SciencesPo Computational Economics
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1 Numerical Differentiation and Integration

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1.1 Derivatives

1. Finite Differencing: a numerical approximation
   - Based on Taylor's Theorem
   - Observe variation in function values from evaluating it at "close" points.
   - Forward Differencing and Central Differencing
2. Automatic Differentiation
   - Breaks down the actual `code` that defines a function and performs elementary differentiation rules, after disecting expressions via the chain rule.
   - This produces **analytic** derivatives, i.e. there is **no** approximation error.
   - This is the future.
3. Symbolic Differentiation
   - Some languages (most notably Mathematica) support symbolic algebra. Very useful sometimes if one needs to work through complicated expressions.
   - Not very useful for high computational demands, i.e. repeated computation of derivatives in an optimization routine.

1.2 Finite Differences

- Consider the definition of the derivative of f at point x:

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

- The simplest way to calculate a numerical derivative is to replicate this computation for small h with:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}, \quad h \text{ small.}$$

- This is known as the Forward Difference approach.

- There are different approaches, e.g. the central difference approach does

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}, \quad h \text{ small.}$$

- How does this perform?

```
In [1]: using Plots
        pyplot()
        f(x) = 2 - x^2
        c = -0.75
        sec_line(h) = x -> f(c) + (f(c + h) - f(c))/h * (x - c)
        plot([f, sec_line(1), sec_line(.5), sec_line(.25), sec_line(.05)], -1, 1)
```

```
/Users/florian.oswald/.julia/v0.5/Conda/deps/usr/lib/python2.7/site-packages/matplotlib/font_man
  warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment.')
```

- What's the problem? Well, what is *small*?

1.2.1 Finite Differences: what's the right step size h?

- Theoretically, we would like to have h as small as possible, since we want to approximate the limit at zero.
- In practice, on a computer, there is a limit to this. There is a smallest representable number, as we know.
- `eps()`.
- One can show that the optimal step size is $h = \sqrt{\texttt{eps()}}$

1.3 Automatic Differentiation (AD)

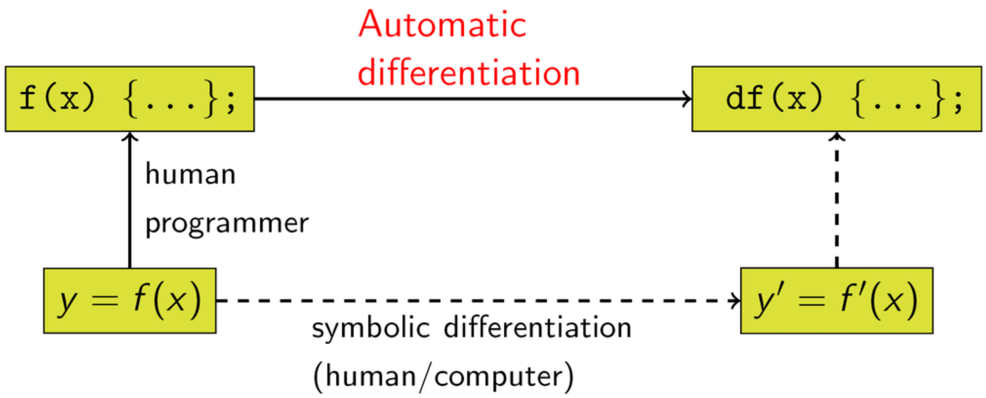
- 2 modes: Forward and Reverse Mode.
- The basic idea is that the derivative of any function can be decomposed into some basic algebraic operations.
- The wikipedia page is informative

1.4 Example

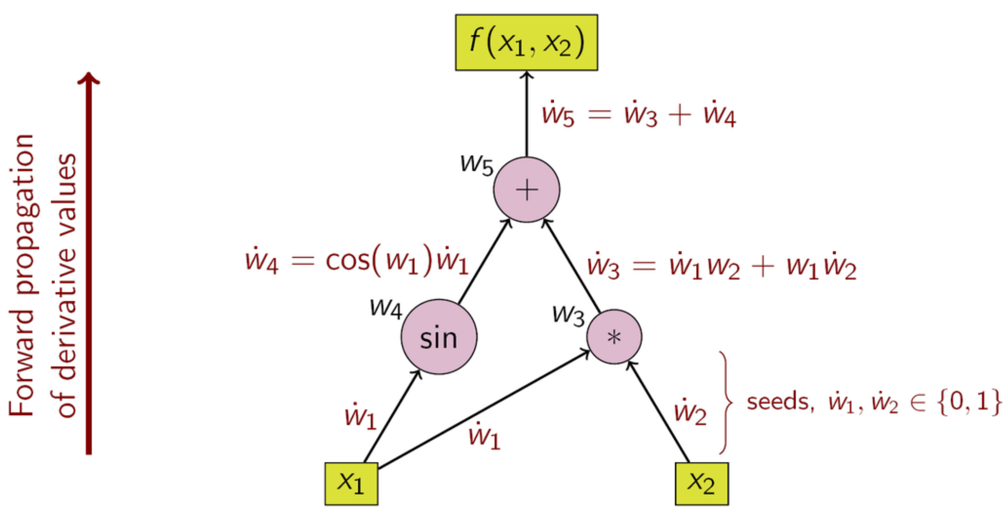
- Suppose we want to differentiate $f(x_1, x_2) = x_1 x_2 + \sin x_1$
- We label subexpressions by w_i as follows:

