

Automatic Differentiation: CES example

Symbolic derivatives are more accurate than finite differences, but they can be expensive to evaluate without a lot of work. We shall illustrate the points in a simple example.

We write an expression corresponding to four inputs in a CES utility function

```
In[77]:= vars = {x, y, z, w};
```

```
In[79]:= utility = Sum[a_i vars[[i]]^σ, {i, 1, 4}]^φ
```

```
Out[79]= (x^σ a_1 + y^σ a_2 + z^σ a_3 + w^σ a_4)^φ
```

This takes five powers, three additions, and four multiplications: 12 flops

Compute the gradient

```
In[81]:= gradutility = Table[D[utility, vars[[i]]], {i, 1, 4}];  
gradutility // TableForm
```

```
Out[82]//TableForm=
```

$$\begin{aligned} & x^{-1+\sigma} \sigma \phi a_1 (x^\sigma a_1 + y^\sigma a_2 + z^\sigma a_3 + w^\sigma a_4)^{-1+\phi} \\ & y^{-1+\sigma} \sigma \phi a_2 (x^\sigma a_1 + y^\sigma a_2 + z^\sigma a_3 + w^\sigma a_4)^{-1+\phi} \\ & z^{-1+\sigma} \sigma \phi a_3 (x^\sigma a_1 + y^\sigma a_2 + z^\sigma a_3 + w^\sigma a_4)^{-1+\phi} \\ & w^{-1+\sigma} \sigma \phi a_4 (x^\sigma a_1 + y^\sigma a_2 + z^\sigma a_3 + w^\sigma a_4)^{-1+\phi} \end{aligned}$$

Each gradient uses six powers, five additions, and eight multiplications: $19 \times 4 = 95$ flops

So, computing the four terms in the gradient vector costs EIGHT time the cost of one function evaluation!

However, note that the function and its gradient contains many common elements. Let's use this to reduce the computational burden.

The following term appears in utility and its appearance in each gradient can be avoided by the following substitution

```
In[83]:= sub1 = (xσ a1 + yσ a2 + zσ a3 + wσ a4) → v1
```

```
Out[83]= xσ a1 + yσ a2 + zσ a3 + wσ a4 → v1
```

```
In[84]:= grad = gradf /. sub1
```

```
Out[84]= {v1-1+φ x-1+σ σ φ a1, v1-1+φ y-1+σ σ φ a2, v1-1+φ z-1+σ σ φ a3, v1-1+φ w-1+σ σ φ a4}
```

We now compute the $-1+\sigma$, $-1+\phi$ and $\sigma\phi$ terms: 3 new flops
but then substitute them out in grad

```
In[87]:= sub2 = {-1 +  $\phi$  →  $\phi m1$ , -1 +  $\sigma$  →  $\sigma m1$ ,  $\sigma\phi$  →  $\sigma\phi$ }
```

```
Out[87]:= {-1 +  $\phi$  →  $\phi m1$ , -1 +  $\sigma$  →  $\sigma m1$ ,  $\sigma\phi$  →  $\sigma\phi$ }
```

```
In[88]:= grad = grad /. sub2
```

```
Out[88]:= { $v1^{\phi m1} x^{\sigma m1} \sigma\phi a_1$ ,  $v1^{\phi m1} y^{\sigma m1} \sigma\phi a_2$ ,  $v1^{\phi m1} z^{\sigma m1} \sigma\phi a_3$ ,  $v1^{\phi m1} w^{\sigma m1} \sigma\phi a_4$ }
```

The next substitution requires one power and one multiplication: 2 flops

```
In[89]:= sub4 =  $\sigma\phi v1^{\phi m1}$  → v2
```

```
Out[89]:=  $v1^{\phi m1} \sigma\phi$  → v2
```

```
In[90]:= grad = grad /. sub4
```

```
Out[90]:= { $v2 x^{\sigma m1} a_1$ ,  $v2 y^{\sigma m1} a_2$ ,  $v2 z^{\sigma m1} a_3$ ,  $v2 w^{\sigma m1} a_4$ }
```

This expression now needs two multiplications and one power per gradient. So the marginal cost of the gradient is $5+4 \times 3=17$ flops -- BASICALLY THE SAME COST AS ONE EVALUATION OF THE FUNCTION!

