

# Lec 13 - Numerical optimization (cont.)

**Statistical Computing and Computation**

**Sta 663 | Spring 2022**

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# Method Summary

SciPy Method	Description	Gradient	Hessian
---	Newton's method (naive)	✓	✓
---	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	✗

# Methods collection

```
def define_methods(x0, f, grad, hess, tol=1e-8):
    return {
        "naive_newton": lambda: newtons_method(x0, f, grad, hess, tol=tol),
        "naive_cg": lambda: conjugate_gradient(x0, f, grad, hess, tol=tol),
        "cg": lambda: optimize.minimize(f, x0, jac=grad, method="CG", tol=tol),
        "newton-cg": lambda: optimize.minimize(f, x0, jac=grad, hess=None, method="Newton-CG", tol=tol),
        "newton-cg w/ H": lambda: optimize.minimize(f, x0, jac=grad, hess=hess, method="Newton-CG", tol=tol),
        "bfgs": lambda: optimize.minimize(f, x0, jac=grad, method="BFGS", tol=tol),
        "bfgs w/o G": lambda: optimize.minimize(f, x0, method="BFGS", tol=tol),
        "l-bfgs": lambda: optimize.minimize(f, x0, method="L-BFGS-B", tol=tol),
        "nelder-mead": lambda: optimize.minimize(f, x0, method="Nelder-Mead", tol=tol)
    }
```

# Method Timings

```
x0 = (1.6, 1.1)
f, grad, hess = mk_quad(0.7)
methods = define_methods(x0, f, grad, hess)

df = pd.DataFrame({
    key: timeit.Timer(methods[key]).repeat(10, 100) for key in methods
})

df
```

```
##      naive_newton  naive_cg        cg  ...   bfgs w/o G   1-bfgs nelder-mead
## 0      0.023537  0.039970  0.011881  ...  0.066303  0.036481  0.147036
## 1      0.022836  0.040031  0.011484  ...  0.066409  0.036509  0.145659
## 2      0.023006  0.040840  0.011460  ...  0.065983  0.036171  0.146303
## 3      0.023108  0.040619  0.011740  ...  0.065224  0.036673  0.146443
## 4      0.022910  0.040613  0.011933  ...  0.065597  0.036137  0.146067
## 5      0.022782  0.040496  0.011701  ...  0.066092  0.036383  0.147324
## 6      0.022979  0.040472  0.011504  ...  0.065924  0.036287  0.146281
## 7      0.023019  0.040539  0.011490  ...  0.066140  0.036171  0.146400
## 8      0.022744  0.039657  0.011497  ...  0.065693  0.036117  0.145820
## 9      0.022946  0.039879  0.011523  ...  0.065842  0.036078  0.146332
##
## [10 rows x 9 columns]
```

```
g = sns.catplot(data=df.melt(), y="variable", x="value", aspect=2)
g.ax.set_xlabel("Time (100 iter)")
g.ax.set_ylabel("")
plt.show()
```



# Timings across cost functions

```
def time_cost_func(x0, name, cost_func, *args):
    x0 = (1.6, 1.1)
    f, grad, hess = cost_func(*args)
    methods = define_methods(x0, f, grad, hess)

    return ( pd.DataFrame({
        key: timeit.Timer(methods[key]).repeat(10, 20) for key in
    })
    .melt()
    .assign(cost_func = name)
)

df = pd.concat([
    time_cost_func(x0, "Well-cond quad", mk_quad, 0.7),
    time_cost_func(x0, "Ill-cond quad", mk_quad, 0.02),
    time_cost_func(x0, "Rosenbrock", mk_rosenbrock)
])
```

```
df
##      variable     value      cost_func
## 0  naive_newton  0.004699 Well-cond quad
## 1  naive_newton  0.004590 Well-cond quad
## 2  naive_newton  0.004567 Well-cond quad
## 3  naive_newton  0.004557 Well-cond quad
## 4  naive_newton  0.004553 Well-cond quad
## ...
## 85 nelder-mead  0.047754 Rosenbrock
## 86 nelder-mead  0.047654 Rosenbrock
## 87 nelder-mead  0.047935 Rosenbrock
## 88 nelder-mead  0.047746 Rosenbrock
## 89 nelder-mead  0.047725 Rosenbrock
##
## [270 rows x 3 columns]
```

```
g = sns.catplot(data=df, y="variable", x="value", hue="cost_func", alpha=0.5, aspect=2)
g.ax.set_xlabel("Time (20 iter)")
g.ax.set_ylabel("")
plt.show()
```



