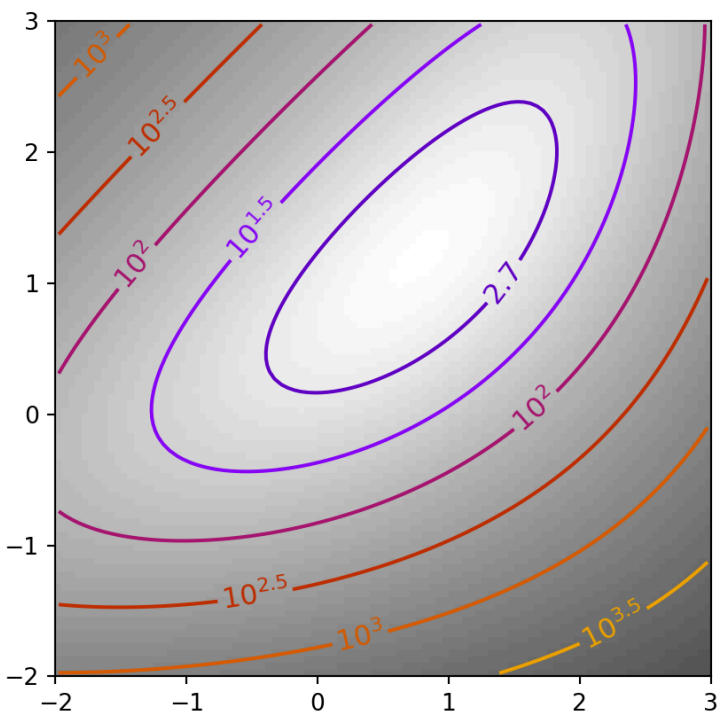
Runtimes | Function calls



Exercise 1

Try minimizing the following function using different optimization methods starting from $x_0 = [0, 0]$, which method(s) appear to work best?

$$f(x) = \exp(x_1 - 1) + \exp(-x_2 + 1) + (x_1 - x_2)^2$$



MVN Example

MVN density cost function

For an n-dimensional multivariate normal we define the $n \times 1$ vectors x and μ and the $n \times n$ covariance matrix Σ,

$$f(x) = \det(2\pi\Sigma)^{-1/2} \exp\left[-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right]$$

$$\nabla f(x) = -f(x)\Sigma^{-1}(x-\mu)$$

$$\nabla^2 f(x) = f(x)\left(\Sigma^{-1}(x-\mu)(x-\mu)^T\Sigma^{-1} - \Sigma^{-1}\right)$$

Our goal will be to find the mode (maximum) of this density.

```python
def mk_mvn(mu, Sigma):
  Sigma_inv = np.linalg.inv(Sigma)
  norm_const = 1 / (np.sqrt(np.linalg.det(2>

  # Returns the negative density (since we v
  def f(x):
    x_m = x - mu
    return -(norm_const *
      np.exp(
        -0.5 * x_m.T @ Sigma_inv @ x_m
      )
    ).item()

  def grad(x):
    return (-f(x) * Sigma_inv @ (x - mu))

  def hess(x):
    n = len(x)
    x_m = x - mu
    return f(x) * (
      (Sigma_inv @ x_m).reshape((n,1))
      @ (x_m.T @ Sigma_inv).reshape((1,n))
      - Sigma_inv
    )
```

Gradient checking

One of the most common issues when implementing an optimizer is to get the gradient calculation wrong which can produce problematic results. It is possible to numerically check the gradient function by comparing results between the gradient function and finite differences from the objective function via `optimize.check_grad()`.

```
# 5d
f, grad, hess = mk_mvn(
  np.zeros(5), np.eye(5,5)
)
```

```
optimize.check_grad(f, grad, np.zeros(5))
```

```
np.float64(2.6031257322754127e-10)
```

```
optimize.check_grad(f, grad, np.ones(5))
```

```
np.float64(1.725679820308689e-11)
```

```
# 10d
f, grad, hess = mk_mvn(
  np.zeros(10), np.eye(10)
)
```

```
optimize.check_grad(f, grad, np.zeros(10))
```

```
np.float64(2.8760747774580336e-12)
```

```
optimize.check_grad(f, grad, np.ones(10))
```

```
np.float64(2.850398669793798e-14)
```

