FEniCS Course

Lecture 12: Computing sensitivities

Contributors
Simon Funke

Adjoints are key ingredients for sensitivity analysis, PDE-constrained optimization, ...

So far we have focused on solving forward PDEs.

But we want to do (and can do) more than that!

Maybe we are interested in ...

- the sensitivity with respect to certain parameters
    - initial conditions,
    - forcing terms,
    - unknown coefficients.
- PDE-constrained optimization
    - data assimilation
    - optimal control
- goal-oriented error control

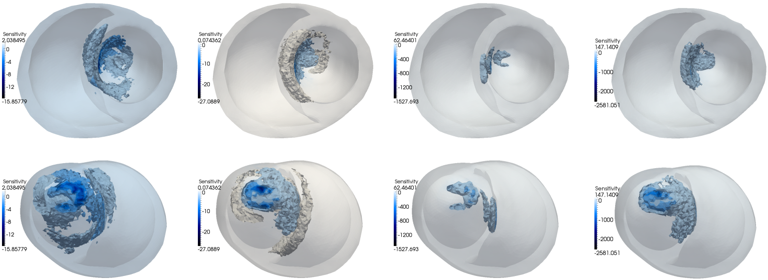
For this we want to compute functional derivatives and adjoints provide an efficient way of doing so.

What is the sensitivity of the abnormal wave propagation to the local tissue conductivities?

The wave propagation abnormality at a given time T:

$$J(v, s, u) = \|v(T) - v_{\text{obs}}(T)\|^2, \quad \frac{\partial J}{\partial g_{\text{e|i|l|t}}} = ?$$

```
v_d = Function(V, "healthy_obs_200.xml.gz")
J = Functional(inner(v - v_d, v - v_d)*dx*dt[T])
dJdg_s = compute_gradient(J, gs)
```



The Hello World of functional derivatives

Consider the Poisson's equation

$$\begin{aligned} -\nu \Delta u &= m \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega, \end{aligned}$$

together with the *objective functional*

$$J(u) = \frac{1}{2} \int_\Omega \|u - u_d\|^2 \,\mathrm{d}x,$$

where u_d is a known function.

Goal

Compute the sensitivity of J with respect to the *parameter* m: $\mathrm{d}J/\mathrm{d}m$.

Computing functional derivatives (Part 1/3)

Given

- Parameter m,
- PDE $F(u, m) = 0$ with solution u.
- Objective functional $J(u, m) \to \mathbb{R}$,

Goal

Compute $\mathrm{d}J/\mathrm{d}m$.

Reduced functional

Consider u as an implicit function of m by solving the PDE.
With that we define the *reduced functional* R:

$$R(m) = J(u(m), m)$$

Computing functional derivatives (Part 1/3)

Given

- Parameter m,
- PDE $F(u, m) = 0$ with solution u.
- Objective functional $J(u, m) \to \mathbb{R}$,

Goal

Compute $\mathrm{d}J/\mathrm{d}m$.

Reduced functional

Consider u as an implicit function of m by solving the PDE.
With that we define the *reduced functional* R:

$$R(m) = J(u(m), m)$$

Computing functional derivatives (Part 1/3)

Given

- Parameter m,
- PDE $F(u, m) = 0$ with solution u.
- Objective functional $J(u, m) \to \mathbb{R}$,

Goal

Compute $\mathrm{d}J/\mathrm{d}m$.

Reduced functional

Consider u as an implicit function of m by solving the PDE.
With that we define the *reduced functional* R:

$$R(m) = J(u(m), m)$$

Computing functional derivatives (Part 2/3)

Reduced functional:

$$R(m) \equiv J(u(m), m).$$

Taking the derivative of with respect to m yields:

$$\frac{\mathrm{d}R}{\mathrm{d}m} = \frac{\mathrm{d}J}{\mathrm{d}m} = \frac{\partial J}{\partial u}\frac{\mathrm{d}u}{\mathrm{d}m} + \frac{\partial J}{\partial m}.$$

Computing $\frac{\partial J}{\partial u}$ and $\frac{\partial J}{\partial m}$ is straight-forward, but how handle $\frac{\mathrm{d}u}{\mathrm{d}m}$?

Computing functional derivatives (Part 2/3)

Reduced functional:

$$R(m) \equiv J(u(m), m).$$

Taking the derivative of with respect to m yields:

$$\frac{\mathrm{d}R}{\mathrm{d}m} = \frac{\mathrm{d}J}{\mathrm{d}m} = \frac{\partial J}{\partial u}\frac{\mathrm{d}u}{\mathrm{d}m} + \frac{\partial J}{\partial m}.$$

Computing $\frac{\partial J}{\partial u}$ and $\frac{\partial J}{\partial m}$ is straight-forward, but how handle $\frac{\mathrm{d}u}{\mathrm{d}m}$?