# Profiling - BFGS

```
import cProfile

f, grad, hess = mk_quad(0.7)

def run():
    for i in range(100):
        optimize.minimize(fun = f, x0 = (1.6, 1.1), jac=grad, method="BFGS", tol=1e-11)

cProfile.run('run()', sort="totime")

##           112904 function calls (112804 primitive calls) in 0.047 seconds
##
## Ordered by: internal time
##
##   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
##      100    0.010    0.000    0.046    0.000 _optimize.py:1253(_minimize_bfgs)
## 13700/13600    0.004    0.000    0.015    0.000 {built-in method numpy.core._multiarray_umath.implement_array_function}
##     4200    0.003    0.000    0.003    0.000 {method 'reduce' of 'numpy.ufunc' objects}
##     1000    0.002    0.000    0.003    0.000 <string>:8(gradient)
##     1000    0.002    0.000    0.006    0.000 <string>:2(f)
##      900    0.002    0.000    0.025    0.000 _linesearch.py:91(scalar_search_wolfe1)
##     2000    0.002    0.000    0.004    0.000 numeric.py:2388(array_equal)
##     2100    0.001    0.000    0.004    0.000 fromnumeric.py:69(_wrapreduction)
##      900    0.001    0.000    0.010    0.000 _linesearch.py:77(derphi)
##     5200    0.001    0.000    0.004    0.000 <__array_function__ internals>:177(dot)
##      900    0.001    0.000    0.013    0.000 _linesearch.py:73(phi)
##     2100    0.001    0.000    0.001    0.000 shape_base.py:23(atleast_1d)
##     1000    0.001    0.000    0.008    0.000 _differentiable_functions.py:132(fun_wrapped)
##     1000    0.001    0.000    0.005    0.000 _differentiable_functions.py:162(grad_wrapped)
##      900    0.001    0.000    0.026    0.000 _linesearch.py:31(line_search_wolfe1)
```

# Profiling - Nelder-Mead

```
def run():
    for i in range(100):
        optimize.minimize(fun = f, x0 = (1.6, 1.1), method="Nelder-Mead", tol=1e-11)

cProfile.run('run()', sort="tottime")

##             756504 function calls in 0.270 seconds
##
## Ordered by: internal time
##
##   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
##      100    0.071    0.001    0.269    0.003 _optimize.py:635(_minimize_neldermead)
##    18600    0.034    0.000    0.087    0.000 <string>:2(f)
##    38000    0.028    0.000    0.028    0.000 {method 'reduce' of 'numpy.ufunc' objects}
##    86400    0.017    0.000    0.108    0.000 {built-in method numpy.core._multiarray_umath.implement_array_function}
##    28500    0.013    0.000    0.040    0.000 fromnumeric.py:69(_wrapreduction)
##    18600    0.011    0.000    0.117    0.000 _optimize.py:491(function_wrapper)
##    18600    0.008    0.000    0.035    0.000 fromnumeric.py:2160(sum)
##    29400    0.007    0.000    0.019    0.000 fromnumeric.py:51(_wrapfunc)
##    19600    0.006    0.000    0.006    0.000 {method 'take' of 'numpy.ndarray' objects}
##    28500    0.005    0.000    0.005    0.000 fromnumeric.py:70(<dictcomp>)
##    18800    0.005    0.000    0.005    0.000 {built-in method numpy.array}
##    19600    0.005    0.000    0.025    0.000 <__array_function__ internals>:177(take)
##    19600    0.005    0.000    0.016    0.000 fromnumeric.py:93(take)
##    18600    0.004    0.000    0.044    0.000 <__array_function__ internals>:177(sum)
##    18600    0.004    0.000    0.004    0.000 {built-in method numpy.arange}
##    18600    0.004    0.000    0.016    0.000 <__array_function__ internals>:177(copy)
##    9800     0.004    0.000    0.004    0.000 {method 'argsort' of 'numpy.ndarray' objects}
##    9700     0.003    0.000    0.017    0.000 fromnumeric.py:2675(amax)
##    9600     0.003    0.000    0.006    0.000 fromnumeric.py:1755(ravel)
```