Gradient checking (wrong gradient)

```
1 wrong_grad = lambda x: 5*grad(x)
```

```
1 # 5d
2 f, grad, hess = mk_mvn(
3   np.zeros(5), np.eye(5)
4 )
```

```
1 optimize.check_grad(f, wrong_grad, np.zeros
```

```
np.float64(2.6031257322754127e-10)
```

```
1 optimize.check_grad(f, wrong_grad, np.ones(5
```

```
np.float64(0.007419234855235744)
```

```
1 # 10d
2 f, grad, hess = mk_mvn(
3   np.zeros(10), np.eye(10)
4 )
```

```
1 optimize.check_grad(f, wrong_grad, np.zeros(
```

```
np.float64(2.8760747774580336e-12)
```

```
1 optimize.check_grad(f, wrong_grad, np.ones(1
```

```
np.float64(8.703385925704049e-06)
```

Why does `np.ones()` detect an issue but `np.zeros()` does not?

Hessian checking

Note since the gradient of the gradient is the hessian we can use this function to check our implementation of the hessian as well, just use `grad()` as `func` and `hess()` as `grad`.

```
# 5d
f, grad, hess = mk_mvn(np.zeros(5), np.eye(5
```

```
optimize.check_grad(grad, hess, np.zeros(5)
```

```
np.float64(3.878959614448864e-18)
```

```
optimize.check_grad(grad, hess, np.ones(5))
```

```
np.float64(3.8156075963144067e-11)
```

```
# 10d
f, grad, hess = mk_mvn(np.zeros(10), np.eye(
```

```
optimize.check_grad(grad, hess, np.zeros(10)
```

```
np.float64(4.2856853864461685e-20)
```

```
optimize.check_grad(grad, hess, np.ones(10))
```