Computing functional derivatives (Part 2/3)

Reduced functional:

$$R(m) \equiv J(u(m), m).$$

Taking the derivative of with respect to m yields:

$$\frac{\mathrm{d}R}{\mathrm{d}m} = \frac{\mathrm{d}J}{\mathrm{d}m} = \frac{\partial J}{\partial u}\frac{\mathrm{d}u}{\mathrm{d}m} + \frac{\partial J}{\partial m}.$$

Computing $\frac{\partial J}{\partial u}$ and $\frac{\partial J}{\partial m}$ is straight-forward, but how handle $\frac{\mathrm{d}u}{\mathrm{d}m}$?

Computing functional derivatives (Part 3/3)

Taking the derivative of $F(u, m) = 0$ with respect to m yields:

$$\frac{\mathrm{d}F}{\mathrm{d}m} = \frac{\partial F}{\partial u}\frac{\mathrm{d}u}{\mathrm{d}m} + \frac{\partial F}{\partial m} = 0$$

Hence:

$$\frac{\mathrm{d}u}{\mathrm{d}m} = -\left(\frac{\partial F}{\partial u}\right)^{-1}\frac{\partial F}{\partial m}$$

Final formula for functional derivative

$$\frac{\mathrm{d}J}{\mathrm{d}m} = -\overbrace{\frac{\partial J}{\partial u}\underbrace{\left(\frac{\partial F}{\partial u}\right)^{-1}}_{}}^{\text{adjoint PDE}}\!\!\!\!\!\!\!\!\underbrace{\phantom{\left(\frac{\partial F}{\partial u}\right)^{-1}}\frac{\partial F}{\partial m}}_{\text{tangent linear PDE}} + \frac{\partial J}{\partial m},$$

Computing functional derivatives (Part 3/3)

Taking the derivative of $F(u, m) = 0$ with respect to m yields:

$$\frac{\mathrm{d}F}{\mathrm{d}m} = \frac{\partial F}{\partial u}\frac{\mathrm{d}u}{\mathrm{d}m} + \frac{\partial F}{\partial m} = 0$$

Hence:

$$\frac{\mathrm{d}u}{\mathrm{d}m} = -\left(\frac{\partial F}{\partial u}\right)^{-1}\frac{\partial F}{\partial m}$$

Final formula for functional derivative

$$\frac{\mathrm{d}J}{\mathrm{d}m} = -\overbrace{\frac{\partial J}{\partial u}\left(\frac{\partial F}{\partial u}\right)^{-1}}^{\text{adjoint PDE}}\!\!\!\!\!\!\!\!\underbrace{\phantom{\left(\frac{\partial F}{\partial u}\right)^{-1}}\frac{\partial F}{\partial m}}_{\text{tangent linear PDE}} + \frac{\partial J}{\partial m},$$

Computing functional derivatives (Part 3/3)

Taking the derivative of $F(u, m) = 0$ with respect to m yields:

$$\frac{\mathrm{d}F}{\mathrm{d}m} = \frac{\partial F}{\partial u}\frac{\mathrm{d}u}{\mathrm{d}m} + \frac{\partial F}{\partial m} = 0$$

Hence:

$$\frac{\mathrm{d}u}{\mathrm{d}m} = -\left(\frac{\partial F}{\partial u}\right)^{-1}\frac{\partial F}{\partial m}$$

Final formula for functional derivative

$$\frac{\mathrm{d}J}{\mathrm{d}m} = -\overbrace{\frac{\partial J}{\partial u}\left(\frac{\partial F}{\partial u}\right)^{-1}}^{\text{adjoint PDE}}\underbrace{\left(\frac{\partial F}{\partial u}\right)^{-1}\frac{\partial F}{\partial m}}_{\text{tangent linear PDE}} + \frac{\partial J}{\partial m},$$

Dimensions of a finite dimensional example

$$\frac{\mathrm{d}J}{\mathrm{d}m} = \overbrace{\boxed{-\frac{\partial J}{\partial u}} \times \underbrace{\boxed{\left(\frac{\partial F}{\partial u}\right)^{-1}}}_{}}^{\text{discretised adjoint PDE}} \underbrace{\times \boxed{\frac{\partial F}{\partial m}}}_{\text{discretised tangent linear PDE}} + \boxed{\frac{\partial J}{\partial m}}$$

The tangent linear solution is a matrix of dimension $|u| \times |m|$ and requires the solution of m linear systems.

The adjoint solution is a vector of dimension $|u|$ and requires the solution of one linear system.

Adjoint approach

1. Solve the adjoint equation for λ

$$\frac{\partial F}{\partial u}^* \lambda = -\frac{\partial J^*}{\partial u}.$$

2. Compute

$$\frac{\mathrm{d}J}{\mathrm{d}m} = \lambda^* \frac{\partial F}{\partial m} + \frac{\partial J}{\partial m}.$$

The computational expensive part is (1). It requires solving the (linear) adjoint PDE, and its cost is independent of the choice of parameter m.