# optimize.minimize() output

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

```
optimize.minimize(fun = f, x0 = (1.6, 1.1), jac=grad, method="B  
##      fun: 1.2739256453436805e-11  
##  hess_inv: array([[ 1.51494475, -0.00343804],  
##                  [-0.00343804,  3.03497828]])  
##      jac: array([-3.51014018e-07, -2.85996115e-06])  
##  message: 'Optimization terminated successfully.'  
##      nfev: 7  
##      nit: 6  
##      njev: 7  
##      status: 0  
##  success: True  
##      x: array([-5.31839421e-07, -8.84341728e-06])
```

```
optimize.minimize(fun = f, x0 = (1.6, 1.1), jac=grad, hess=hess  
##      fun: 2.3418652989289317e-12  
##      jac: array([0.0000000e+00, 4.10246332e-06])  
##  message: 'Optimization terminated successfully.'  
##      nfev: 12  
##      nhev: 11  
##      nit: 11  
##      njev: 12  
##      status: 0  
##  success: True  
##      x: array([0.0000000e+00, 3.8056246e-06])
```

# Collect

```
def run_collect(name, x0, cost_func, *args, tol=1e-8, skip=[]):
    f, grad, hess = cost_func(*args)
    methods = define_methods(x0, f, grad, hess, tol)

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

        x = methods[method]()

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

    return pd.concat(res)

df = pd.concat([
    run_collect(name, (1.6, 1.1), cost_func, arg, skip=['naive_ne'
    for name, cost_func, arg in zip(
        ("Well-cond quad", "Ill-cond quad", "Rosenbrock"),
        (mk_quad, mk_quad, mk_rosenbrock),
        (1.6, 1.1, 1.1)
    )]]))
```

```
df.drop(["message"], axis=1)
```

		name	method	nit	nfev	nhev	nhev	success
## 1	Well-cond quad		cg	2	5	5	None	True
## 1	Well-cond quad		newton-cg	5	6	13	0	True
## 1	Well-cond quad	newton-cg w/ H		15	15	15	15	True
## 1	Well-cond quad		bfsgs	8	9	9	None	True
## 1	Well-cond quad		bfsgs w/o G	8	27	9	None	True
## 1	Well-cond quad		l-bfgs	6	21	7	None	True
## 1	Well-cond quad		nelder-mead	76	147	None	None	True
## 1	Ill-cond quad		cg	9	17	17	None	True
## 1	Ill-cond quad		newton-cg	3	4	9	0	True
## 1	Ill-cond quad	newton-cg w/ H		54	106	106	54	True
## 1	Ill-cond quad		bfsgs	5	11	11	None	True
## 1	Ill-cond quad		bfsgs w/o G	5	33	11	None	True
## 1	Ill-cond quad		l-bfgs	5	30	10	None	True
## 1	Ill-cond quad		nelder-mead	102	198	None	None	True
## 1	Rosenbrock		cg	17	52	48	None	True
## 1	Rosenbrock		newton-cg	18	22	60	0	True
## 1	Rosenbrock	newton-cg w/ H		17	21	21	17	True
## 1	Rosenbrock		bfsgs	23	26	26	None	True
## 1	Rosenbrock		bfsgs w/o G	23	78	26	None	True
## 1	Rosenbrock		l-bfgs	19	75	25	None	True
## 1	Rosenbrock		nelder-mead	96	183	None	None	True

```
sns.catplot(  
    y = "method", x = "value", hue = "variable", col="name", kind="bar",  
    data = df.melt(id_vars=["name", "method"], value_vars=["nit", "nfev", "njev", "nhev"]).astype({"value":  
})
```



# Exercise 1

Try minimizing the following function using different optimization methods starting from  $x_0 = [0, 0]$ , which appears to work best?

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

# Random starting locations

```
rng = np.random.default_rng(seed=1234)
x0s = rng.uniform(-2,2, (100,2))

df = pd.concat([
    run_collect(name, x0, cost_func, arg, skip=['na'],
    for name, cost_func, arg in zip(
        ("Well-cond quad", "Ill-cond quad", "Rosenbrock",
        (mk_quad, mk_quad, mk_rosenbrock),
        (0.7, 0.02, None)
    )
    for x0 in x0s
])])
```