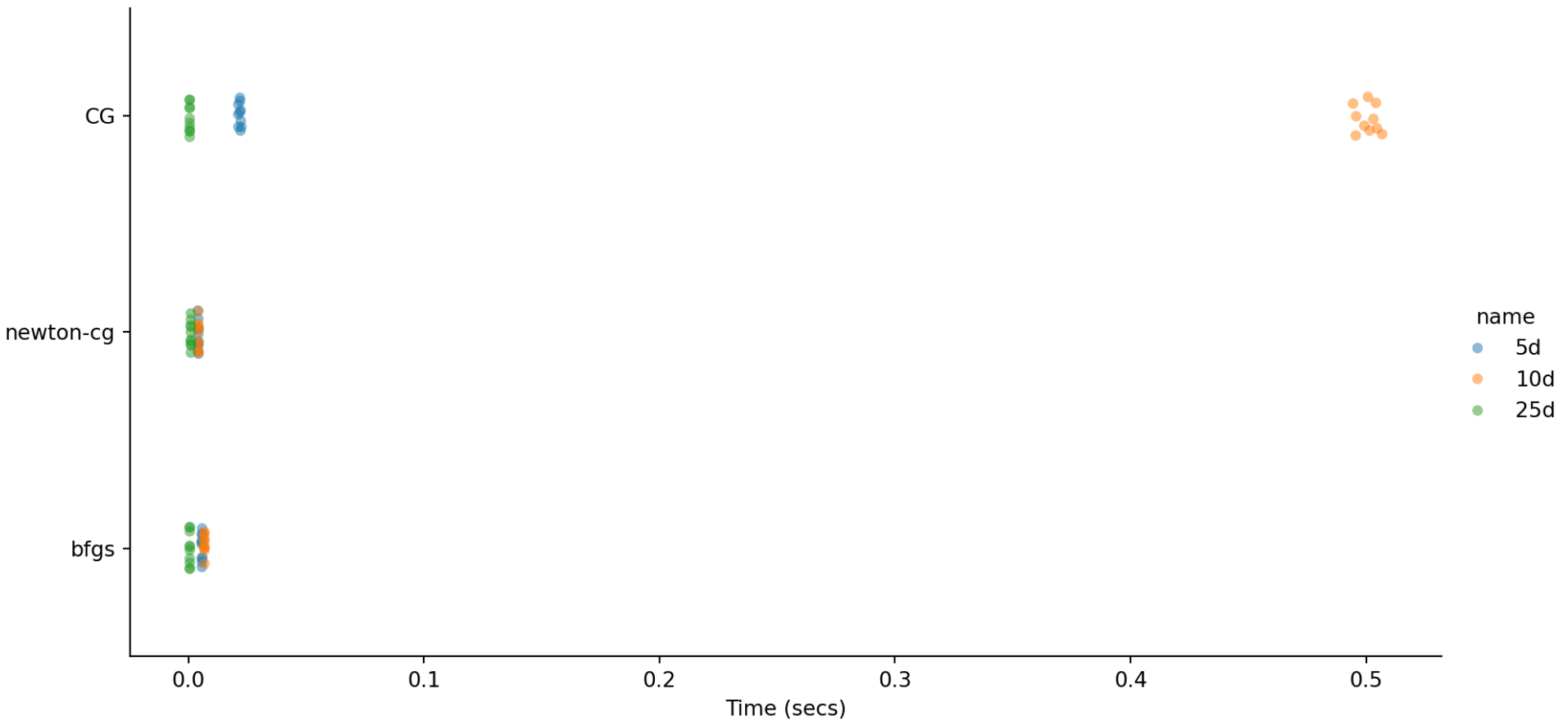
```
np.float64(8.551196009381392e-14)
```

Unit MVNs

```
rng = np.random.default_rng(seed=1234)
runif = rng.uniform(-1,1, size=25)

df = pd.concat([
  run_collect(
    name, runif[:n], mk_mvn,
    np.zeros(n), np.eye(n),
    tol=1e-10,
    skip=['naive_newton', 'naive_cg', 'bfgs w/o G', 'newton-cg w/ H', 'l-bfgs-b', 'nelder-mea
  )
  for name, n in zip(
    ("5d", "10d", "25d"),
    (5, 10, 25)
  )
])
```

Performance (Unit MVNs)

Run times | Function calls



What's going on? (good)

```
n = 5
f, grad, hess = mk_mvn(np.zeros(n), np.eye(n))
```

```
optimize.minimize(
  f, runif[:n], jac=grad,
  method="newton-cg", tol=1e-10
)
```

```
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: -0.010105326013811651
       x: [ 5.071e-11 -1.274e-11  4.502e-11
-2.535e-11 -1.924e-11]
     nit: 4
     jac: [ 5.125e-13 -1.288e-13  4.550e-13
-2.562e-13 -1.945e-13]
    nfev: 5
    njev: 9
    nhev: 0
```

```
optimize.minimize(
  f, runif[:n], jac=grad,
  method="bfgs", tol=1e-10
)
```

```
  message: Optimization terminated
successfully.
  success: True
   status: 0
      fun: -0.010105326013811651
        x: [-2.482e-13  6.237e-14 -2.203e-13
1.240e-13  9.422e-14]
      nit: 4
      jac: [-2.508e-15  6.303e-16 -2.227e-15
1.253e-15  9.521e-16]
 hess_inv: [[ 4.463e+01 -1.096e+01 ...
-2.181e+01 -1.656e+01]
            [-1.096e+01  3.756e+00 ...
5.481e+00  4.161e+00]
            ...
            [-2.181e+01  5.481e+00 ...
1.190e+01  8.276e+00]
            [-1.656e+01  4.161e+00
```