Let's now consider the Hessian. We first define it and then eliminate repetitions due to symmetry

```
In[91]:= hessf = Table[D[gradf, vars[[i]]], {i, 1, 4}];
```

```
hess = hessf // Flatten // Union
```

```
Out[92]= {x-1+σ y-1+σ σ2 (-1+φ) φ a1 a2 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-2+φ, x-1+σ z-1+σ σ2 (-1+φ) φ a1 a3 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-2+φ,  
y-1+σ z-1+σ σ2 (-1+φ) φ a2 a3 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-2+φ, w-1+σ x-1+σ σ2 (-1+φ) φ a1 a4 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-2+φ,  
w-1+σ y-1+σ σ2 (-1+φ) φ a2 a4 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-2+φ, w-1+σ z-1+σ σ2 (-1+φ) φ a3 a4 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-2+φ,  
x-2+2σ σ2 (-1+φ) φ a12 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-2+φ + x-2+σ (-1+σ) σ φ a1 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-1+φ,  
y-2+2σ σ2 (-1+φ) φ a22 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-2+φ + y-2+σ (-1+σ) σ φ a2 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-1+φ,  
z-2+2σ σ2 (-1+φ) φ a32 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-2+φ + z-2+σ (-1+σ) σ φ a3 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-1+φ,  
w-2+2σ σ2 (-1+φ) φ a42 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-2+φ + w-2+σ (-1+σ) σ φ a4 (xσ a1 + yσ a2 + zσ a3 + wσ a4)-1+φ}
```

First we use the substitutions we used for the gradient; these require no new flops.

```
In[99]:= hess = hess /. sub1 /. sub2 /. sub3;
% // TableForm
```

```
Out[100]//TableForm=
```

```

v1-2+φ xσm1 yσm1 σ2 φ φm1 a1 a2
v1-2+φ xσm1 zσm1 σ2 φ φm1 a1 a3
v1-2+φ yσm1 zσm1 σ2 φ φm1 a2 a3
v1-2+φ wσm1 xσm1 σ2 φ φm1 a1 a4
v1-2+φ wσm1 yσm1 σ2 φ φm1 a2 a4
v1-2+φ wσm1 zσm1 σ2 φ φm1 a3 a4
v1φm1 x-2+σ σm1 σ φ a1 + v1-2+φ x-2+2 σ σ2 φ φm1 a12
v1φm1 y-2+σ σm1 σ φ a2 + v1-2+φ y-2+2 σ σ2 φ φm1 a22
v1φm1 z-2+σ σm1 σ φ a3 + v1-2+φ z-2+2 σ σ2 φ φm1 a32
v1φm1 w-2+σ σm1 σ φ a4 + v1-2+φ w-2+2 σ σ2 φ φm1 a42

```

Let's now eliminate repeated terms. The next substitution requires one power and one addition (2 extra flops)

```
In[101]:= hess /. v1-2+σ1 → v3
```

```

Out[101]= {v1-2+φ xσm1 yσm1 σ2 φ φm1 a1 a2, v1-2+φ xσm1 zσm1 σ2 φ φm1 a1 a3, v1-2+φ yσm1 zσm1 σ2 φ φm1 a2 a3,
v1-2+φ wσm1 xσm1 σ2 φ φm1 a1 a4, v1-2+φ wσm1 yσm1 σ2 φ φm1 a2 a4, v1-2+φ wσm1 zσm1 σ2 φ φm1 a3 a4,
v1φm1 x-2+σ σm1 σ φ a1 + v1-2+φ x-2+2 σ σ2 φ φm1 a12, v1φm1 y-2+σ σm1 σ φ a2 + v1-2+φ y-2+2 σ σ2 φ φm1 a22,
v1φm1 z-2+σ σm1 σ φ a3 + v1-2+φ z-2+2 σ σ2 φ φm1 a32, v1φm1 w-2+σ σm1 σ φ a4 + v1-2+φ w-2+2 σ σ2 φ φm1 a42}