$$\begin{aligned} f(x_1, x_2) &= x_1 x_2 + \sin x_1 \\ &= w_1 w_2 + sin w_1 \\ &= w_3 + w_4 \\ &= w_5 \end{aligned}$$

- Computation of the partial derivative starts with the seed value, i.e. $\dot{w}_1 = \frac{\partial x_1}{\partial x_1} = 1$.
- We store for each subexpression both the value and the derivative, i.e. $(w_i, \dot{w}_i)$
- We then sweep through the expression tree as in this picture:



By Berland at en.wikipedia [Public domain], from Wikimedia Commons



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1.5 AD in Julia

- The organisation here is http://www.juliadiff.org
- There are many packages to perform differentiation with Julia here.
- Many packages rely on the machinery here.
- Let's quickly look at https://github.com/JuliaDiff/ForwardDiff.jl

In [3]:
```julia
# from ForwardDiff's readme:
using ForwardDiff
f(x::Vector) = sum(sin, x) + prod(tan, x) * sum(sqrt, x);
x = rand(5) # small size for example's sake
g = x -> ForwardDiff.gradient(f, x); # g = f
g(x)
ForwardDiff.hessian(f, x)
```

```
WARNING: Method definition f(Array{T<:Any, 1}) in module Main at In[2]:3 overwritten at In[3]:3.
```

Out[3]:
```
5Œ5 Array{Float64,2}:
 -0.0976779   0.582799   0.539911  2.13939    0.602214
  0.582799   -0.271656   0.397163  1.57396    0.44295
  0.539911    0.397163  -0.347212  1.45755    0.410393
  2.13939     1.57396    1.45755   0.426115   1.62638
  0.602214    0.44295    0.410393  1.62638   -0.249782
```

- The authors provide some benchmarks. Let's run those:

```julia
include(joinpath(Pkg.dir("ForwardDiff"),"benchmark","ForwardDiffBenchmarks.jl"))
```

1.6 Numerical Approximation of Integrals

- We will focus on methods that represent integrals as weighted sums.
- The typical representation will look like:

$$E[G(\epsilon)] = \int_{\mathbb{R}^N} G(\epsilon)w(\epsilon)d\epsilon \approx \sum_{j=1}^{J} \omega_j G(\epsilon_j)$$

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- N is the dimensionality of the integration problem.
- $G : \mathbb{R}^N \mapsto \mathbb{R}$ is the function we want to integrate wrt $\epsilon \in \mathbb{R}^N$.
- w is a density function s.t. $\int_{\mathbb{R}^n} w(\epsilon)d\epsilon = 1$.
- ω are weights such that (most of the time) $\sum_{j=1}^{J} \omega_j = 1$.
- We will look at normal shocks $\epsilon \sim N(0_N, I_N)$
- in that case, $w(\epsilon) = (2\pi)^{-N/2} \exp\left(-\frac{1}{2}\epsilon^T\epsilon\right)$
- I_N is the n by n identity matrix, i.e. there is no correlation among the shocks for now.
- Other random processes will require different weighting functions, but the principle is identical.
- For now, let's say that $N = 1$

1.7 Quadrature Rules

- We focus exclusively on those and leave Simpson and Newton Cowtes formulas out.
  - This is because Quadrature is the method that in many situations gives highes accuracy with lowest computational cost.
- Quadrature provides a rule to compute weights w_j and nodes ϵ_j.
- There are many different quadrature rules.
- They differ in their domain and weighting function.
- https://en.wikipedia.org/wiki/Gaussian_quadrature
- In general, we can convert our function domain to a rule-specific domain with change of variables.