What's going on? (okay)

```python
n = 10
f, grad, hess = mk_mvn(np.zeros(n), np.eye(n))
```

```python
optimize.minimize(
  f, runif[:n], jac=grad,
  method="newton-cg", tol=1e-10
)
```

```
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: -0.00010211745783654051
       x: [-8.223e-04  2.067e-04 -7.301e-04
4.111e-04  3.120e-04
            6.588e-04  4.454e-04  3.130e-04
-8.005e-04  4.077e-04]
     nit: 3
     jac: [-8.397e-08  2.110e-08 -7.455e-08
4.198e-08  3.186e-08
            6.727e-08  4.549e-08  3.196e-08
-8.174e-08  4.163e-08]
    nfev: 6
    njev: 9
    nhev: 0
```

```python
optimize.minimize(
  f, runif[:n], jac=grad,
  method="bfgs", tol=1e-10
)
```

```
  message: Optimization terminated
successfully.
  success: True
   status: 0
      fun: -0.00010211761384541865
        x: [-2.347e-09  5.898e-10 -2.084e-09
1.173e-09  8.906e-10
             1.880e-09  1.271e-09  8.933e-10
-2.285e-09  1.164e-09]
      nit: 2
      jac: [-2.396e-13  6.023e-14 -2.128e-13
1.198e-13  9.094e-14
             1.920e-13  1.298e-13  9.122e-14
-2.333e-13  1.188e-13]
 hess_inv: [[ 1.685e+04 -4.235e+03 ...
1.641e+04 -8.356e+03]
            [-4.235e+03  1.065e+03 ...
-4.123e+03  2.100e+03]
```

What's going on? (bad)

```
n = 25
f, grad, hess = mk_mvn(np.zeros(n), np.eye(n))
```

```
optimize.minimize(
  f, runif[:n], jac=grad,
  method="newton-cg", tol=1e-10
)
```

```
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: -1.2867324357023428e-12
       x: [ 9.534e-01 -2.396e-01 ...  2.220e-01
-8.797e-01]
     nit: 1
     jac: [ 1.227e-12 -3.083e-13 ...  2.857e-13
-1.132e-12]
    nfev: 1
    njev: 1
    nhev: 0
```

```
optimize.minimize(
  f, runif[:n], jac=grad,
  method="bfgs", tol=1e-10
)
```

```
  message: Optimization terminated
successfully.
  success: True
   status: 0
      fun: -1.2867324357023428e-12
        x: [ 9.534e-01 -2.396e-01 ...  2.220e-
01 -8.797e-01]
      nit: 0
      jac: [ 1.227e-12 -3.083e-13 ...  2.857e-
13 -1.132e-12]
 hess_inv: [[1 0 ... 0 0]
            [0 1 ... 0 0]
            ...
            [0 0 ... 1 0]
            [0 0 ... 0 1]]
     nfev: 1
     njev: 1
```

All bad?

```
1 optimize.minimize(
2   f, runif[:n], jac=grad,
3   method="nelder-mead", tol=1e-10
4 )
```

```
      message: Maximum number of function evaluations has been exceeded.
      success: False
       status: 1
          fun: -5.2161537392613975e-11
            x: [ 7.181e-02 -3.136e-01 ...  3.193e-01  3.222e-02]
          nit: 4136
         nfev: 5000
 final_simplex: (array([[ 7.181e-02, -3.136e-01, ...,  3.193e-01,
                          3.222e-02],
                        [ 7.275e-02, -3.237e-01, ...,  3.218e-01,
                          2.192e-02],
                        ...,
                        [ 8.238e-02, -3.143e-01, ...,  3.247e-01,
                          2.232e-02],
                        [ 8.105e-02, -3.178e-01, ...,  3.119e-01,
                          3.078e-02]], shape=(26, 25)), array([-5.216e-11, -5.216e-11, ...,
-5.213e-11, -5.213e-11],
                       shape=(26,)))
```