```

one extra addition (cumulative total of 3 flops)

```
In[102]:= % /. -2 + σ → σm2
```

```

Out[102]= {v1-2+φ xσm1 yσm1 σ2 φ φm1 a1 a2, v1-2+φ xσm1 zσm1 σ2 φ φm1 a1 a3, v1-2+φ yσm1 zσm1 σ2 φ φm1 a2 a3,
v1-2+φ wσm1 xσm1 σ2 φ φm1 a1 a4, v1-2+φ wσm1 yσm1 σ2 φ φm1 a2 a4, v1-2+φ wσm1 zσm1 σ2 φ φm1 a3 a4,
v1φm1 xσm2 σm1 σ φ a1 + v1-2+φ x-2+2 σ σ2 φ φm1 a12, v1φm1 yσm2 σm1 σ φ a2 + v1-2+φ y-2+2 σ σ2 φ φm1 a22,
v1φm1 zσm2 σm1 σ φ a3 + v1-2+φ z-2+2 σ σ2 φ φm1 a32, v1φm1 wσm2 σm1 σ φ a4 + v1-2+φ w-2+2 σ σ2 φ φm1 a42}

```

one extra addition and one multiplication (total 5 flops)

$$\ln[103]:= \% /. -2 + \phi \rightarrow \phi m2$$
$$\text{Out}[103]=\left\{v_1^{\phi m^2} x^{\phi m^1} y^{\phi m^1} \sigma^2 \phi \phi m^1 a_1 a_2, v_1^{\phi m^2} x^{\phi m^1} z^{\phi m^1} \sigma^2 \phi \phi m^1 a_1 a_3, v_1^{\phi m^2} y^{\phi m^1} z^{\phi m^1} \sigma^2 \phi \phi m^1 a_2 a_3, \right. \\ v_1^{\phi m^2} w^{\phi m^1} x^{\phi m^1} \sigma^2 \phi \phi m^1 a_1 a_4, v_1^{\phi m^2} w^{\phi m^1} y^{\phi m^1} \sigma^2 \phi \phi m^1 a_2 a_4, v_1^{\phi m^2} w^{\phi m^1} z^{\phi m^1} \sigma^2 \phi \phi m^1 a_3 a_4, \\ v_1^{\phi m^1} x^{\phi m^2} \phi m^1 \sigma \phi a_1 + v_1^{\phi m^2} x^{-2+2 \sigma} \sigma^2 \phi \phi m^1 a_1^2, v_1^{\phi m^1} y^{\phi m^2} \phi m^1 \sigma \phi a_2 + v_1^{\phi m^2} y^{-2+2 \sigma} \sigma^2 \phi \phi m^1 a_2^2, \\ \left. v_1^{\phi m^1} z^{\phi m^2} \phi m^1 \sigma \phi a_3 + v_1^{\phi m^2} z^{-2+2 \sigma} \sigma^2 \phi \phi m^1 a_3^2, v_1^{\phi m^1} w^{\phi m^2} \phi m^1 \sigma \phi a_4 + v_1^{\phi m^2} w^{-2+2 \sigma} \sigma^2 \phi \phi m^1 a_4^2\right\}$$
$$\ln[105] := \% / . - 2 + 2 \sigma \rightarrow \sigma^2 m^2$$
$$\text{Out}[105]= \left\{ v1^{\phi m2} x^{\sigma m1} y^{\sigma m1} \sigma^2 \phi \phi m1 a_1 a_2, v1^{\phi m2} x^{\sigma m1} z^{\sigma m1} \sigma^2 \phi \phi m1 a_1 a_3, v1^{\phi m2} y^{\sigma m1} z^{\sigma m1} \sigma^2 \phi \phi m1 a_2 a_3, v1^{\phi m2} w^{\sigma m1} x^{\sigma m1} \sigma^2 \phi \phi m1 a_1 a_4, \right. \\ v1^{\phi m2} w^{\sigma m1} y^{\sigma m1} \sigma^2 \phi \phi m1 a_2 a_4, v1^{\phi m2} w^{\sigma m1} z^{\sigma m1} \sigma^2 \phi \phi m1 a_3 a_4, v1^{\phi m1} x^{\sigma m2} \sigma m1 \sigma \phi a_1 + v1^{\phi m2} x^{\sigma 2 m2} \sigma^2 \phi \phi m1 a_1^2, \\ \left. v1^{\phi m1} y^{\sigma m2} \sigma m1 \sigma \phi a_2 + v1^{\phi m2} y^{\sigma 2 m2} \sigma^2 \phi \phi m1 a_2^2, v1^{\phi m1} z^{\sigma m2} \sigma m1 \sigma \phi a_3 + v1^{\phi m2} z^{\sigma 2 m2} \sigma^2 \phi \phi m1 a_3^2, v1^{\phi m1} w^{\sigma m2} \sigma m1 \sigma \phi a_4 + v1^{\phi m2} w^{\sigma 2 m2} \sigma^2 \phi \phi m1 a_4^2 \right\}$$

