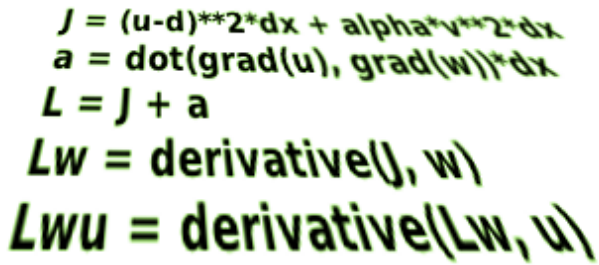
Automation of PDE constrained optimization

Algorithmic differentiation as abstract building blocks in high level algorithms



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Overview of talk

The algorithmic differentiation of variational forms as implemented in FEniCS (UFL) can be a powerful building block for high level optimization algorithms.

- Example PDE constrained optimization problem
- Automation of gradient based optimization algorithms
- Automation of Lagrangian based optimization algorithms
- Algorithmic differentiation in FEniCS explained

Example weak forms in the Unified Form Language showing tensor algebra and index notation

$$u : x \mapsto R^d, \qquad v : x \mapsto R^d, \qquad M : x \mapsto R^{d,d}. \tag{1}$$

$$a_1(u, v; M) = \int_\Omega (\operatorname{grad} u \cdot M) : \operatorname{grad} v \, \mathrm{d}x, \tag{2}$$

$$a_2(u, v; M) = \int_\Omega M_{ij} u_{k,i} v_{k,j} \, \mathrm{d}x \tag{3}$$

```
1 V = VectorElement("Lagrange", triangle, 3)
2 T = TensorElement("Lagrange", triangle, 1)
3 u = TrialFunction(V);  v = TestFunction(V);  M = Coefficient(T)
4 a1 = inner(dot(grad(u), M), grad(v))*dx
5 a2 = M[i,j] * u[k].dx(i) * v[k].dx(j) * dx
```

Example PDE constrained optimization problem

Minimize a cost functional J of the control $v \in V$ and state $u = u(v) \in U$

$$J(v) = \hat{J}(v, u(v)) = \int_{\Omega_D} (u - z)^2 \,\mathrm{d}x + \alpha \int_{\Omega_C} v^2 \,\mathrm{d}x, \tag{4}$$

constrained by the state equation (PDE)

$$a(u, w) = b(v; w), \qquad \forall w \in U, \tag{5}$$

$$u = 0, \qquad \text{on} \quad \partial\Omega. \tag{6}$$

For examples later I'll use

$$a(u, w) = \int_{\Omega} uw + \operatorname{grad} u \cdot \operatorname{grad} w \,\mathrm{d}x, \tag{7}$$

$$b(v; w) = \int_{\Omega} vw \,\mathrm{d}x. \tag{8}$$

V, J, a, b, etc. must be part of a problem definition.

Example problem class

```
1  class Problem:
2      def __init__(self, n=128, alpha=1e-4,
3                   zexpr="1.0+3.0*x[0]+exp(x[1])",
4                   v0expr="0.0"):
5          self.mesh = UnitSquare(128, 128)
6          self.V = FunctionSpace(self.mesh, "Lagrange", 1)
7          self.z = Function(self.V)
8          self.z.interpolate(Expression(zexpr))
9          # ... some more lines
10     def J(self, v, u):
11         return 0.5*(u-self.z)**2*dx + 0.5*self.alpha*v**2*dx
12     def a(self, u, w):
13         return (u*w + dot(grad(u), grad(w)))*dx
14     def b(self, v, w):
15         return v*w*dx
16     def a_adjoint(self, u, w):
17         return self.a(w, u)
```

Gradient based iterative methods require the computation of $D_{v,\eta}J(v)$ via duality arguments

$$D_{v,\eta}J(v) \equiv \frac{d}{d\tau}\left[J(v+\tau\eta)\right]_{\tau=0}, \qquad \forall \eta \in V_h, \tag{9}$$

which can be split into

$$D_{v,\eta}J = D_{v,\eta}\hat{J} + D_{u,\bar{u}}\hat{J}, \qquad \bar{u} \equiv D_{v,\eta}u(v). \tag{10}$$