Options (newton-cg)

```
1 optimize.show_options(solver="minimize", method="newton-cg")
```

```
Minimization of scalar function of one or more variables using the
Newton-CG algorithm.

Note that the `jac` parameter (Jacobian) is required.

Options
-------
disp : bool
    Set to True to print convergence messages.
xtol : float
    Average relative error in solution `xopt` acceptable for
    convergence.
maxiter : int
    Maximum number of iterations to perform.
eps : float or ndarray
    If `hessp` is approximated, use this value for the step size.
return_all : bool, optional
    Set to True to return a list of the best solution at each of the
```

Options (bfgs)

```
1 optimize.show_options(solver="minimize", method="bfgs")
```

```
Minimization of scalar function of one or more variables using the
BFGS algorithm.

Options
-------
disp : bool
    Set to True to print convergence messages.
maxiter : int
    Maximum number of iterations to perform.
gtol : float
    Terminate successfully if gradient norm is less than `gtol`.
norm : float
    Order of norm (Inf is max, -Inf is min).
eps : float or ndarray
    If `jac is None` the absolute step size used for numerical
    approximation of the jacobian via forward differences.
return_all : bool, optional
    Set to True to return a list of the best solution at each of the
```

Options (Nelder-Mead)

```
1 optimize.show_options(solver="minimize", method="newton-cg")
```

```
Minimization of scalar function of one or more variables using the
Newton-CG algorithm.

Note that the `jac` parameter (Jacobian) is required.

Options
-------
disp : bool
    Set to True to print convergence messages.
xtol : float
    Average relative error in solution `xopt` acceptable for
    convergence.
maxiter : int
    Maximum number of iterations to perform.
eps : float or ndarray
    If `hessp` is approximated, use this value for the step size.
return_all : bool, optional
    Set to True to return a list of the best solution at each of the
```

SciPy implementation

The following code comes from SciPy's `minimize()` implementation:

```
if tol is not None:
  options = dict(options)
  if meth == 'nelder-mead':
      options.setdefault('xatol', tol)
      options.setdefault('fatol', tol)
  if meth in ('newton-cg', 'powell', 'tnc'):
      options.setdefault('xtol', tol)
  if meth in ('powell', 'l-bfgs-b', 'tnc', 'slsqp'):
      options.setdefault('ftol', tol)
  if meth in ('bfgs', 'cg', 'l-bfgs-b', 'tnc', 'dogleg',
              'trust-ncg', 'trust-exact', 'trust-krylov'):
      options.setdefault('gtol', tol)
  if meth in ('cobyla', '_custom'):
      options.setdefault('tol', tol)
  if meth == 'trust-constr':
      options.setdefault('xtol', tol)
      options.setdefault('gtol', tol)
      options.setdefault('barrier_tol', tol)
```

Fixing our tolerances?

```
n = 25
f, grad, hess = mk_mvn(np.zeros(n), np.eye(n))
```

```
optimize.minimize(
  f, runif[:n], jac=grad,
  method="newton-cg", tol=1e-16
)
```

```
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: -1.2867324357023428e-12
       x: [ 9.534e-01 -2.396e-01 ...  2.220e-01
-8.797e-01]
     nit: 1
     jac: [ 1.227e-12 -3.083e-13 ...  2.857e-13
-1.132e-12]
    nfev: 1
    njev: 1
    nhev: 0
```

```
optimize.minimize(
  f, runif[:n], jac=grad,
  method="bfgs", tol=1e-16
)
```

```
  message: Optimization terminated
successfully.
  success: True
   status: 0
      fun: -1.0537841099018322e-10
        x: [-2.645e-08  6.648e-09 ... -6.160e-
09  2.441e-08]
      nit: 3
      jac: [-2.788e-18  7.006e-19 ... -6.492e-
19  2.572e-18]
 hess_inv: [[ 9.790e+08 -2.461e+08 ...
2.280e+08 -9.034e+08]
            [-2.461e+08  6.184e+07 ...
-5.730e+07  2.270e+08]
            ...
            [ 2.280e+08 -5.730e+07 ...
5.310e+07 -2.104e+08]
            [-9.034e+08  2.270e+08
```