one multiplication (total 6 flops)

```
In[106]:= % /.  $\sigma m1 \sigma \phi \rightarrow \sigma m1 \sigma \phi$ 
```

$$\text{Out}\{106\} = \{v1^{\phi m2} x^{\sigma m1} y^{\sigma m1} \sigma^2 \phi \phi m1 a_1 a_2, v1^{\phi m2} x^{\sigma m1} z^{\sigma m1} \sigma^2 \phi \phi m1 a_1 a_3, v1^{\phi m2} y^{\sigma m1} z^{\sigma m1} \sigma^2 \phi \phi m1 a_2 a_3, v1^{\phi m2} w^{\sigma m1} x^{\sigma m1} \sigma^2 \phi \phi m1 a_1 a_4, \\ v1^{\phi m2} w^{\sigma m1} y^{\sigma m1} \sigma^2 \phi \phi m1 a_2 a_4, v1^{\phi m2} w^{\sigma m1} z^{\sigma m1} \sigma^2 \phi \phi m1 a_3 a_4, v1^{\phi m1} x^{\sigma m2} \sigma m1 \sigma \phi a_1 + v1^{\phi m2} x^{\sigma 2 m2} \sigma^2 \phi \phi m1 a_1^2, \\ v1^{\phi m1} y^{\sigma m2} \sigma m1 \sigma \phi a_2 + v1^{\phi m2} y^{\sigma 2 m2} \sigma^2 \phi \phi m1 a_2^2, v1^{\phi m1} z^{\sigma m2} \sigma m1 \sigma \phi a_3 + v1^{\phi m2} z^{\sigma 2 m2} \sigma^2 \phi \phi m1 a_3^2, v1^{\phi m1} w^{\sigma m2} \sigma m1 \sigma \phi a_4 + v1^{\phi m2} w^{\sigma 2 m2} \sigma^2 \phi \phi m1 a_4^2\}$$
$$\ln[107] := \% /. v1^{\phi m2} \rightarrow v2$$
$$\text{Out}\{107\} = \left\{ \begin{aligned} &v_2 x^{\sigma m_1} y^{\sigma m_1} \sigma^2 \phi \phi m_1 a_1 a_2, v_2 x^{\sigma m_1} z^{\sigma m_1} \sigma^2 \phi \phi m_1 a_1 a_3, v_2 y^{\sigma m_1} z^{\sigma m_1} \sigma^2 \phi \phi m_1 a_2 a_3, v_2 w^{\sigma m_1} x^{\sigma m_1} \sigma^2 \phi \phi m_1 a_1 a_4, \\ &v_2 w^{\sigma m_1} y^{\sigma m_1} \sigma^2 \phi \phi m_1 a_2 a_4, v_2 w^{\sigma m_1} z^{\sigma m_1} \sigma^2 \phi \phi m_1 a_3 a_4, v_1 \phi m_1 x^{\sigma m_2} \sigma m_1 \sigma \phi a_1 + v_2 x^{\sigma 2 m_2} \sigma^2 \phi \phi m_1 a_1^2, \\ &v_1 \phi m_1 y^{\sigma m_2} \sigma m_1 \sigma \phi a_2 + v_2 y^{\sigma 2 m_2} \sigma^2 \phi \phi m_1 a_2^2, v_1 \phi m_1 z^{\sigma m_2} \sigma m_1 \sigma \phi a_3 + v_2 z^{\sigma 2 m_2} \sigma^2 \phi \phi m_1 a_3^2, v_1 \phi m_1 w^{\sigma m_2} \sigma m_1 \sigma \phi a_4 + v_2 w^{\sigma 2 m_2} \sigma^2 \phi \phi m_1 a_4^2 \end{aligned} \right\}$$
$$\text{In}[108]:= \% /. v1^{\phi m1} \rightarrow v3$$
$$\text{Out[108]} = \left\{ v_2 x^{\sigma m_1} y^{\sigma m_1} \sigma^2 \phi \phi m_1 a_1 a_2, v_2 x^{\sigma m_1} z^{\sigma m_1} \sigma^2 \phi \phi m_1 a_1 a_3, v_2 y^{\sigma m_1} z^{\sigma m_1} \sigma^2 \phi \phi m_1 a_2 a_3, v_2 w^{\sigma m_1} x^{\sigma m_1} \sigma^2 \phi \phi m_1 a_1 a_4, \right. \\ \left. v_2 w^{\sigma m_1} y^{\sigma m_1} \sigma^2 \phi \phi m_1 a_2 a_4, v_2 w^{\sigma m_1} z^{\sigma m_1} \sigma^2 \phi \phi m_1 a_3 a_4, v_3 x^{\sigma m_2} \sigma m_1 \sigma \phi a_1 + v_2 x^{\sigma 2 m_2} \sigma^2 \phi \phi m_1 a_1^2, \right. \\ \left. v_3 y^{\sigma m_2} \sigma m_1 \sigma \phi a_2 + v_2 y^{\sigma 2 m_2} \sigma^2 \phi \phi m_1 a_2^2, v_3 z^{\sigma m_2} \sigma m_1 \sigma \phi a_3 + v_2 z^{\sigma 2 m_2} \sigma^2 \phi \phi m_1 a_3^2, v_3 w^{\sigma m_2} \sigma m_1 \sigma \phi a_4 + v_2 w^{\sigma 2 m_2} \sigma^2 \phi \phi m_1 a_4^2 \right\}$$