1.8 Gauss-Hermite: Expectation of a Normally Distributed Variable

- There are many different rules, all specific to a certain random process.
- Gauss-Hermite is designed for an integral of the form

$$\int_{-\infty}^{+\infty} e^{-x^2} G(x) dx$$

and where we would approximate

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x) dx \approx \sum_{i=1}^{n} \omega_i G(x_i)$$

- Now, let's say we want to approximate the expected value of function f when it's argument $z \sim N(\mu, \sigma^2)$:

$$E[f(z)] = \int_{-\infty}^{+\infty} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(z-\mu)^2}{2\sigma^2}\right) f(z) dz$$

1.9 Gauss-Hermite: Expectation of a Normally Distributed Variable

- The rule is defined for x however. We need to transform z:

$$x = \frac{(z-\mu)^2}{2\sigma^2} \Rightarrow z = \sqrt{2}\sigma x + \mu$$

- This gives us now (just plug in for z)

$$E[f(z)] = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{\pi}} \exp\left(-x^2\right) f(\sqrt{2}\sigma x + \mu) dx$$

- And thus, our approximation to this, using weights ω_i and nodes x_i is

$$E[f(z)] \approx \sum_{j=1}^{J} \frac{1}{\sqrt{\pi}} \omega_j f(\sqrt{2}\sigma x_j + \mu)$$

1.10 Using Quadrature in Julia

- https://github.com/ajt60gaibb/FastGaussQuadrature.jl

```
In [5]: #Pkg.add("FastGaussQuadrature")

        using FastGaussQuadrature

        np = 3

        rules = Dict("hermite" => gausshermite(np),
                     "chebyshev" => gausschebyshev(np),
                     "legendre" => gausslegendre(np),
                     "lobatto" => gausslobatto(np))


        using DataFrames

        integ = DataFrame(Rule=Symbol[Symbol(x) for x in keys(rules)],nodes=[x[1] for x in value
```

```
Out[5]: 4Œ3 DataFrames.DataFrame
         Row   Rule        nodes

         1     lobatto     [-1.0,0.0,1.0]
         2     hermite     [-1.22474,-8.88178e-16,1.22474]
         3     legendre    [-0.774597,0.0,0.774597]
         4     chebyshev   [-0.866025,6.12323e-17,0.866025]

         Row   weights

         1     [0.333333,1.33333,0.333333]
         2     [0.295409,1.18164,0.295409]
         3     [0.555556,0.888889,0.555556]
         4     [1.0472,1.0472,1.0472]
```

1.11 Quadrature in more dimensions: Product Rule

- If we have $N > 1$, we can use the product rule: this just takes the kronecker product of all univariate rules.
- This works well as long as N is not too large. The number of required function evaluations grows exponentially.

$$E[G(\epsilon)] = \int_{\mathbb{R}^N} G(\epsilon)w(\epsilon)d\epsilon \approx \sum_{j_1=1}^{J_1} \cdots \sum_{j_N=1}^{J_N} \omega_{j_1}^1 \cdots \omega_{j_N}^N G(\epsilon_{j_1}^1, \ldots, \epsilon_{j_N}^N)$$

  where $\omega_{j_1}^1$ stands for weight index j_1 in dimension 1, same for ϵ.
- Total number of nodes: $J = J_1 J_2 \cdots J_N$, and J_i can differ from J_k.

1.11.1 Example for $N = 3$

- Suppose we have $\epsilon^i \sim N(0,1), i = 1,2,3$ as three uncorrelated random variables.
- Let's take $J = 3$ points in all dimensions, so that in total we have $J^N = 27$ points.
- We have the nodes and weights from before in `rules["hermite"]`.

In [9]:
```
rules["hermite"][1]
repeat(rules["hermite"][1],inner=[1],outer=[9])
```

Out[9]:
```
27-element Array{Float64,1}:
 -1.22474
 -8.88178e-16
  1.22474
 -1.22474
 -8.88178e-16
  1.22474
 -1.22474
 -8.88178e-16
  1.22474
 -1.22474
 -8.88178e-16
  1.22474
 -1.22474

 -1.22474
 -8.88178e-16
  1.22474
 -1.22474
 -8.88178e-16
  1.22474
 -1.22474
 -8.88178e-16
  1.22474
 -1.22474
 -8.88178e-16
  1.22474
```

In [6]:
```
nodes = Any[]
push!(nodes,repeat(rules["hermite"][1],inner=[1],outer=[9]))  # dim1
push!(nodes,repeat(rules["hermite"][1],inner=[3],outer=[3]))  # dim2
push!(nodes,repeat(rules["hermite"][1],inner=[9],outer=[1]))  # dim3
weights = kron(rules["hermite"][2],kron(rules["hermite"][2],rules["hermite"][2]))
df = hcat(DataFrame(weights=weights),DataFrame(nodes,[:dim1,:dim2,:dim3]))
```