Limits of floating point precision

Every type of floating point value has finite precision due to the limitations of how it is represented. This value is typically refered to as the machine epsilon value, this is the smallest possible spacing between 1.0 and the next representable floating-point number.

```
1 np.finfo(np.float64).eps
```

```
np.float64(2.220446049250313e-16)
```

```
1 np.finfo(np.float32).eps
```

```
np.float32(1.1920929e-07)
```

```
1 np.finfo(np.float16).eps
```

```
np.float16(0.000977)
```

```
1 1+np.finfo(np.float64).eps > 1
```

```
np.True_
```

```
1 1+np.finfo(np.float64).eps/2 > 1
```

```
np.False_
```

Fixes?

```
def mk_prop_mvn(mu, Sigma):
  Sigma_inv = np.linalg.inv(Sigma)
  #norm_const = 1 / (np.sqrt(np.linalg.det(2*np.pi*Sigma)))
  norm_const = 1

  # Returns the negative density (since we want the max not min)
  def f(x):
    x_m = x - mu
    return -(norm_const *
      np.exp(
        -0.5 * x_m.T @ Sigma_inv @ x_m
      )
    ).item()

  def grad(x):
    return (-f(x) * Sigma_inv @ (x - mu))

  def hess(x):
    n = len(x)
    x_m = x - mu
    return f(x) * (
      (Sigma_inv @ x_m).reshape((n,1))
      @ (x_m.T @ Sigma_inv).reshape((1,n))
      - Sigma_inv
```

```python
n = 25
f, grad, hess = mk_prop_mvn(np.zeros(n), np.eye(n))
```

```python
optimize.minimize(
  f, runif[:n], jac=grad,
  method="newton-cg", tol=1e-10
)
```