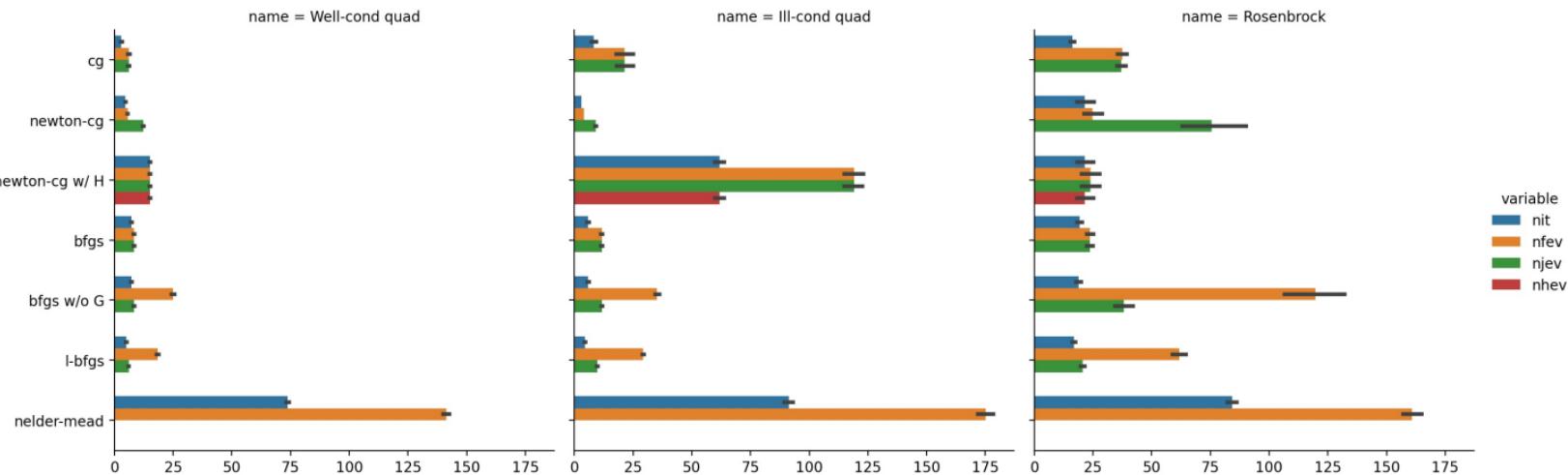
```
df.drop(["message"], axis=1)
```

		name	method	nit	nfev	njev	nhev	success
## 1	Well-cond	quad	cg	2	5	5	None	True
## 1	Well-cond	quad	newton-cg	5	6	13	0	True
## 1	Well-cond	quad	newton-cg w/ H	15	15	15	15	True
## 1	Well-cond	quad	bfsgs	6	7	7	None	True
## 1	Well-cond	quad	bfsgs w/o G	6	21	7	None	True
## ..	...	...	...	...	...	...	...	...
## 1	Rosenbrock		newton-cg w/ H	17	17	17	17	True
## 1	Rosenbrock		bfsgs	26	31	31	None	True
## 1	Rosenbrock		bfsgs w/o G	26	93	31	None	True
## 1	Rosenbrock		l-bfgs	18	57	19	None	True
## 1	Rosenbrock		nelder-mead	75	145	None	None	True
##								

```
## [2100 rows x 7 columns]
```

# Performance (random start)

```
sns.catplot(  
    y = "method", x = "value", hue = "variable", col="name", kind="bar",  
    data = df.melt(id_vars=["name", "method"], value_vars=["nit", "nfev", "njev", "nhev"]).astype({"value":  
}).set(  
    xlabel="", ylabel=""  
)
```



# MVN Cost Function

For an  $n$ -dimensional multivariate normal we have the  $n \times 1$  vectors  $x$  and  $\mu$  and the  $n \times n$  covariance matrix  $\Sigma$ ,

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

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

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

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

    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 @
                                                       x_m))

    return f, grad, hess
```

# 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()`.

```
# 2d  
f, grad, hess = mk_mvн(np.zeros(2), np.eye(2,2))  
optimize.check_grad(f, grad, [0,0])
```

```
## 1.0536712127723509e-08
```

```
optimize.check_grad(f, grad, [1,1])
```

```
## 2.8653603296584263e-09
```

```
# 4d  
f, grad, hess = mk_mvн(np.zeros(4), np.eye(4,4))  
optimize.check_grad(f, grad, [0,0,0,0])
```

```
## 1.4901161193847656e-08
```

```
# 20d  
f, grad, hess = mk_mvн(np.zeros(20), np.eye(20))  
optimize.check_grad(f, grad, np.zeros(20))
```