Out[6]: 27Œ4 DataFrames.DataFrame

Row	weights	dim1	dim2	dim3
1	0.0257793	-1.22474	-1.22474	-1.22474
2	0.103117	-8.88178e-16	-1.22474	-1.22474

```
3     0.0257793  1.22474       -1.22474      -1.22474
4     0.103117   -1.22474      -8.88178e-16  -1.22474
5     0.412469   -8.88178e-16  -8.88178e-16  -1.22474
6     0.103117   1.22474       -8.88178e-16  -1.22474
7     0.0257793  -1.22474      1.22474       -1.22474
8     0.103117   -8.88178e-16  1.22474       -1.22474
9     0.0257793  1.22474       1.22474       -1.22474
10    0.103117   -1.22474      -1.22474      -8.88178e-16
11    0.412469   -8.88178e-16  -1.22474      -8.88178e-16

16    0.103117   -1.22474      1.22474       -8.88178e-16
17    0.412469   -8.88178e-16  1.22474       -8.88178e-16
18    0.103117   1.22474       1.22474       -8.88178e-16
19    0.0257793  -1.22474      -1.22474      1.22474
20    0.103117   -8.88178e-16  -1.22474      1.22474
21    0.0257793  1.22474       -1.22474      1.22474
22    0.103117   -1.22474      -8.88178e-16  1.22474
23    0.412469   -8.88178e-16  -8.88178e-16  1.22474
24    0.103117   1.22474       -8.88178e-16  1.22474
25    0.0257793  -1.22474      1.22474       1.22474
26    0.103117   -8.88178e-16  1.22474       1.22474
27    0.0257793  1.22474       1.22474       1.22474
```

- Imagine you had a function g defined on those 3 dims: in order to approximate the integral, you would have to evaluate g at all combinations of `dimx`, multiply with the corresponding weight, and sum.

1.11.2 Alternatives to the Product Rule

- Monomial Rules: They grow only linearly.
- Please refer to [juddbook] [1] for more details.

1.12 Monte Carlo Integration

- A widely used method is to just draw N points randomly from the space of the shock ϵ, and to assign equal weights $\omega_j = \frac{1}{N}$ to all of them.
- The expectation is then

$$E[G(\epsilon)] \approx \frac{1}{N} \sum_{j=1}^{N} G(\epsilon_j)$$

- This in general a very inefficient method.
- Particularly in more than 1 dimensions, the number of points needed for good accuracy is very large.

1.13 Quasi Monte Carlo Integration

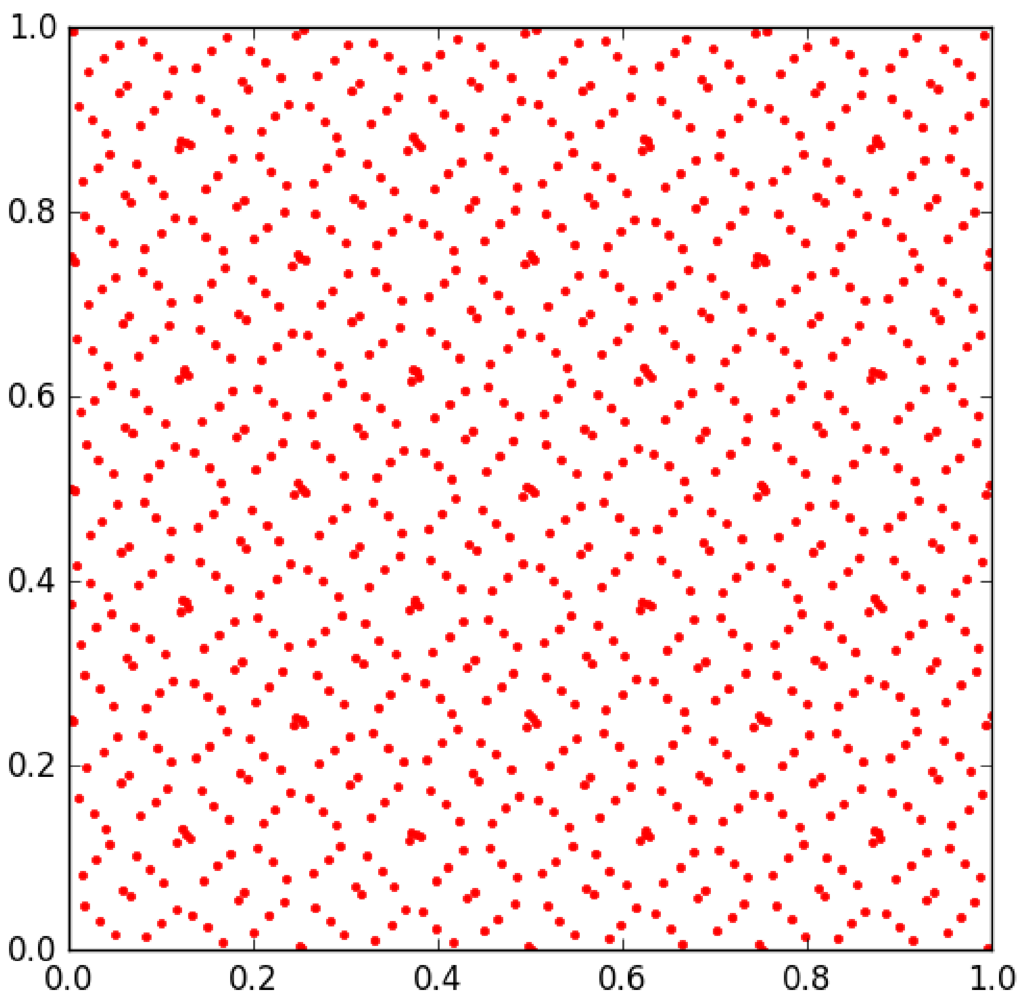
- Uses non-product techniques to construct a grid of uniformly spaced points.
- The researcher controlls the number of points.
- We need to construct equidistributed points.