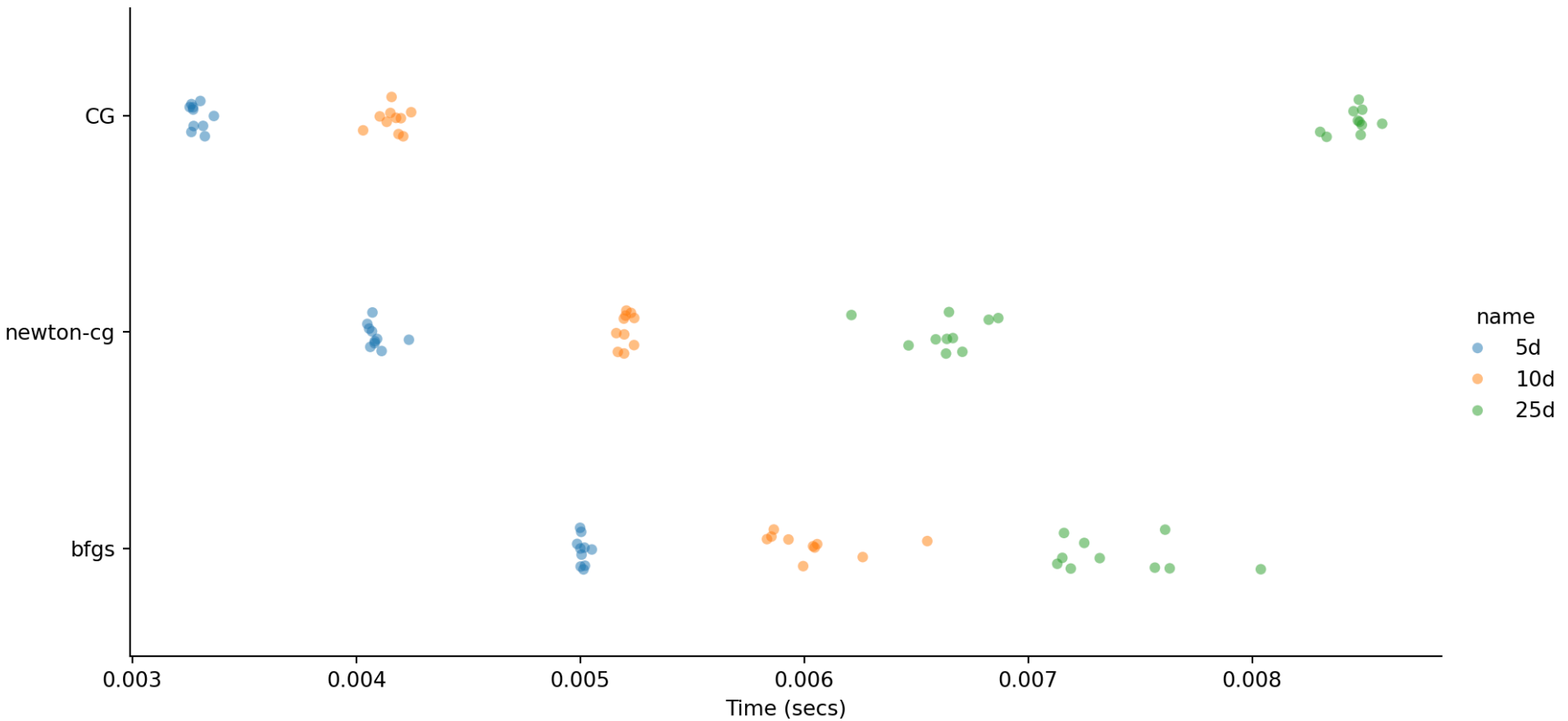
```
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: -1.0
       x: [-3.701e-16  9.302e-17 ... -8.619e-17
3.415e-16]
     nit: 4
     jac: [-3.701e-16  9.302e-17 ... -8.619e-17
3.415e-16]
    nfev: 10
    njev: 14
    nhev: 0
```

```python
optimize.minimize(
  f, runif[:n], jac=grad,
  method="bfgs", tol=1e-10
)
```

```
  message: Optimization terminated
successfully.
  success: True
   status: 0
      fun: -1.0
        x: [-3.040e-15  7.639e-16 ... -7.079e-
16  2.805e-15]
      nit: 4
      jac: [-3.040e-15  7.639e-16 ... -7.079e-
16  2.805e-15]
 hess_inv: [[ 1.000e+00 -6.660e-09 ...  6.171e-
09 -2.445e-08]
            [-6.660e-09  1.000e+00 ... -1.551e-
09  6.145e-09]
            ...
            [ 6.171e-09 -1.551e-09 ...
1.000e+00 -5.694e-09]
            [-2.445e-08  6.145e-09 ...
```

Performance

Run times | Function calls



Some general advice

- Having access to the gradient is almost always helpful / necessary
- Having access to the hessian can be helpful, but usually does not significantly improve things
- The curse of dimensionality is real
  - Be careful with `tol` - it means different things for different methods
- In general, **BFGS** or **L-BFGS** should be a first choice for most problems (either well- or ill-conditioned)
  - **CG** can perform better for well-conditioned problems with cheap function evaluations

Maximum Likelihood example

Normal MLE

```
1 from scipy.stats import norm
2
3 n = norm(-3.2, 1.25)
4 x = n.rvs(size=100, random_state=1234)
5 {'μ': x.mean(), 'σ': x.std()}
```

```
{'μ': np.float64(-3.156109646093205), 'σ':
np.float64(1.2446060629192537)}
```

```
1 mle_norm = lambda θ: -np.sum(
2   norm.logpdf(x, loc=θ[0], scale=θ[1])
3 )
```

```
1 mle_norm([0,1])
```

```
np.float64(667.3974708213642)
```

```
1 mle_norm([-3, 1])
```

```
np.float64(170.56457699340282)
```

```
1 mle_norm([-3.2, 1.25])
```

```
np.float64(163.83926813257395)
```

```
1 mle_norm([-3.3, 1.25])
```

```
np.float64(164.44016639757749)
```