First solve the dual equation for w, where $a^*(u,v) \equiv a(v,u)$,

$$a^*(w,\psi) = D_{u,\psi}\hat{J}, \qquad \forall \psi, \tag{11}$$

$$w = 0, \qquad \text{on} \quad \partial\Omega. \tag{12}$$

Then

$$D_{u,\bar{u}}\hat{J} = a^*(w,\bar{u}) = a(\bar{u},w) = b(\eta;w) \tag{13}$$

Example computation of gradient via adjoint equation

```
1  # Callback for scipy.optimize.fmin_l_bfgs_b
2  def func(x):
3      global p, u, v, w, phi, psi
4      v.vector()[:] = x
5      solve(p.a(phi, psi) == p.b(v, psi), u, p.bcu)
6
7      J = p.J(v, u)
8      dJdu = derivative(J, u, psi)
9      dJdv = derivative(J, v, psi)
10     Jvalue = assemble(J)
11
12     solve(p.a_adjoint(phi, psi) == dJdu, w, p.bcw)
13     DJ = assemble(dJdv + p.b(psi, w))
14
15     return Jvalue, DJ.array().copy()
```

One shot methods can be automated through differentiation of the Lagrangian functional

Define the Lagrangian functional

$$L(v, w, u) = J(v, u) + a(u, w) - b(v, w), \tag{14}$$

and differentiate it to find the optimality conditions for (v, w, u),

$$L_v = D_{v,\hat{v}} L(u, v, w) = 0, \qquad \forall \hat{v} \in V, \tag{15}$$

$$L_w = D_{w,\hat{w}} L(u, v, w) = 0, \qquad \forall \hat{w} \in U, \tag{16}$$

$$L_u = D_{u,\hat{u}} L(u, v, w) = 0, \qquad \forall \hat{u} \in U. \tag{17}$$

Then differentiate again to build the block system

$$\begin{bmatrix} L_{vv} & L_{vw} & 0 \\ L_{wv} & 0 & L_{wu} \\ 0 & L_{uw} & L_{uu} \end{bmatrix} \begin{bmatrix} v \\ w \\ u \end{bmatrix} = \begin{bmatrix} \alpha M & B^* & 0 \\ B & 0 & A \\ 0 & A^* & M \end{bmatrix} \begin{bmatrix} v \\ w \\ u \end{bmatrix} = \begin{bmatrix} -L_v \\ -L_w \\ -L_u \end{bmatrix} \tag{18}$$

Automation of one shot method preconditioning

Define the preconditioning norm

$$P(v, w, u) = \|v\|^2 + \|w\|^2 + \|u\|^2 + a(u, u) + a(w, w) \tag{19}$$

and differentiate it twice to find the block preconditioner system

$$\begin{bmatrix} M & 0 & 0 \\ 0 & M + A & 0 \\ 0 & 0 & M + A \end{bmatrix} \tag{20}$$

Choice of preconditioner not obvious, more work needed.

Example one shot solver

```
1  M = MixedFunctionSpace([p.V, p.V, p.V])
2  uvw = Function(M); u, v, w = split(uvw)
3  bcs = [DirichletBC(M.sub(0), 0, DomainBoundary()),
4         DirichletBC(M.sub(2), 0, DomainBoundary())]
5
6  L = p.J(v, u) + p.a(u, w) - p.b(v, w)
7  precnorm = 0.5*(u**2 + v**2 + w**2)*dx + p.a(u,u) + p.a(w,w)
8
9  F = derivative(L, uvw)
10 A, b = assemble_system(derivative(F, uvw), -F, bcs)
11 Pform = derivative(derivative(precnorm, uvw))
12 P, _ = assemble_system(Pform, -F, bcs)
13
14 solver = KrylovSolver("tfqmr", "amg")
15 solver.set_operators(A, P)
16 solver.solve(uvw.vector(), b)
```

Automatic functional differentiation is (almost) just differentiation of expressions

With no loss of generality w.r.t. multiple integrals or additional independent coefficients, we can consider a functional

$$F(g) = \int_D E(g)\,\mathrm{d}\mu. \tag{21}$$

The Gateaux derivative of F w.r.t. $g \in V$ in a direction $\phi \in V$ is

$$D_{g,\phi}F(g) \equiv \frac{\mathrm{d}}{\mathrm{d}\tau}\left[F(g+\tau\phi)\right]_{\tau=0} = \int_D \frac{\mathrm{d}}{\mathrm{d}\tau}\left[E(g+\tau\phi)\right]_{\tau=0}, \tag{22}$$

assuming the domain D is independent of g.