```
## 3.332000937312528e-08
```

```
optimize.check_grad(f, grad, np.ones(20))
```

```
## 7.079924060068647e-13
```

```
# 50d  
f, grad, hess = mk_mvн(np.zeros(50), np.eye(50))  
optimize.check_grad(f, grad, np.zeros(50))
```

```
## 5.268356063861754e-08
```

# Testing optimizers

```
f, grad, hess = mk_mvnp(np.zeros(4), np.eye(4,4))
optimize.minimize(fun=f, x0=[1,1,1,1], jac=grad, method="CG", t
##      fun: -1.0
##      jac: array([6.46744384e-16, 6.46744384e-16, 6.46744384e-
## message: 'Optimization terminated successfully.'
##      nfev: 8
##      nit: 3
##      njev: 8
##      status: 0
##      success: True
##      x: array([6.46744384e-16, 6.46744384e-16, 6.46744384e-
optimize.minimize(fun=f, x0=[1,1,1,1], jac=grad, method="BFGS",
##      fun: -1.0
##      hess_inv: array([[1.00000001e+00, 1.32716307e-08, 1.32716307
##                      [1.32716307e-08, 1.00000001e+00, 1.32716306e-08, 1.327
##                      [1.32716307e-08, 1.32716306e-08, 1.00000001e+00, 1.327
##                      [1.32716306e-08, 1.32716306e-08, 1.32716306e-08, 1.000
##      jac: array([9.80523384e-16, 9.80523381e-16, 9.80523384e
##      message: 'Optimization terminated successfully.'
##      nfev: 10
##      nit: 5
##      njev: 10
##      status: 0
##      success: True
##      x: array([9.80523384e-16, 9.80523381e-16, 9.80523384e
```

```
n = 20
f, grad, hess = mk_mvnp(np.zeros(n), np.eye(n,n))
optimize.minimize(fun=f, x0=np.ones(n), jac=grad, method="CG",
##      fun: -1.0
##      jac: array([3.67929936e-19, 3.67929936e-19, 3.67929936e-19,
##                  3.67929936e-19, 3.67929936e-19, 3.67929936e-19,
##      message: 'Optimization terminated successfully.'
##      nfev: 14
##      nit: 2
##      njev: 14
##      status: 0
##      success: True
##      x: array([3.67929936e-19, 3.67929936e-19, 3.67929936e-19,
##                  3.67929936e-19, 3.67929936e-19, 3.67929936e-19,
##                  3.67929936e-19, 3.67929936e-19, 3.67929936e-19,
##                  3.67929936e-19, 3.67929936e-19, 3.67929936e-19,
##                  3.67929936e-19, 3.67929936e-19, 3.67929936e-19,
```

# Unit MVNs

```
df = pd.concat([
    run_collect(
        name, np.ones(n), mk_mvns,
        np.zeros(n), np.eye(n),
        tol=1e-10,
        skip=['naive_newton', 'naive_cg']
    )
    for name, n in zip(
        ("2d", "5d", "10d", "20d", "50d"),
        (2, 5, 10, 20, 50)
    )
])
```

```
df.drop(["message"], axis=1)
```

##	name	method	nit	nfev	njev	nhev	success
## 1	2d	cg	3	6	6	None	True
## 1	2d	newton-cg	2	3	5	0	True
## 1	2d	newton-cg w/ H	2	2	2	2	True
## 1	2d	bfsgs	4	8	8	None	True
## 1	2d	bfsgs w/o G	4	24	8	None	True
## 1	2d	l-bfgs	5	21	7	None	True
## 1	2d	nelder-mead	75	157	None	None	True
## 1	5d	cg	3	8	8	None	True
## 1	5d	newton-cg	4	8	12	0	True
## 1	5d	newton-cg w/ H	4	7	7	4	True
## 1	5d	bfsgs	5	11	11	None	True
## 1	5d	bfsgs w/o G	5	72	12	None	True
## 1	5d	l-bfgs	4	54	9	None	True
## 1	5d	nelder-mead	297	529	None	None	True
## 1	10d	cg	2	24	22	None	True
## 1	10d	newton-cg	3	9	12	0	True
## 1	10d	newton-cg w/ H	3	8	8	3	True
## 1	10d	bfsgs	3	12	12	None	True
## 1	10d	bfsgs w/o G	2	121	11	None	True
## 1	10d	l-bfgs	3	110	10	None	True
## 1	10d	nelder-mead	1408	2000	None	None	False
## 1	20d	cg	2	14	14	None	True
## 1	20d	newton-cg	3	10	13	0	True
## 1	20d	newton-cg w/ H	3	9	9	3	True
## 1	20d	bfsgs	2	15	15	None	True
## 1	20d	bfsgs w/o G	2	315	15	None	True
## 1	20d	l-bfgs	3	210	10	None	True

# Adding correlation