- Typically one uses a low-discrepancy sequence of points, e.g. the Weyl sequence:
- $x_n = {nv}$ where v is an irrational number and {} stands for the fractional part of a number. for $v = \sqrt{2}$,

$$x_1 = \{1\sqrt{2}\} = \{1.4142\} = 0.4142, x_2 = \{2\sqrt{2}\} = \{2.8242\} = 0.8242, ...$$

- Other low-discrepancy sequences are Niederreiter, Haber, Baker or Sobol.

In [2]:
```
# Pkg.add("Sobol")
using Sobol
using PyPlot
s = SobolSeq(2)
p = hcat([next(s) for i = 1:1024]...)'
subplot(111, aspect="equal")
plot(p[:,1], p[:,2], "r.")
```



```
INFO: No packages to install, update or remove
INFO: Package database updated
INFO: METADATA is out-of-date  you may not have the latest version of Sobol
INFO: Use `Pkg.update()` to get the latest versions of your packages
```

```
Out[2]: 1-element Array{Any,1}:
         PyObject <matplotlib.lines.Line2D object at 0x323fb92d0>
```

Correlated Shocks

- We often face situations where the shocks are in fact correlated.
  - One very typical case is an AR1 process:

$$z_{t+1} = \rho z_t + \varepsilon_t, \varepsilon \sim N(0, \sigma^2)$$

- The general case is again:

$$E[G(\epsilon)] = \int_{\mathbb{R}^N} G(\epsilon) w(\epsilon) d\epsilon \approx \sum_{j_1=1}^{J_1} \cdots \sum_{j_N=1}^{J_N} \omega_{j_1}^1 \cdots \omega_{j_N}^N G(\epsilon_{j_1}^1, \dots, \epsilon_{j_N}^N)$$

- Now $\epsilon \sim N(\mu, \Sigma)$ where Σ is an N by N variance-covariance matrix.
- The multivariate density is

$$w(\epsilon) = (2\pi)^{-N/2} det(\Sigma)^{-1/2} \exp\left(-\frac{1}{2}(\epsilon - \mu)^T (\epsilon - \mu)\right)$$

- We need to perform a change of variables before we can integrate this.
- Given Σ is symmetric and positive semi-definite, it has a Cholesky decomposition,

$$\Sigma = \Omega \Omega^T$$

  where Ω is a lower-triangular with strictly positive entries.
- The linear change of variables is then

$$v = \Omega^{-1}(\epsilon - \mu)$$

- Plugging this in gives

$$\sum_{j=1}^{J} \omega_j G(\Omega v_j + \mu) \equiv \sum_{j=1}^{J} \omega_j G(\epsilon_j)$$

  where $v \sim N(0, I_N)$.
- So, we can follow the exact same steps as with the uncorrelated shocks, but need to adapt the nodes.

1.14 References

- The Integration part of these slides are based on [@maliar-maliar] [2] chapter 5

References

[1] Kenneth L. Judd. *Numerical methods in economics*. The MIT Press, 1998.

[2] Lilia Maliar and Serguei Maliar. Numerical methods for large scale dynamic economic models. *Handbook of Computational Economics*, 3:325, 2013.