Algorithmic differentiation of an expression tree is the chain rule plus differentiation rules for each type and operator

- Algorithm structure equivalent to forward mode AD.
- The innermost derivatives are computed first, recursively.
- Function gradients still represented after differentiation.

$$\operatorname{grad}(v * u) = \operatorname{grad} v * u + v * \operatorname{grad} u \tag{23}$$

Directional derivatives w.r.t. functions requires differentiation rules for $D_{g,\phi}t$ for all types of terminal expression t

Assuming coefficient functions g, h, we have

$$D_{g,\phi}g = \frac{\mathrm{d}}{\mathrm{d}\tau}\left[g + \tau\phi\right]_{\tau=0} = \phi, \tag{24}$$

$$D_{g,\phi}\nabla g = \frac{\mathrm{d}}{\mathrm{d}\tau}\left[\nabla(g + \tau\phi)\right]_{\tau=0} = \nabla\phi, \tag{25}$$

$$D_{g,\phi}\nabla h = \frac{\partial h}{\partial g}\phi. \tag{26}$$

The user can provide $\frac{\partial h}{\partial g}$, which by default is 0.

Algorithms for each differentiation variable type differ only by the terminal differentiation rules

```
1  V = FiniteElement("Lagrange", triangle, 1)
2  u = Coefficient(V)
3  w = TestFunction(V)
4  v = variable(u)
5  f = diff(v**2, v)                  # == 2*v
6  g = derivative(u**2*dx, u, w)      # == 2*u*w
```

Or considering nested differentiation,

$$\text{grad}\,(vu)] = \text{grad}\,(v)u + v\text{grad}\,(u), \tag{27}$$

$$f = \frac{d}{dv}[\text{grad}\,(vu)] = \text{grad}\,u, \tag{28}$$

$$g = D_{u,w}[\text{grad}\,(vu)] = \text{grad}\,(v)w + v\text{grad}\,(w). \tag{29}$$

Ways to use differentiation features of UFL

- Computing cost functional gradient.
- Differentiation of Lagrangian functional.

- Sensitivity analysis or parameter estimation.
- Exact linearization of nonlinear residual equation.
- Differentiation of e.g. hyperelasticity material laws.
- Computing a source term for validation of a solver.

Thank you!

Software links:

- *http://www.fenicsproject.org*
- *http://www.launchpad.net/ufl*
- *http://launchpad.net/cbc.block*
- *http://www.dolfin-adjoint.org*

Preconditioning papers:

- J. Schöberl and W. Zulehner, SJMAEL (2010)
- B.F. Nielsen and K.-A. Mardal, SISC (2012)

Questions:

- *https://answers.launchpad.net/fenics*
- *martinal@simula.no*

A simple example equation

$$a(u, v) = \int_\Omega \operatorname{grad} u \cdot \operatorname{grad} v \, \mathrm{d}x, \tag{30}$$

$$L(v; f, g) = \int_\Omega f \, v \, \mathrm{d}x + \int_{\partial\Omega} g \, v \, \mathrm{d}s \tag{31}$$

```
1  cell = tetrahedron
2  V = FiniteElement("Lagrange", cell, 1)
3
4  f = Coefficient(V)
5  g = Coefficient(V)
6  u = TrialFunction(V)
7  v = TestFunction(V)
8
9  a = dot(grad(u), grad(v)) * dx
10 L = f*v*dx + g*v*ds
```

Tree representation of the weak Laplace form

```
1  a = dot(grad(u), grad(v)) * dx
2  print ufl.algorithms.tree_format(a)
```

```
1  Form:
2      Integral:
3          domain type: cell
4          domain id: 0
5          integrand:
6              Dot
7              (
8                  Grad
9                      Argument(FiniteElement(...), -1)
10                 Grad
11                     Argument(FiniteElement(...), -2)
12             )
```

Some expression simplifications are carried out when constructing expression objects

Canonical ordering of sum and product terms:

- `a*b` $\rightarrow$ `a*b`, `b*a` $\rightarrow$ `a*b`

Simplification of identity and zero terms:

- `1*f` $\rightarrow$ `f`, `0*f` $\rightarrow$ `0`, `0+f` $\rightarrow$ `f`

Constant folding:

- `cos(0)` $\rightarrow$ `1`

Tensor component cancellations:

- `as_tensor(A[i,j], (i,j))` $\rightarrow$ `A`

Note how these simplifications work together with the differentiation chain rule:

- $\frac{d}{dx}(xy) = 1y + x0 \rightarrow y + 0 \rightarrow y$.