Automatic differentiation: The most criminally underused tool in probabilistic numerics

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Do we know the function we're integrating?

Do we know the function we’re integrating?

- Me: We treat the integrand as an unknown function –
- FB: But we do know what the function is.
- Me: OK, we know how to evaluate it, but we don’t know its integral.
- FB: If you can write it down and evaluate it, how is that different than knowing what the function is?
- Me: ...
- FB: ...

How to exploit our knowledge of integrand?

- Naive quadrature hopeless in high dimensions.
- Control flow can help break up the domain. Or, can find additivity. Can incorporate into custom kernels.
- What about continuous models, or physical simulations?
- Look mostly like compositions of many vector-valued, differentiable operations. f(g(h(x)))
- What to do with this sort of structure?
- Can model each function separately, but this gives deep (intractable) model.

Let's use gradient observations

- Bayesian Quadrature motivated by expense of evaluating function
- Gradients and higher derivatives are available cheaply!
- Even if function isn't everywhere differentiable, if it's continuous and differentiable almost everywhere, then gradients help find high/low regions.
- Chain rule combines info about all elements of composition
- Higher-order gradients give non-local information (Taylor expansion)

Common examples have (stochastic) gradients available

- Physical simulations
- Model hyperparameters (GPs, neural nets)
- Bayesian Quadrature itself! Might want to optimize based on output.
- Solar system models for expolanet detection
- Models of prawn behavior

Price List

	Time cost	num observations
function evaluation	$O(1)$	1
gradient evaluation	$O(2)$	D
Hessian-vector product	$O(4)$	D
full Hessian	$O(4D)$	D^2

How to condition on a Hessian-vector product?

- Automatic differentiation to the rescue again:

$$\mathrm{cov}(f(\mathbf{x}), Af(\mathbf{x}')) = A\,\mathrm{cov}(f(\mathbf{x}), f(\mathbf{x}'))$$

- Holds true for Hess-vec product: $A = \mathbf{v}^T \nabla_{\mathbf{x}} \nabla_{\mathbf{x}}^T$
- So

$$\mathrm{cov}(f(\mathbf{x}), \left[\mathbf{v}^T \nabla_{\mathbf{x}'} \nabla_{\mathbf{x}'}^T f(\mathbf{x}')\right]_d) = \left[\mathbf{v}^T \nabla_{\mathbf{x}'} \nabla_{\mathbf{x}'}^T k(\mathbf{x}, \mathbf{x}')|_{\mathbf{x}'}\right]_d$$

How to code a Hessian-vector product?

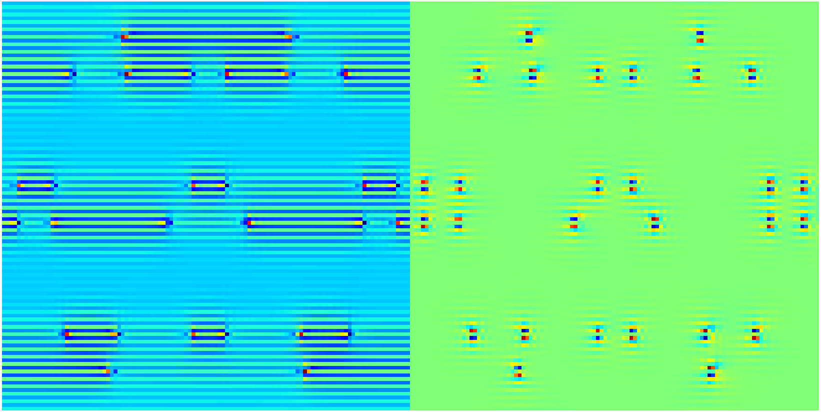
```python
from autograd import grad
from autograd.numpy import np

def hessian_vector_product(fun):
    fun_grad = grad(fun)
    def vector_dot_grad(arg, vector):
        return np.dot(vector, fun_grad(arg))
    return grad(vector_dot_grad)
```

- No explicit Hessian
- Can call HVP on complicated integrand
- Can call HVP on complicated kernel
- Can construct higher-order products

Example: Taking gradient through fluid sim

[Show code and demo]



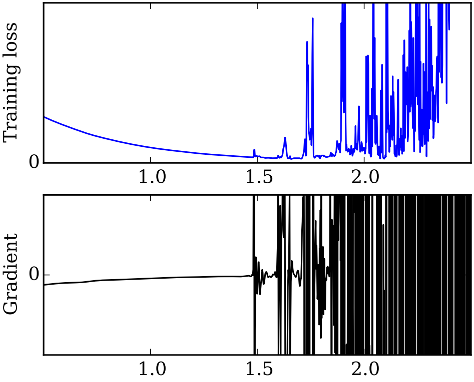
through fluid sim

Memory limitations for large simulations

- If you can reverse dynamics exactly, no need for intermediate storage.
- If you can reverse dynamics approximately, store only lost bits
- Obvious applications are physical simulations, learning dynamics

When will gradients be meaningful?

- Chaotic dynamics → gradient very noisy
- Smooth dynamics → meaningful gradient even for long sims
- Heteroskedastic noise model could gently back off to gradient-free case



learning rate

Autodiff makes the codebase small

- BBQ code was at least half derivatives
- Needed Hessians for Laplace approx
- Changing model or kernel means re-doing all derivatives
- Spearmint uses slice sampling for hyperparameters. Doesn’t scale to high dimensions. Use HMC or BBSVI instead. (more autodiff)

Summary

- Gradient or HVP provide D times more info at only twice the cost
- Ridiculous to say we care about expensive evaluations and ignore this
- HVPs and higher derivatives provide non-local-info
- Can ask which direction is most informative
- Autodiff makes code base simpler + less error prone