```
def build_Sigma(n):
    S = np.full((n,n), 0.5)
    np.fill_diagonal(S, 1)
    return S

df = pd.concat([
    run_collect(
        name, np.ones(n), mk_mvN,
        np.zeros(n), build_Sigma(n),
        tol=1e-9/n,
        skip=['naive_newton', 'naive_cg'])
    )
    for name, n in zip(
        ("2d", "5d", "10d", "20d", "50d"),
        (2, 5, 10, 20, 50)
    )
])
])
```

```
df.drop(["message"], axis=1)
```

##	name	method	nit	nfev	njev	nhev	success
## 1	2d	cg	15	18	18	None	False
## 1	2d	newton-cg	5	7	12	0	True
## 1	2d	newton-cg w/ H	5	6	6	5	True
## 1	2d	bfsgs	3	7	7	None	True
## 1	2d	bfsgs w/o G	3	24	8	None	False
## 1	2d	l-bfgs	5	21	7	None	True
## 1	2d	nelder-mead	73	145	None	None	True
## 1	5d	cg	5	19	19	None	True
## 1	5d	newton-cg	5	7	12	0	True
## 1	5d	newton-cg w/ H	5	6	6	5	True
## 1	5d	bfsgs	5	8	8	None	True
## 1	5d	bfsgs w/o G	7	528	86	None	False
## 1	5d	l-bfgs	4	54	9	None	True
## 1	5d	nelder-mead	224	421	None	None	True
## 1	10d	cg	10	23	23	None	False
## 1	10d	newton-cg	5	6	11	0	True
## 1	10d	newton-cg w/ H	5	5	5	5	True
## 1	10d	bfsgs	4	9	9	None	True
## 1	10d	bfsgs w/o G	6	132	12	None	True
## 1	10d	l-bfgs	4	99	9	None	True
## 1	10d	nelder-mead	1151	1754	None	None	True
## 1	20d	cg	5	25	25	None	True
## 1	20d	newton-cg	4	5	9	0	True
## 1	20d	newton-cg w/ H	4	4	4	4	True
## 1	20d	bfsgs	5	9	9	None	True
## 1	20d	bfsgs w/o G	6	210	10	None	False
## 1	20d	l-bfgs	5	189	9	None	True

df

##	name	method	nit	nfev	njev	nhev	success	message
## 1	2d	cg	15	18	18	None	False	Desired error not necessarily achieved due to ...
## 1	2d	newton-cg	5	7	12	0	True	Optimization terminated successfully.
## 1	2d	newton-cg w/ H	5	6	6	5	True	Optimization terminated successfully.
## 1	2d	bfgs	3	7	7	None	True	Optimization terminated successfully.
## 1	2d	bfgs w/o G	3	24	8	None	False	Desired error not necessarily achieved due to ...
## 1	2d	l-bfgs	5	21	7	None	True	CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=PGTOL
## 1	2d	nelder-mead	73	145	None	None	True	Optimization terminated successfully.
## 1	5d	cg	5	19	19	None	True	Optimization terminated successfully.
## 1	5d	newton-cg	5	7	12	0	True	Optimization terminated successfully.
## 1	5d	newton-cg w/ H	5	6	6	5	True	Optimization terminated successfully.
## 1	5d	bfgs	5	8	8	None	True	Optimization terminated successfully.
## 1	5d	bfgs w/o G	7	528	86	None	False	Desired error not necessarily achieved due to ...
## 1	5d	l-bfgs	4	54	9	None	True	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
## 1	5d	nelder-mead	224	421	None	None	True	Optimization terminated successfully.
## 1	10d	cg	10	23	23	None	False	Desired error not necessarily achieved due to ...
## 1	10d	newton-cg	5	6	11	0	True	Optimization terminated successfully.
## 1	10d	newton-cg w/ H	5	5	5	5	True	Optimization terminated successfully.
## 1	10d	bfgs	4	9	9	None	True	Optimization terminated successfully.
## 1	10d	bfgs w/o G	6	132	12	None	True	Optimization terminated successfully.
## 1	10d	l-bfgs	4	99	9	None	True	CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
## 1	10d	nelder-mead	1151	1754	None	None	True	Optimization terminated successfully.
## 1	20d	cg	5	25	25	None	True	Optimization terminated successfully.
## 1	20d	newton-cg	4	5	9	0	True	Optimization terminated successfully.
## 1	20d	newton-cg w/ H	4	4	4	4	True	Optimization terminated successfully.

# What's going on?