one multiplication (7 flops)

In[109]:= % /. $\sigma^2 \phi \phi m1 \rightarrow \text{SFF}$ // Expand

Out[109]= $\{ \text{SFF } v2 x^{\sigma m1} y^{\sigma m1} a_1 a_2, \text{SFF } v2 x^{\sigma m1} z^{\sigma m1} a_1 a_3, \text{SFF } v2 y^{\sigma m1} z^{\sigma m1} a_2 a_3, \\ \text{SFF } v2 w^{\sigma m1} x^{\sigma m1} a_1 a_4, \text{SFF } v2 w^{\sigma m1} y^{\sigma m1} a_2 a_4, \text{SFF } v2 w^{\sigma m1} z^{\sigma m1} a_3 a_4, v3 x^{\sigma m2} \sigma m1 \sigma \phi a_1 + \text{SFF } v2 x^{\sigma 2 m2} a_1^2, \\ v3 y^{\sigma m2} \sigma m1 \sigma \phi a_2 + \text{SFF } v2 y^{\sigma 2 m2} a_2^2, v3 z^{\sigma m2} \sigma m1 \sigma \phi a_3 + \text{SFF } v2 z^{\sigma 2 m2} a_3^2, v3 w^{\sigma m2} \sigma m1 \sigma \phi a_4 + \text{SFF } v2 w^{\sigma 2 m2} a_4^2 \}$

In[112]:= % /. v2 SFF \rightarrow v2SFF // Expand

Out[112]= $\{ v2\text{SFF } x^{\sigma m1} y^{\sigma m1} a_1 a_2, v2\text{SFF } x^{\sigma m1} z^{\sigma m1} a_1 a_3, v2\text{SFF } y^{\sigma m1} z^{\sigma m1} a_2 a_3, v2\text{SFF } w^{\sigma m1} x^{\sigma m1} a_1 a_4, v2\text{SFF } w^{\sigma m1} y^{\sigma m1} a_2 a_4, v2\text{SFF } w^{\sigma m1} z^{\sigma m1} a_3 a_4, \\ v3 x^{\sigma m2} \sigma m1 \sigma \phi a_1 + v2\text{SFF } x^{\sigma 2 m2} a_1^2, v3 y^{\sigma m2} \sigma m1 \sigma \phi a_2 + v2\text{SFF } y^{\sigma 2 m2} a_2^2, v3 z^{\sigma m2} \sigma m1 \sigma \phi a_3 + v2\text{SFF } z^{\sigma 2 m2} a_3^2, v3 w^{\sigma m2} \sigma m1 \sigma \phi a_4 + v2\text{SFF } w^{\sigma 2 m2} a_4^2 \}$

This last set requires

4 flops in 6 cases = 24

7 flops in 4 cases = 28

So the total is 12+24+28 = 64 flops, WHICH IS LESS THAN FOUR TIMES THE COST OF THE FUNCTION!