### Optimization Services and Nonlinear Programming

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November 6, 2007



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### Outline

The Context

The OS API

Algorithmic Differentiation API

Postfix (and Prefix)



Here is the context.





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Here is what is happening on the solver.





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### The Solver Side

On the solver end there is an executable **OSSolverService** that communicates with specific solver. Here is what it does.

Step 1: Create an **OSiLReader** object.

Step 2: Have the **OSiLReader** object parse the OSiL XML instance and create an in-memory **OSInstance** object.

Step 3: Create an object in the specific solver class (e.g. create an IpoptSolver, LindoSolver, or KnitroSolver).

Step 4: Have the solver specific object **work with** the a generic **OSInstance** and the solver library to solve the problem.



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#### Here is another view of solver side





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## **OS Customized Solver Interfaces**

CoinSolver

Ipopt Solver

Knitro Solver

Lindo Solver



## **OS Supported Solvers**

- Clp using CoinSolver
- Cbc using CoinSolver
- Cplex using CoinSolver
- Dylp using CoinSolver
- Glpk using CoinSolver
- Ipopt using IpoptSolver
- Knitro using KnitroSolver
- Lindo using KnitroSolver
- SYMPHONY using CoinSolver
- Vol using CoinSolver



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**Objective:** Create an API that is as flexible as possible and can deal with numerous solver APIs

In this talk we focus on the nonlinear aspects of the API.



## The OS API

The **OSIIb** provides in-memory representation of optimization instance, **OSInstance**. It is an API that has three types of methods:

- get() methods: a set of methods to get information about the problem instance including the problem in a postfix or prefix format
- set() methods: a set of methods to create/modify a problem instance
- calculate() methods: a set of methods for performing Algorithmic Differentiation (based upon the COIN-OR CppAD by Brad Bell).



### **Algorithmic Differentiation**

The OS API has both *high level* and *low level* calls for algorithmic differentiation.

Both the high level and low level calls are public methods but **the** high level calls

- are meant to be user friendly the user does not need to know anything about forward sweeps or reverse sweeps or any other aspect of algorithmic differentiation
- the high level calls are similar in nature to calls that the nonlinear solver codes use



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### **Algorithmic Differentiation – Sparsity Patterns**

Many derivative-based solvers want to know the sparsity pattern of the constraint Jacobian.

sparseJac = osinstance->getJacobianSparsityPattern();

- store non zero elements by row in sparse format
- the first conVals correspond to variables with constant derivative
- variables with a constant derivative are never sent to gradient and Hessian calculators



#### Algorithmic Differentiation – Sparsity Patterns

Similarly for Hessian of Lagrangian

osinstance->getLagrangianHessianSparsityPattern( );

Here our code is not real smart smart at this point. For example,

$$x_1^2 + x_2^2 + \dots + x_n^2$$

will generate a dense Hessian.



### Algorithmic Differentiation – some motivation

Key Idea: The API of nonlinear solvers not really setup to maximize the efficient use of AD.

A typical API will have methods such as:

- get an objective function value
- get constraint values
- get objective gradient
- get constraint Jacobian
- get Hessian of Lagrangian

**An Issue:** from an AD perspective, when, for example, calculating first derivatives it would be nice to know if a second derivative is also required.



#### Here is another view of solver side





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### Algorithmic Differentiation – some motivation

The Problem: Many nonlinear algorithms, such as interior point methods **do not** calculate all orders of derivatives for the current iterate.

For example, they may do a simple line search and not use any second derivative information.

In the API method calls for function evaluations they **do not communicate if a higher order derivative is required for the current iterate.** 



# Algorithmic Differentiation – gradient calculation

#### calculateAllConstraintFunctionGradients()

The method arguments are:

- double\* x
- double\* objLambda
- double\* conLambda
- bool new\_x
- int highestOrder



# Algorithmic Differentiation – gradient calculation

Assume, for example, only first derivative information required.

If a call has been placed to
calculateAllConstraintFunctionValues with highestOrder
= 0, then the appropriate call to get gradient evaluations is

calculateAllConstraintFunctionGradients( x, NULL, NULL, false, 1);

Note that in this function call  $new_x = false$ . This prevents a call to forwardAD() with order 0 to get the function values.



# Algorithmic Differentiation – gradient calculation

If, at the current iterate, the Hessian of the Lagrangian function is also desired then an appropriate call is

In this case, if there was a prior call

calculateAllConstraintFunctionValues(x, w, z, true, 0);

then only first and second derivatives are calculated, not function values.



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# Algorithmic Differentiation – Hessian calculation

In our implementation, there are **exactly two** conditions that require a new function or derivative evaluation. A new evaluation is required if and only if

1. The value of  $new_x$  is true

-OR-

 For the callback function the value of the input parameter highestOrder is strictly greater than the current value of m\_iHhighestOrderEvaluated.

In the code we keep track of the highest order derivative calculation that has been made.



# Algorithmic Differentiation – Hessian calculation

```
for(index = 0; index < n; index++){
    unit_col_vec[ index] = 1;
    // calculate column i of the Jacobian matrix
    gradVals = f.Forward(1, unit_col_vec);
    unit_col_vec[ index] = 0;
    // get row i of the Lagrangian function!!!
    f.Reverse(2, lagMultipliers);
}</pre>
```

In a bad implementation, I could end up doing a forward sweep three times.



#### The OS API – Postfix

Postfix is an excellent way to represent a wide variety of optimization problems.

By defining enough operators you can model very generic nonlinear optimization.

A good structure for implementing algorithmic differentiation.

As an example, the internal representation of an optimization instance in LINDO is a postfix instruction list.



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### The OS API – Postfix





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#### The OS API – Postfix

Key Postfix related methods.

In order to get the problem in postfix use the method:

getNonlinearExpressionTreeInPostfix( int rowIdx);

This returns a vector of pointers to **OSnLNode** objects.

There is an OSnLNode for every operator.



## **OS Supported Operators**

- OSnLNodeVariable
- OSnLNodeTimes
- OSnLNodePlus
- OSnLNodeSum
- OSnLNodeMinus
- OSnLNodeNegate
- OSnLNodeDivide
- OSnLNodePower
- OSnLNodeProduct
- OSnLNodeLn
- OSnLNodeSqrt
- OSnLNodeSquare
- OSnLNodeSin
- OSnLNodeCos
- OSnLNodeExp
- OSnLNodeif
- OSnLNodeAbs
- OSnLNodeMax
- OSnLNodeMin
- OSnLNodeE
- OSnLNodePI
- OSnLNodeAllDiff



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## **Using Lindo**

**Step 1:** For each row and the objective function convert the expression tree into a list of OSnLNodes in postfix.

**Step 2:** Loop over the list of OSnLNodes and create a Lindo instructions list (map between OS operators and Lindo operator codes).

Step 3: Call the Lindo LSaddInstruct() method.

Step 4: Solve!



#### Here is another view of solver side





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