```
n = 50
```

```
f, grad, hess = mk_mvnp(np.zeros(n), build_Sigma(n))
```

```
optimize.minimize(f, np.ones(n), jac=grad, method="CG", tol=1e-
```

```
##      fun: -1.0
##      jac: array([ 1.12332277e-10,  8.72935916e-11, -3.3297223
##                    8.69788321e-11, -4.18555930e-11,  2.10910902e-11, -1.
##                   -1.56070646e-10, -1.73949531e-11, -2.46648960e-10, -9.
##                  -2.69689780e-10, -2.53304579e-10, -2.14723226e-10, -2.
##                 -6.02970488e-11, -2.62054475e-10, -1.88641458e-10,  1.
##                -1.37095135e-10, -1.99919295e-10, -1.62557241e-10, -1.
##               -1.82270787e-10, -1.70384755e-10, -1.70436047e-10, -1.
##              -2.19757053e-10, -1.52952018e-10, -2.13786756e-10, -1.
##             -2.04463656e-10, -2.43201436e-10, -2.04465933e-10, -2.
##            -2.78825917e-10, -1.90142568e-10, -2.29375511e-10, -2.
##           -2.43124923e-10, -2.29273546e-10, -2.27412666e-10, -2.
##          -2.63387506e-10, -2.38475808e-10, -2.78480808e-10, -2.
##         -2.58275285e-10, -2.50752825e-10])
##      message: 'Desired error not necessarily achieved due to prec
##      nfev: 35
##      nit: 12
##      njev: 35
##      status: 2
##      success: False
##      x: array([-4.12110457e-09, -4.13362391e-09, -4.3437568
##                -4.13378129e-09, -4.19819851e-09, -4.16672516e-09, -4.
```

```
optimize.minimize(f, np.ones(n), jac=grad, method="BFGS", tol=1
```

```
##      fun: -1.0
##      hess_inv: array([[1.49000053, 0.49000053, 0.49000053, ..., 0.490000
##                        0.49000053],
##                      [0.49000053, 1.49000053, 0.49000053, ..., 0.49000053, 0.490000
##                        0.49000053],
##                      [0.49000053, 0.49000053, 1.49000053, ..., 0.49000053, 0.490000
##                        0.49000053],
##                      ...,
##                      [0.49000053, 0.49000053, 0.49000053, ..., 1.49000053, 0.490000
##                        0.49000053],
##                      [0.49000053, 0.49000053, 0.49000053, ..., 0.49000053, 1.490000
##                        0.49000053],
##                      [0.49000053, 0.49000053, 0.49000053, ..., 0.49000053, 0.490000
##                        1.49000053]])
##      jac: array([-2.73970642e-12, -2.74307089e-12, -2.79949727e-12,
##                  -2.74292110e-12, -2.76027528e-12, -2.75166780e-12, -2.7565265
##                  -2.77555684e-12, -2.75705655e-12, -2.78801410e-12, -2.7668121
##                  -2.79098818e-12, -2.78892573e-12, -2.78363550e-12, -2.7839237
##                  -2.76262526e-12, -2.78983521e-12, -2.77993127e-12, -2.7531132
##                  -2.77310882e-12, -2.78152071e-12, -2.77661830e-12, -2.7730126
##                  -2.77931259e-12, -2.77777327e-12, -2.77782252e-12, -2.7743122
##                  -2.78416334e-12, -2.77532276e-12, -2.78339434e-12, -2.7801260])
```

```

sns.catplot(
    y = "method", x = "value", hue = "variable", col="name", kind="bar",
    data = df.melt(
        id_vars=["name", "method"], value_vars=["nit", "nfev", "njev", "nhev"]
    ).astype(
        {"value": "float64"}
    ).query(
        "name != '2d'"
    )
).set(
    xscale="log", xlabel="", ylabel=""
)

```



# 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
- 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