Minimizing

```
1 optimize.minimize(mle_norm, x0=[0,1], method="bfgs")
```

```
  message: Desired error not necessarily achieved due to precision loss.
  success: False
   status: 2
      fun: nan
        x: [-1.436e+04 -3.533e+03]
      nit: 2
      jac: [       nan        nan]
hess_inv: [[ 9.443e-01  2.340e-01]
           [ 2.340e-01  5.905e-02]]
     nfev: 339
     njev: 113
```

Adding constraints

```python
def mle_norm2(θ):
  if θ[1] <= 0:
    return np.inf
  else:
    return -np.sum(
      norm.logpdf(x, loc=θ[0], scale=θ[1])
    )
```

```python
optimize.minimize(mle_norm2, x0=[0,1], metho
```

```
  message: Optimization terminated
successfully.
  success: True
   status: 0
      fun: 163.77575977255518
        x: [-3.156e+00  1.245e+00]
      nit: 9
      jac: [ 0.000e+00  0.000e+00]
 hess_inv: [[ 1.475e-02 -1.179e-04]
            [-1.179e-04  7.723e-03]]
     nfev: 43
     njev: 14
```

```python
{'μ': x.mean(), 'σ': x.std()}
```

```
{'μ': np.float64(-3.156109646093205), 'σ': np.float64(1.2446060629192537)}
```

Specifying Bounds

It is also possible to specify bounds via `bounds` but this is only available for certain optimization methods (i.e. Nelder-Mead & L-BFGS-B).

```
optimize.minimize(
  mle_norm, x0=[0,1], method="l-bfgs-b",
  bounds = [(-1e16, 1e16), (1e-16, 1e16)]
)
```

```
  message: CONVERGENCE: RELATIVE REDUCTION OF F <= FACTR*EPSMCH
  success: True
   status: 0
      fun: 163.77575977287245
        x: [-3.156e+00  1.245e+00]
      nit: 10
      jac: [ 2.046e-04  0.000e+00]
     nfev: 69
     njev: 23
 hess_inv: <2x2 LbfgsInvHessProduct with dtype=float64>
```

Exercise 2

Using `optimize.minimize()` recover the shape and scale parameters for these data using MLE.

```
1  from scipy.stats import gamma
2
3  g = gamma(a=2.0, scale=2.0)
4  x = g.rvs(size=100, random_state=1234)
5  x.round(2)
```

```
array([ 4.7 ,  1.11,  1.8 ,  6.19,  3.37,  0.25,  6.45,  0.36,  4.49,
        4.14,  2.84,  1.91,  8.03,  2.26,  2.88,  6.88,  6.84,  6.83,
        6.1 ,  3.03,  3.67,  2.57,  3.53,  2.07,  4.01,  1.51,  5.69,
        3.92,  6.01,  0.82,  2.11,  2.97,  5.02,  9.13,  4.19,  2.82,
       11.81,  1.17,  1.69,  4.67,  1.47, 11.67,  5.25,  3.44,  8.04,
        3.74,  5.73,  6.58,  3.54,  2.4 ,  1.32,  2.04,  2.52,  4.89,
        4.14,  5.02,  4.75,  8.24,  7.6 ,  1.  ,  6.14,  0.58,  2.83,
        2.88,  5.42,  0.5 ,  3.46,  4.46,  1.86,  4.59,  2.24,  2.62,
        3.99,  3.74,  5.27,  1.42,  0.56,  7.54,  5.5 ,  1.58,  5.49,
        6.57,  4.79,  5.84,  8.21,  1.66,  1.53,  4.27,  2.57,  1.48,
        5.23,  3.84,  3.15,  2.1 ,  3.71,  2.79,  0.86,  8.52,  4.36,
        3.3 ])
```